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Supporting Information

Generation of an Aromatic Amide-Derived Phosphane (Aphos) Library via Self-Assisted Molecular Editing and Applications of Aphos in Room-Temperature Suzuki–Miyura Reactions

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Contents

Experimental

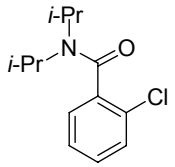
General method.

All microwave reactions were carried out in closed 10 mL pressurized process vials on a technical microwave reactor (Emrys™ creator from Personal Chemistry AB or Initiator™ from Biotage AB, Uppsala, Sweden) with the reaction temperature measured by an IR sensor. NMR spectra were recorded on a 300, 400, or 500 MHz instrument in $CDCl_3$ using residual $CHCl_3$ as the internal reference for ^1H (δ 7.26) and ^{13}C (δ 77.2) or a routine external reference for ^{31}P. IR spectra were taken on a FT-IR spectrophotometer. Mass spectra (MS) were measured by the +CI or +ESI method. Elemental analyses were performed by Zhejiang University, Hangzhou, China. Melting points are uncorrected. Silica gel plates 60 F-254 (0.25-mm, E. Merck) were used for thin-layer chromatography using UV light, or 7% ethanolic phosphomolybdic acid and heating as the visualizing methods. Silica gel 60 (particle size 0.040–0.063 mm, E. Merck) was used for flash column chromatography. Yields refer to chromatographically and spectroscopically (^1H NMR) homogeneous materials. Aryl boronic acids and other reagents were obtained commercially and used as received. Dry THF and Toluene were freshly distilled from sodium and benzophenone under a nitrogen atmosphere. Toluene was degassed before use in all microwave-assisted reactions.

General procedure for synthesis of chloro-substituted benzamides 13.

A solution of 2-, 3-, or 4-chlorobenzoic acid (1.566 g, 10 mmol) in $SOCl_2$ (20 mL) was heated at reflux for 4 h, then the excess $SOCl_2$ was removed by distillation. CH_2Cl_2 (20 mL) was added to the residue and the resultant solution was cooled in an ice-water bath (0 °C), followed by adding Et_3N (1.41 mL, 11 mmol) dropwise via a syringe. After stirring for 5 min at the same temperature, *i*-Pr_2NH (1.54 mL, 11 mmol) was added dropwise via a syringe. The mixture was then stirred at room temperature for 2 h. Water (20 mL) was added to the reaction mixture and the aqueous phase was extracted with EtOAc (2 x 20 mL). The combined organic layer was washed with water (1 x 50 mL) and brine (1 x 50 mL), dried over anhydrous $MgSO_4$, and concentrated under reduced pressure. The residue was purified by flash column chromatography (silica gel, 10% EtOAc–hexane) to give the amide **13**.

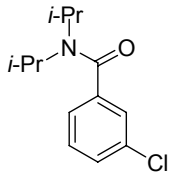
N,*N*-Diisopropyl 2-Chlorobenzamide.



13 (2-)

Prepared in 91% yield. IR (film) 2971, 1627, 1441, 1342 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.40–7.16 (m, 4 H), 3.63–3.46 (m, 2 H), 1.56 (d, *J* = 6.8 Hz, 3 H), 1.55 (d, *J* = 6.8 Hz, 3 H), 1.19 (d, *J* = 6.8 Hz, 3 H), 1.05 (d, *J* = 6.8 Hz, 3 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 1.67.3, 138.0, 130.0, 129.6, 129.2, 127.0, 126.6, 51.0, 45.9, 20.7, 20.6, 20.6, 20.1.

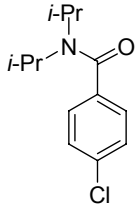
***N*,*N*-Diisopropyl 3-Chlorobenzamide.**



13 (3-)

Prepared in 90% yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.40–7.18 (m, 4 H), 3.79 (br s, 1 H), 3.53 (br s, 1 H), 1.53 (br s, 6 H), 1.18 (br s, 6 H).

***N*,*N*-Diisopropyl 4-Chlorobenzamide.**[1]

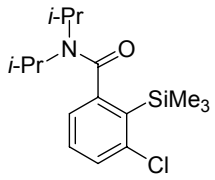


13 (4-)

Prepared in 92% yield as a white solid; mp 89–90 °C (EtOAc–hexane); R_f = 0.30 (9.1% EtOAc–hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 7.29–7.16 (m, 4 H), 3.85–3.40 (br s, 2 H), 1.85–0.70 (br s, 12 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.9, 137.4, 134.6, 128.8 (x 2), 127.3 (x 2), 21.0 (x 4) (The carbon in N–*C*H was not observed due to peak broadening as the result of amide rotation).

[1] U. Gerardo, C. Nadege, C. H. B. Dennis, *Synthesis* **1986**, 1286–1288.

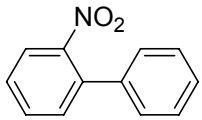
***N*,*N*-Diisopropyl 3-Chloro-2-trimethylsilylbenzamide.**[2]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (dd, *J* = 8.4, 1.6 Hz, 1 H), 7.24 (d, *J* = 8.0 Hz, 1 H), 6.97 (dd, *J* = 7.6, 1.6 Hz, 1 H), 3.71 (septet, *J* = 6.4 Hz, 1 H), 3.49 (septet, *J* = 6.8 Hz, 1 H), 1.55 (d, *J* = 6.8 Hz, 3 H), 1.51 (d, *J* = 6.4 Hz, 3 H), 1.17 (d, *J* = 6.4 Hz, 3 H), 1.09 (d, *J* = 6.8 Hz, 3 H), 0.43 (s, 9 H).

Characterization of Suzuki–Miyaura coupling products.

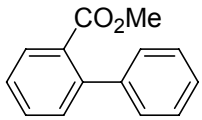
2-Nitrobiphenyl.[3]



[Table 4, entry 1]

Prepared in 94% yield from 2-chloro-1-nitrobenzene and phenylboronic acid as a yellow oil; R_f = 0.47 (4.8% EtOAc–hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 7.8, 0.9 Hz, 1 H), 7.61 (td, *J* = 7.5, 1.5 Hz, 1 H), 7.50–7.40 (m, 5 H), 7.37–7.33 (m, 2 H).

2-Carbomethoxybiphenyl.[4]



[Table 4, entry 2]

Prepared in 90% yield from methyl 2-chlorobenzoate and phenylboronic acid as a colorless oil; R_f = 0.40 (4.8% EtOAc–hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.5 Hz, 1 H), 7.53 (t, *J* = 7.5 Hz, 1 H), 7.44–7.30 (m, 7 H), 3.64 (s, 3 H).

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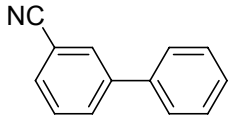
[2] P. A. Brough, S. Fisher, B. Zhao, R. C. Thomas, V. Snieckus, *Tetrahedron Lett.* **1996**, *37*, 2915–2918.
[3] J.-H. Li, W.-J., Liu, Y.-X. Xie, *J. Org. Chem.* **2005**, *70*, 5409–5412.
[4] D. Zim, V. R. Lando, J. Dupont, A. L. Monteiro, *Org. Lett.* **2001**, *3*, 3049–3051.

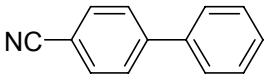
3-Cyanobiphenyl.[5]



[Table 4, entry 3]

Prepared in 87% yield from 3-chlorobenzonitrile and phenylboronic acid as a colorless oil; R_f = 0.39 (4.8% EtOAc–hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.87–7.80 (m, 2 H), 7.65–7.39 (m, 7 H).

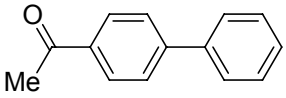
4-Cyanobiphenyl.[6]



[Table 4, entry 4]

Prepared in 97% yield from 4-chlorobenzonitrile and phenylboronic acid as a white solid; R_f = 0.39 (4.8% EtOAc–hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.74–7.67 (m, 4 H), 7.60–7.43 (m, 5 H).

4-Acetobiphenyl.[7]

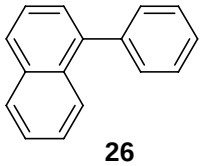


[Table 4, entry 5]

Prepared in 92% yield from 4-chloroacetophenone and phenylboronic acid as a white solid; R_f = 0.32 (4.8% EtOAc–hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06–8.03 (m, 2 H), 7.71–7.63 (m, 4 H), 7.51–7.38 (m, 3 H), 2.66 (s, 3 H).

1-Phenylnaphthalene (26).[4]

[5] B. Tao, D. W. Boykin, *J. Org. Chem.* **2004**, *69*, 4330–4335.
[6] J. P. Wolfe, R. A. Singer, B. H. Yang, S. L. Buchwald, *J. Am. Chem. Soc.* **1999**, *121*, 9550–9561.
[7] I. Barba, R. Chinchilla, C. Gomez, *Tetrahedron* **1990**, *46*, 7813–7822.



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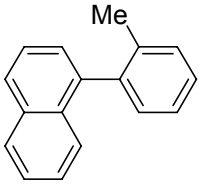
[Table 5, entry 1 & Table 6, entry 1]

Prepared in 82% and 98% yields from 1-chloronaphthalene and phenylboronic acid as a white solid; R_f = 0.70 (hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.94 (d, J = 8.1 Hz, 2 H), 7.90 (d, J = 8.4 Hz, 1 H), 7.58–7.44 (m, 9 H).

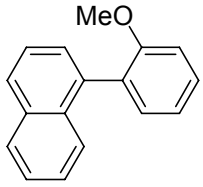
1-*o*-Tolylnaphtalene.[8]



[Table 5, entry 2 & Table 6, entry 2]

Prepared in 94% and 99% yields from 1-chloronaphthalene and 2-tolueneboronic acid as a white solid; R_f = 0.66 (hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.94–7.87 (m, 2 H), 7.57–7.47 (m, 3 H), 7.42–7.25 (m, 6 H), 2.06 (s, 3 H).

1-(2-Methoxyphenyl)naphthalene.[9]

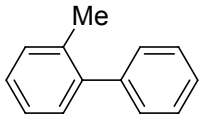


[Table 5, entry 3 & Table 6, entry 3]

Prepared in 95% and 96% yields from 1-chloronaphthalene and 2-methoxybenzeneboronic acid as a white solid; R_f = 0.19 (hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.90 (t, J = 7.5 Hz, 2 H), 7.63–7.38 (m, 6 H), 7.32 (d, J = 7.5 Hz, 1 H), 7.14–7.06 (m, 2 H), 3.73 (s, 3 H).

[8] Y. Terao, H. Wakui, T. Satoh, M. Miura, M. Nomura, *J. Am. Chem. Soc.* **2001**, *123*, 10407–10408.
[9] Y. Terao, H. Wakui, M. Nomoto, T. Satoh, M. Miura, M. Nomura, *J. Org. Chem.* **2003**, *68*, 5236–5243.

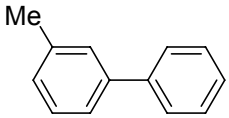
2-Methylbiphenyl.[10]



[Table 5, entry 4 & Table 6, entry 4]

Prepared in 90% and 99% yields from 2-chlorotoulene and phenylboronic acid as a colorless oil; R_f = 0.76 (hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44–7.25 (m, 9 H), 2.31 (s, 3 H).

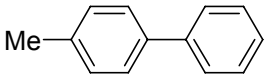
3-Methylbiphenyl.[4]



[Table 5, entry 5 & Table 6, entry 5]

Prepared in 87% and 99% yields from 3-chlorotoulene and phenylboronic acid as a colorless oil; R_f = 0.73 (hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.66–7.21 (m, 9 H), 2.49 (s, 3 H).

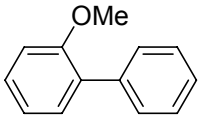
4-Methylbiphenyl.[11]



[Table 5, entry 6 & Table 6, entry 6]

Prepared in 82% and 98% yields from 4-chlorotoulene and phenylboronic acid as a white solid; R_f = 0.71 (hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.68–7.32 (m, 9 H), 2.49 (s, 3 H).

2-Methoxybiphenyl (28).[6]



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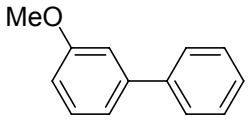
[Table 5, entry 7 & Table 6, entry 7]

[10] X. Bei, H. W. Turner, W. H. Weinberg, A. S. Guram, J. L. Peterson, *J. Org. Chem.* **1999**, *64*, 6797–6803.
[11] M. S. C. Rao, G. S. K. Rao, *Synthesis* **1987**, 231–233.

Prepared in 88% and 92% yields from 2-chloroanisole and phenylboronic acid as a colorless oil; R_f = 0.32 (hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59–7.56 (m, 2 H), 7.48–7.42 (m, 2 H), 7.38–7.33 (m, 3 H), 7.07–7.01 (m, 2 H), 3.85 (s, 3 H).

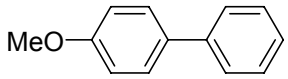
3-Methoxybiphenyl.[12]



[Table 5, entry 8 & Table 6, entry 8]

Prepared in 75% and 99% yields from 3-chloroanisole and phenylboronic acid as a colorless oil; R_f = 0.45 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64–7.62 (m, 2 H), 7.49–7.45 (m, 2 H), 7.41–7.37 (m, 2 H), 7.24–7.16 (m, 2 H), 6.95–6.92 (m, 1 H), 3.89 (s, 3 H).

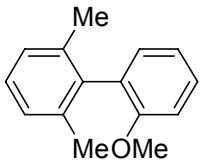
4-Methoxybiphenyl.[6]



[Table 6, entry 9]

Prepared in 80% yield from 4-chloroanisole and phenylboronic acid as a colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57–7.51 (m, 4 H), 7.44–7.40 (m, 2 H), 7.33–7.28 (m, 1 H), 7.01–6.96 (m, 2 H), 3.86 (s, 3 H).

2-Methoxyl-2',6'-dimethylbiphenyl.[13]



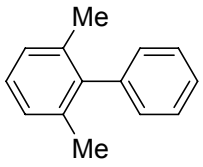
[Table 5, entry 9 & Table 6, entry 11]

Prepared in 84% and 91% yields from 2-chloro-1,3-dimethylbenzene and 2-methoxybenzeneboronic acid as a colorless oil; R_f = 0.40 (hexane); ^{1}H NMR (400 MHz,

[12] T. Mino, Y. Shirae, M. Sakamoto, T. Fujita, *J. Org. Chem.* **2005**, *70*, 2191–2194.
[13] J. M. Saa, G. Martrorell, A. Garcia-Roso, *J. Org. Chem.* **1992**, *57*, 678–685.

$CDCl_3$) δ 7.25–7.21 (m, 1 H), 7.08–6.99 (m, 3 H), 6.94–6.86 (m, 3 H), 3.61 (s, 3 H), 1.92 (s, 6 H).

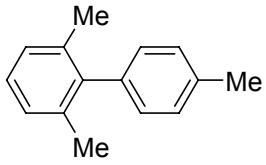
2,6-Dimethylbiphenyl.[6]



[Table 5, entry 10 & Table 6, entry 10]

Prepared in 53% and 94% yields from 2-chloro-1,3-dimethylbenzene and phenylboronic acid as a colorless oil; R_f = 0.82 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34–7.24 (m, 3 H), 7.07–6.98 (m, 5 H), 1.93 (s, 6 H).

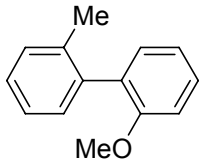
2,6,4'-Trimethylbiphenyl.[14]



[Table 5, entry 11]

Prepared in 28% yield from 2-chloro-1,3-dimethylbenzene and 4-tolueneboronic acid as a colorless oil; R_f = 0.62 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33–7.12 (m, 7 H), 2.50 (s, 3 H), 2.14 (s, 6 H).

2-Methoxy-2'-methylbiphenyl.[15]



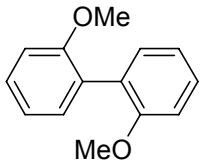
[Table 5, entries 12 and 16 & Table 6, entry 12]

Prepared in 86% and 85% yields from 2-chlorotoulene and 2-methoxybenzeneboronic acid as a white solid; R_f = 0.32 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41–7.35 (m, 1 H), 7.30–

[14] R. Singh, M. S. Viciu, N. Kramareva, O. Navarro, S. P. Nolan, *Org. Lett.* **2005**, *7*, 1829–1832.
[15] D. A. Widdowson, Y.-Z. Zhang, *Tetrahedron* **1986**, *42*, 2111–2116.

7.18 (m, 5 H), 7.08–6.99 (m, 2 H), 3.77 (s, 3 H), 2.18 (s, 3 H).

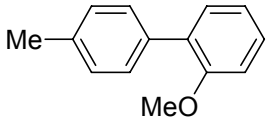
2,2'-Dimethoxybiphenyl.[16]



[Table 5, entry 13 & Table 6, entry 13]

Prepared in 47% and 78% yields from 1-chloro-2-anisole and 2-methoxybenzeneboronic acid as a white solid; R_f = 0.30 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41–7.30 (m, 4 H), 7.09–7.02 (m, 4 H), 3.83 (s, 6 H).

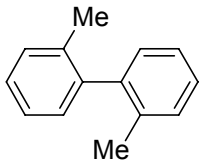
2-Methoxy-4'-methylbiphenyl.[6]



[Table 5, entry 14 & Table 6, entry 14]

Prepared in 54% and 92% yields from 4-chlorotoluene and 2-methoxybenzeneboronic acid as a colorless oil; R_f = 0.38 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52–7.28 (m, 6 H), 7.09–7.02 (m 2 H), 3.86 (s, 3 H), 2.46 (s, 3 H).

2,2'-Dimethylbiphenyl.[17]

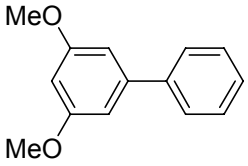


[Table 5, entry 15]

Prepared in 35% yield from 2-chlorotoluene and 2-toluneboronic acid as a colorless oil; R_f = 0.53 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.7.30–7.10 (m, 8 H), 2.07 (s, 6 H).

[16] V. Courtois, R. Barhdadi, M. Troupel, J. Périchon, *Tetrahedron* **1997**, *53*, 11569–11576.
[17] A. F. Littke, C. Dai, G. C. Fu, *J. Am. Chem. Soc.* **2000**, *122*, 4020–4028.

3,5-Dimethoxybiphenyl (23).[18]



23 [Table 6, entry 15]

Prepared in 97% yield from 5-chloro-1,3-dimethoxybenzene and phenylboronic acid as a colorless oil; R_f = 0.22 (4.8% EtOAc–hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61–7.36 (m, 5 H), 6.75 (d, *J* = 2.0 H), 6.49 (t, *J* = 2.8 Hz, 1 H), 3.86 (s, 6 H).

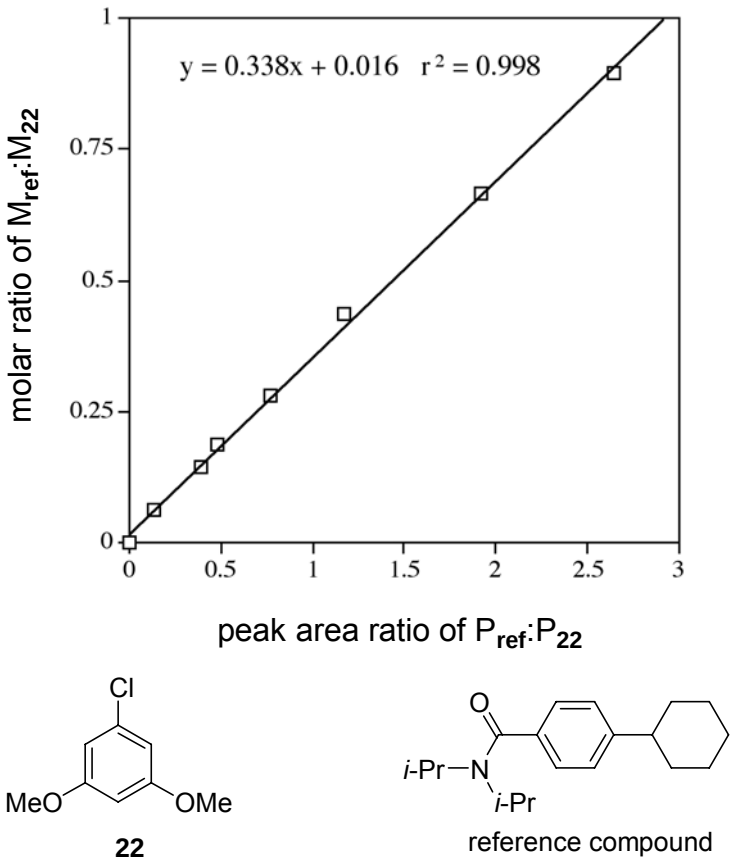
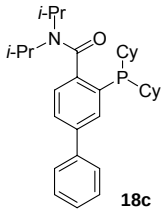


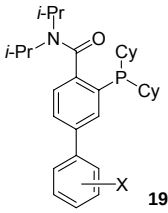
Figure S1. Working curve for quantitative HPLC analysis of **22**.

[18] C. Song, Y. Ma, Q. chai, C. Ma, W. Jiang, M. B. Andrus, *Tetrahedron* **2005**, *61*, 7438–7446.

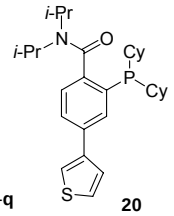
Table S1. Microwave-based high-throughput screening for Aphos ligands[a]



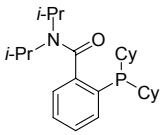
18c



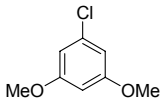
19a-q



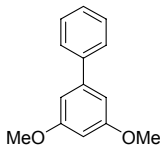
20



21



22

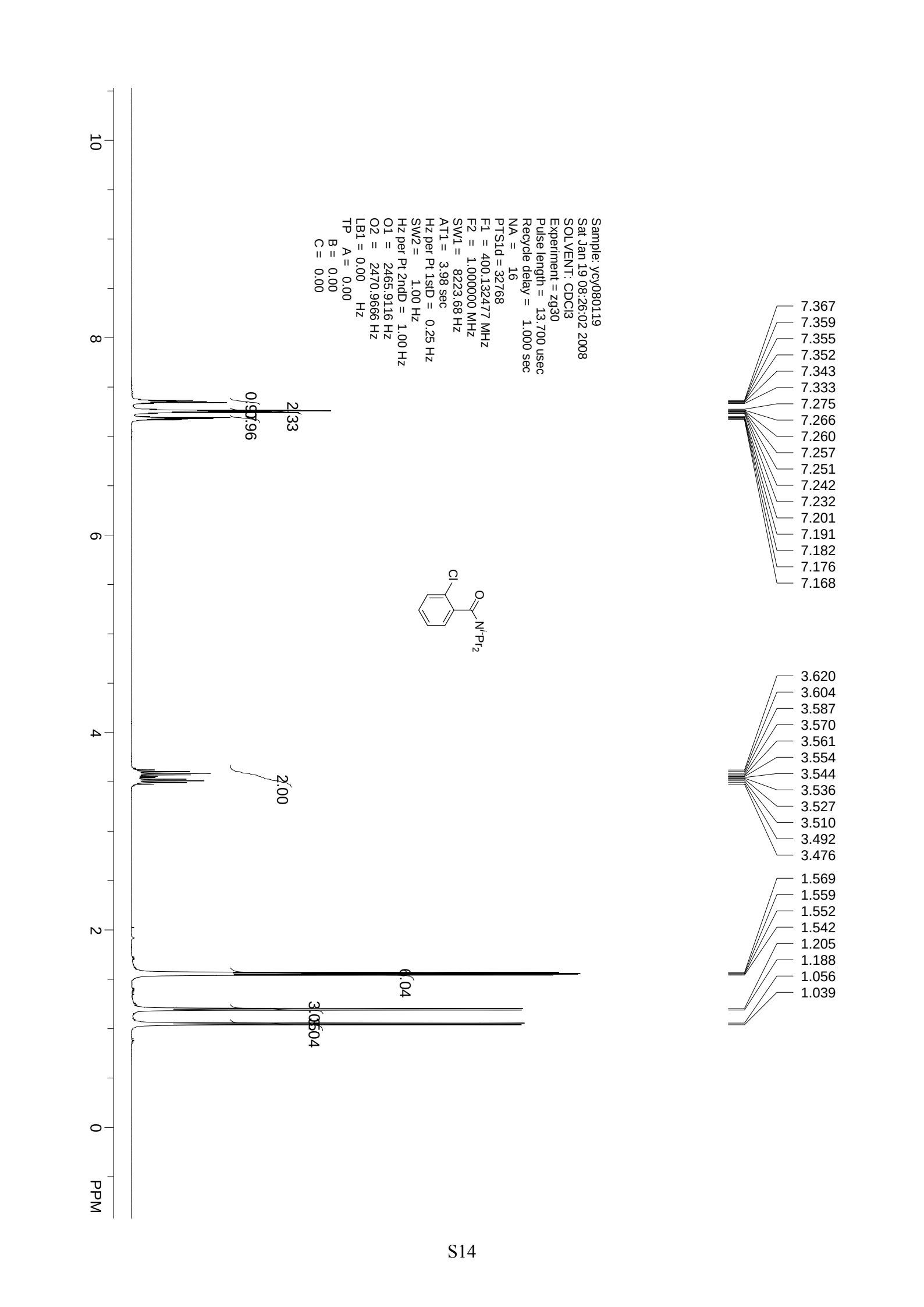


23

Entry	Aphos	Conversion of **22** (%)[b]	**23**: Yield (%)[c]	Calibrated conversion of **22** (%)[d]	Relative efficiency (%)[e]
1	**19a**: X = 3-Ph	63	–	63	–14
2	**20**	70	–	66	–11
3	**19b**: X = 2-OMe	69	68	67	–10
4	**19c**: X = 4-F	74	–	73	–4
5	**19d**: X = 2-Me,4-F	75	–	74	–3
6	**19e**: X = 4-Me	75	75	75	–2
7	**18c**	76	75	76	–1
8	**21**	77	–	77	0
9	**19f**: X = 4-OMe	80	–	80	3
10	**19g**: X = 3-OMe	80	–	80	3
11	**19h**: X = 2,6-Me_2	80	79	81	4
12	**19i**: X = 2-Me	81	80	82	5
13	**19j**: X = 3-CF_3	83	–	83	6
14	**19k**: X = 3-Me,4-F	83	–	83	6
15	**19l**: X = 3,4,5-F_3	84	–	85	8
16	**19m**: X = 3,4-benzo	86	–	87	10
17	**19n**: X = 3-F,4-Ph	85	–	87	10
18	**19o**: X = 2,3-benzo	84	83	89	12
19	**19p**: X = 4-SMe	88	88	90	13
20	**19q**: X = 3-NO_2	90	87	97	20

[a]Aphos ligands were generated via SAME as given in Scheme 3 of the main text. The structures of **18c**, **19a**–**q**, **20**, and **21** were validated by ^{31}P NMR and the purities were estimated by the integration of ^{31}P signals of the catalyst mixture (see Table 1 in the

main text for detail). [b]Determined by HPLC analysis of the reaction mixture. [c]Isolated yield of **23**. [d]Calculated according to the integration of ^{31}P signals of the Aphos mixture by the formula of [calibrated conversion %] = {[conversion %] – [(integrations of **21** and **17a**) x 77%]} / [integration of Aphos (**18c**, **19a**–**q**, **20**)]. It is assumed that during the reaction of **22** with $PhB(OH)_2$, **17a** remained in the catalyst mixture is converted into the Aphos **18c**, which has a similar efficiency as the Aphos **21**. [e]Defined as the difference in calibrated conversions between the Aphos (**18c**, **19a**–**q**, **20**) and **21**. The negative values indicate a diminished efficiency of the new Aphos ligands and *vice versa*.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SOLVENT: CDCl3
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NA = 16
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F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 3.98 sec
Hz per Pt 1stD = 0.25 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2465.9116 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
Cl
O
N^{i}Pr$_2$
7.367
7.359
7.355
7.352
7.343
7.333
7.275
7.266
7.260
7.257
7.251
7.242
7.232
7.201
7.191
7.182
7.176
7.168
3.620
3.604
3.587
3.570
3.561
3.554
3.544
3.536
3.527
3.510
3.492
3.476
1.569
1.559
1.552
1.542
1.205
1.188
1.056
1.039
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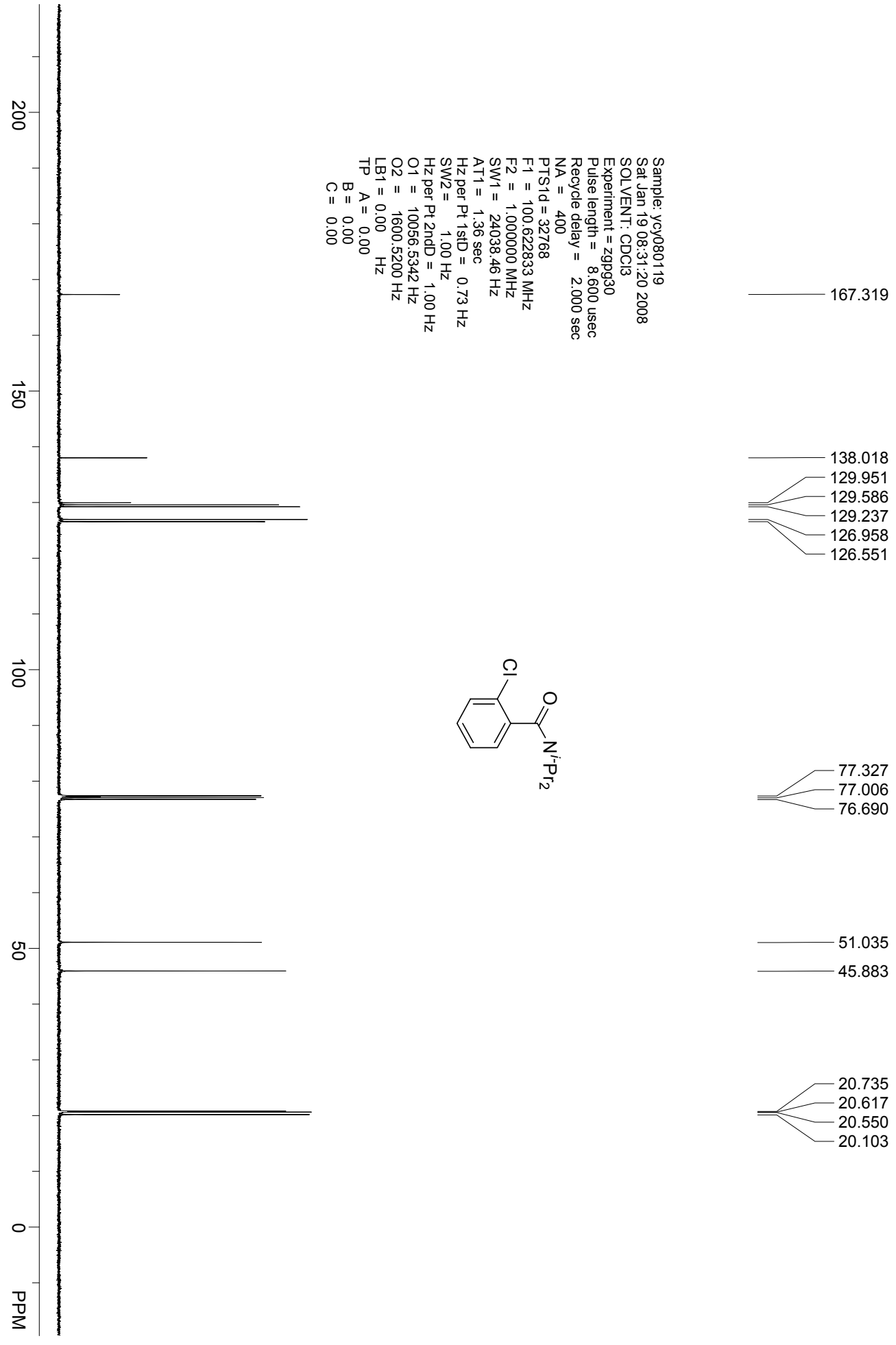
0.96
2.00
6.04
3.05
3.04
10
8
6
4
2
0
PPM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Recycle delay = 2.000 sec
NA = 400
PTS1d = 32768
F1 = 100.622833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10056.5342 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
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O
N-iPr2
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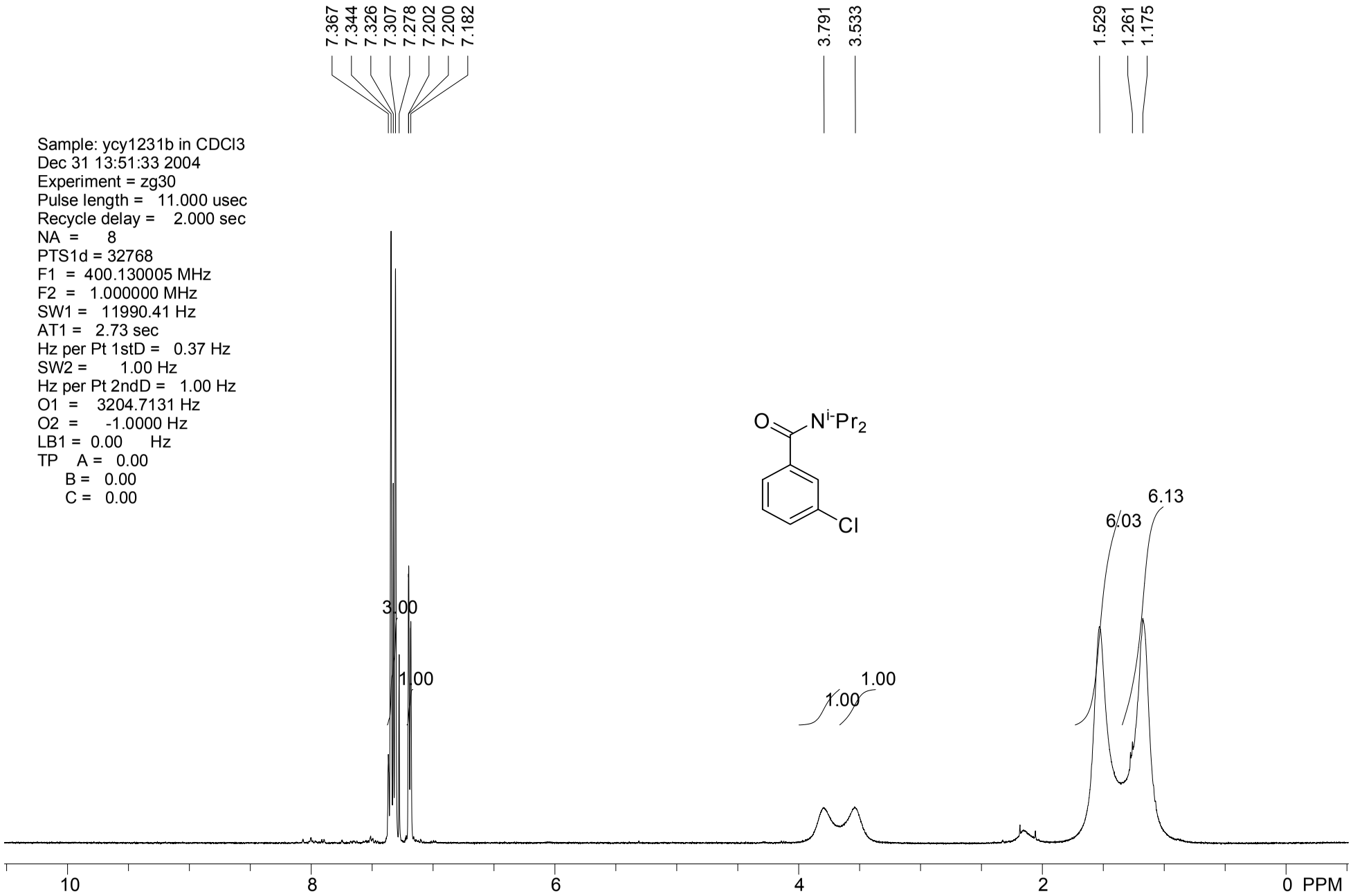
138.018
129.951
129.586
129.237
126.958
126.551
77.327
77.006
76.690
51.035
45.883
20.735
20.617
20.550
20.103
200
150
100
50
0
PPM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7.344
7.326
7.307
7.278
7.202
7.200
7.182
3.791
3.533
1.529
1.261
1.175
Sample: ycy1231b in CDCl3
Dec 31 13:51:33 2004
Experiment = zg30
Pulse length = 11.000 usec
Recycle delay = 2.000 sec
NA = 8
PTS1d = 32768
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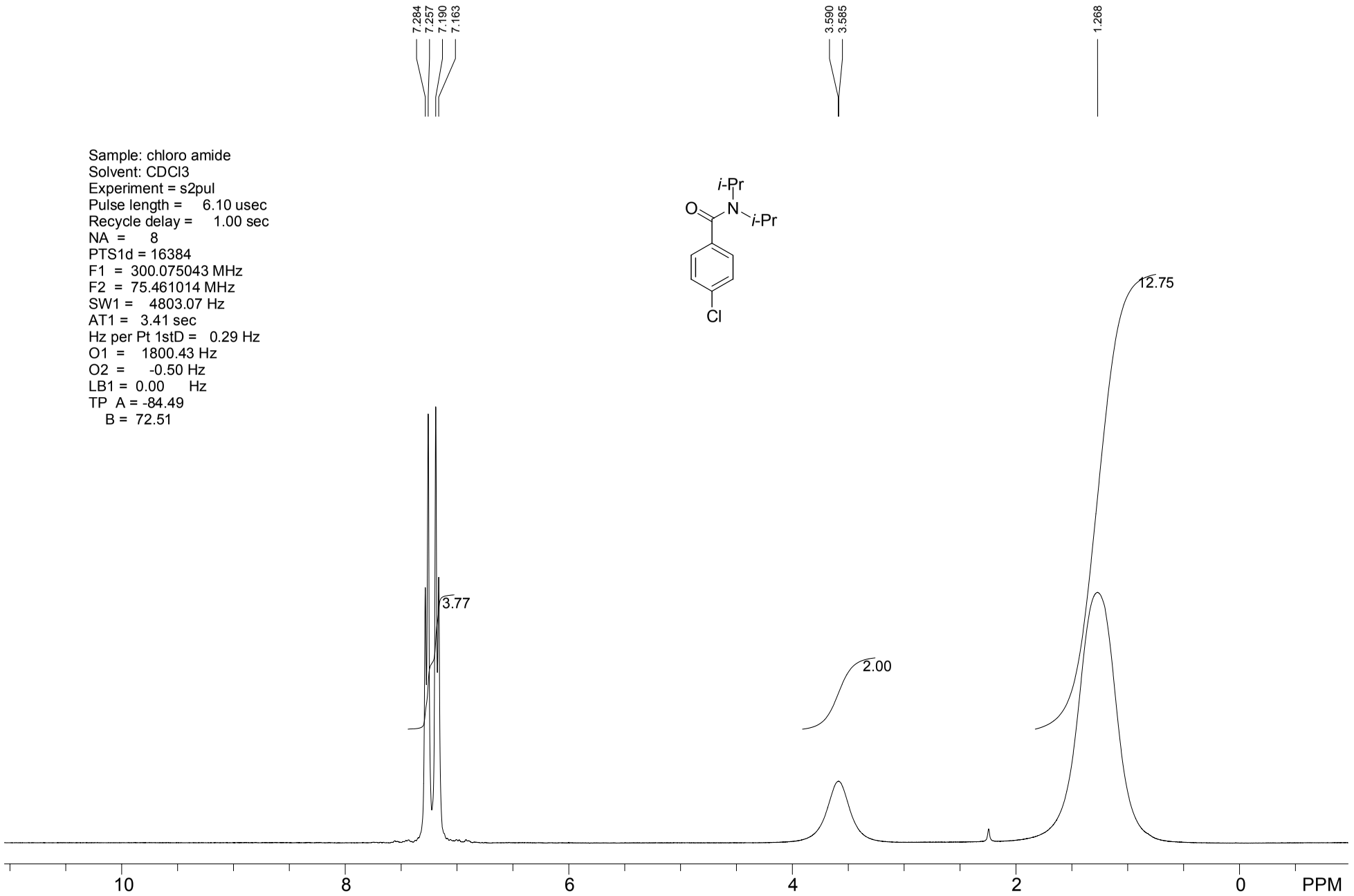
F2 = 1.000000 MHz
SW1 = 11990.41 Hz
AT1 = 2.73 sec
Hz per Pt 1stD = 0.37 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 3204.7131 Hz
O2 = -1.0000 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
N^i-Pr2
Cl
3.00
1.00
1.00
1.00
6.03
6.13
10
8
6
4
2
0 PPM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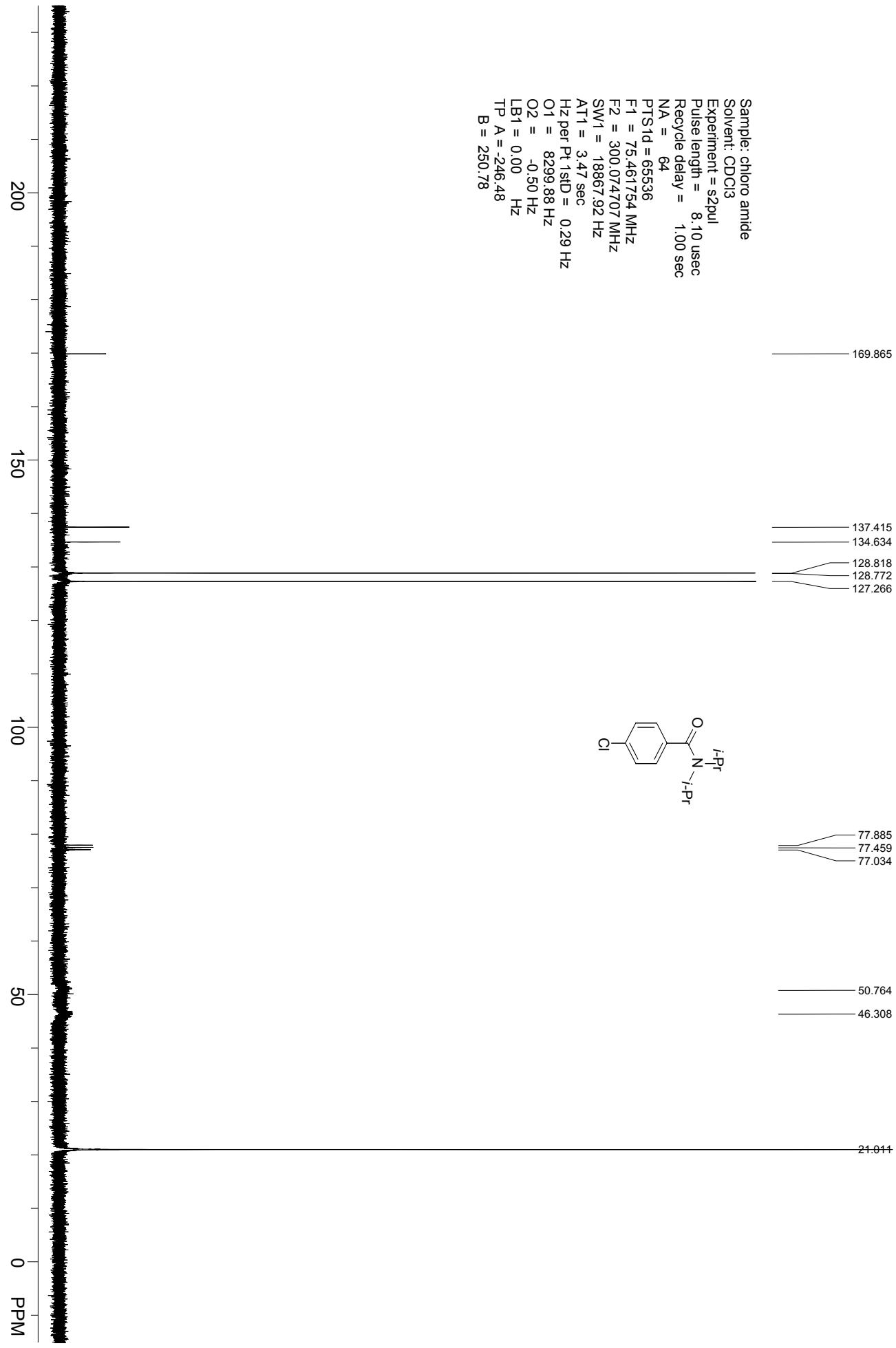
7.257
7.190
7.163
3.590
3.585
1.268
Sample: chloro amide
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1800.43 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -84.49
B = 72.51
i-Pr
O
N
i-Pr
Cl
12.75
3.77
2.00
10
8
6
4
2
0
PPM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Solvent: CDCl3
Experiment = s2pul
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Recycle delay = 1.00 sec
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PTS1d = 65536
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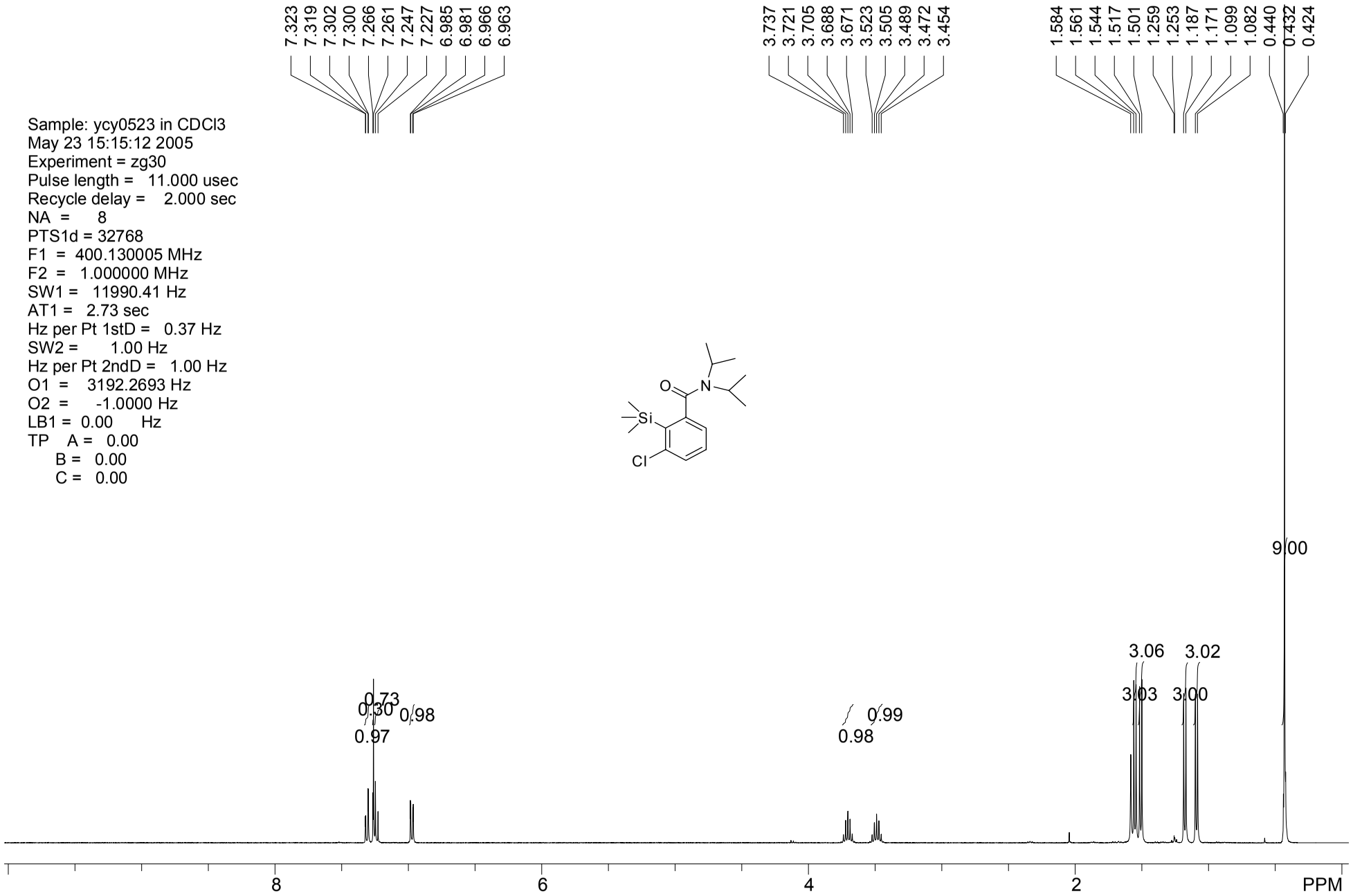
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -246.48
B = 250.78
169.865
137.415
134.634
128.818
128.772
127.266
77.885
77.459
77.034
50.764
46.308
21.011
Cl
O
N
i-Pr
i-Pr
200
150
100
50
0
PPM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7.300
7.266
7.261
7.247
7.227
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6.981
6.966
6.963
3.737
3.721
3.705
3.688
3.671
3.523
3.505
3.489
3.472
3.454
1.584
1.561
1.544
1.517
1.501
1.259
1.253
1.187
1.171
1.099
1.082
0.440
0.432
0.424
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May 23 15:15:12 2005
Experiment = zg30
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Recycle delay = 2.000 sec
NA = 8
PTS1d = 32768
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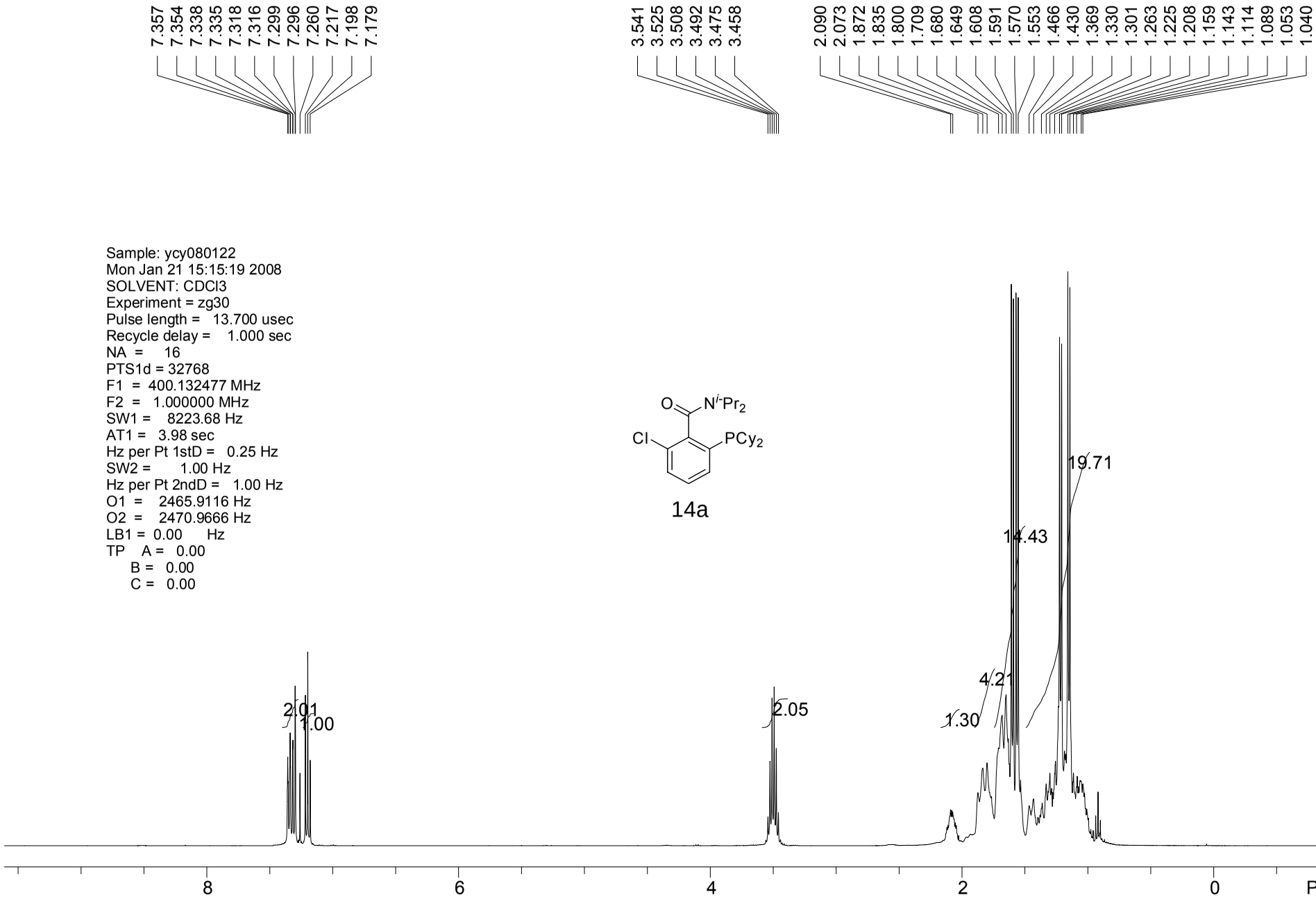
F2 = 1.000000 MHz
SW1 = 11990.41 Hz
AT1 = 2.73 sec
Hz per Pt 1stD = 0.37 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 3192.2693 Hz
O2 = -1.0000 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
N
Si
Cl
9.00
3.06
3.02
3.03
3.00
0.73
0.30
0.98
0.97
0.99
0.98
8
6
4
2
PPM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7.198
7.179
3.541
3.525
3.508
3.492
3.475
3.458
2.090
2.073
1.872
1.835
1.800
1.709
1.680
1.649
1.608
1.591
1.570
1.553
1.466
1.430
1.369
1.330
1.301
1.263
1.225
1.208
1.159
1.143
1.114
1.089
1.053
1.040
Sample: ycy080122
Mon Jan 21 15:15:19 2008
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 13.700 usec
Recycle delay = 1.000 sec
NA = 16
PTS1d = 32768
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 3.98 sec
Hz per Pt 1stD = 0.25 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2465.9116 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
N^{i}Pr$_2$
Cl
PCy$_2$
14a
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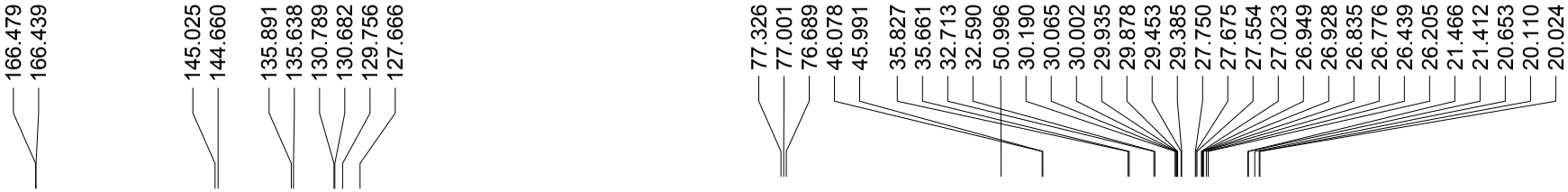
1.00
2.05
1.30
4.21
14.43
19.71
8
6
4
2
0
PPM
S20



