

**Reactivity of (2-Alkenyl-3-pentene-1,5-diy)iron Complexes:**

**Preparation of Functionalized Vinylcyclopropanes and Cycloheptadienes**

Rajesh K. Pandey, Lizhu Wang, Nathaniel J. Wallock, Sergey Lindeman,

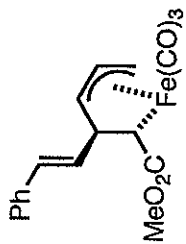
and William A. Donaldson\*

*Supporting Information*

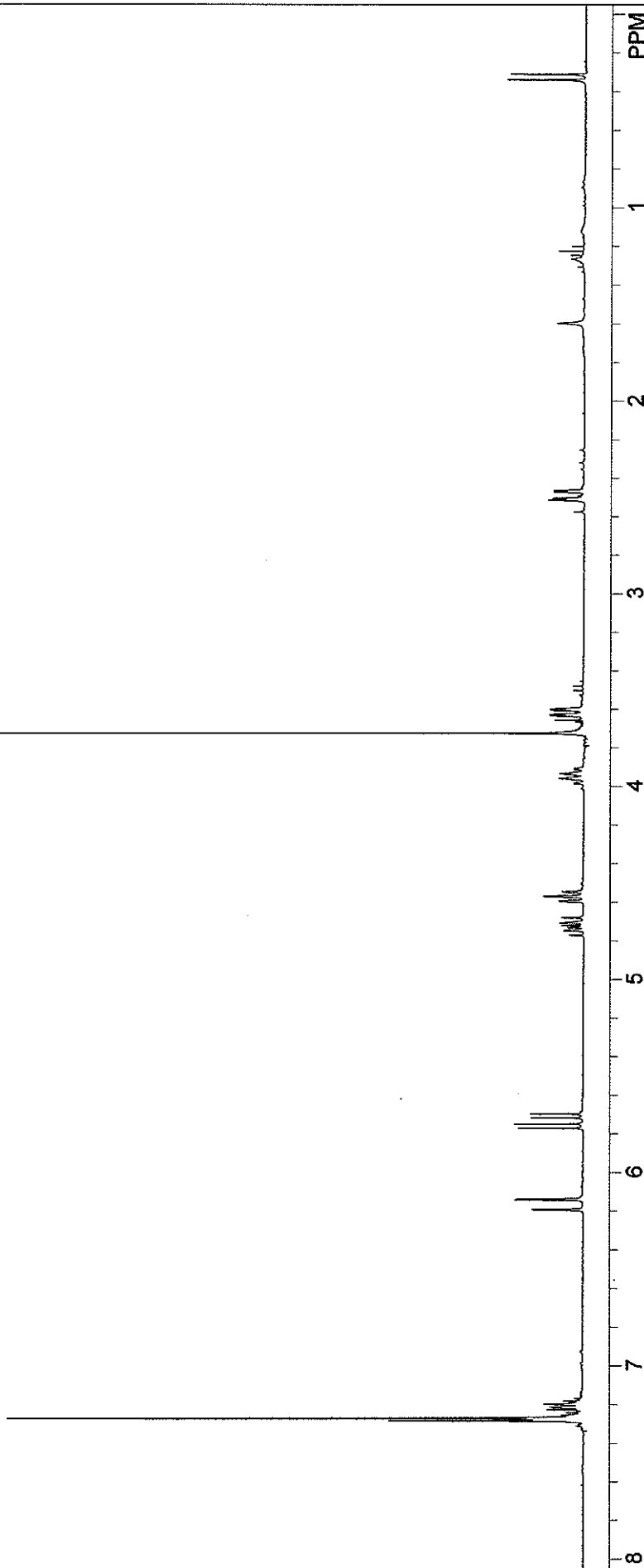
All spectra in CDCl<sub>3</sub> unless otherwise noted

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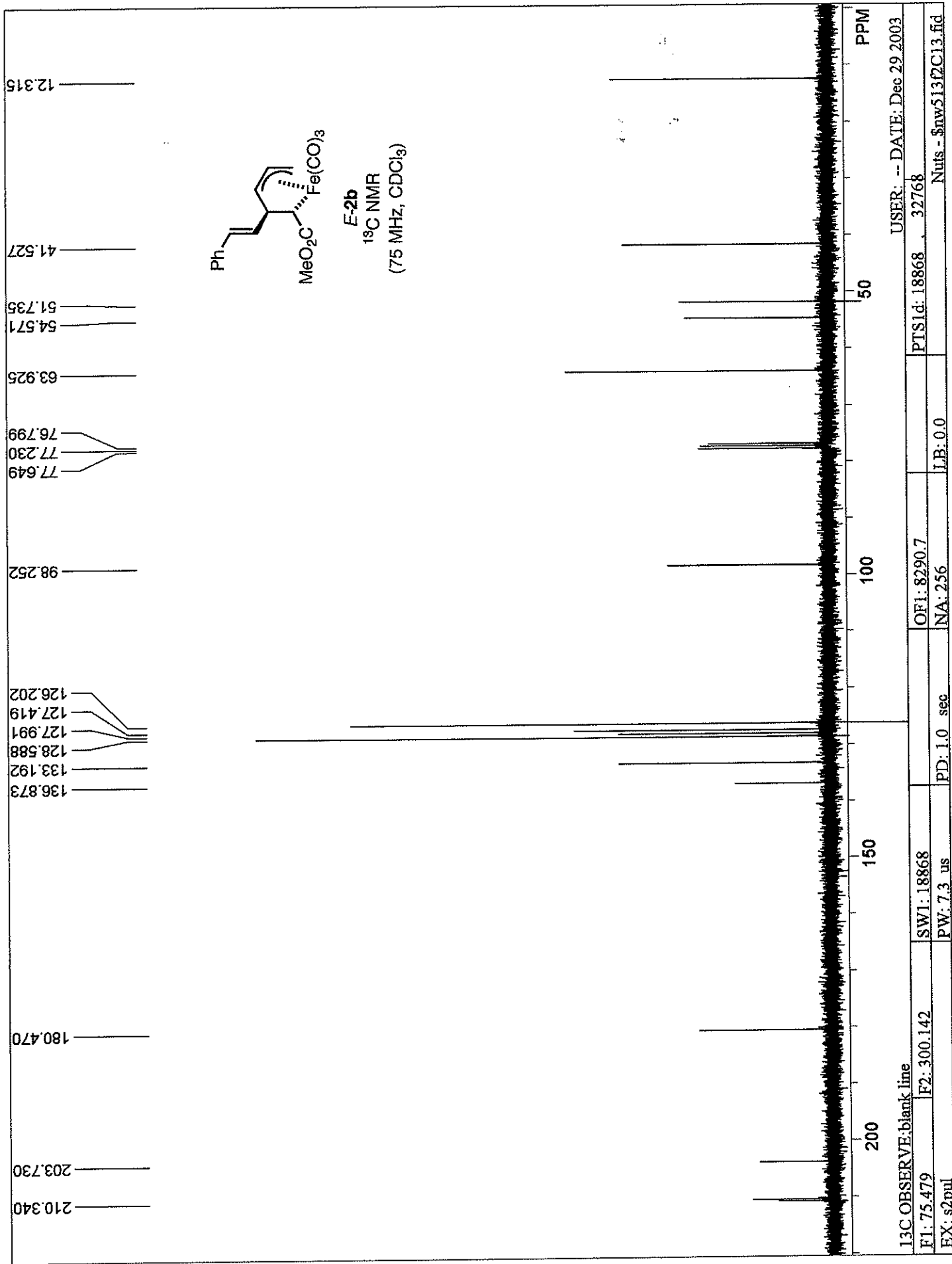
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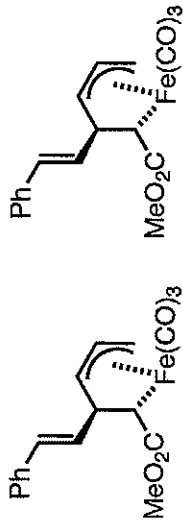


**E-2b**  
<sup>1</sup>H NMR  
 (300 MHz, CDCl<sub>3</sub>)



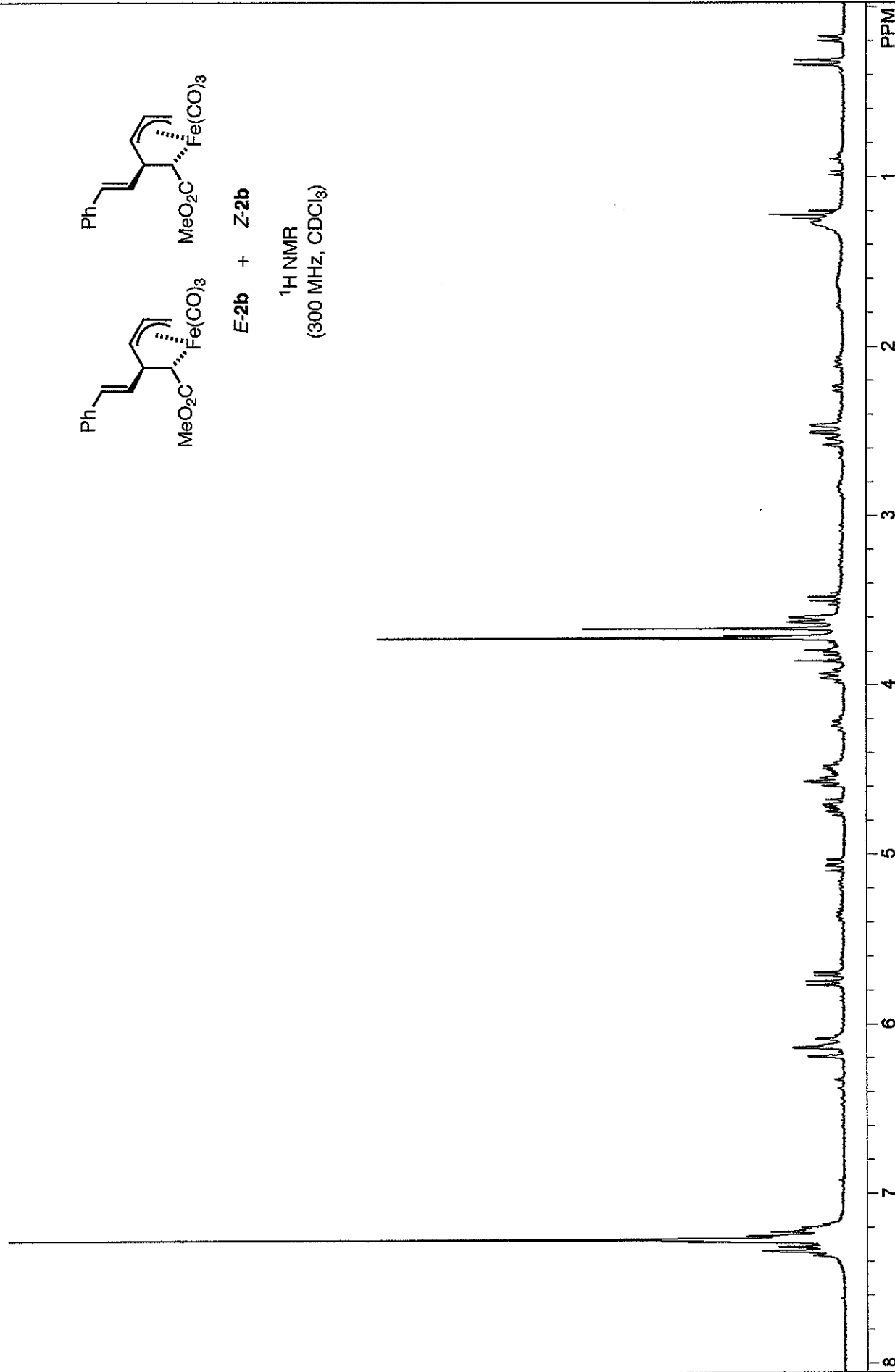
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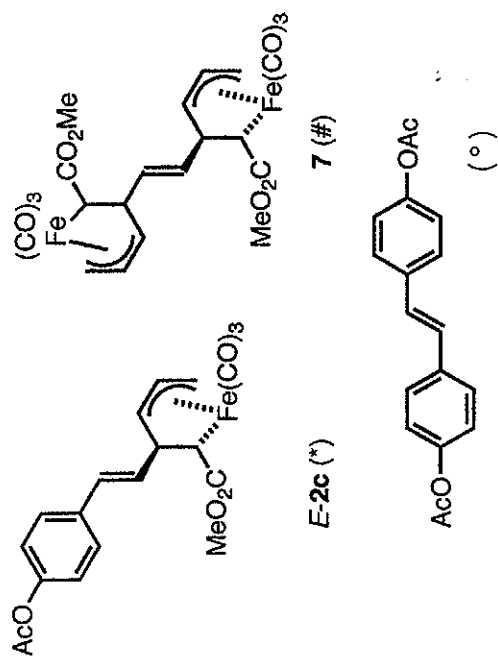


**E-2b + Z-2b**

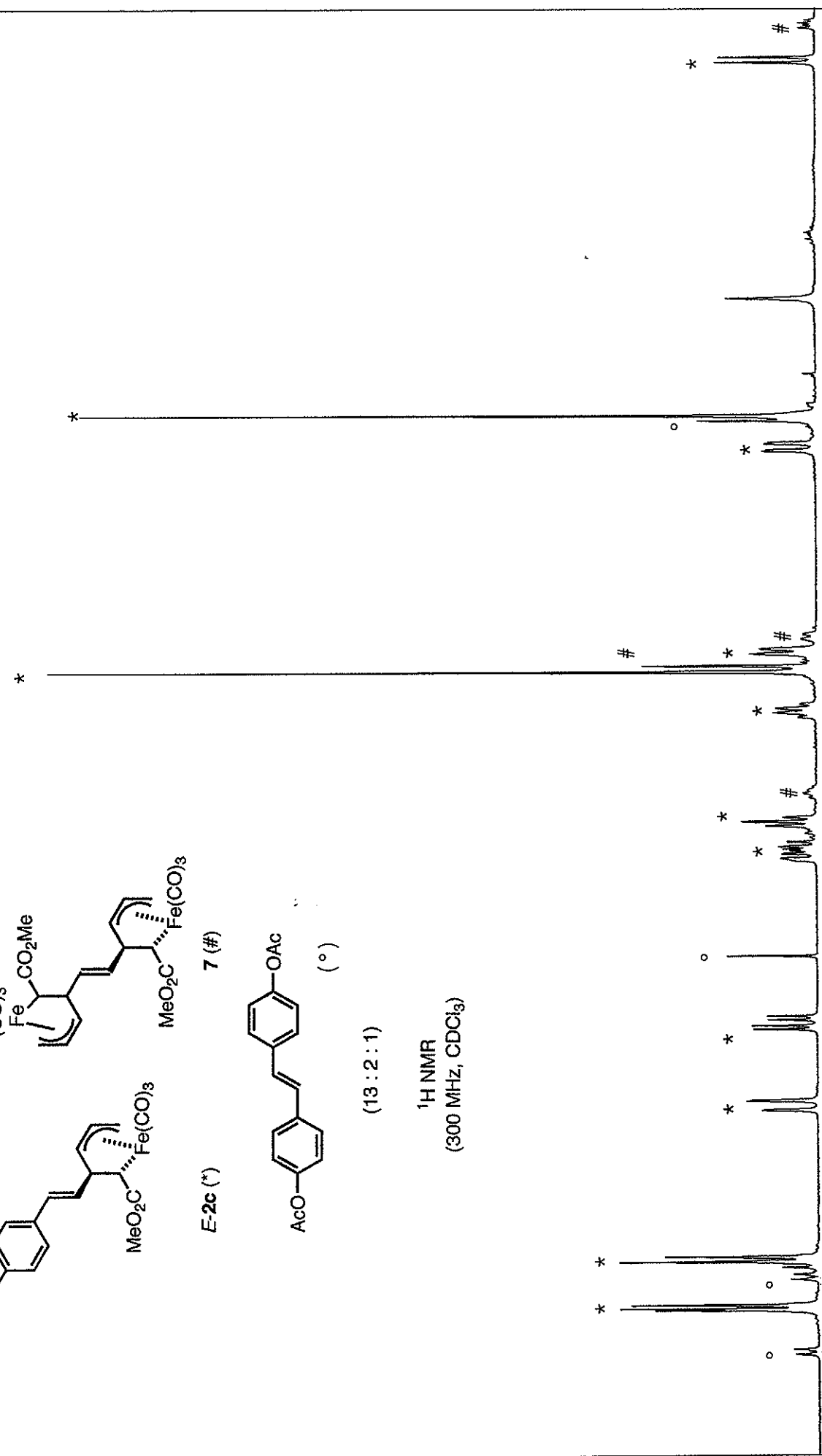
<sup>1</sup>H NMR  
(300 MHz, CDCl<sub>3</sub>)



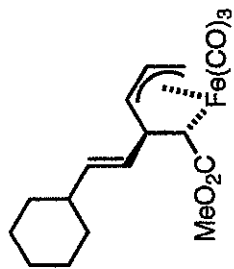
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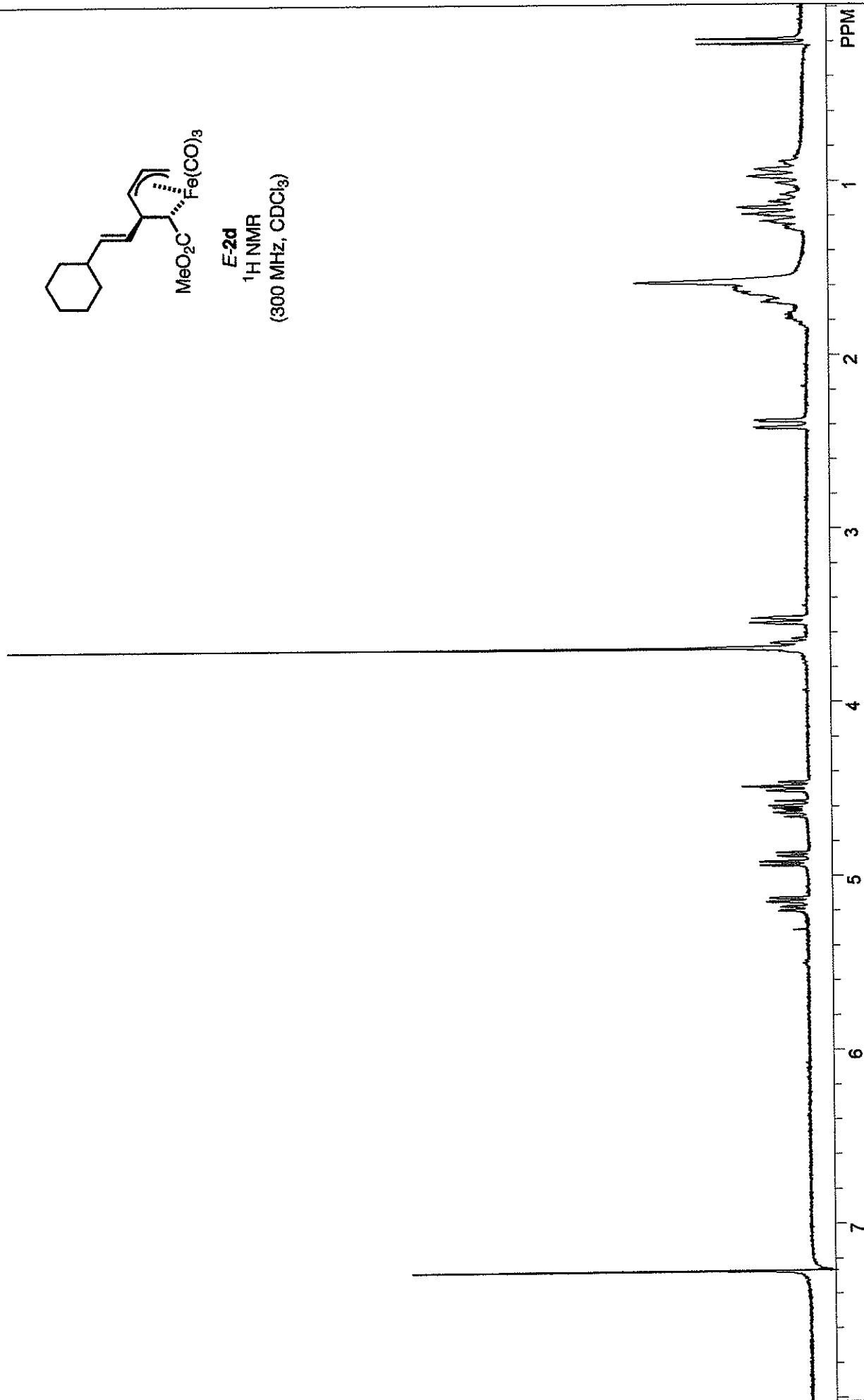
(13 : 2 : 1)  
<sup>1</sup>H NMR  
 (300 MHz, CDCl<sub>3</sub>)



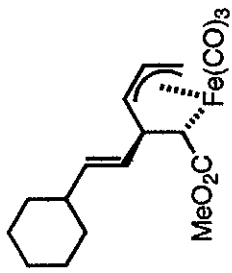
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6	F2: 75.479	OF1: 1792.1
5	PW: 6.3 usec	NA: 8
4	PD: 1.0 sec	LB: 0.0
3		WinNuts - \$rkp031.fid
2		
1		
0		



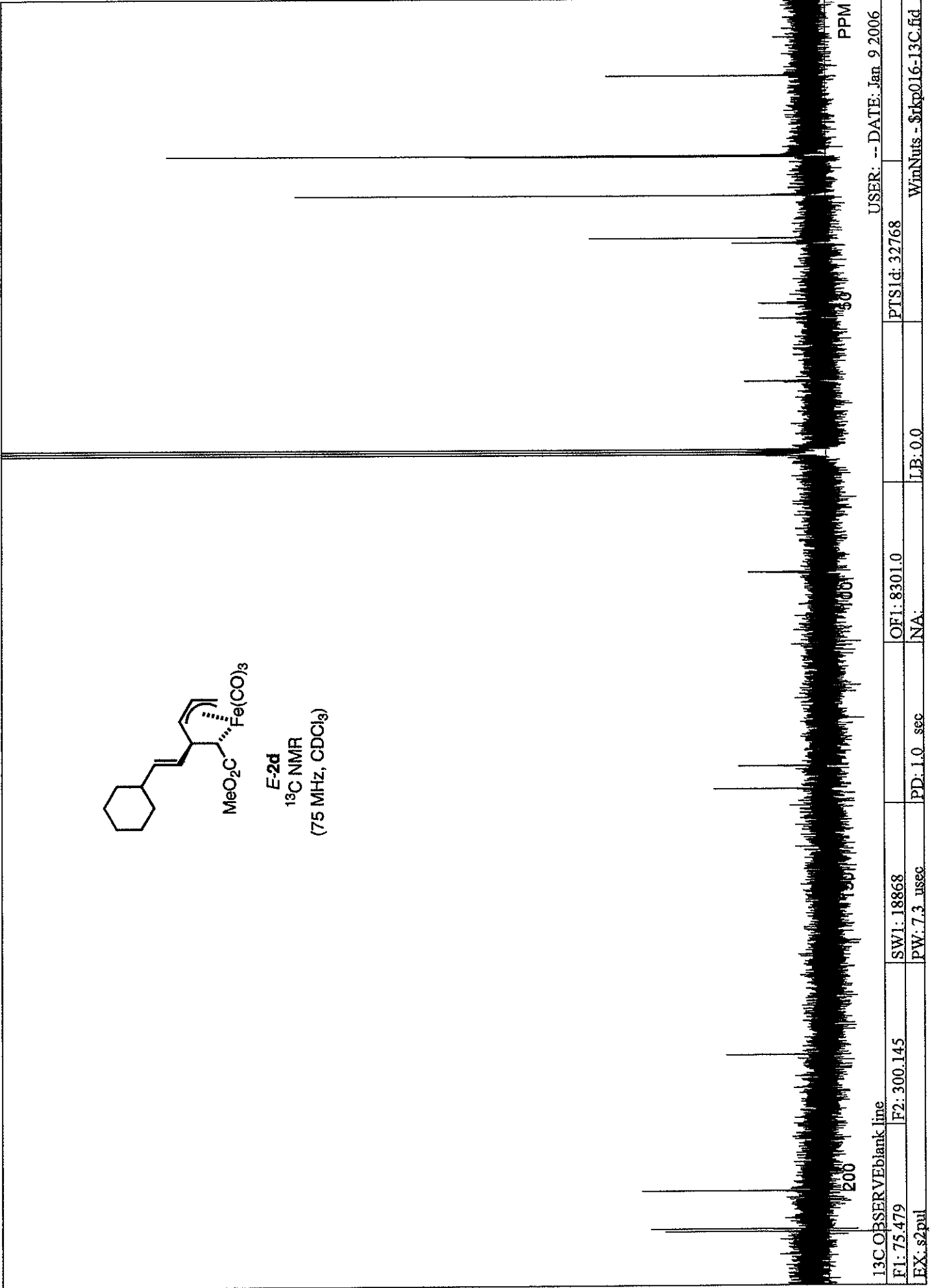
**E-2d**  
 $^1\text{H NMR}$   
 (300 MHz,  $\text{CDCl}_3$ )



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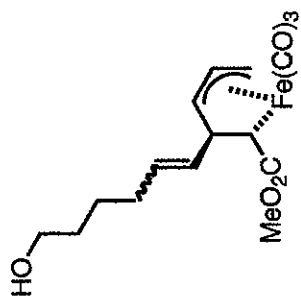


**E-2d**  
<sup>13</sup>C NMR  
 (75 MHz, CDCl<sub>3</sub>)

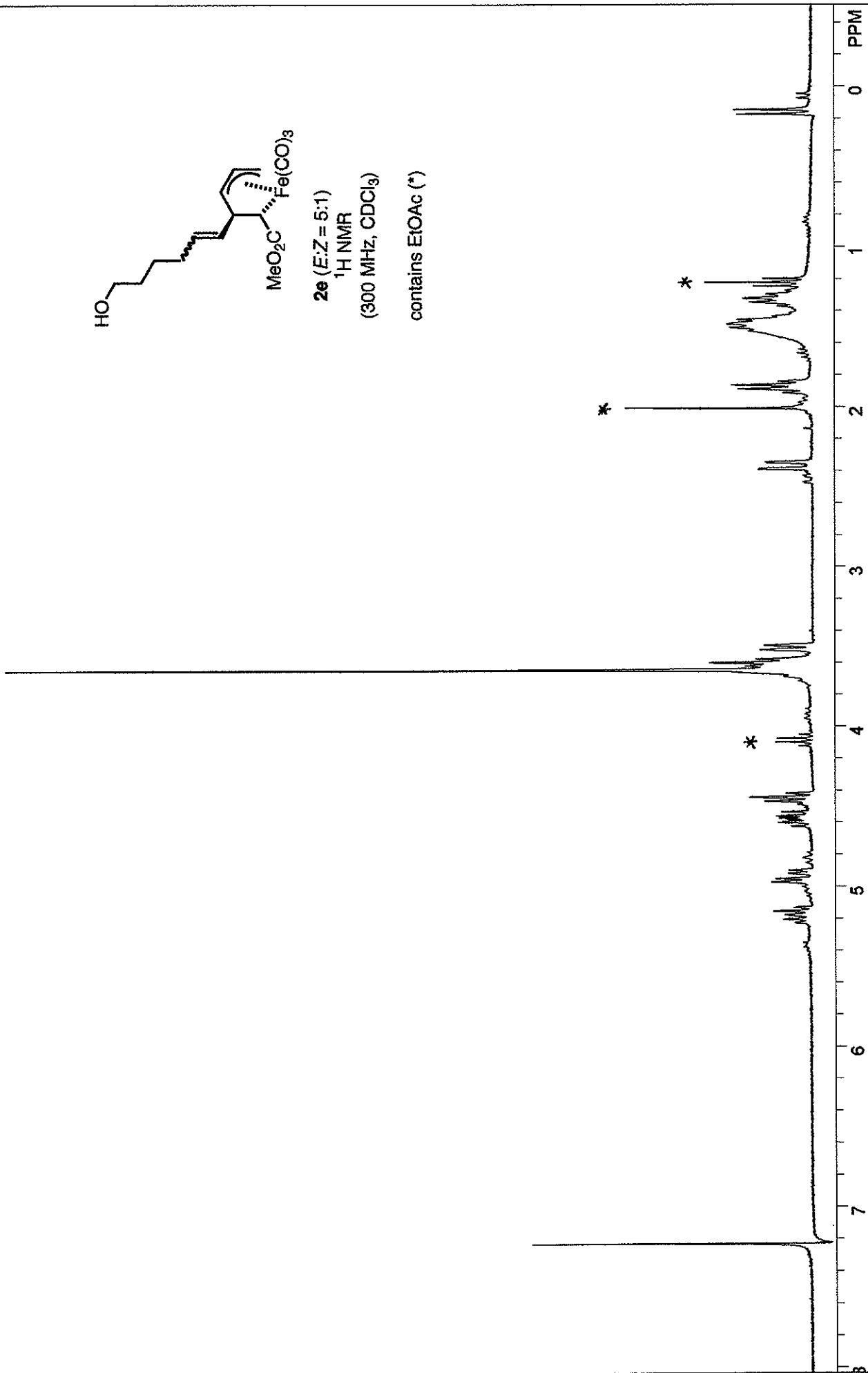


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	PD: 1.0 sec		

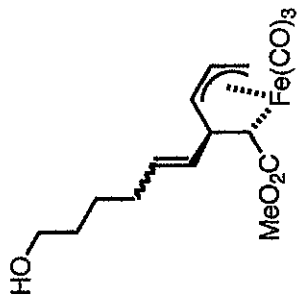




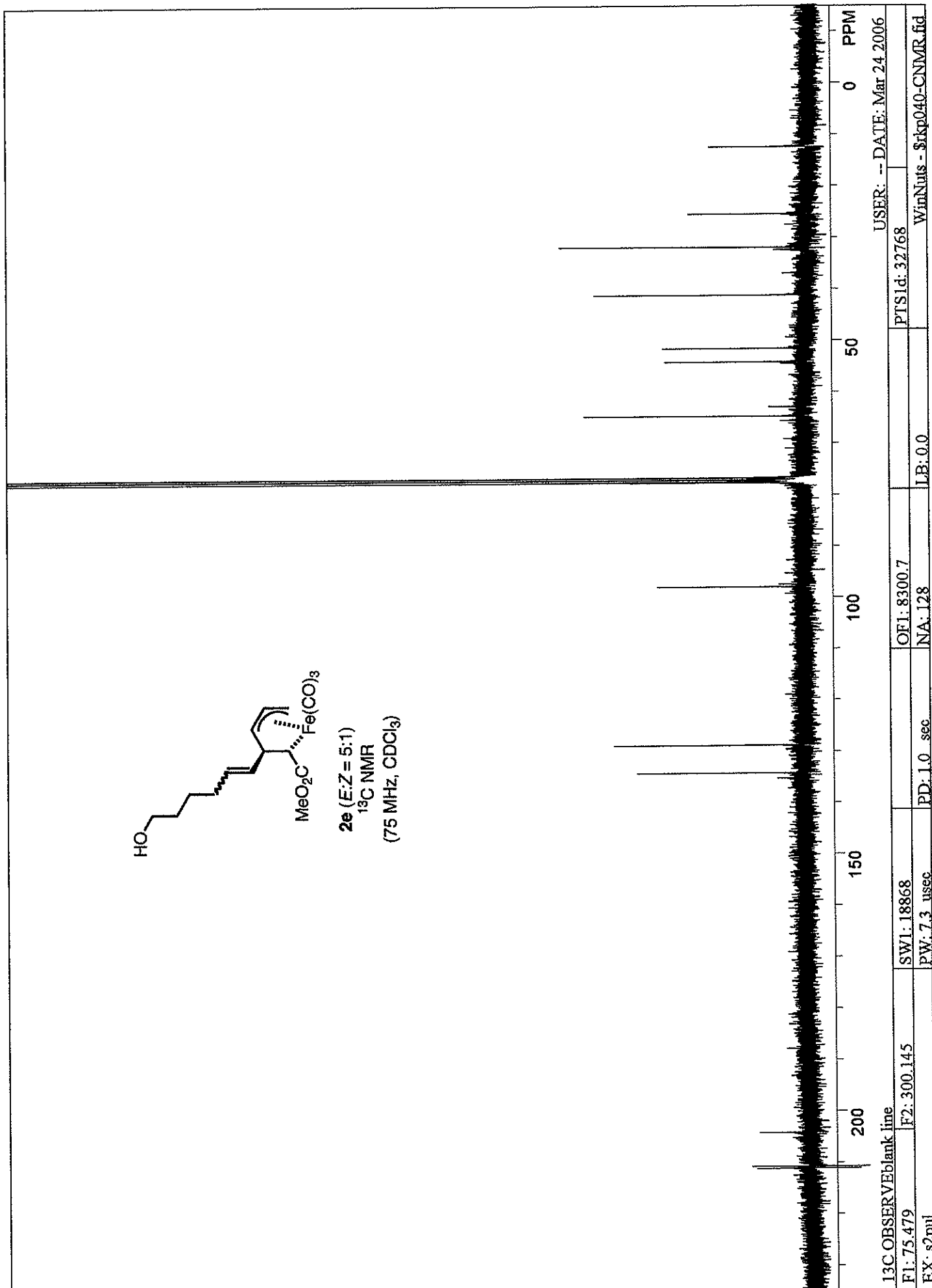
**2e** (E:Z = 5:1)  
<sup>1</sup>H NMR  
 (300 MHz, CDCl<sub>3</sub>)  
 contains EtOAc (\*)



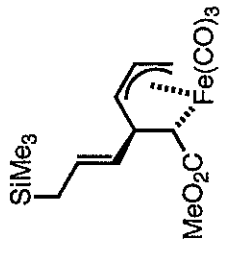
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	PW: 6.3 usec	NA: 8	
	PD: 1.0 sec		



**2e** (E:Z = 5:1)  
<sup>18</sup>C NMR  
 (75 MHz, CDCl<sub>3</sub>)



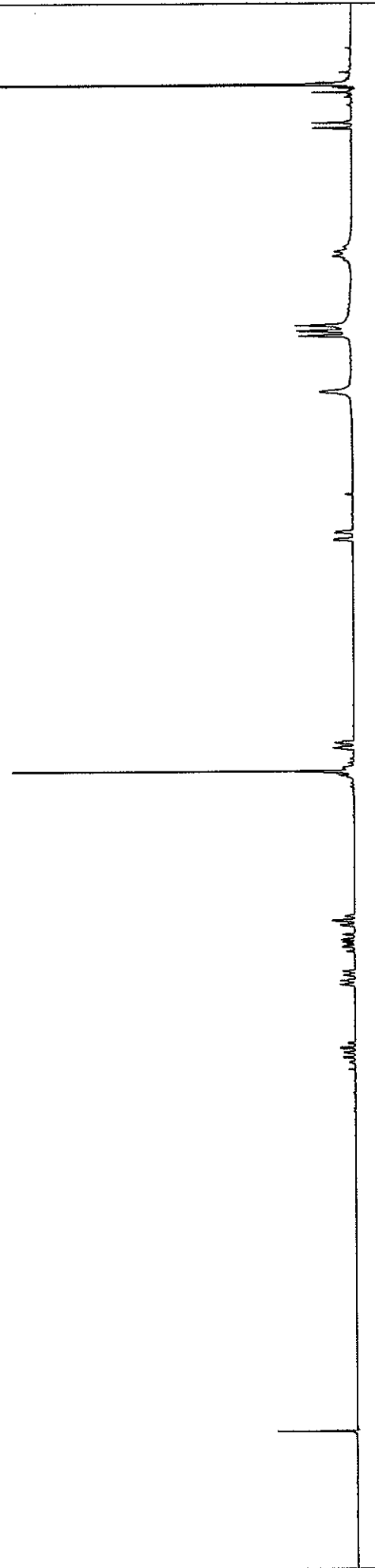
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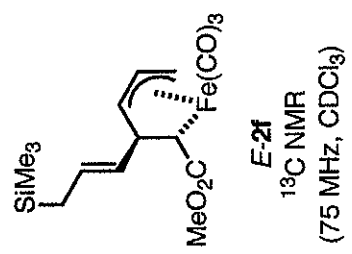
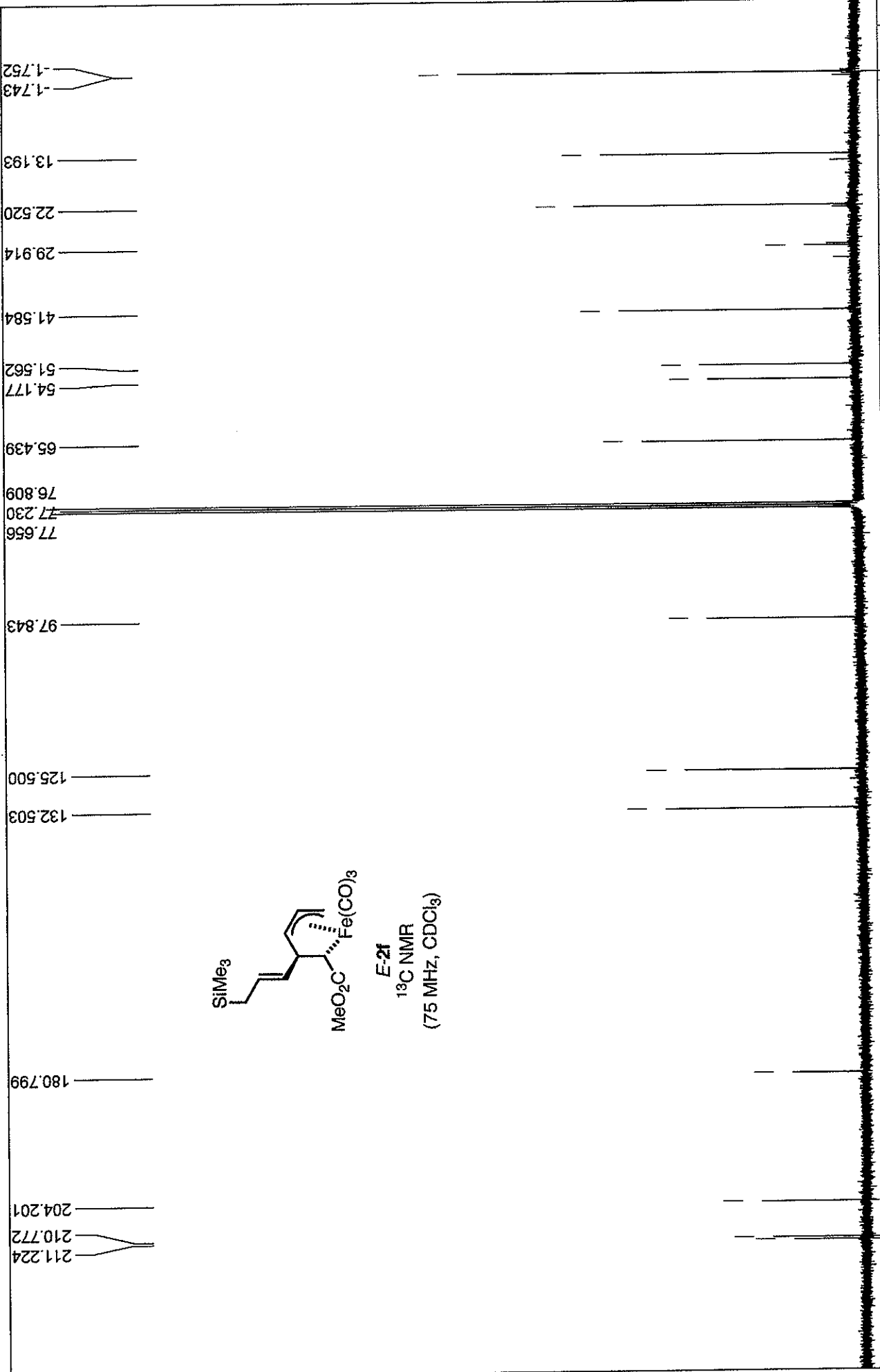
**E-2f**

<sup>1</sup>H NMR

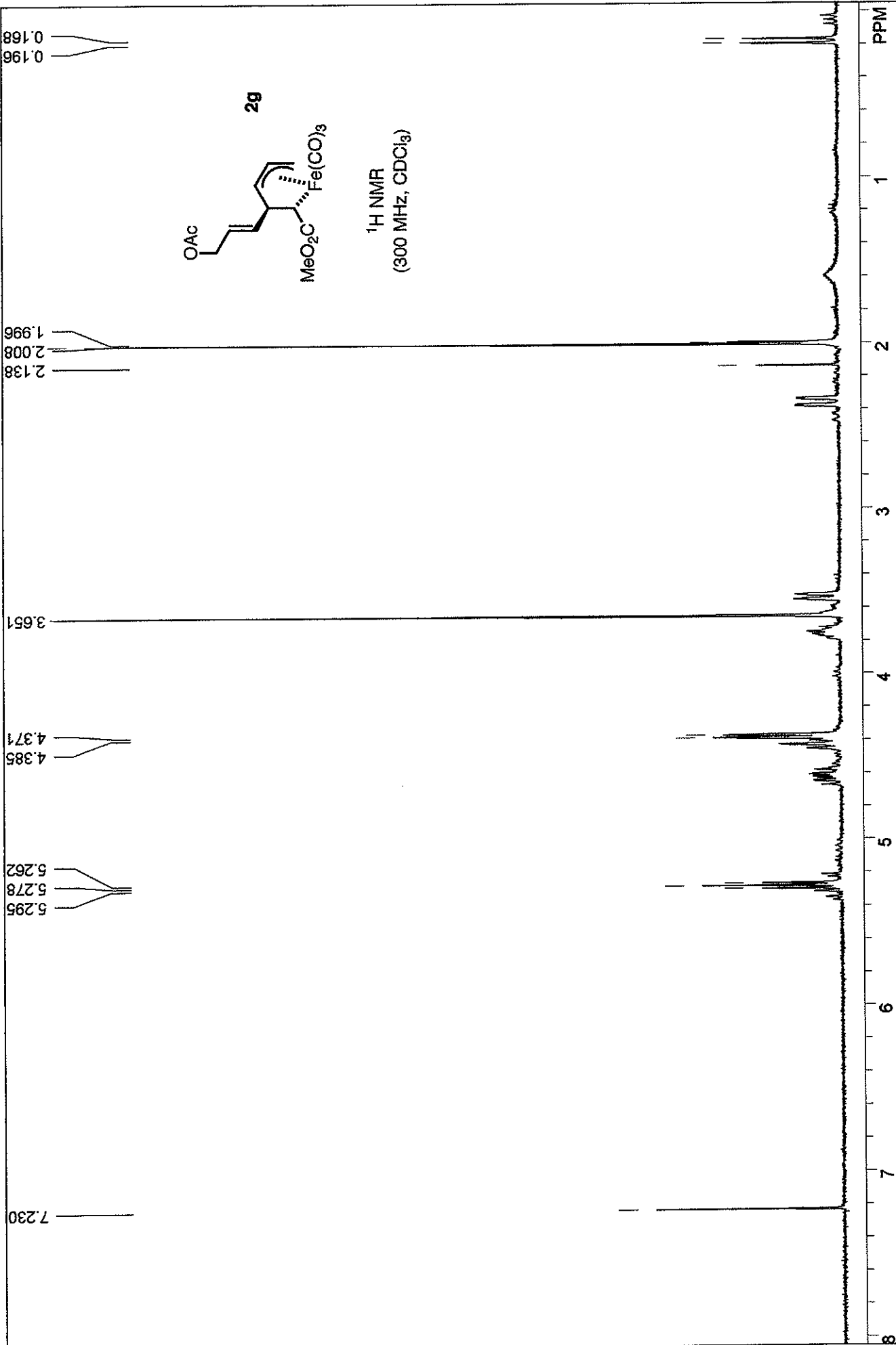
(300 MHz, CDCl<sub>3</sub>)



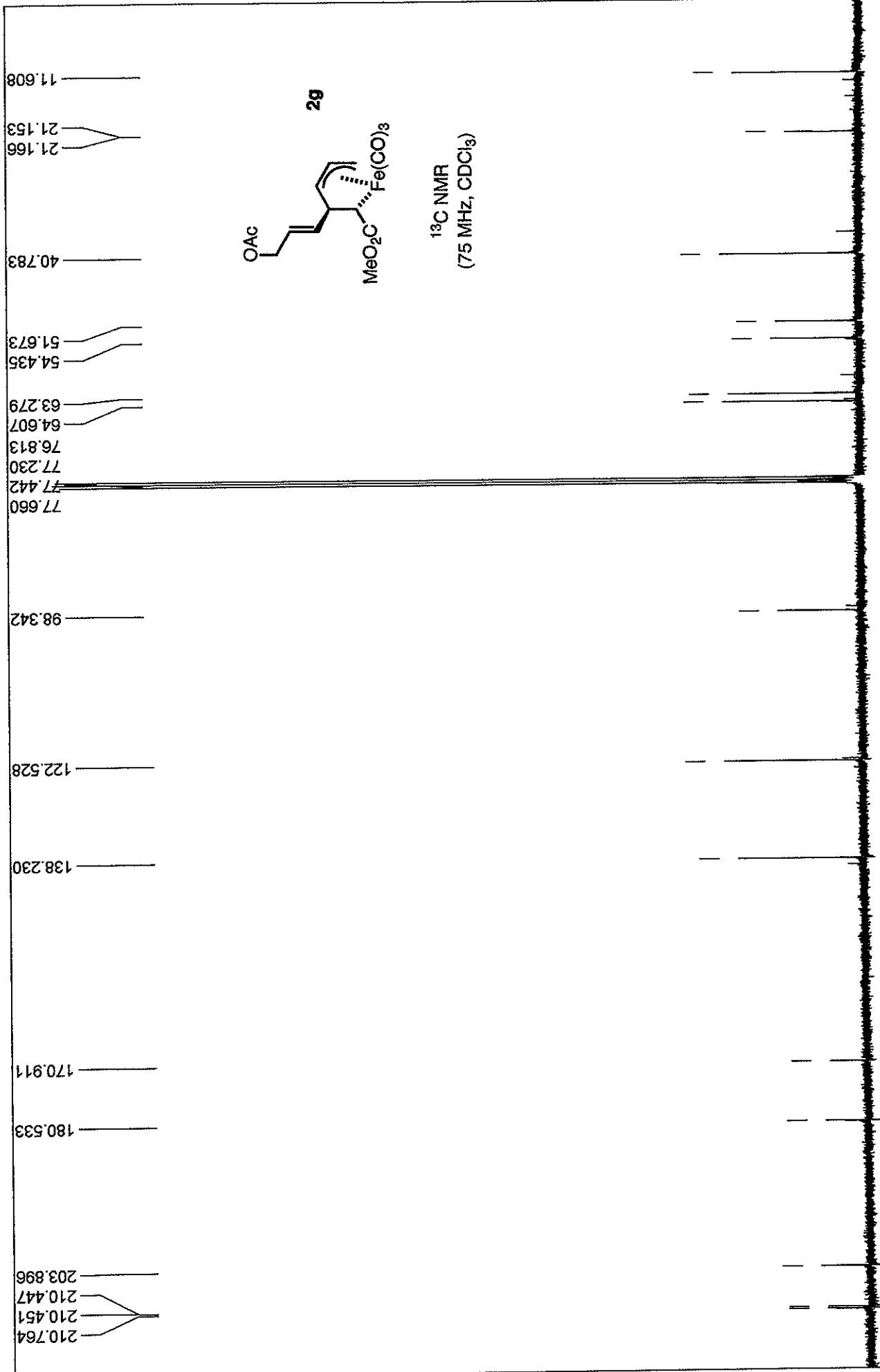
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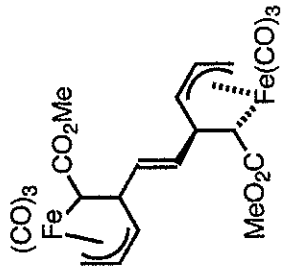
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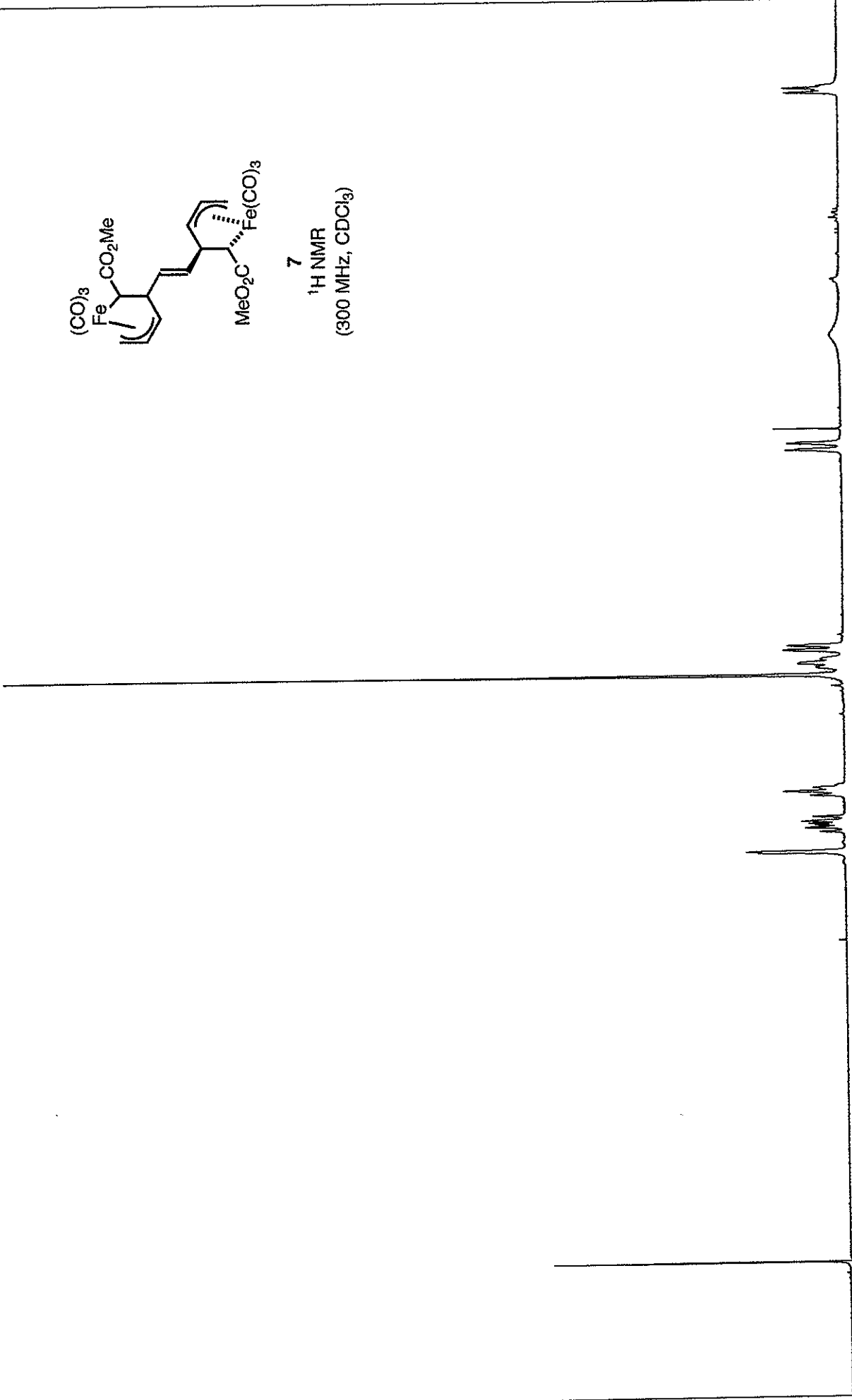
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	PW: 6.3 usec	PD: 1.0 sec	WinNuts - \$rkp026.fid



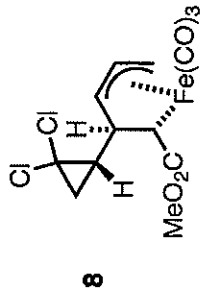
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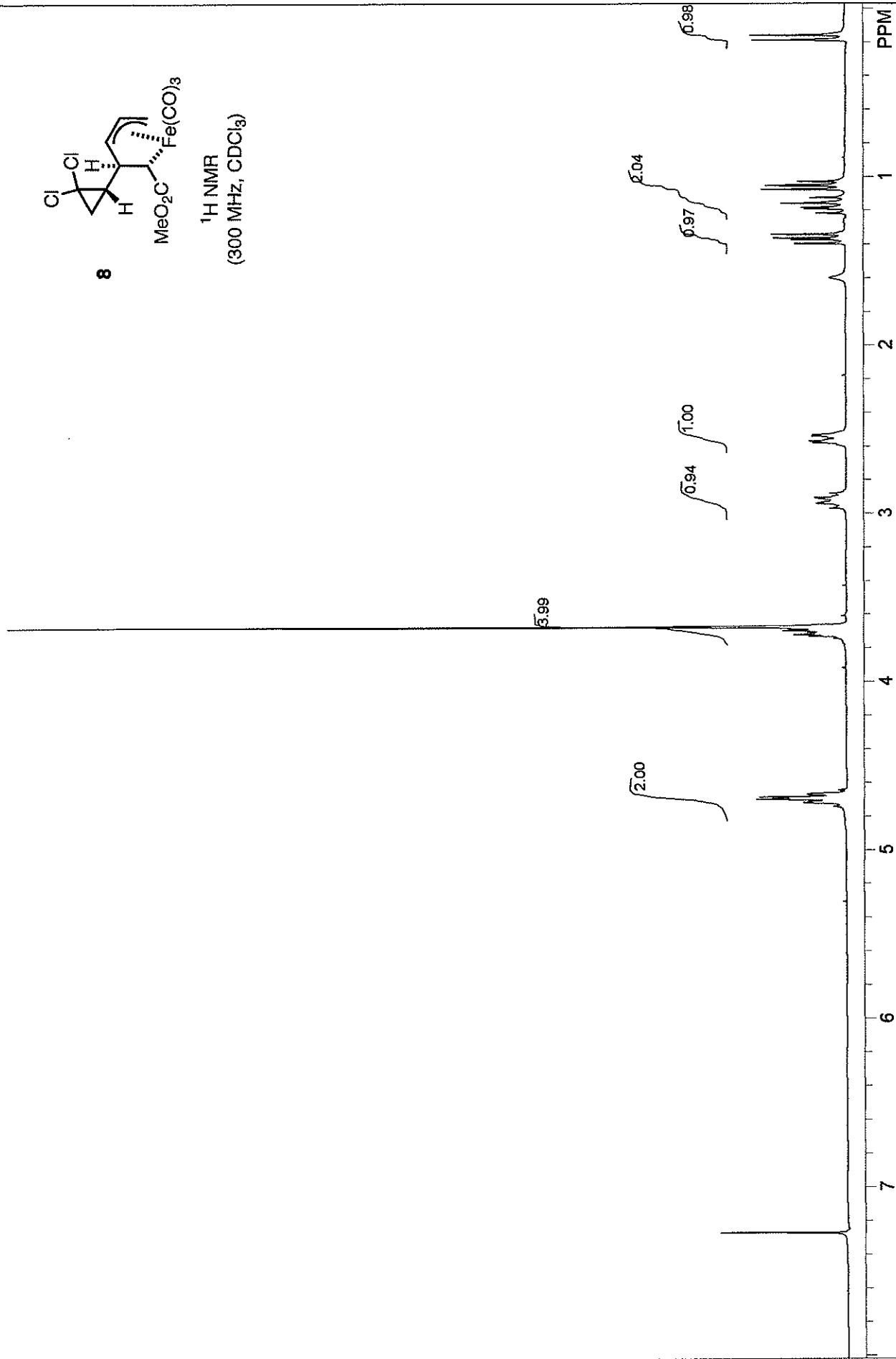
7  
<sup>1</sup>H NMR  
(300 MHz, CDCl<sub>3</sub>)



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F2: 75.479	NA: 8	
EX: s2pul	PD: 1.0 sec	LB: 0.0
	PW: 6.3 ussec	



<sup>1</sup>H NMR  
(300 MHz, CDCl<sub>3</sub>)



STANDARD 1H OBSERVE:blank.jine

F1: 300.136

F2: 75.476

SWI: 4803

PW: 6.3 us

OF1: 1804.5

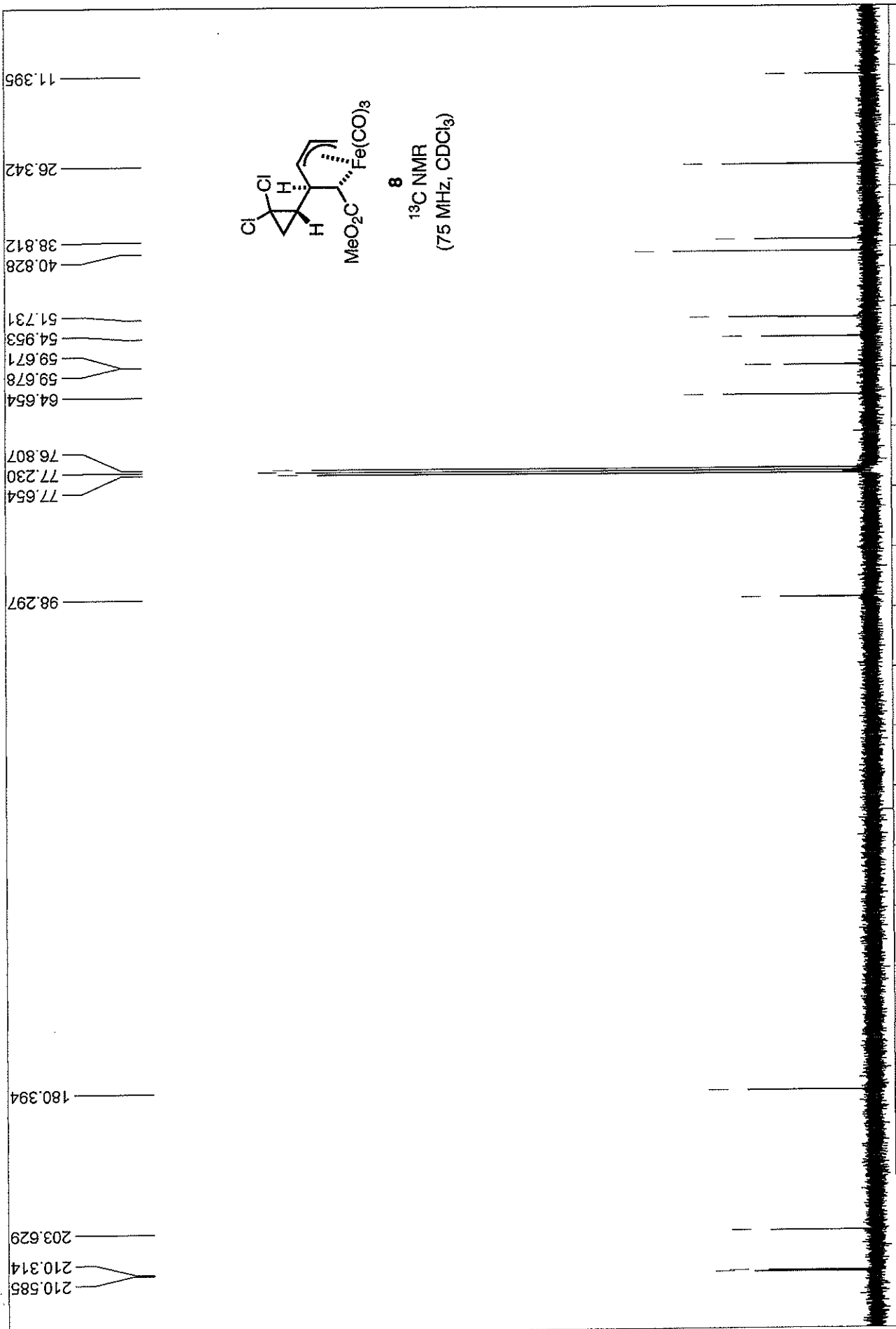
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PTS1d: 9596 . 16384