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Mon Jan 21 15:29:25 2008
SOLVENT: CDCl3
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Recycle delay = 2.000 sec
NA = 11003
PTS1d = 32768
F1 = 100.622833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
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O2 = 1600.5200 Hz
LB1 = 0.00 Hz
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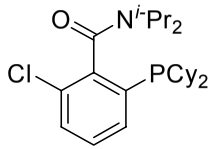
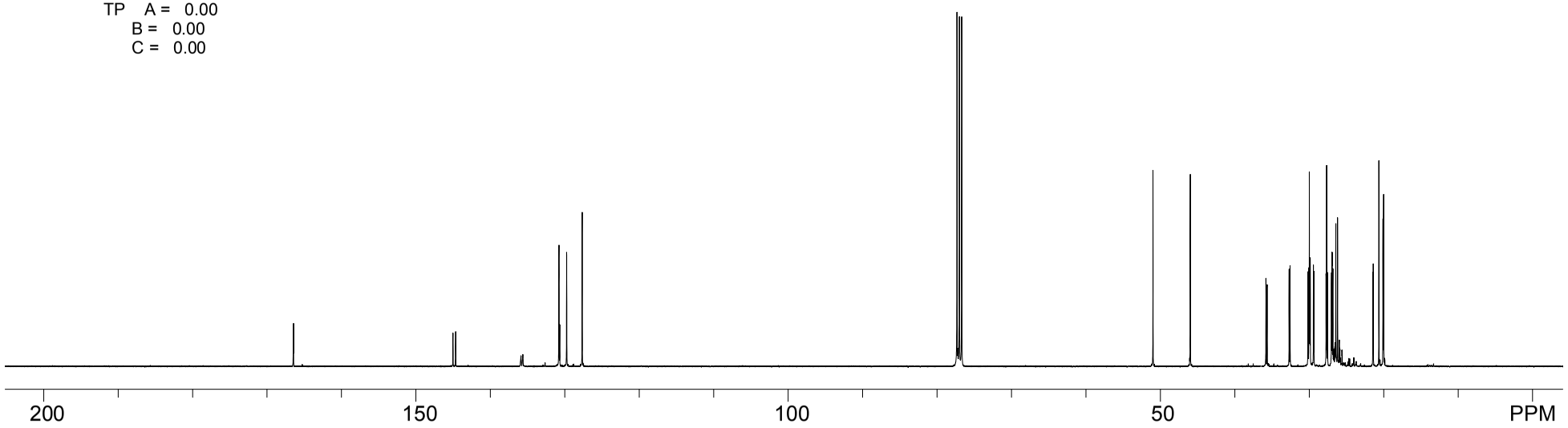
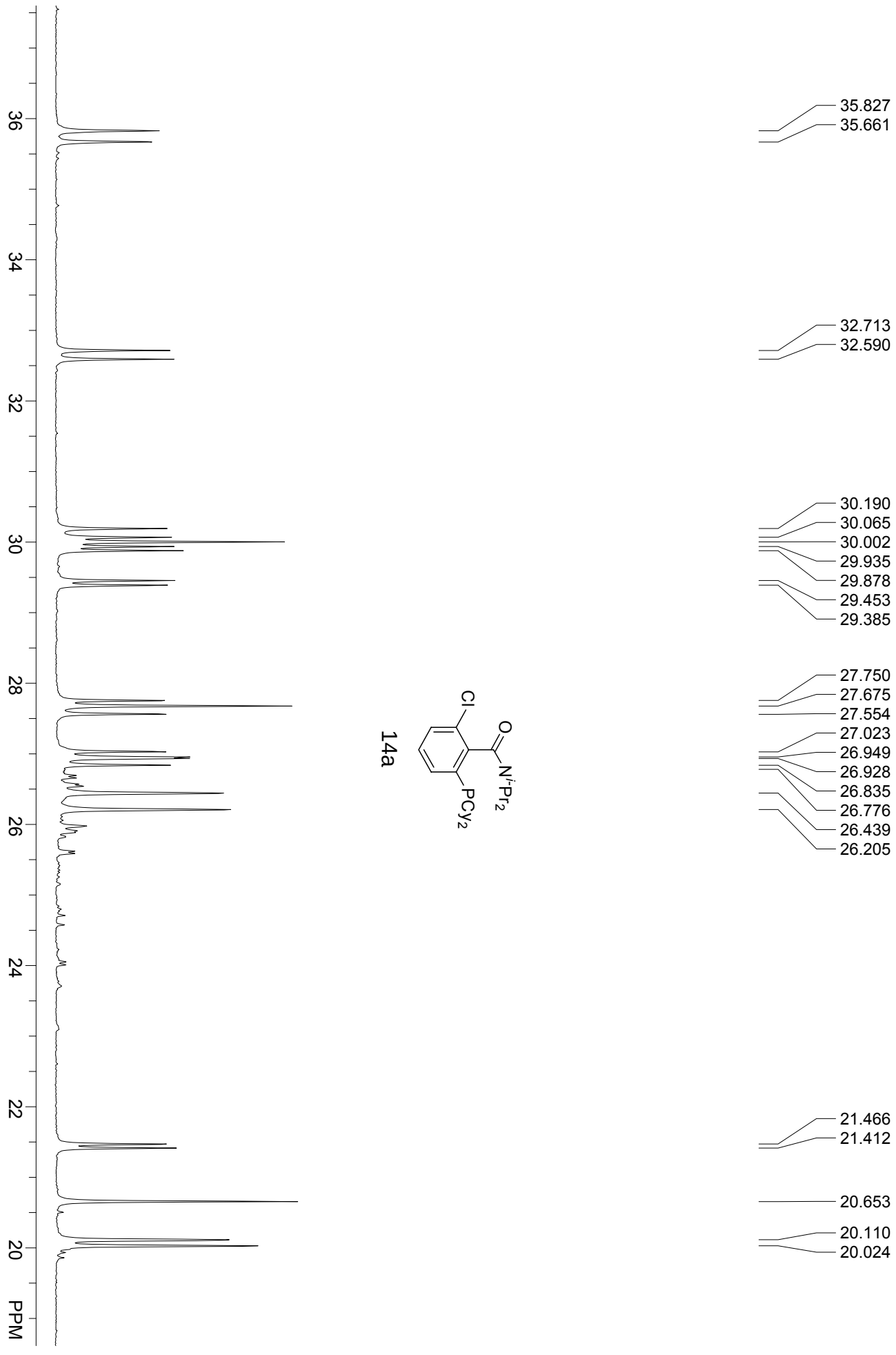
B = 0.00
C = 0.00



14a

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30.190
30.065
30.002
29.935
29.878
29.453
29.385
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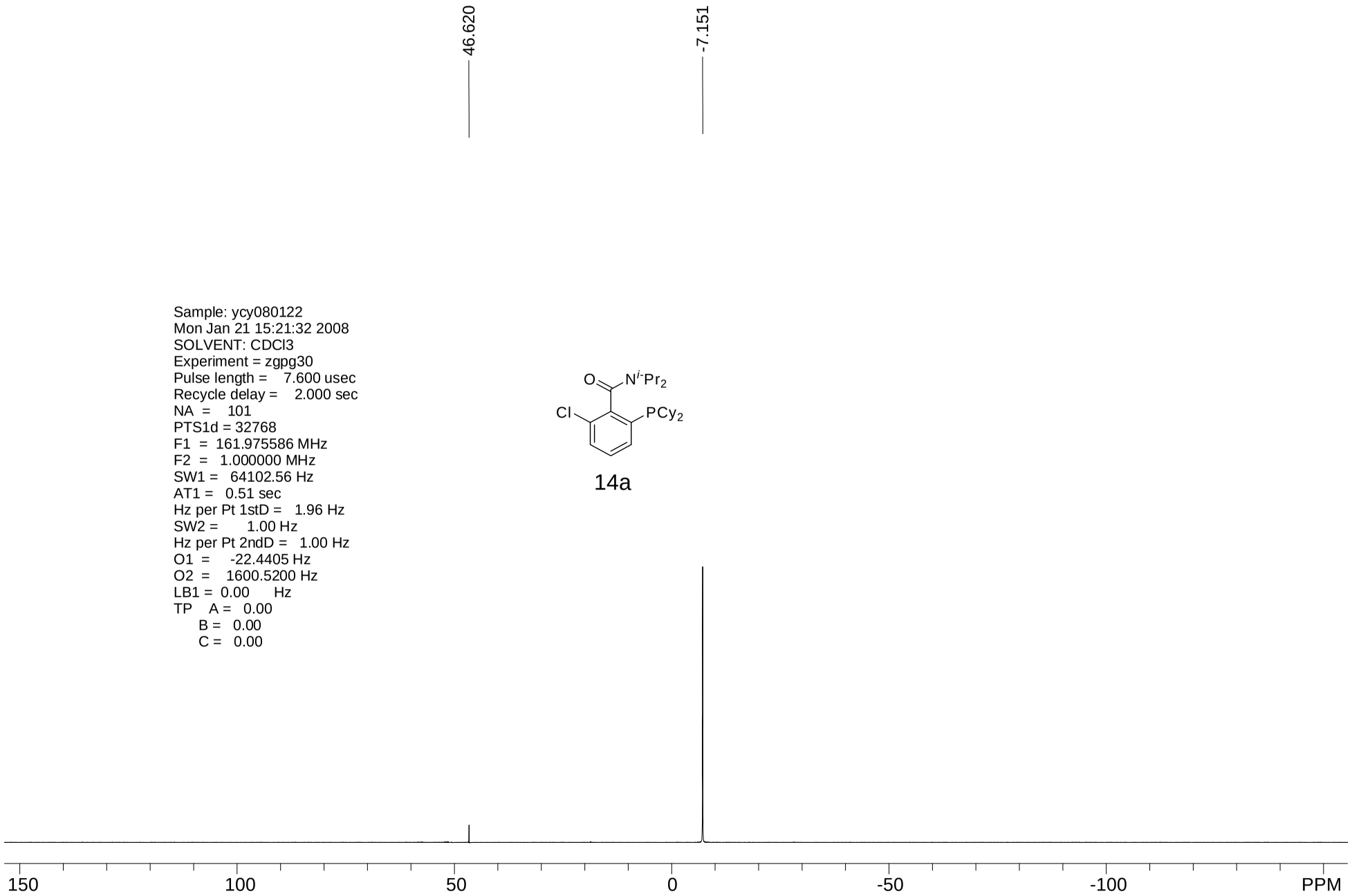
27.554
27.023
26.949
26.928
26.835
26.776
26.439
26.205
21.466
21.412
20.653
20.110
20.024
36
34
32
30
28
26
24
22
20
PPM
Cl
O
N^{i}Pr$_2$
PCy$_2$
14a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-7.151
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Mon Jan 21 15:21:32 2008
SOLVENT: CDCl3
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Pulse length = 7.600 usec
Recycle delay = 2.000 sec
NA = 101
PTS1d = 32768
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F2 = 1.000000 MHz
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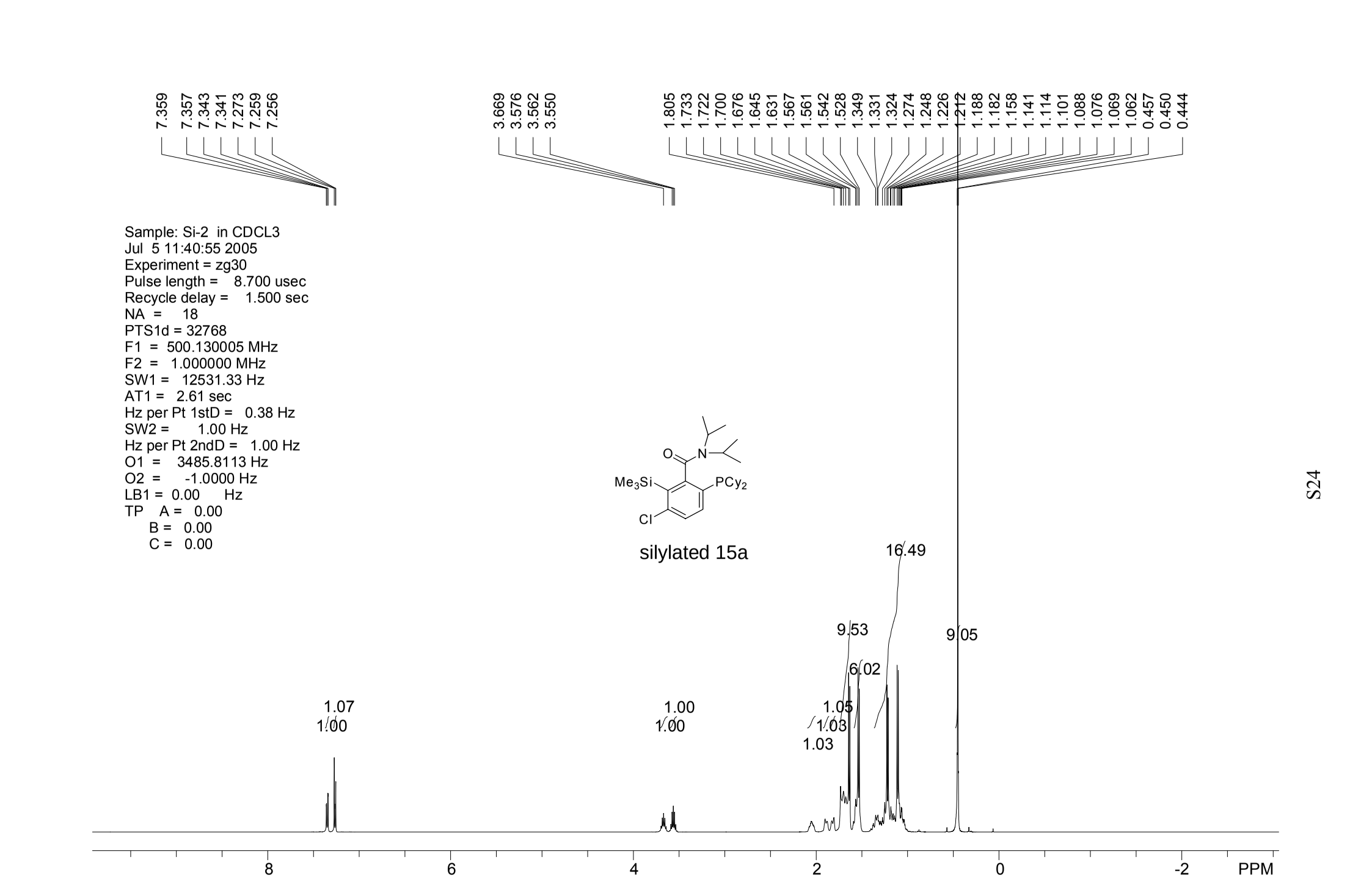
AT1 = 0.51 sec
Hz per Pt 1stD = 1.96 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = -22.4405 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
N^{i}Pr$_2$
Cl
PCy$_2$
14a
150
100
50
0
-50
-100
PPM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7.259
7.256
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3.576
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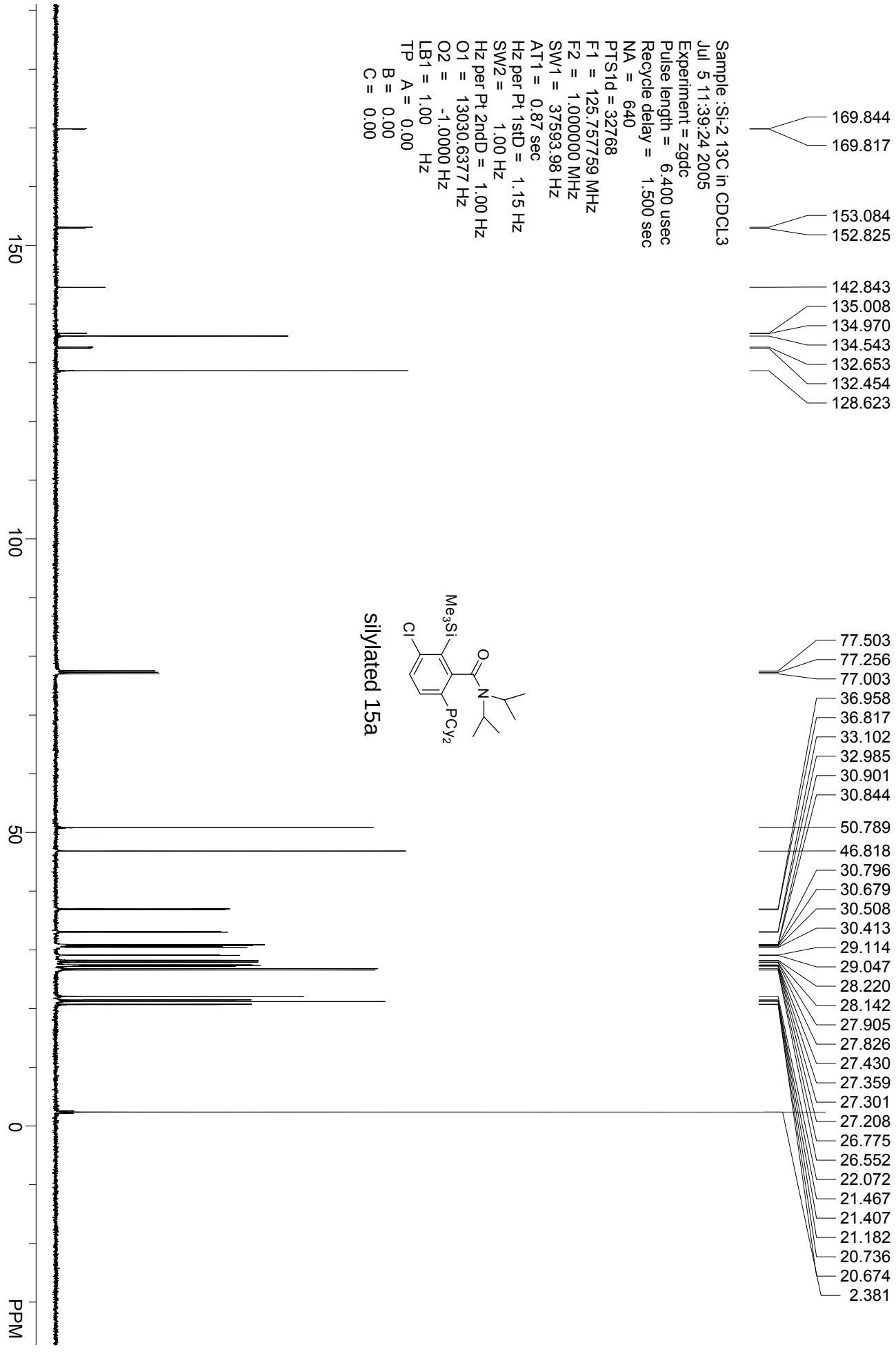
3.550
1.805
1.733
1.722
1.700
1.676
1.645
1.631
1.567
1.561
1.542
1.528
1.349
1.331
1.324
1.274
1.248
1.226
1.212
1.188
1.182
1.158
1.141
1.114
1.101
1.088
1.076
1.069
1.062
0.457
0.450
0.444
Sample: Si-2 in CDCL3
Jul 5 11:40:55 2005
Experiment = zg30
Pulse length = 8.700 usec
Recycle delay = 1.500 sec
NA = 18
PTS1d = 32768
F1 = 500.130005 MHz
F2 = 1.000000 MHz
SW1 = 12531.33 Hz
AT1 = 2.61 sec
Hz per Pt 1stD = 0.38 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 3485.8113 Hz
O2 = -1.0000 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
N
Me3Si
PCy2
Cl
silylated 15a
16.49
9.53
9.05
6.02
1.07
1.00
1.00
1.00
1.05
1.03
1.03
8
6
4
2
0
-2
PPM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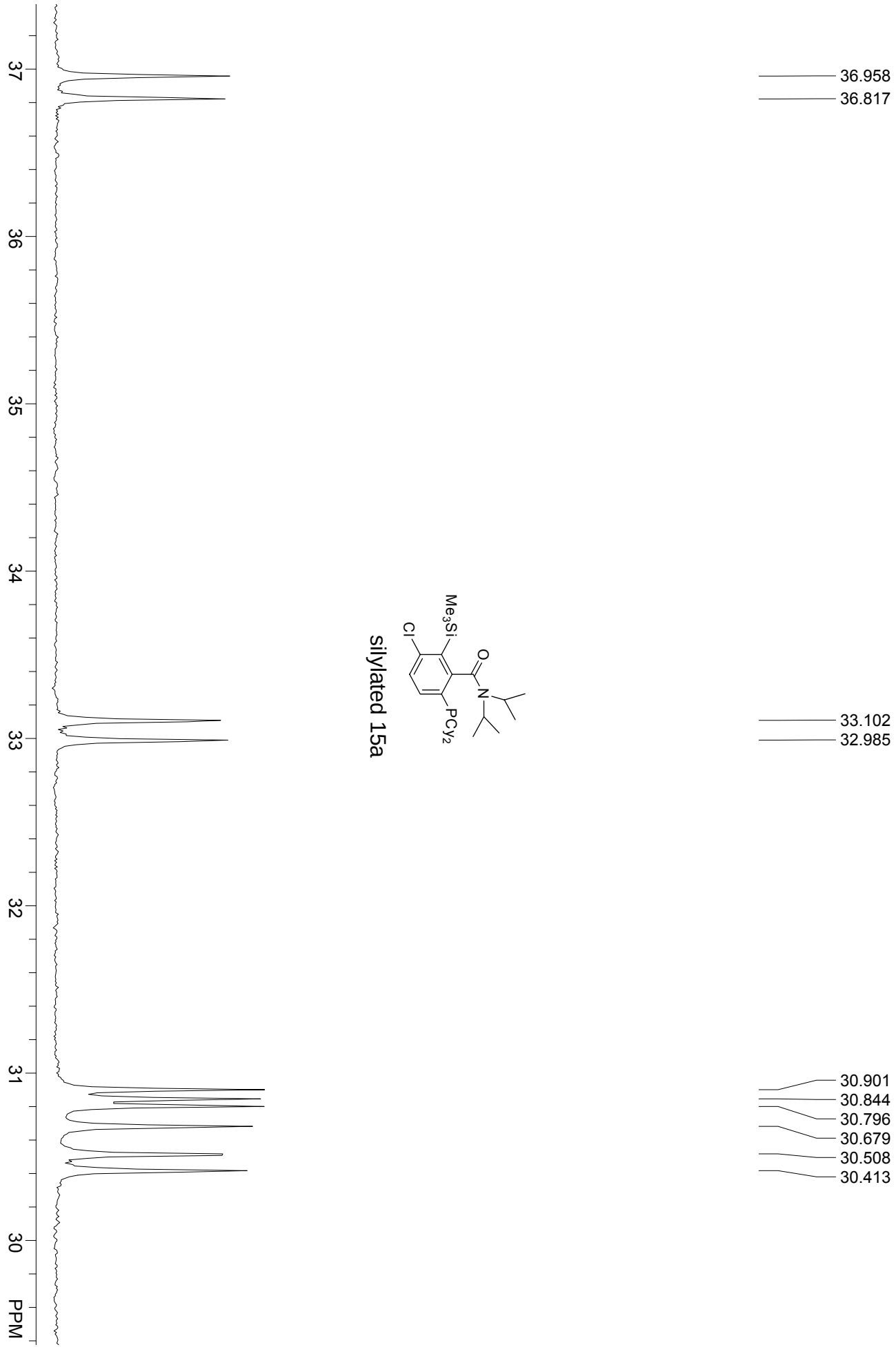
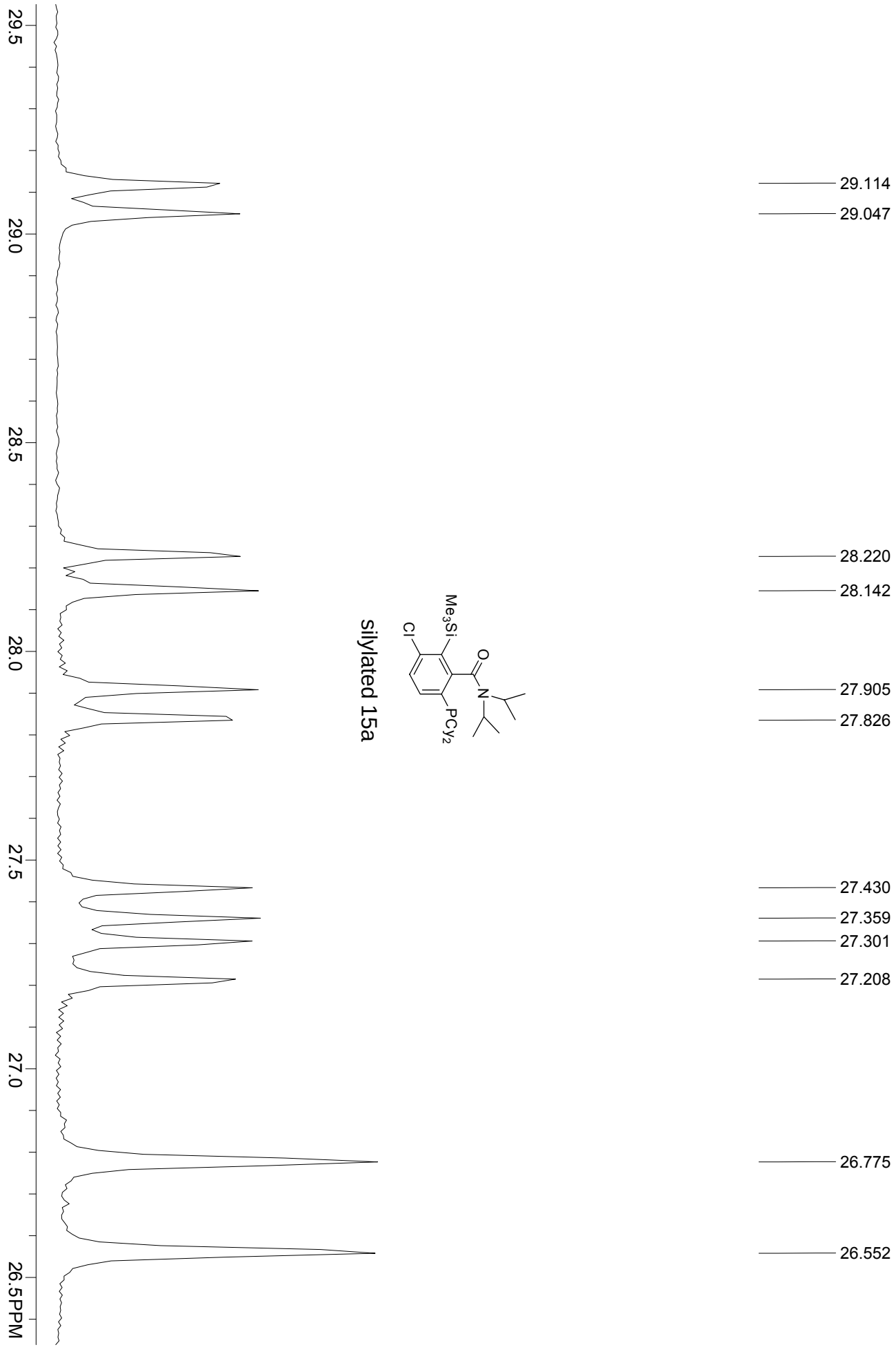
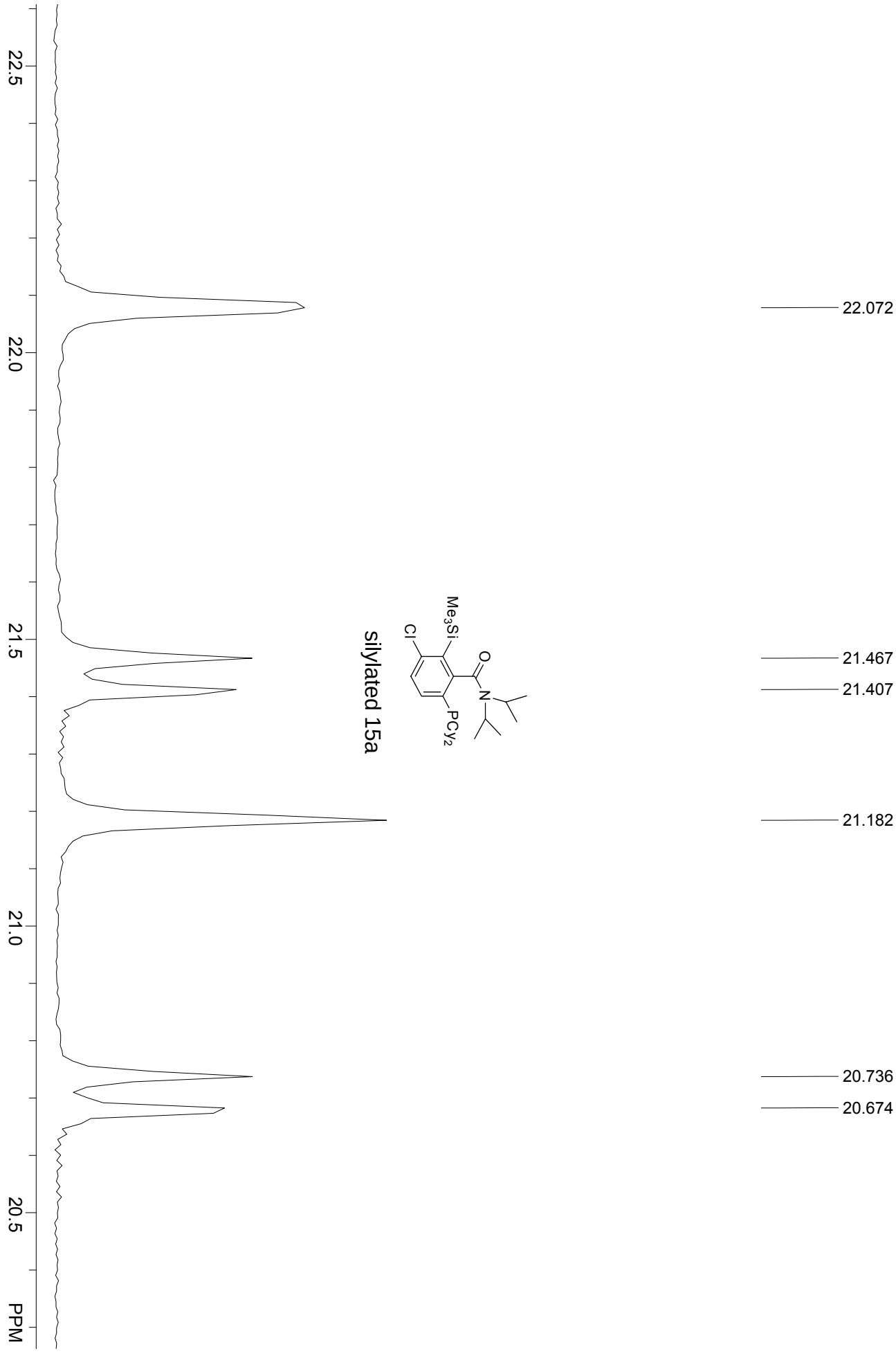
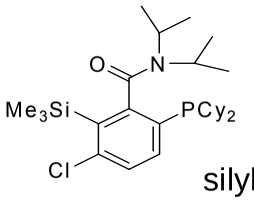
Jul 5 11:39:24 2005
Experiment = zgdc
Pulse length = 6.400 usec
Recycle delay = 1.500 sec
NA = 640
PTS1d = 32768
F1 = 125.757759 MHz
F2 = 1.000000 MHz
SW1 = 37593.98 Hz
AT1 = 0.87 sec
Hz per Pt 1stD = 1.15 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 13030.6377 Hz
O2 = -1.0000 Hz
LB1 = 1.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
169.844
169.817
153.084
152.825
142.843
135.008
134.970
134.543
132.653
132.454
128.623
77.503
77.256
77.003
36.958
36.817
33.102
32.985
30.901
30.844
50.789
46.818
30.796
30.679
30.508
30.413
29.114
29.047
28.220
28.142
27.905
27.826
27.430
27.359
27.301
27.208
26.775
26.552
22.072
21.467
21.407
21.182
20.736
20.674
2.381
Me3Si
Cl
O
N
PCy2
silylated 15a
150
100
50
0
PPM


37
36
35
34
33
32
31
30
PPM
36.958
36.817
33.102
32.985
30.901
30.844
30.796
30.679
30.508
30.413
silylated 15a
Me3Si
Cl
O
N
PCy2

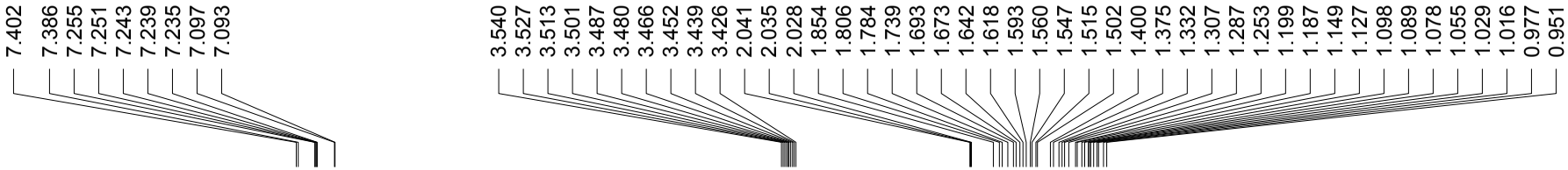

29.5
29.0
28.5
28.0
27.5
27.0
26.5PPM
29.114
29.047
28.220
28.142
27.905
27.826
27.430
27.359
27.301
27.208
26.775
26.552
silylated 15a
Me3Si
Cl
O
N
PCy2


22.5
22.0
21.5
21.0
20.5
PPM
22.072
21.467
21.407
21.182
20.736
20.674
silylated 15a
Me3Si
Cl
O
N
PCy2

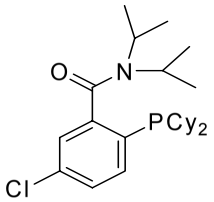
Sample :Si-2 31P in CDCL3
Jul 4 17:18:01 2005
Experiment = zgdc
Pulse length = 4.000 usec
Recycle delay = 3.000 sec
NA = 124
PTS1d = 32768
F1 = 202.456039 MHz
F2 = 1.000000 MHz
SW1 = 60606.06 Hz
AT1 = 0.54 sec
Hz per Pt 1stD = 1.85 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 42.5390 Hz
O2 = -1.0000 Hz
LB1 = 2.00 Hz
TP A = 0.00
B = 0.00
C = 0.00



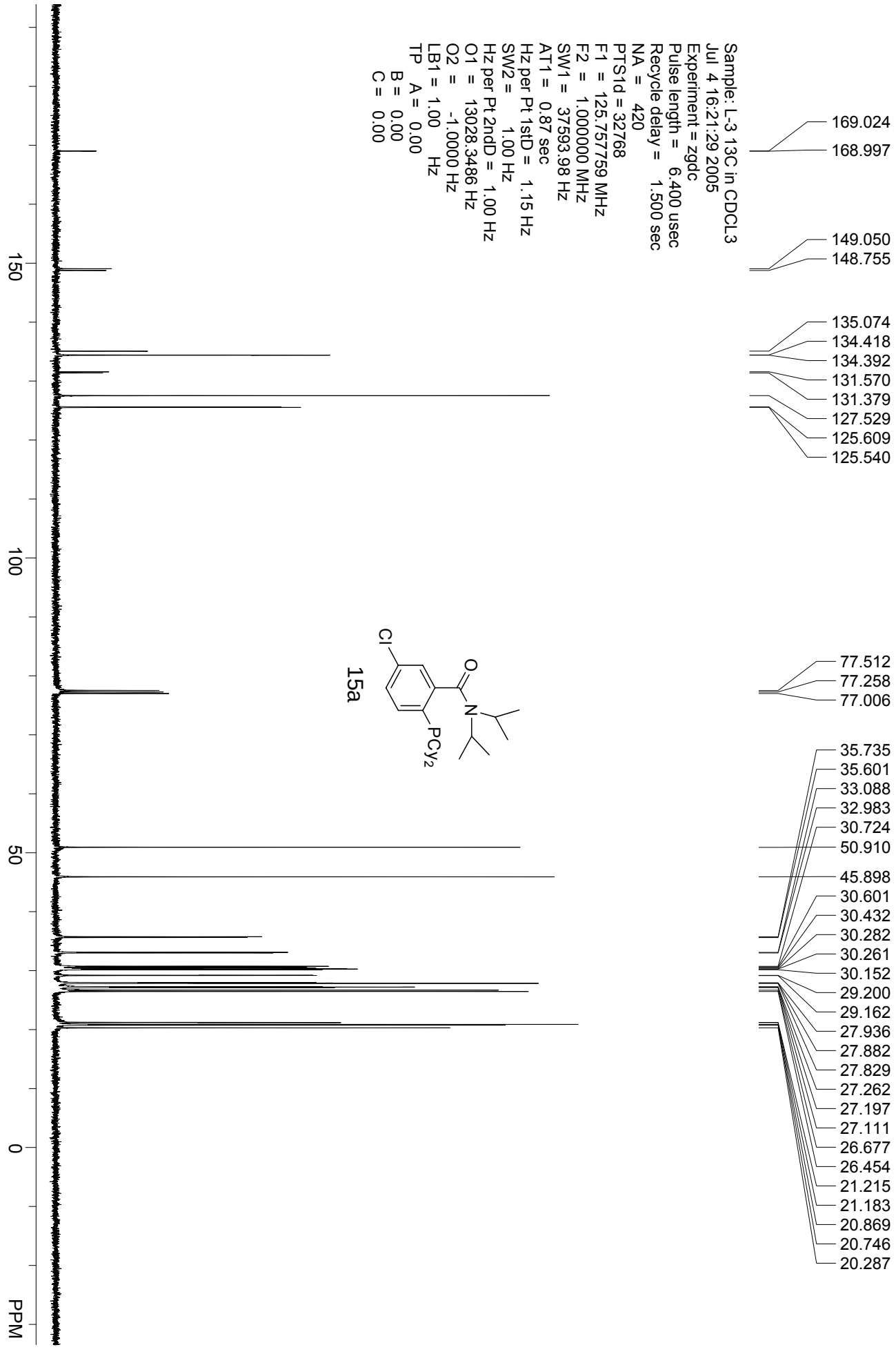
silylated 15a

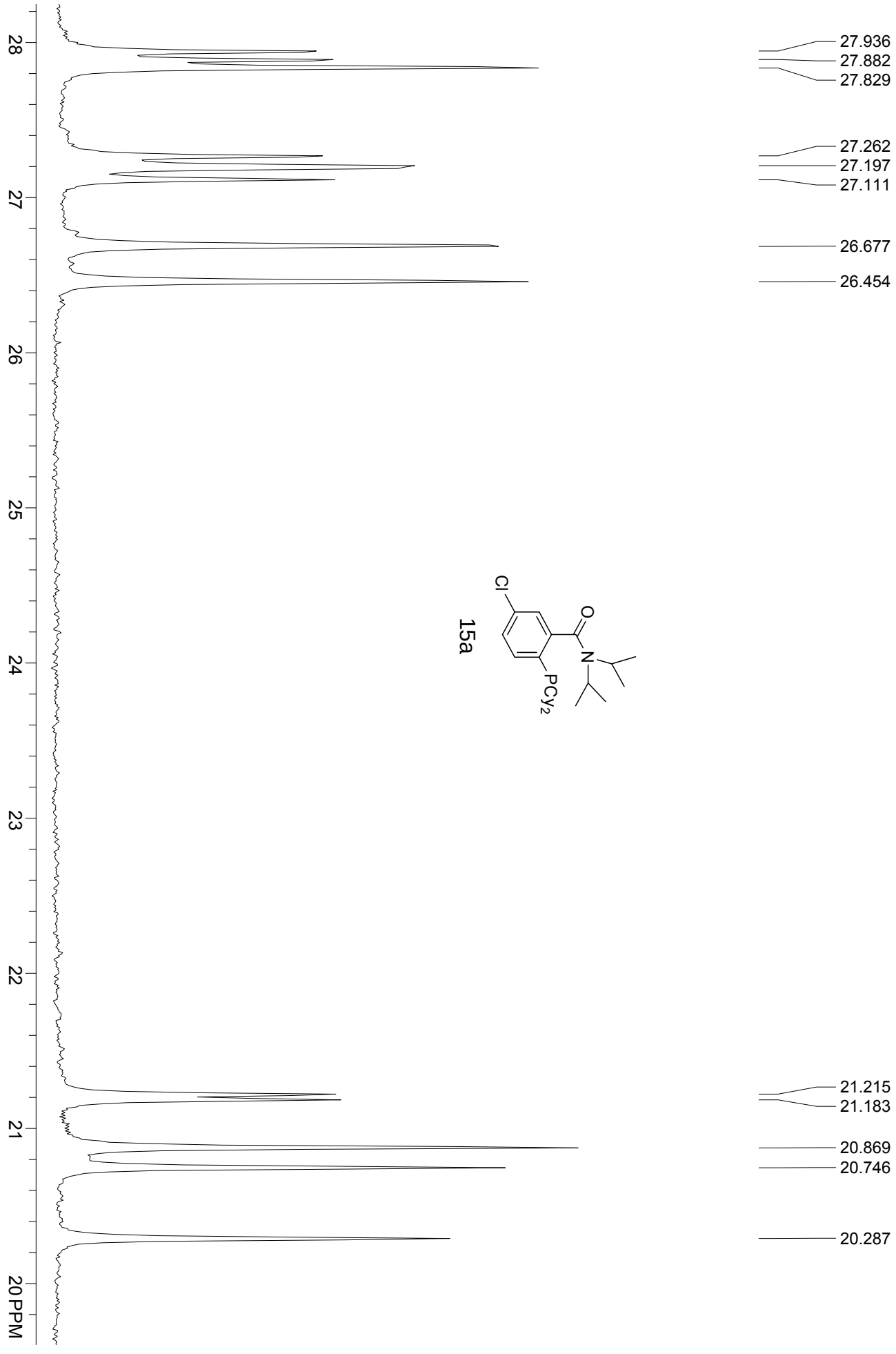


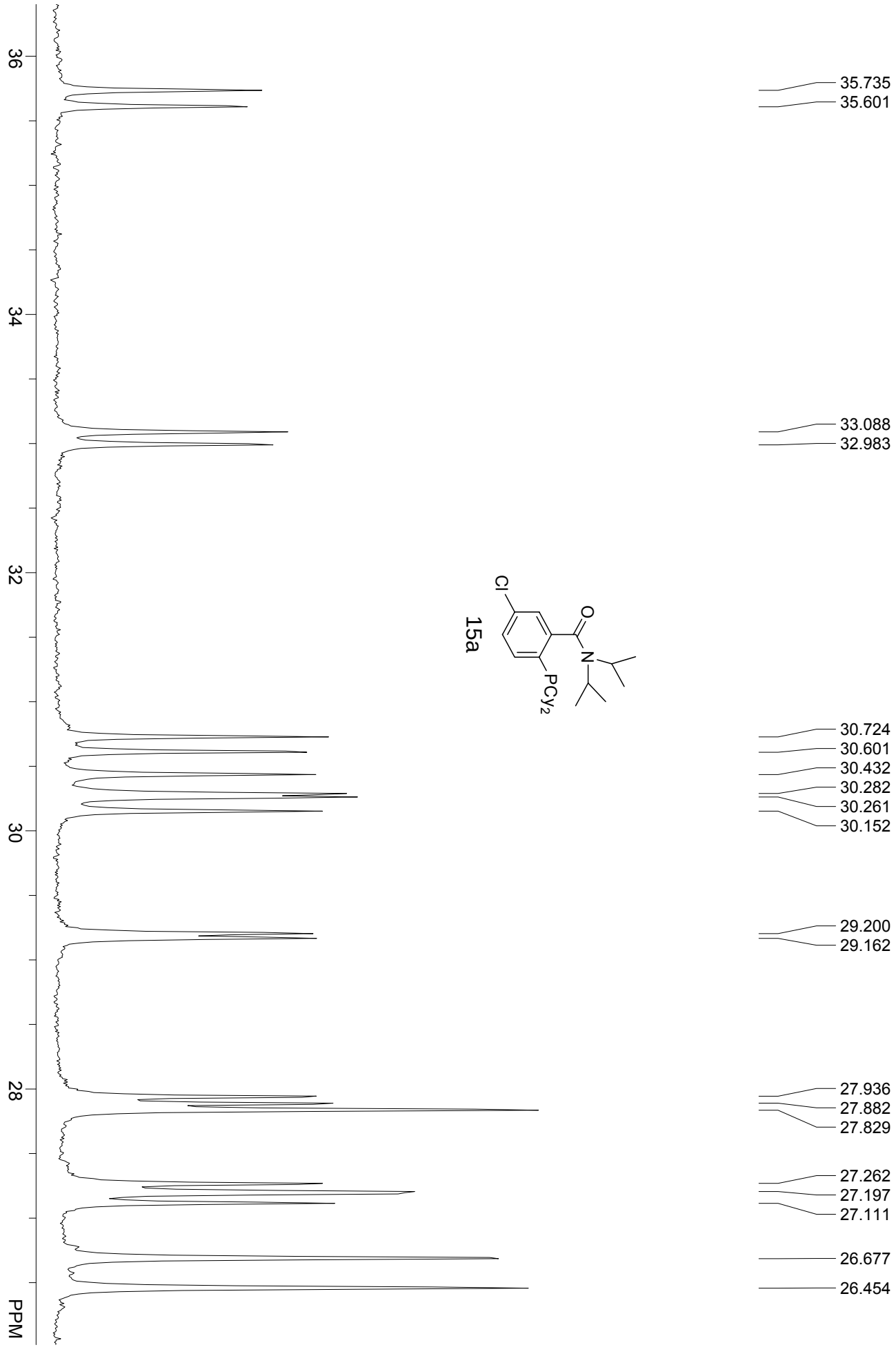
Sample: L-3 in CDCL3
Jul 4 16:43:40 2005
Experiment = zg30
Pulse length = 8.700 usec
Recycle delay = 1.500 sec
NA = 16
PTS1d = 32768
F1 = 500.130035 MHz
F2 = 1.000000 MHz
SW1 = 12531.33 Hz
AT1 = 2.61 sec
Hz per Pt 1stD = 0.38 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 3478.5496 Hz
O2 = -1.0000 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00



15a

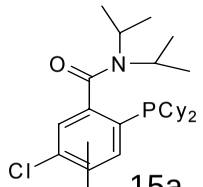

Sample: L-3 13C in CDCL3
Jul 4 16:21:29 2005
Experiment = zgdc
Pulse length = 6.400 usec
Recycle delay = 1.500 sec
NA = 420
PTS1d = 32768
F1 = 125.757759 MHz
F2 = 1.000000 MHz
SW1 = 37593.98 Hz
AT1 = 0.87 sec
Hz per Pt 1stD = 1.15 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 13028.3486 Hz
O2 = -1.0000 Hz
LB1 = 1.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
169.024
168.997
149.050
148.755
135.074
134.418
134.392
131.570
131.379
127.529
125.609
125.540
77.512
77.258
77.006
35.735
35.601
33.088
32.983
30.724
50.910
45.898
30.601
30.432
30.282
30.261
30.152
29.200
29.162
27.936
27.882
27.829
27.262
27.197
27.111
26.677
26.454
21.215
21.183
20.869
20.746
20.287
150
100
50
0
PPM
Cl
O
N
PCy2
15a


28
27
26
25
24
23
22
21
20 PPM
27.936
27.882
27.829
27.262
27.197
27.111
26.677
26.454
21.215
21.183
20.869
20.746
20.287
15a
Cl
O
N
PCy2


36
34
32
30
28
PPM
35.735
35.601
33.088
32.983
30.724
30.601
30.432
30.282
30.261
30.152
29.200
29.162
27.936
27.882
27.829
27.262
27.197
27.111
26.677
26.454
Cl
O
N
PCy2
15a

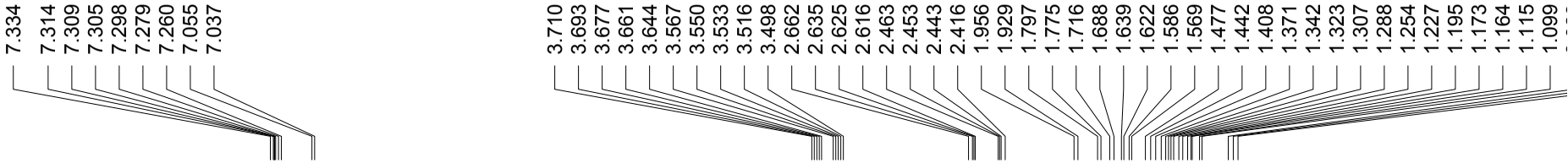
Sample L-3 31P in CDCL3
Jul 4 16:56:25 2005
Experiment = zgdc
Pulse length = 4.000 usec
Recycle delay = 3.000 sec
NA = 227
PTS1d = 32768
F1 = 202.456039 MHz
F2 = 1.000000 MHz
SW1 = 60606.06 Hz
AT1 = 0.54 sec
Hz per Pt 1stD = 1.85 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 42.5390 Hz
O2 = -1.0000 Hz
LB1 = 2.00 Hz
TP A = 0.00
B = 0.00
C = 0.00

-8.833

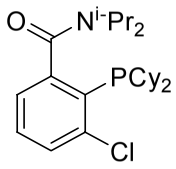


15a

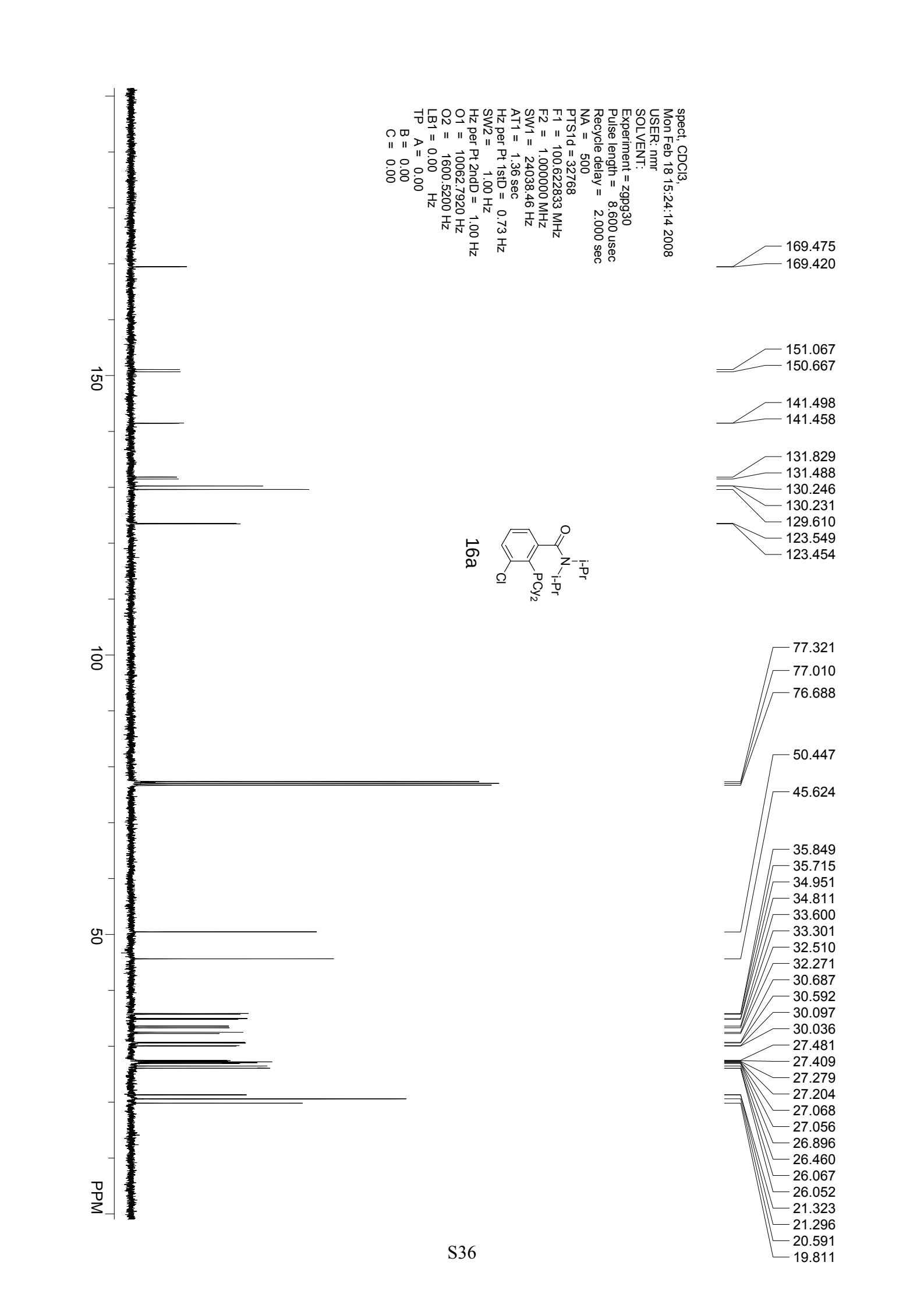
100 50 0 -50 -100 PPM

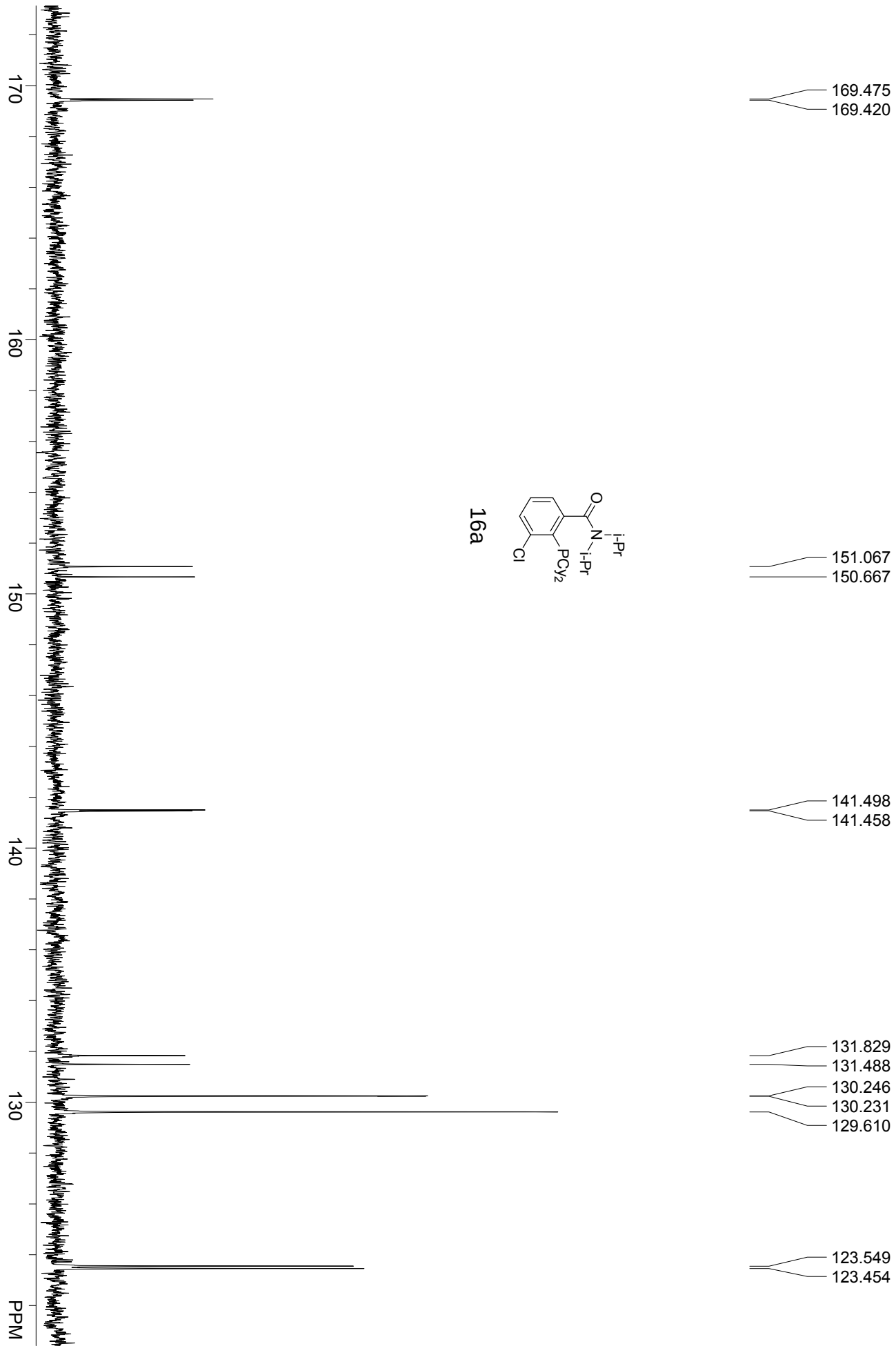


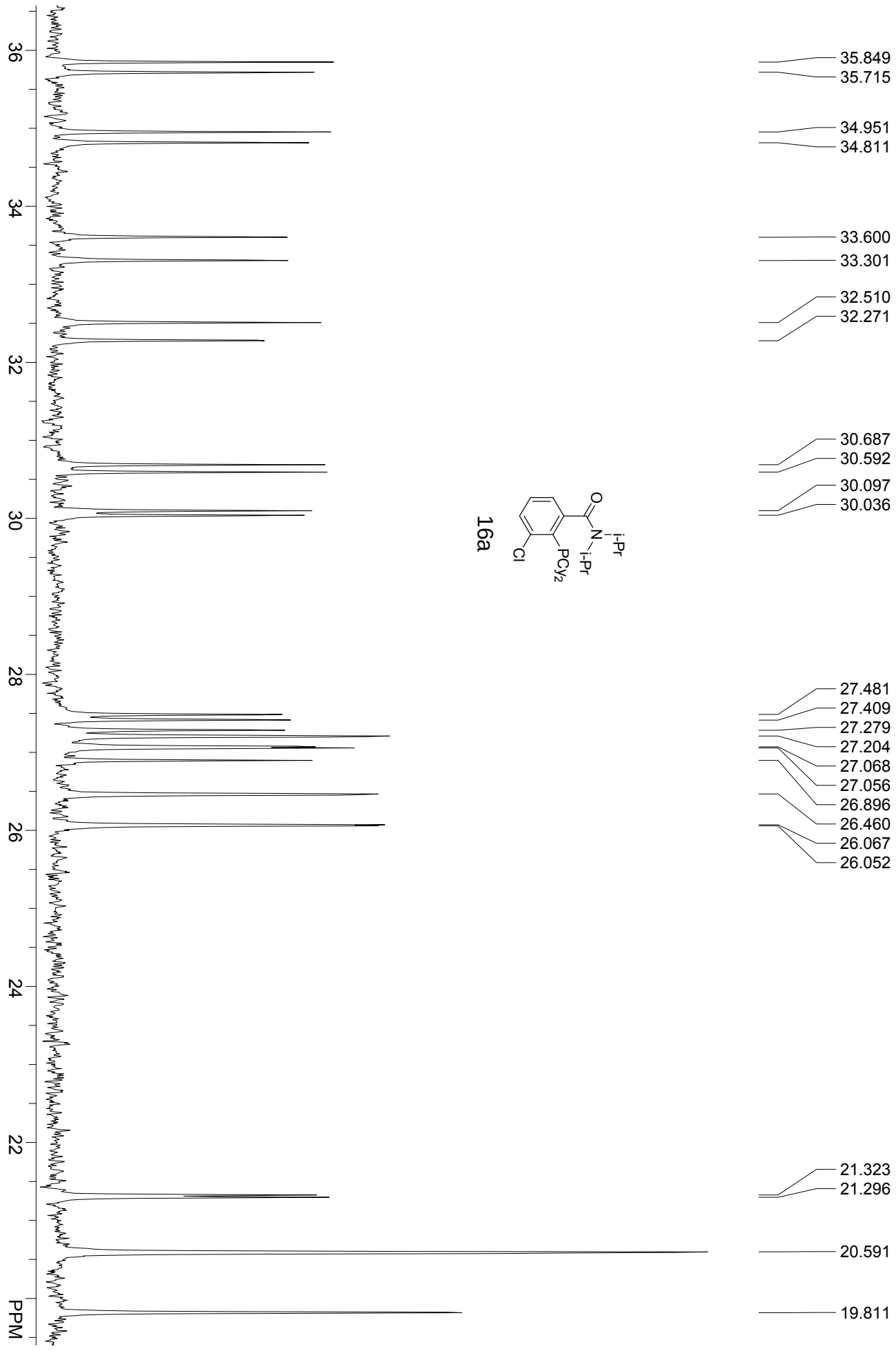
Sample: ycy0106-L in CDCl3
Jan 6 13:42:19 2005
Experiment = zg30
Pulse length = 11.000 usec
Recycle delay = 2.000 sec
NA = 8
PTS1d = 32768
F1 = 400.130005 MHz
F2 = 1.000000 MHz
SW1 = 11990.41 Hz
AT1 = 2.73 sec
Hz per Pt 1stD = 0.37 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 3198.4917 Hz
O2 = -1.0000 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00



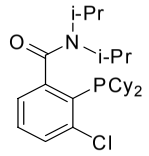
16a


spect, CDCl3,
Mon Feb 18 15:24:14 2008
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 8.600 usec
Recycle delay = 2.000 sec
NA = 500
PTS1d = 32768
F1 = 100.622833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10062.7920 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
16a
i-Pr
i-Pr
PCy2
Cl
169.475
169.420
151.067
150.667
141.498
141.458
131.829
131.488
130.246
130.231
129.610
123.549
123.454
77.321
77.010
76.688
50.447
45.624
35.849
35.715
34.951
34.811
33.600
33.301
32.510
32.271
30.687
30.592
30.097
30.036
27.481
27.409
27.279
27.204
27.068
27.056
26.896
26.460
26.067
26.052
21.323
21.296
20.591
19.811
150
100
50
PPM

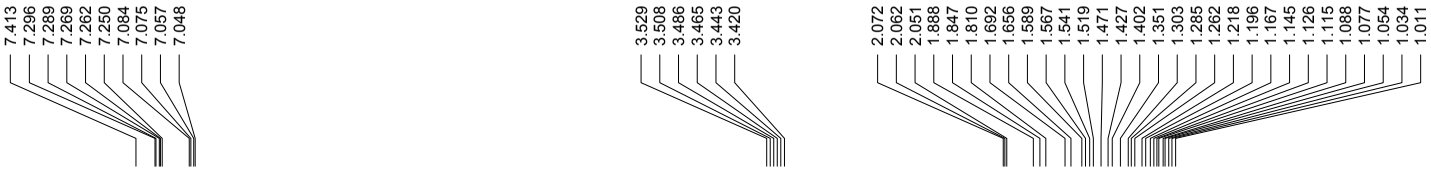

169.475
169.420
151.067
150.667
141.498
141.458
131.829
131.488
130.246
130.231
129.610
123.549
123.454
170
160
150
140
130
PPM
16a
O
N
i-Pr
i-Pr
PCy2
Cl


36
34
32
30
28
26
24
22
PPM
35.849
35.715
34.951
34.811
33.600
33.301
32.510
32.271
30.687
30.592
30.097
30.036
27.481
27.409
27.279
27.204
27.068
27.056
26.896
26.460
26.067
26.052
21.323
21.296
20.591
19.811
16a
O
N
i-Pr
i-Pr
PCy2
Cl

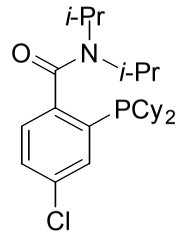
spect, CDCl3,
Mon Feb 18 15:13:55 2008
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 7.600 usec
Recycle delay = 2.000 sec
NA = 18
PTS1d = 32768
F1 = 161.975586 MHz
F2 = 1.000000 MHz
SW1 = 64102.56 Hz
AT1 = 0.51 sec
Hz per Pt 1stD = 1.96 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = -22.4405 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00



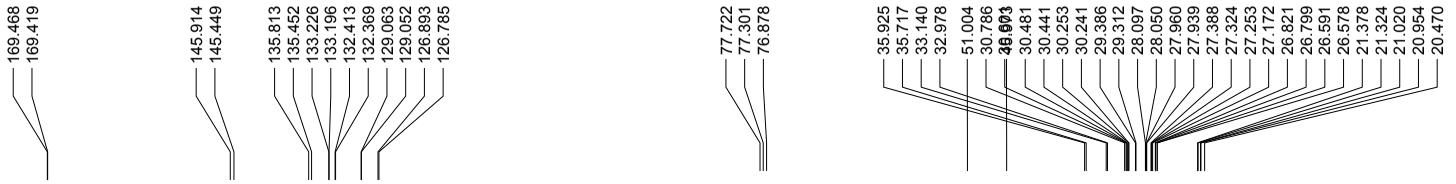
16a



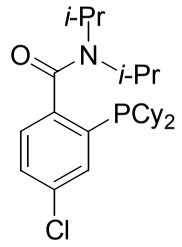
Sample: chloro ligand
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1800.43 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -79.10
B = 57.96



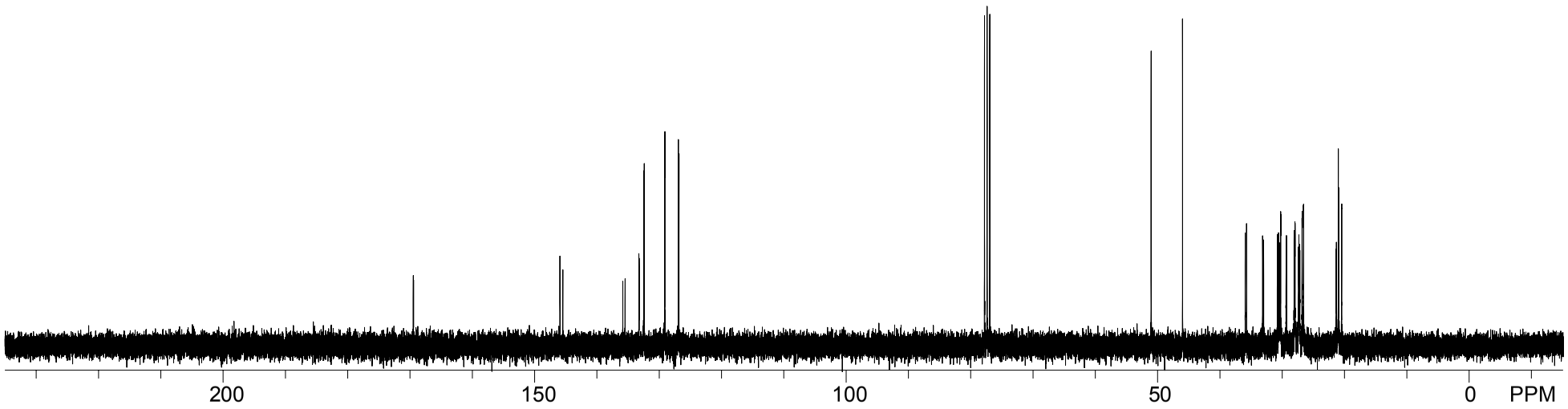
17a

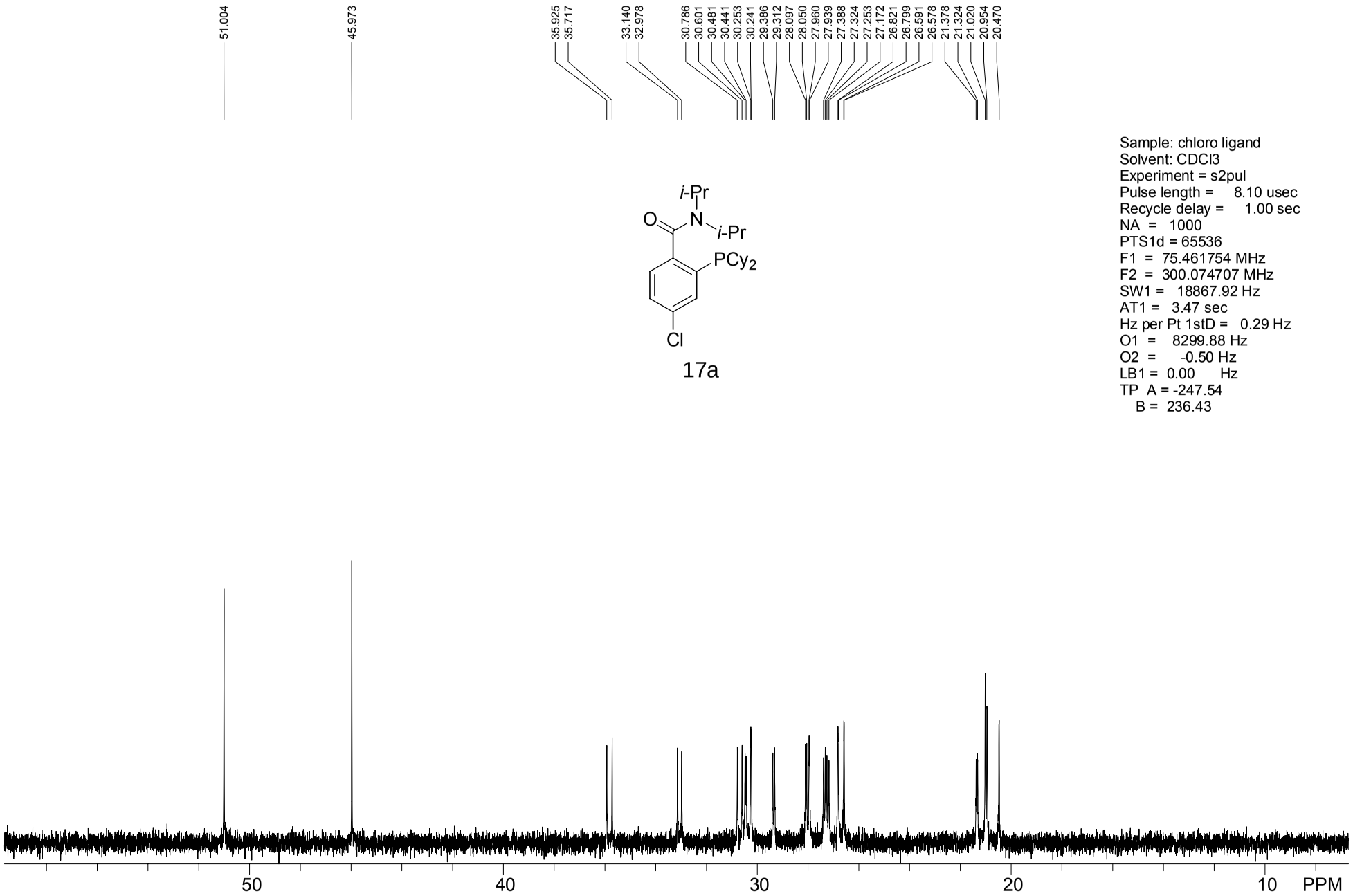


Sample: chloro ligand
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 1000
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -247.54
B = 236.43

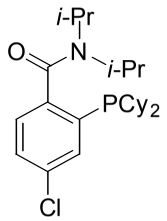


17a

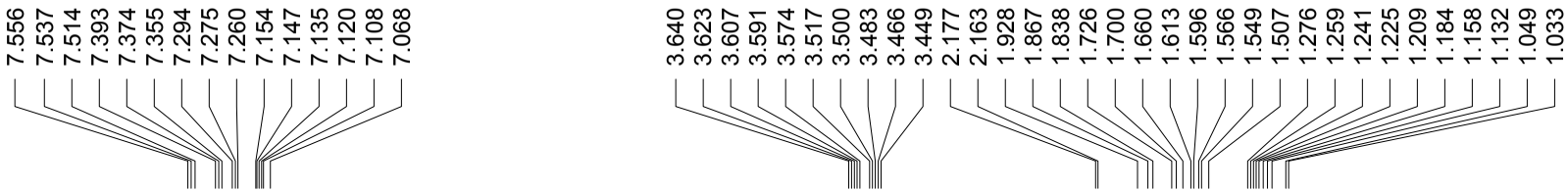



51.004
45.973
35.925
35.717
33.140
32.978
30.786
30.601
30.481
30.441
30.253
30.241
29.386
29.312
28.097
28.050
27.960
27.939
27.388
27.324
27.253
27.172
26.821
26.799
26.591
26.578
21.378
21.324
21.020
20.954
20.470
i-Pr
O
N
i-Pr
PCy2
Cl
17a
Sample: chloro ligand
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 1000
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -247.54
B = 236.43
50
40
30
20
10
PPM

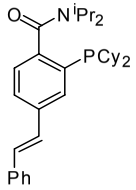
Sample: chloro ligand
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 32
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 2703.04
B = -2838.40



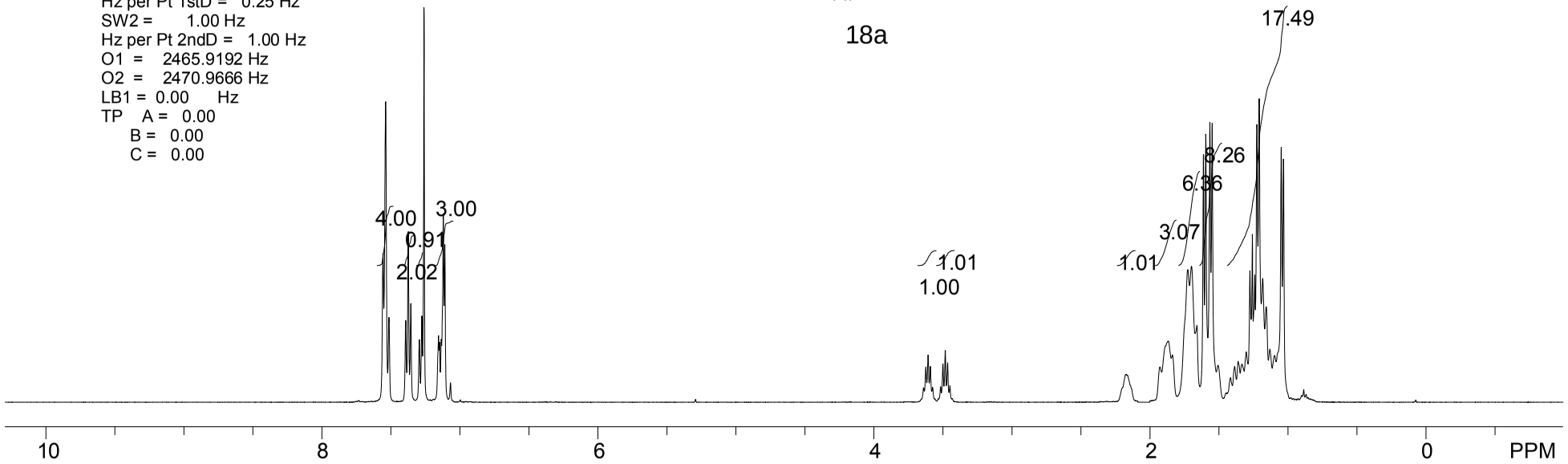
17a

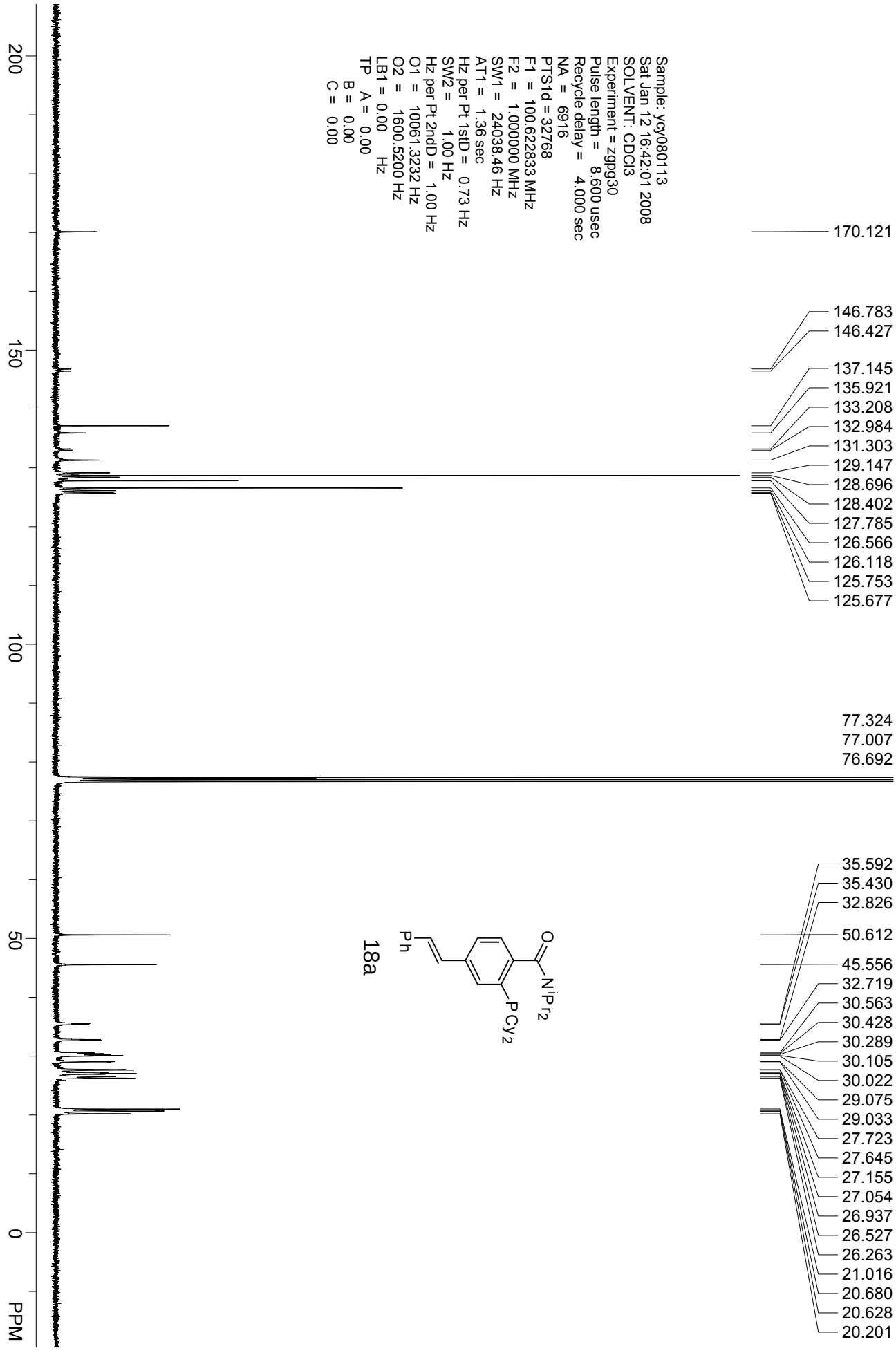


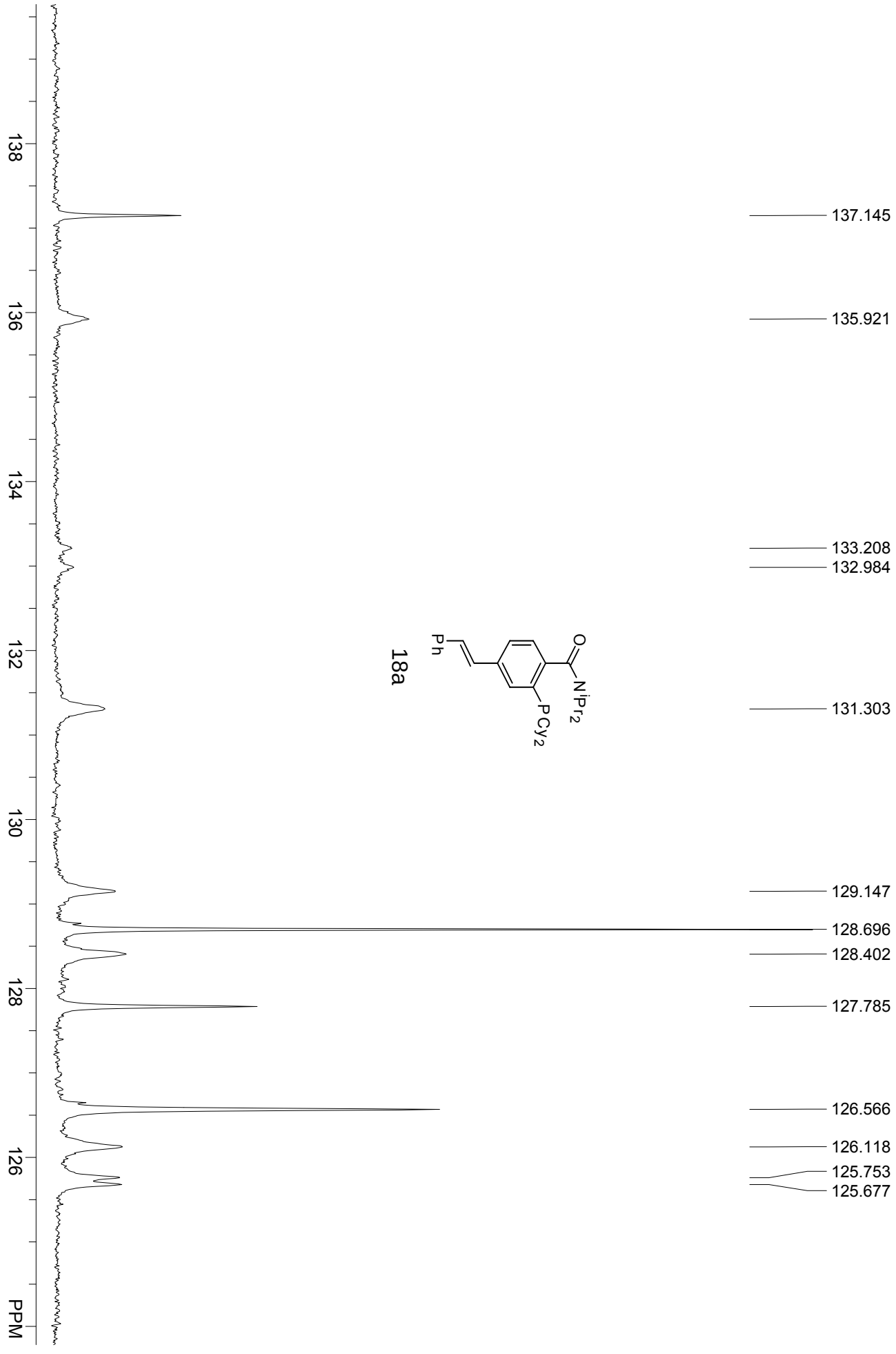
Sample: ycy080113
Sat Jan 12 16:30:15 2008
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 13.700 usec
Recycle delay = 1.000 sec
NA = 16
PTS1d = 32768
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 3.98 sec
Hz per Pt 1stD = 0.25 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2465.9192 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00

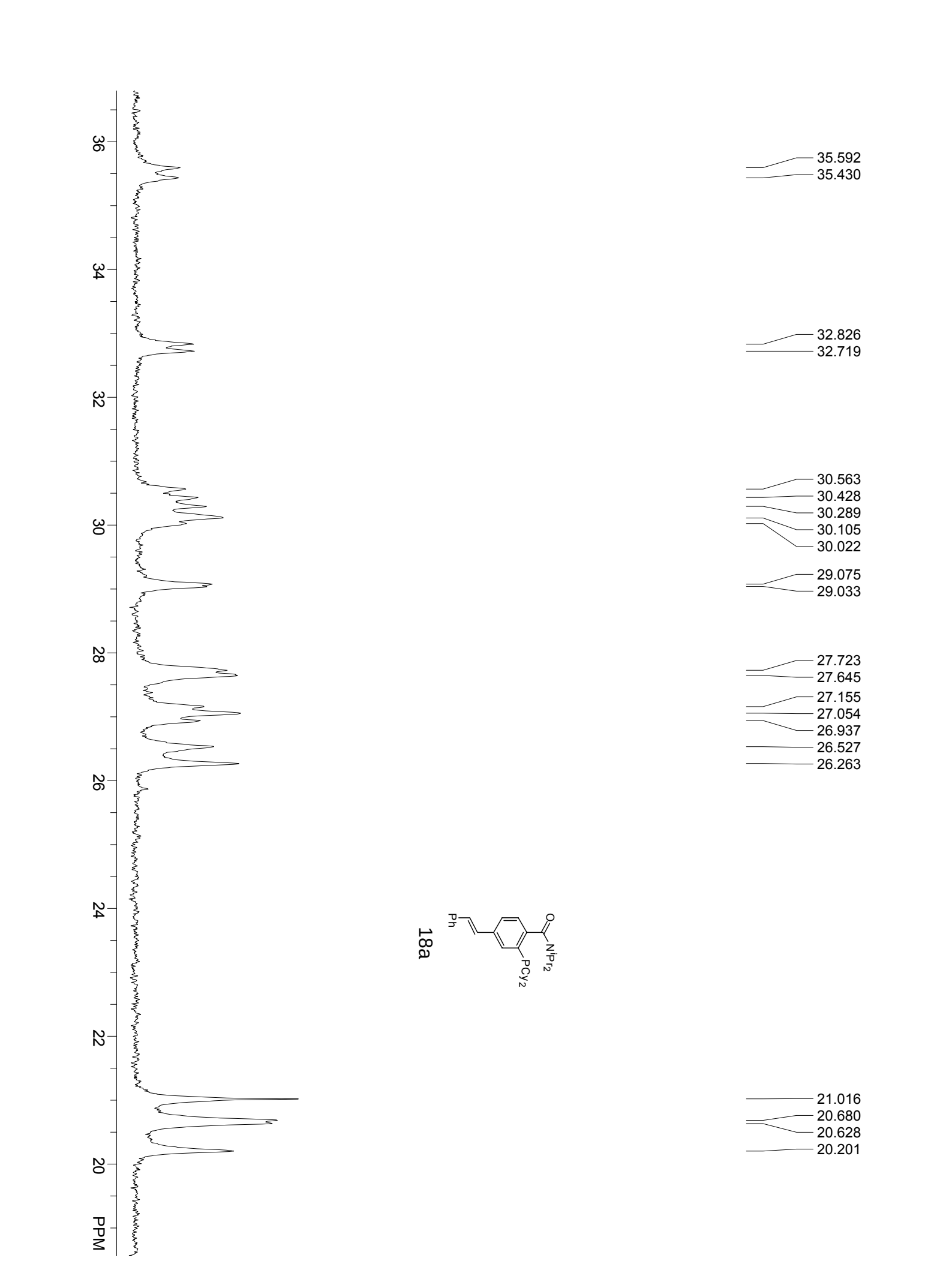


18a

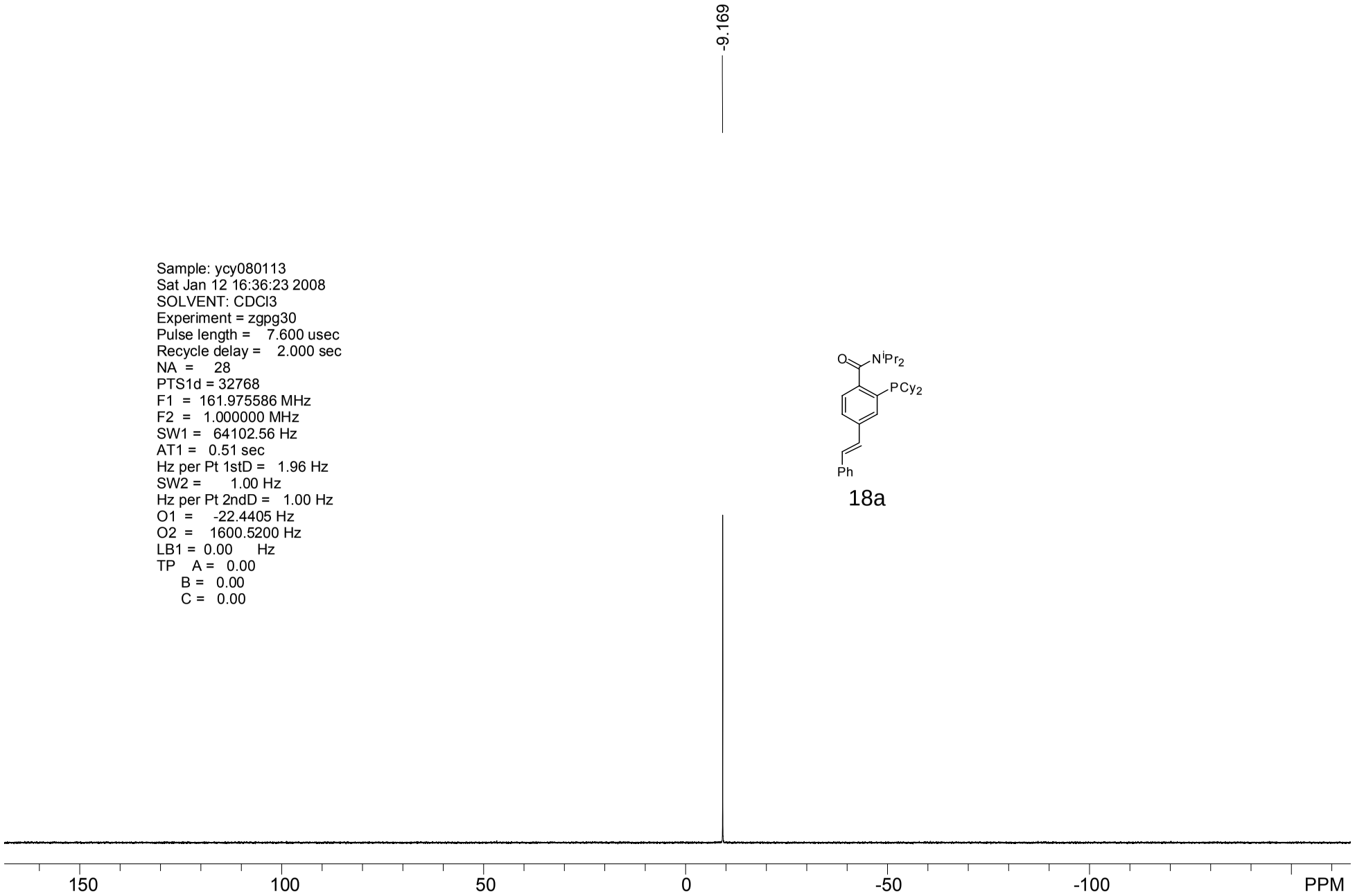


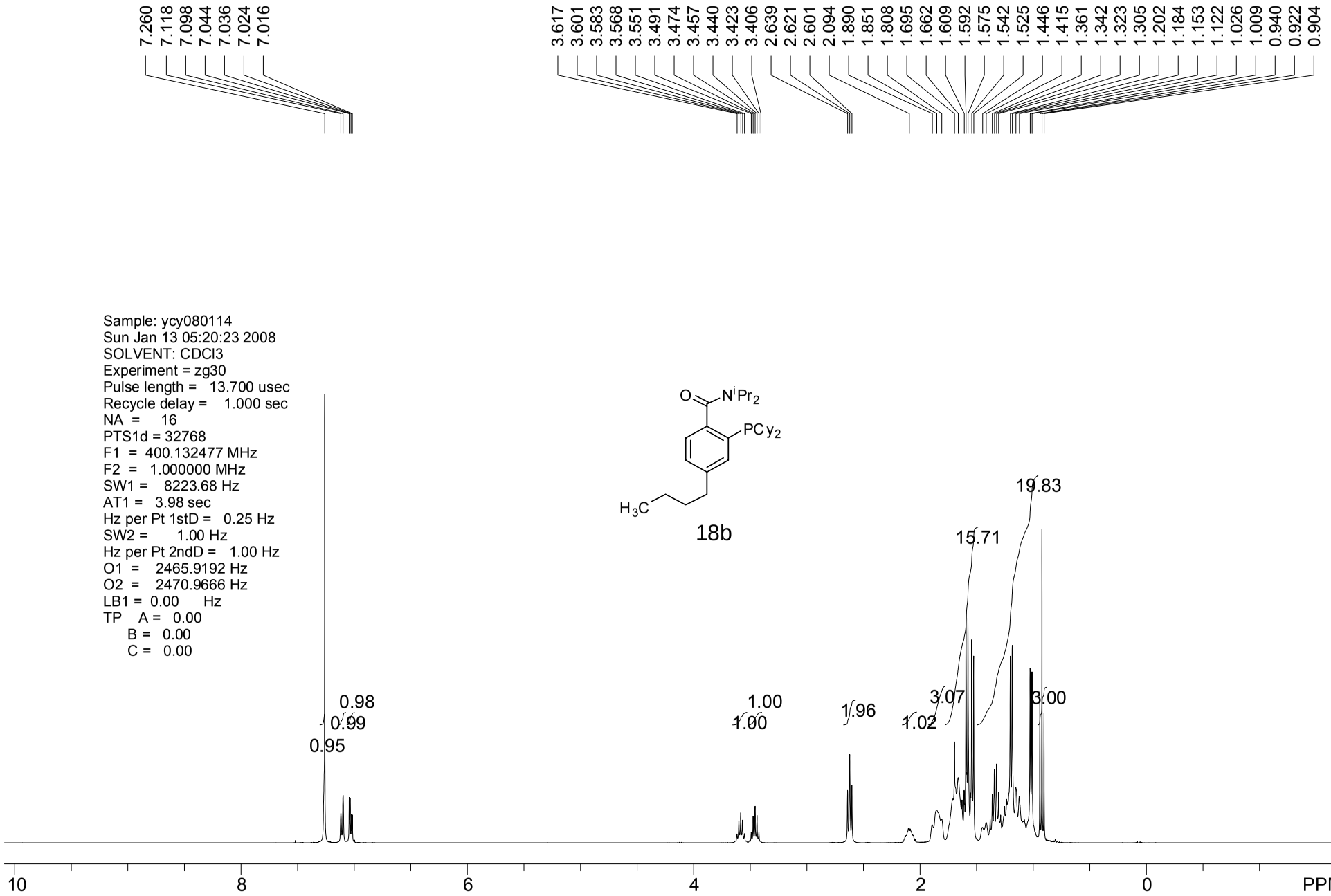

Sample: ycy080113
Sat Jan 12 16:42:01 2008
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.600 usec
Recycle delay = 4.000 sec
NA = 6916
PTS1d = 32768
F1 = 100.622833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10061.3232 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
170.121
146.783
146.427
137.145
135.921
133.208
132.984
131.303
129.147
128.696
128.402
127.785
126.566
126.118
125.753
125.677
77.324
77.007
76.692
35.592
35.430
32.826
50.612
45.556
32.719
30.563
30.428
30.289
30.105
30.022
29.075
29.033
27.723
27.645
27.155
27.054
26.937
26.527
26.263
21.016
20.680
20.628
20.201
18a
Ph
O
N iPr2
PCy2
200
150
100
50
0
PPM

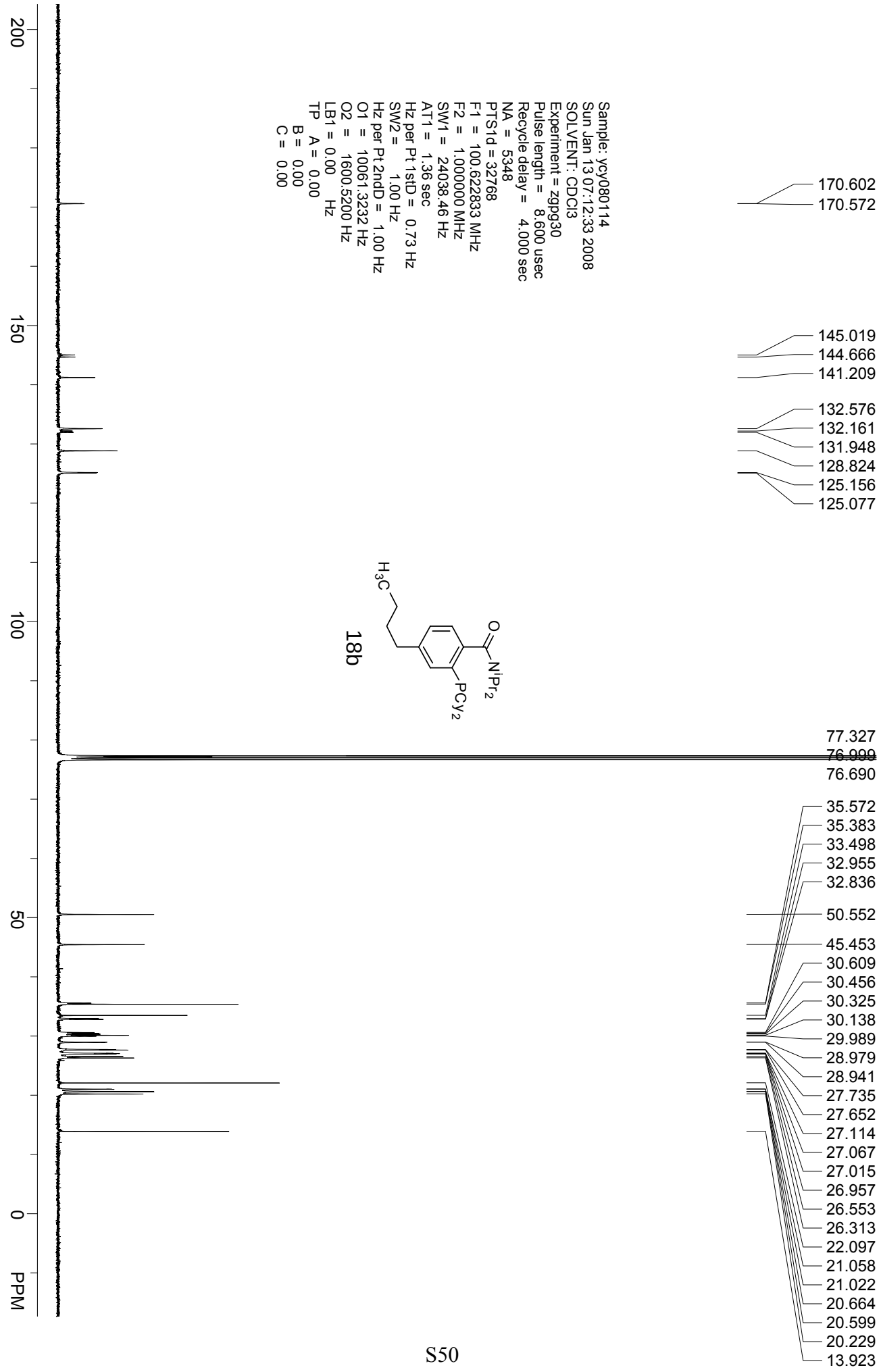

138
136
134
132
130
128
126
PPM
137.145
135.921
133.208
132.984
131.303
129.147
128.696
128.402
127.785
126.566
126.118
125.753
125.677
18a
Ph
O
N^{i}Pr$_2$
PCy$_2$

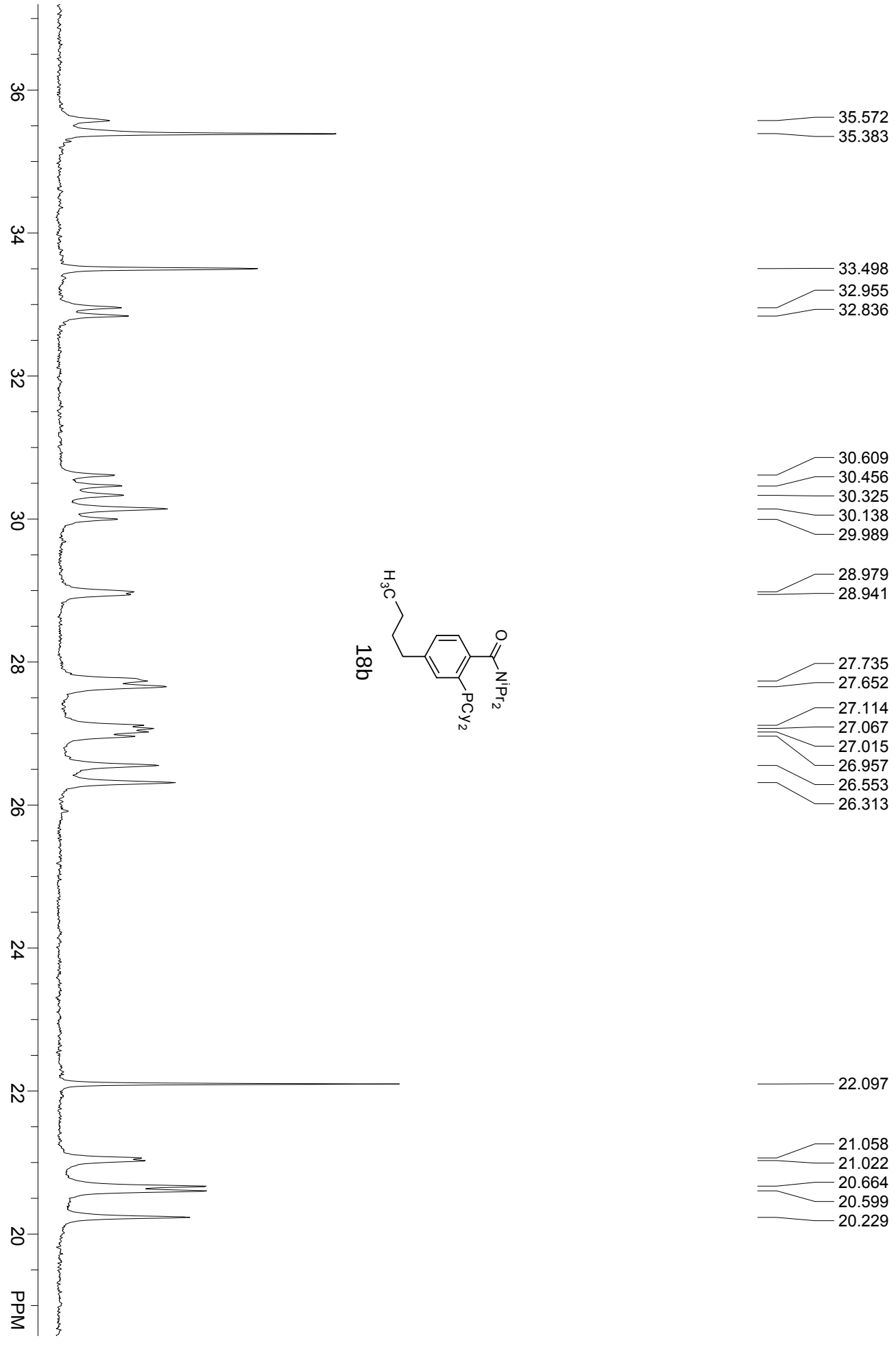

36
34
32
30
28
26
24
22
20
PPM
35.592
35.430
32.826
32.719
30.563
30.428
30.289
30.105
30.022
29.075
29.033
27.723
27.645
27.155
27.054
26.937
26.527
26.263
21.016
20.680
20.628
20.201
Ph
O
N^{i}Pr$_2$
PCy$_2$

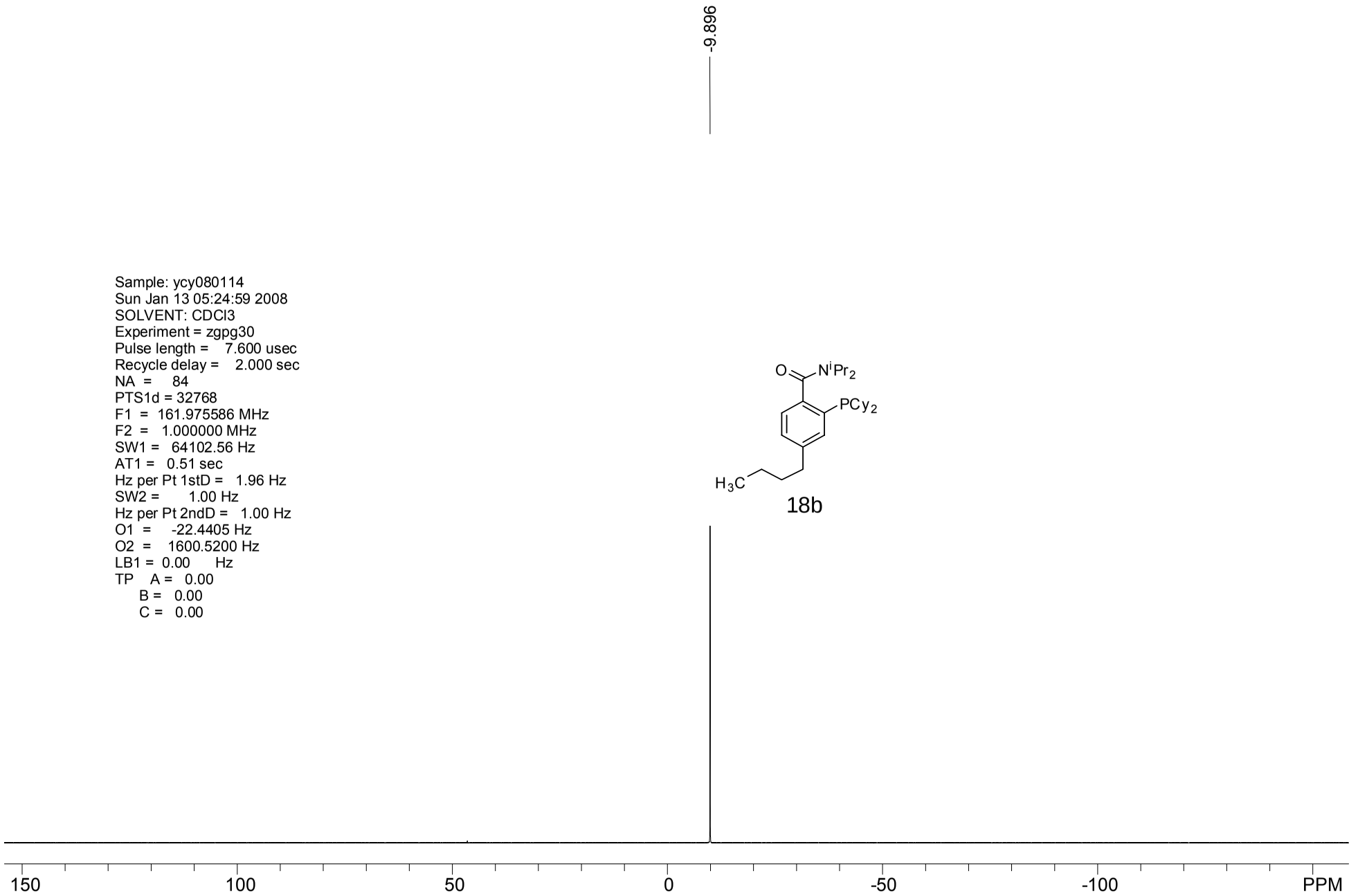
18a

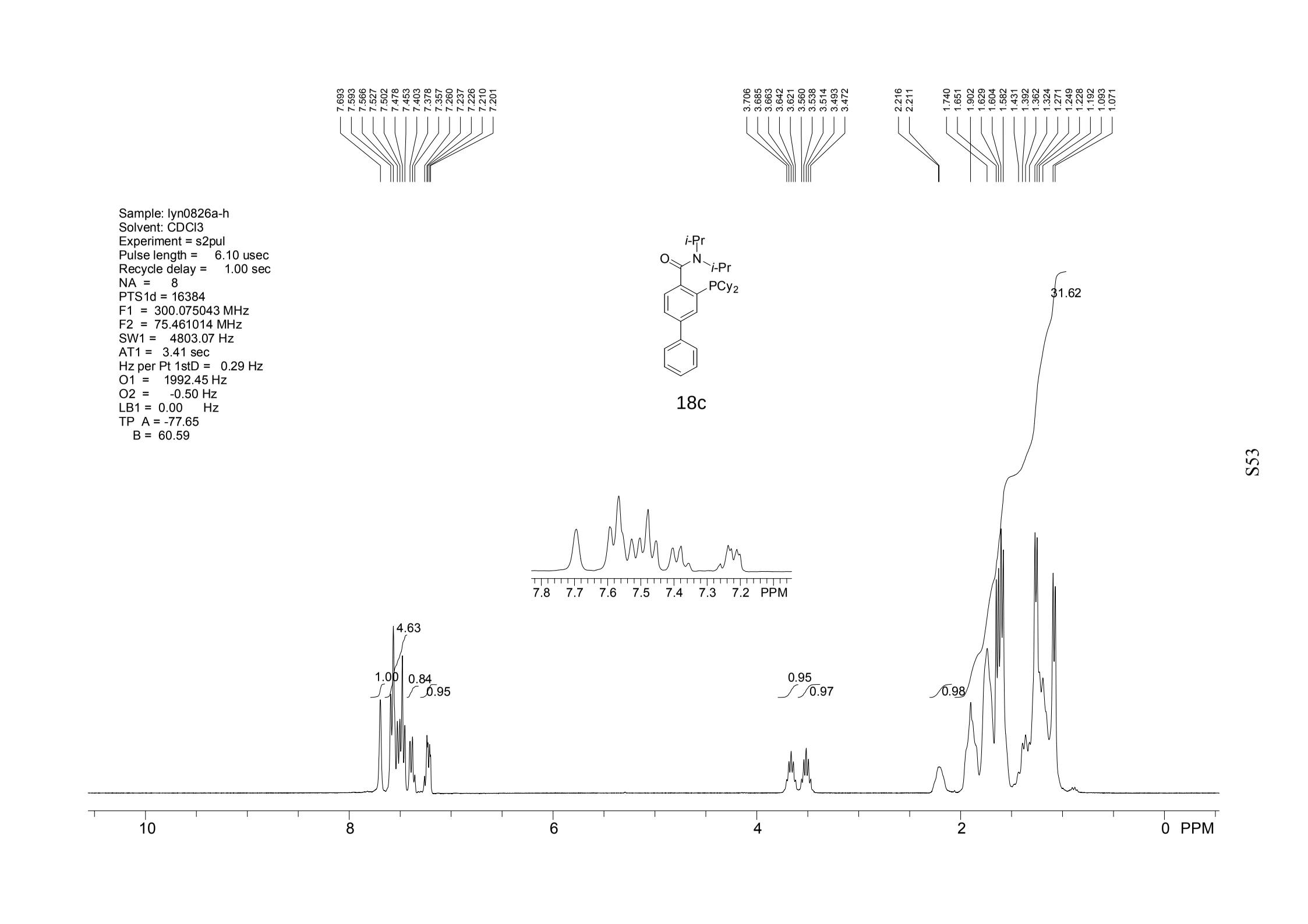

-9.169
Sample: ycy080113
Sat Jan 12 16:36:23 2008
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 7.600 usec
Recycle delay = 2.000 sec
NA = 28
PTS1d = 32768
F1 = 161.975586 MHz
F2 = 1.000000 MHz
SW1 = 64102.56 Hz
AT1 = 0.51 sec
Hz per Pt 1stD = 1.96 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = -22.4405 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
N^{i}Pr$_2$
PCy$_2$
Ph
18a
150
100
50
0
-50
-100
PPM