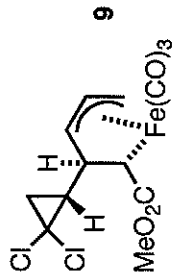
USER: -- DATE: Apr 20 2007

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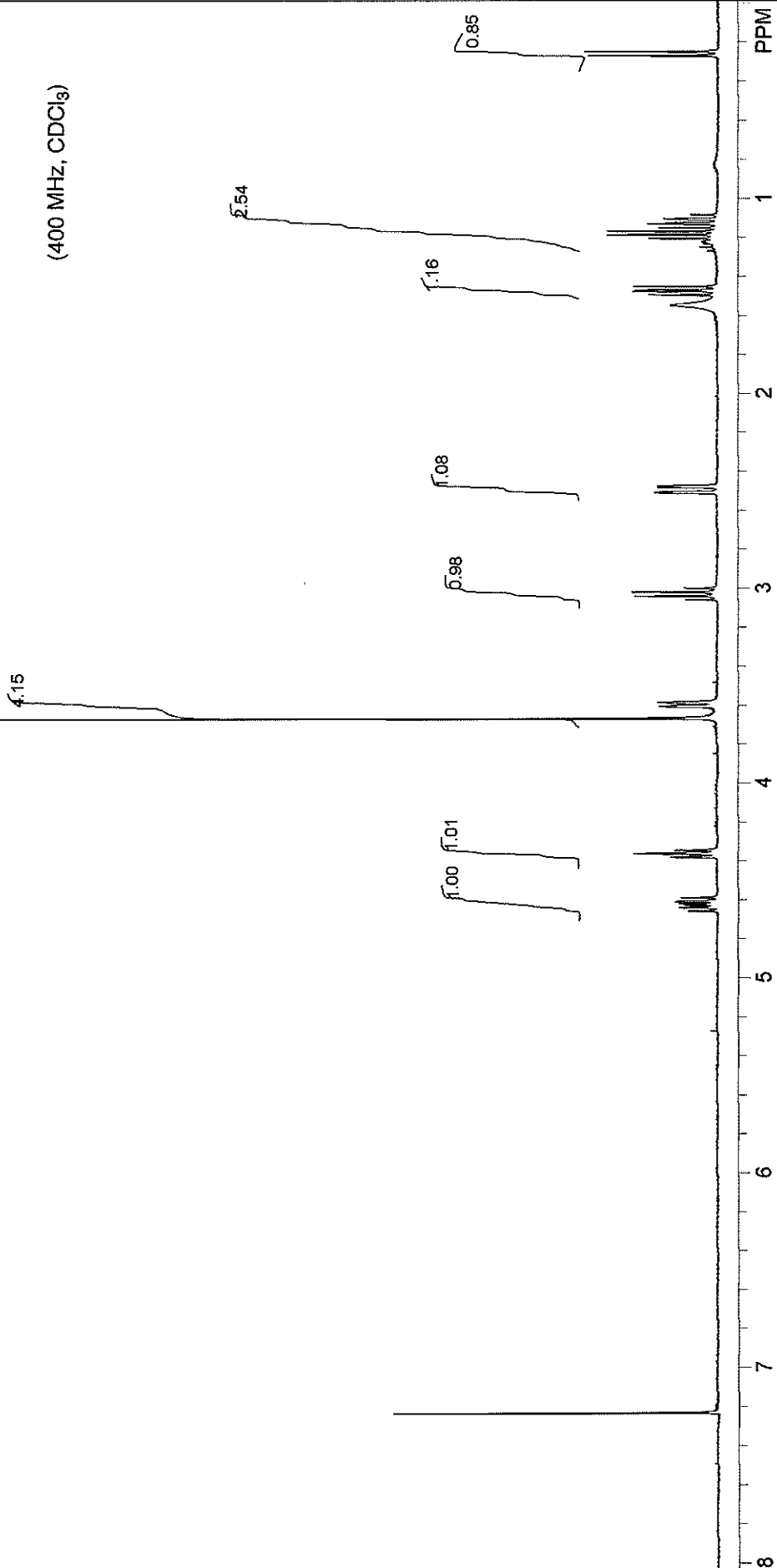


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EX: s2pul			



<sup>1</sup>H NMR

(400 MHz, CDCl<sub>3</sub>)

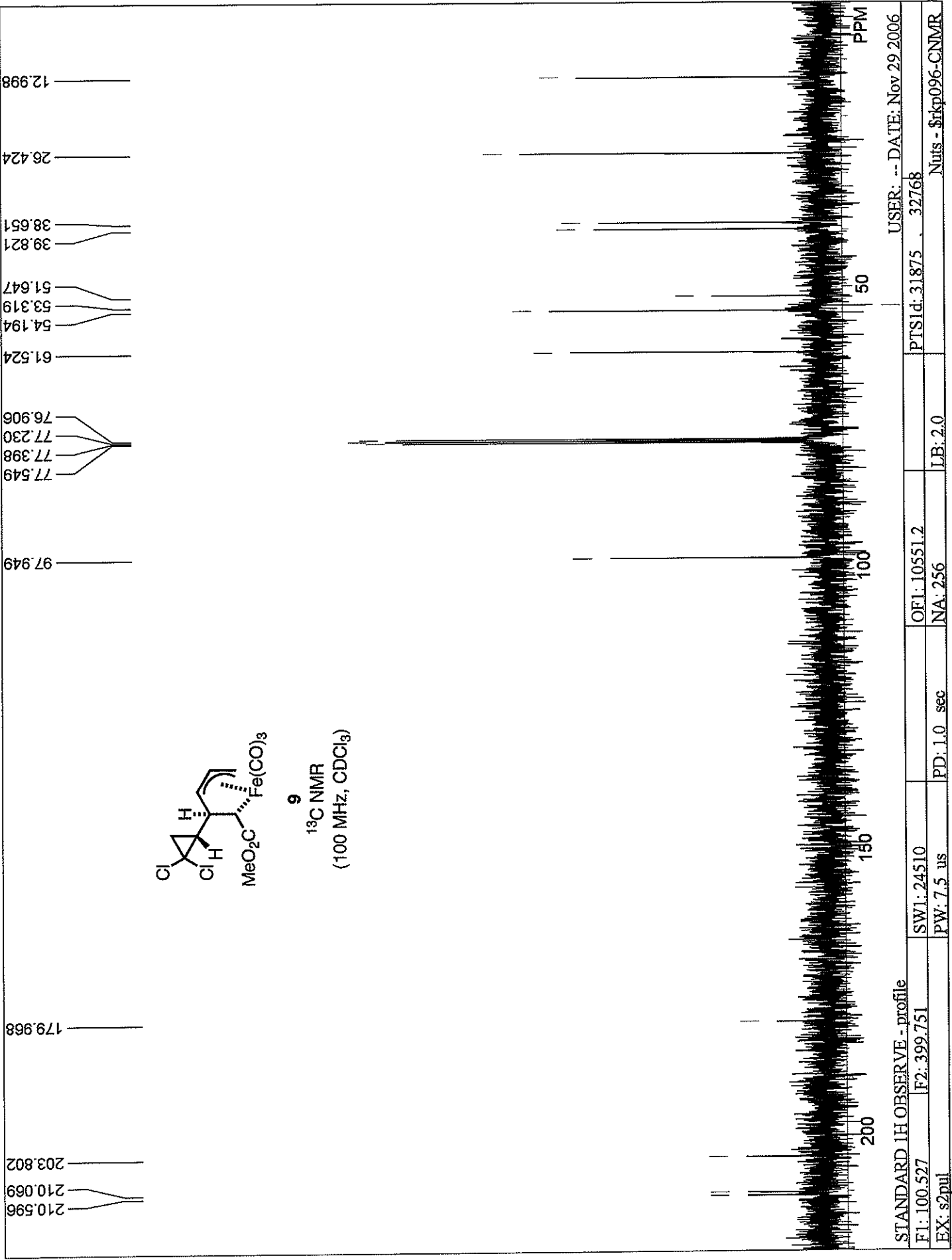


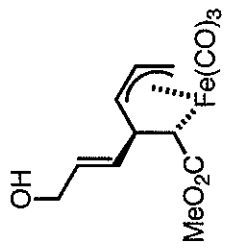
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 EX: s2pul

OF1: 2385.5  
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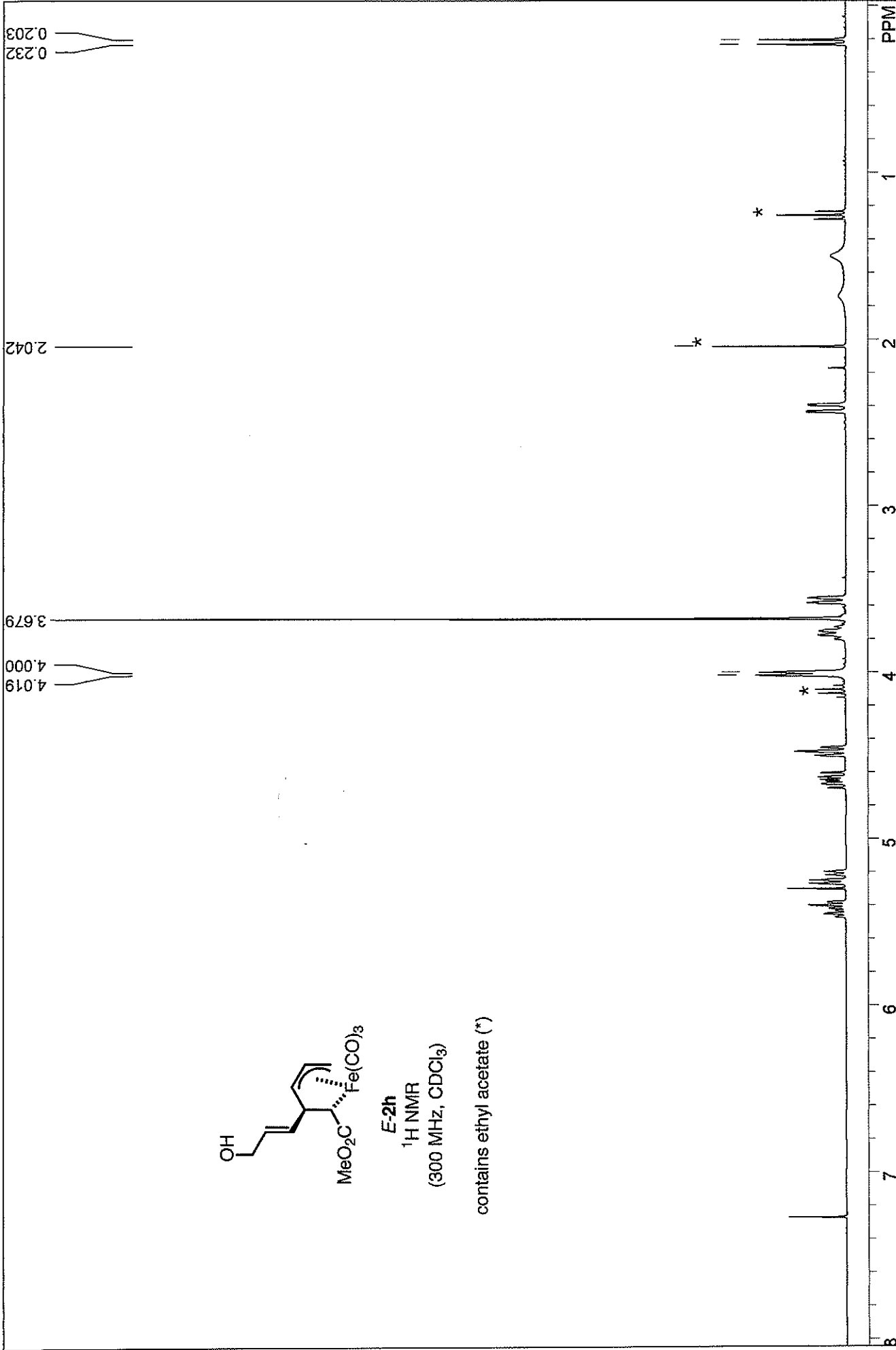
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USER: -- DATE: Apr 17 2007  
 16384  
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E-2h  
<sup>1</sup>H NMR  
 (300 MHz, CDCl<sub>3</sub>)  
 contains ethyl acetate (\*)



STANDARD 1H OBSERVEblank line

F1: 300.145

F2: 75.479

SW1: 4810

PW: 6.3 usec

NA:

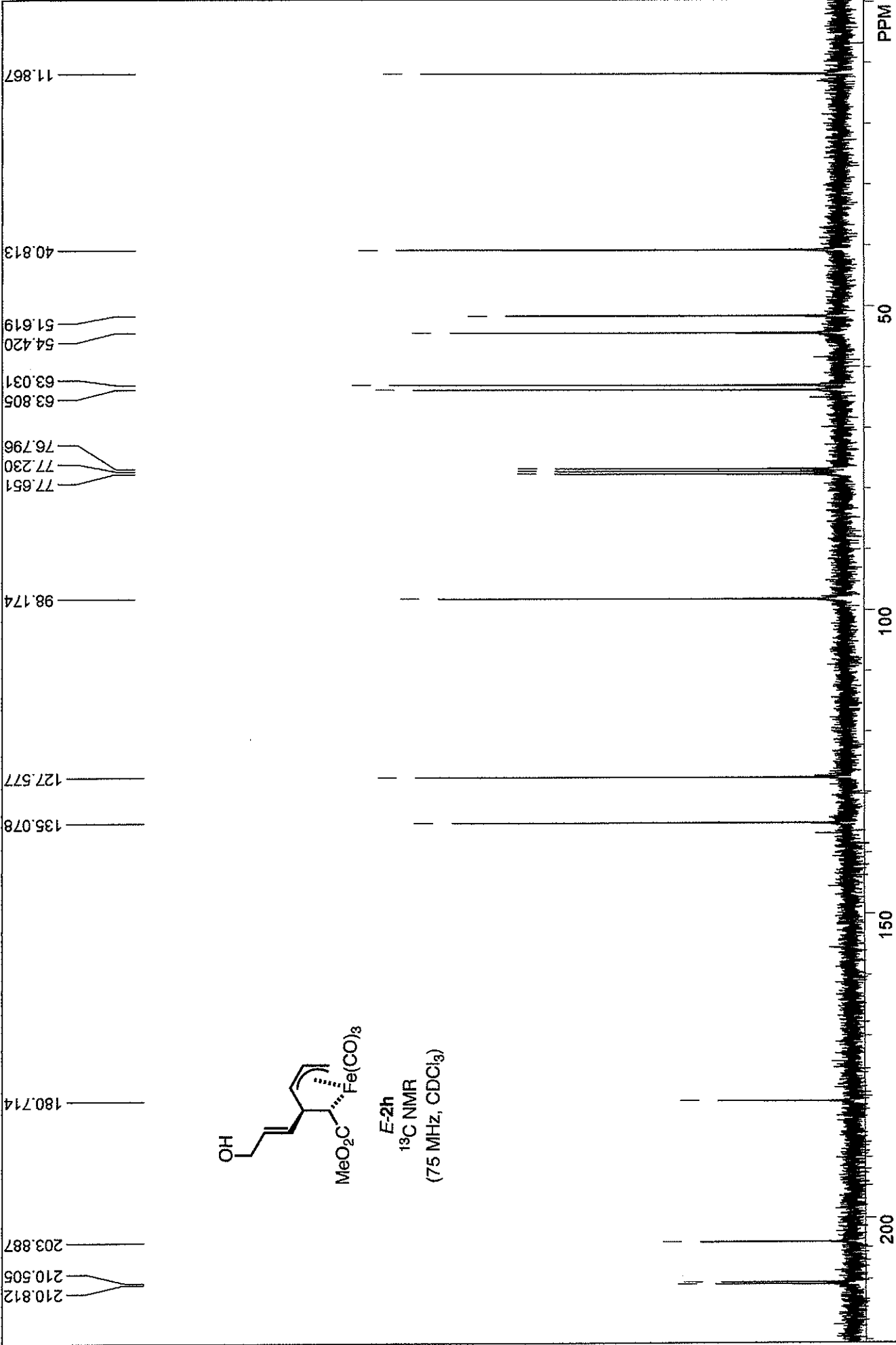
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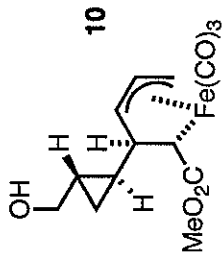
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PTS1d: 16384

USER: -- DATE: Aug 8 2006

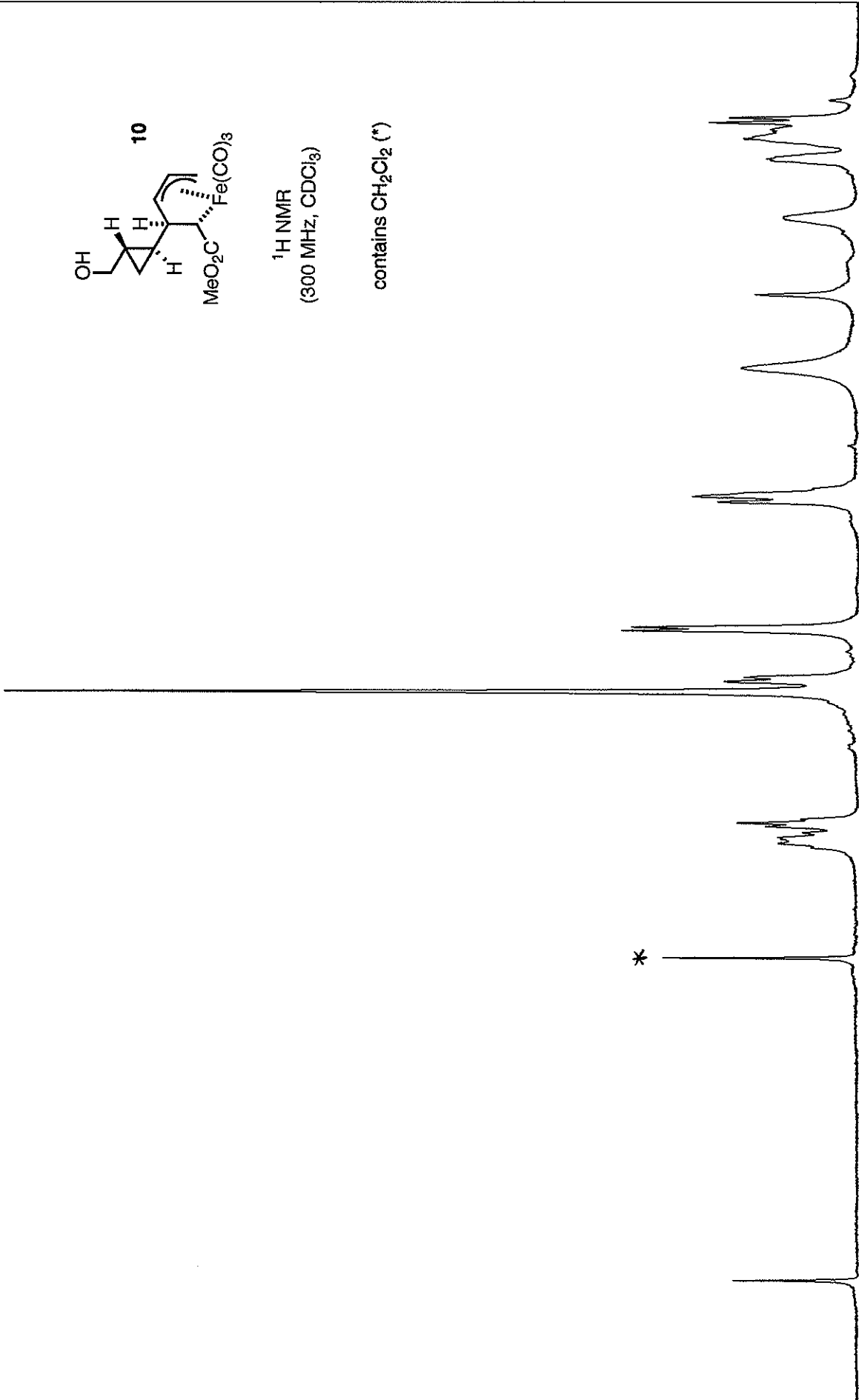
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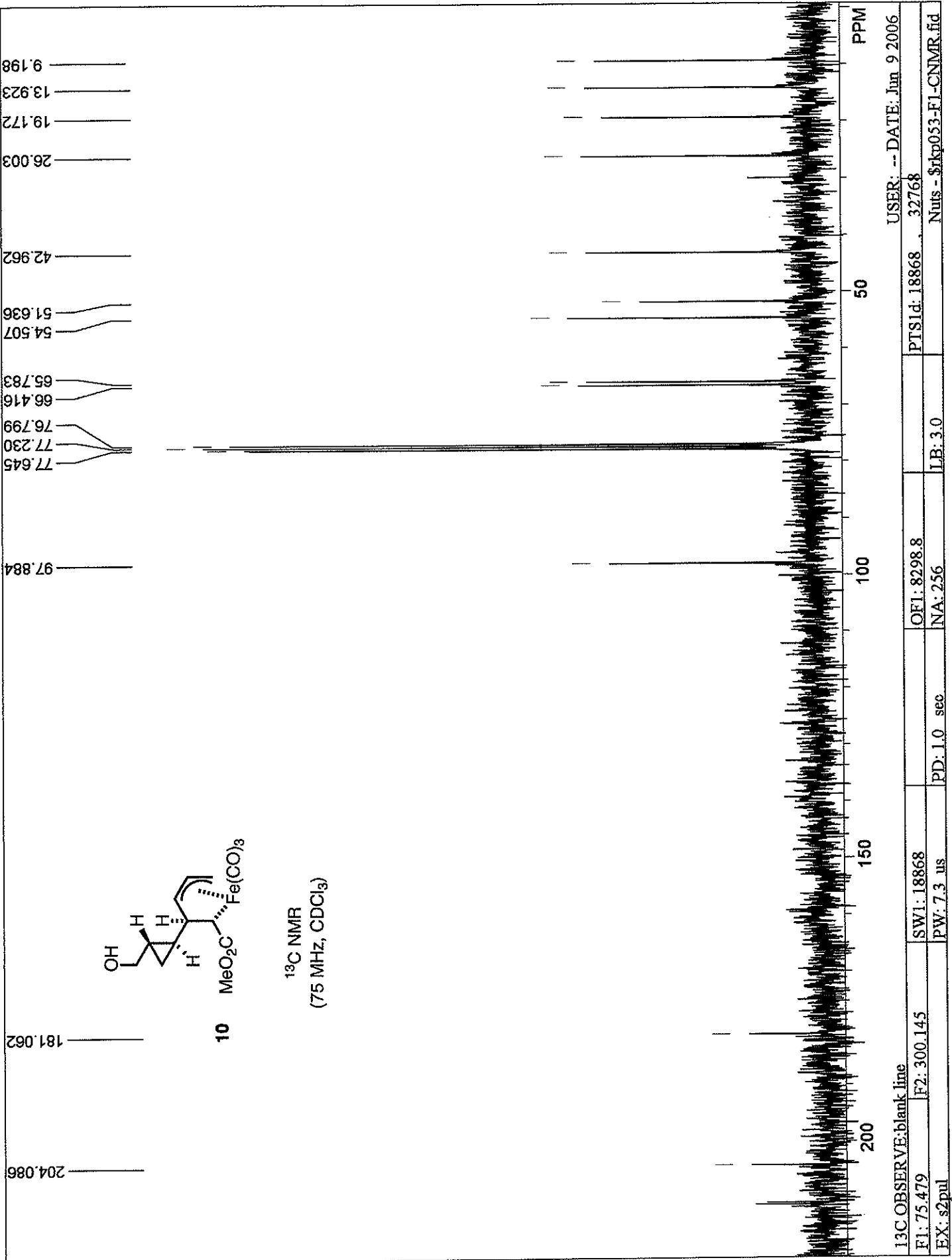


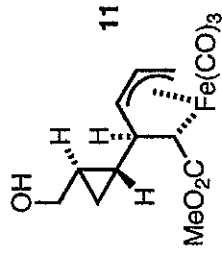
<sup>1</sup>H NMR  
(300 MHz, CDCl<sub>3</sub>)

contains CH<sub>2</sub>Cl<sub>2</sub> (\*)



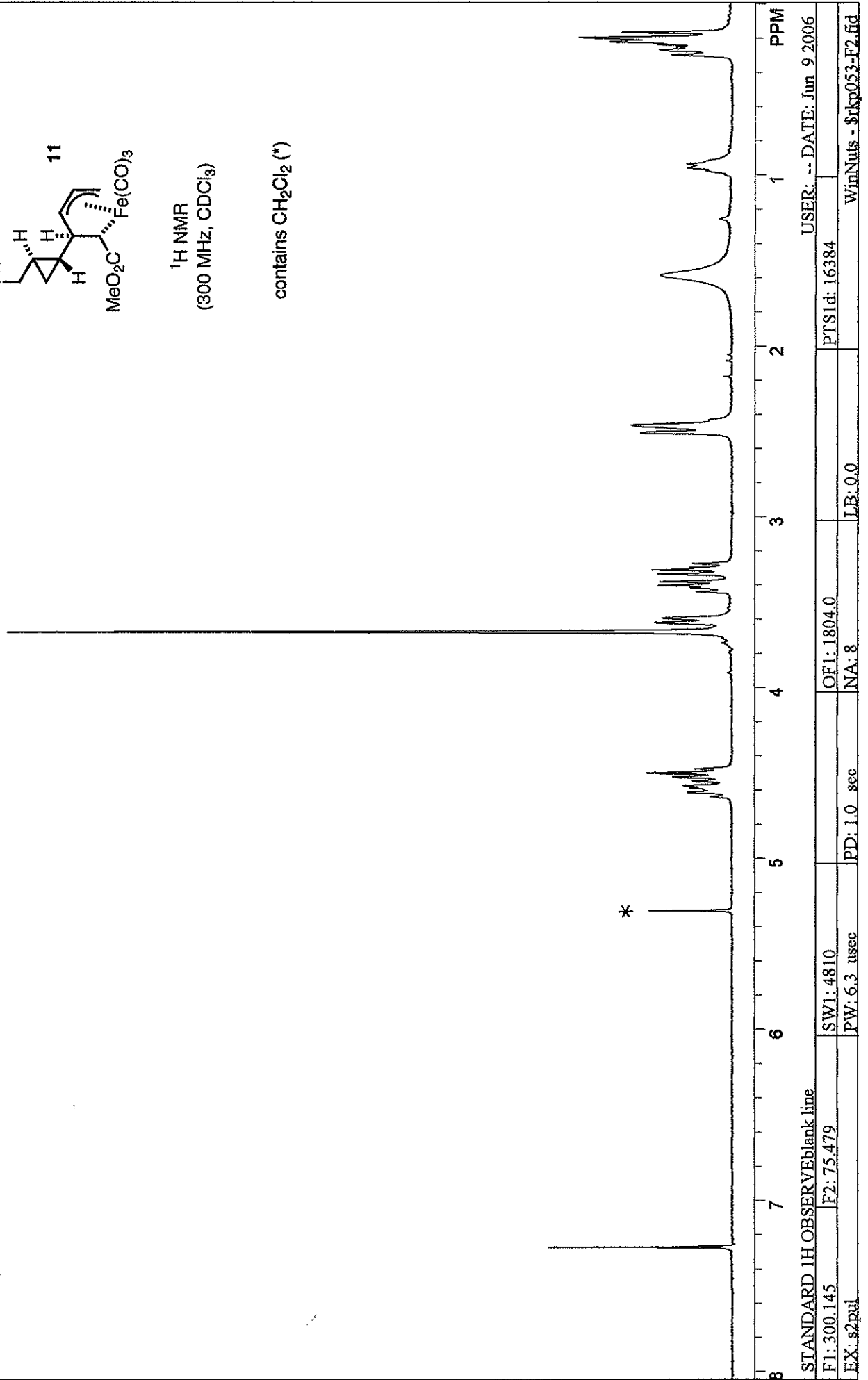
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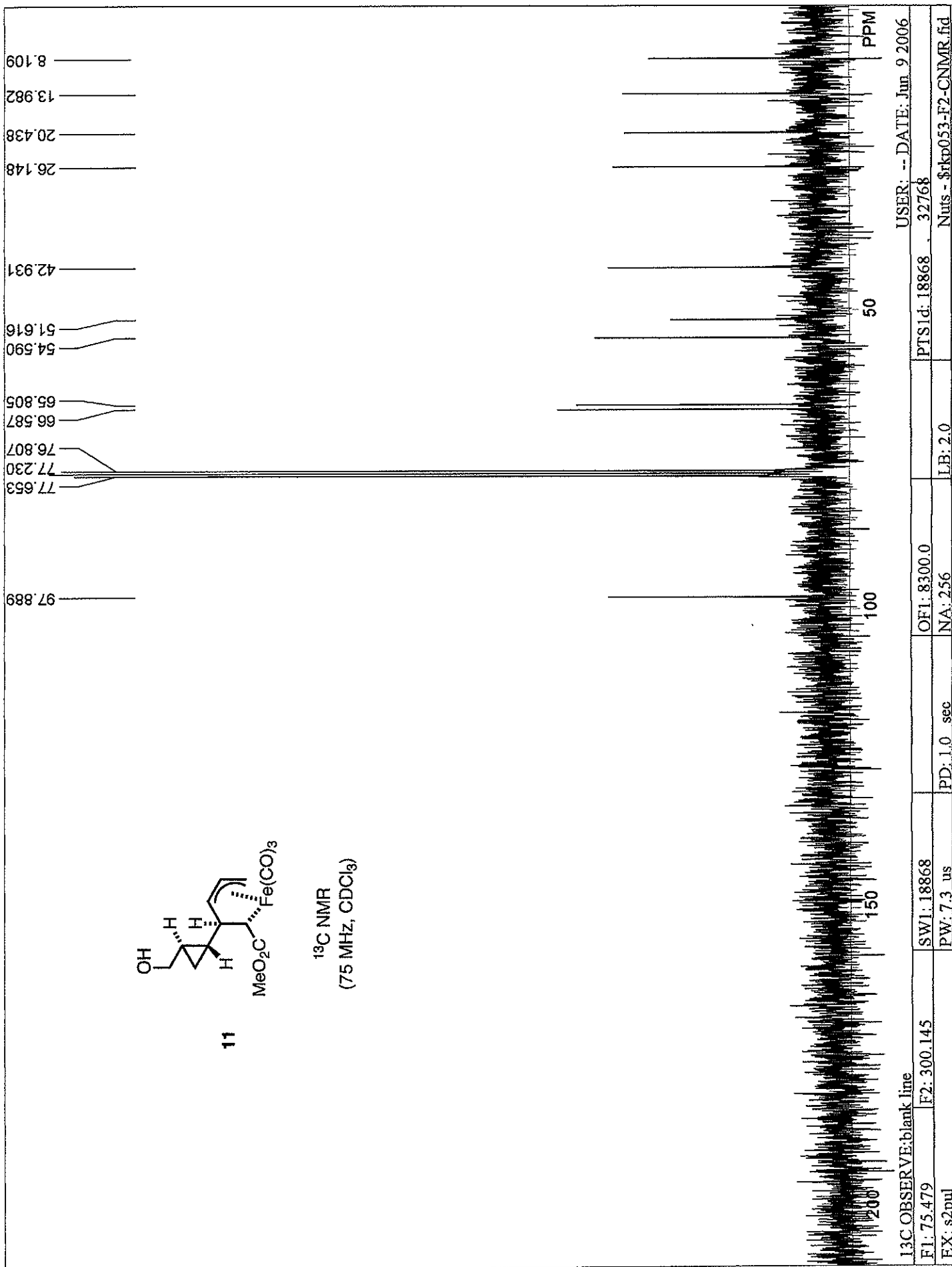