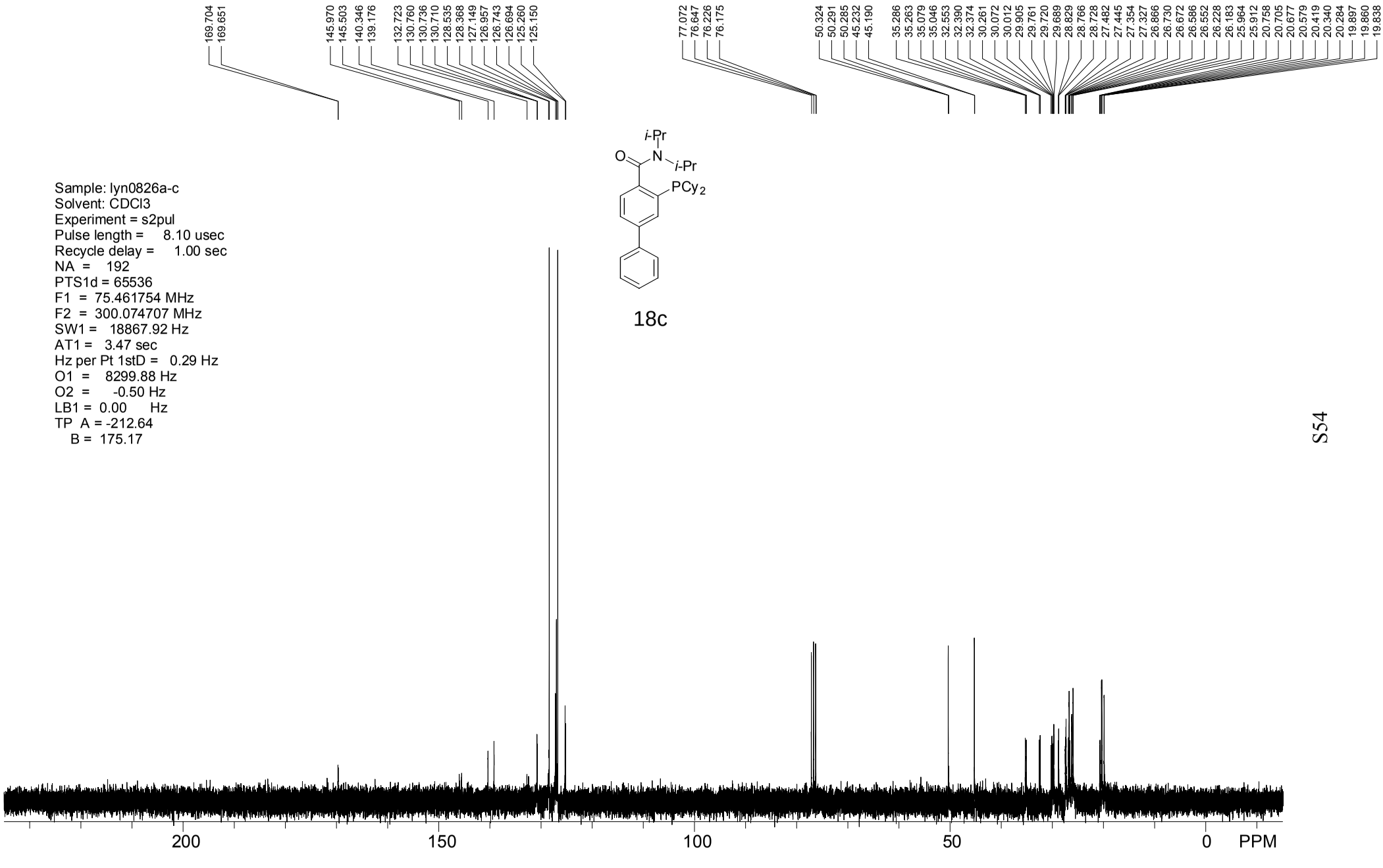

7.260
7.118
7.098
7.044
7.036
7.024
7.016
3.617
3.601
3.583
3.568
3.551
3.491
3.474
3.457
3.440
3.423
3.406
2.639
2.621
2.601
2.094
1.890
1.851
1.808
1.695
1.662
1.609
1.592
1.575
1.542
1.525
1.446
1.415
1.361
1.342
1.323
1.305
1.202
1.184
1.153
1.122
1.026
1.009
0.940
0.922
0.904
Sample: ycy080114
Sun Jan 13 05:20:23 2008
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 13.700 usec
Recycle delay = 1.000 sec
NA = 16
PTS1d = 32768
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 3.98 sec
Hz per Pt 1stD = 0.25 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2465.9192 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
N^{i}Pr$_2$
PCy$_2$
H$_3$C
18b
0.95
0.99
0.98
1.00
1.00
1.96
1.02
3.07
15.71
19.83
3.00
10
8
6
4
2
0
PPM


Sample: ycy080114
Sun Jan 13 07:12:33 2008
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.600 usec
Recycle delay = 4.000 sec
NA = 5348
PTS1d = 32768
F1 = 100.622833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10061.3232 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
18b
170.602
170.572
145.019
144.666
141.209
132.576
132.161
131.948
128.824
125.156
125.077
77.327
76.999
76.690
35.572
35.383
33.498
32.955
32.836
50.552
45.453
30.609
30.456
30.325
30.138
29.989
28.979
28.941
27.735
27.652
27.114
27.067
27.015
26.957
26.553
26.313
22.097
21.058
21.022
20.664
20.599
20.229
13.923
200
150
100
50
0
PPM

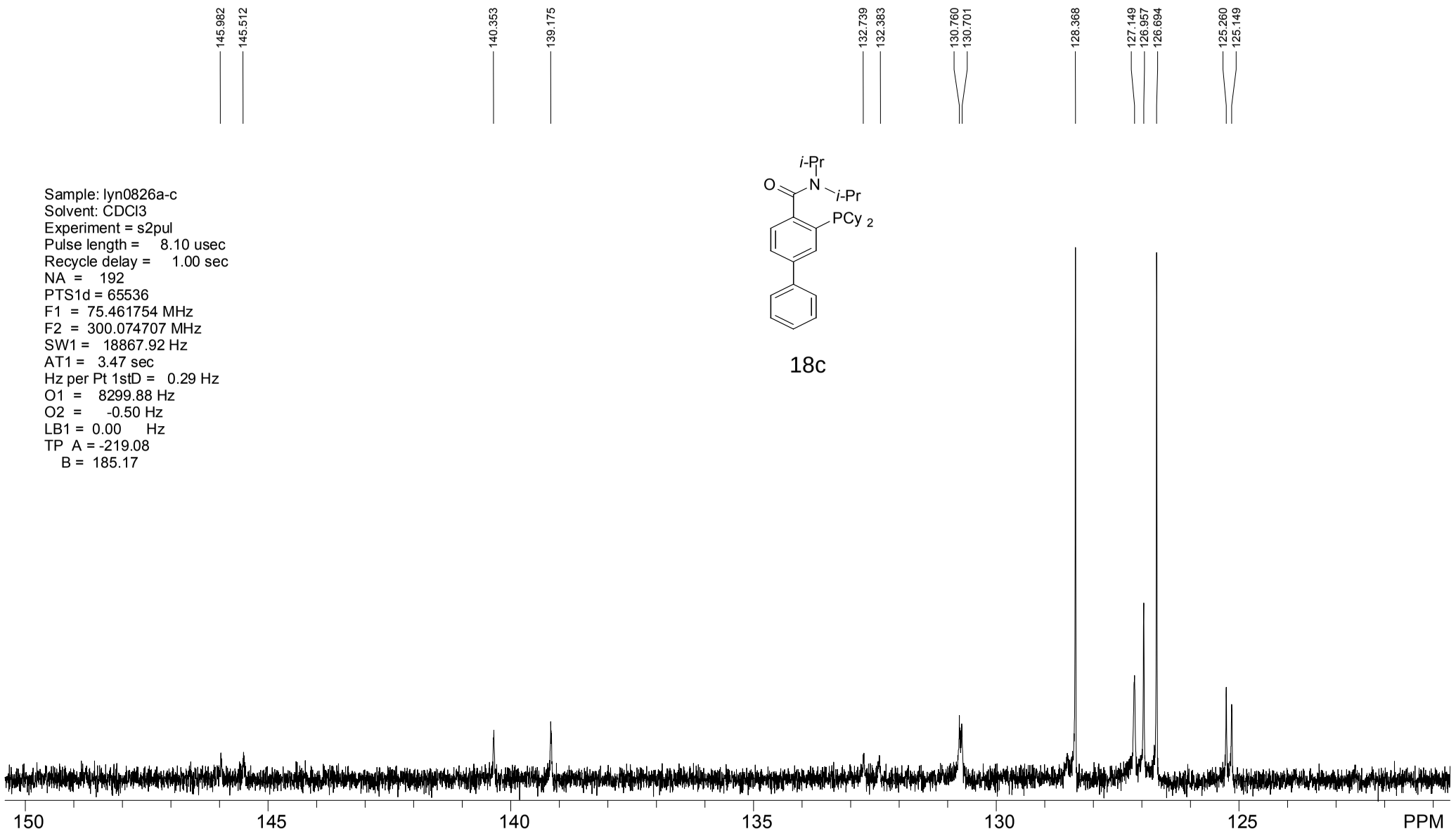

36
34
32
30
28
26
24
22
20
PPM
35.572
35.383
33.498
32.955
32.836
30.609
30.456
30.325
30.138
29.989
28.979
28.941
27.735
27.652
27.114
27.067
27.015
26.957
26.553
26.313
22.097
21.058
21.022
20.664
20.599
20.229
H3C
O
NiPr2
PCy2
18b

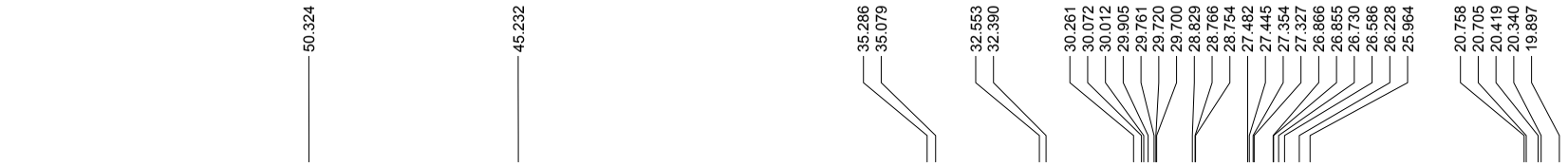

-9.896
Sample: ycy080114
Sun Jan 13 05:24:59 2008
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 7.600 usec
Recycle delay = 2.000 sec
NA = 84
PTS1d = 32768
F1 = 161.975586 MHz
F2 = 1.000000 MHz
SW1 = 64102.56 Hz
AT1 = 0.51 sec
Hz per Pt 1stD = 1.96 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = -22.4405 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
NiPr2
PCy2
H3C
18b
150
100
50
0
-50
-100
PPM


7.693
7.593
7.566
7.527
7.502
7.478
7.453
7.403
7.378
7.357
7.260
7.237
7.226
7.210
7.201
3.706
3.685
3.663
3.642
3.621
3.560
3.538
3.514
3.493
3.472
2.216
2.211
1.740
1.651
1.902
1.629
1.604
1.582
1.431
1.392
1.362
1.324
1.271
1.249
1.228
1.192
1.093
1.071
Sample: lyn0826a-h
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1992.45 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -77.65
B = 60.59
i-Pr
N
i-Pr
PCy2
18c
31.62
4.63
1.00
0.84
0.95
0.95
0.97
0.98
7.8 7.7 7.6 7.5 7.4 7.3 7.2 PPM
10 8 6 4 2 0 PPM

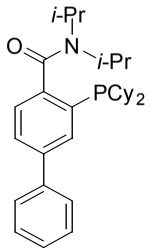

169.704
169.651
145.970
145.503
140.346
139.176
132.723
130.760
130.736
130.710
128.535
128.368
127.149
126.957
126.743
126.694
125.260
125.150
77.072
76.647
76.226
76.175
50.324
50.291
50.285
45.232
45.190
35.286
35.263
35.079
35.046
32.553
32.390
32.374
30.261
30.072
30.012
29.905
29.761
29.720
29.689
28.829
28.766
28.728
27.482
27.445
27.354
27.327
26.866
26.730
26.672
26.586
26.552
26.228
26.183
25.964
25.912
20.758
20.705
20.677
20.579
20.419
20.340
20.284
19.897
19.860
19.838
i-Pr
N
i-Pr
O
PCy2
Sample: lyn0826a-c
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 192
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -212.64
B = 175.17
200
150
100
50
0
PPM

18c

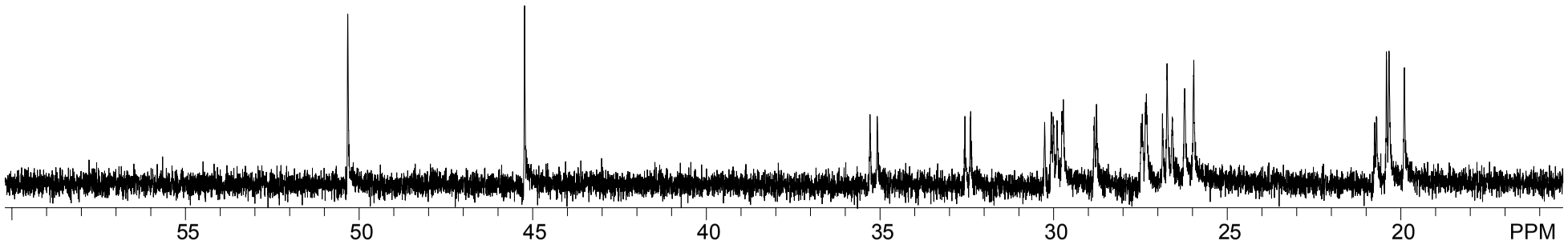

145.982
145.512
140.353
139.175
132.739
132.383
130.760
130.701
128.368
127.149
126.957
126.694
125.260
125.149
i-Pr
O
N
i-Pr
PCy 2
18c
Sample: lyn0826a-c
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 192
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -219.08
B = 185.17
150
145
140
135
130
125
PPM



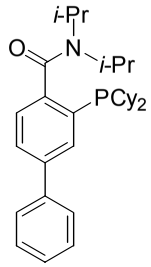
Sample: lyn0826a-c
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 192
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -212.64
B = 175.17



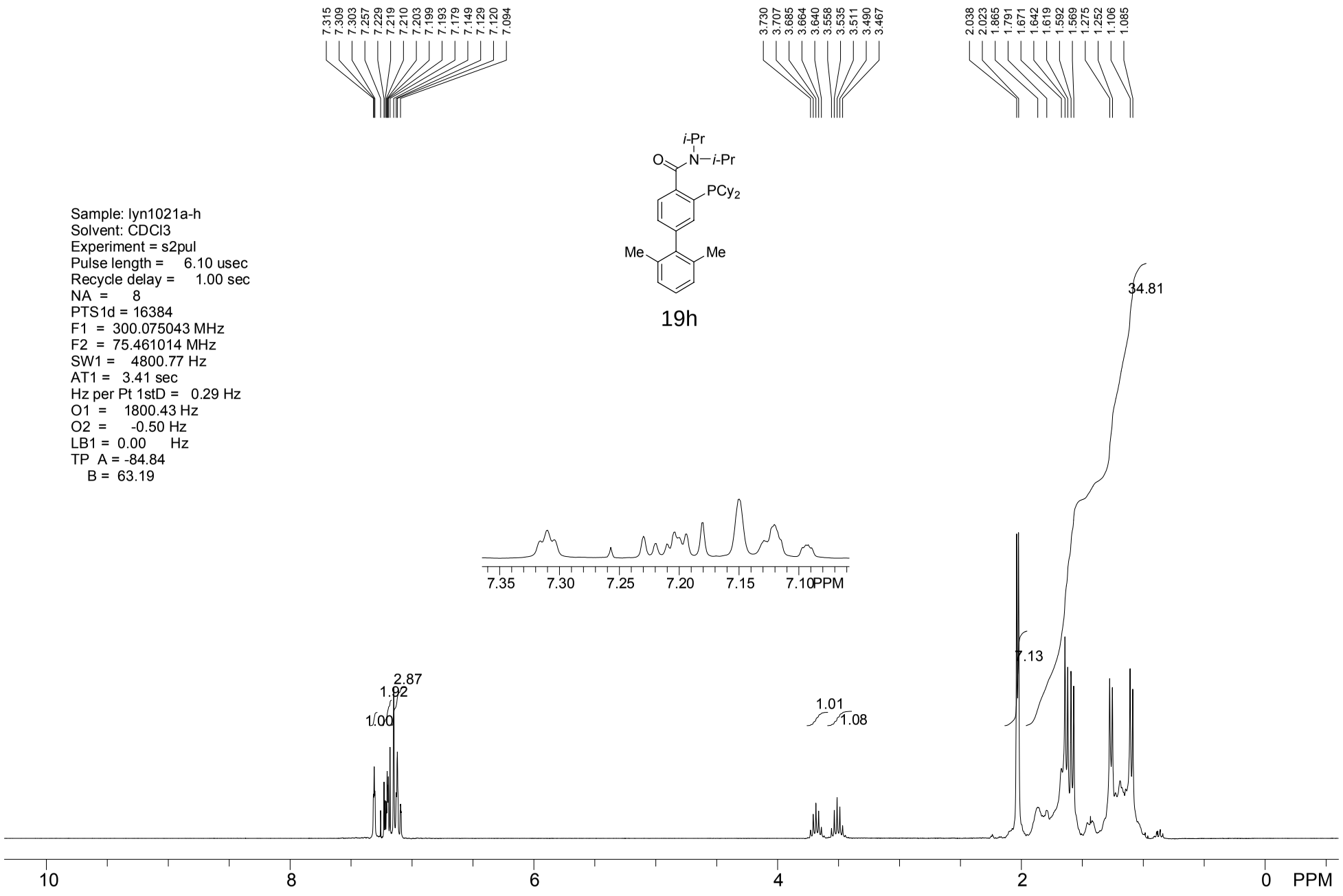
18c

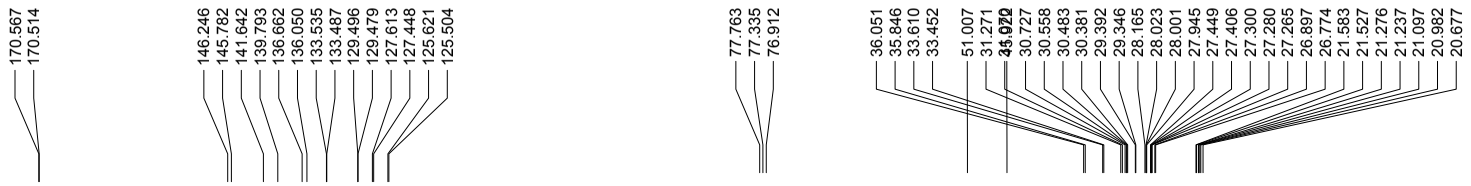


Sample: A-phos-3
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.14 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.477806 MHz
F2 = 300.074707 MHz
SW1 = 36496.35 Hz
AT1 = 1.80 sec
Hz per Pt 1stD = 0.56 Hz
O1 = 6073.59 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 1996.69
B = -2889.82

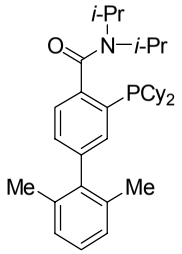


18c

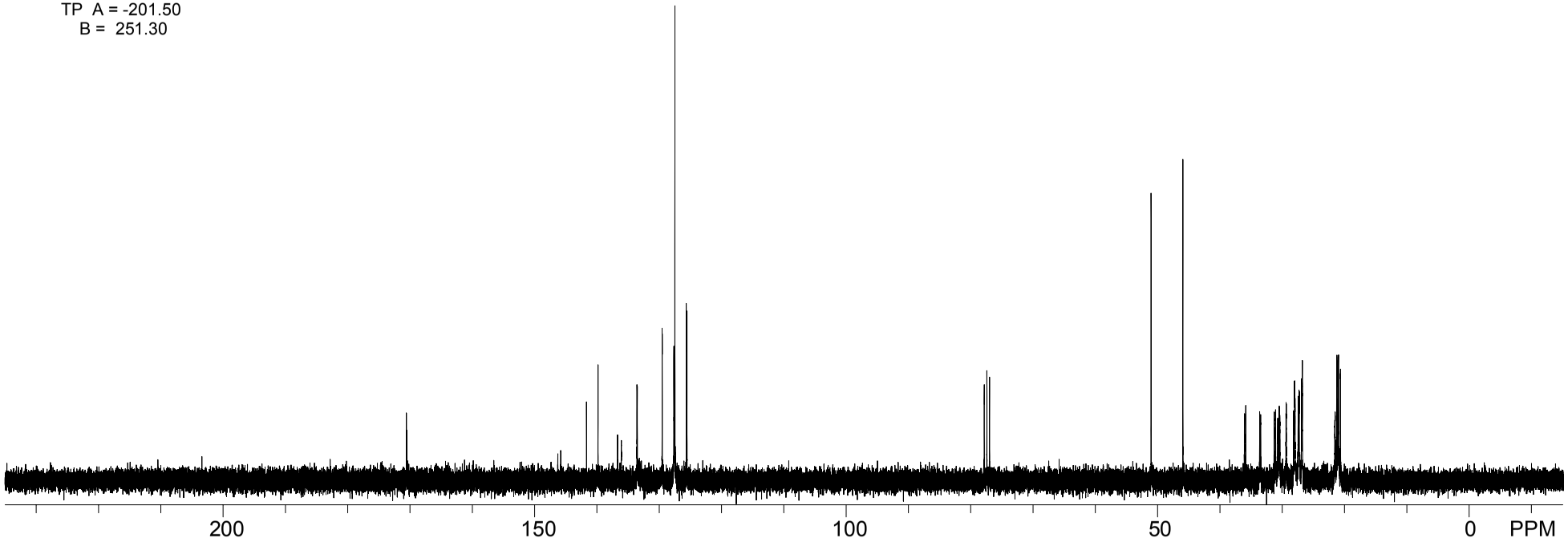

7.315
7.309
7.303
7.257
7.229
7.219
7.210
7.203
7.199
7.193
7.179
7.149
7.129
7.120
7.094
3.730
3.707
3.685
3.664
3.640
3.558
3.535
3.511
3.490
3.467
2.038
2.023
1.865
1.791
1.671
1.642
1.619
1.592
1.569
1.275
1.252
1.106
1.085
i-Pr
N—i-Pr
PCy2
Me
Me
19h
Sample: lyn1021a-h
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4800.77 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1800.43 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -84.84
B = 63.19
34.81
7.13
2.87
1.92
1.00
1.01
1.08
7.35
7.30
7.25
7.20
7.15
7.10
PPM
10
8
6
4
2
0
PPM

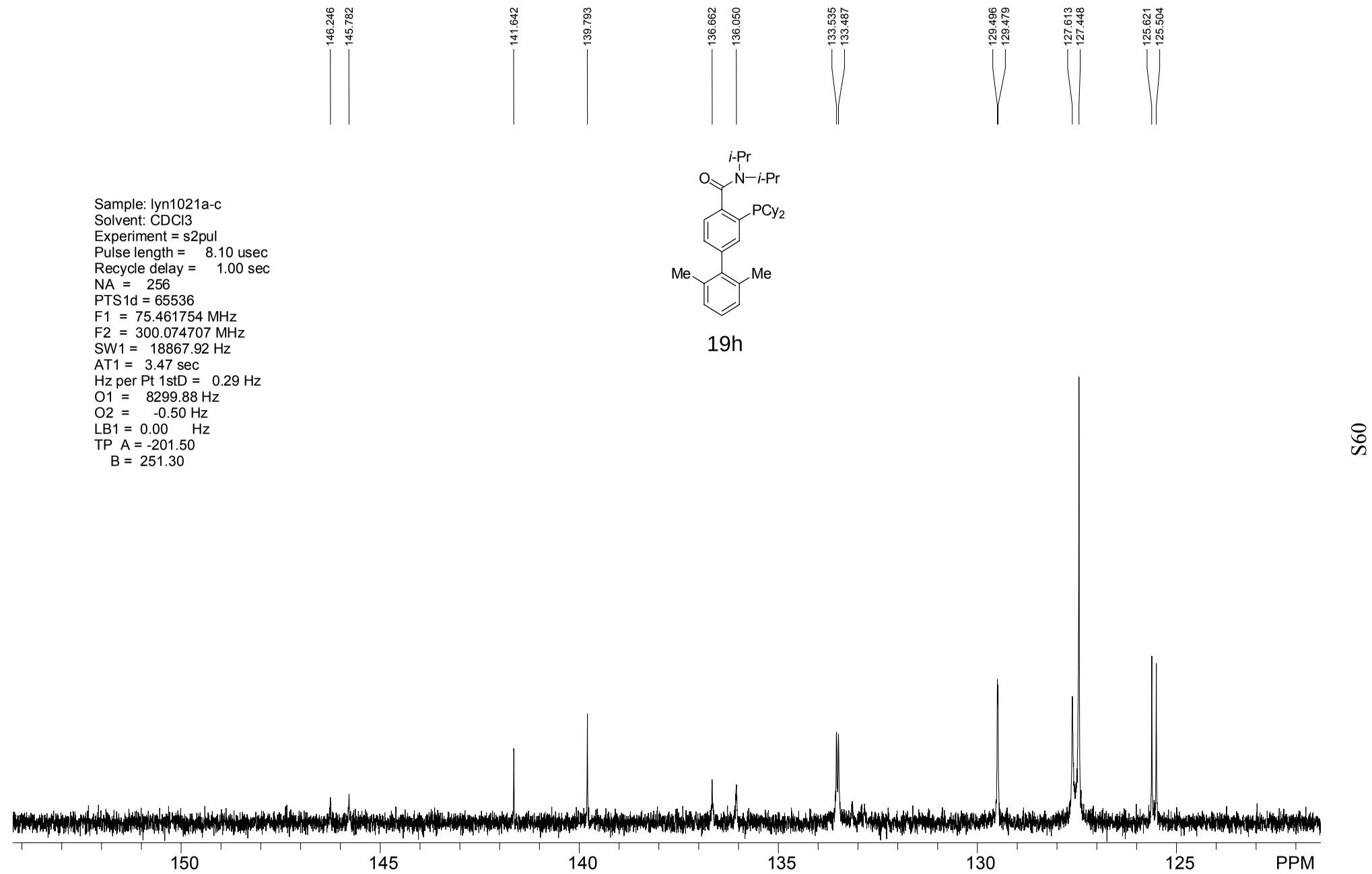


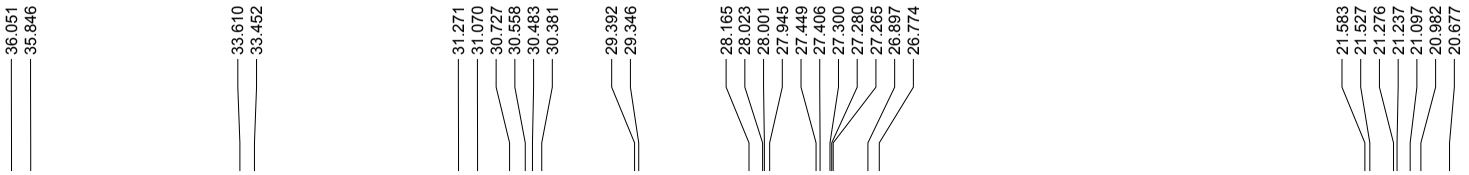
Sample: lyn1021a-c
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 256
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -201.50
B = 251.30

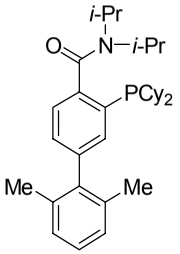


19h



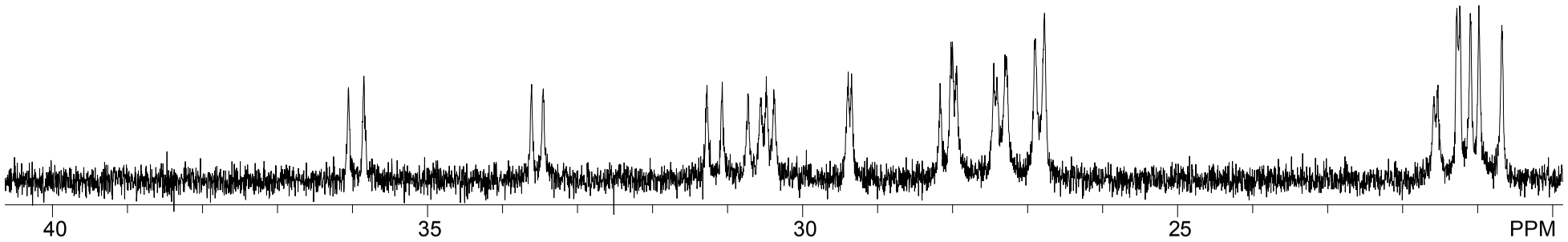

146.246
145.782
141.642
139.793
136.662
136.050
133.535
133.487
129.496
129.479
127.613
127.448
125.621
125.504
i-Pr
O
N—i-Pr
PCy2
Me
Me
19h
Sample: lyn1021a-c
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 256
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -201.50
B = 251.30
150
145
140
135
130
125
PPM

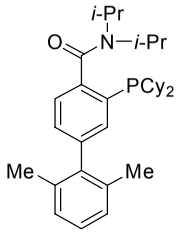




19h

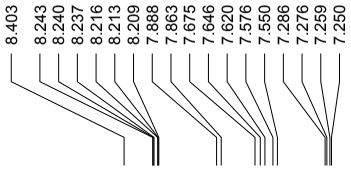
Sample: lyn1021a-c
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 256
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -201.50
B = 251.30

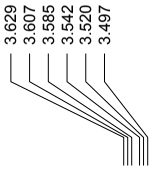


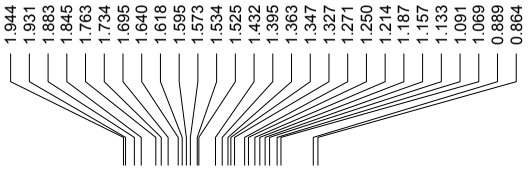


19h

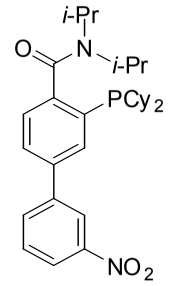
Sample: lyn0506c-p
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 82.16
B = -45.71



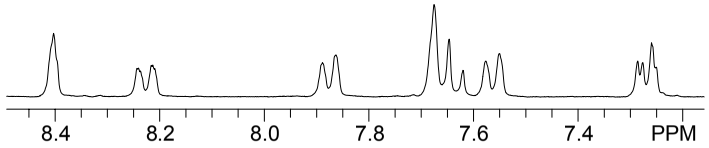


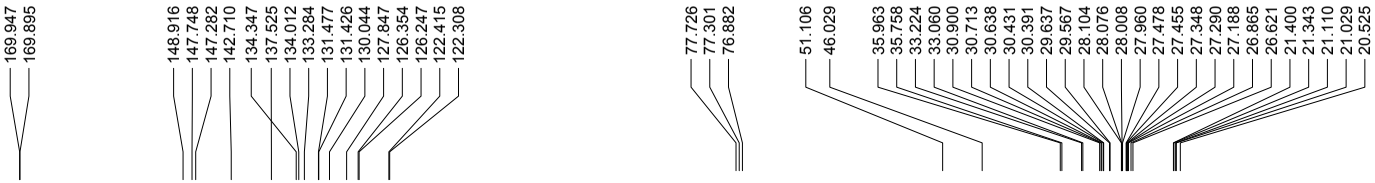


Sample: 3-NO2 ligand
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1800.43 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -81.69
B = 63.49

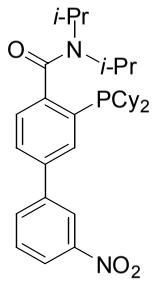


19q

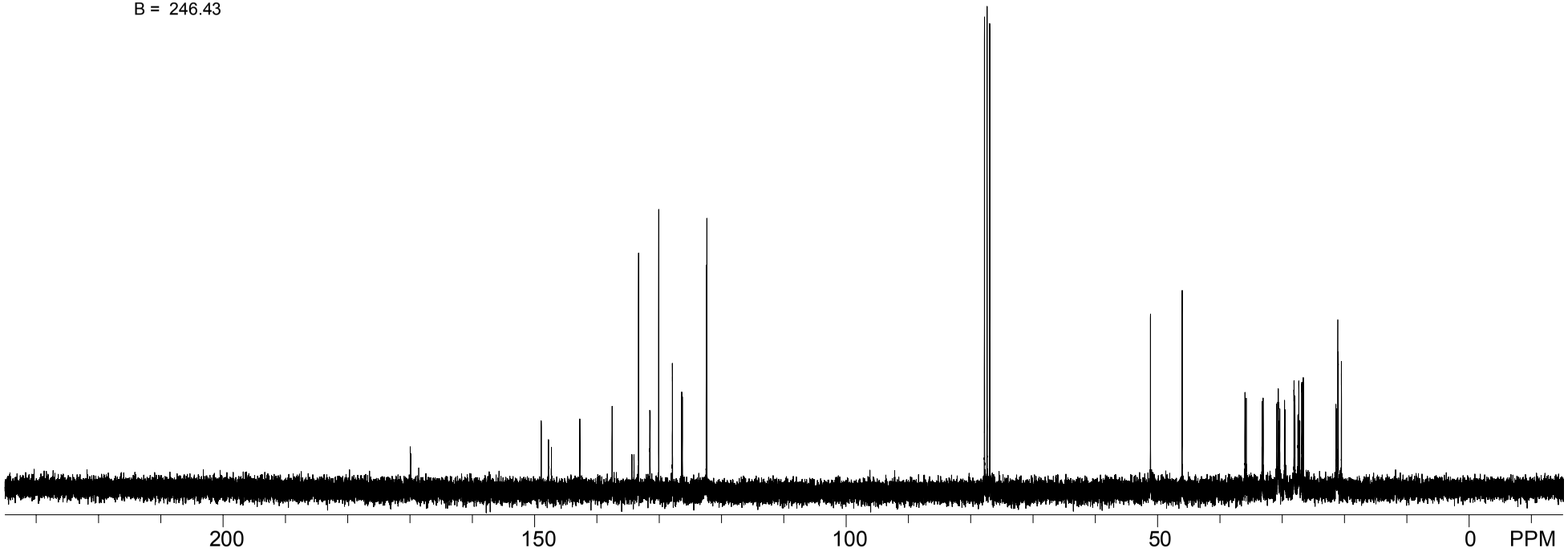


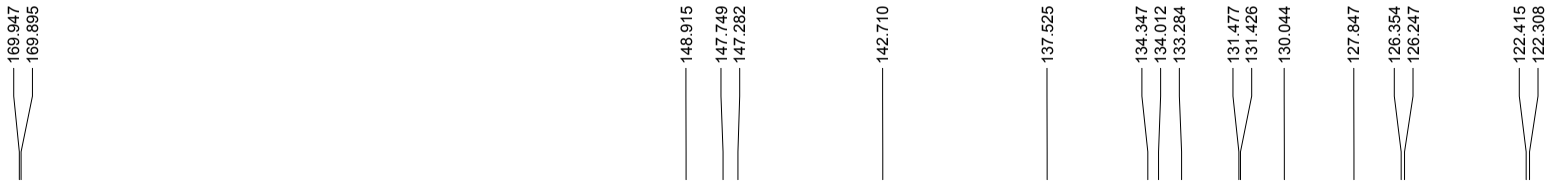


Sample: 3-NO2 ligand
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 2000
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -251.55
B = 246.43

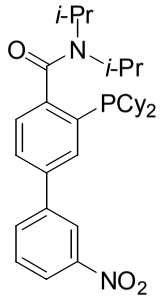


19q

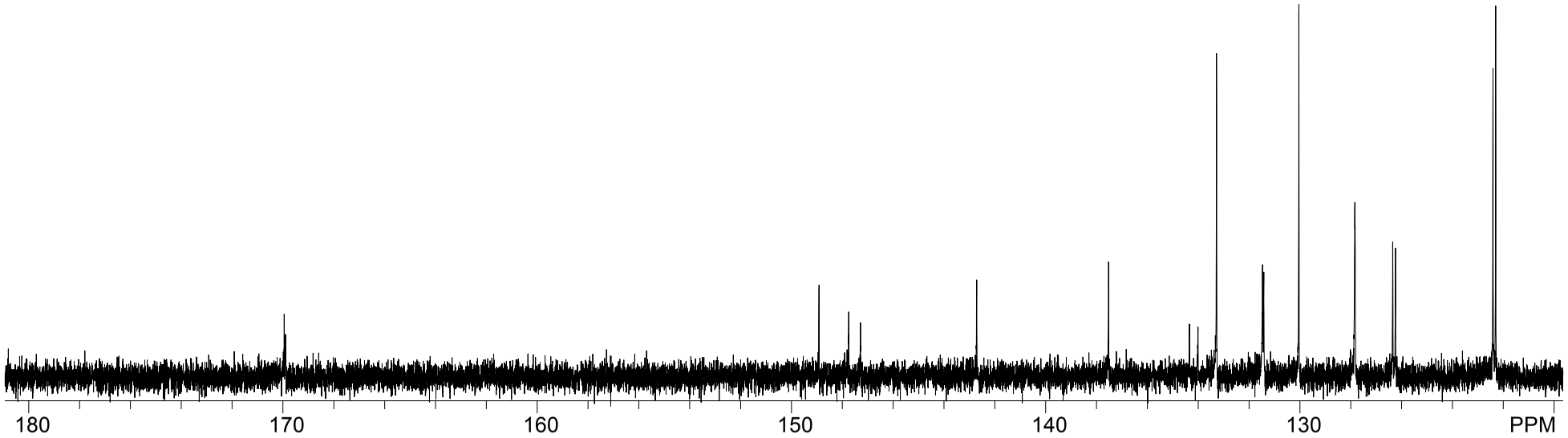


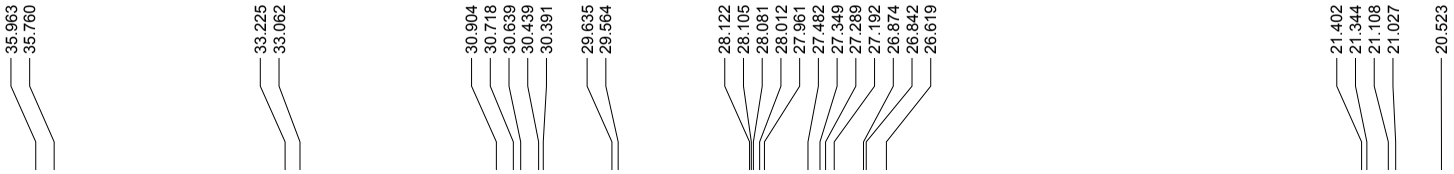


Sample: ligand
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 2000
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -258.76
B = 264.63

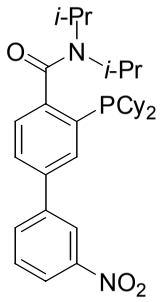


19q

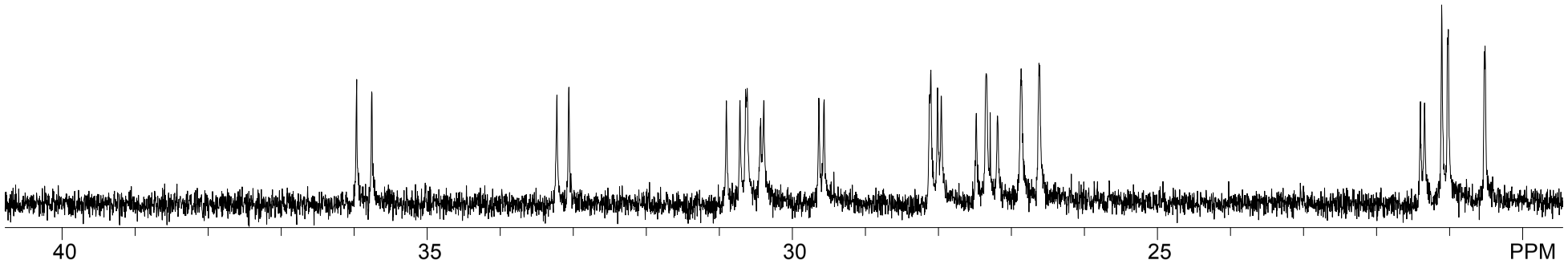




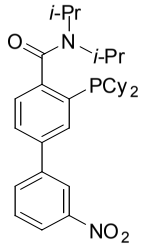
Sample: ligand
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 2000
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -258.76
B = 264.63



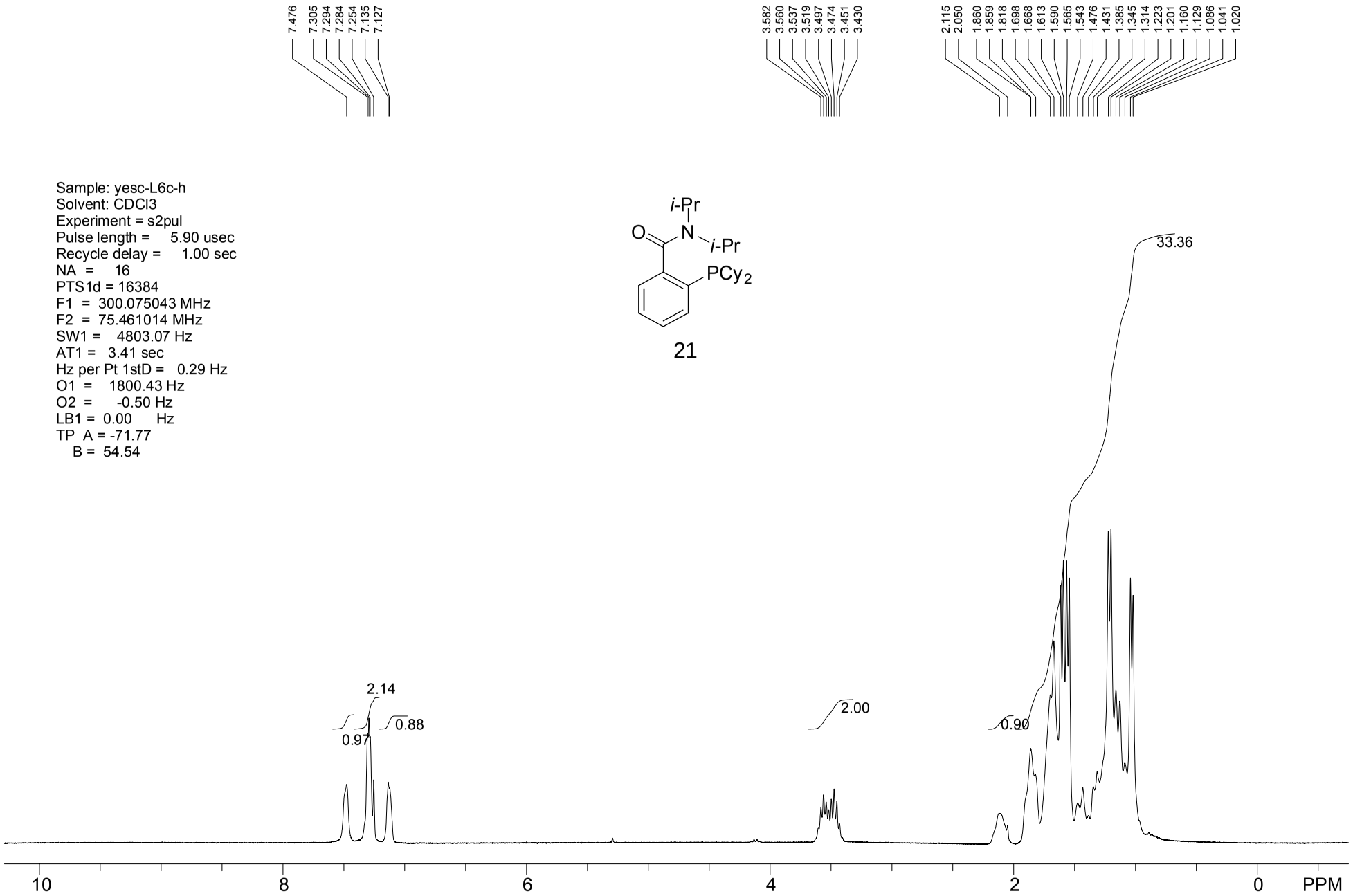
19q

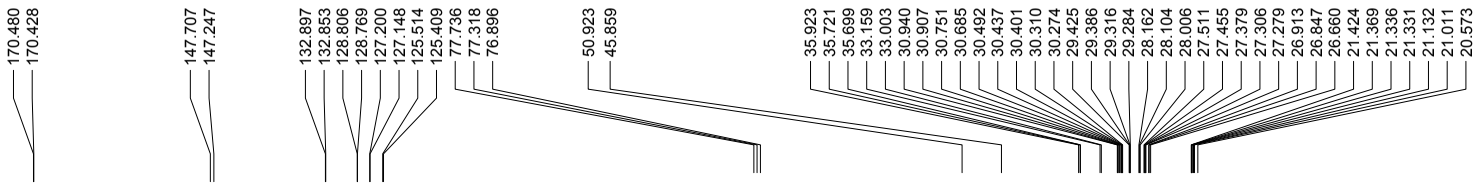


Sample: ligand
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 32
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 25.75
B = 11.69

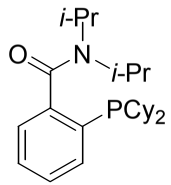


19q

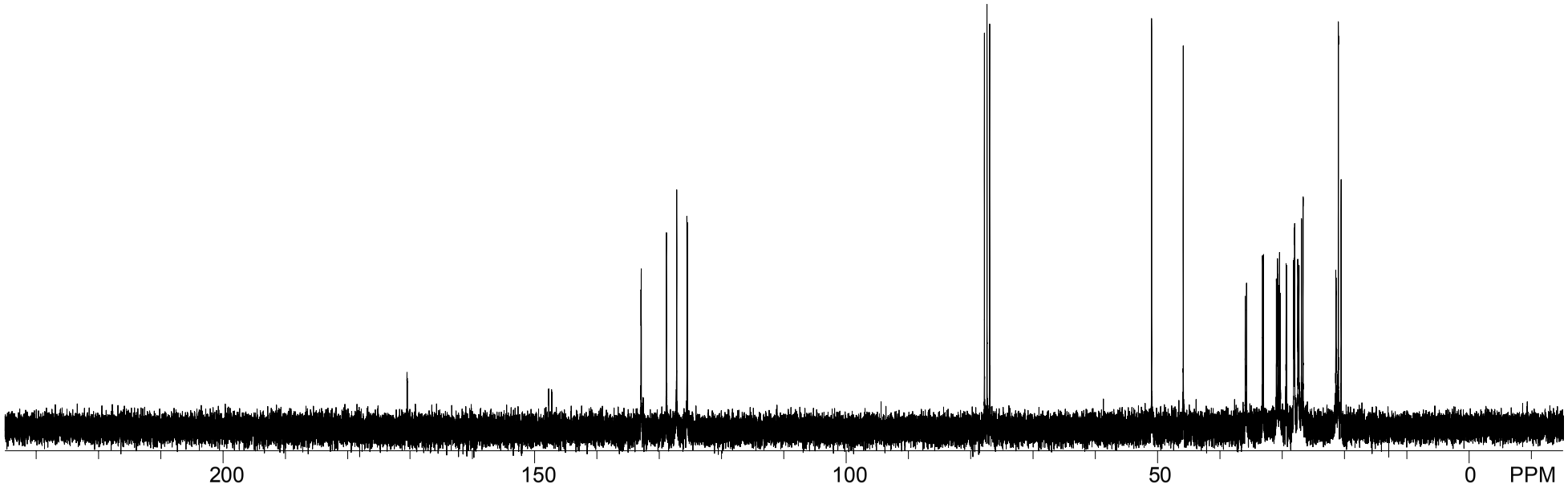

7.476
7.305
7.294
7.284
7.254
7.135
7.127
3.582
3.560
3.537
3.519
3.497
3.474
3.451
3.430
2.115
2.050
1.860
1.859
1.818
1.698
1.668
1.613
1.590
1.565
1.543
1.476
1.431
1.385
1.345
1.314
1.223
1.201
1.160
1.129
1.086
1.041
1.020
Sample: yesc-L6c-h
Solvent: CDCl3
Experiment = s2pul
Pulse length = 5.90 usec
Recycle delay = 1.00 sec
NA = 16
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1800.43 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -71.77
B = 54.54
i-Pr
O
N
i-Pr
PCy2
21
33.36
2.14
0.88
0.97
2.00
0.90
10
8
6
4
2
0
PPM

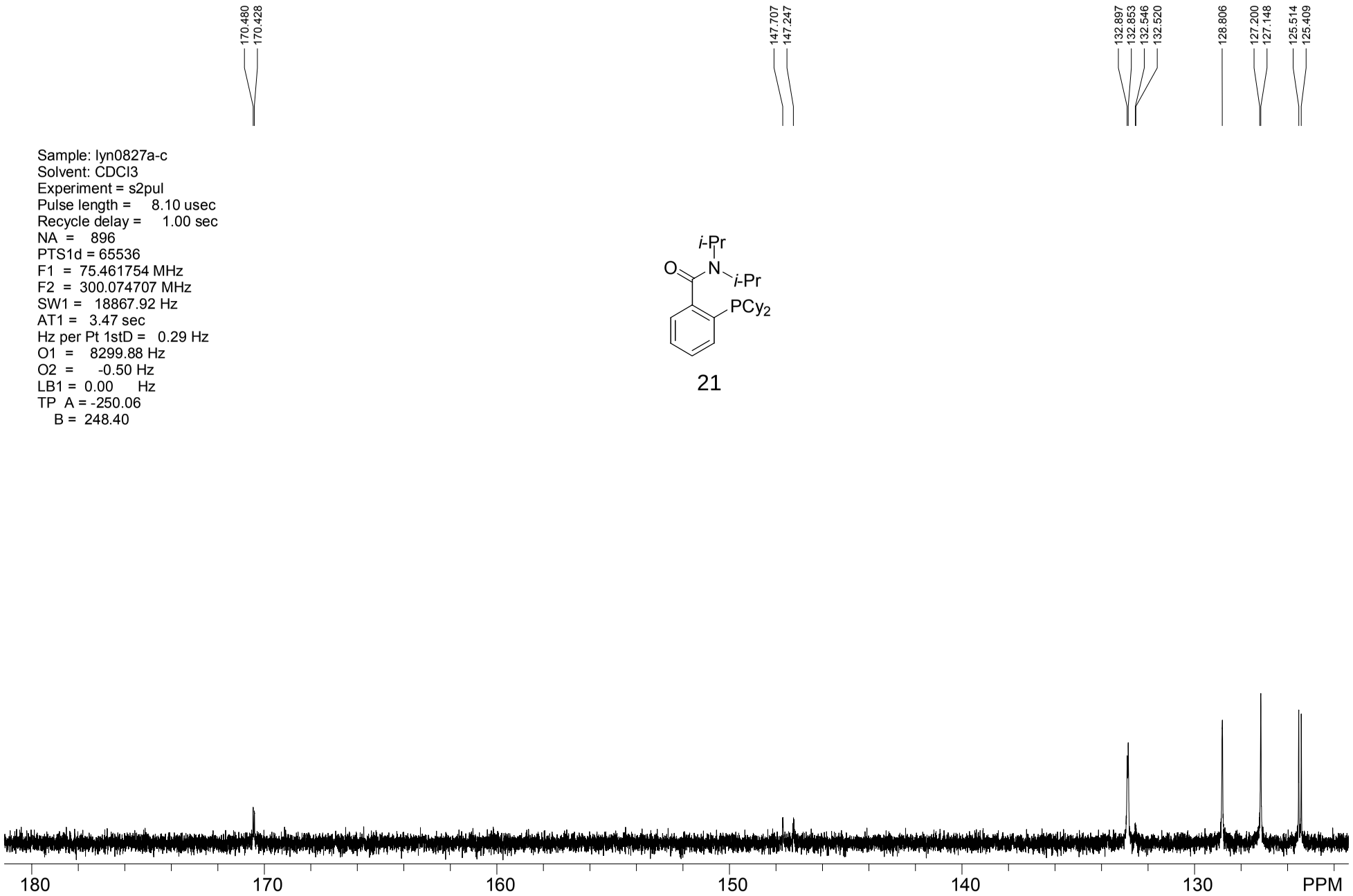


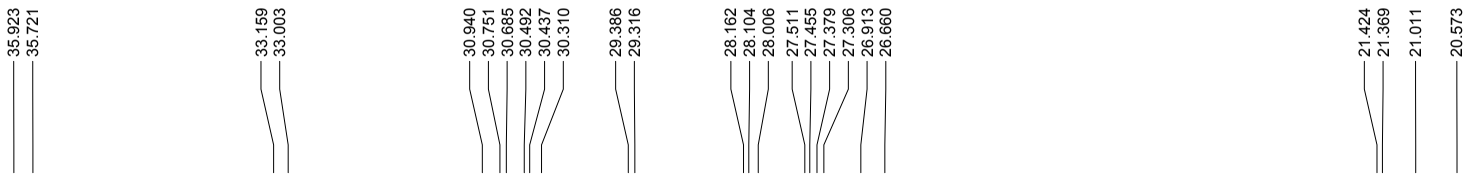
Sample: lyn0827a-c
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 896
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -250.06
B = 248.40



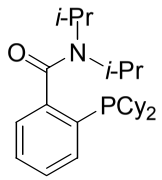
21



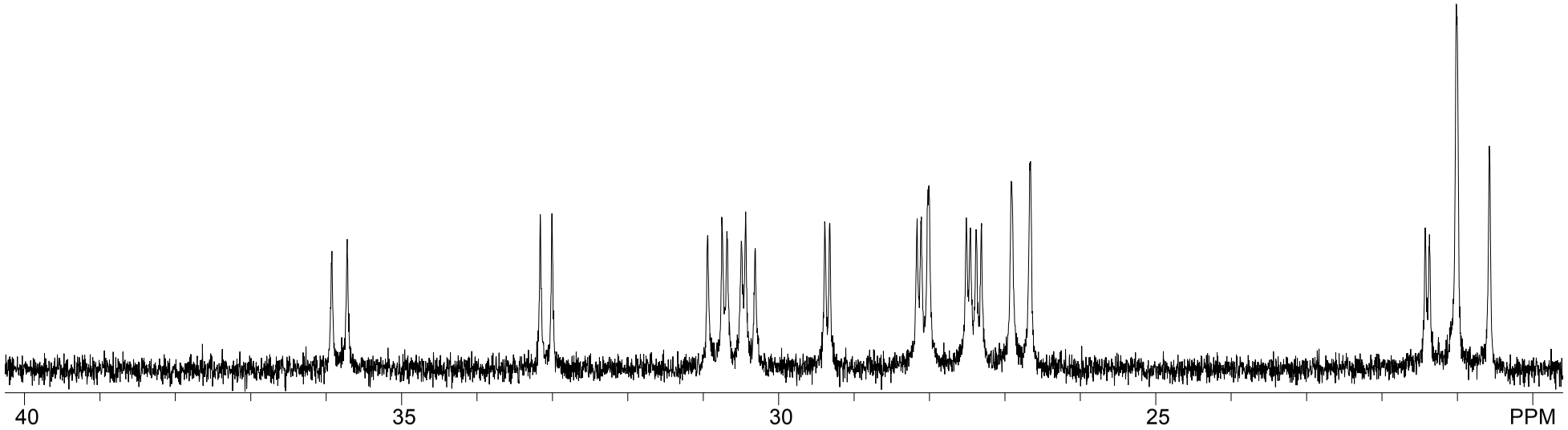

170.480
170.428
147.707
147.247
132.897
132.853
132.546
132.520
128.806
127.200
127.148
125.514
125.409
Sample: lyn0827a-c
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 896
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -250.06
B = 248.40
i-Pr
O
N
i-Pr
PCy2
21
180
170
160
150
140
130
PPM



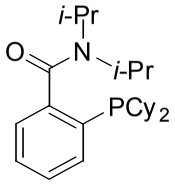
Sample: lyn0827a-c
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 896
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -250.06
B = 248.40



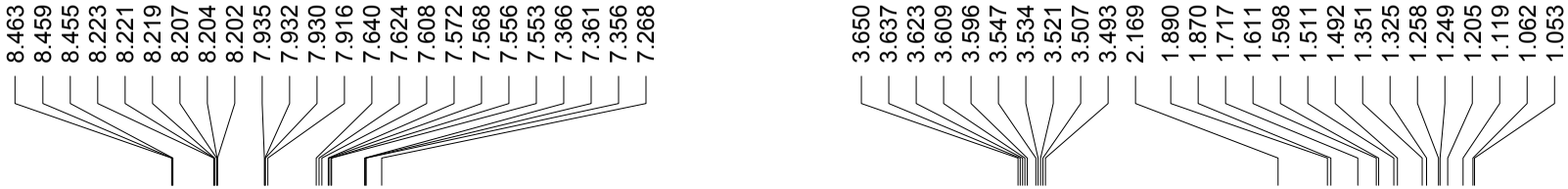
21



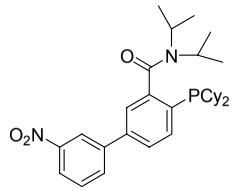
Sample: A-phos-2
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.14 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.477806 MHz
F2 = 300.074707 MHz
SW1 = 36496.35 Hz
AT1 = 1.80 sec
Hz per Pt 1stD = 0.56 Hz
O1 = 6073.59 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 2004.90
B = -2891.62



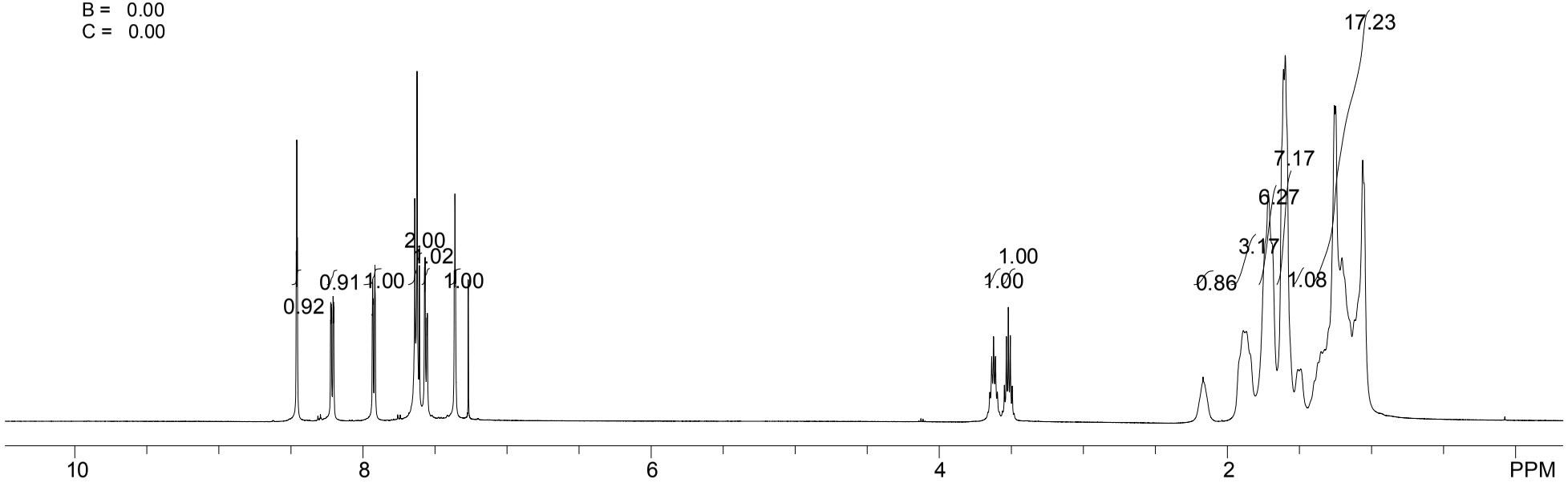
21

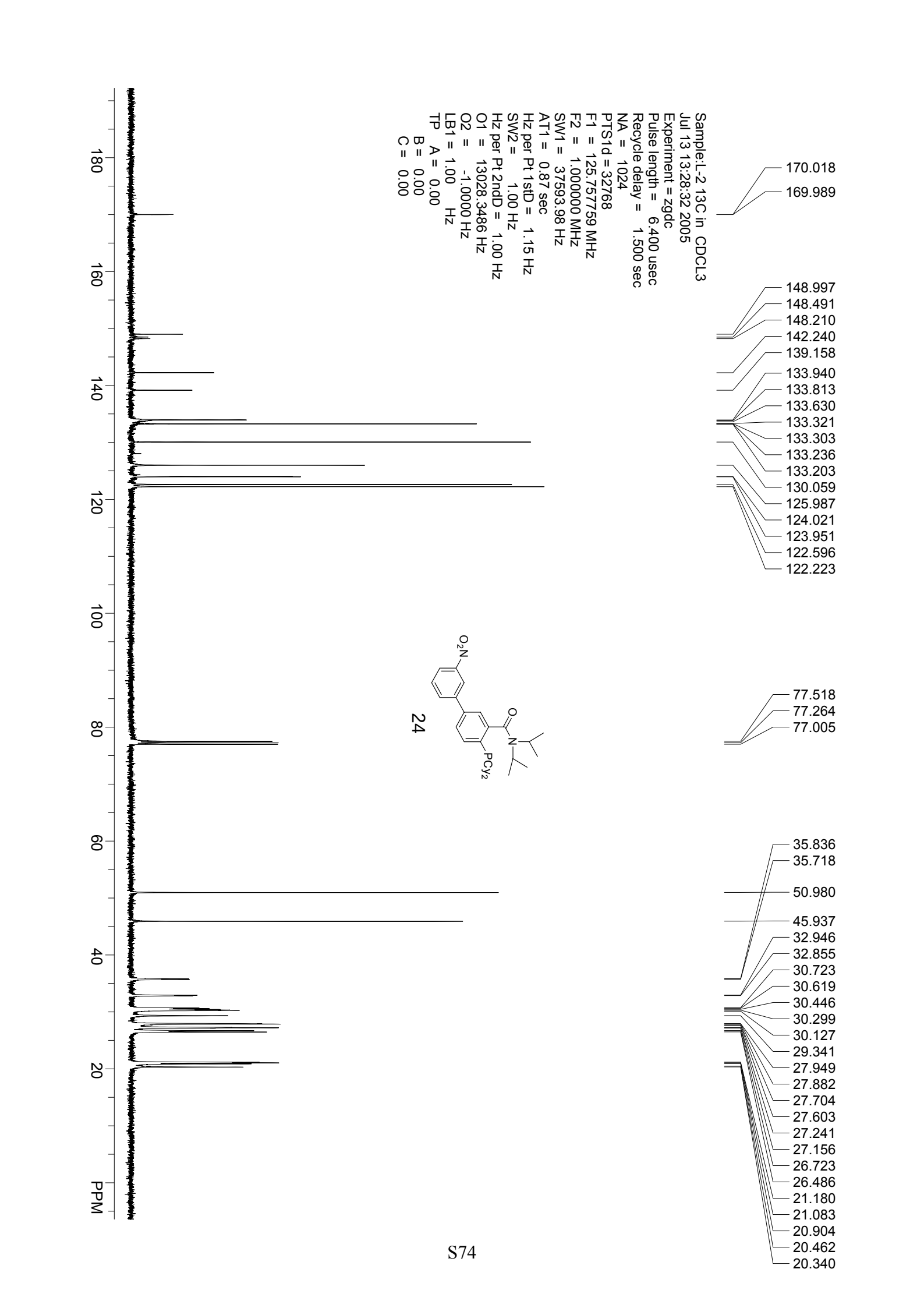


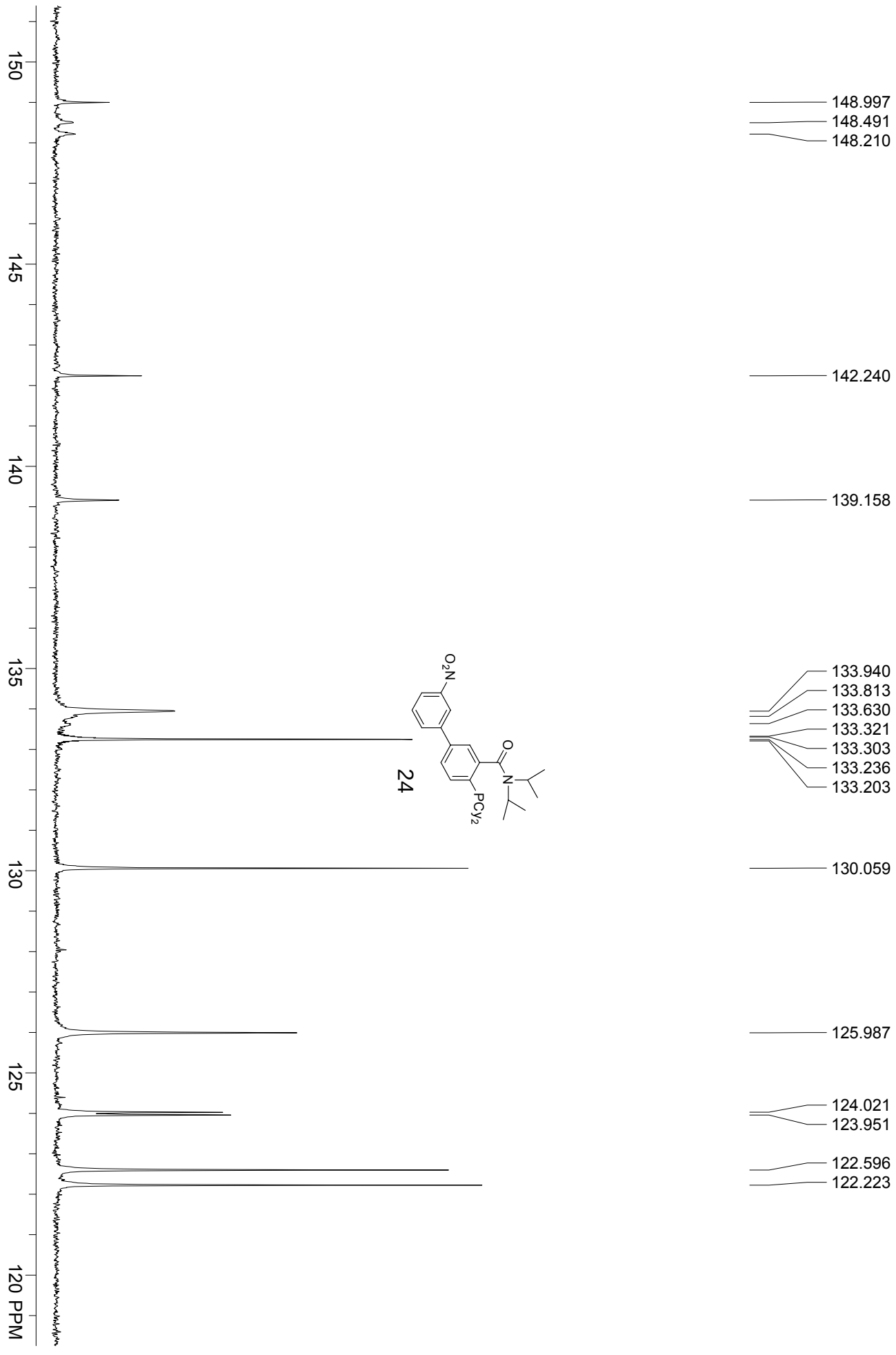
Sample:L-2 in CDCL3
Jul 13 13:33:26 2005
Experiment = zg30
Pulse length = 8.700 usec
Recycle delay = 1.500 sec
NA = 16
PTS1d = 32768
F1 = 500.130005 MHz
F2 = 1.000000 MHz
SW1 = 12531.33 Hz
AT1 = 2.61 sec
Hz per Pt 1stD = 0.38 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 3590.4385 Hz
O2 = -1.0000 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00

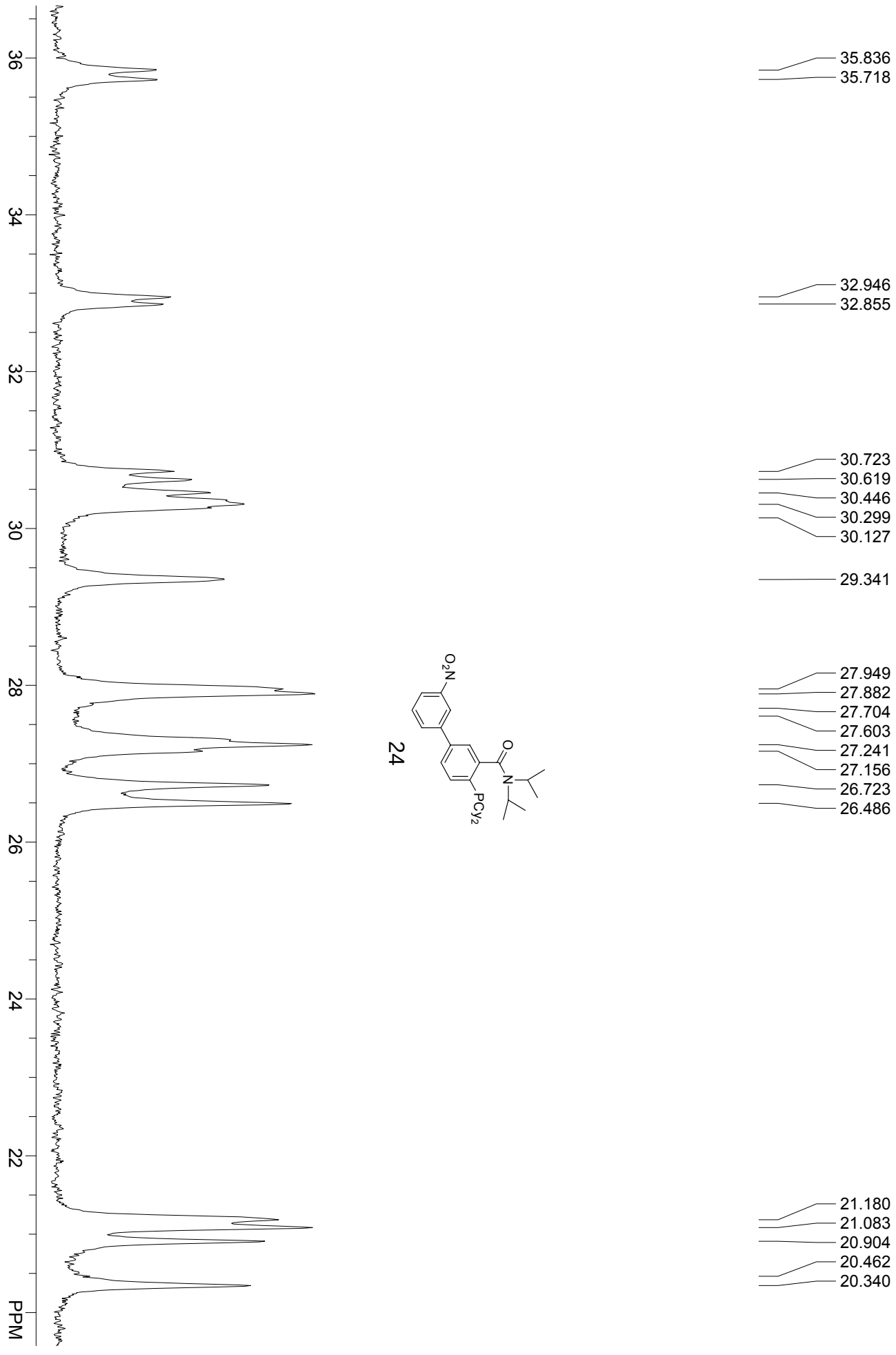


24

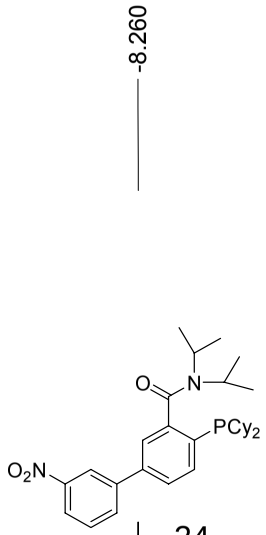



Sample:L-2 13C in CDCL3
Jul 13 13:28:32 2005
Experiment = zgdc
Pulse length = 6.400 usec
Recycle delay = 1.500 sec
NA = 1024
PTS1d = 32768
F1 = 125.757759 MHz
F2 = 1.000000 MHz
SW1 = 37593.98 Hz
AT1 = 0.87 sec
Hz per Pt 1stD = 1.15 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 13028.3486 Hz
O2 = -1.0000 Hz
LB1 = 1.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
170.018
169.989
148.997
148.491
148.210
142.240
139.158
133.940
133.813
133.630
133.321
133.303
133.236
133.203
130.059
125.987
124.021
123.951
122.596
122.223
77.518
77.264
77.005
35.836
35.718
50.980
45.937
32.946
32.855
30.723
30.619
30.446
30.299
30.127
29.341
27.949
27.882
27.704
27.603
27.241
27.156
26.723
26.486
21.180
21.083
20.904
20.462
20.340
O2N
O
N
PCy2
24
180
160
140
120
100
80
60
40
20
PPM


150
145
140
135
130
125
120 PPM
148.997
148.491
148.210
142.240
139.158
133.940
133.813
133.630
133.321
133.303
133.236
133.203
130.059
125.987
124.021
123.951
122.596
122.223
24
O2N
O
N
PCy2


36
34
32
30
28
26
24
22
PPM
35.836
35.718
32.946
32.855
30.723
30.619
30.446
30.299
30.127
29.341
27.949
27.882
27.704
27.603
27.241
27.156
26.723
26.486
21.180
21.083
20.904
20.462
20.340
O2N
O
N
PCy2
24

Sample:L-2 31P in CDCL3 31P
Jul 13 13:37:06 2005
Experiment = zgdc
Pulse length = 4.000 usec
Recycle delay = 3.000 sec
NA = 105
PTS1d = 32768
F1 = 202.456039 MHz
F2 = 1.000000 MHz
SW1 = 60606.06 Hz
AT1 = 0.54 sec
Hz per Pt 1stD = 1.85 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 42.5390 Hz
O2 = -1.0000 Hz
LB1 = 2.00 Hz
TP A = 0.00
B = 0.00
C = 0.00



24

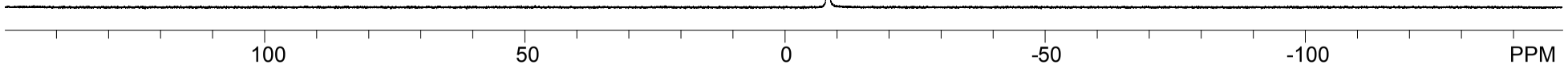
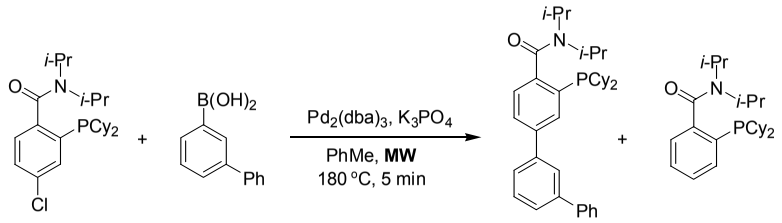


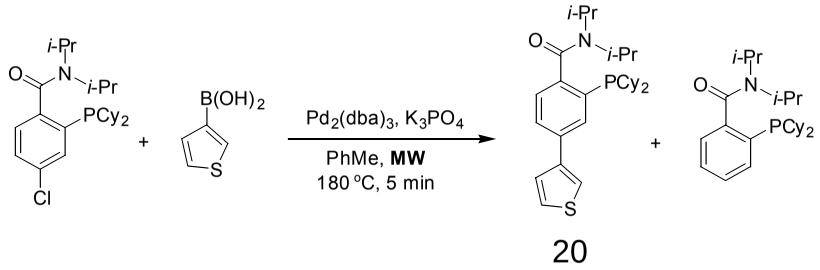
Table 1, entry 1:



19a

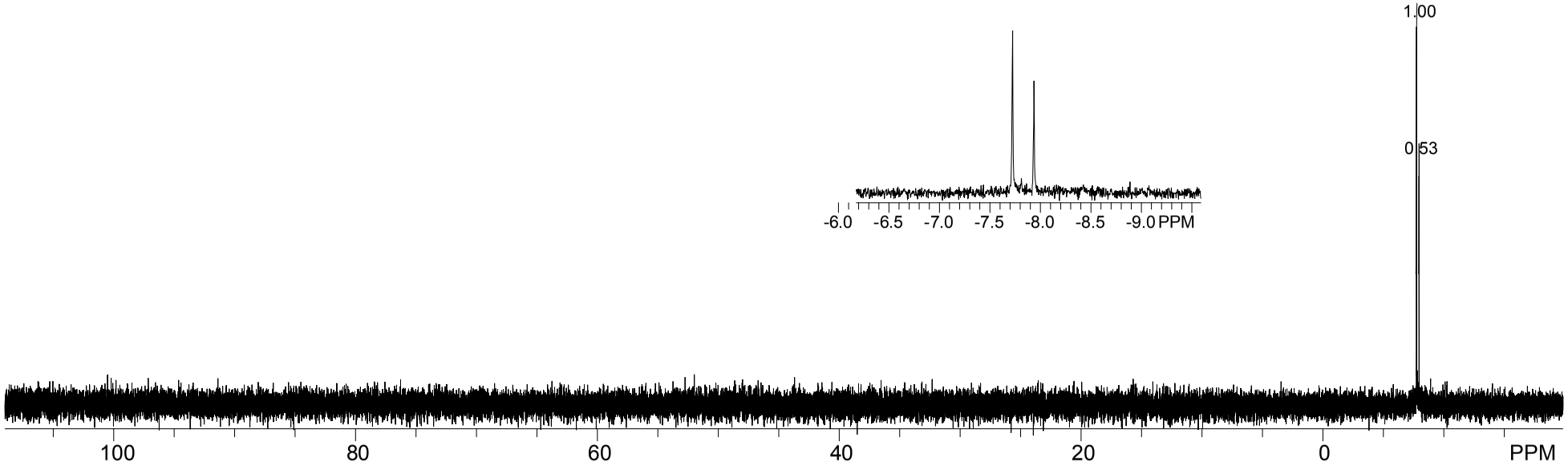
Sample: 3-Ph
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 34.80
B = 2.76

Table 1, entry 2:



20

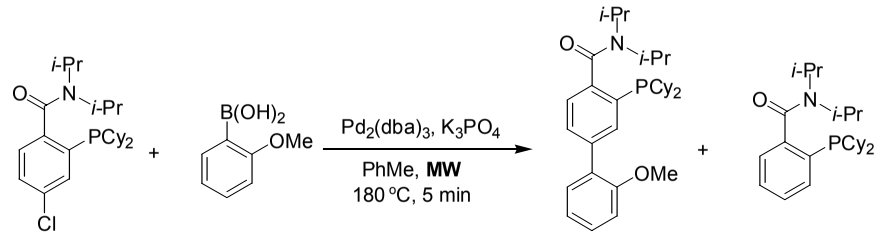
Sample: 3-thienyl
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 94.55
B = -57.02



47.793

-7.322
-7.926

Table 1, entry 3:



19b

Sample: 2-OMe
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 59.08
B = -28.94

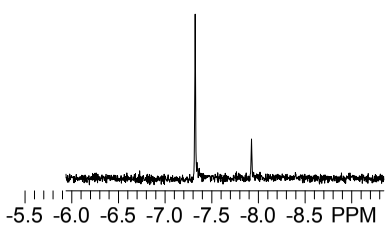
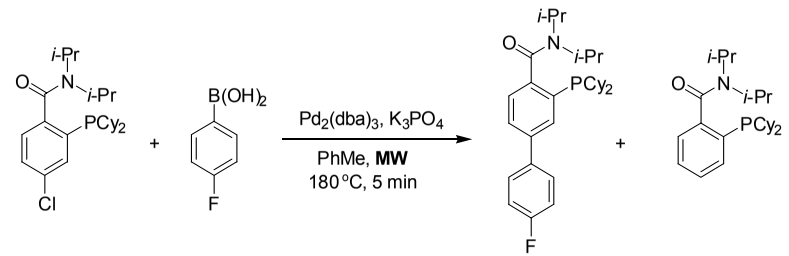


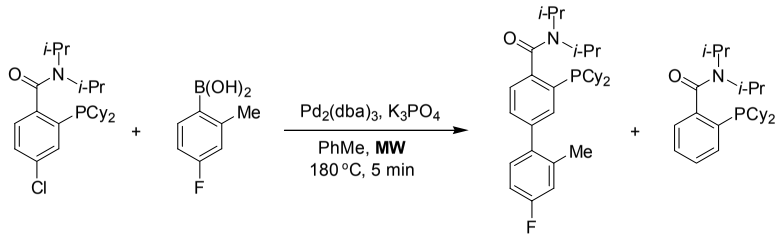
Table 1, entry 4:



19c

Sample: 4-F
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -158.29
B = 219.13

Table 1, entry 5:



19d

Sample: 2-Me,4-F
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 84.52
B = -40.99

Table 1, entry 6:

19e

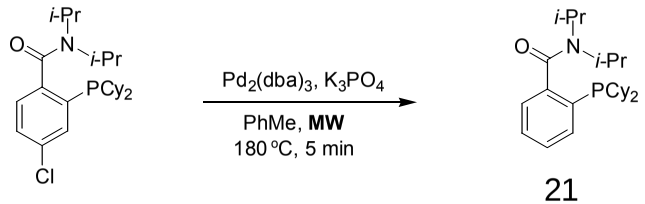
Sample: 4-Me
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 76.72
B = -40.66

Table 1, entry 7:

18c

Sample: H
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -154.67
B = 213.10

Table 1, entry 8:



21

Sample: -
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 33.40
B = 1.45

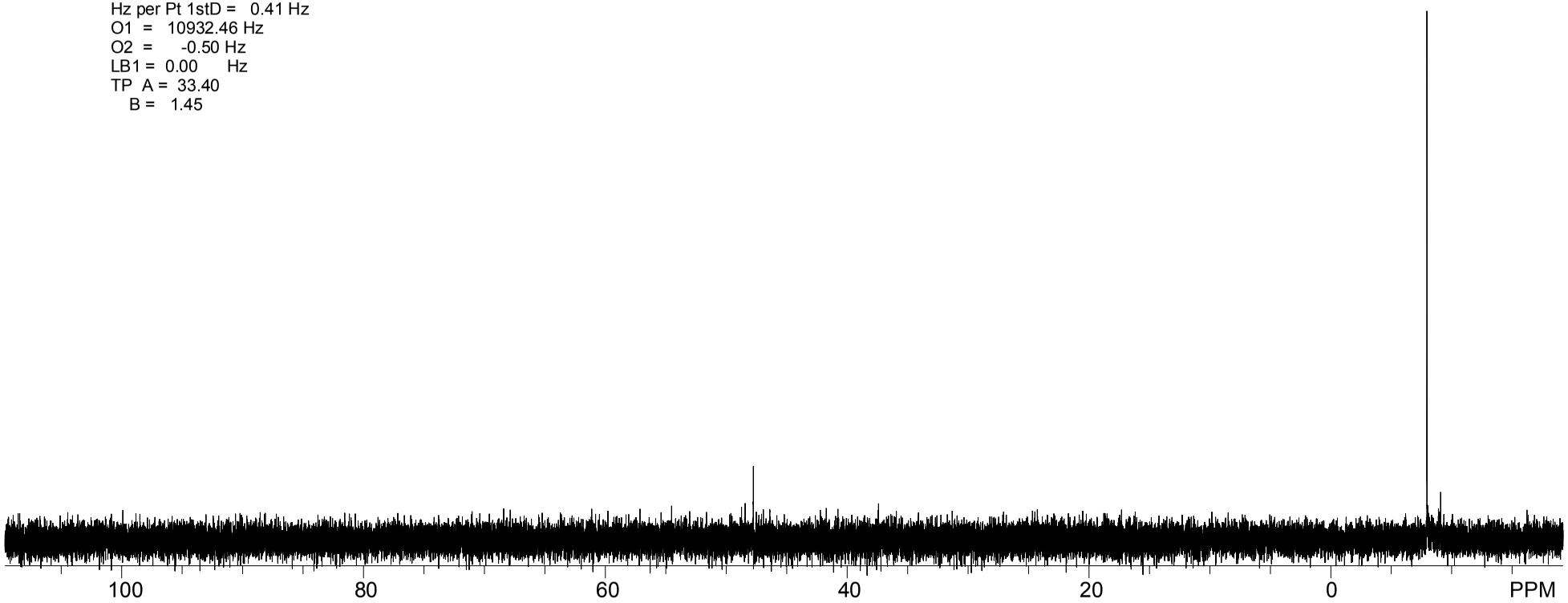
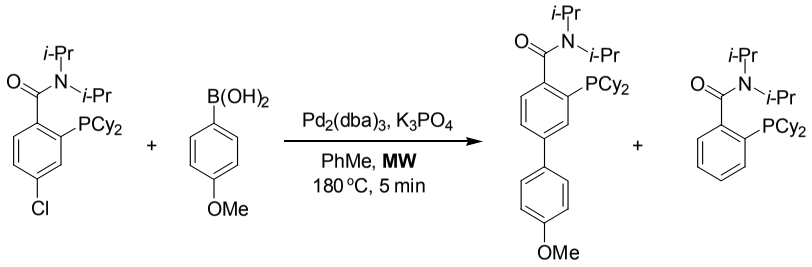


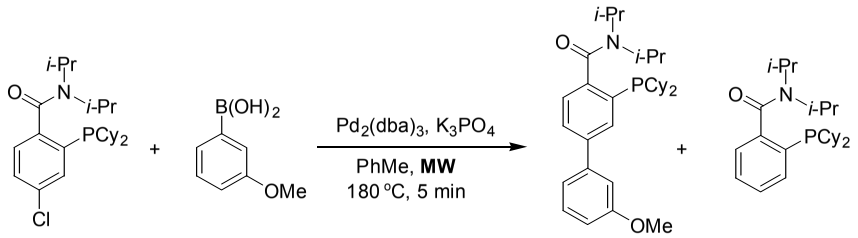
Table 1, entry 9:



19f

Sample: 4-OMe
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 26.81
B = 14.86

Table 1, entry 10:



19g

Sample: 3-OMe
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 1.78
B = 40.34

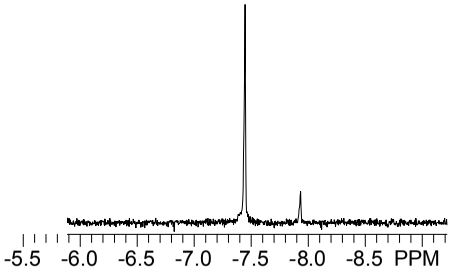
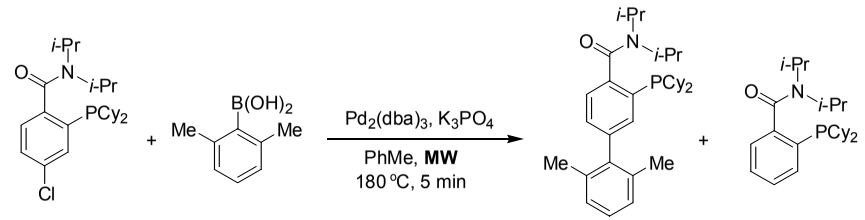


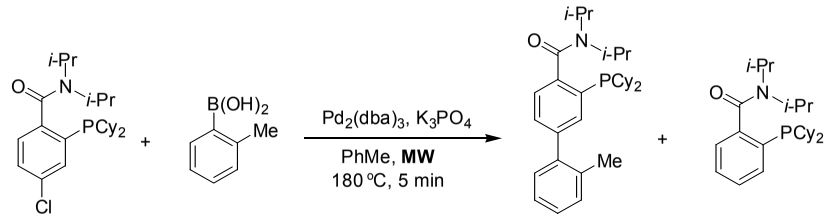
Table 1, entry 11:



19h

Sample: 2,6-Me
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 1.97
B = 37.81

Table 1, entry 12:



19i

Sample: 2-Me
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 177.47
B = -143.47

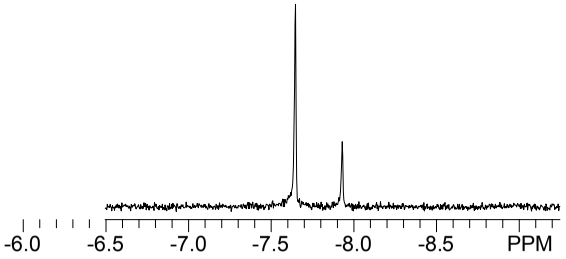
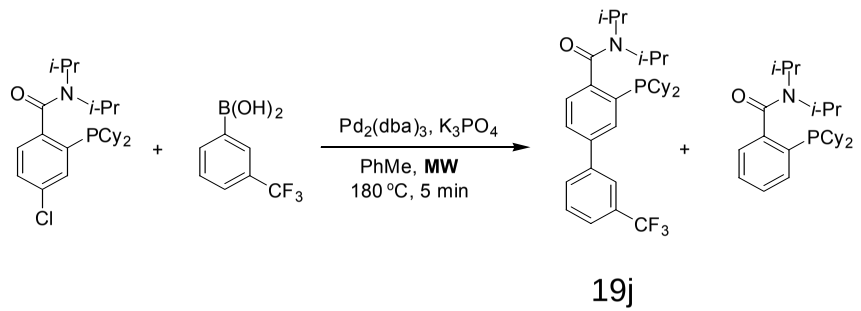


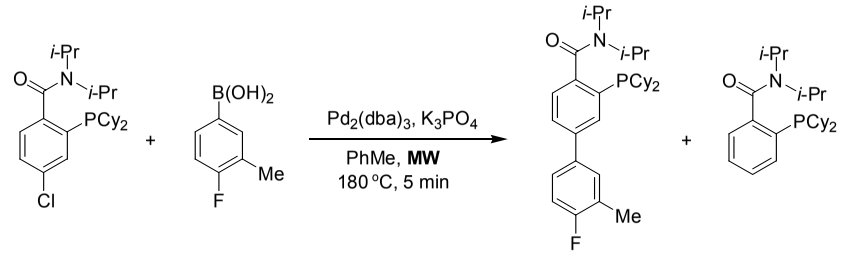
Table 1, entry 13:



19j

Sample: 3-CF3
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -4.37
B = 55.65

Table 1, entry 14:



19k

Sample: 3-Me,4-F
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 71.89
B = -36.18

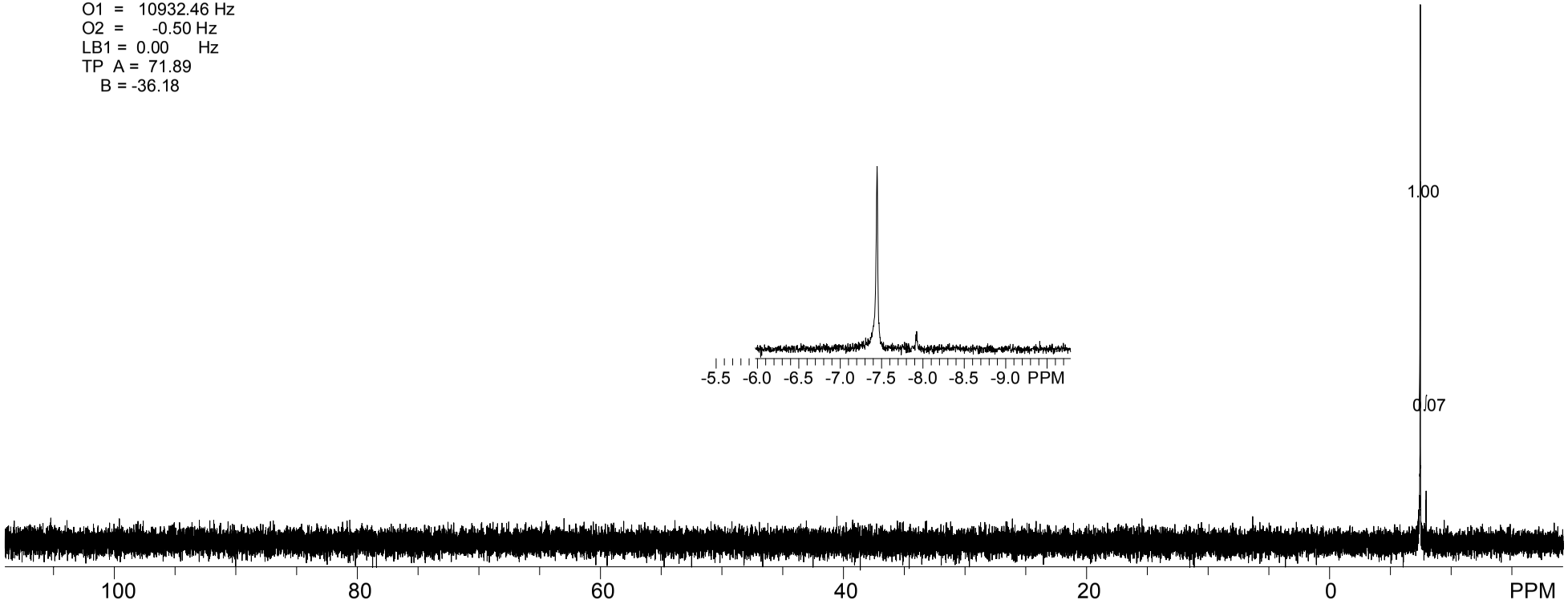
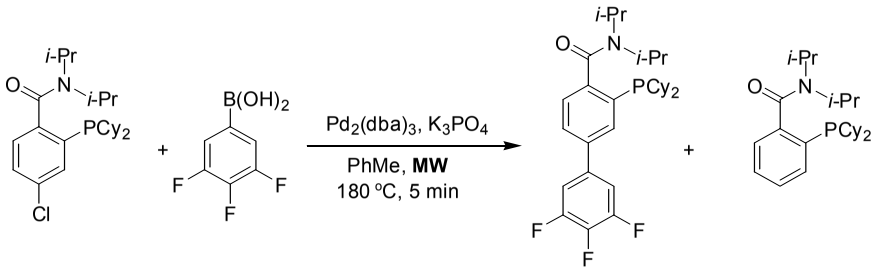


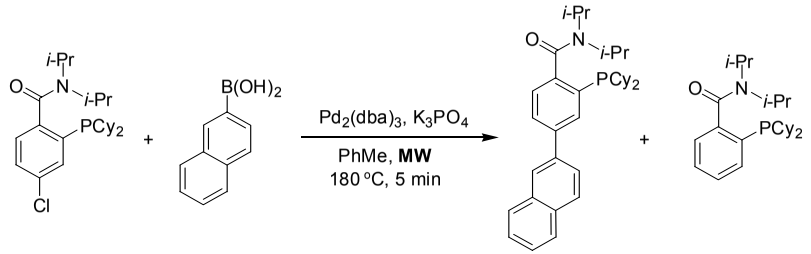
Table 1, entry 15:



19l

Sample: 3,4,5-F
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 109.72
B = -65.55

Table 1, entry 16:



19m

Sample: 3,4-benzo
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 45.79
B = -3.78

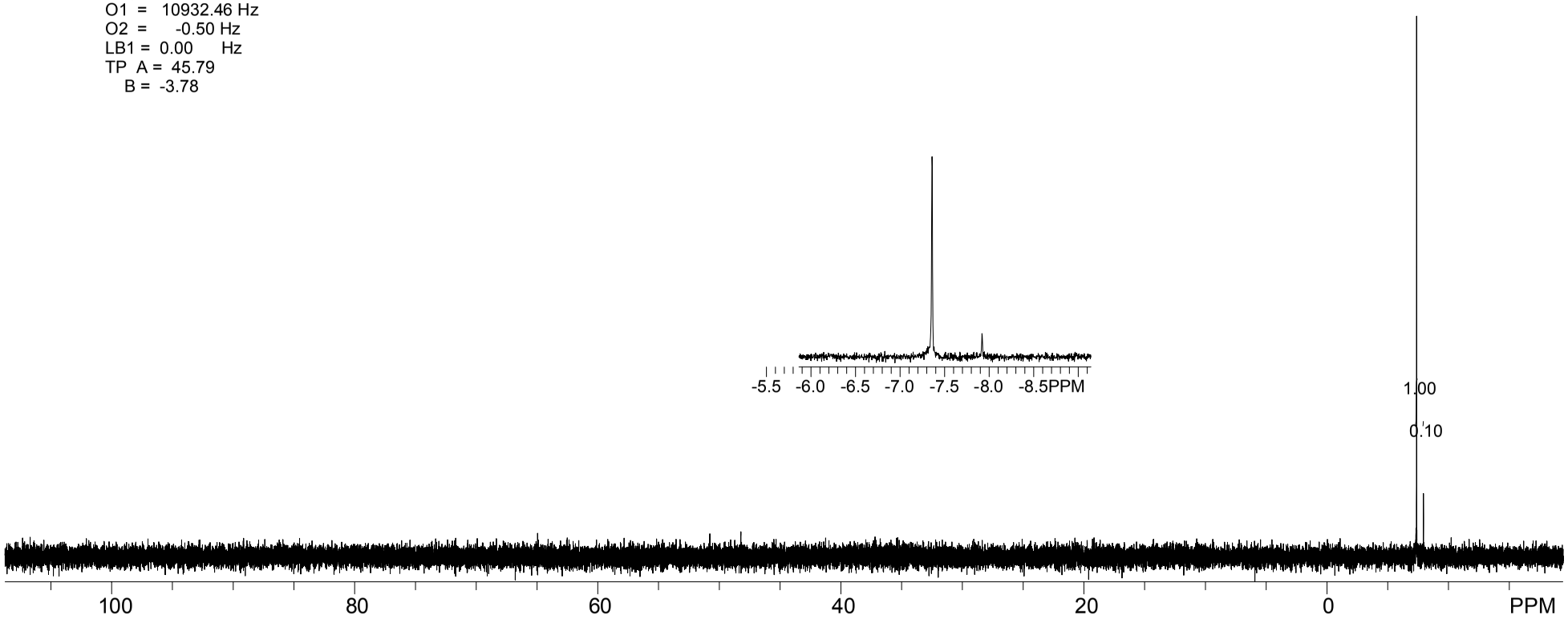
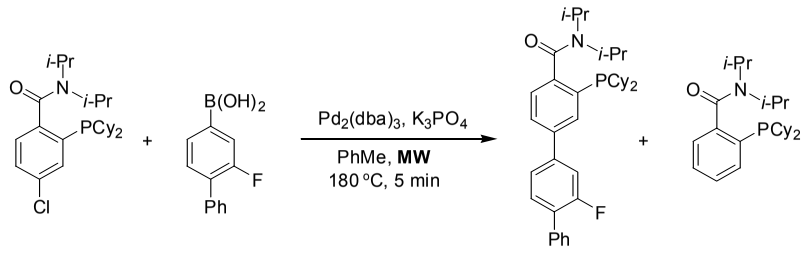


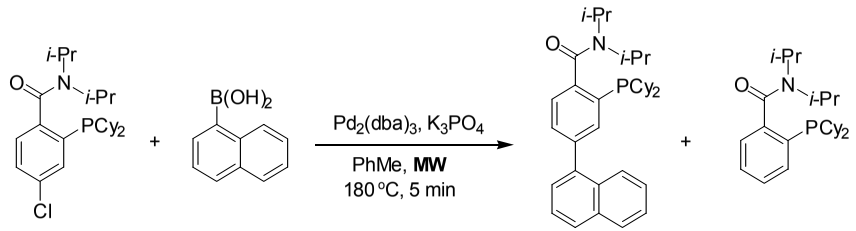
Table 1, entry 17:



19n

Sample: 3-F,4-phenyl
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -72.42
B = 123.02

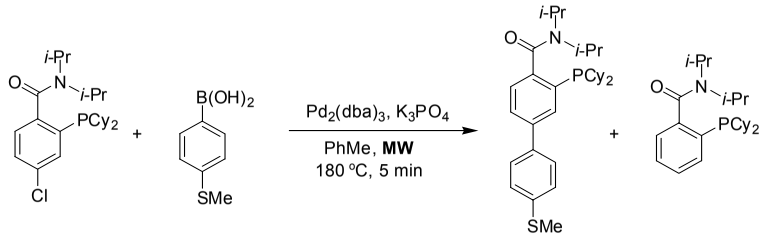
Table 1, entry 18:



19o

Sample: 2,3-benzo
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 92.57
B = -62.49

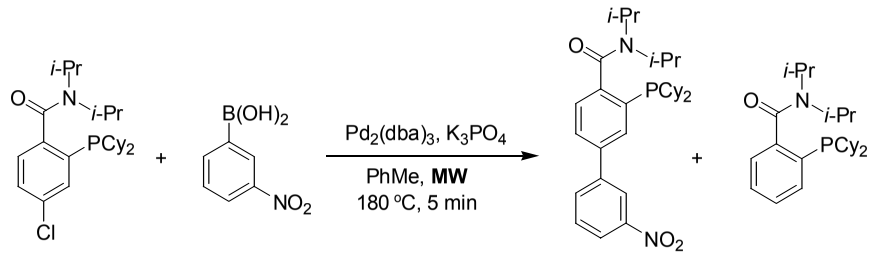
Table 1, entry 19:



19p

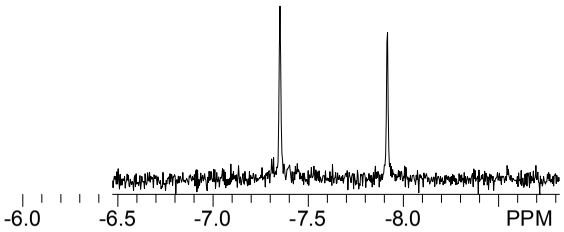
Sample: 4-SMe
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 142.62
B = -108.94

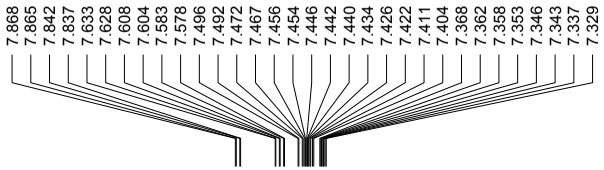
Table 1, entry 20:



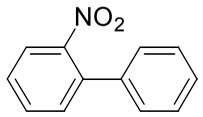
19q

Sample: 3-NO2
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.53 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 121.482666 MHz
F2 = 300.074707 MHz
SW1 = 26737.97 Hz
AT1 = 2.45 sec
Hz per Pt 1stD = 0.41 Hz
O1 = 10932.46 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = 85.88
B = -46.33

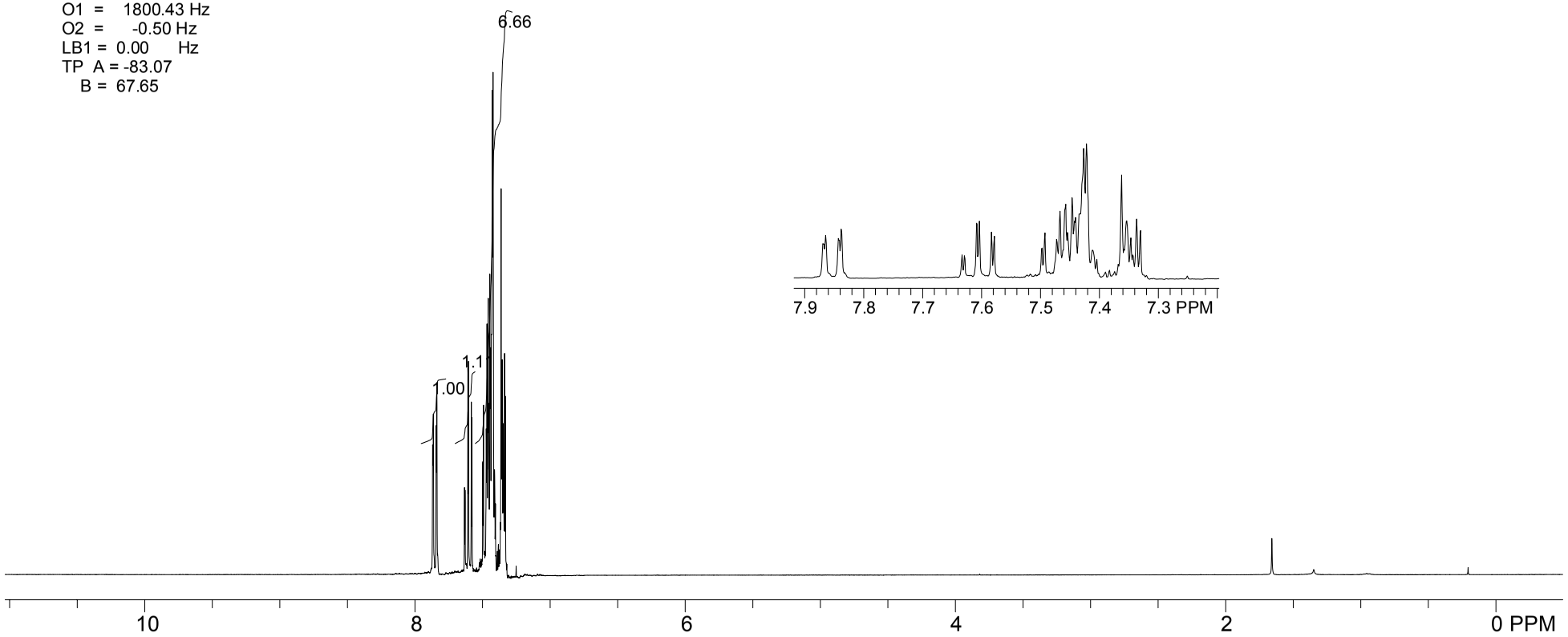


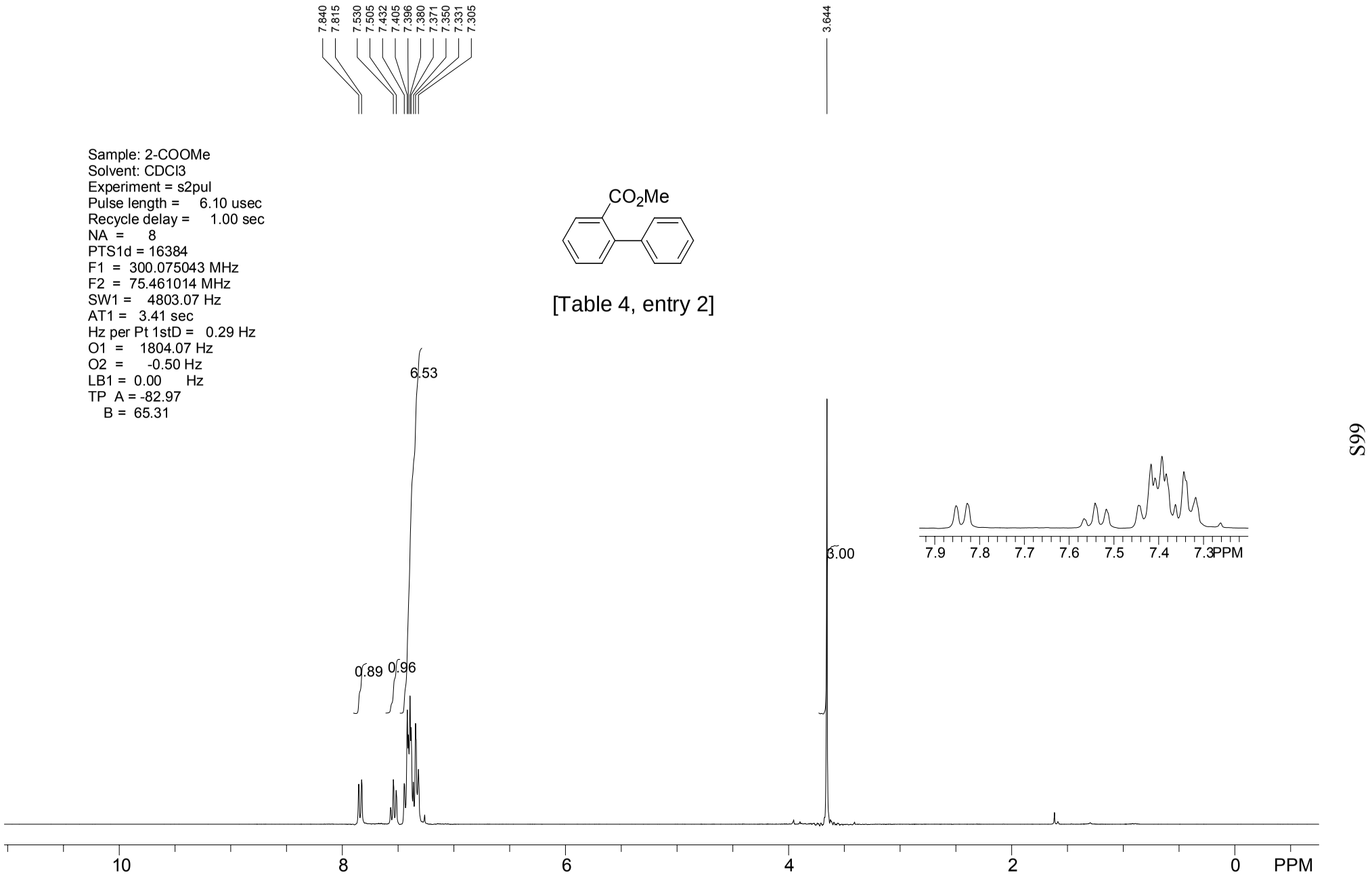


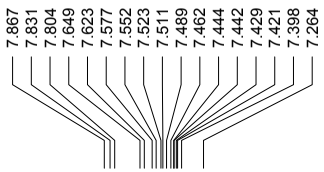
Sample: 2-NO2
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1800.43 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -83.07
B = 67.65



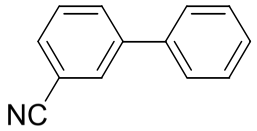
[Table 4, entry 1]