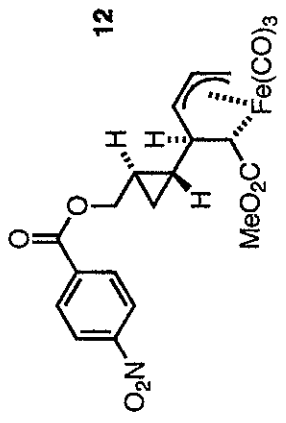
<sup>1</sup>H NMR  
(300 MHz, CDCl<sub>3</sub>)

contains CH<sub>2</sub>Cl<sub>2</sub> (\*)

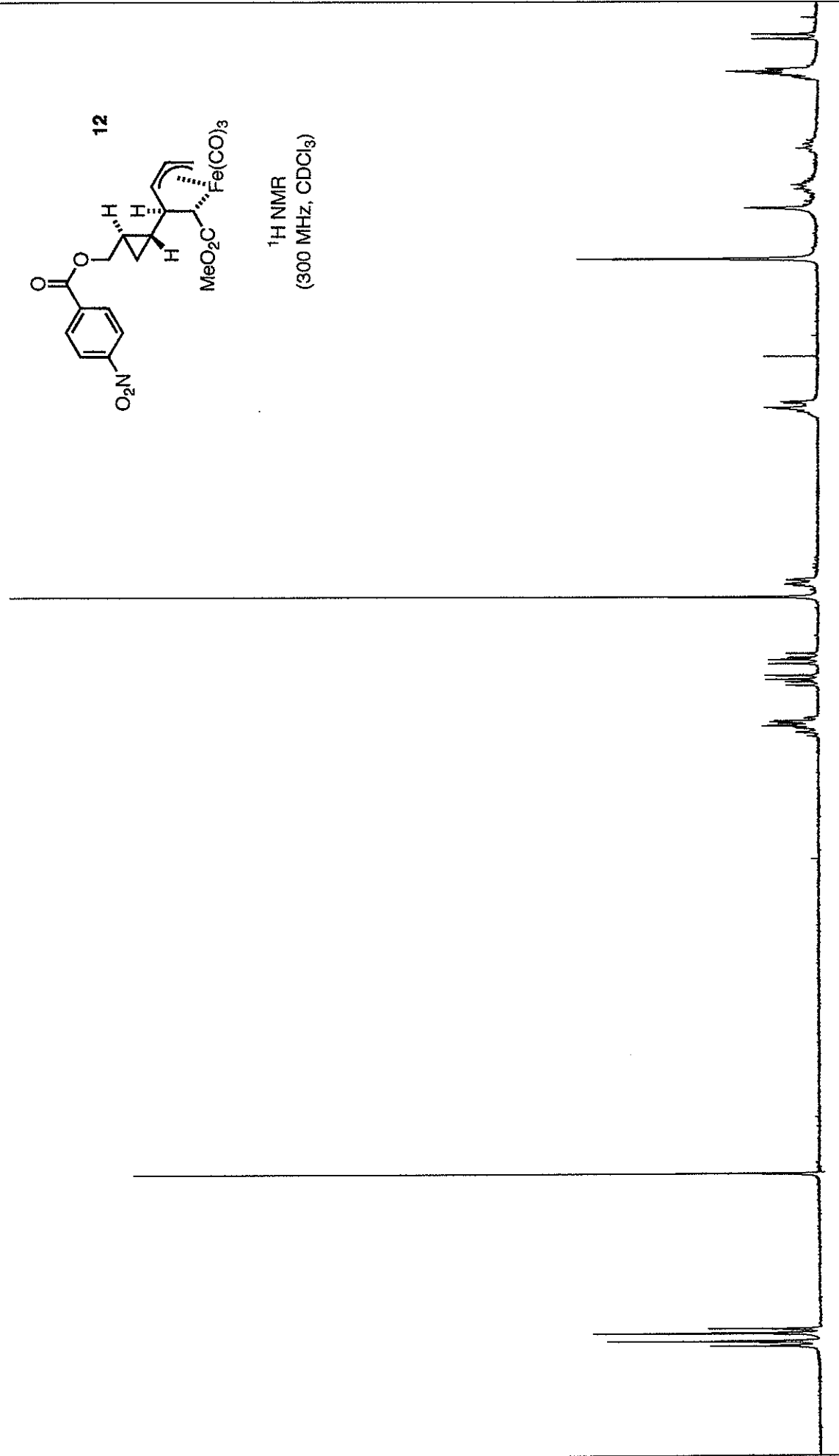




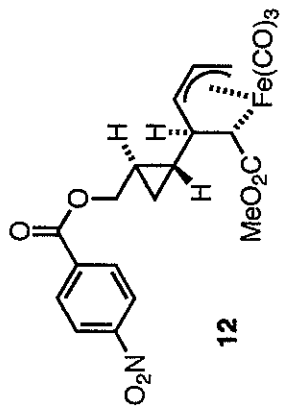
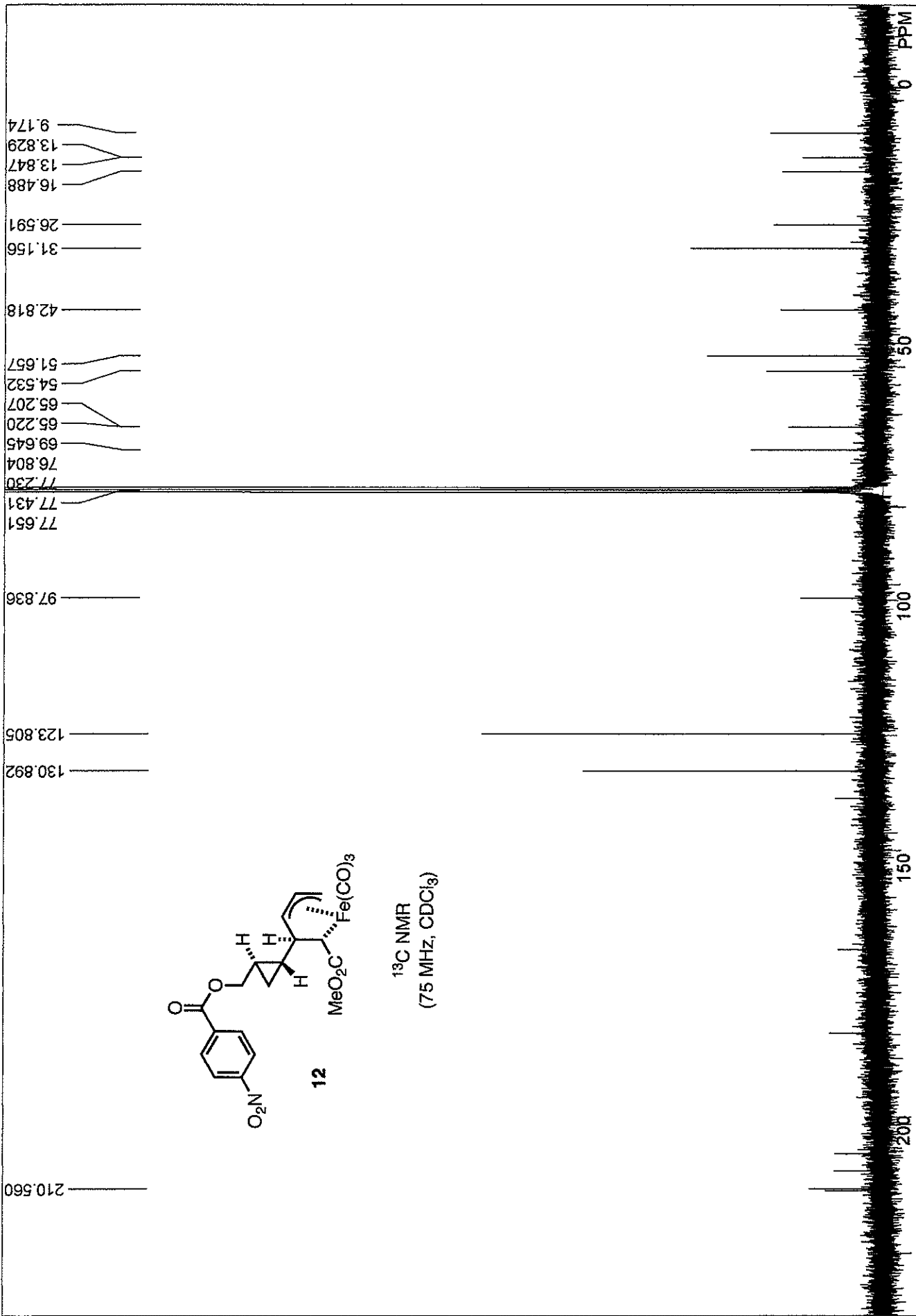




<sup>1</sup>H NMR  
(300 MHz, CDCl<sub>3</sub>)

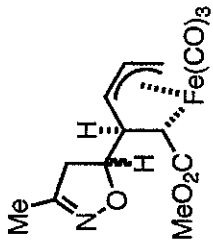


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PW: 6.3 usec	NA: 8		
PD: 1.0 sec			

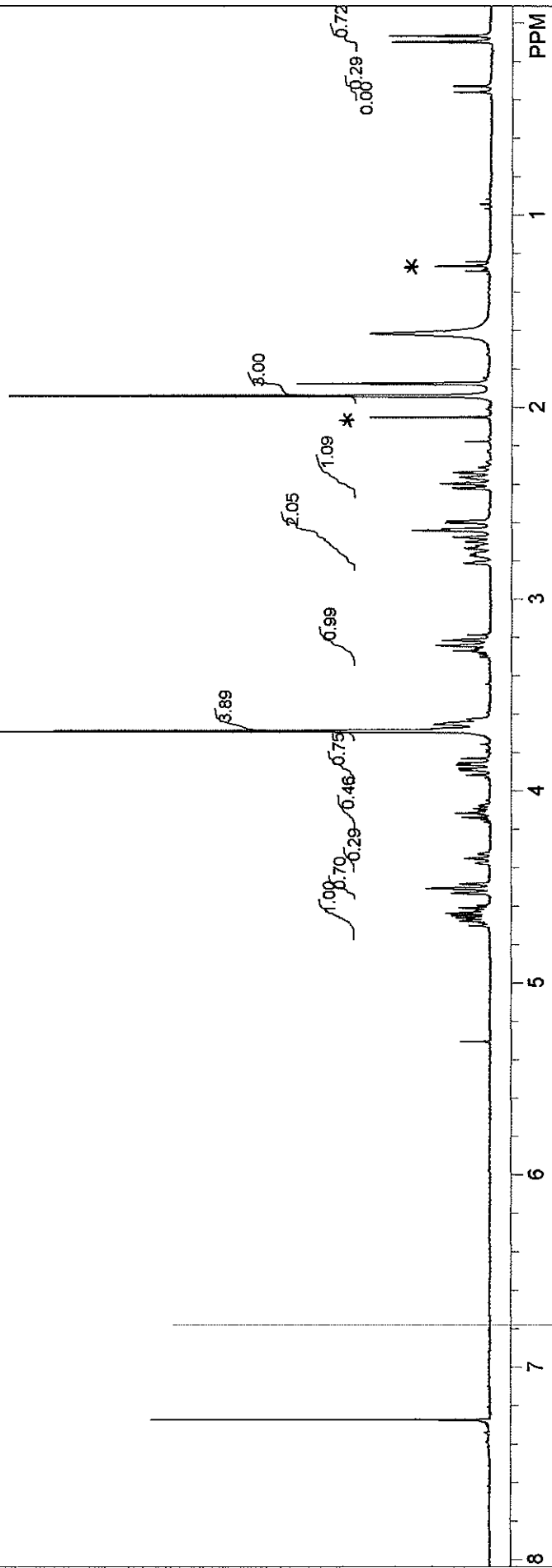


<sup>13</sup>C NMR  
(75 MHz, CDCl<sub>3</sub>)

13C OBSERVE: blank line		USER: -- DATE: Sep 27 2006	
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EX: s2pul	PW: 7.3 us	OF1: 8284.6	LB: 0.0
	PD: 1.0 sec	NA:	Nuts - \$rkp056-CNMR.fid

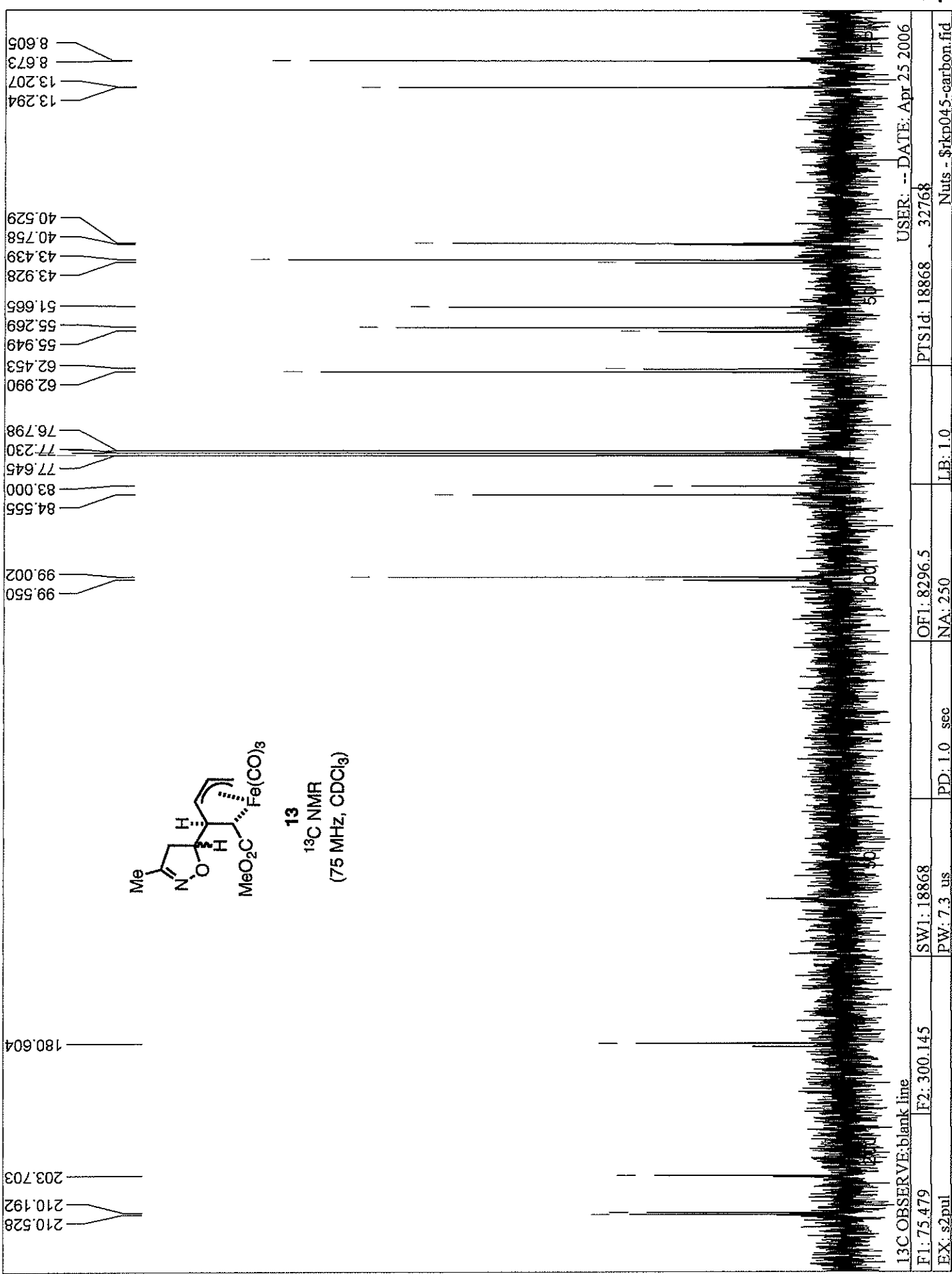


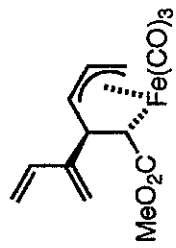
**13**  
<sup>1</sup>H NMR  
 (300 MHz, CDCl<sub>3</sub>)  
 contains EtOAc (\*)



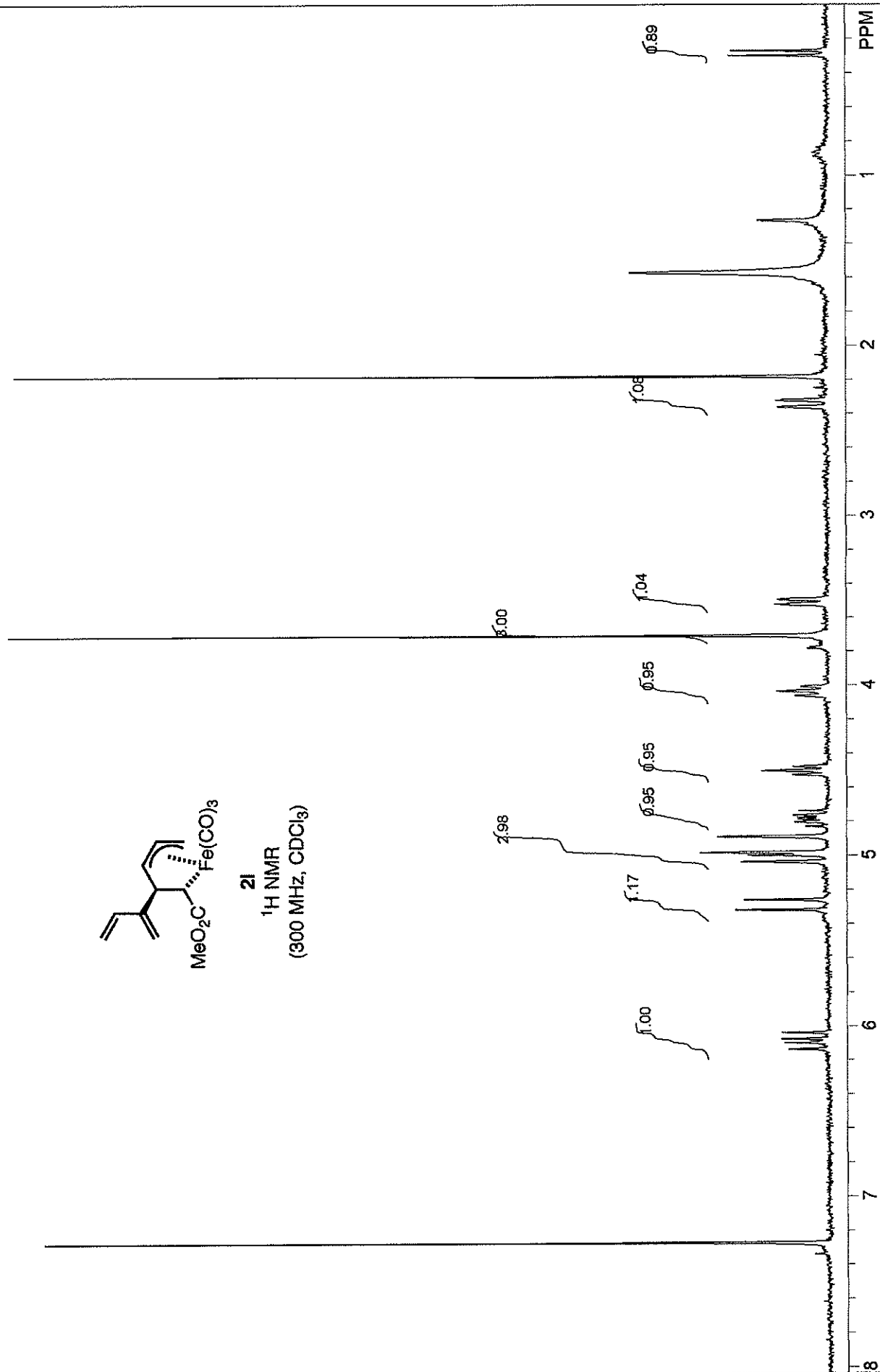
STANDARD 1H OBSERVE: blank line

FI: 300.145	F2: 75.479	SW1: 4810	OF1: 1803.9	PTS1d: 14409	16384	USER: -- DATE: Apr 17 2006
EX: s2pul	PW: 6.3 us	PD: 1.0 sec	NA: 8	LB: 0.0	Nuts - \$rpk045-column.fid	





**21**  
<sup>1</sup>H NMR  
 (300 MHz, CDCl<sub>3</sub>)



STANDARD 1H OBSERVE:blank line

F1: 300.136 F2: 75.476 SW1: 4810

EX: s2pul PW: 6.3 us PD: 1.0 sec

OF1: 1803.9

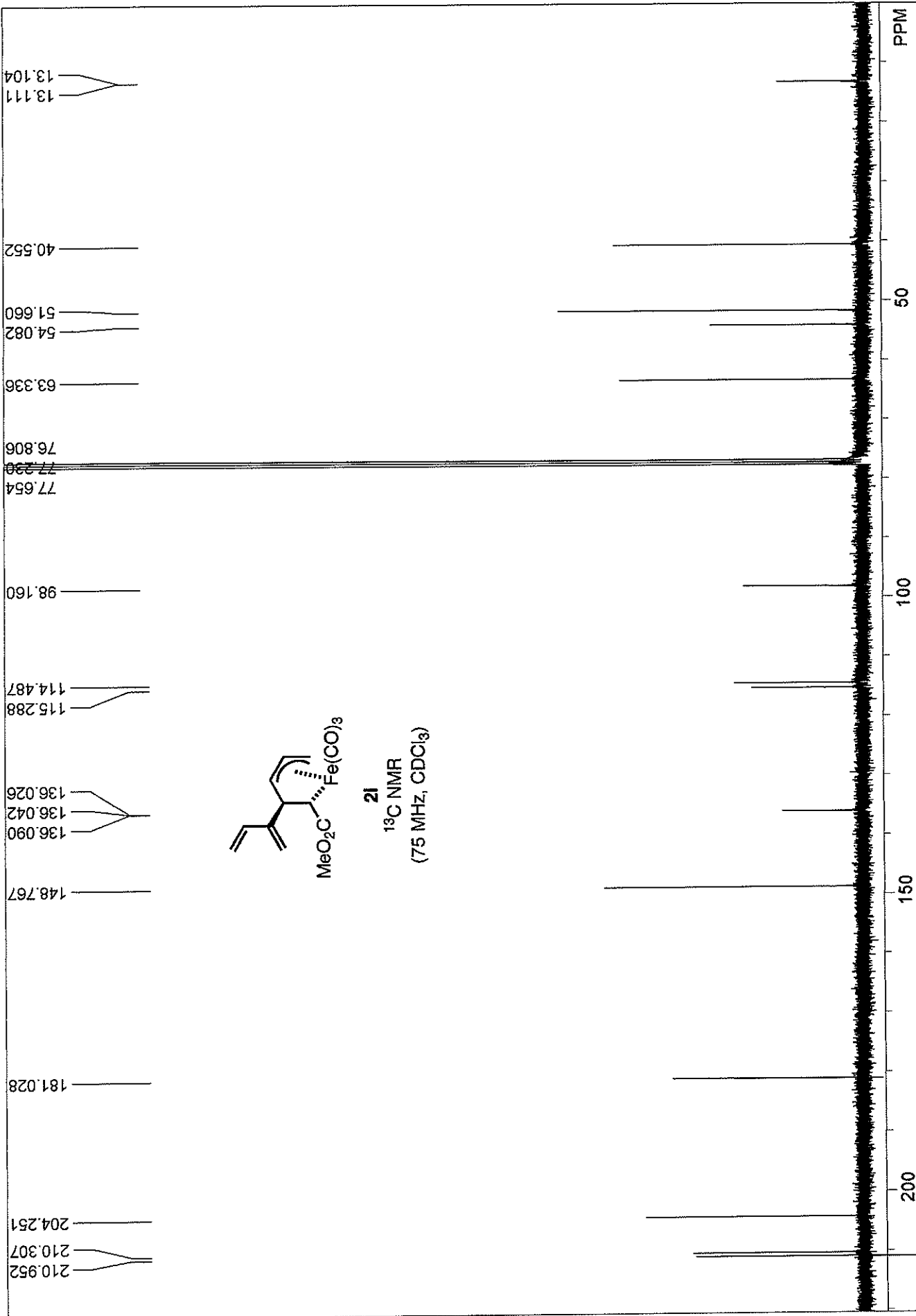
NA: 8

LB: 0.5

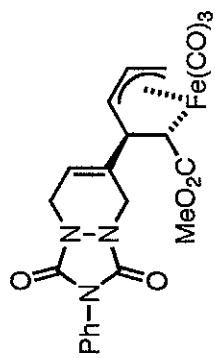
PTS1d: 14430 16384

Nuts: \$1w17-product2.fid

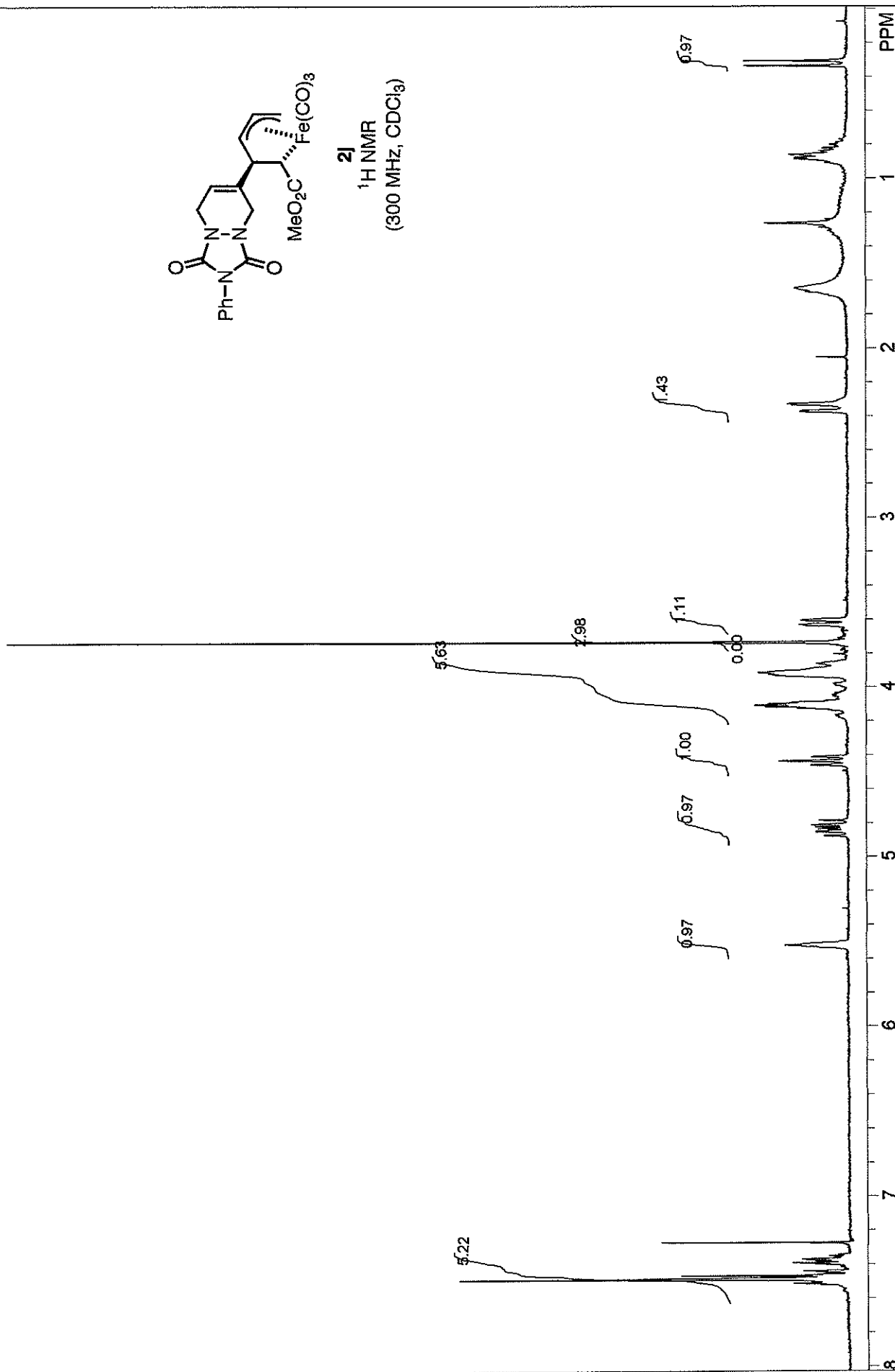
USER: -- DATE: Jan 30 2007



13C OBSERVE: blank line  
 F1: 75.477 F2: 300.135 SW1: 18868 PD: 1.0 sec OF1: 8300.3 LB: 0.0  
 EX: s2pul PW: 7.3 us NA: 16384  
 USER: -- DATE: Mar 18 2007  
 PTSId: 34246 65536  
 Nuts - \$lw17C13.fid