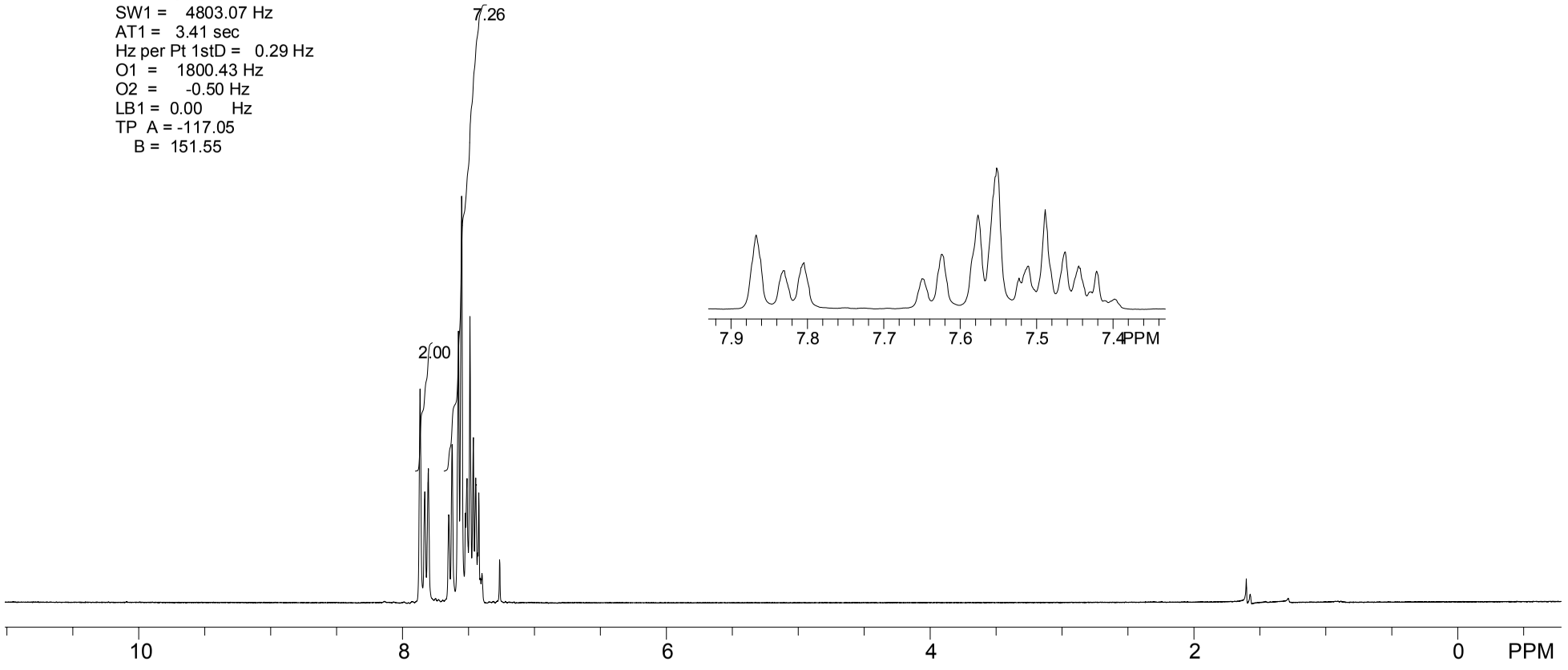

7.840
7.815
7.530
7.505
7.432
7.405
7.396
7.380
7.371
7.350
7.331
7.305
3.644
Sample: 2-COOMe
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1804.07 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -82.97
B = 65.31
CO2Me
[Table 4, entry 2]
6.53
0.89
0.96
3.00
7.9
7.8
7.7
7.6
7.5
7.4
7.3PPM
10
8
6
4
2
0
PPM

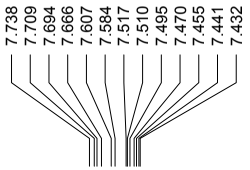


Sample: 3-CN
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1800.43 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -117.05
B = 151.55

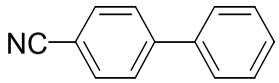


[Table 4, entry 3]

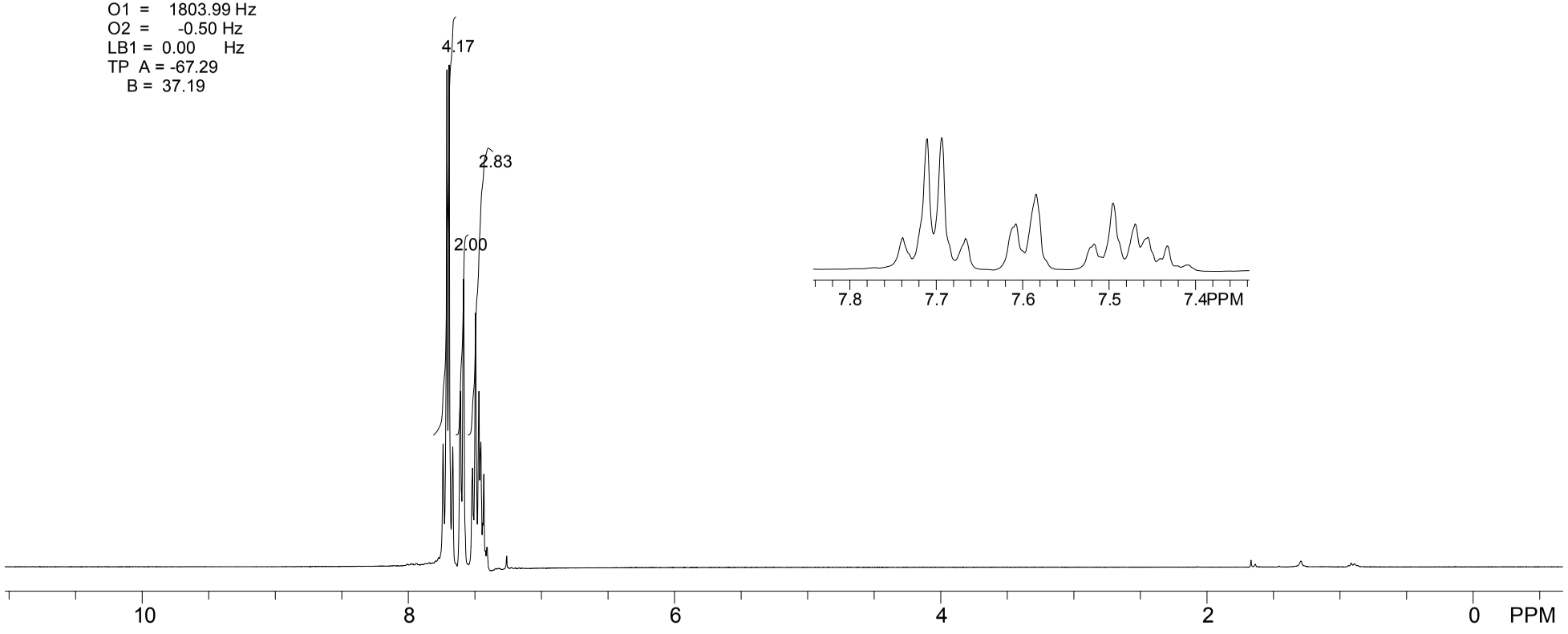


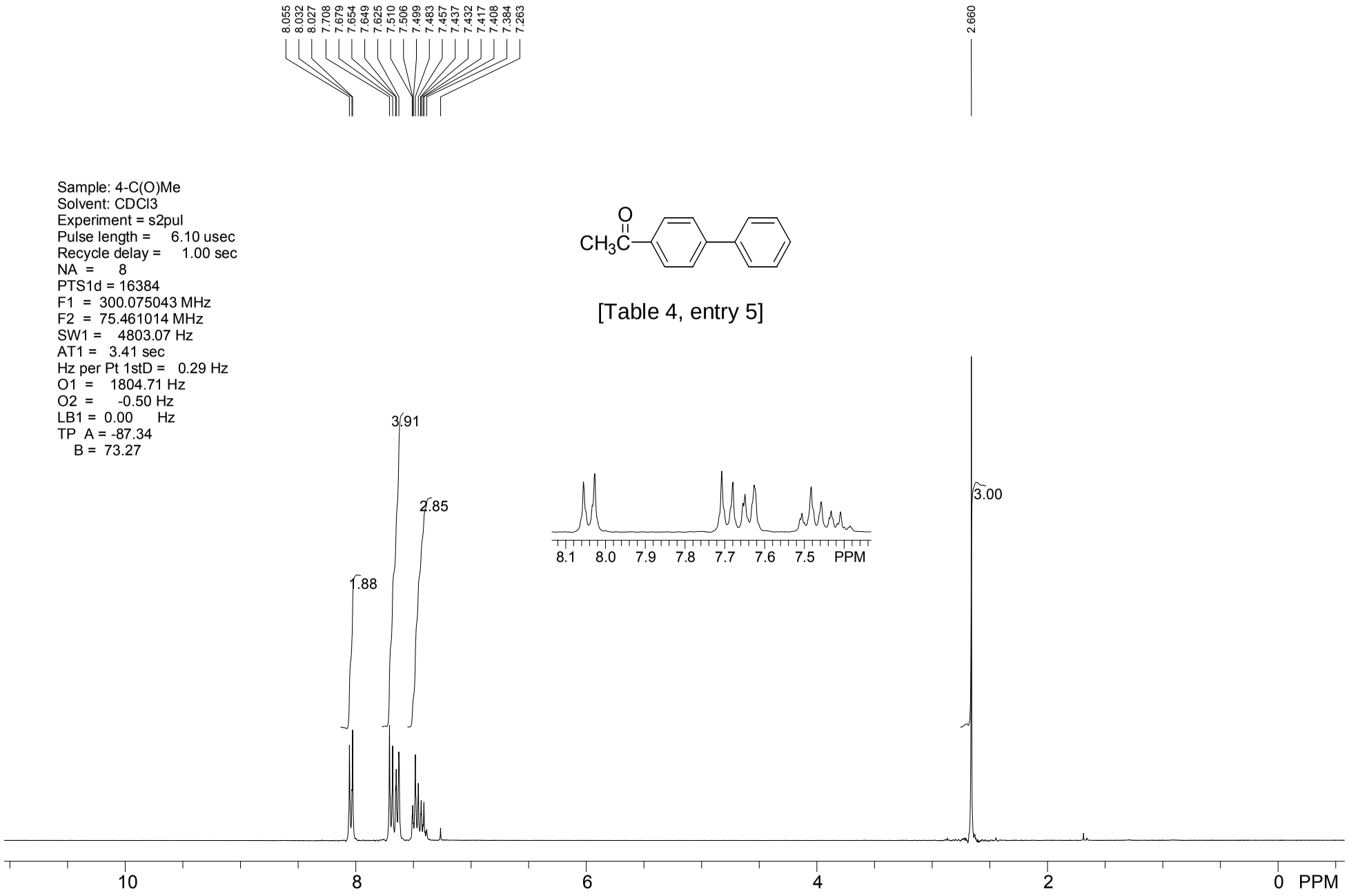


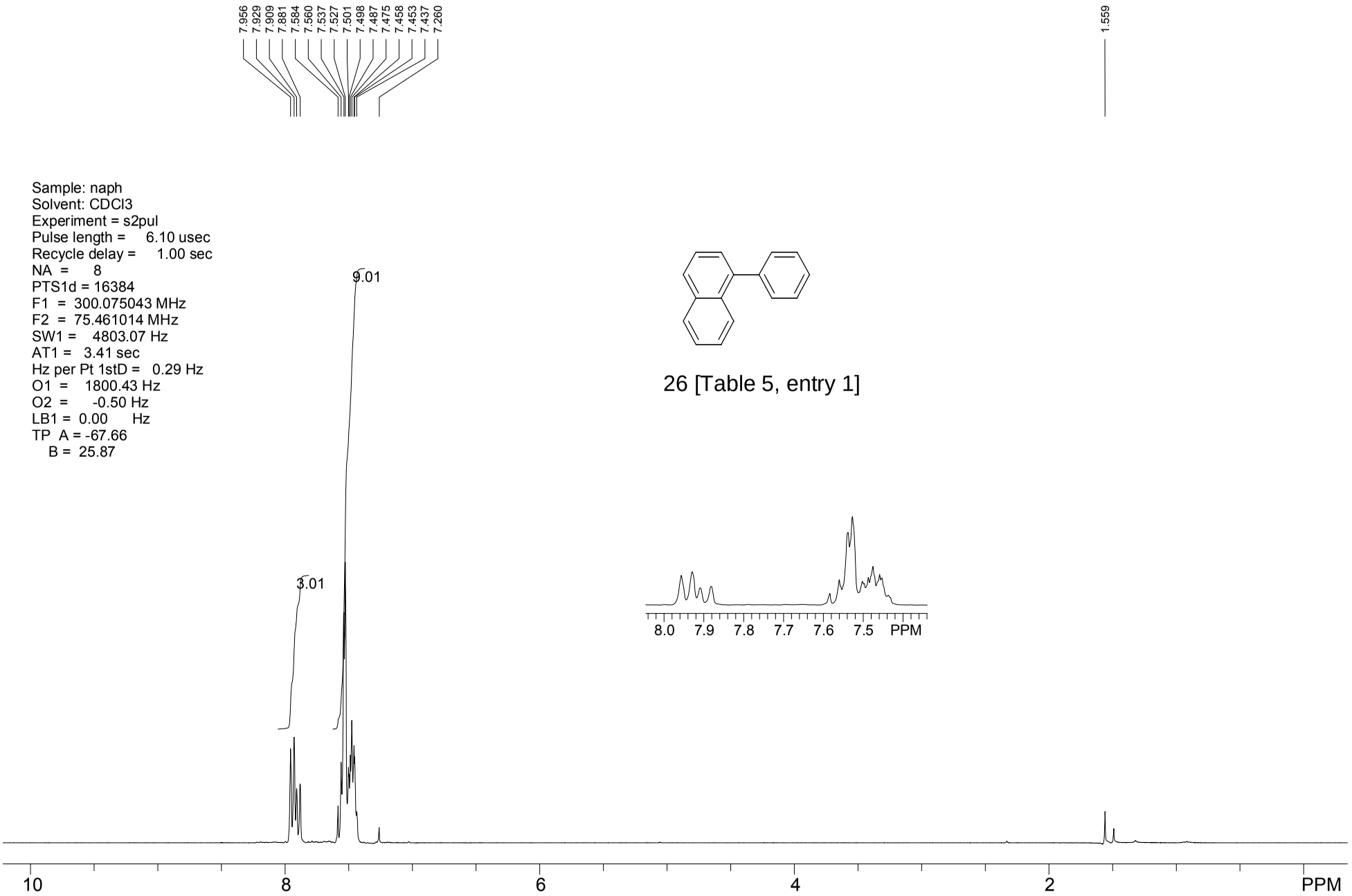
Sample: 4-CN
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1803.99 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -67.29
B = 37.19

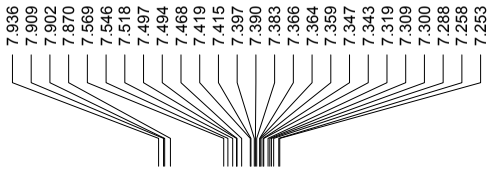


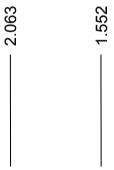
[Table 4, entry 4]



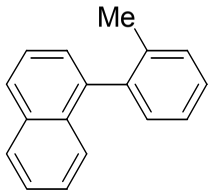

8.055
8.032
8.027
7.708
7.679
7.654
7.649
7.625
7.510
7.506
7.499
7.483
7.457
7.437
7.432
7.417
7.408
7.384
7.263
2.660
Sample: 4-C(O)Me
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1804.71 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -87.34
B = 73.27
O
CH3C
[Table 4, entry 5]
3.91
2.85
1.88
3.00
8.1 8.0 7.9 7.8 7.7 7.6 7.5 PPM
10 8 6 4 2 0 PPM


7.956
7.929
7.909
7.881
7.584
7.560
7.537
7.527
7.501
7.498
7.487
7.475
7.458
7.453
7.437
7.260
1.559
Sample: naph
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1800.43 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -67.66
B = 25.87
9.01
3.01
26 [Table 5, entry 1]
8.0 7.9 7.8 7.7 7.6 7.5 PPM
10 8 6 4 2 PPM

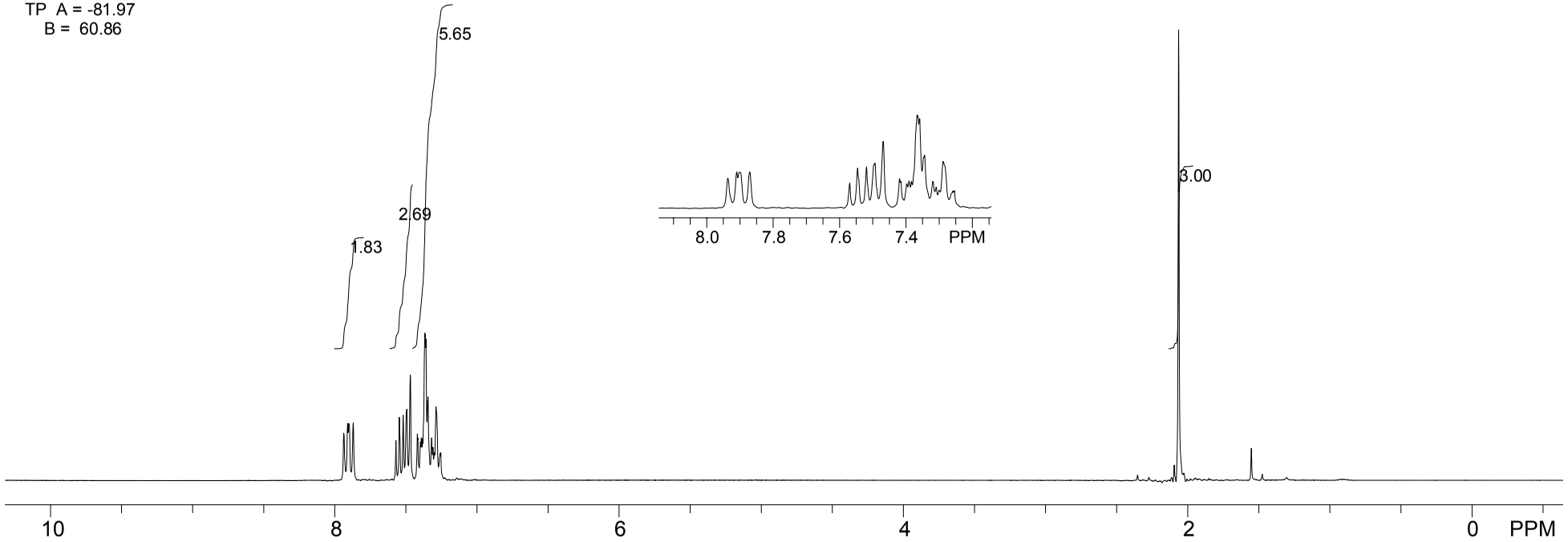


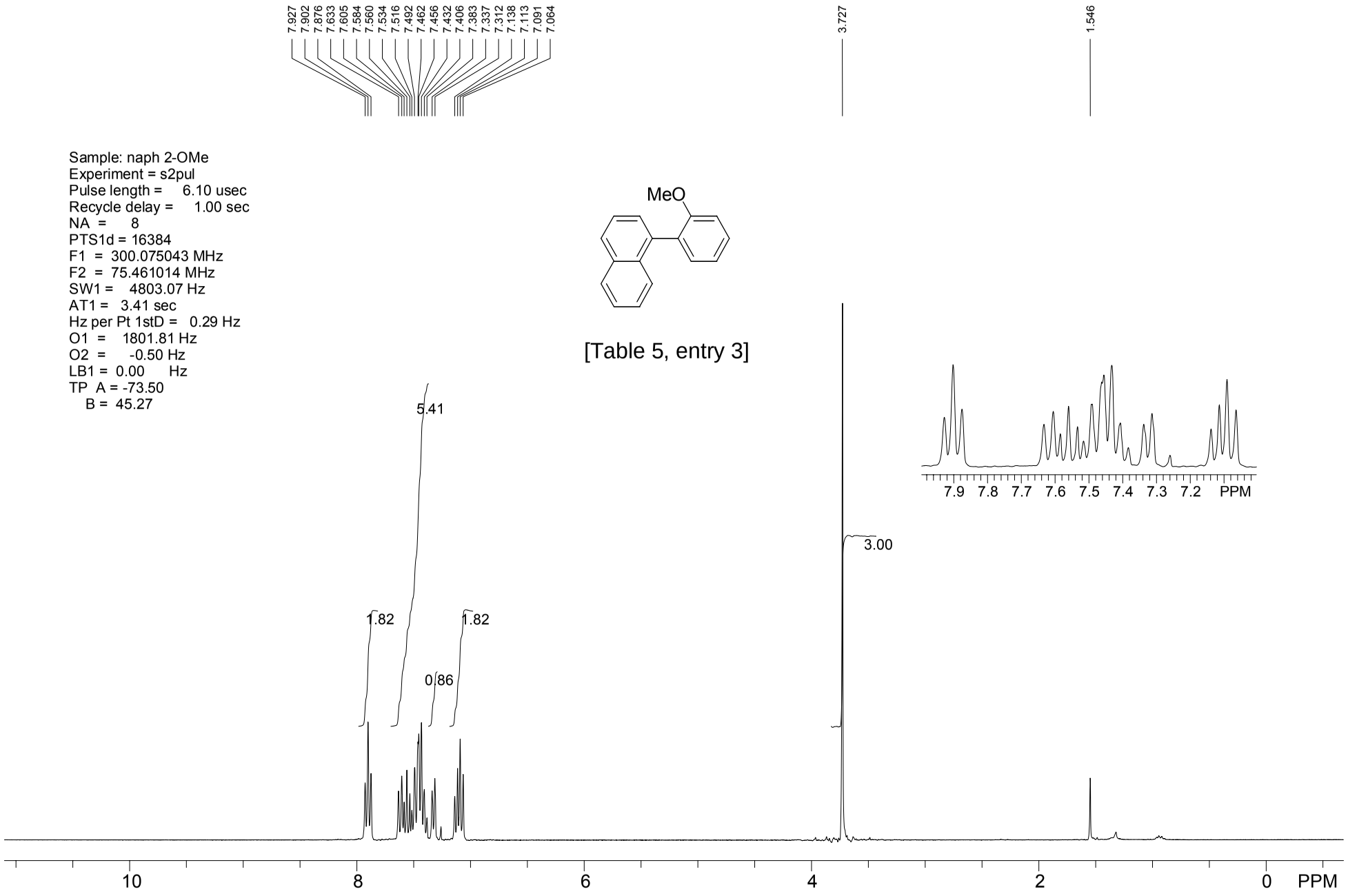


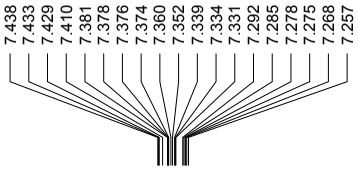
Sample: naph 2-Me
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1800.43 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -81.97
B = 60.86

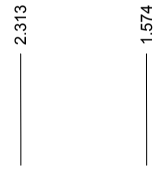


[Table 5, entry 2]

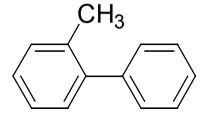



7.927
7.902
7.876
7.633
7.605
7.584
7.560
7.534
7.516
7.492
7.462
7.456
7.432
7.406
7.383
7.337
7.312
7.138
7.113
7.091
7.064
3.727
1.546
Sample: naph 2-OMe
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1801.81 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -73.50
B = 45.27
MeO
[Table 5, entry 3]
5.41
1.82
1.82
0.86
3.00
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 PPM
10 8 6 4 2 0 PPM

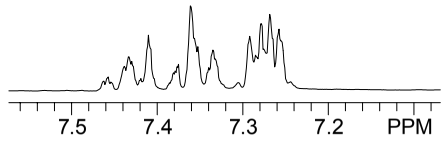




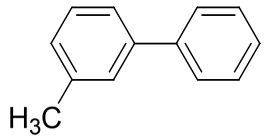
Sample: 2-Me
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 16
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1800.43 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -95.96
B = 78.67



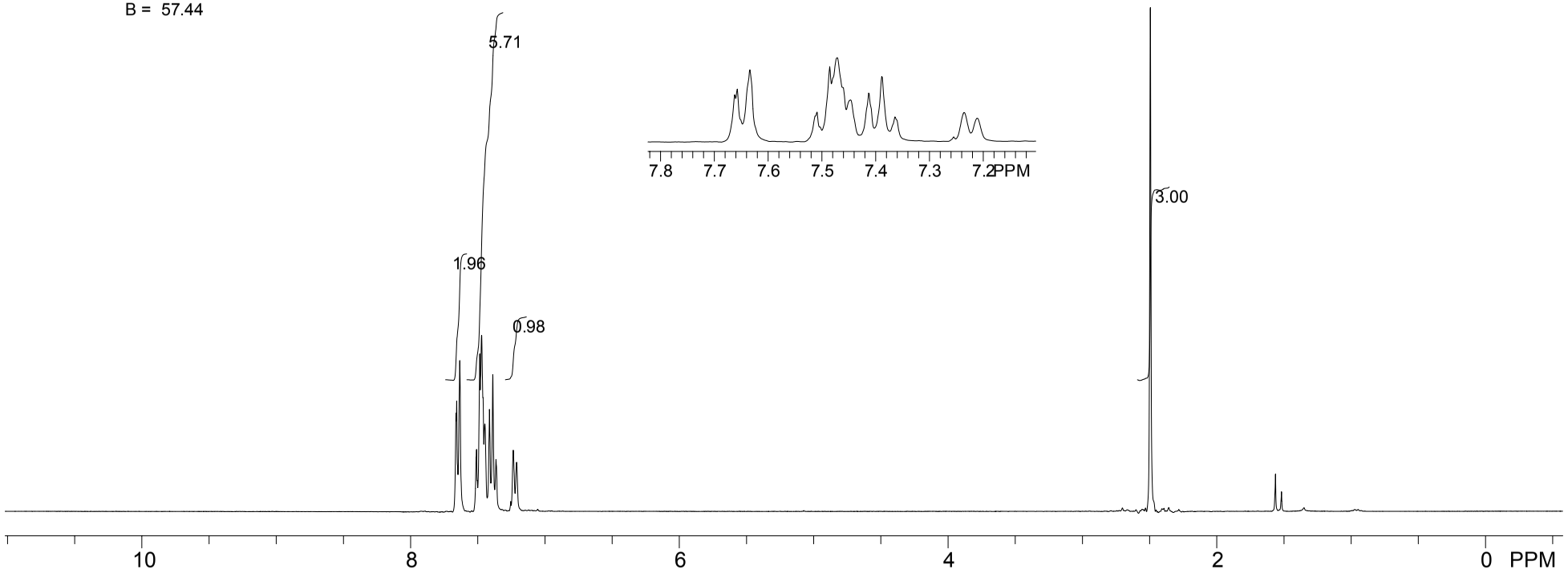
[Table 5, entry 4]

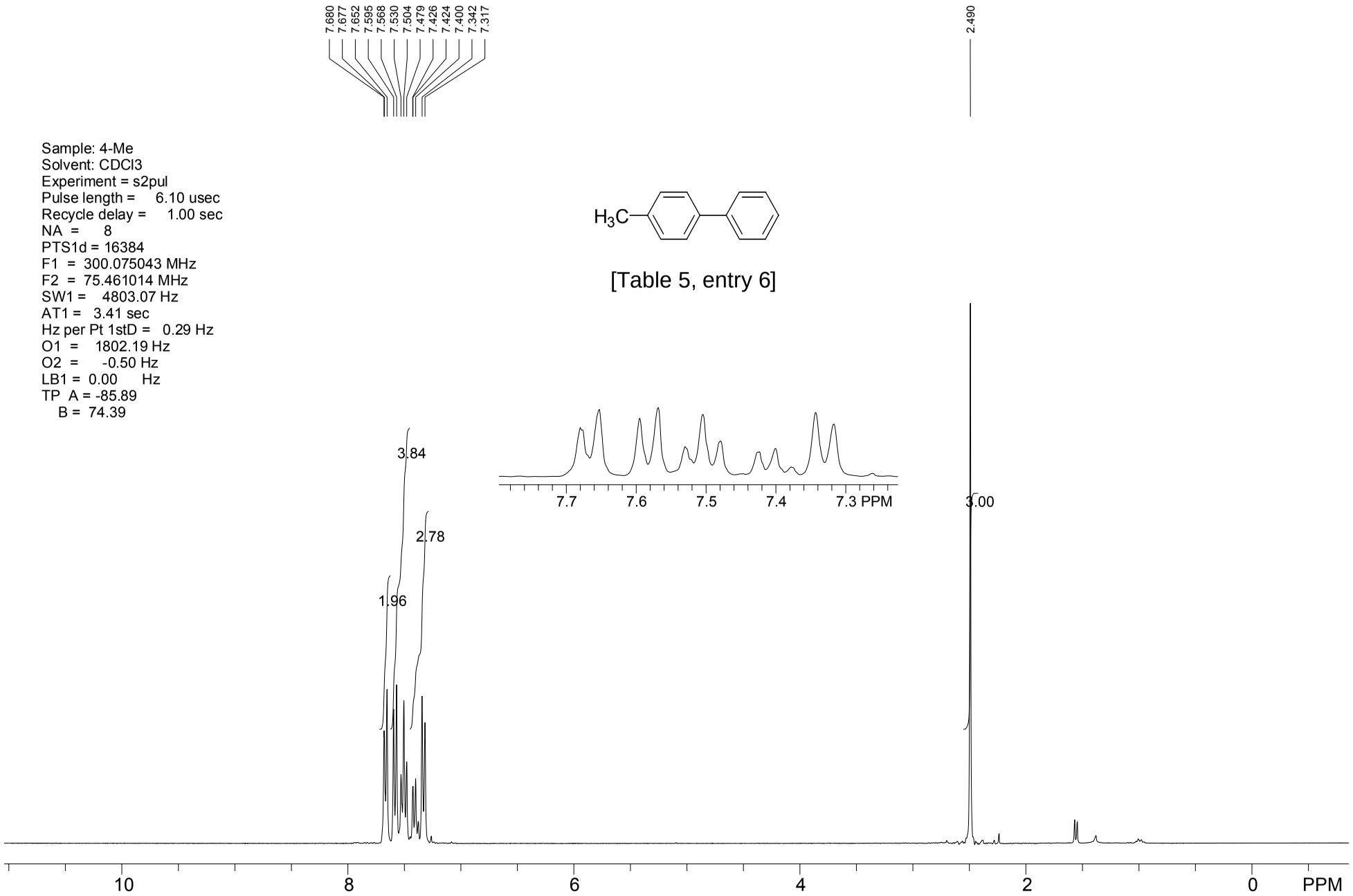


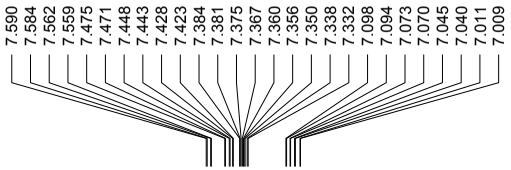
Sample: 3-Me
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1800.43 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -74.50
B = 57.44



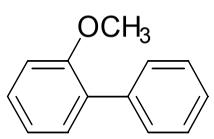
[Table 5, entry 5]



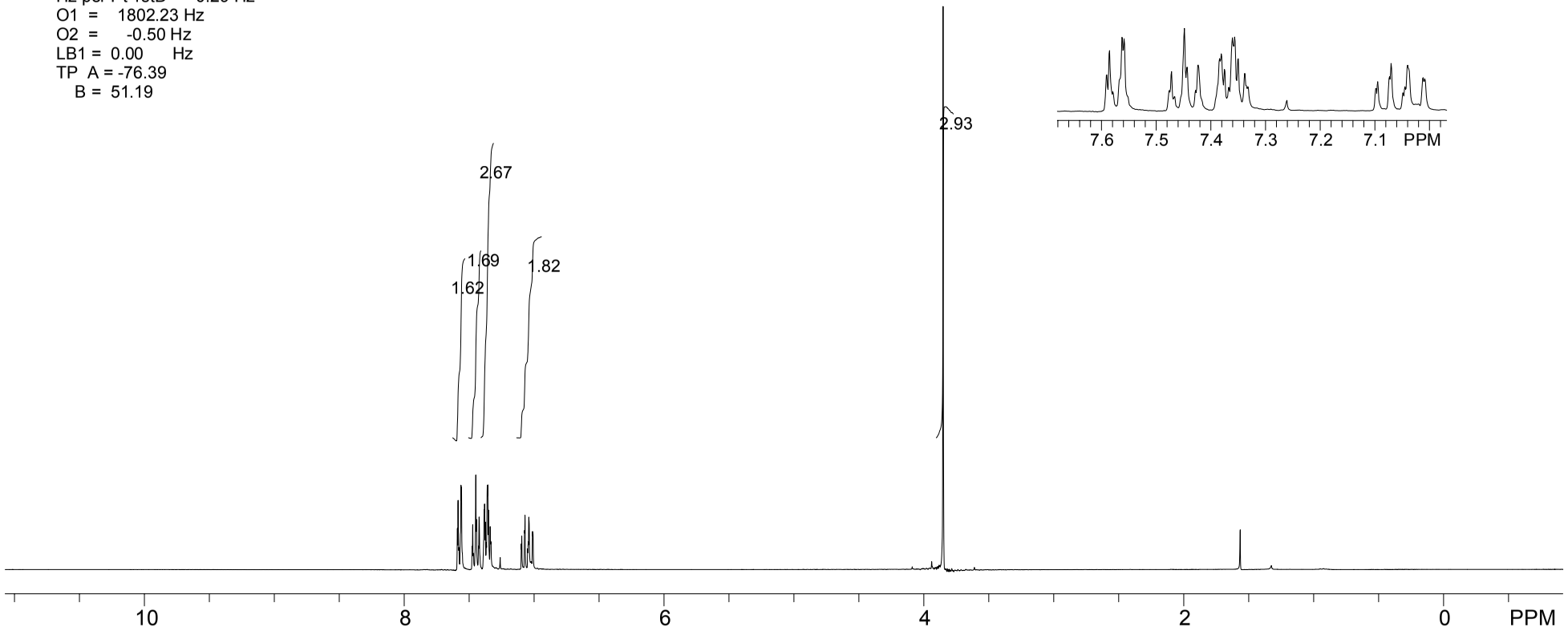

7.680
7.677
7.652
7.595
7.568
7.530
7.504
7.479
7.426
7.424
7.400
7.342
7.317
2.490
Sample: 4-Me
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1802.19 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -85.89
B = 74.39
H3C
[Table 5, entry 6]
3.84
2.78
1.96
3.00
7.7
7.6
7.5
7.4
7.3 PPM
10
8
6
4
2
0
PPM

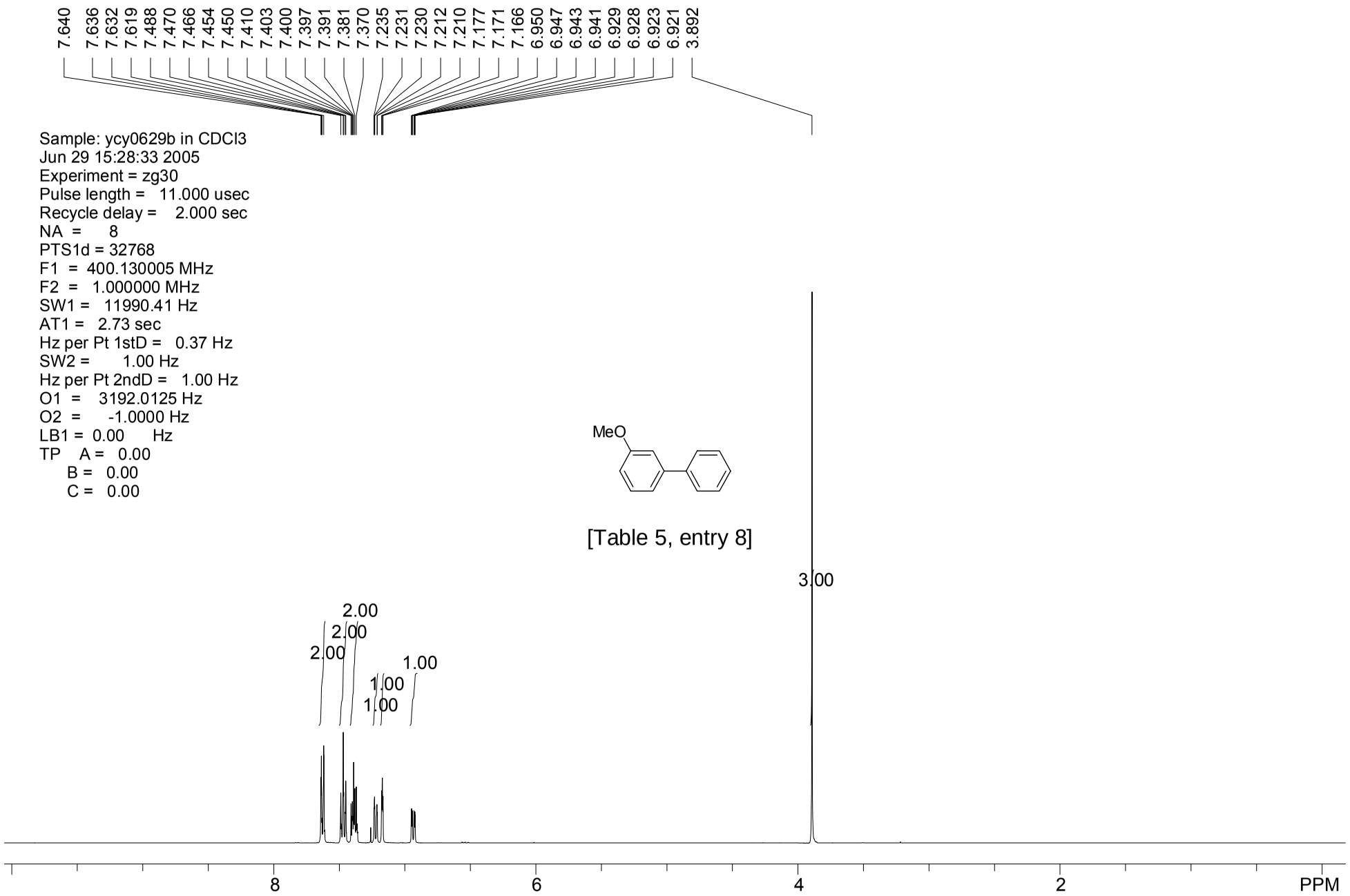


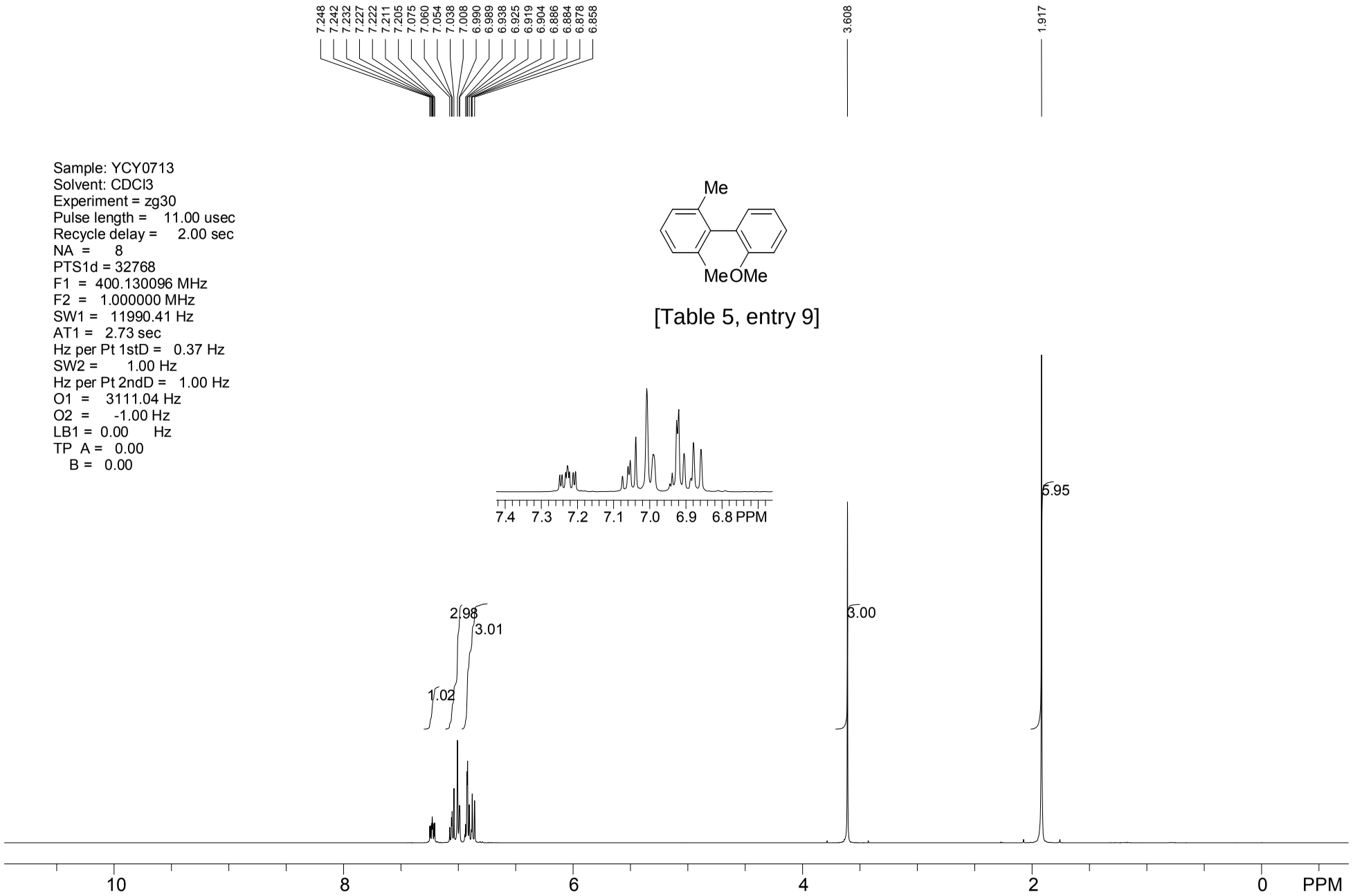
Sample: 2-OMe
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 16
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1802.23 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -76.39
B = 51.19

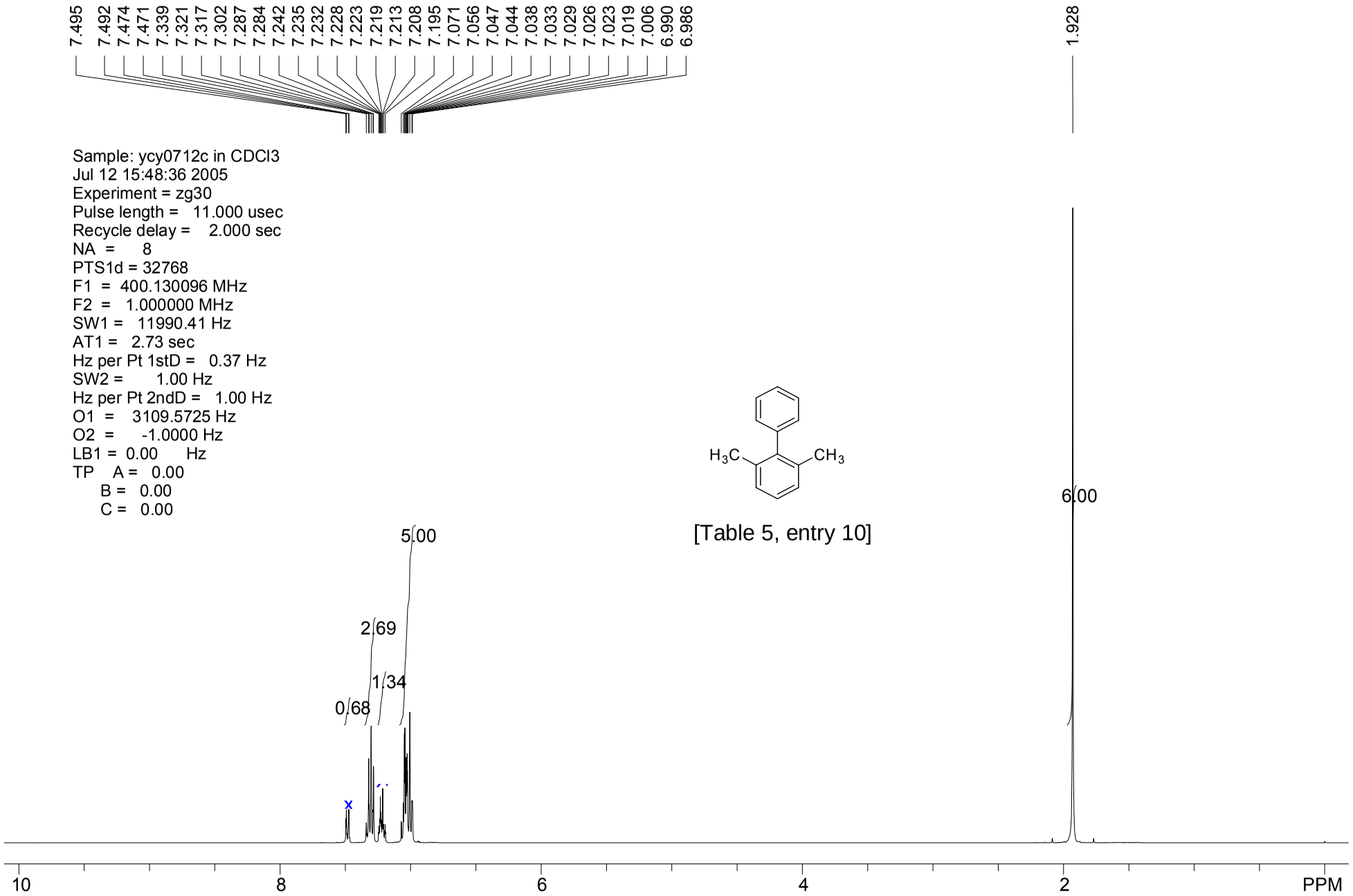


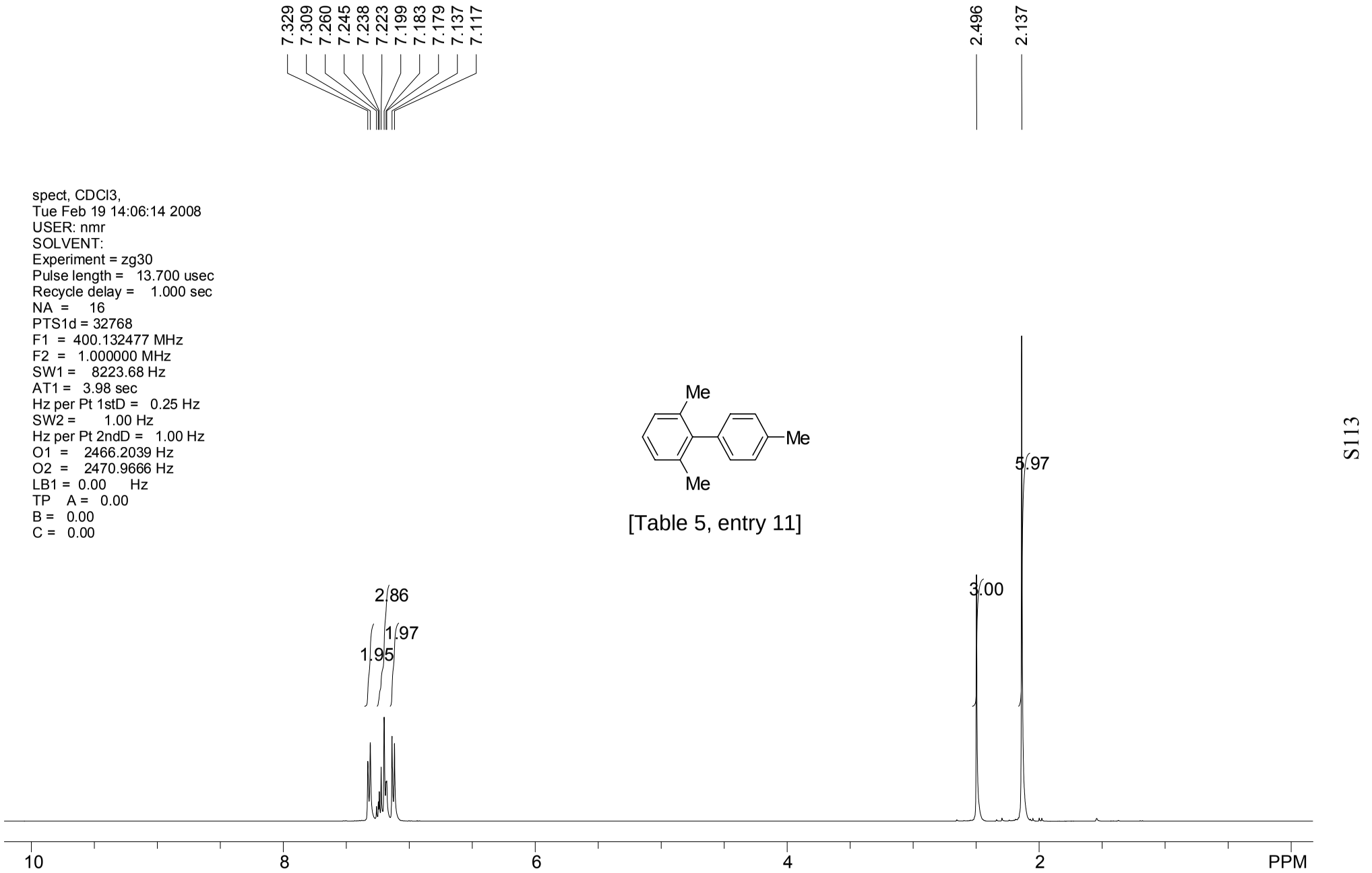
28 [Table 5, entry 7]

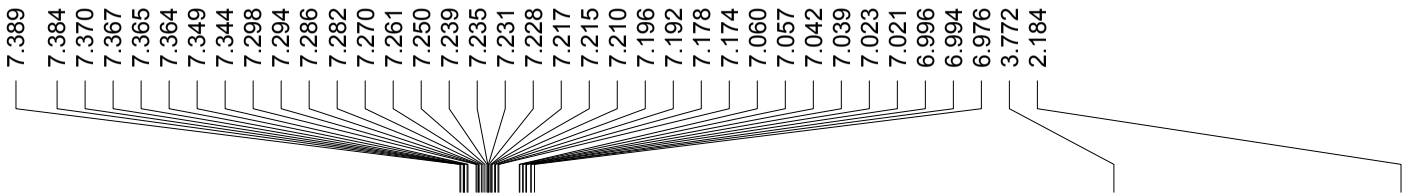



7.640
7.636
7.632
7.619
7.488
7.470
7.466
7.454
7.450
7.410
7.403
7.400
7.397
7.391
7.381
7.370
7.235
7.231
7.230
7.212
7.210
7.177
7.171
7.166
6.950
6.947
6.943
6.941
6.929
6.928
6.923
6.921
3.892
Sample: ycy0629b in CDCl3
Jun 29 15:28:33 2005
Experiment = zg30
Pulse length = 11.000 usec
Recycle delay = 2.000 sec
NA = 8
PTS1d = 32768
F1 = 400.130005 MHz
F2 = 1.000000 MHz
SW1 = 11990.41 Hz
AT1 = 2.73 sec
Hz per Pt 1stD = 0.37 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 3192.0125 Hz
O2 = -1.0000 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
MeO
[Table 5, entry 8]
3.00
2.00
2.00
2.00
1.00
1.00
1.00
8
6
4
2
PPM

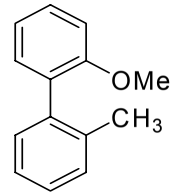

7.248
7.242
7.232
7.227
7.222
7.211
7.205
7.075
7.060
7.054
7.038
7.008
6.990
6.989
6.938
6.925
6.919
6.904
6.886
6.884
6.878
6.858
3.608
1.917
Sample: YCY0713
Solvent: CDCl3
Experiment = zg30
Pulse length = 11.00 usec
Recycle delay = 2.00 sec
NA = 8
PTS1d = 32768
F1 = 400.130096 MHz
F2 = 1.000000 MHz
SW1 = 11990.41 Hz
AT1 = 2.73 sec
Hz per Pt 1stD = 0.37 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 3111.04 Hz
O2 = -1.00 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
Me
MeOMe
[Table 5, entry 9]
7.4 7.3 7.2 7.1 7.0 6.9 6.8 PPM
2.98
3.01
1.02
3.00
6.95
10
8
6
4
2
0
PPM


7.495
7.492
7.474
7.471
7.339
7.321
7.317
7.302
7.287
7.284
7.242
7.235
7.232
7.228
7.223
7.219
7.213
7.208
7.195
7.071
7.056
7.047
7.044
7.038
7.033
7.029
7.026
7.023
7.019
7.006
6.990
6.986
1.928
Sample: ycy0712c in CDCl3
Jul 12 15:48:36 2005
Experiment = zg30
Pulse length = 11.000 usec
Recycle delay = 2.000 sec
NA = 8
PTS1d = 32768
F1 = 400.130096 MHz
F2 = 1.000000 MHz
SW1 = 11990.41 Hz
AT1 = 2.73 sec
Hz per Pt 1stD = 0.37 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 3109.5725 Hz
O2 = -1.0000 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
H3C
CH3
[Table 5, entry 10]
6.00
5.00
2.69
1.34
0.68
10
8
6
4
2
PPM

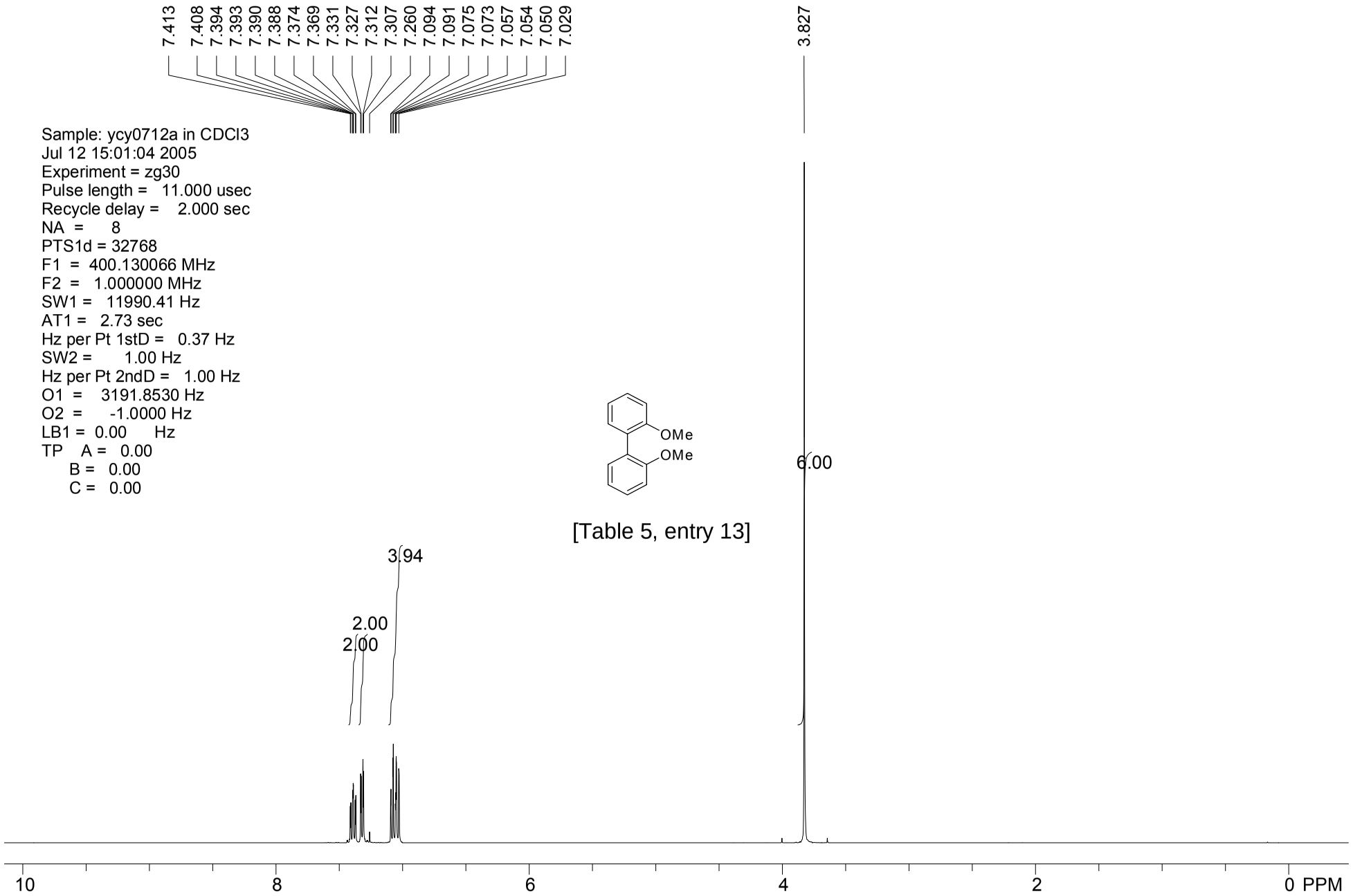

7.329
7.309
7.260
7.245
7.238
7.223
7.199
7.183
7.179
7.137
7.117
2.496
2.137
spect, CDCl3,
Tue Feb 19 14:06:14 2008
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 13.700 usec
Recycle delay = 1.000 sec
NA = 16
PTS1d = 32768
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 3.98 sec
Hz per Pt 1stD = 0.25 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2466.2039 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
Me
Me
Me
[Table 5, entry 11]
2.86
1.97
1.95
3.00
5.97
10
8
6
4
2
PPM

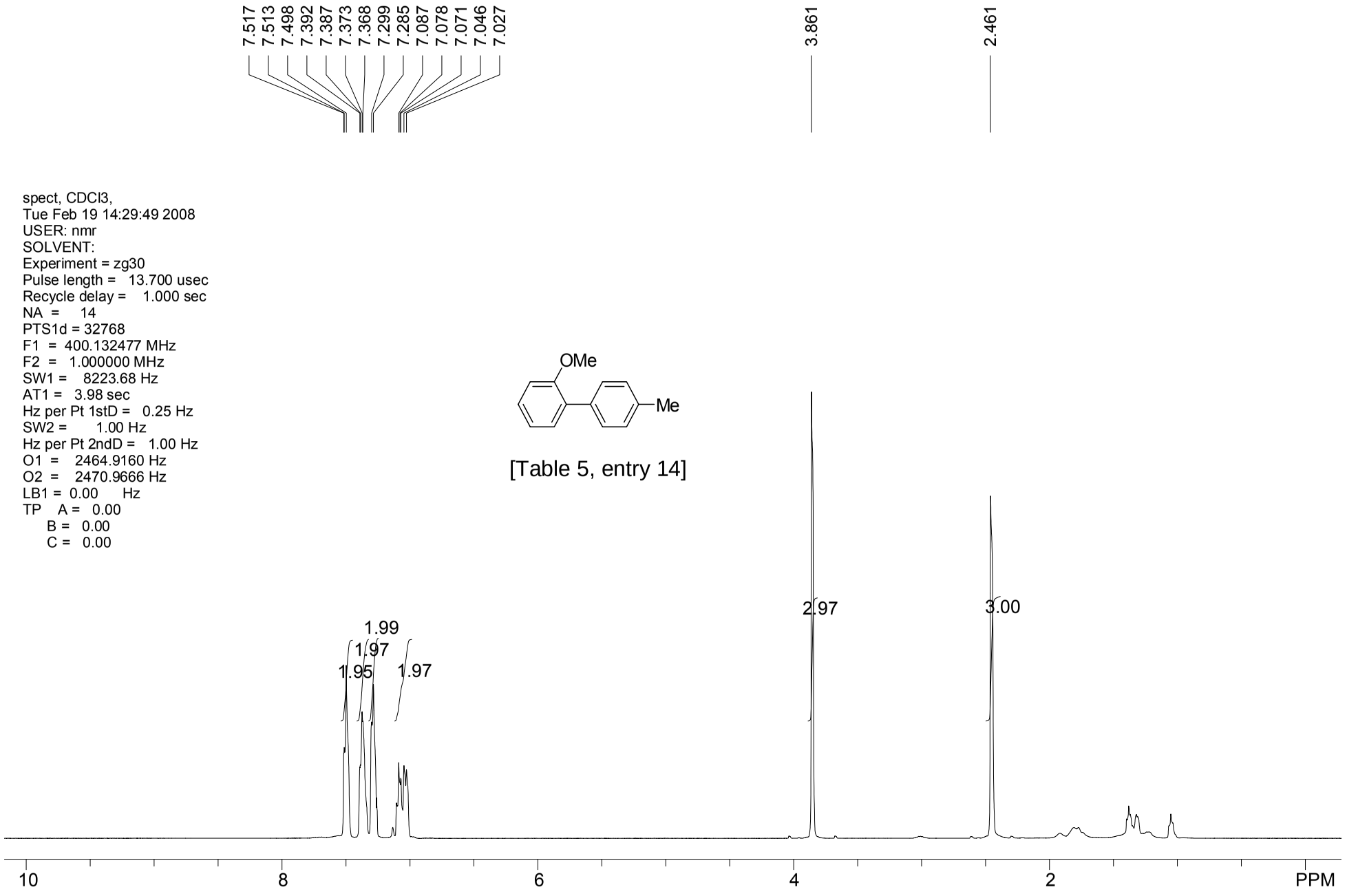


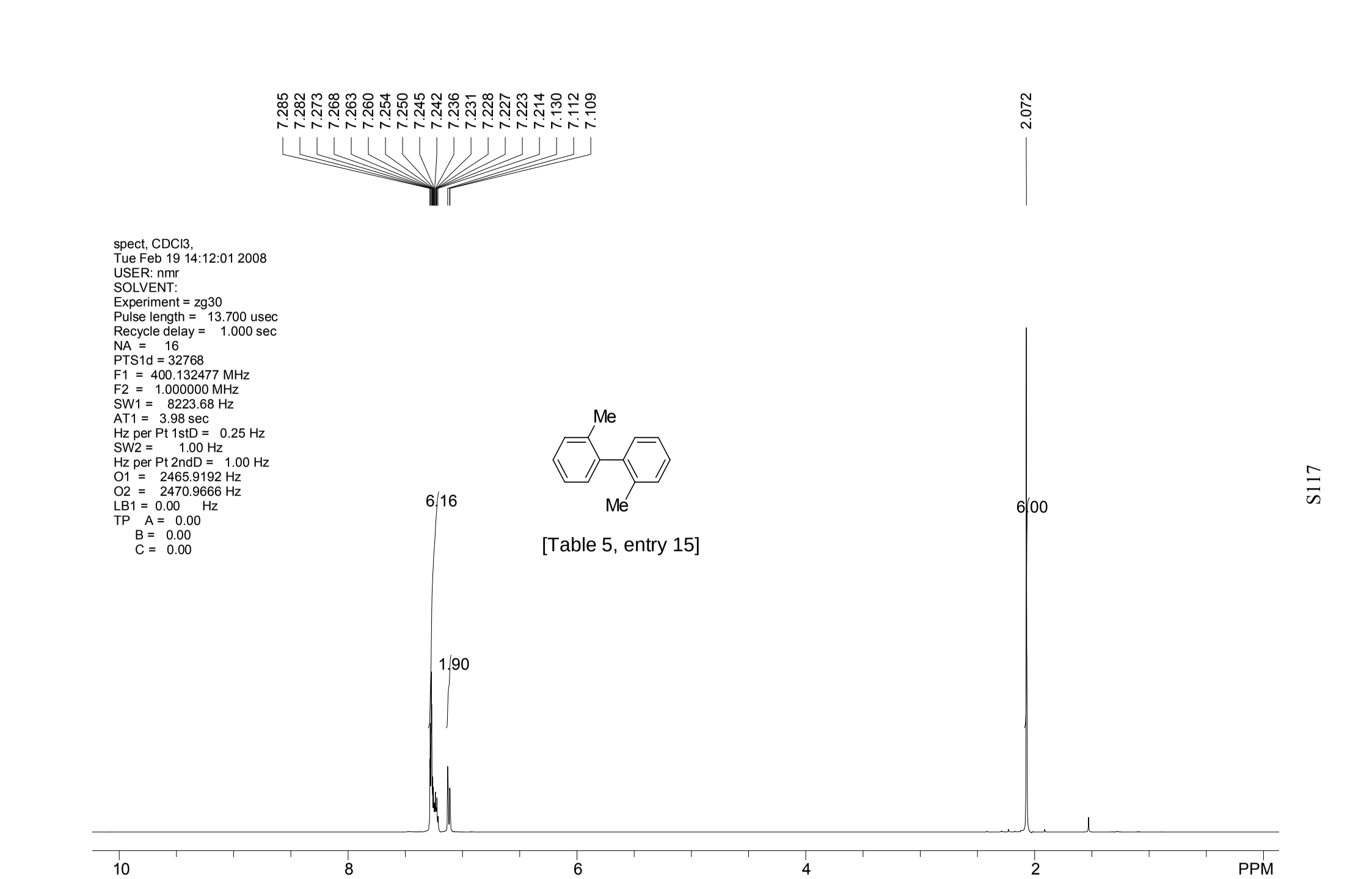
Sample: ycy0704 in CDCl3
Jul 5 11:31:44 2005
Experiment = zg30
Pulse length = 11.000 usec
Recycle delay = 2.000 sec
NA = 2
PTS1d = 32768
F1 = 400.130035 MHz
F2 = 1.000000 MHz
SW1 = 11990.41 Hz
AT1 = 2.73 sec
Hz per Pt 1stD = 0.37 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 3166.6536 Hz
O2 = -1.0000 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00

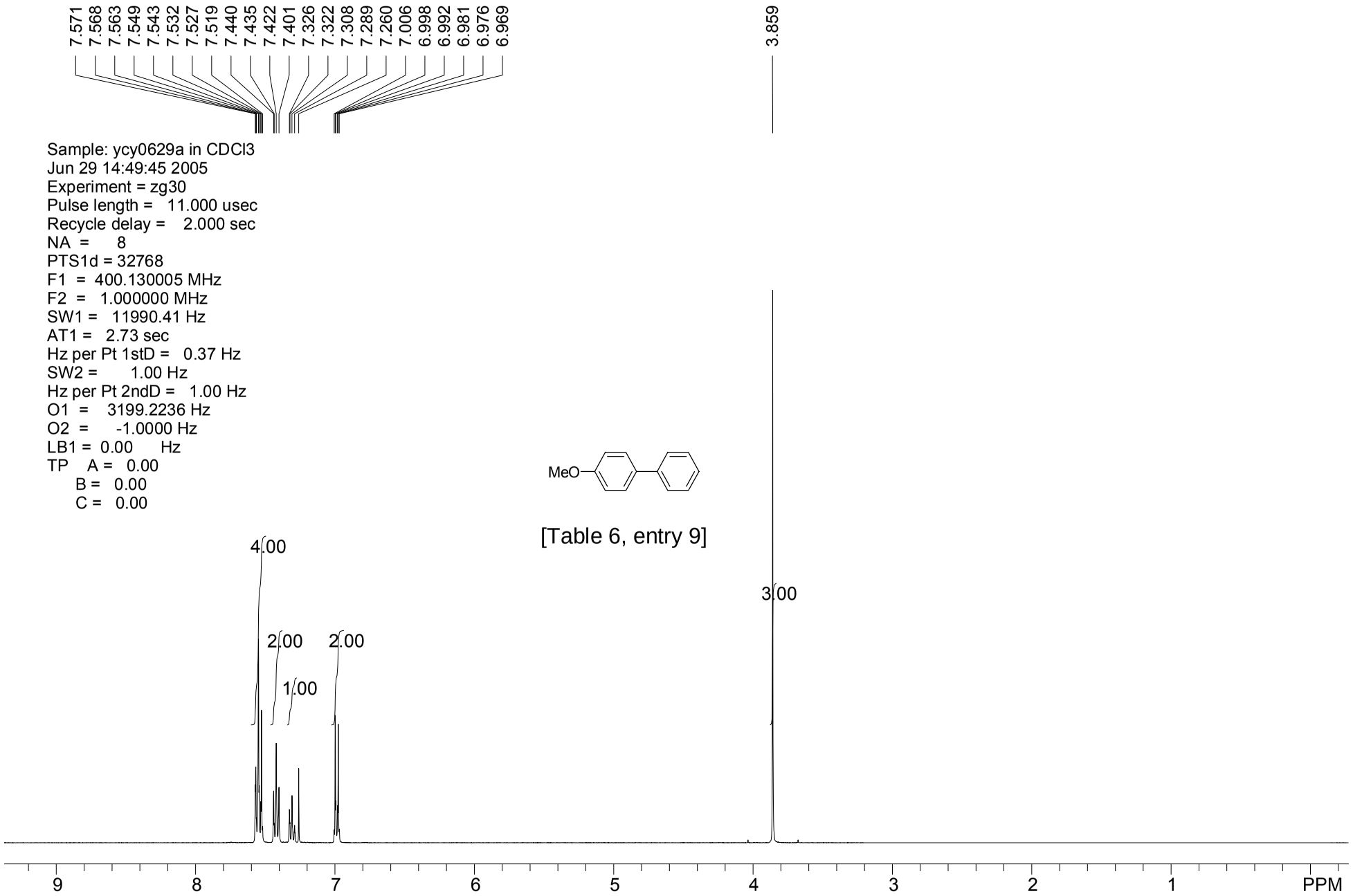


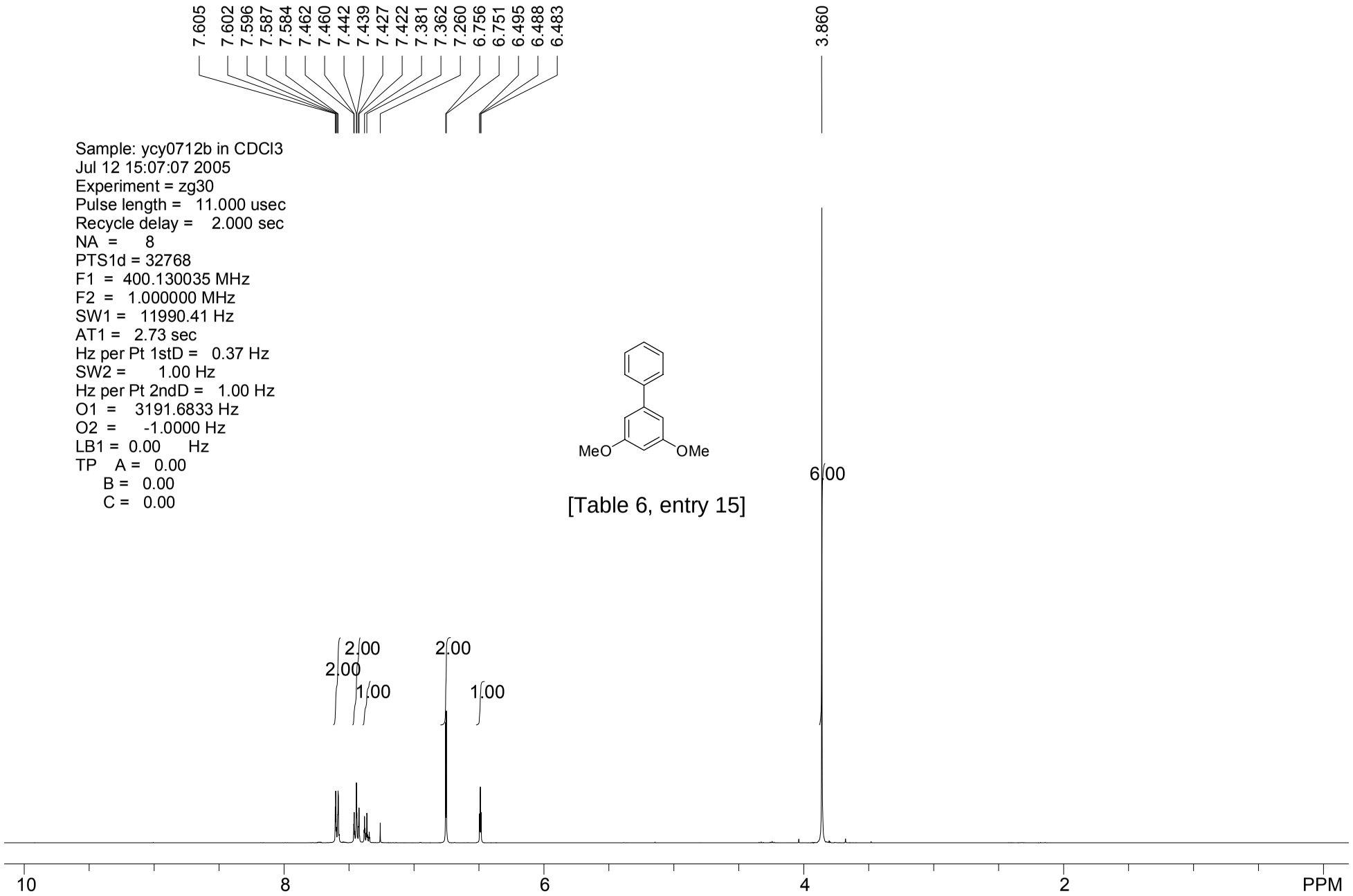
[Table 5, entries 12 & 16]

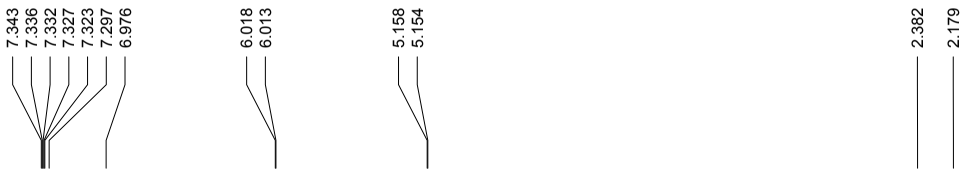

7.413
7.408
7.394
7.393
7.390
7.388
7.374
7.369
7.331
7.327
7.312
7.307
7.260
7.094
7.091
7.075
7.073
7.057
7.054
7.050
7.029
3.827
Sample: ycy0712a in CDCl3
Jul 12 15:01:04 2005
Experiment = zg30
Pulse length = 11.000 usec
Recycle delay = 2.000 sec
NA = 8
PTS1d = 32768
F1 = 400.130066 MHz
F2 = 1.000000 MHz
SW1 = 11990.41 Hz
AT1 = 2.73 sec
Hz per Pt 1stD = 0.37 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 3191.8530 Hz
O2 = -1.0000 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
OMe
OMe
[Table 5, entry 13]
6.00
3.94
2.00
2.00
10
8
6
4
2
0 PPM


7.517
7.513
7.498
7.392
7.387
7.373
7.368
7.299
7.285
7.087
7.078
7.071
7.046
7.027
3.861
2.461
spect, CDCl3,
Tue Feb 19 14:29:49 2008
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 13.700 usec
Recycle delay = 1.000 sec
NA = 14
PTS1d = 32768
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 3.98 sec
Hz per Pt 1stD = 0.25 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2464.9160 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
OMe
Me
[Table 5, entry 14]
1.99
1.97
1.95
1.97
2.97
3.00
10
8
6
4
2
PPM

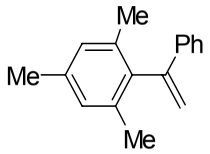

7.285
7.282
7.273
7.268
7.263
7.260
7.254
7.250
7.245
7.242
7.236
7.231
7.228
7.227
7.223
7.214
7.130
7.112
7.109
2.072
spect, CDCl3,
Tue Feb 19 14:12:01 2008
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 13.700 usec
Recycle delay = 1.000 sec
NA = 16
PTS1d = 32768
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 3.98 sec
Hz per Pt 1stD = 0.25 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2465.9192 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
Me
Me
[Table 5, entry 15]
6.16
1.90
6.00
10
8
6
4
2
PPM


7.571
7.568
7.563
7.549
7.543
7.532
7.527
7.519
7.440
7.435
7.422
7.401
7.326
7.322
7.308
7.289
7.260
7.006
6.998
6.992
6.981
6.976
6.969
3.859
Sample: ycy0629a in CDCl3
Jun 29 14:49:45 2005
Experiment = zg30
Pulse length = 11.000 usec
Recycle delay = 2.000 sec
NA = 8
PTS1d = 32768
F1 = 400.130005 MHz
F2 = 1.000000 MHz
SW1 = 11990.41 Hz
AT1 = 2.73 sec
Hz per Pt 1stD = 0.37 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 3199.2236 Hz
O2 = -1.0000 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
MeO
[Table 6, entry 9]
4.00
2.00
2.00
1.00
3.00
9
8
7
6
5
4
3
2
1
PPM

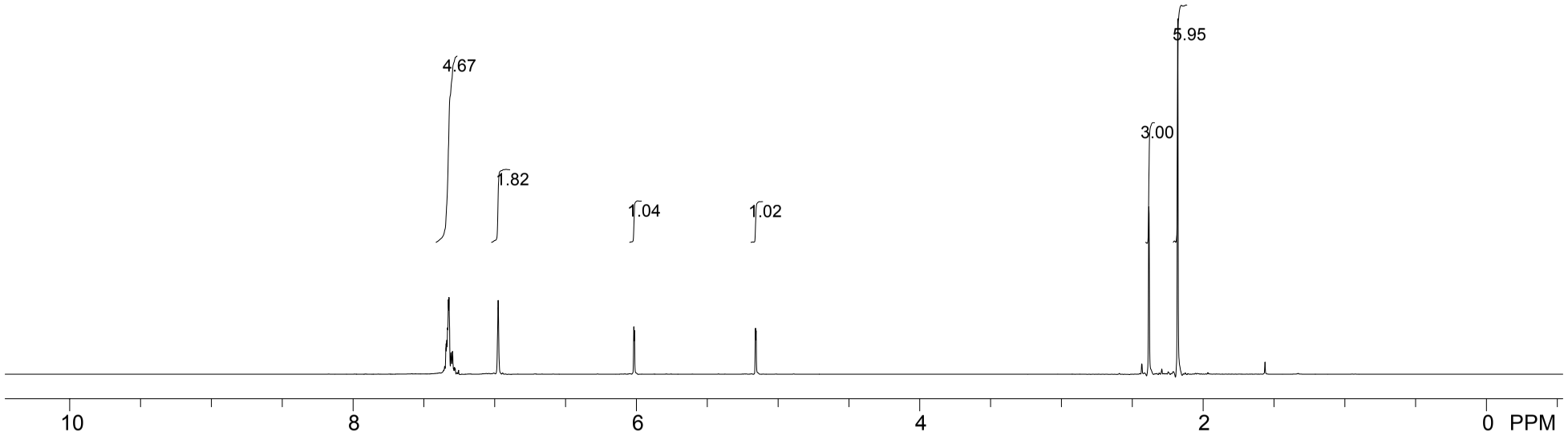

7.605
7.602
7.596
7.587
7.584
7.462
7.460
7.442
7.439
7.427
7.422
7.381
7.362
7.260
6.756
6.751
6.495
6.488
6.483
3.860
Sample: ycy0712b in CDCl3
Jul 12 15:07:07 2005
Experiment = zg30
Pulse length = 11.000 usec
Recycle delay = 2.000 sec
NA = 8
PTS1d = 32768
F1 = 400.130035 MHz
F2 = 1.000000 MHz
SW1 = 11990.41 Hz
AT1 = 2.73 sec
Hz per Pt 1stD = 0.37 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 3191.6833 Hz
O2 = -1.0000 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
MeO
OMe
[Table 6, entry 15]
6.00
2.00
2.00
2.00
1.00
1.00
10
8
6
4
2
PPM

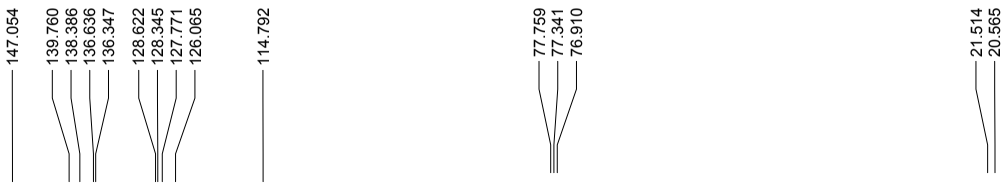


Sample: lyn1013b-h
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4800.77 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1800.43 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -83.49
B = 58.76

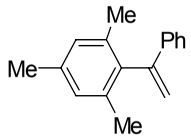


31a

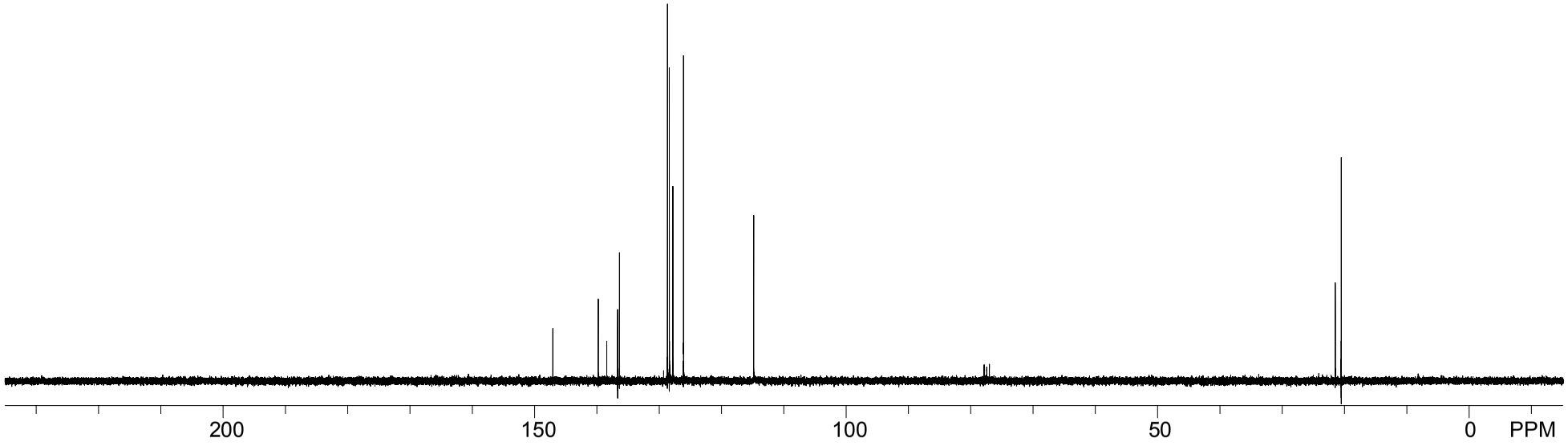




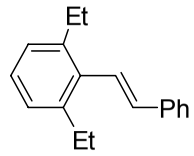
Sample: lyn1013b-c
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -213.37
B = 241.67



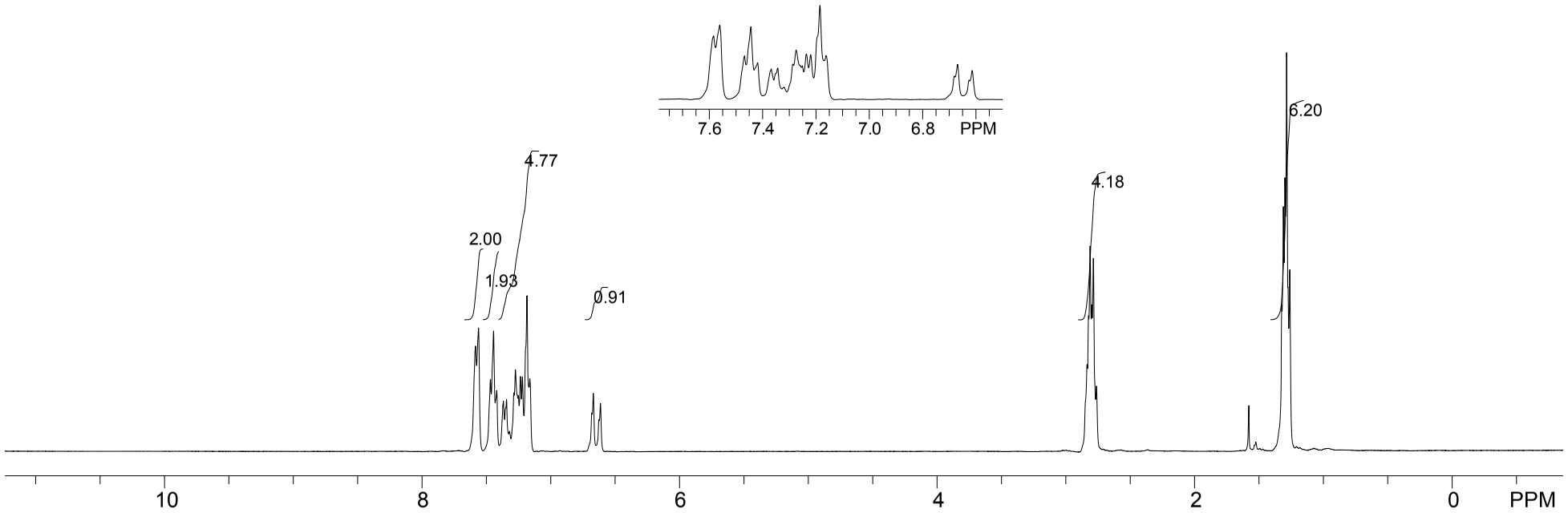
31a

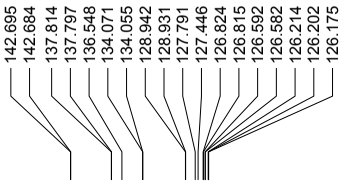


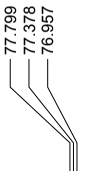
Sample: lyn0813a-h
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4803.07 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1800.43 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -80.11
B = 62.57

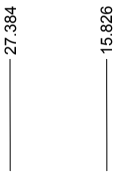


31b

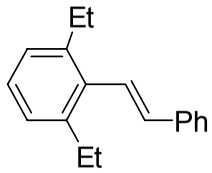




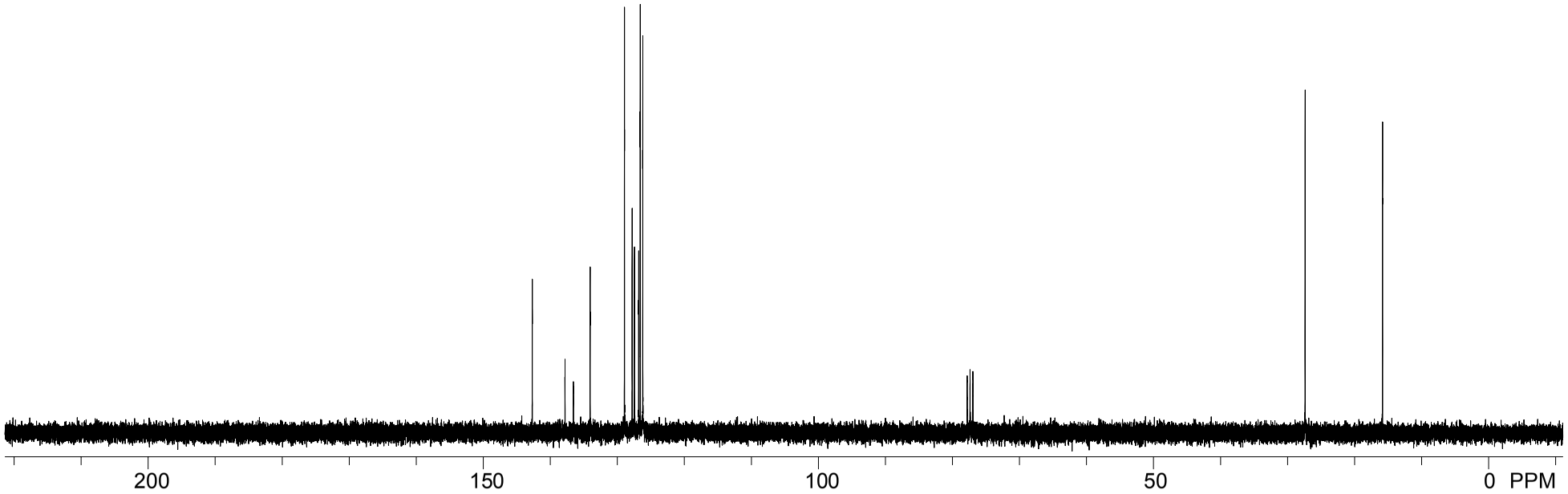


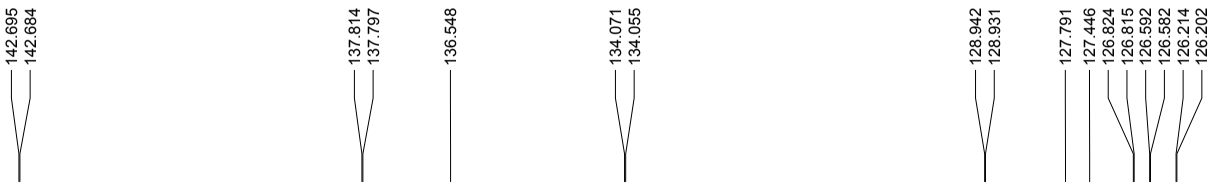


Sample: lyn0813a-c
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 128
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -261.29
B = 250.15

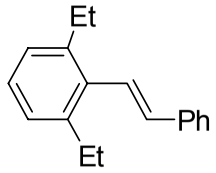


31b

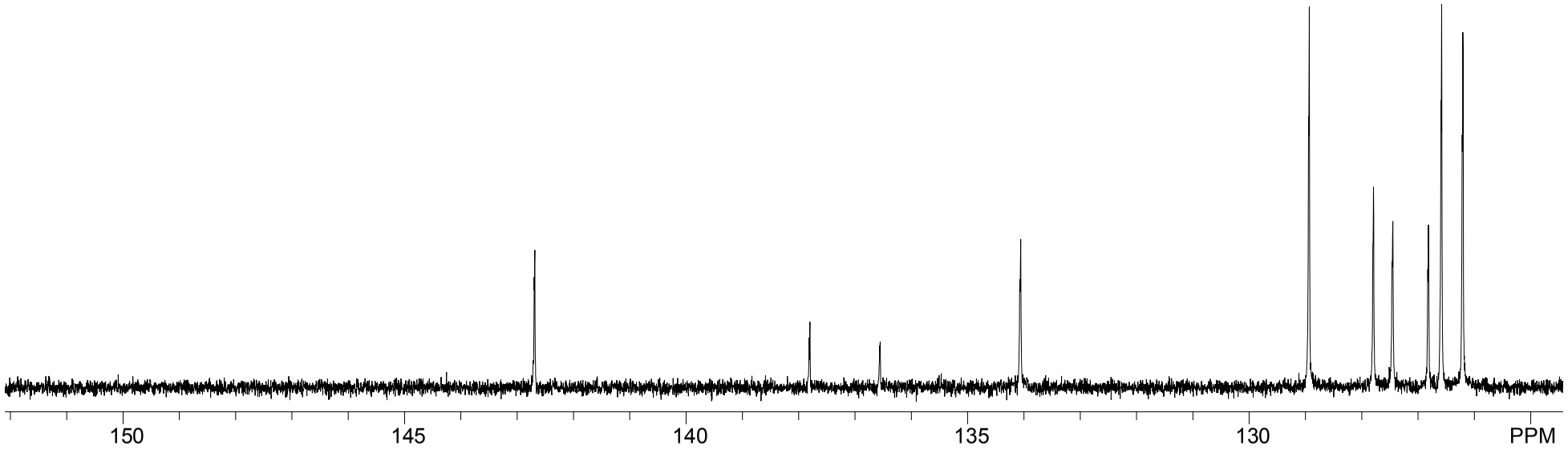


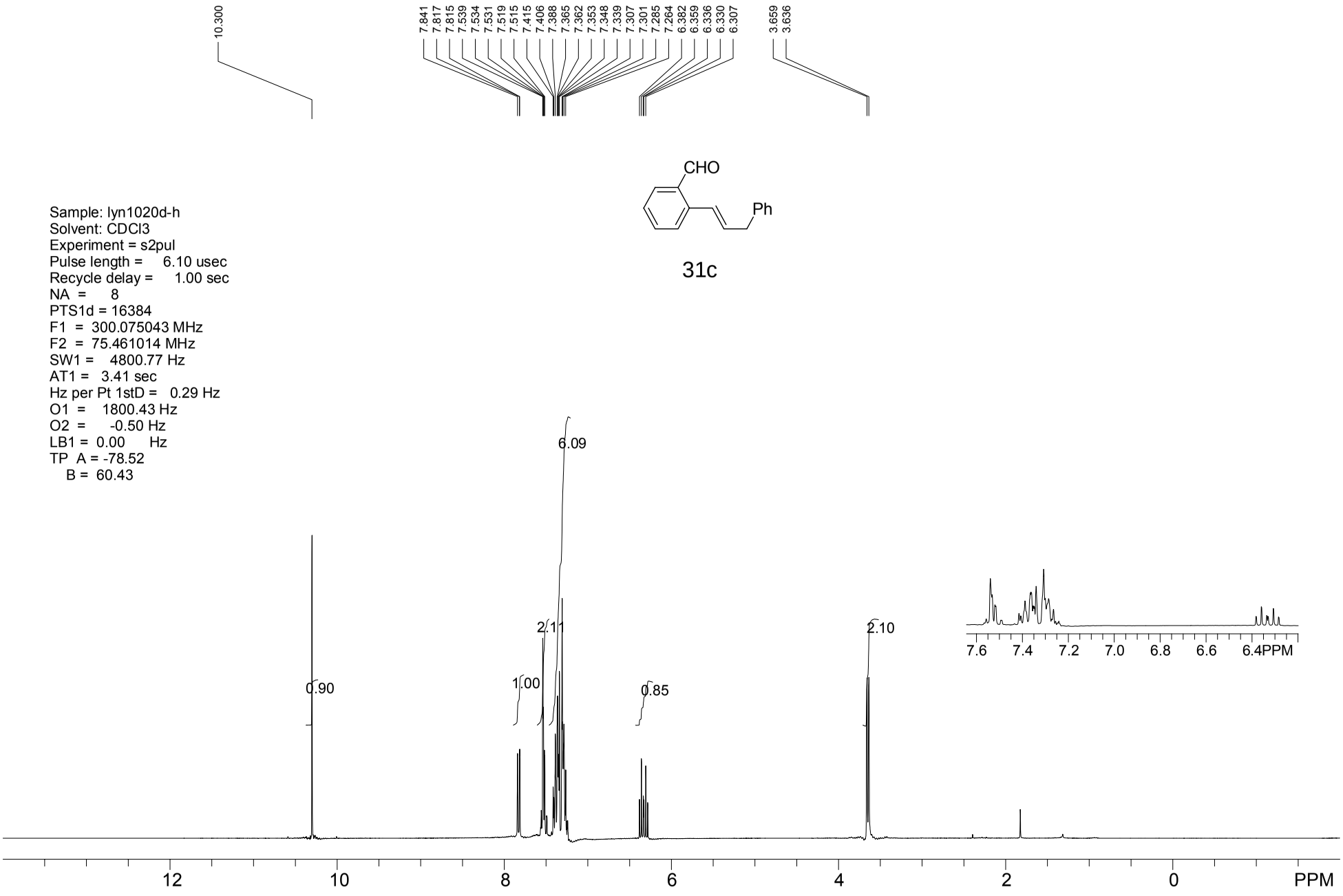


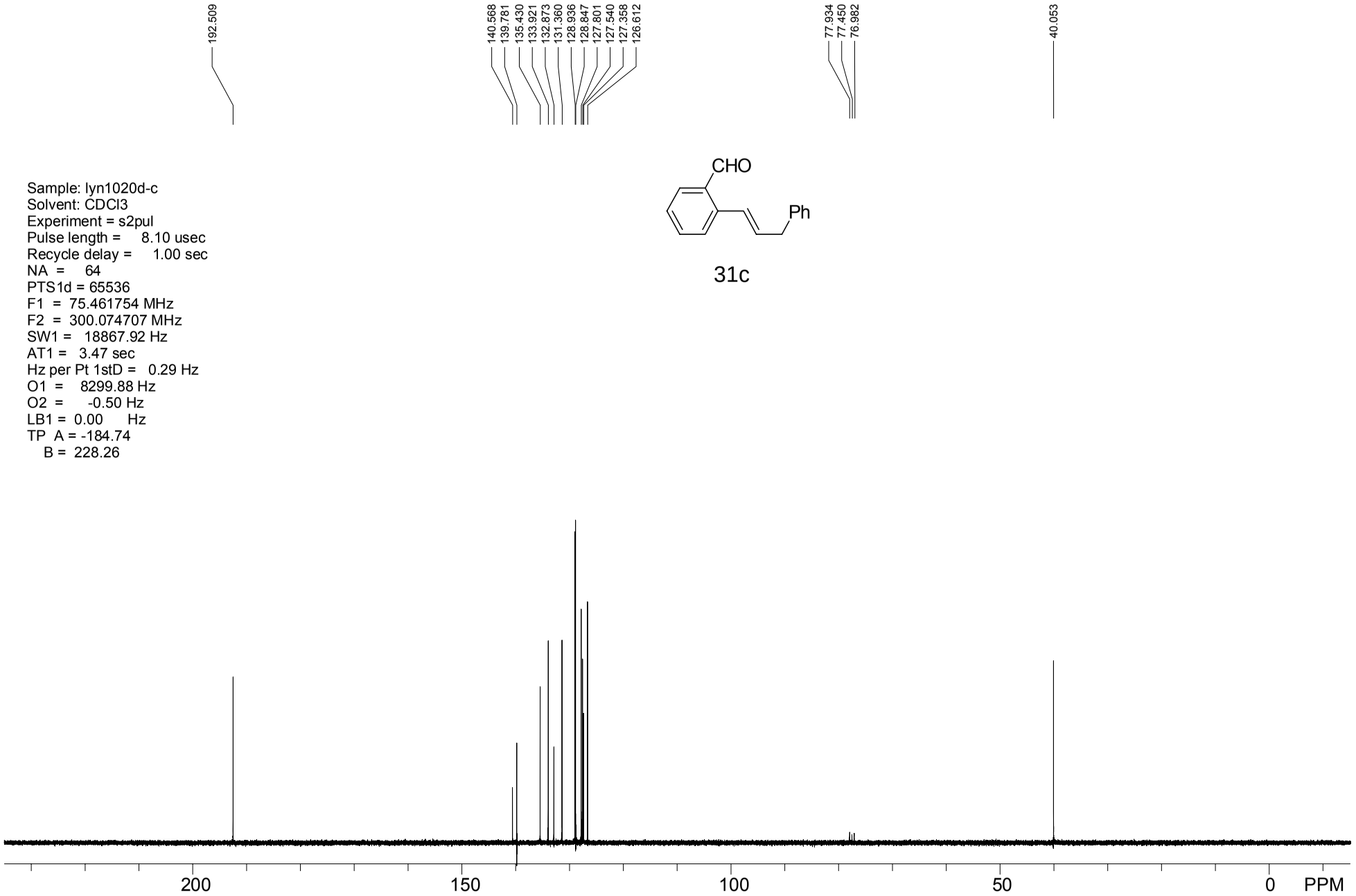
Sample: lyn0813a-c
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 128
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -261.29
B = 250.15

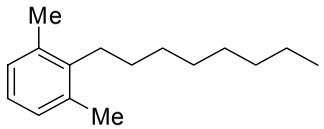


31b



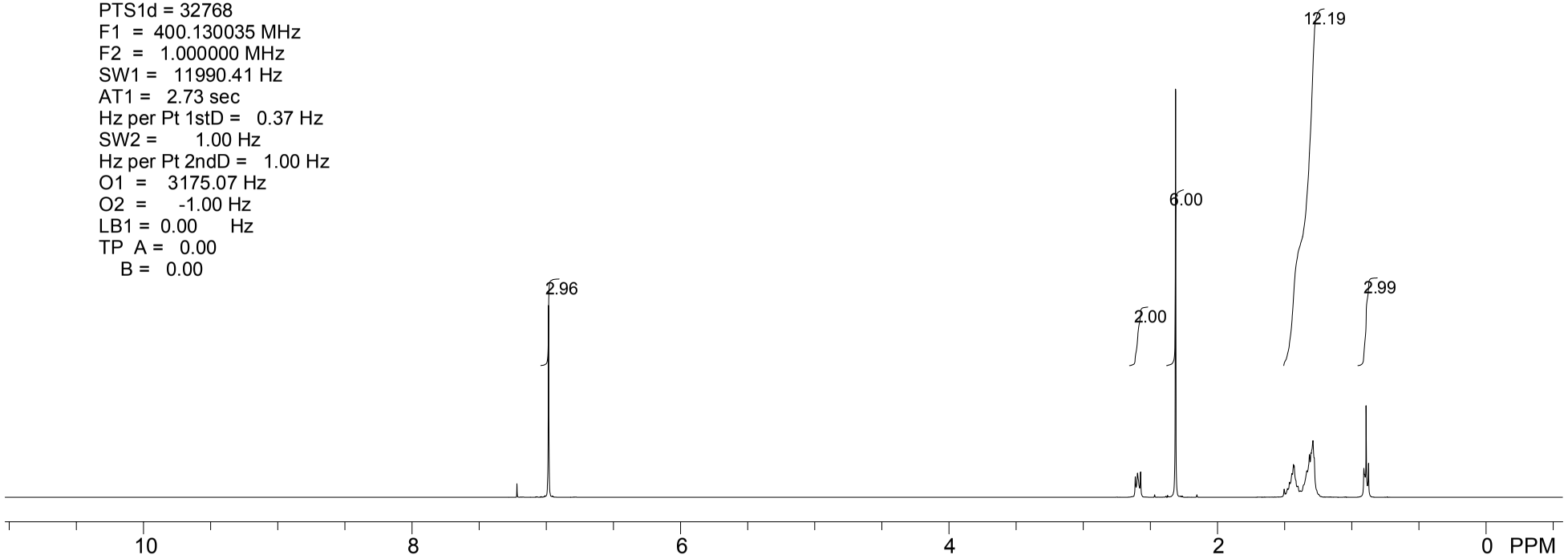

10.300
7.841
7.817
7.815
7.539
7.534
7.531
7.519
7.515
7.415
7.406
7.388
7.365
7.362
7.353
7.348
7.339
7.307
7.301
7.285
7.264
6.382
6.359
6.336
6.330
6.307
3.659
3.636
CHO
Ph
31c
Sample: lyn1020d-h
Solvent: CDCl3
Experiment = s2pul
Pulse length = 6.10 usec
Recycle delay = 1.00 sec
NA = 8
PTS1d = 16384
F1 = 300.075043 MHz
F2 = 75.461014 MHz
SW1 = 4800.77 Hz
AT1 = 3.41 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 1800.43 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -78.52
B = 60.43
6.09
2.11
2.10
0.90
1.00
0.85
7.6
7.4
7.2
7.0
6.8
6.6
6.4PPM
12
10
8
6
4
2
0
PPM

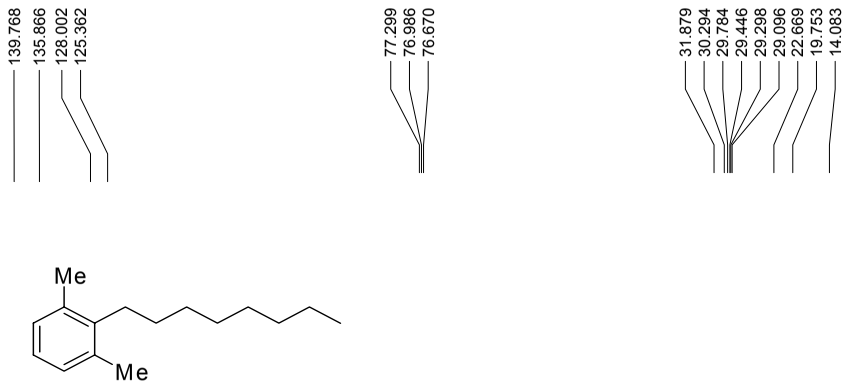

192.509
140.568
139.781
135.430
133.921
132.873
131.360
128.936
128.847
127.801
127.540
127.358
126.612
77.934
77.450
76.982
40.053
CHO
Ph
31c
Sample: lyn1020d-c
Solvent: CDCl3
Experiment = s2pul
Pulse length = 8.10 usec
Recycle delay = 1.00 sec
NA = 64
PTS1d = 65536
F1 = 75.461754 MHz
F2 = 300.074707 MHz
SW1 = 18867.92 Hz
AT1 = 3.47 sec
Hz per Pt 1stD = 0.29 Hz
O1 = 8299.88 Hz
O2 = -0.50 Hz
LB1 = 0.00 Hz
TP A = -184.74
B = 228.26
200
150
100
50
0
PPM



31d

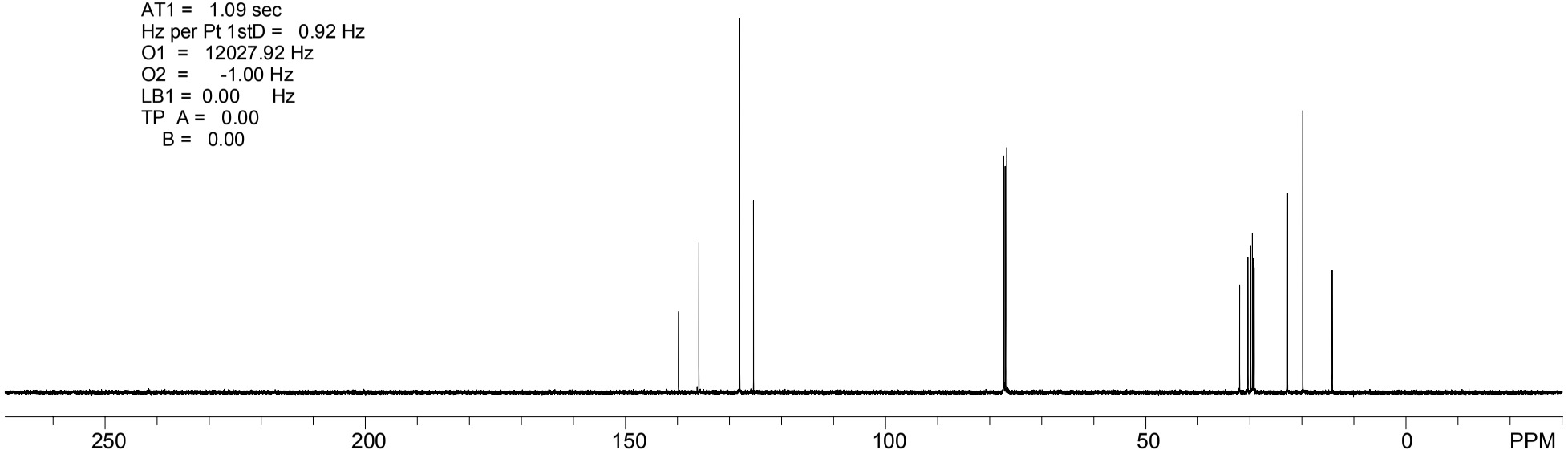
Sample: lyn061007-1-h
Solvent: CDCl3
Experiment = zg30
Pulse length = 11.00 usec
Recycle delay = 2.00 sec
NA = 8
PTS1d = 32768
F1 = 400.130035 MHz
F2 = 1.000000 MHz
SW1 = 11990.41 Hz
AT1 = 2.73 sec
Hz per Pt 1stD = 0.37 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 3175.07 Hz
O2 = -1.00 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00