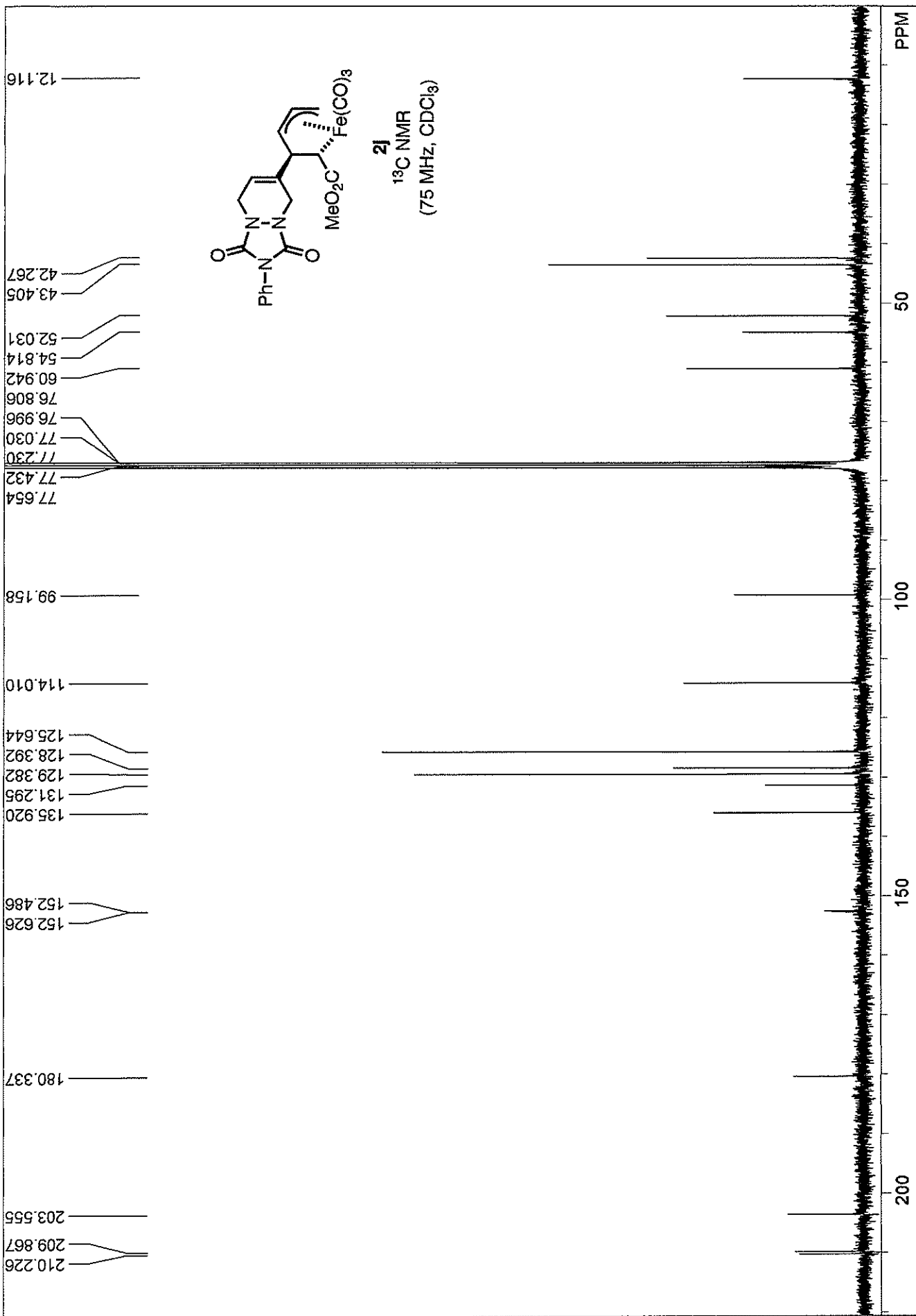


**2j**  
<sup>1</sup>H NMR  
 (300 MHz, CDCl<sub>3</sub>)



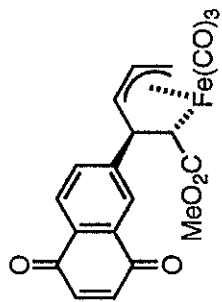
STANDARD 1H OBSERVE: blank line		USER: -- DATE: Mar 24 2007	
F1: 300.136	F2: 75.476	OF1: 1804.1	PTS1d: 9596 , 16384
EX: s2pul	PW: 6.3 us	NA: 8	LB: 0.0
	PD: 1.0 sec		Nuts - \$1w22H1.fid





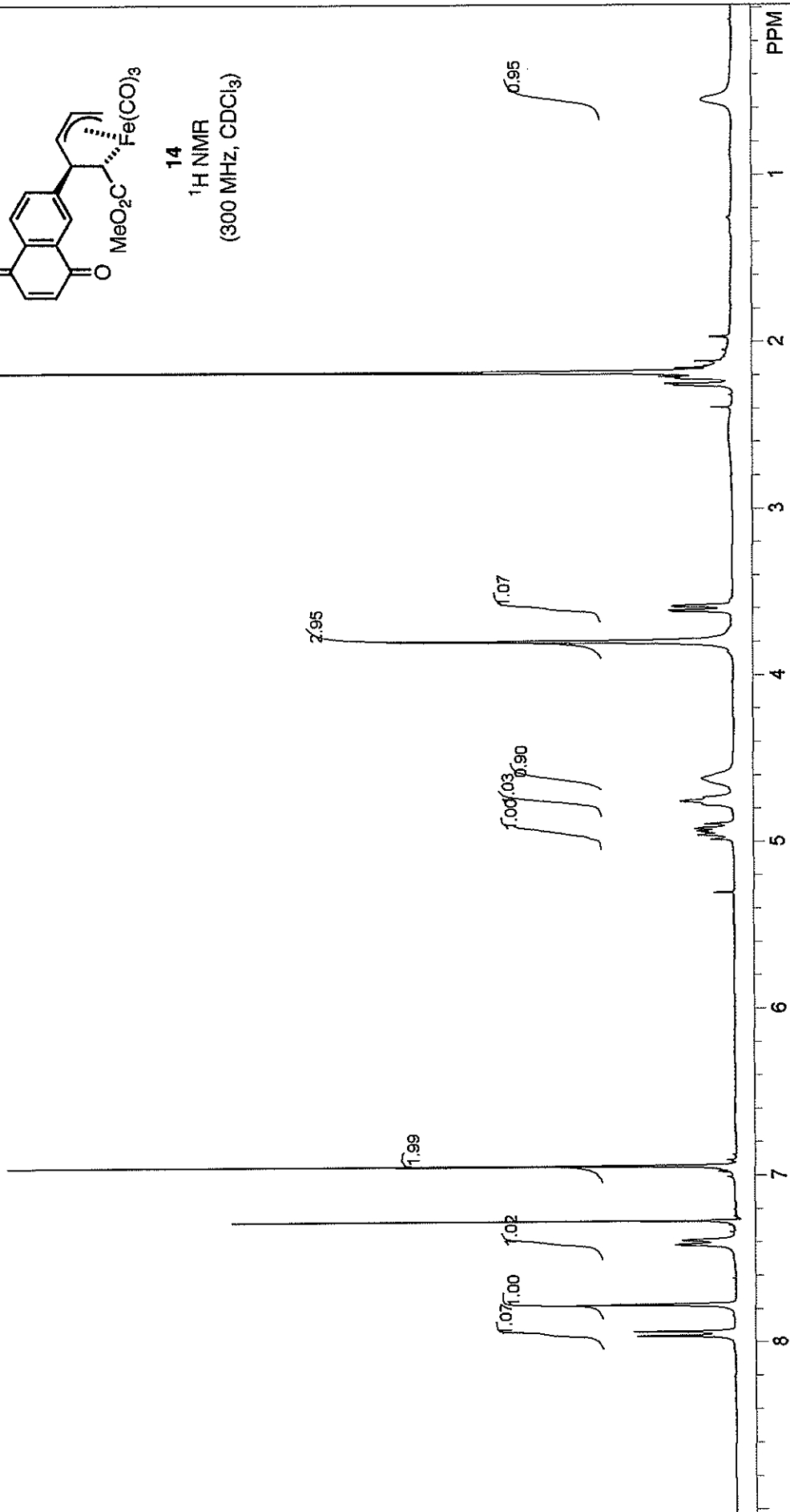
13C OBSERVE, blank line

F1: 75.477	F2: 300.135	SW1: 18868	OF1: 8299.8	PTSD: 34246	USER: -- DATE: Sep 1 2007
EX: s2pul	PW: 7.3 us	PD: 1.0 sec	NA: 16000	65536	
			LB: 0.8		Nuts - \$lv22-C13-300.fid



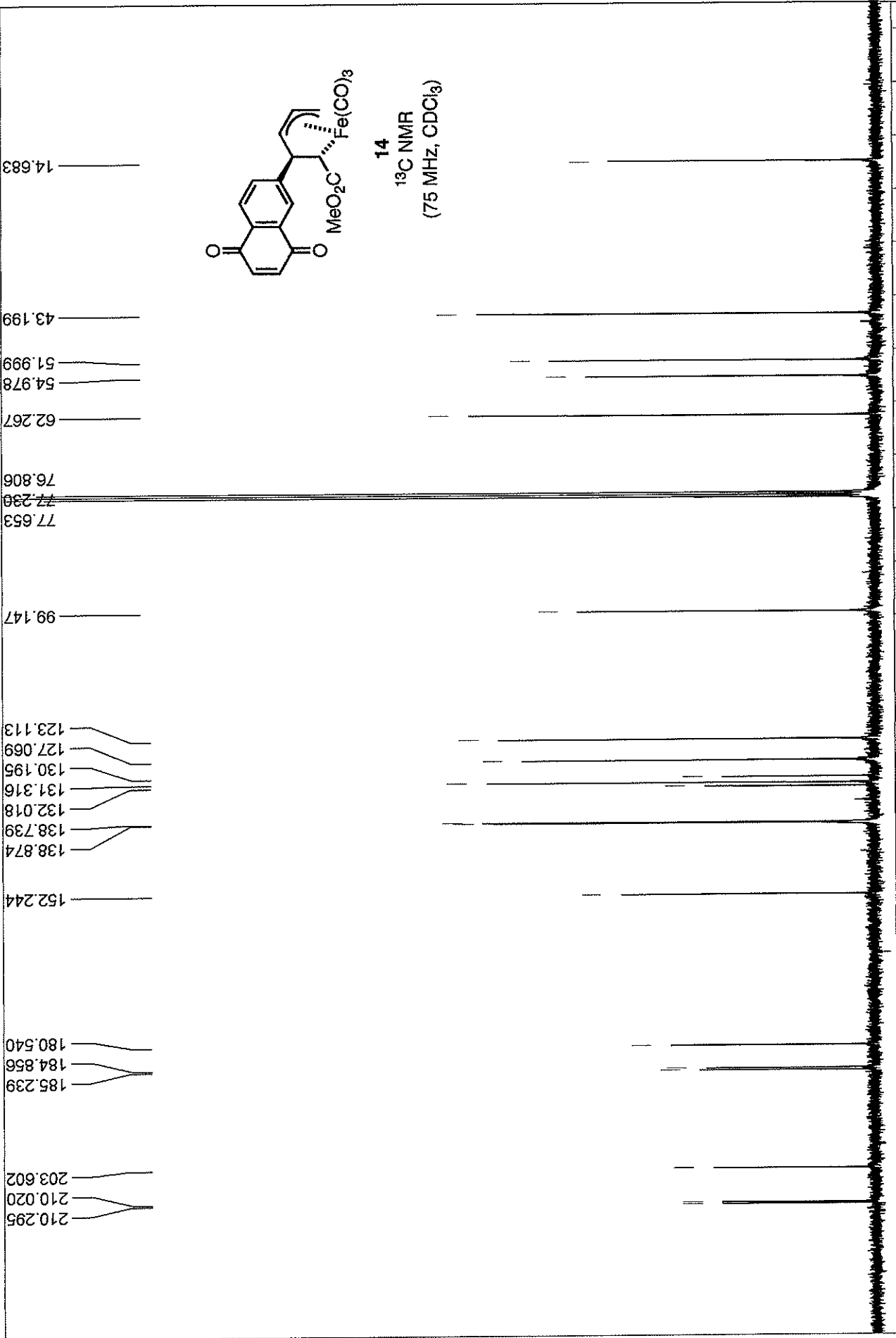
14

<sup>1</sup>H NMR  
(300 MHz, CDCl<sub>3</sub>)

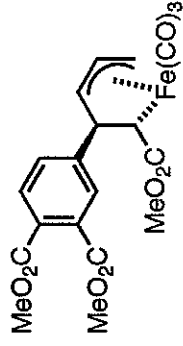


STANDARD 1H OBSERVE:blank line

FI: 300.136	F2: 75.476	SW1: 4803	OF1: 1803.9	PTSID: 9596	DATE: Aug 21 2007
EX: s2pul		PW: 6.3 us	NA: 256	16384	
		PD: 1.0 sec	LB: 0.0		
					Nuts - \$1w66-H1.fid

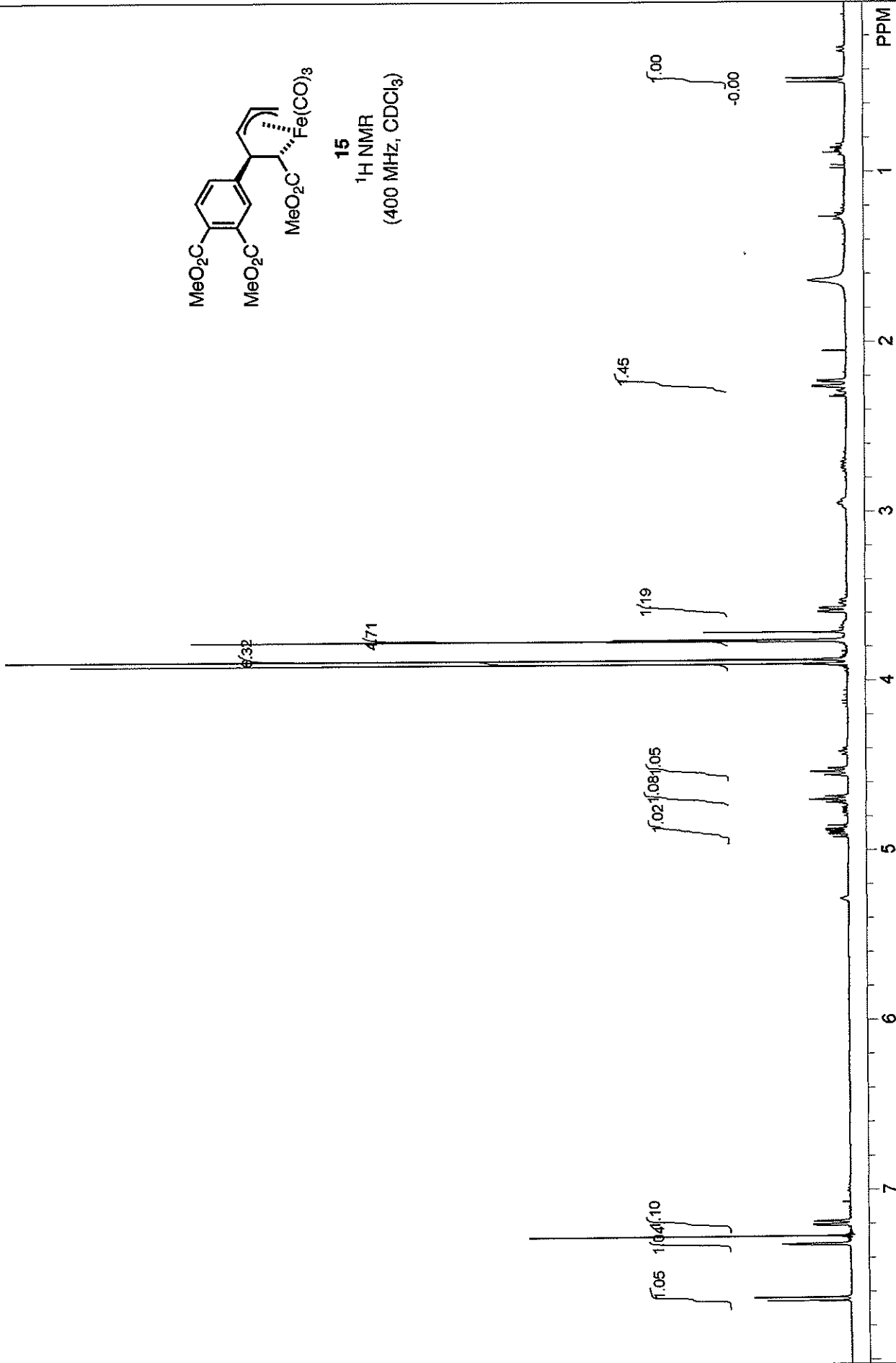


13C OBSERVE: blank line		USER: -- DATE: Oct 31 2007	
F1: 75.477	F2: 300.135	PTSId: 34246	65536
SW1: 18868	OF1: 8298.0	NA: 6080	LB: 0.6
PW: 7.3 us	PD: 1.0 sec	Nuts - \$1w66-C13-300.fid	
EX: s2pul			

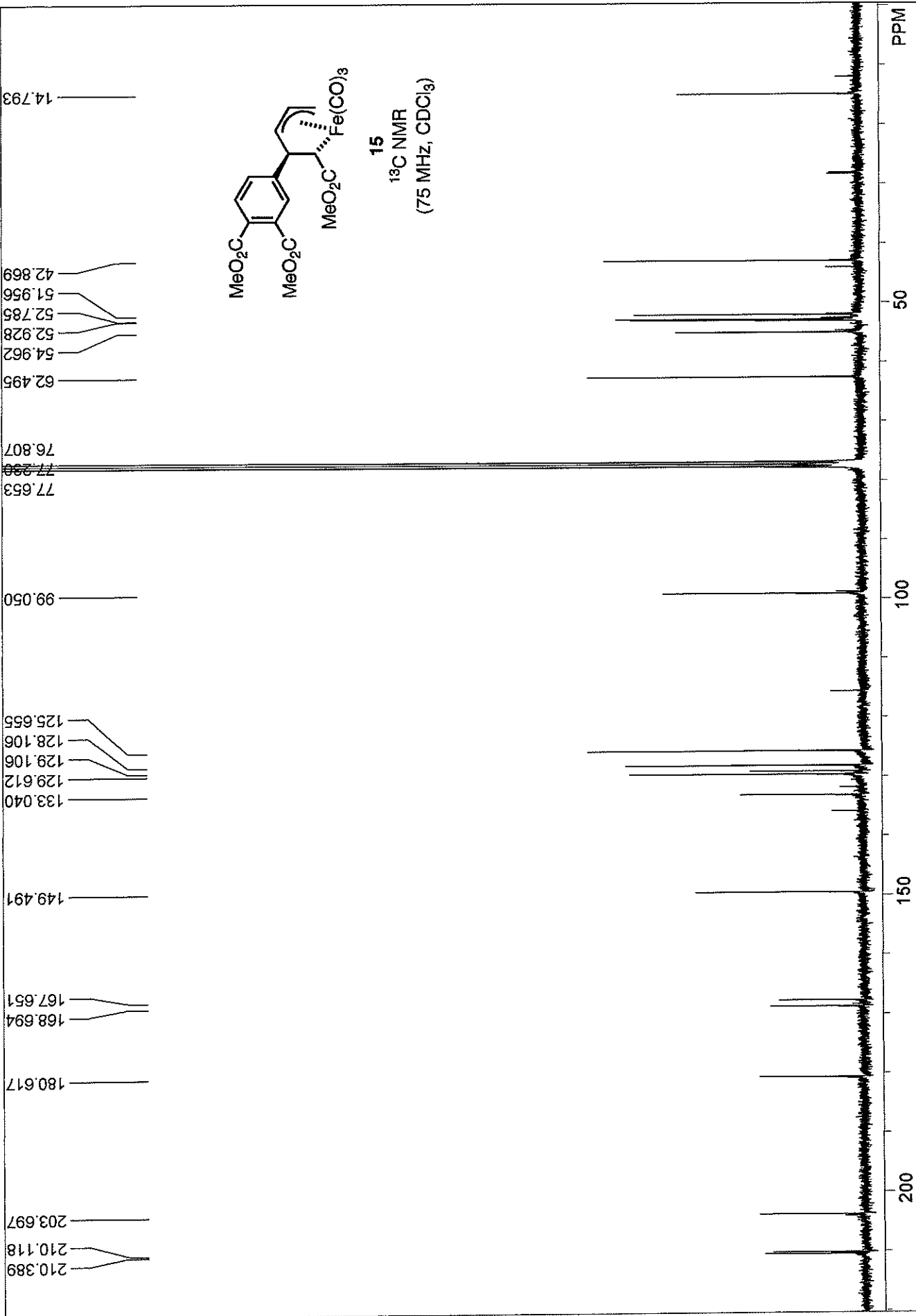


15

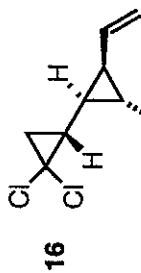
<sup>1</sup>H NMR  
(400 MHz, CDCl<sub>3</sub>)



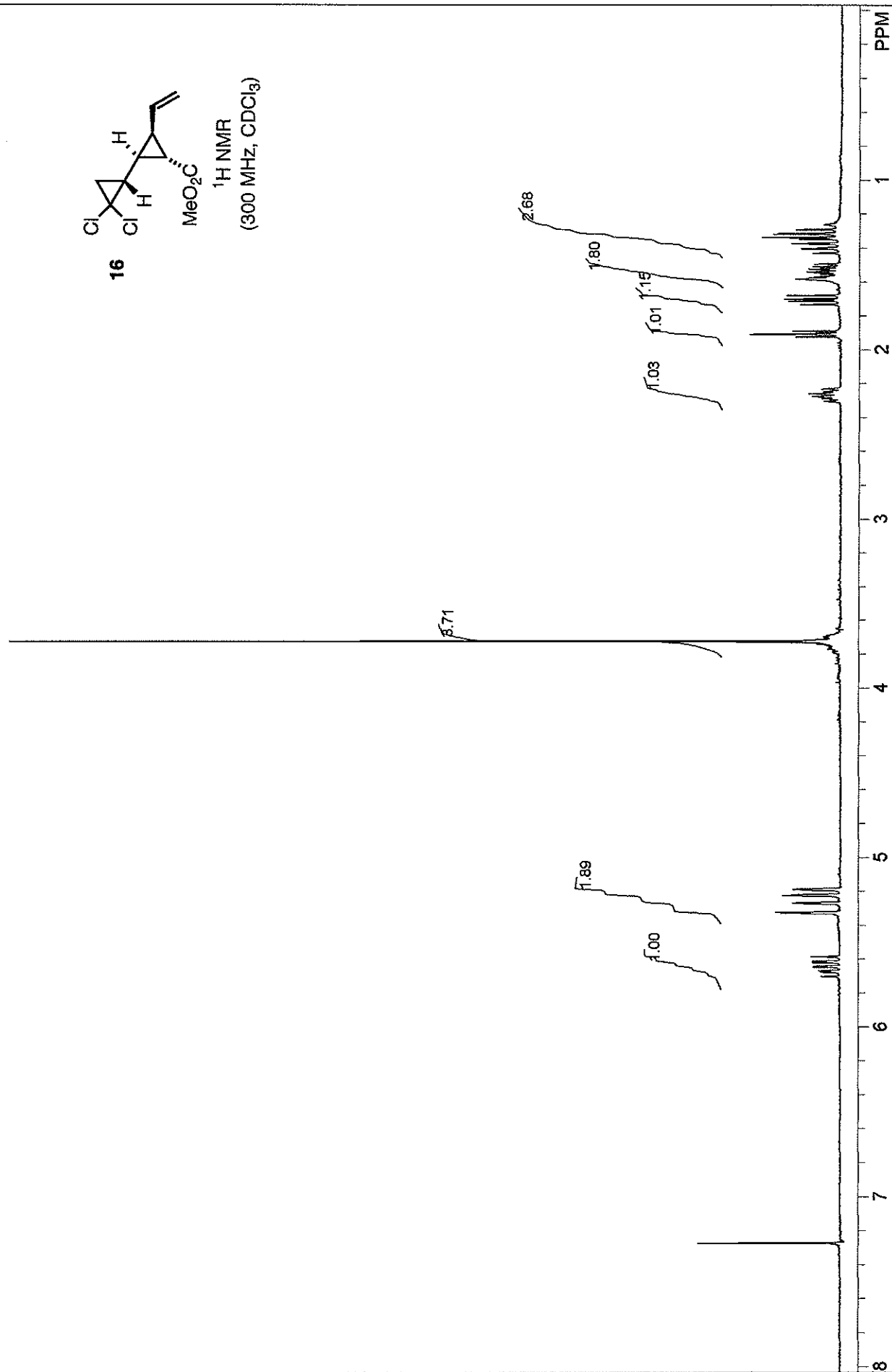
STANDARD_1H_OBSERVE - profile	USER: -- DATE: Aug 17 2007
F1: 399.751	PTSId: 13132 16384
F2: 100.526	OF1: 2403.3
EX: s2pul	NA: 8 LB: 0.0
	PD: 1.0 sec
	PW: 7.7 us
	SW1: 6410
	SW2: 100.526



13C OBSERVE: blank line  
 F1: 75.477 F2: 300.135 SW1: 18868 PW: 7.3 us PD: 1.0 sec  
 EX: s2pul  
 USER: -- DATE: Aug 26 2007  
 PTSId: 34246 65536  
 Nuts - \$hw63-2-C13-300.fid  
 LB: 0.8



<sup>1</sup>H NMR  
(300 MHz, CDCl<sub>3</sub>)



STANDARD 1H OBSERVE:blank line

F1: 300.136 F2: 75.476

EX: s2pul

SW1: 4803

PW: 6.3 us

OF1: 1803.7

PD: 1.0 sec

NA: 8

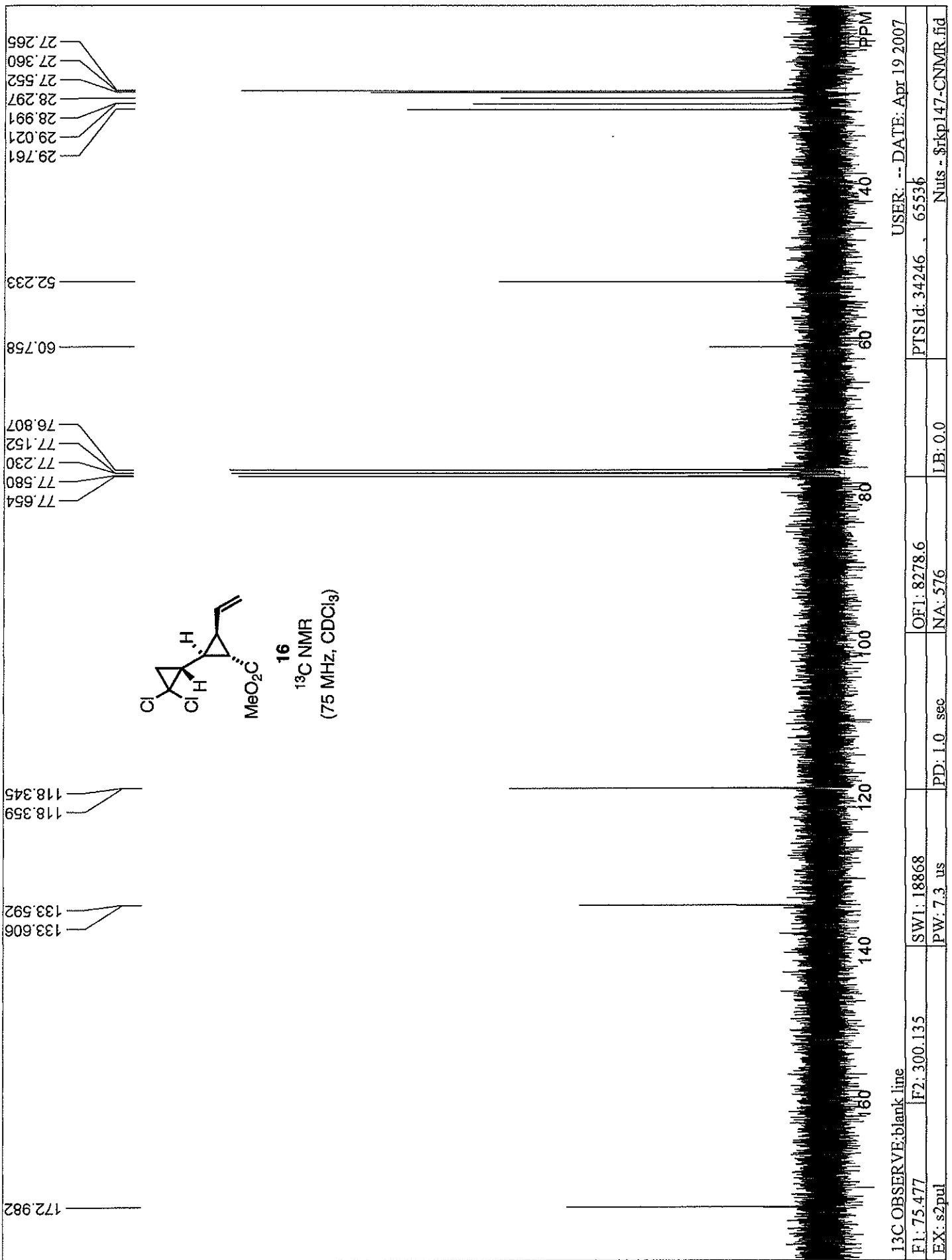
LB: 0.0

PTS1d: 9596

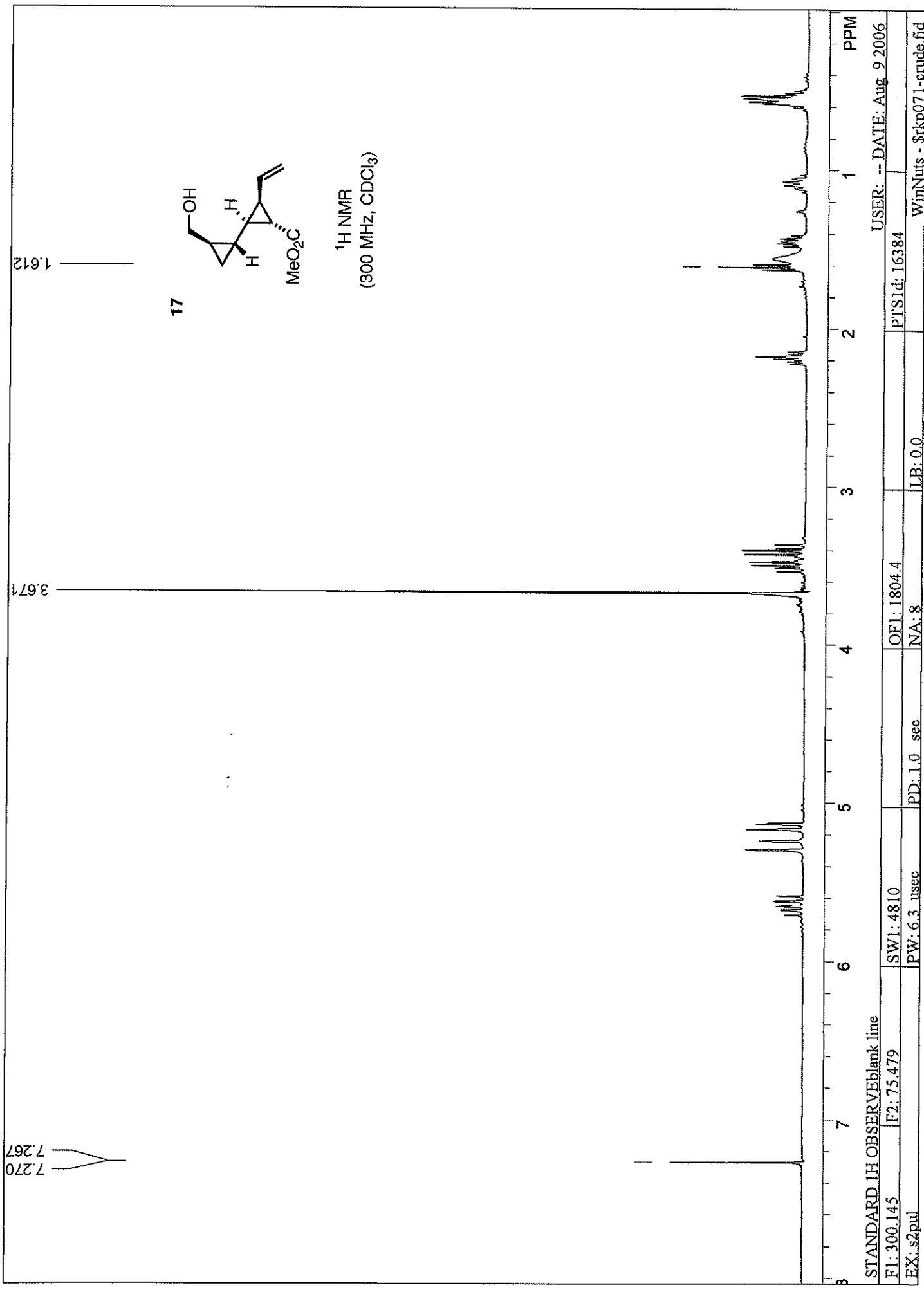
16384

USER: -- DATE: Apr 19 2007

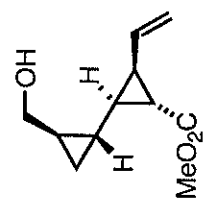
Nuts - \$rkp147-crude.fid



13C OBSERVE: blank line  
 USER: -- DATE: Apr 19 2007  
 F1: 75.477 F2: 300.135 SWH: 18868 PTS1d: 34246 65536  
 EX: s2pul PD: 1.0 sec NA: 576 LB: 0.0 Nuts - \$rkp147-CNMR.fid



17



<sup>1</sup>H NMR  
(300 MHz, CDCl<sub>3</sub>)

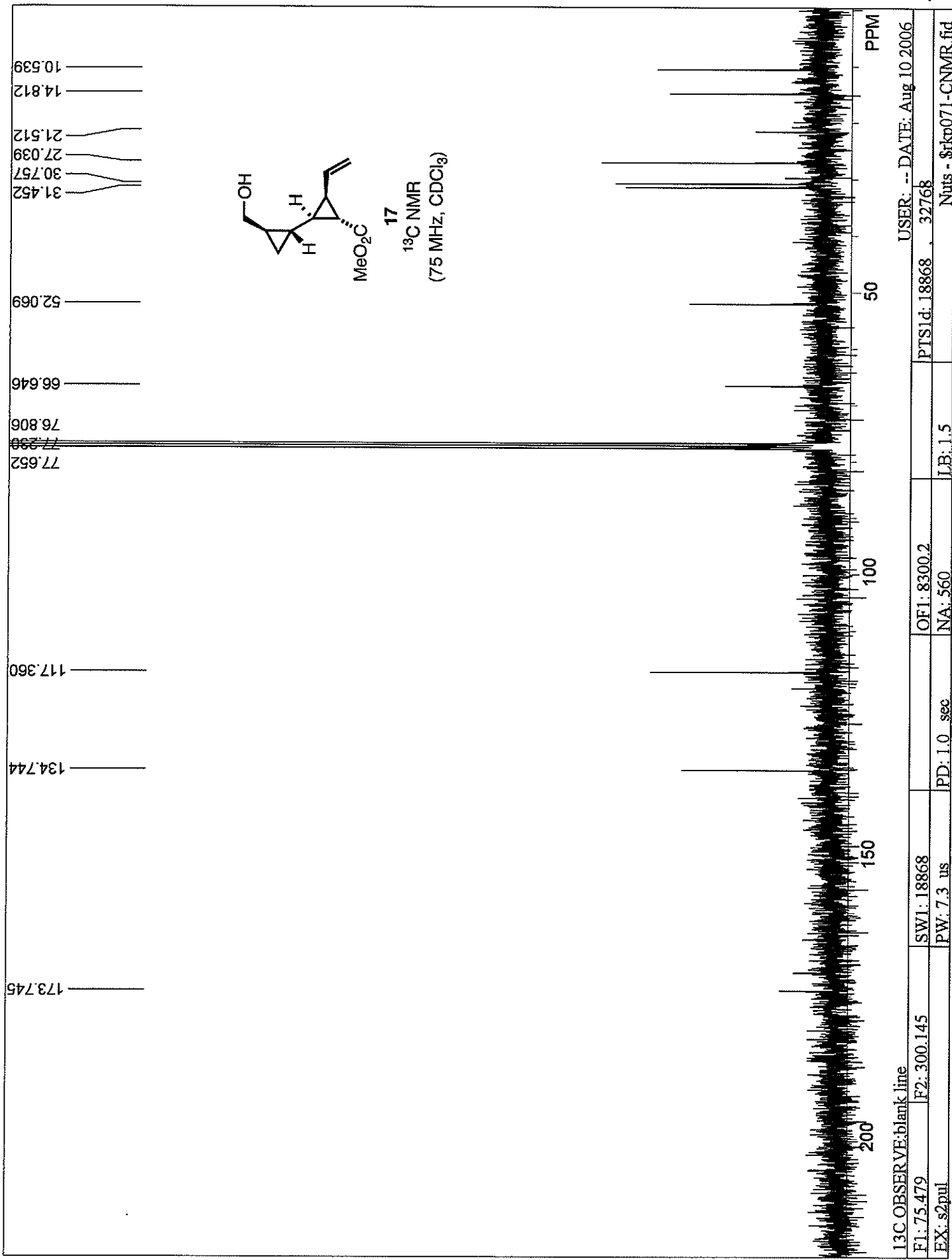
7.270  
7.267

3.671

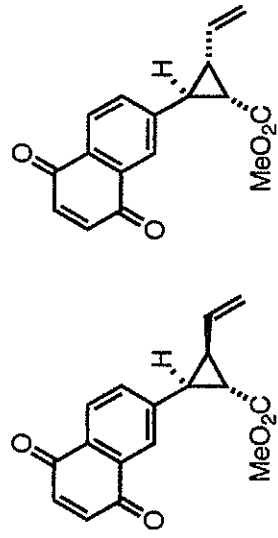
1.612

STANDARD_1H OBSERVE\blank line	
F1: 300.145	F2: 75.479
SW1: 4810	PW: 6.3 usec
PD: 1.0 sec	NA: 8
OF1: 1804.4	LB: 0.0
PTS1d: 16384	USER: -- DATE: Aug 9 2006
EX: s2pul	WinNuis - \$rkp071-crude.fid

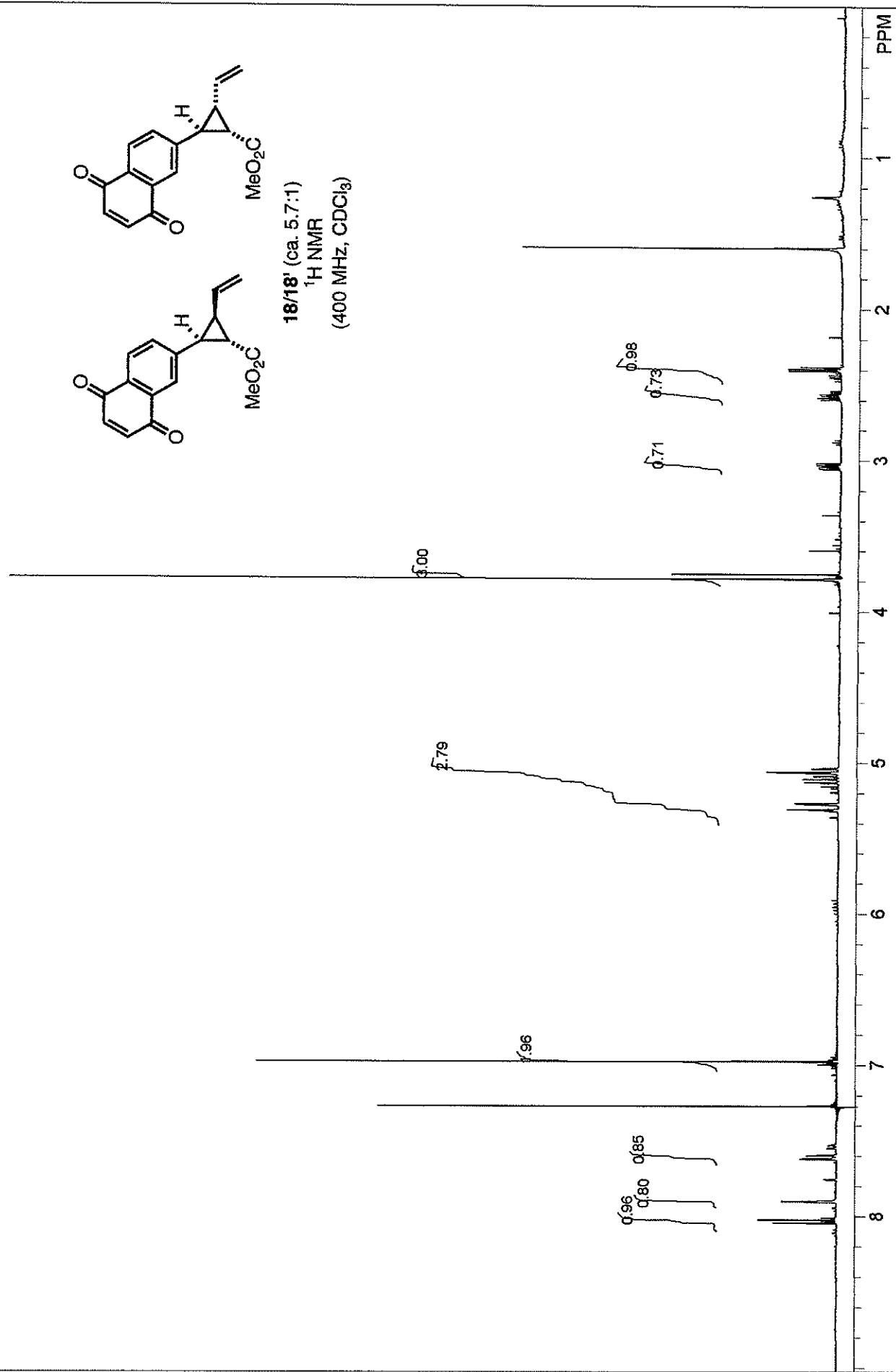




13C.OBSERVE:blank line		USER: -- DATE: Aug 10 2006	
F1: 75.479	F2: 300.145	PTS1d: 18868	32768
EX: s2pul	SW1: 18868	NA: 560	LB: 1.5
	PW: 7.3 us	PD: 1.0 sec	Nuts - \$rkp071-CNNMR.fid

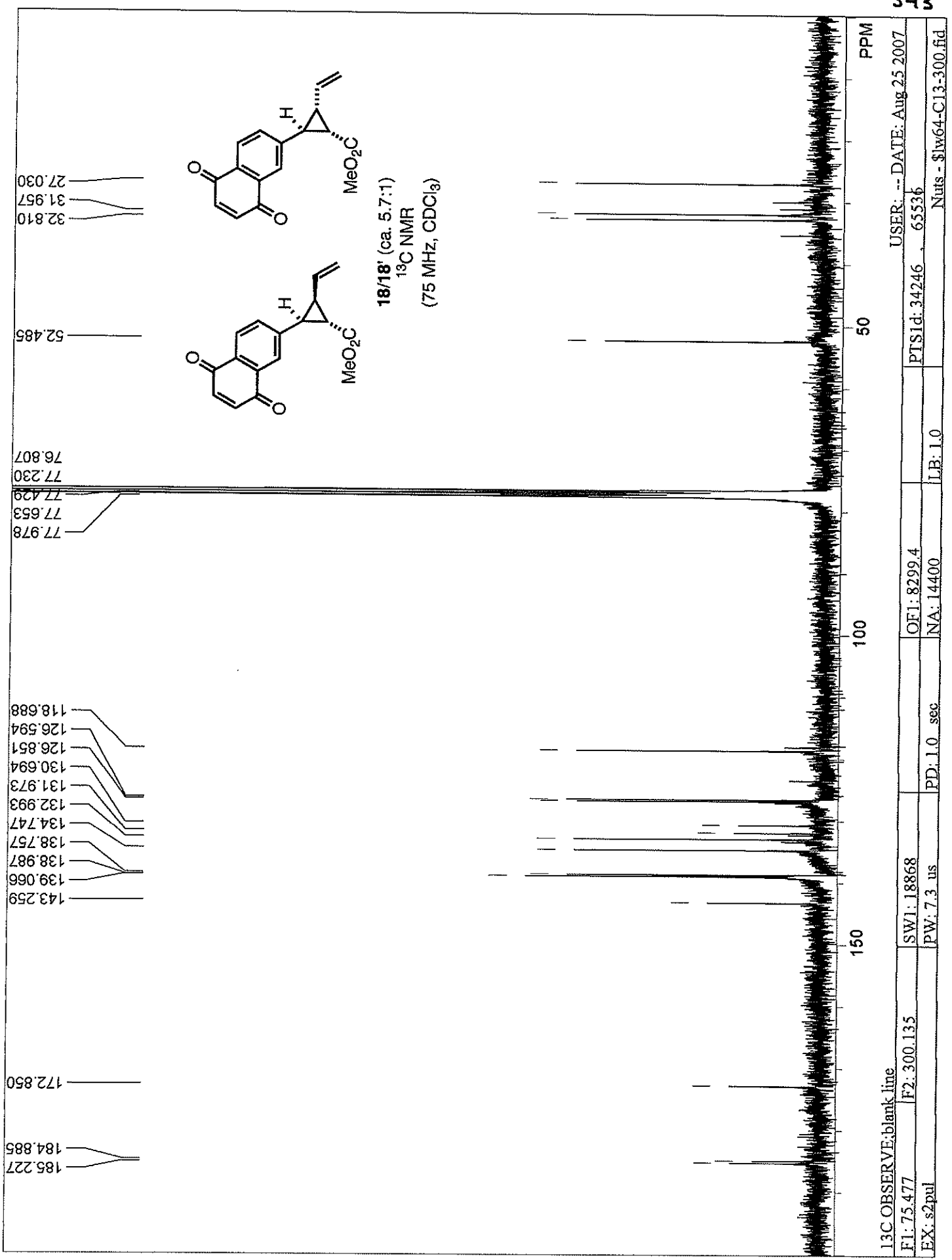


18/18' (ca. 5.7:1)  
<sup>1</sup>H NMR  
(400 MHz, CDCl<sub>3</sub>)



STANDARD 1H OBSERVE - profile

EX: s2pul	SWI: 6410	OF1: 2402.8	PTSD: 13132	USER: -- DATE: Aug 16 2007
PW: 7.7 us	NA: 8	LB: 0.0	16384	
PD: 1.0 sec				Nuts - \$lv64-H1-400.fid



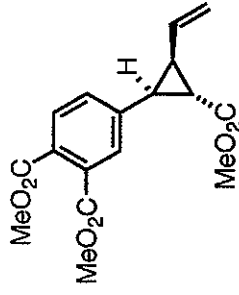
13C OBSERVE: blank line  
 F1: 75.477 F2: 300.135  
 EX: s2pul

SW1: 18868  
 PW: 7.3 us  
 PD: 1.0 sec

OF1: 8299.4  
 NA: 14400

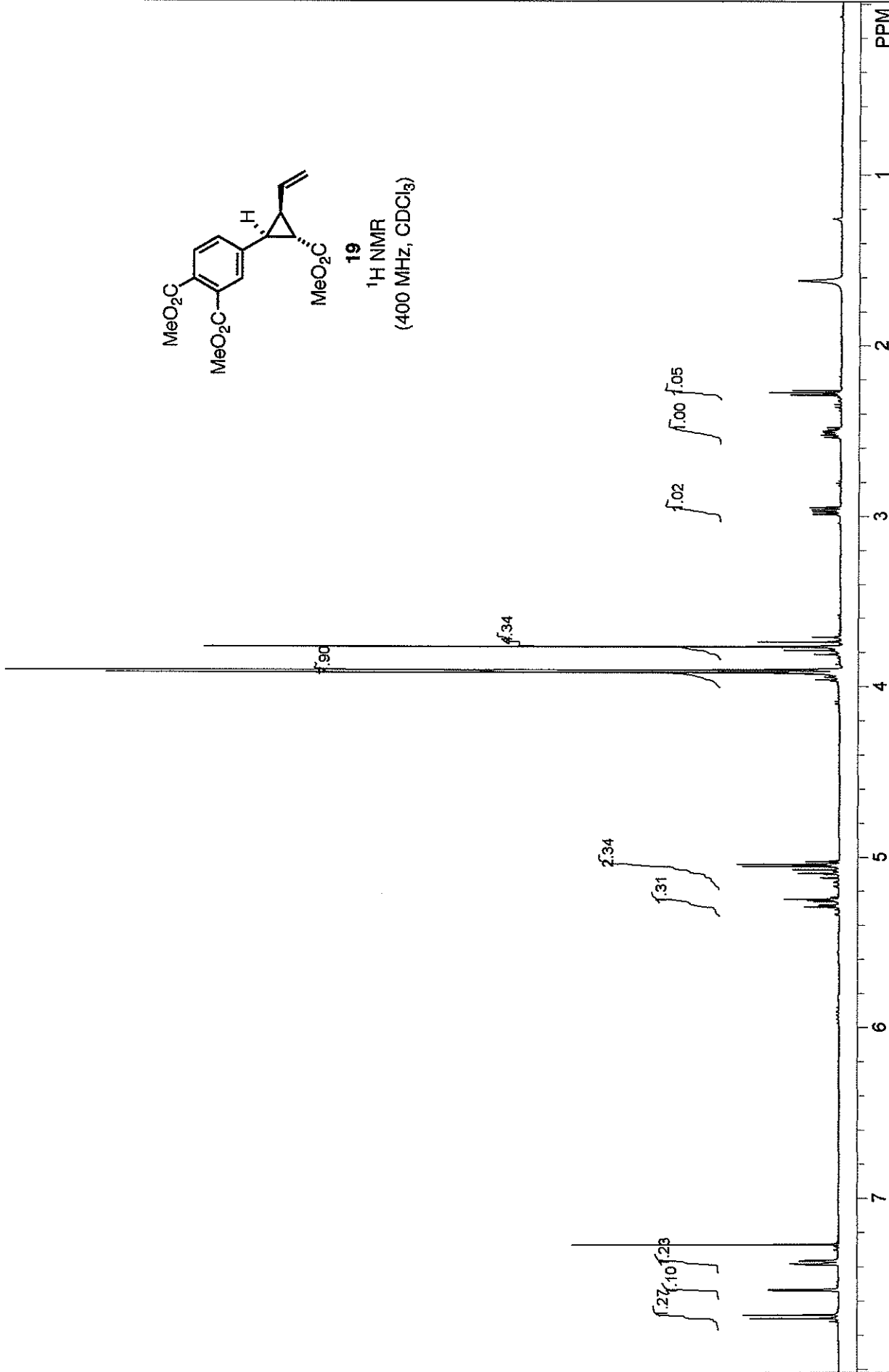
PTS1d: 34246  
 LB: 1.0

USER: -- DATE: Aug 25 2007  
 65536  
 Nuts - \$jw64-CJ3-300.fid



19

<sup>1</sup>H NMR  
(400 MHz, CDCl<sub>3</sub>)



STANDARD 1H OBSERVE - profile

F1: 399.751

F2: 100.526

SW1: 6410

PD: 1.0 sec

OF1: 2403.3

LB: 0.0

PTS1d: 13132

16384

USER: -- DATE: Aug 24 2007

EX: s2pul

NA: 8

NA: 8

NA: 8

NA: 8

NA: 8

NA: 8

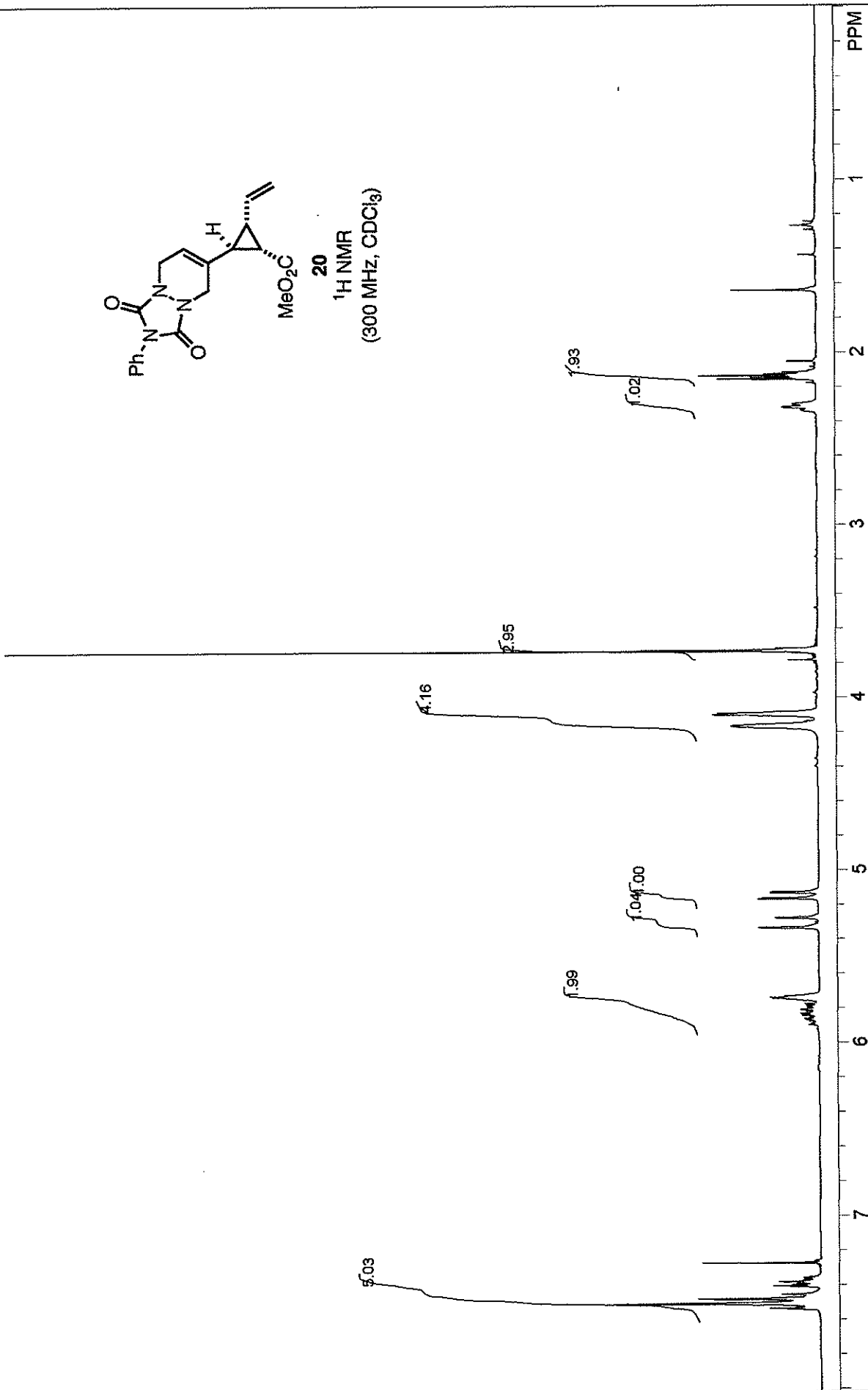
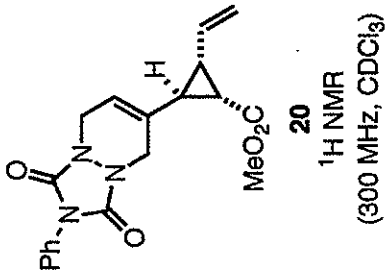
NA: 8