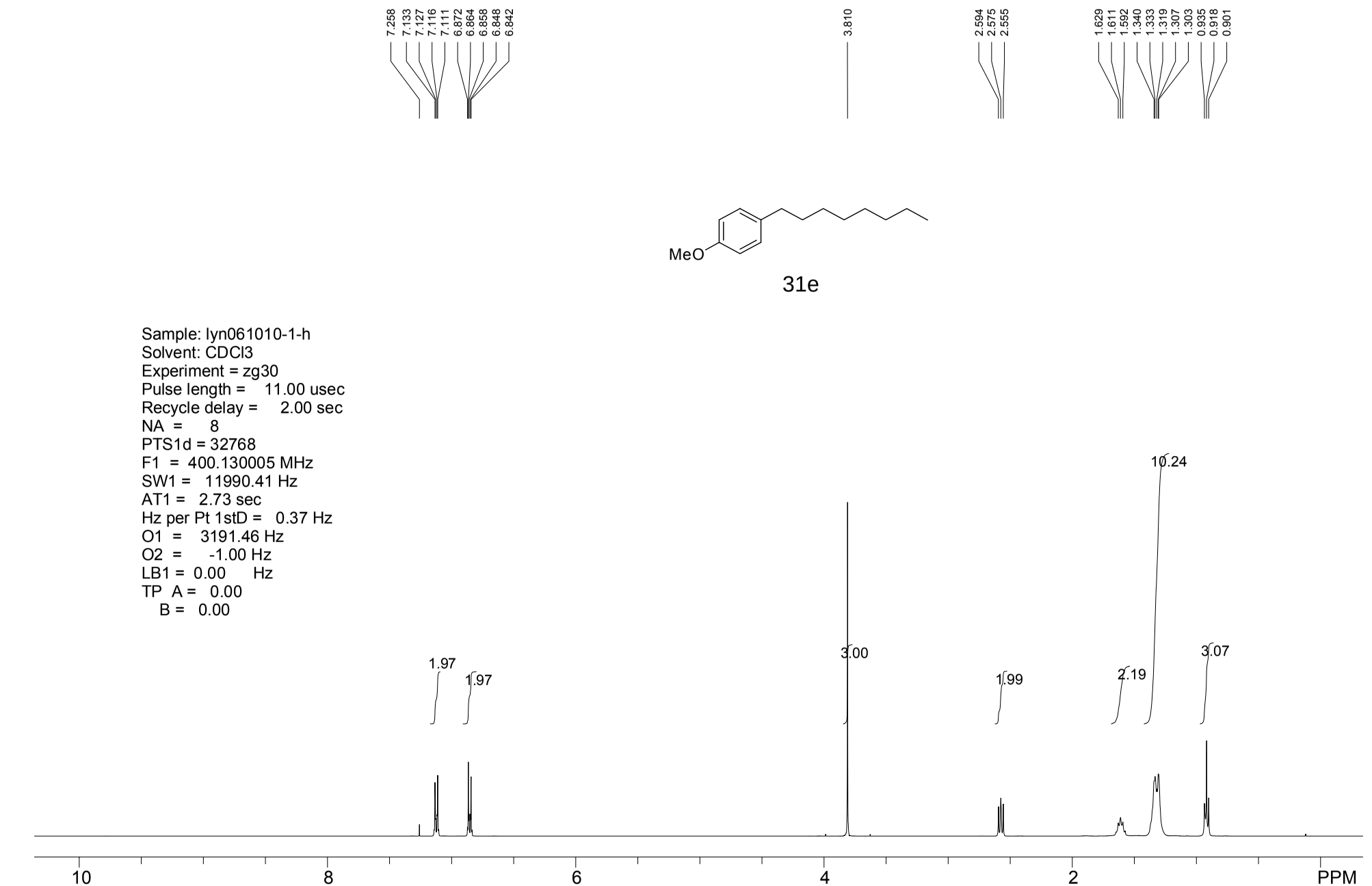


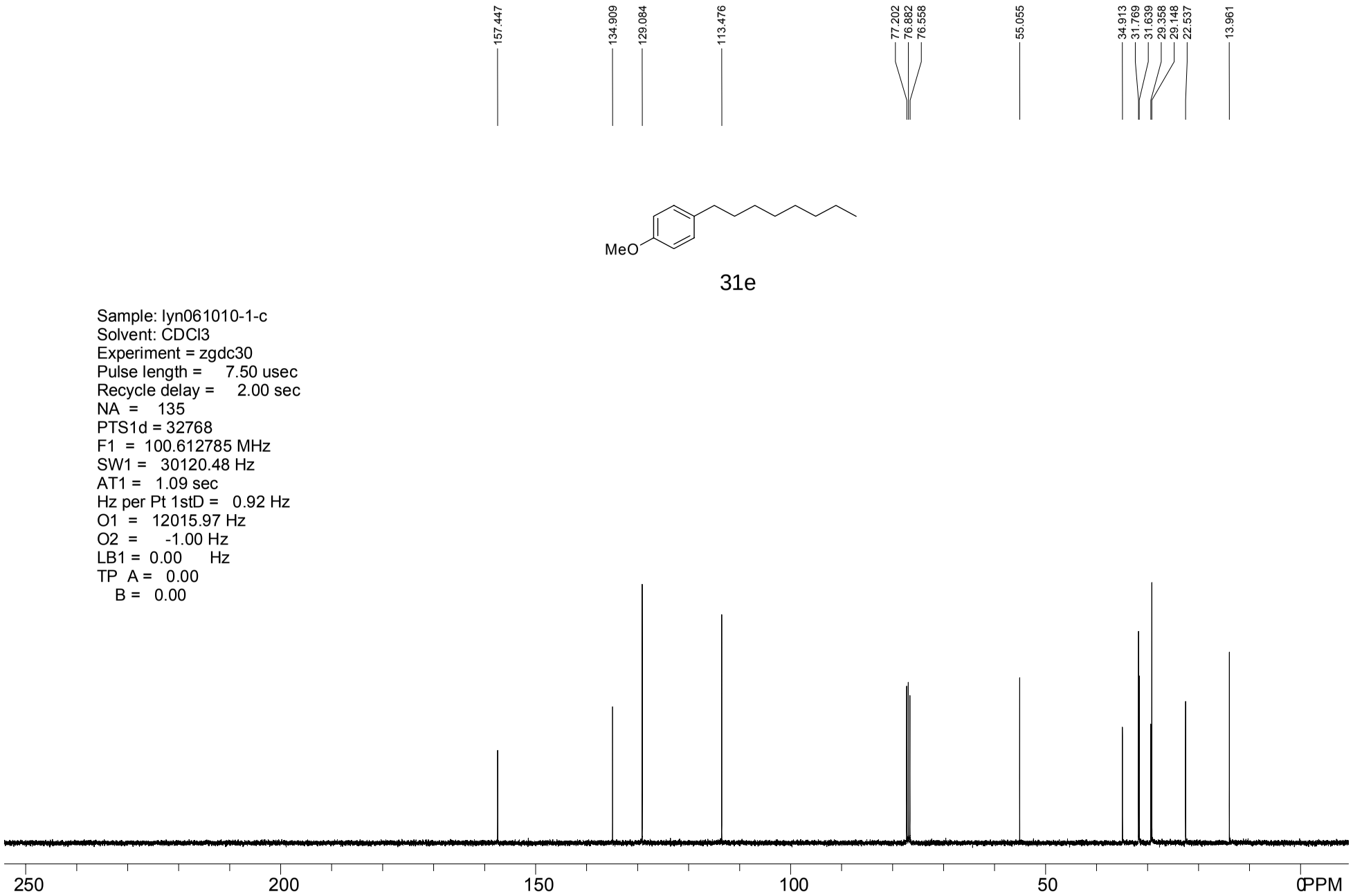


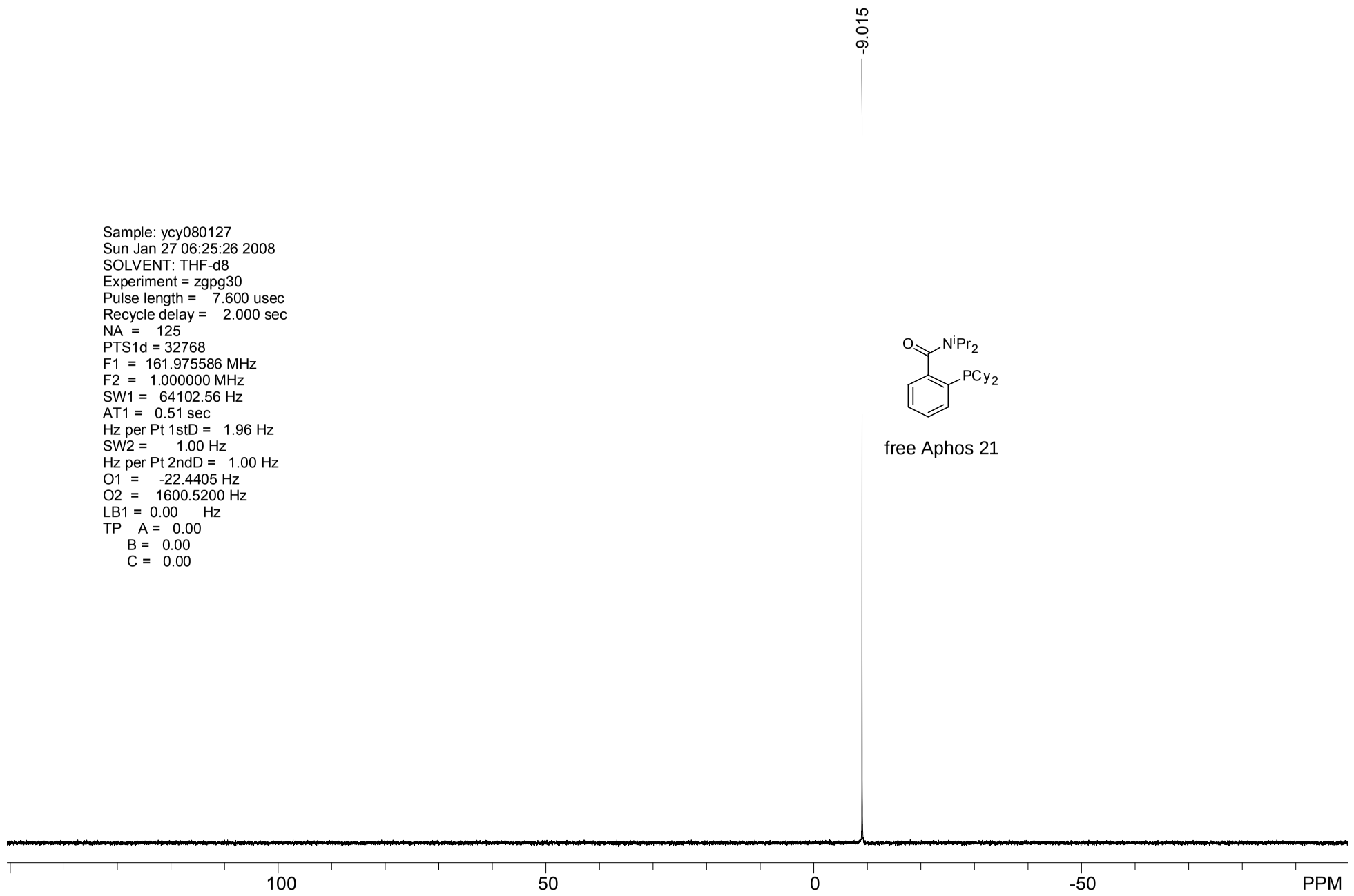
31d

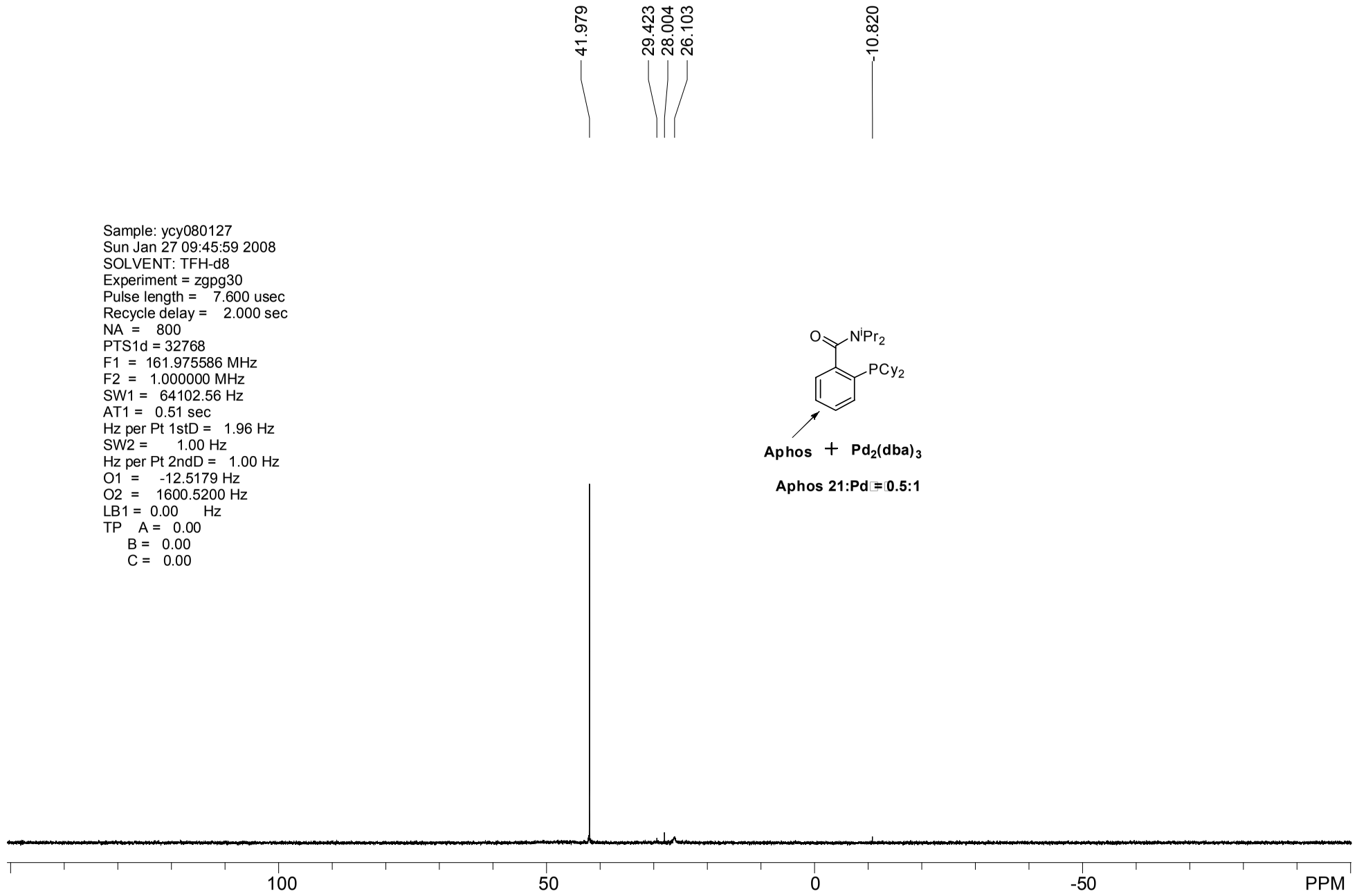
Sample: lyn061007-1-c
Solvent: CDCl3
Experiment = zgdc30
Pulse length = 7.50 usec
Recycle delay = 2.00 sec
NA = 523
PTS1d = 32768
F1 = 100.612778 MHz
SW1 = 30120.48 Hz
AT1 = 1.09 sec
Hz per Pt 1stD = 0.92 Hz
O1 = 12027.92 Hz
O2 = -1.00 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00

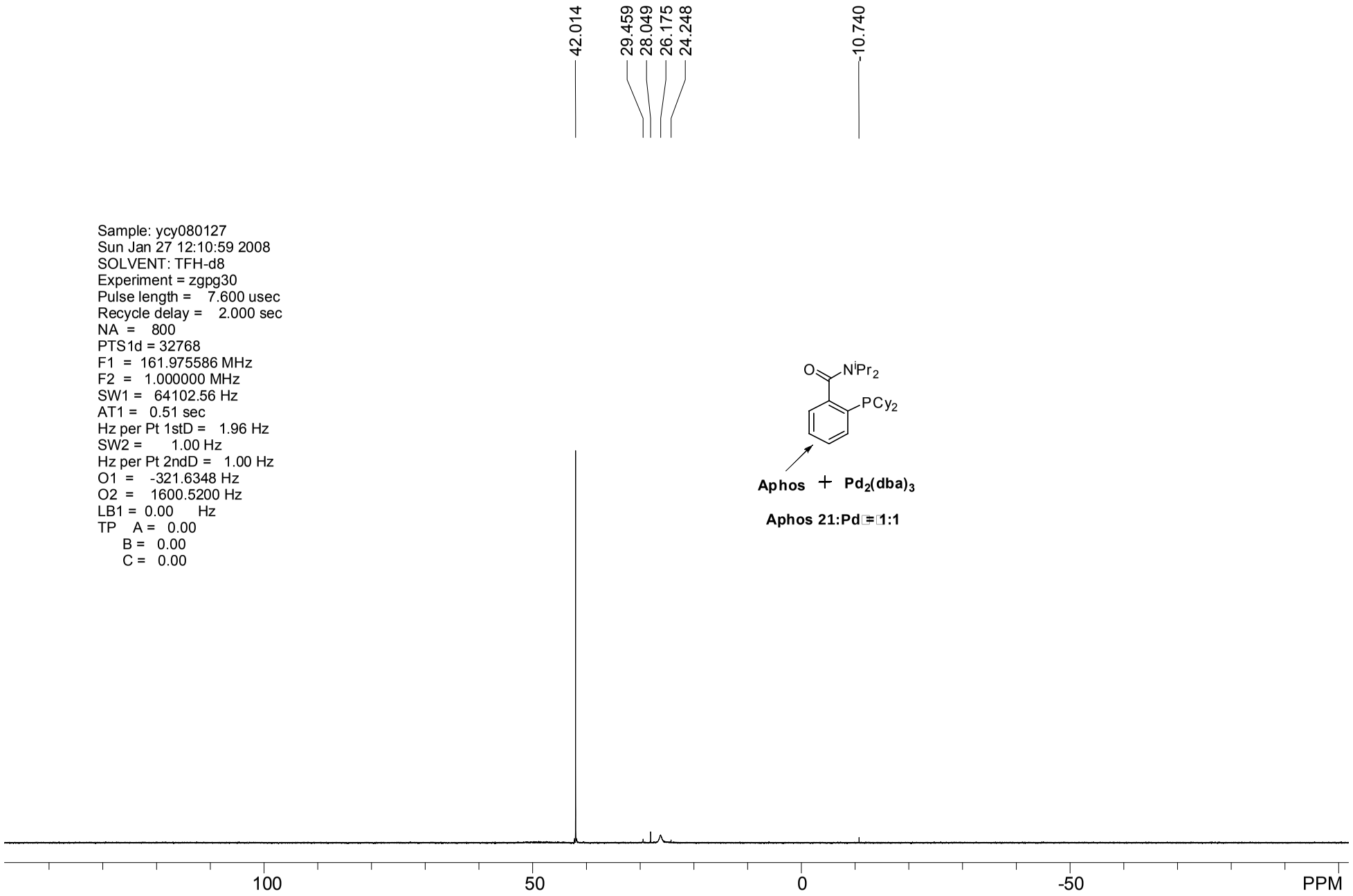


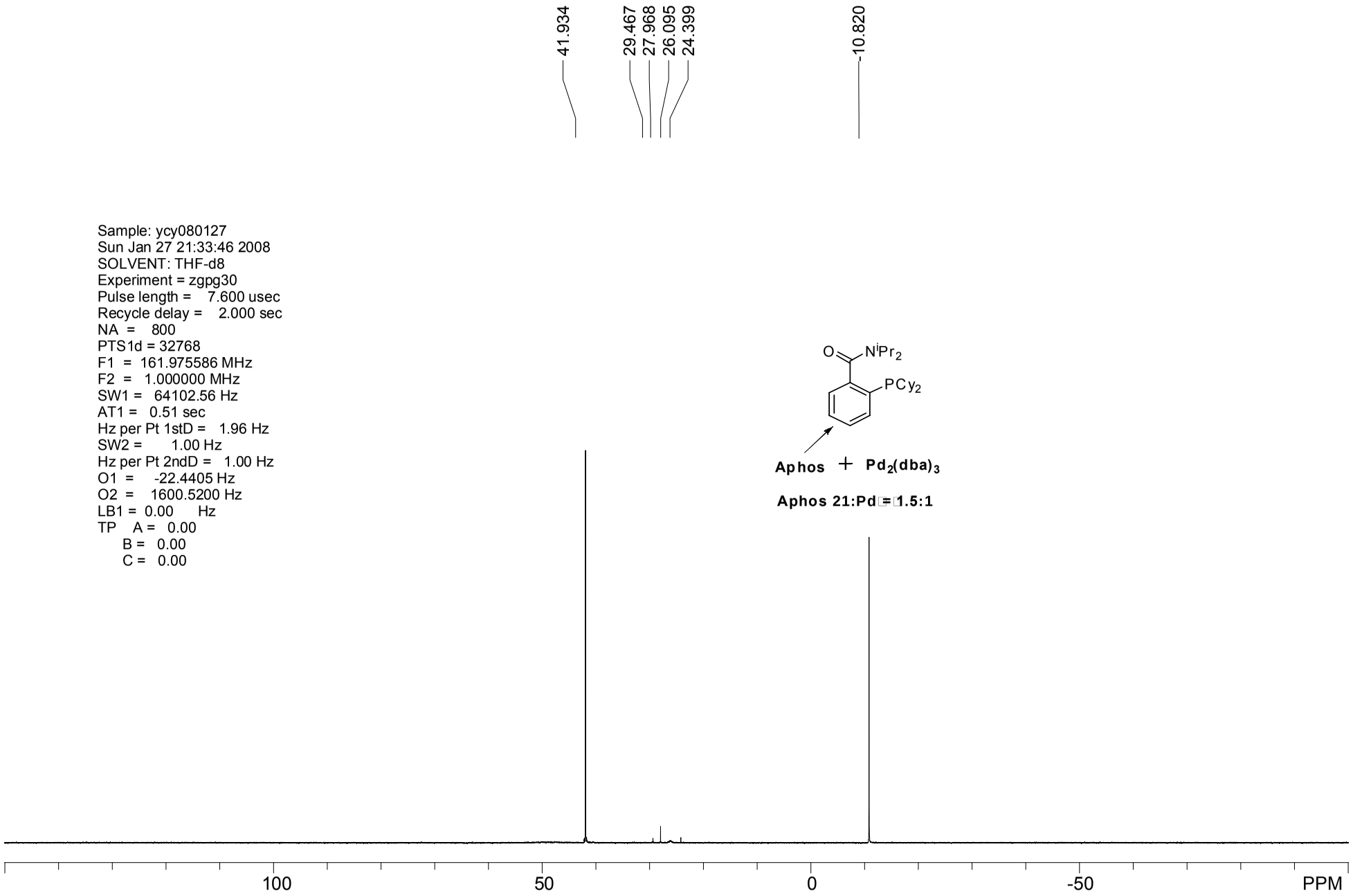

7.258
7.133
7.127
7.116
7.111
6.872
6.864
6.858
6.848
6.842
3.810
2.594
2.575
2.555
1.629
1.611
1.592
1.340
1.333
1.319
1.307
1.303
0.935
0.918
0.901
MeO
31e
Sample: lyn061010-1-h
Solvent: CDCl3
Experiment = zg30
Pulse length = 11.00 usec
Recycle delay = 2.00 sec
NA = 8
PTS1d = 32768
F1 = 400.130005 MHz
SW1 = 11990.41 Hz
AT1 = 2.73 sec
Hz per Pt 1stD = 0.37 Hz
O1 = 3191.46 Hz
O2 = -1.00 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
1.97
1.97
3.00
1.99
2.19
10.24
3.07
10
8
6
4
2
PPM

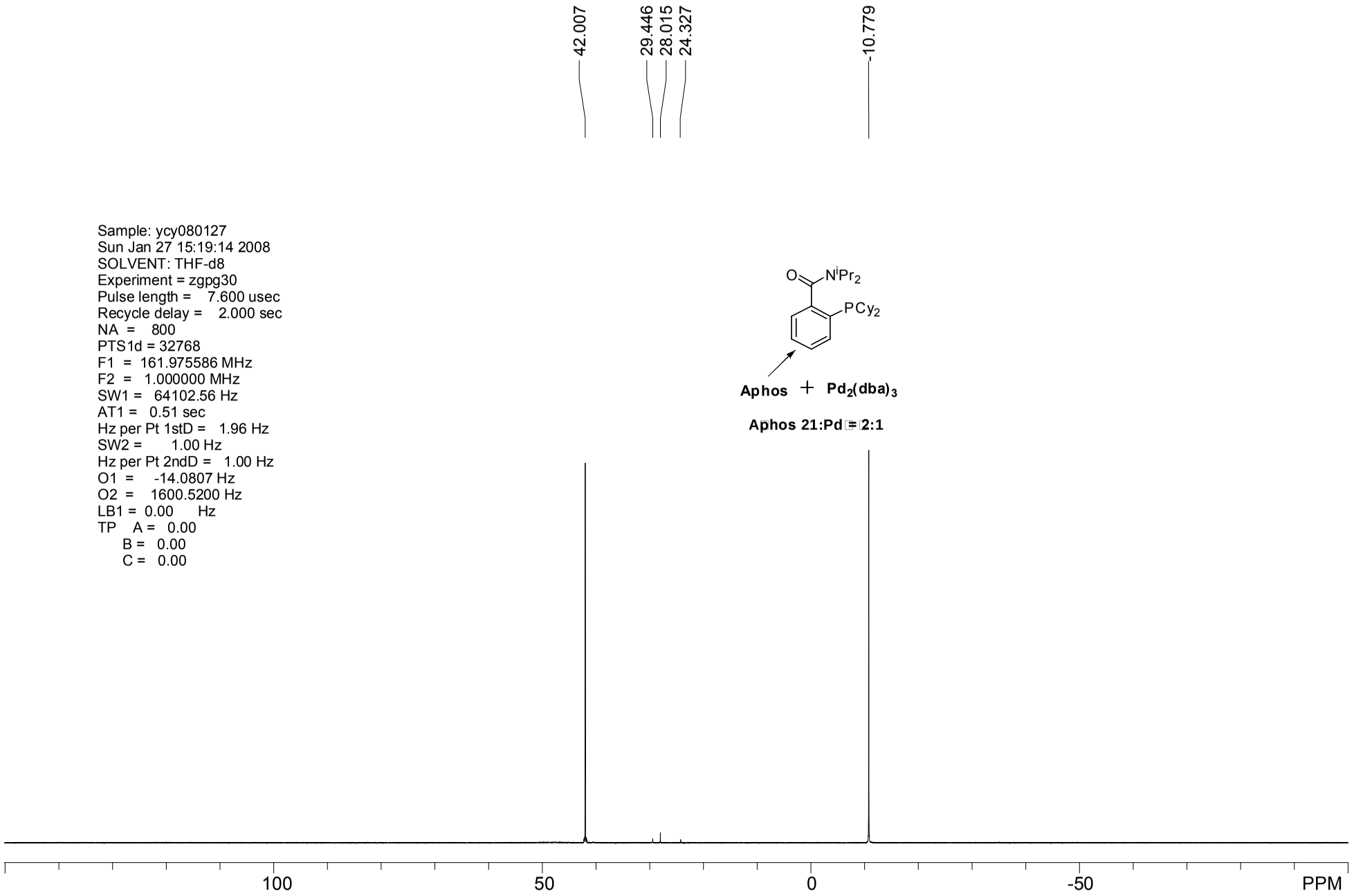

157.447
134.909
129.084
113.476
77.202
76.882
76.558
55.055
34.913
31.769
31.639
29.358
29.148
22.537
13.961
MeO
31e
Sample: lyn061010-1-c
Solvent: CDCl3
Experiment = zgdc30
Pulse length = 7.50 usec
Recycle delay = 2.00 sec
NA = 135
PTS1d = 32768
F1 = 100.612785 MHz
SW1 = 30120.48 Hz
AT1 = 1.09 sec
Hz per Pt 1stD = 0.92 Hz
O1 = 12015.97 Hz
O2 = -1.00 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
250
200
150
100
50
0
PPM

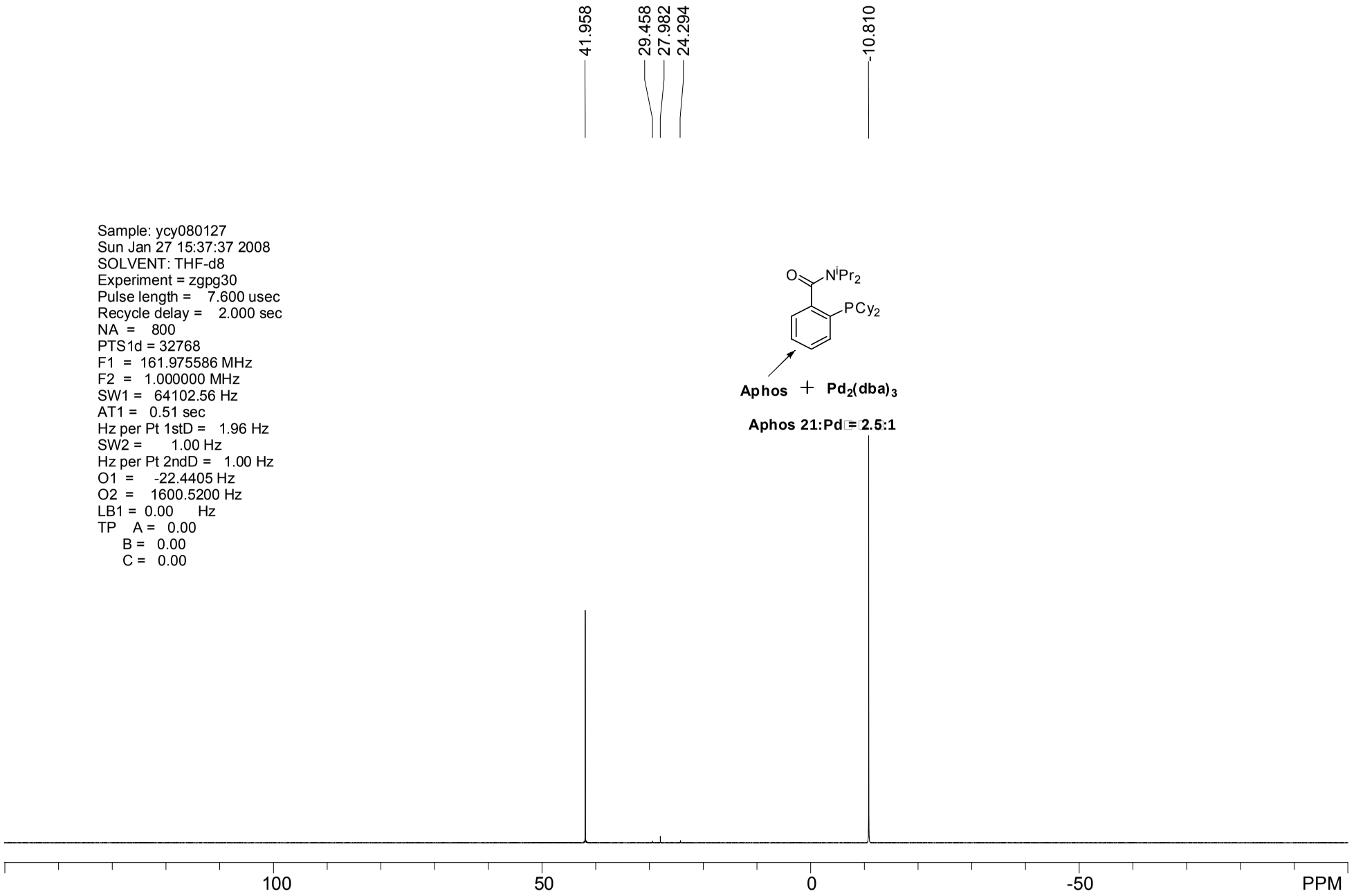

-9.015
Sample: ycy080127
Sun Jan 27 06:25:26 2008
SOLVENT: THF-d8
Experiment = zgpg30
Pulse length = 7.600 usec
Recycle delay = 2.000 sec
NA = 125
PTS1d = 32768
F1 = 161.975586 MHz
F2 = 1.000000 MHz
SW1 = 64102.56 Hz
AT1 = 0.51 sec
Hz per Pt 1stD = 1.96 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = -22.4405 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
NiPr2
PCy2
free Aphos 21
100
50
0
-50
PPM

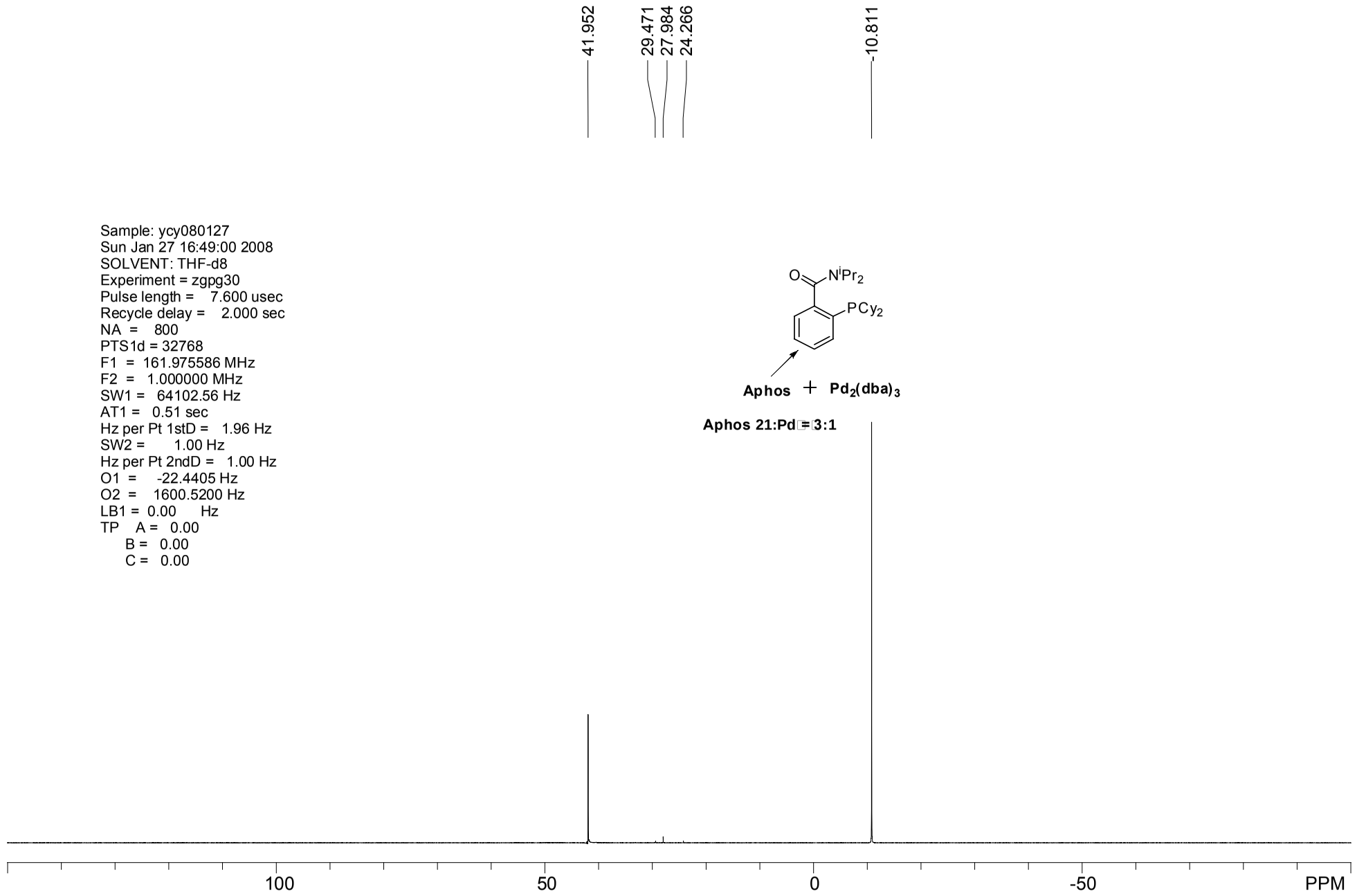

41.979
29.423
28.004
26.103
-10.820
Sample: ycy080127
Sun Jan 27 09:45:59 2008
SOLVENT: TFH-d8
Experiment = zgpg30
Pulse length = 7.600 usec
Recycle delay = 2.000 sec
NA = 800
PTS1d = 32768
F1 = 161.975586 MHz
F2 = 1.000000 MHz
SW1 = 64102.56 Hz
AT1 = 0.51 sec
Hz per Pt 1stD = 1.96 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = -12.5179 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
NiPr2
PCy2
Aphos + Pd2(dba)3
Aphos 21:Pd = 0.5:1
100
50
0
-50
PPM

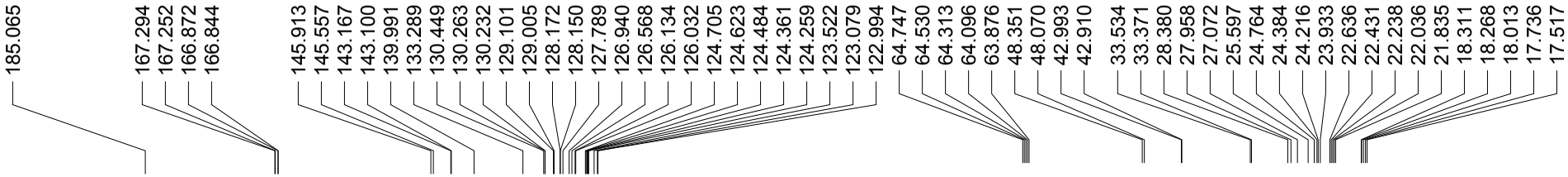

42.014
29.459
28.049
26.175
24.248
-10.740
Sample: ycy080127
Sun Jan 27 12:10:59 2008
SOLVENT: TFH-d8
Experiment = zgpg30
Pulse length = 7.600 usec
Recycle delay = 2.000 sec
NA = 800
PTS1d = 32768
F1 = 161.975586 MHz
F2 = 1.000000 MHz
SW1 = 64102.56 Hz
AT1 = 0.51 sec
Hz per Pt 1stD = 1.96 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = -321.6348 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
NiPr2
PCy2
Aphos + Pd2(dba)3
Aphos 21:Pd = 1:1
100
50
0
-50
PPM


41.934
29.467
27.968
26.095
24.399
-10.820
Sample: ycy080127
Sun Jan 27 21:33:46 2008
SOLVENT: THF-d8
Experiment = zgpg30
Pulse length = 7.600 usec
Recycle delay = 2.000 sec
NA = 800
PTS1d = 32768
F1 = 161.975586 MHz
F2 = 1.000000 MHz
SW1 = 64102.56 Hz
AT1 = 0.51 sec
Hz per Pt 1stD = 1.96 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = -22.4405 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
NiPr2
PCy2
Aphos + Pd2(dba)3
Aphos 21:Pd = 1.5:1
100
50
0
-50
PPM

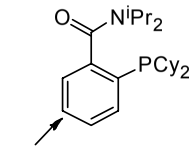

42.007
29.446
28.015
24.327
-10.779
Sample: ycy080127
Sun Jan 27 15:19:14 2008
SOLVENT: THF-d8
Experiment = zgpg30
Pulse length = 7.600 usec
Recycle delay = 2.000 sec
NA = 800
PTS1d = 32768
F1 = 161.975586 MHz
F2 = 1.000000 MHz
SW1 = 64102.56 Hz
AT1 = 0.51 sec
Hz per Pt 1stD = 1.96 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = -14.0807 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
N^{i}Pr$_2$
PCy$_2$
Aphos + Pd$_2$(dba)$_3$
Aphos 21:Pd = 2:1
100
50
0
-50
PPM


41.958
29.458
27.982
24.294
-10.810
Sample: ycy080127
Sun Jan 27 15:37:37 2008
SOLVENT: THF-d8
Experiment = zgpg30
Pulse length = 7.600 usec
Recycle delay = 2.000 sec
NA = 800
PTS1d = 32768
F1 = 161.975586 MHz
F2 = 1.000000 MHz
SW1 = 64102.56 Hz
AT1 = 0.51 sec
Hz per Pt 1stD = 1.96 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = -22.4405 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
NiPr2
PCy2
Aphos + Pd2(dba)3
Aphos 21:Pd = 2.5:1
100
50
0
-50
PPM


41.952
29.471
27.984
24.266
-10.811
Sample: ycy080127
Sun Jan 27 16:49:00 2008
SOLVENT: THF-d8
Experiment = zgpg30
Pulse length = 7.600 usec
Recycle delay = 2.000 sec
NA = 800
PTS1d = 32768
F1 = 161.975586 MHz
F2 = 1.000000 MHz
SW1 = 64102.56 Hz
AT1 = 0.51 sec
Hz per Pt 1stD = 1.96 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = -22.4405 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
N^{i}Pr$_2$
PCy$_2$
Aphos + Pd$_2$(dba)$_3$
Aphos 21:Pd = 3:1
100
50
0
-50
PPM

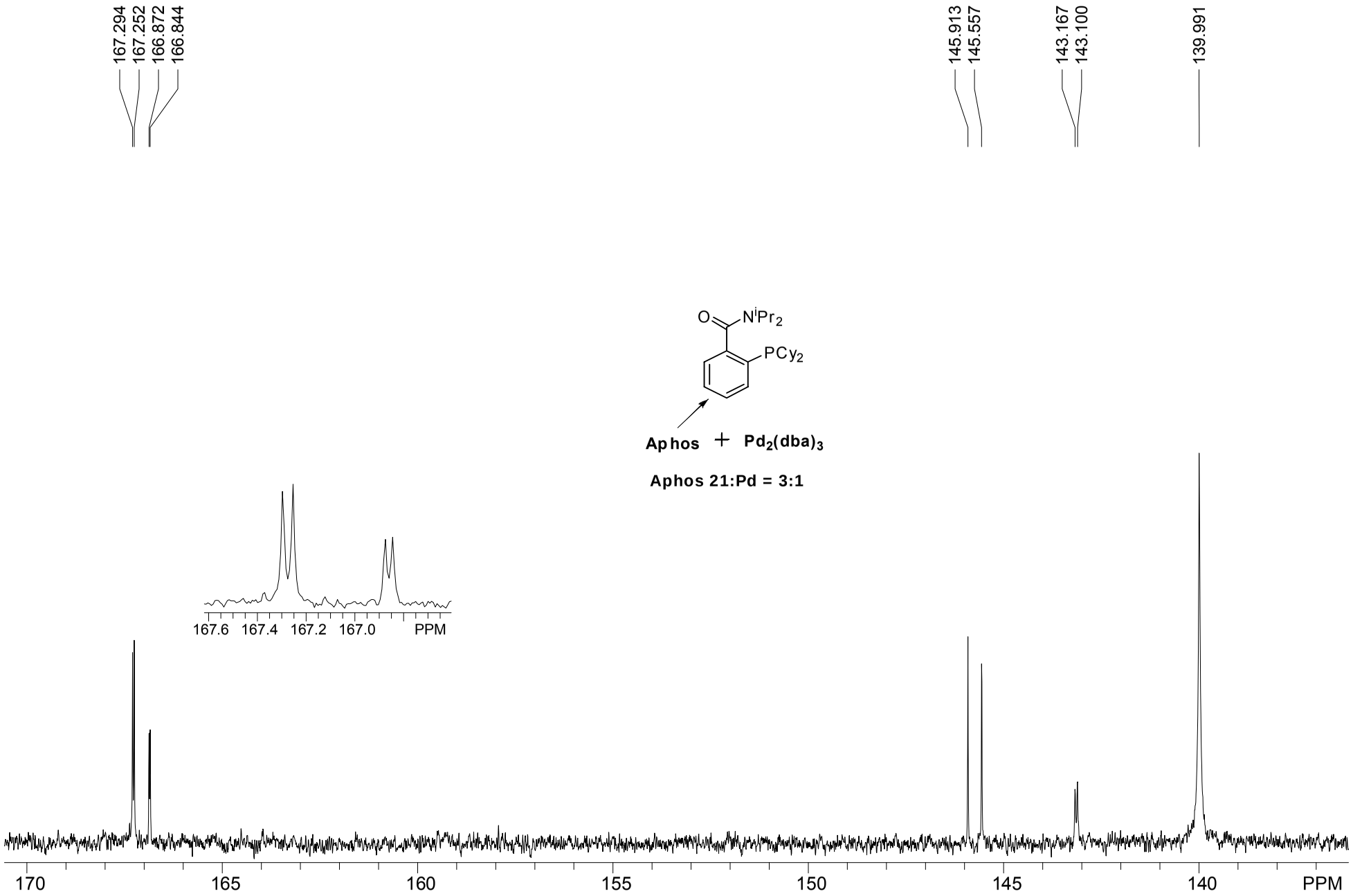


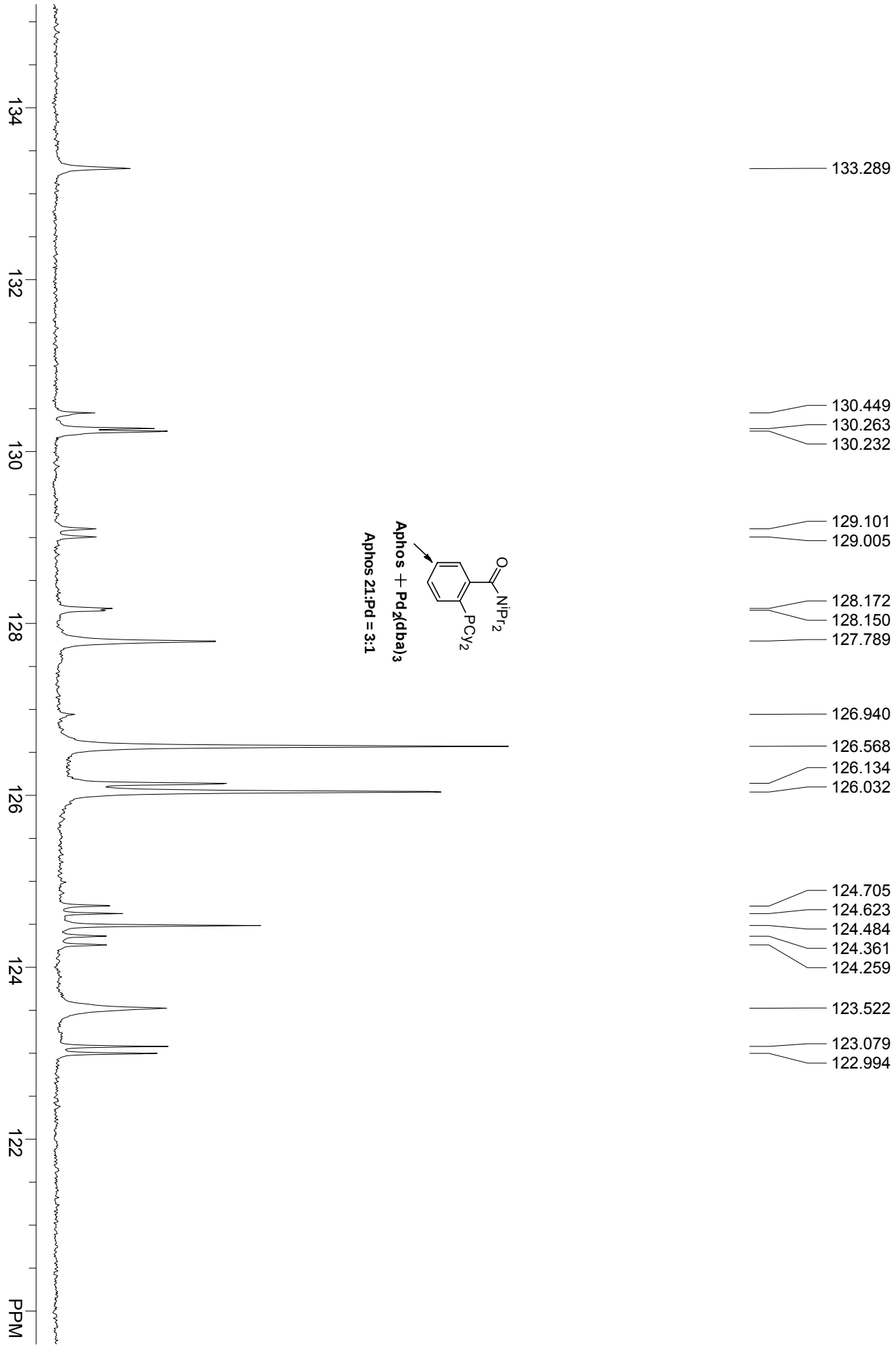
Sample: ycy080127
Mon Jan 28 01:55:14 2008
SOLVENT: THF-d8
Experiment = zgpg30
Pulse length = 8.600 usec
Recycle delay = 2.000 sec
NA = 10804
PTS1d = 32768
F1 = 100.622833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10038.0586 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00

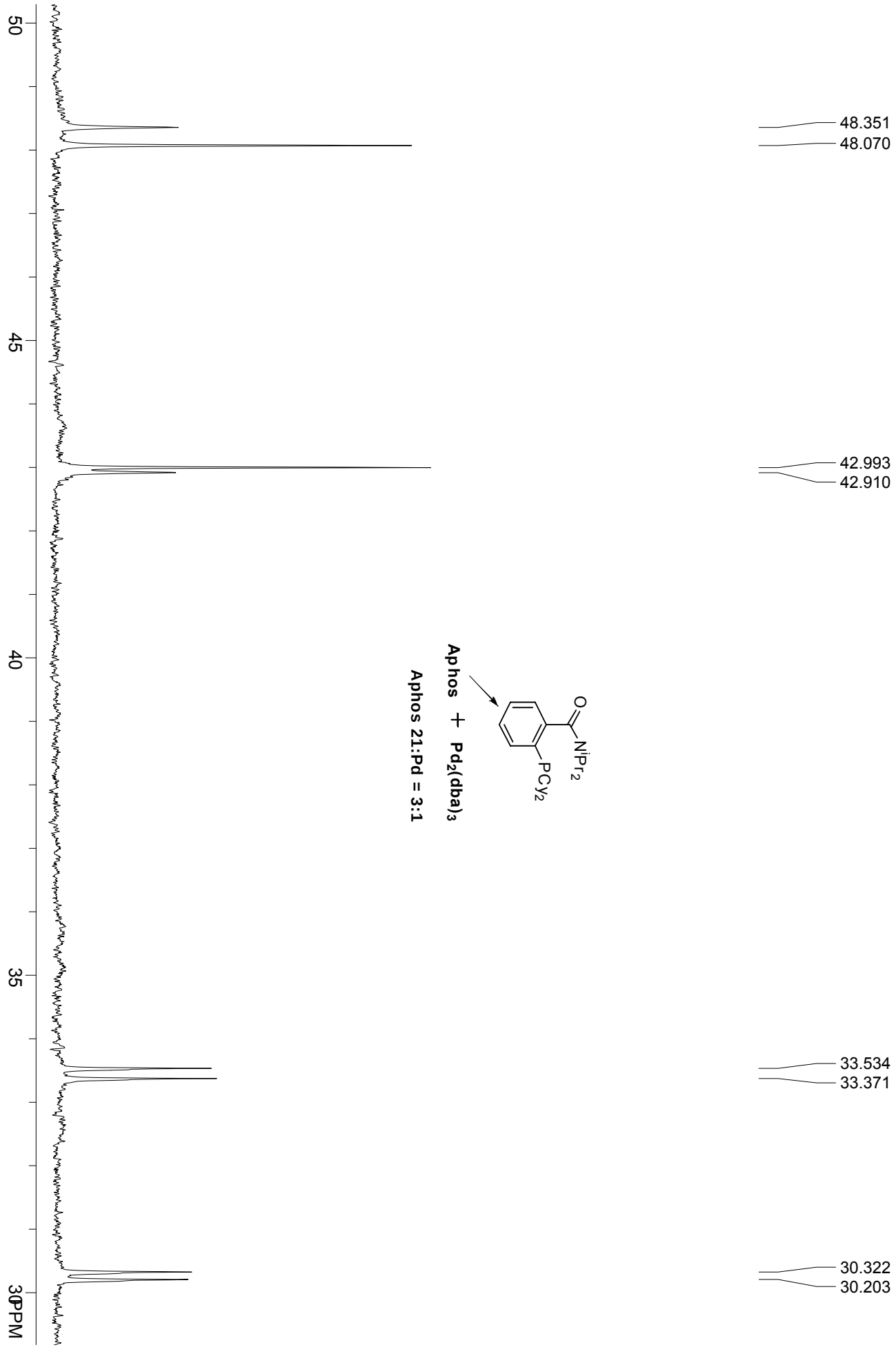


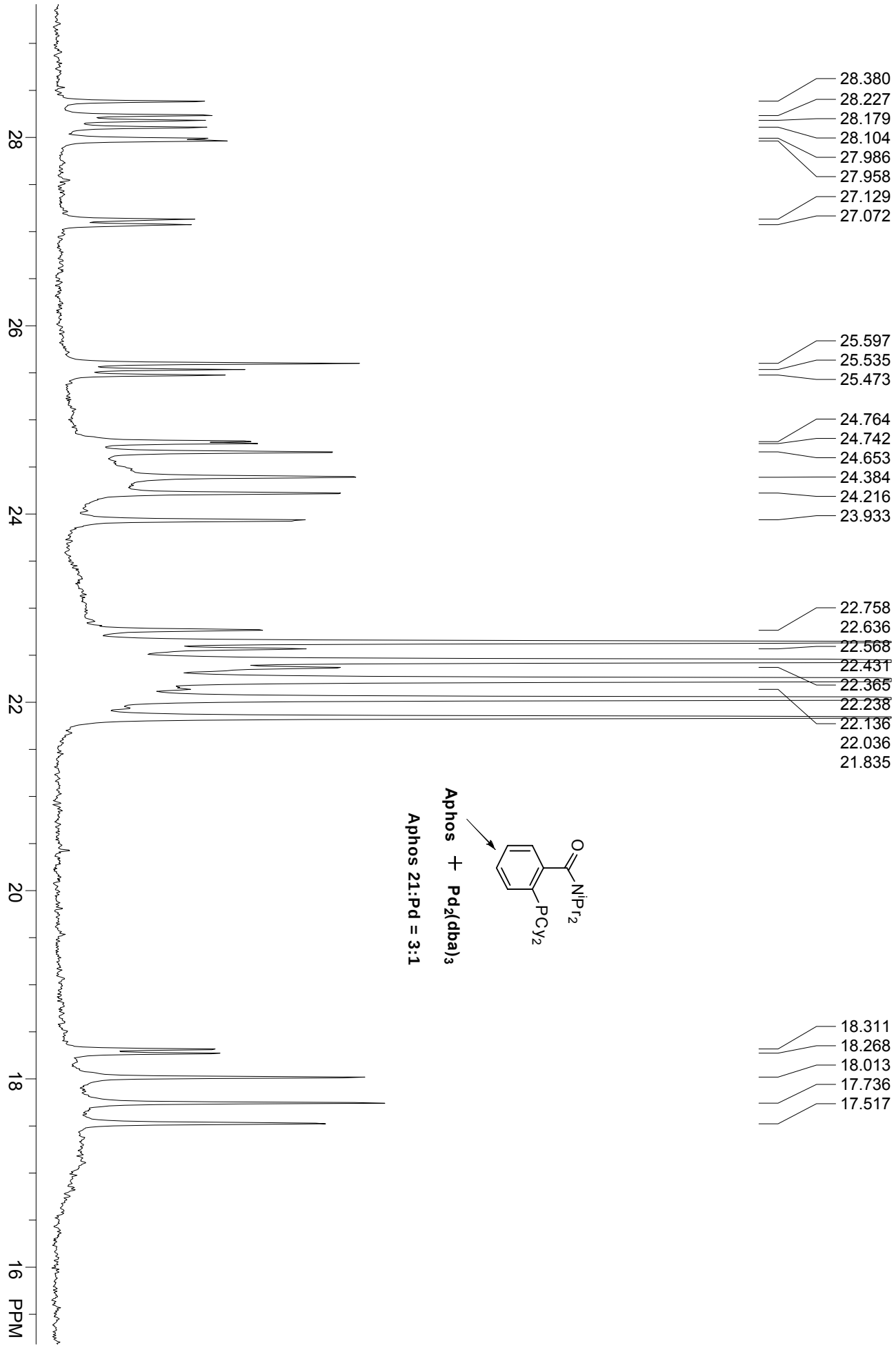
Aphos + $Pd_2(dba)_3$

Aphos 21:Pd = 3:1


167.294
167.252
166.872
166.844
145.913
145.557
143.167
143.100
139.991
O
N^{i}Pr$_2$
PCy$_2$
Aphos + Pd$_2$(dba)$_3$
Aphos 21:Pd = 3:1
167.6 167.4 167.2 167.0 PPM
170 165 160 155 150 145 140 PPM


134
132
130
128
126
124
122
PPM
Aphos + Pd2(dba)3
Aphos 2l:Pd = 3:1
O
NiPr2
PCy2
133.289
130.449
130.263
130.232
129.101
129.005
128.172
128.150
127.789
126.940
126.568
126.134
126.032
124.705
124.623
124.484
124.361
124.259
123.522
123.079
122.994


50
45
40
35
30
PPM
48.351
48.070
42.993
42.910
33.534
33.371
30.322
30.203
Aphos + Pd2(dba)3
Aphos 2:1 Pd = 3:1
O
NiPr2
PCy2


28.380
28.227
28.179
28.104
27.986
27.958
27.129
27.072
25.597
25.535
25.473
24.764
24.742
24.653
24.384
24.216
23.933
22.758
22.636
22.568
22.431
22.365
22.238
22.136
22.036
21.835
18.311
18.268
18.013
17.736
17.517
28
26
24
22
20
18
16 PPM
Aphos + Pd2(dba)3
Aphos 21:Pd = 3:1
O
NiPr2
PCy2