NA: 8

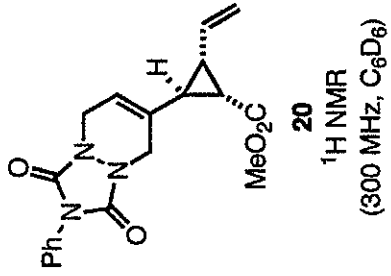
NA: 8



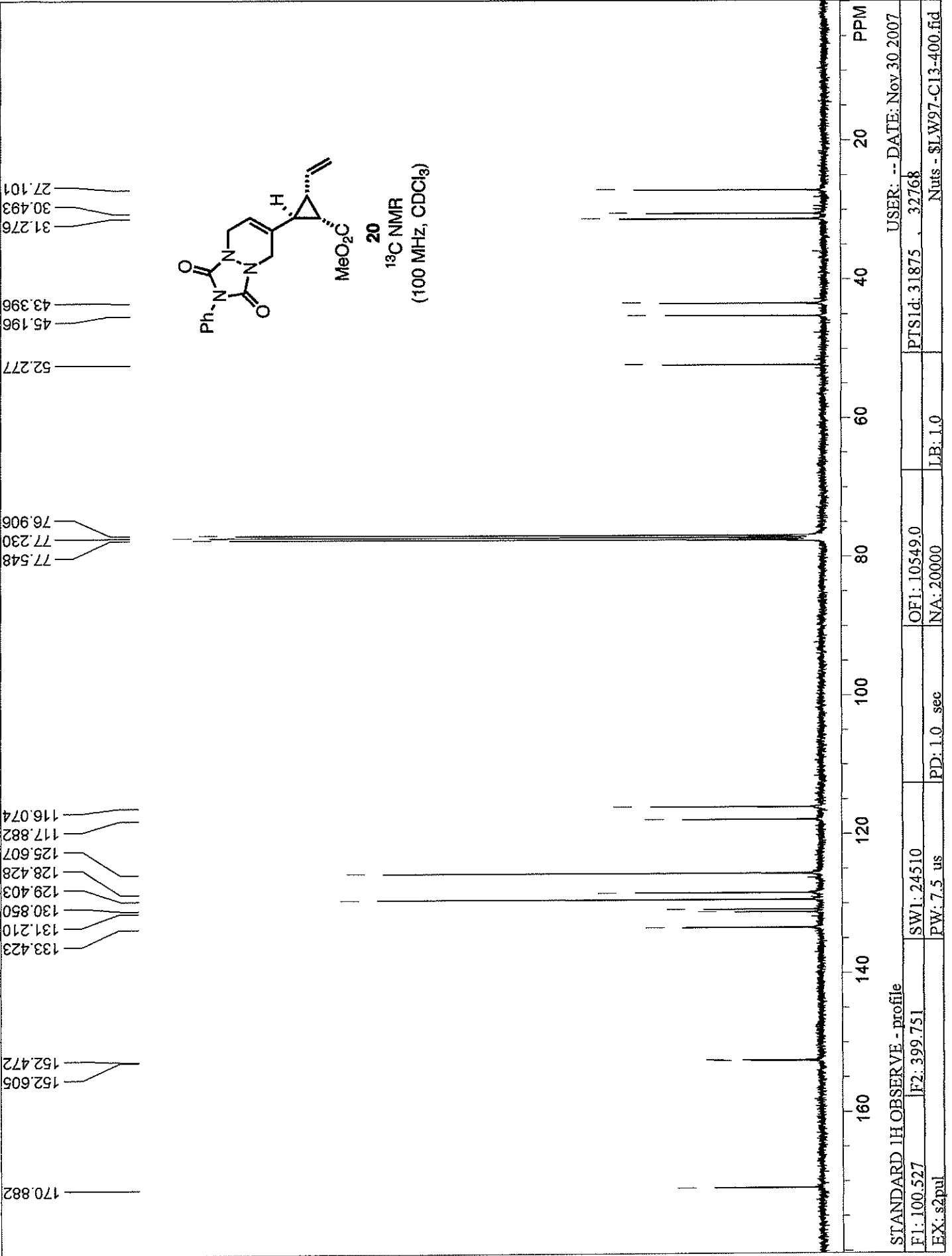
13C OBSERVE: blank line  
 F1: 75.477 F2: 300.135 SW1: 18868 OF1: 8299.9  
 EX: s2pul PD: 1.0 sec NA: 128 LB: 1.0  
 PTS1d: 34246 65536  
 USER: -- DATE: Aug 25 2007  
 Nuts - \$lw65-C13-300.fid



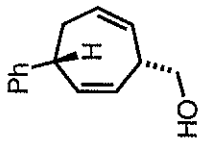
STANDARD 1H OBSERVE:blank line		USER: -- DATE: Nov.30.2007	
F1: 300.136	F2: 75.476	PTS1d: 9596	16384
EX: s2pul		LB: 0.0	Nuts - \$1w97-1-H1-300.fid
	PD: 1.0 sec	NA: 64	
	PW: 6.3 us	OF1: 1804.1	



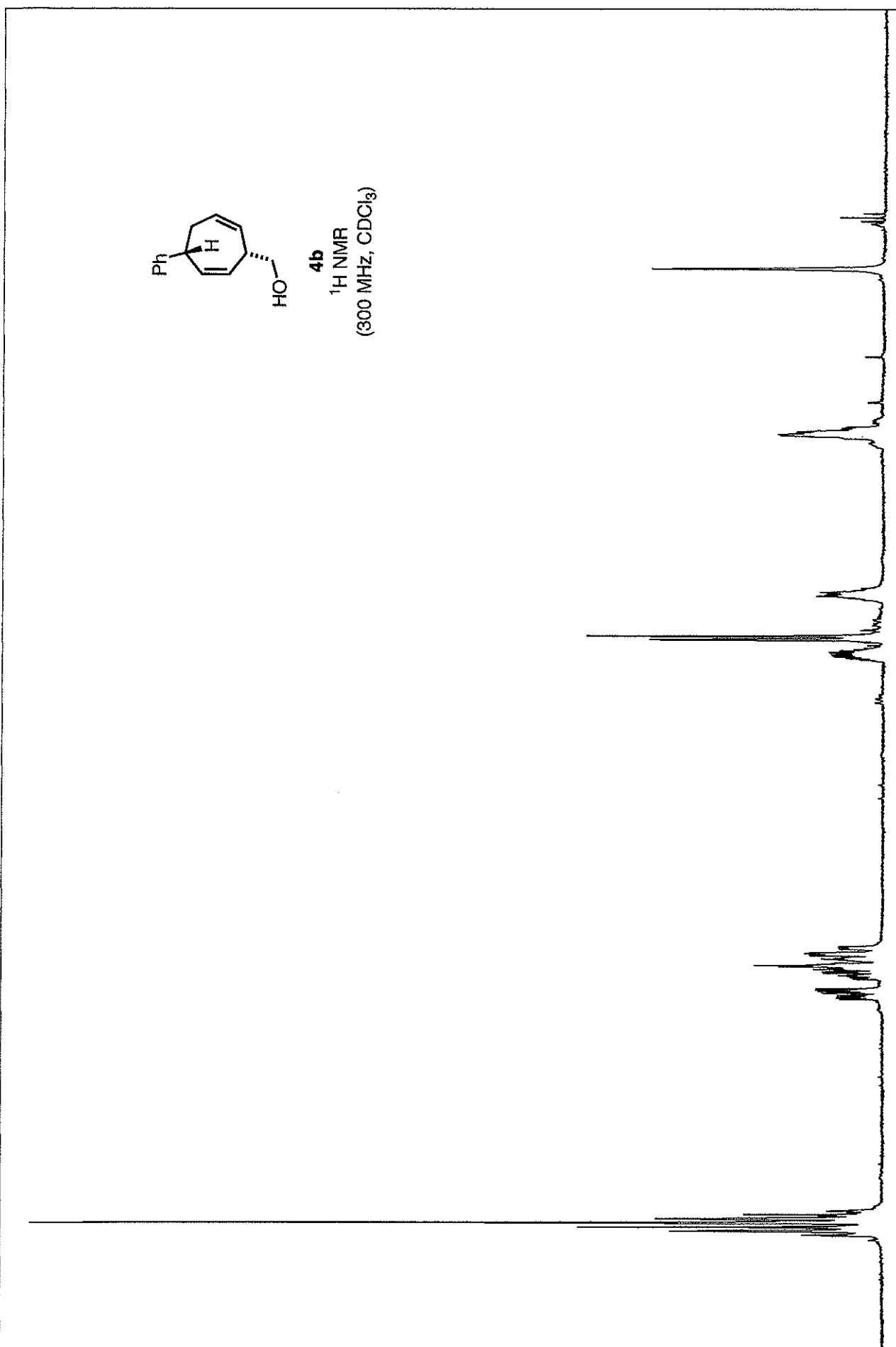
STANDARD 1H OBSERVE:blank line		USER: -- DATE: Dec. 3 2007
FI: 300.136	SW1: 4803	PTS1d: 9596 16384
EX: s2pul	PW: 6.3 us	NA: 256
	PD: 1.0 sec	LB: 0.0
		Nuts - \$1w97-H1-300-DBenzene.fid



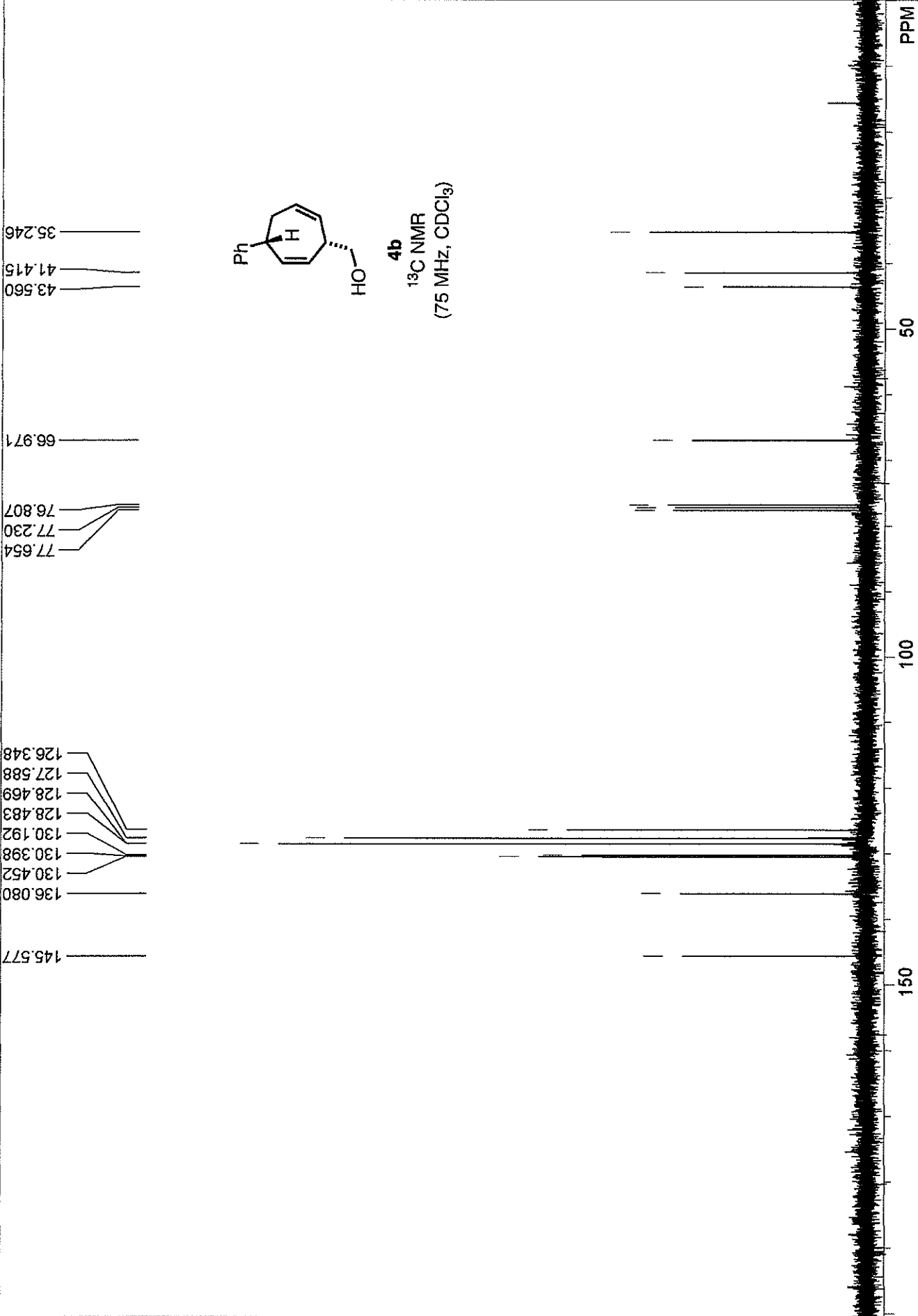




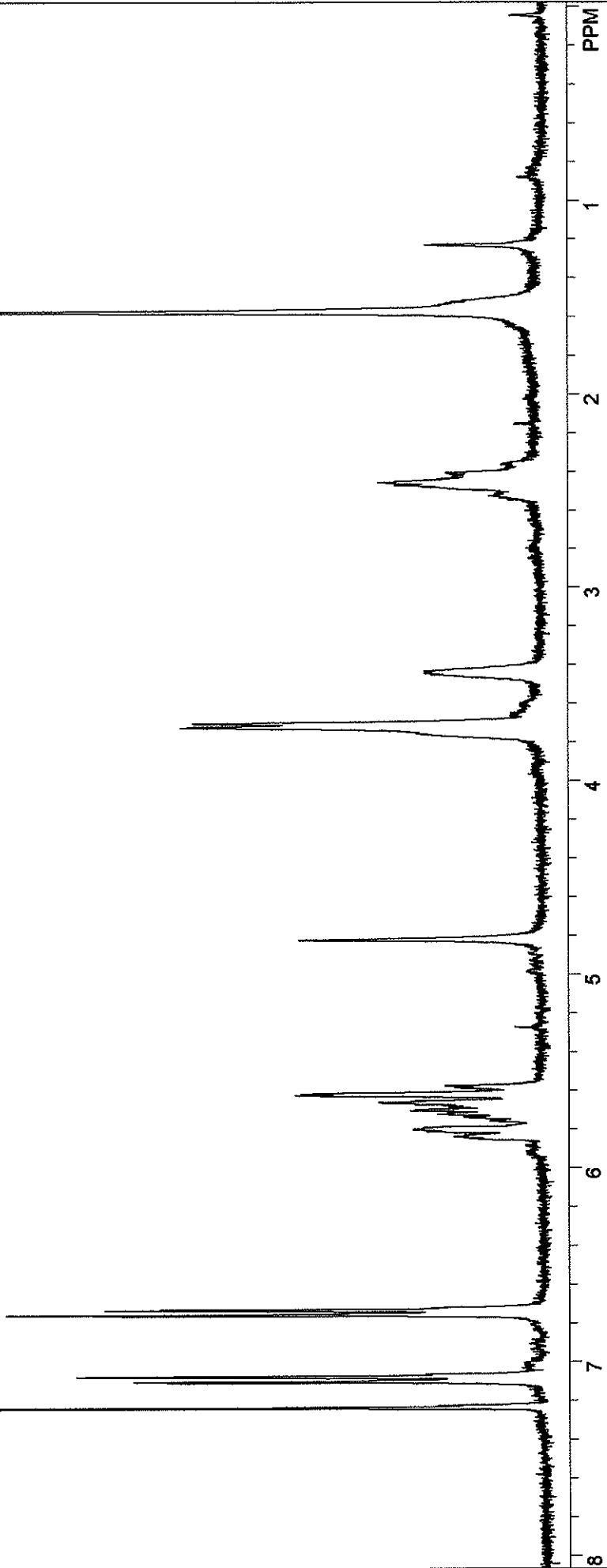
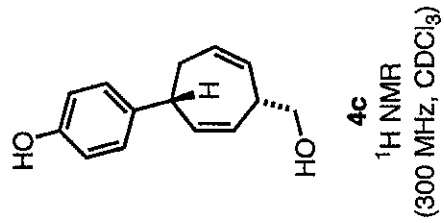
**4b**  
<sup>1</sup>H NMR  
 (300 MHz, CDCl<sub>3</sub>)



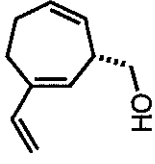
8	7	6	5	4	3	2	1	PPM
STANDARD_1H OBSERVE;blank line								
F1: 300.142		F2: 75.478		SW1: 4803		OF1: 1804.5		USER: -- DATE: May 5 2004
EX: s2pul		PW: 6.0 us		PD: 1.0 sec		NA: 8		PTS1d: 14409 16384
Nuts - \$nw603chromproduct2.fid								



13C OBSERVE: blank line		USER: -- DATE: May 4 2004	
F1: 75.479	F2: 300.142	PTSId: 18868	32768
EX: s2pul	PW: 7.3 us	PD: 1.0 sec	NA: 256
		LB: 0.0	Nus: \$nuv603chromproductC13.fid



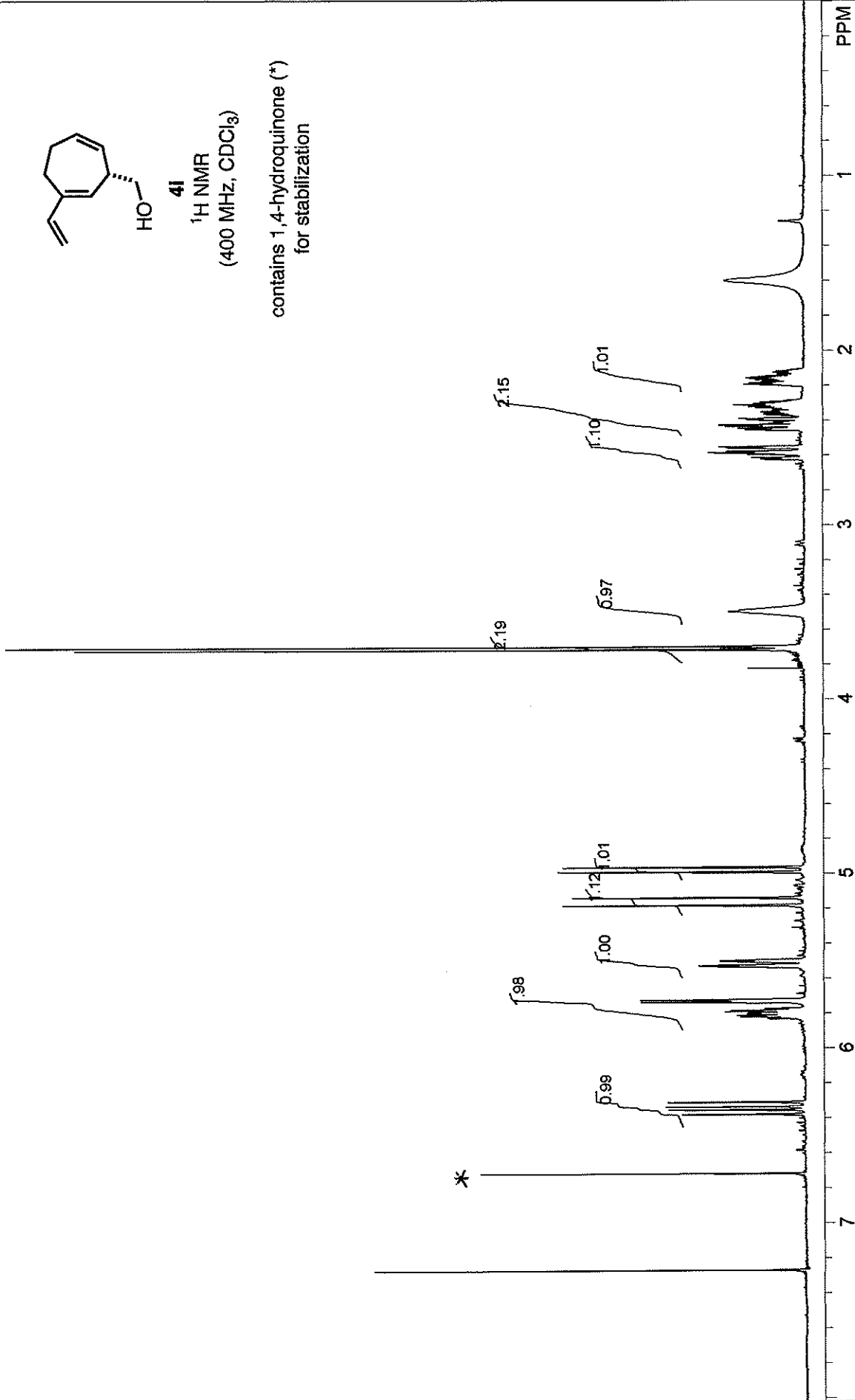
STANDARD 1H OBSERVEblank line		USER: -- DATE: Feb 20 2006	
F1: 300.145	F2: 75.479	PTS1d: 16384	
EX: s2pul	SW1: 4810	OF1: 1794.3	LB: 0.0
	PW: 6.3 usec	PD: 1.0 sec	NA: 8
			WinNuts - \$rkp035e-cryst.fid



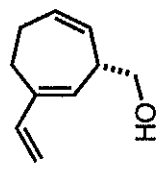
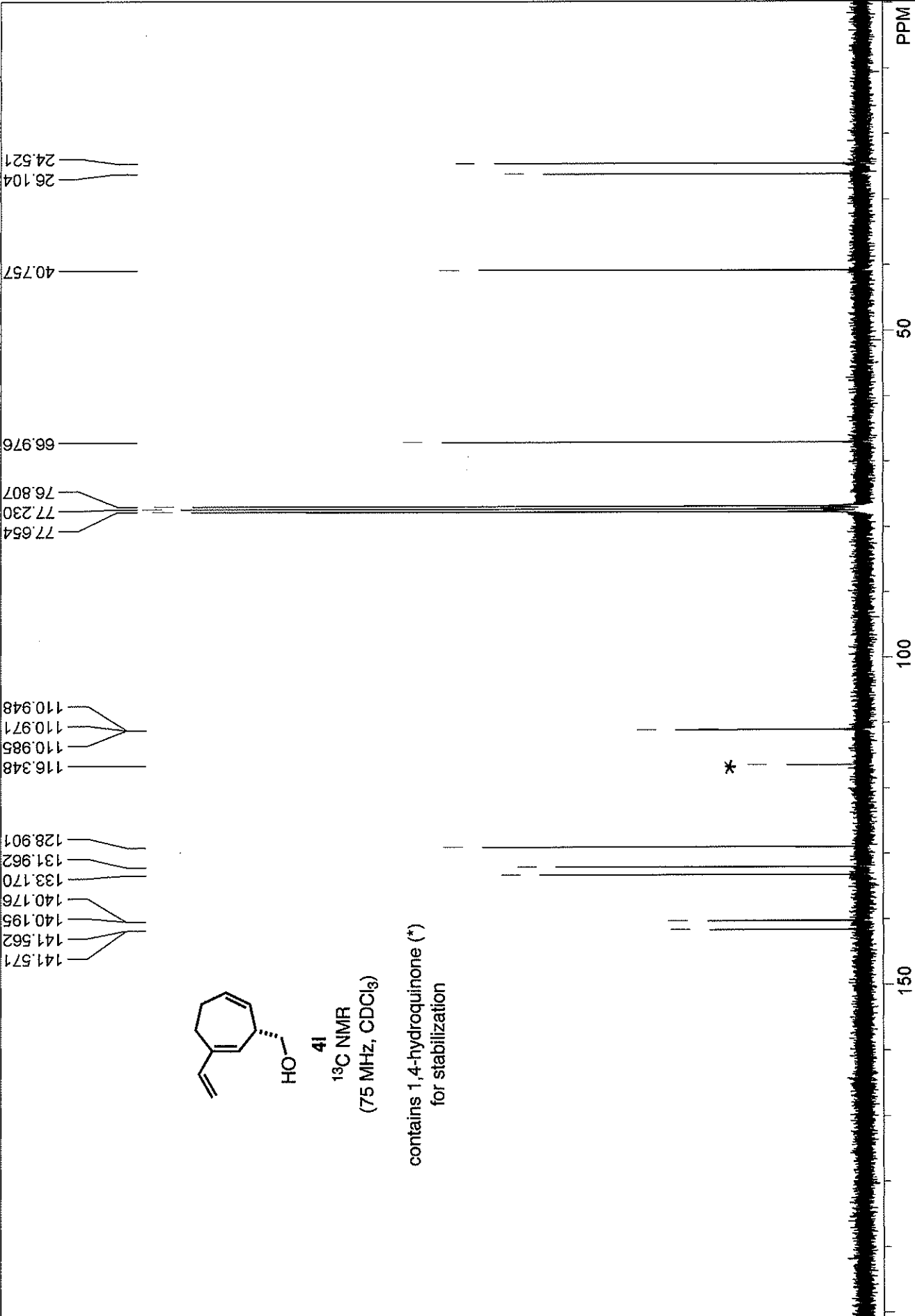
4I

<sup>1</sup>H NMR  
(400 MHz, CDCl<sub>3</sub>)

contains 1,4-hydroquinone (\*)  
for stabilization



.blank ime		USER: -- DATE: Sep 4 2007	
F1: 399.751	F2: 100.526	OF1: 2402.6	PTS1d: 13132 . 16384
EX: s2pul	PW: 7.7 us	NA: 8	LB: 0.0
	PD: 1.0 sec		Nuts - \$lw69-H1-400.fid



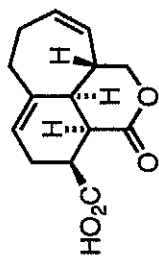
41

<sup>13</sup>C NMR

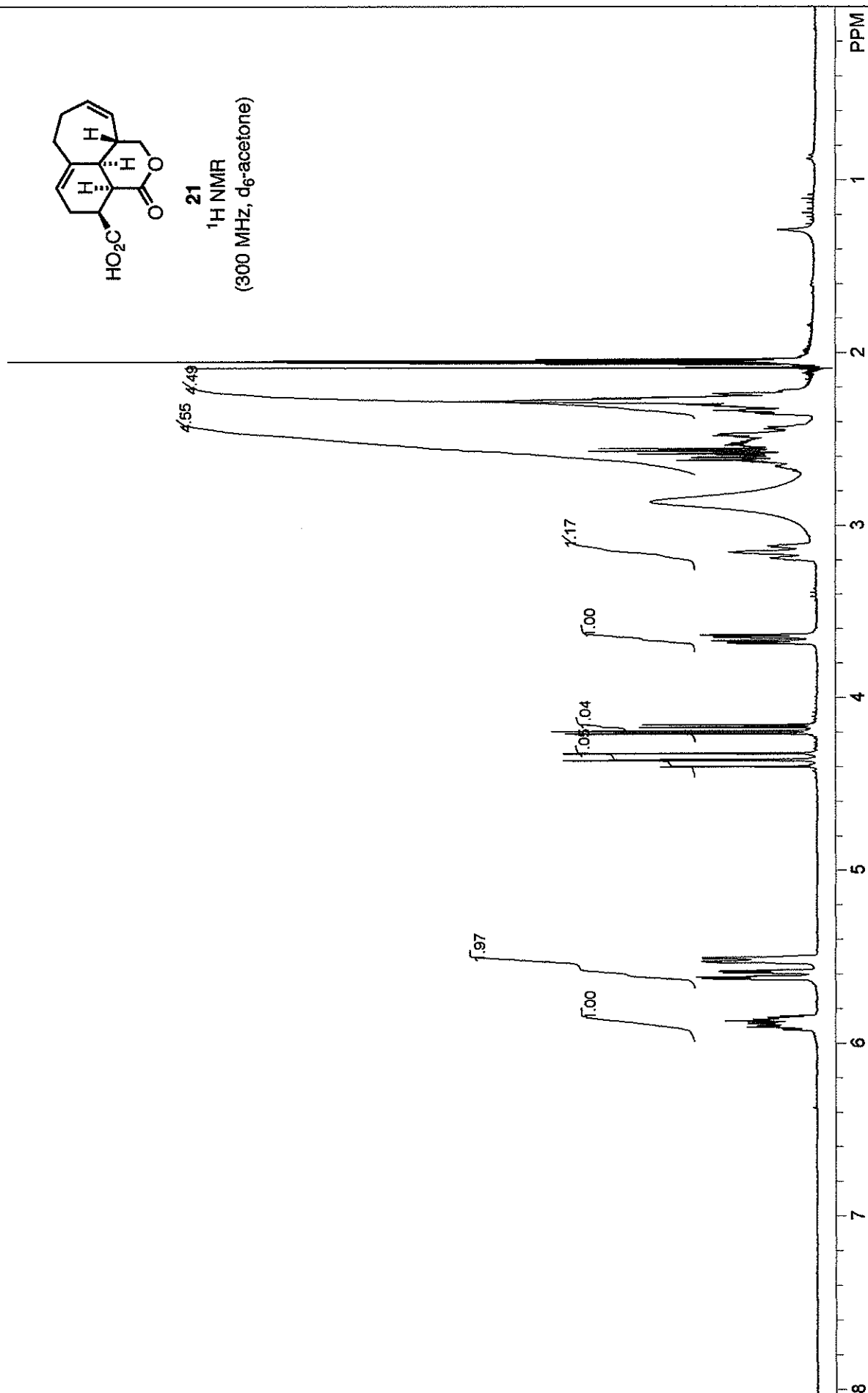
(75 MHz, CDCl<sub>3</sub>)

contains 1,4-hydroquinone (\*)  
for stabilization

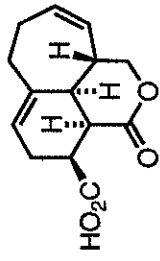
13C OBSERVE: blank_line		USER: -- DATE: Sep 5 2007	
F1: 75.477	F2: 300.135	PTSID: 34246	65536
EX: s2pul	SW1: 18868	OF1: 8299.6	LB: 0.0
	PW: 7.3 us	PD: 1.0 sec	NA:
			Nuis - \$lv69-C13-300.fid



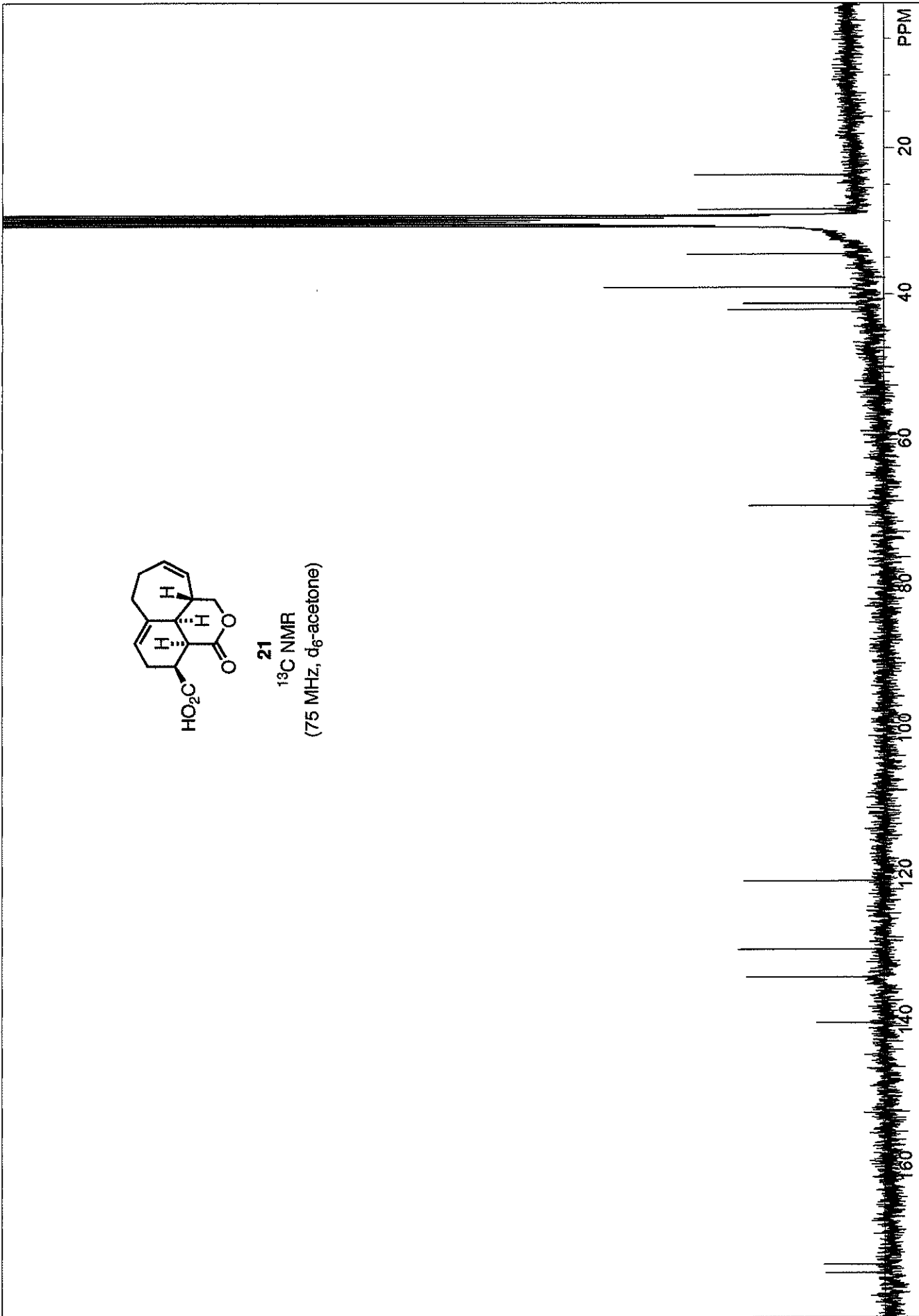
**21**  
<sup>1</sup>H NMR  
 (300 MHz, d<sub>6</sub>-acetone)



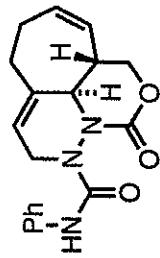
STANDARD 1H OBSERVE: blank\_line  
 F1: 300.137 F2: 75.477 SW1: 4803 OF1: 1800.5  
 EX: s2pul PW: 6.3 us PD: 1.0 sec NA: 256 LB: 0.0  
 PTS1d: 9596 I6384  
 USER: -- DATE: Jul 17 2007  
 Nuts - \$lw46-HI-Ace300.fid



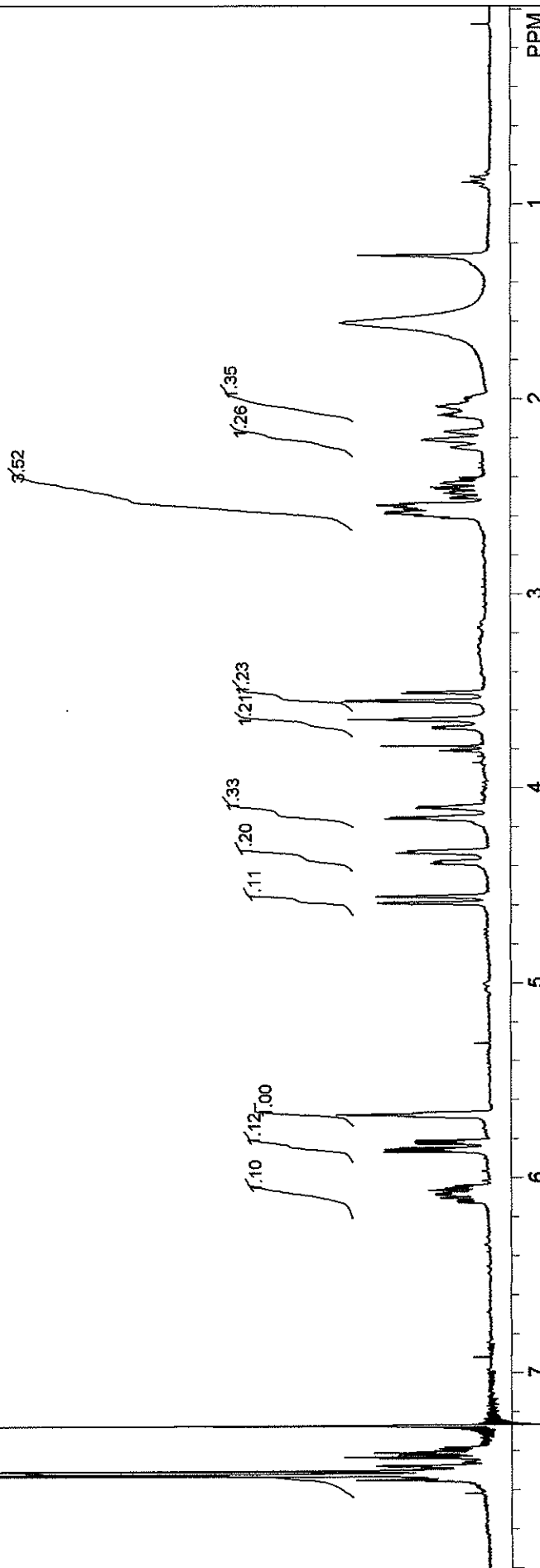
**21**  
<sup>13</sup>C NMR  
 (75 MHz, d<sub>6</sub>-acetone)



13C OBSERVE: blank line		USER: -- DATE: Aug 11 2007	
F1: 75.477	F2: 300.137	PTS1d: 34246	65536
EX: s2pul	SW1: 18568	OF1: 8357.6	LB: 1.5
	PW: 7.3 us	PD: 1.0 sec	NA:
			Nuts - \$lv46-C13-300.fid

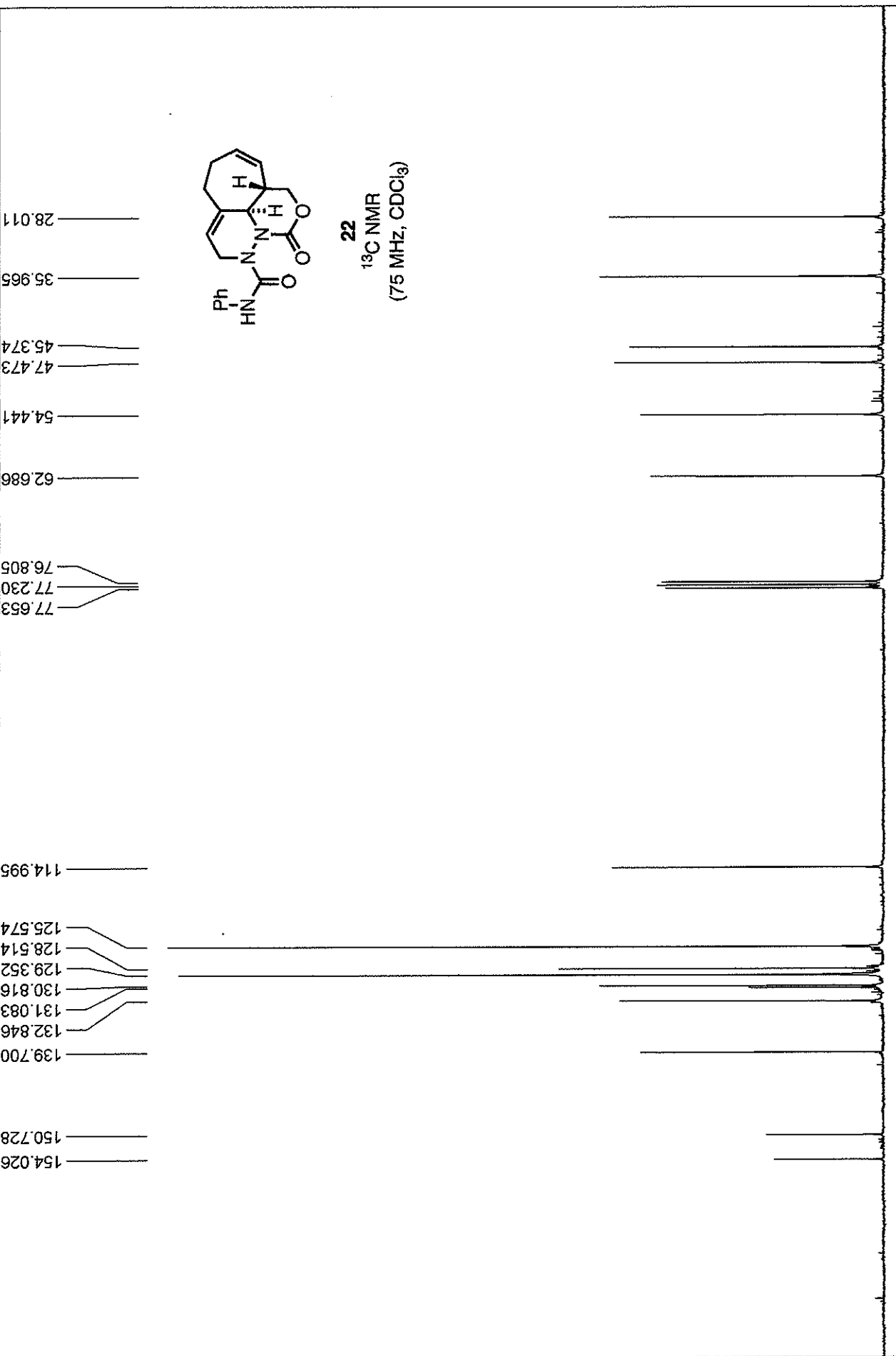


22  
<sup>1</sup>H NMR  
 (300 MHz, CDCl<sub>3</sub>)



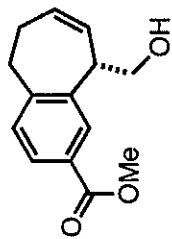
STANDARD 1H OBSERVE:blank line  
 F1: 300.136 F2: 75.476 SW1: 4803  
 EX: s2pul PW: 6.3 us PD: 1.0 sec OF1: 1803.5  
 PTS1d: 9596 , 16384 LB: 0.0 NA: 256  
 USER: -- DATE: Oct 22 2007 Nuis - \$1w86-H1-300.fid



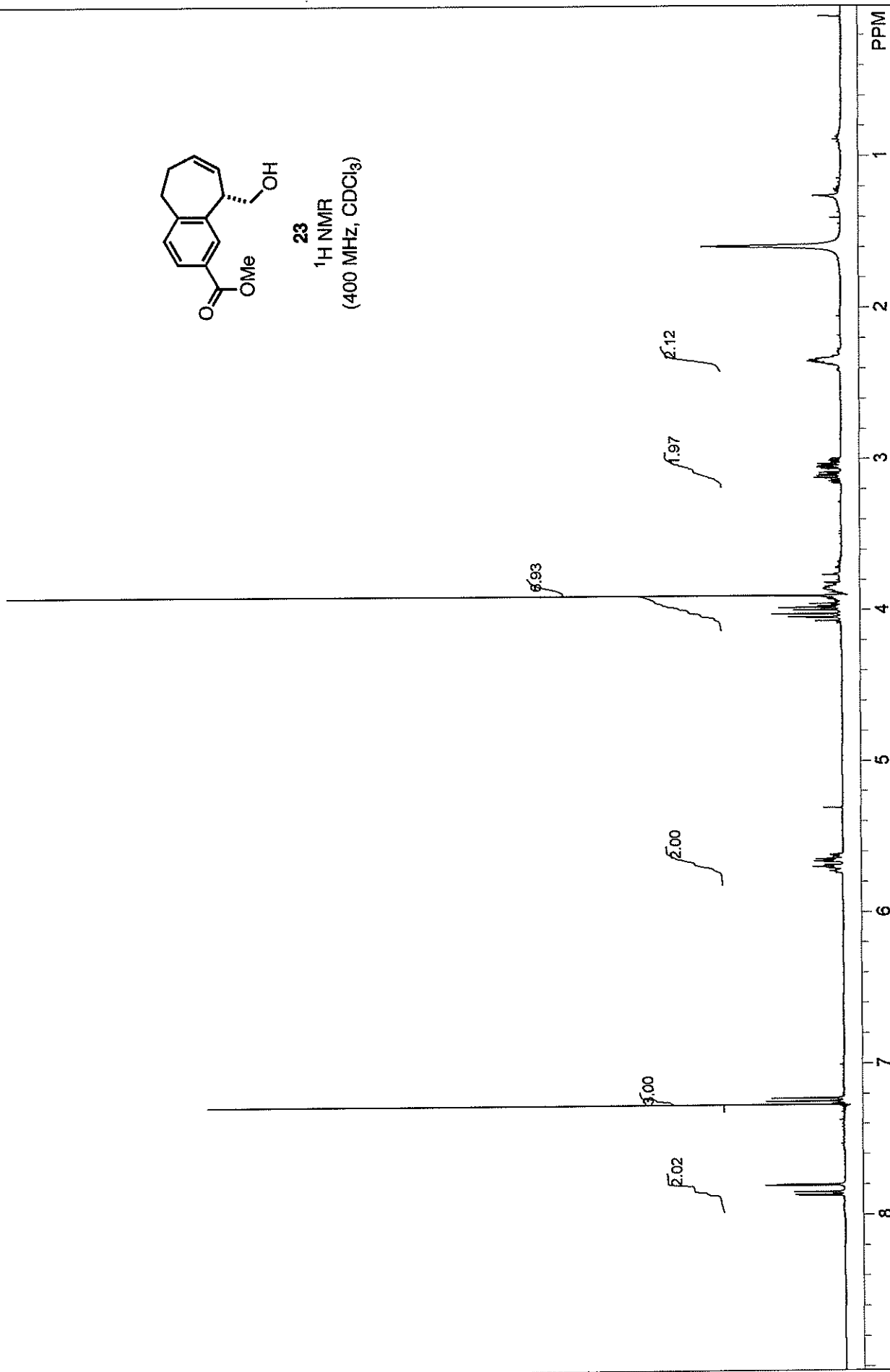


**22**  
<sup>13</sup>C NMR  
(75 MHz, CDCl<sub>3</sub>)

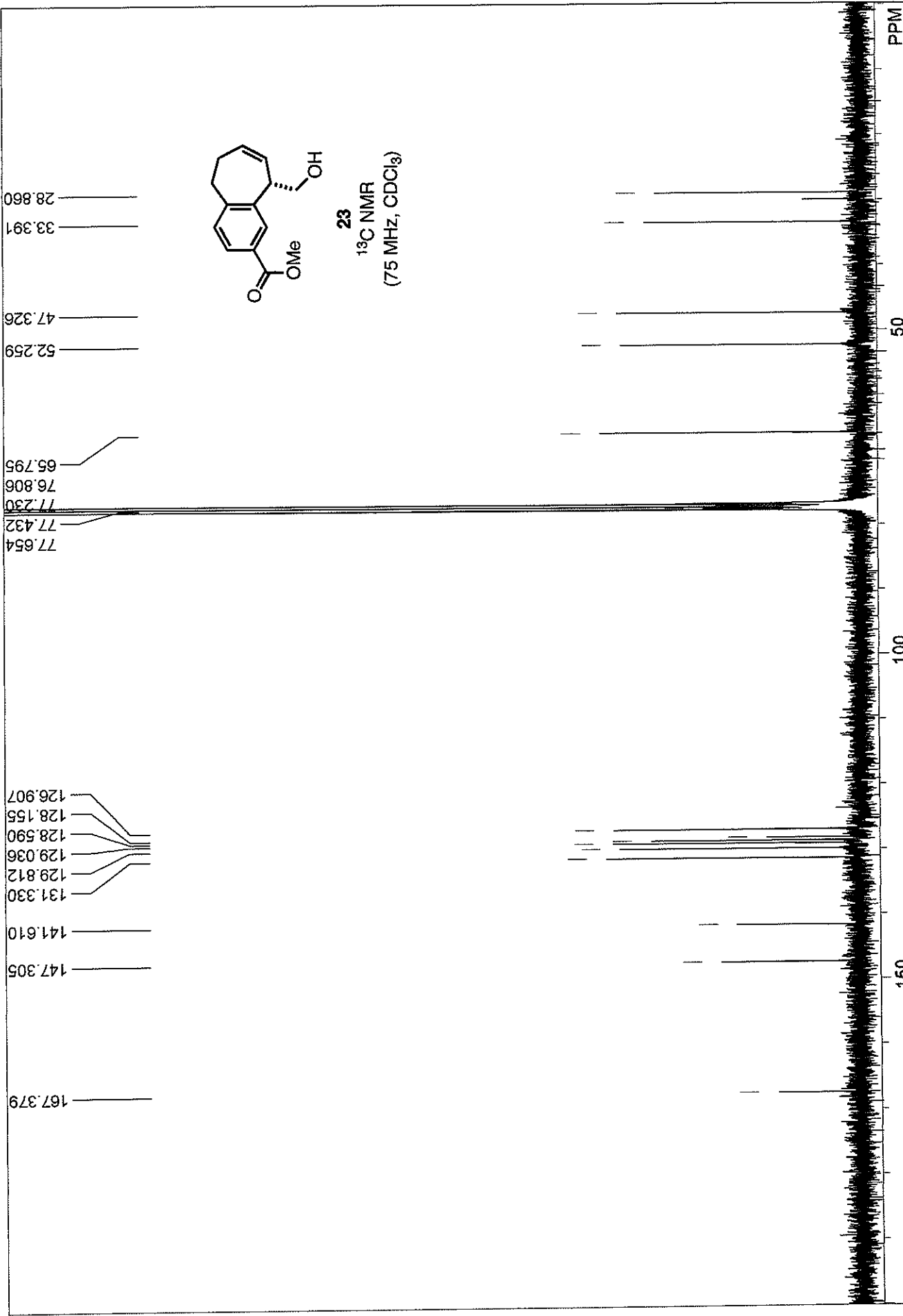
13C OBSERVE: blank line		USER: -- DATE: Nov 5 2007	
F1: 75.477	F2: 300.135	PTS1d: 34246	65336
EX: s2pul	PW: 7.3 us	NA: 12000	LB: 1.0
		Nuts - \$lw86-C13-300.fid	



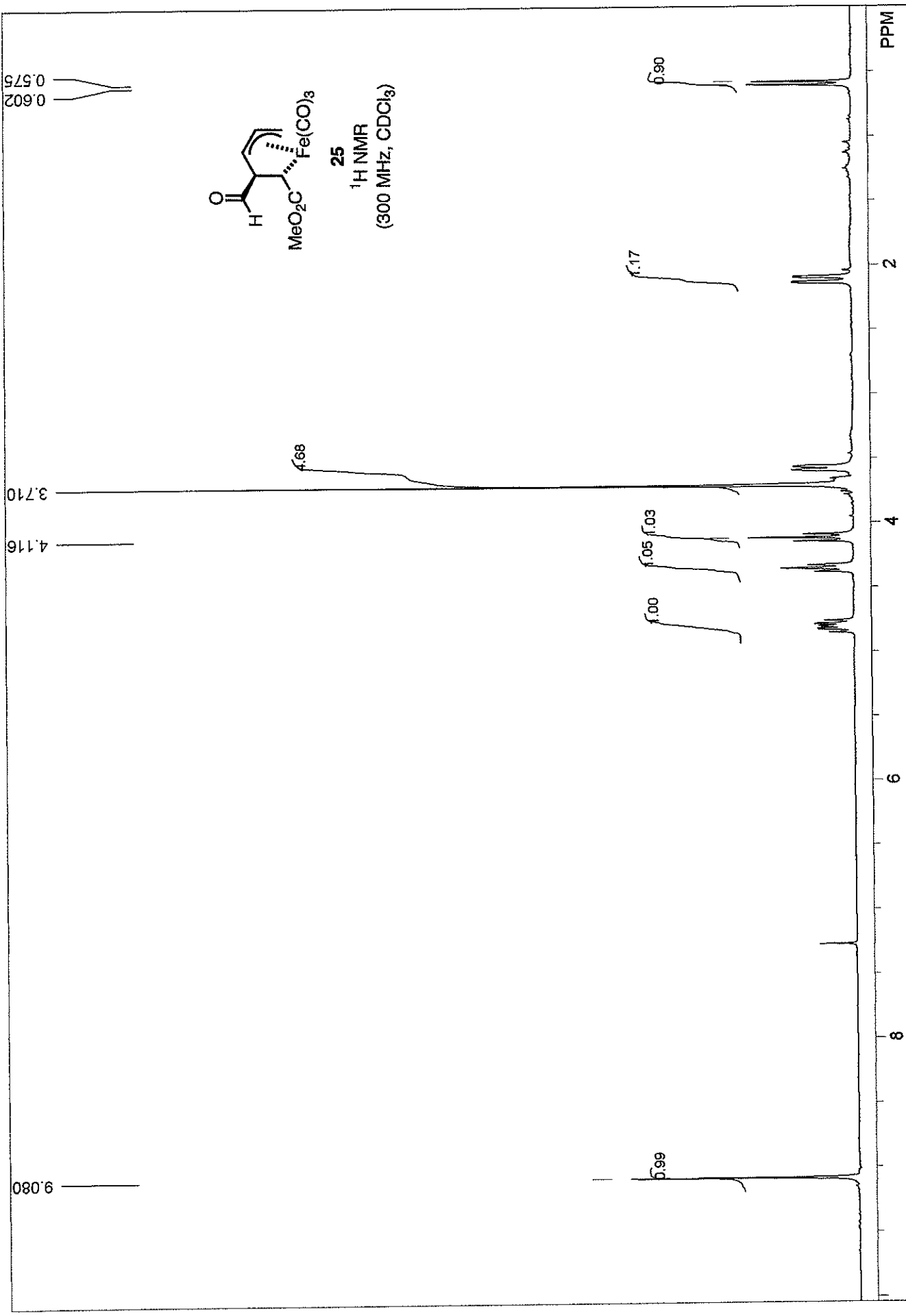
**23**  
<sup>1</sup>H NMR  
 (400 MHz, CDCl<sub>3</sub>)



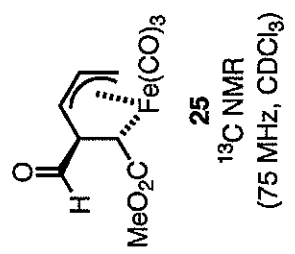
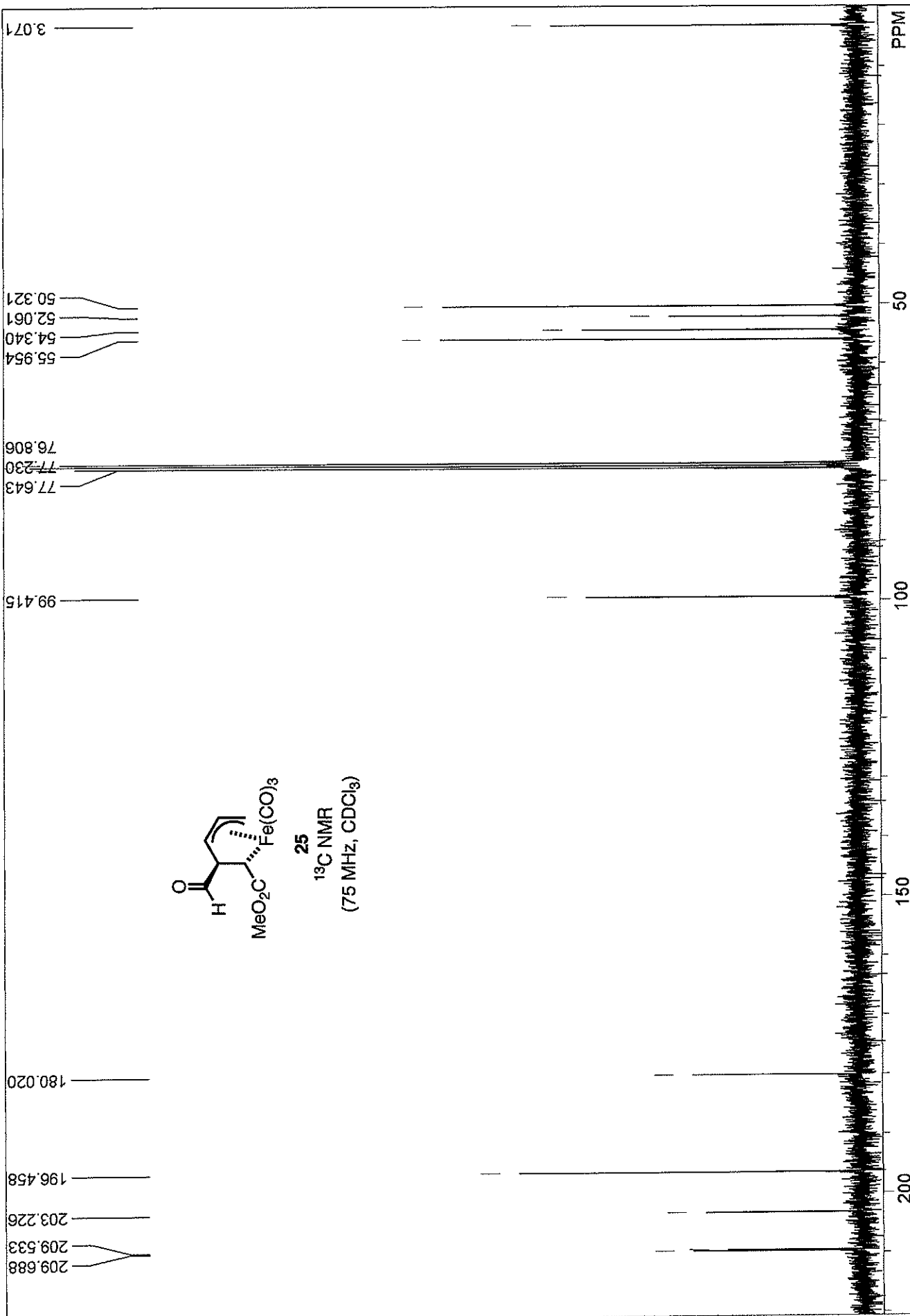
STANDARD 1H OBSERVE - profile		USER: -- DATE: Sep 24 2007	
F1: 399.751	F2: 100.526	PTS1d: 13132	16384
SW1: 6410	OF1: 2402.1	LB: 0.0	Nuts - \$1w76-2H1-400.fid
PW: 8.0 us	NA: 64		
PD: 1.0 sec			
EX: s2pul			



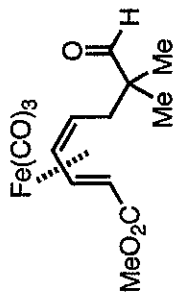
13C OBSERVE: blank line  
 F1: 75.477 F2: 300.135 SW1: 18868  
 EX: s2pul PD: 1.0 sec NA: 15000 OF1: 8300.2  
 PTS1d: 34246 65536 I.B: 0.7  
 USER: -- DATE: Sep 24 2007  
 Nuts - \$lw76-C13-300.fid



STANDARD 1H OBSERVE:blank line  
 F1: 300.142 F2: 75.478 SW1: 4803 PD: 1.0 sec  
 EX: s2pul PW: 6.3 us NA: 8 OF1: 1802.7 LB: 0.0  
 PTS1d: 14409 16384  
 USER: -- DATE: Dec 31 2004  
 Nuts - \$nw11rechrom-2.fid

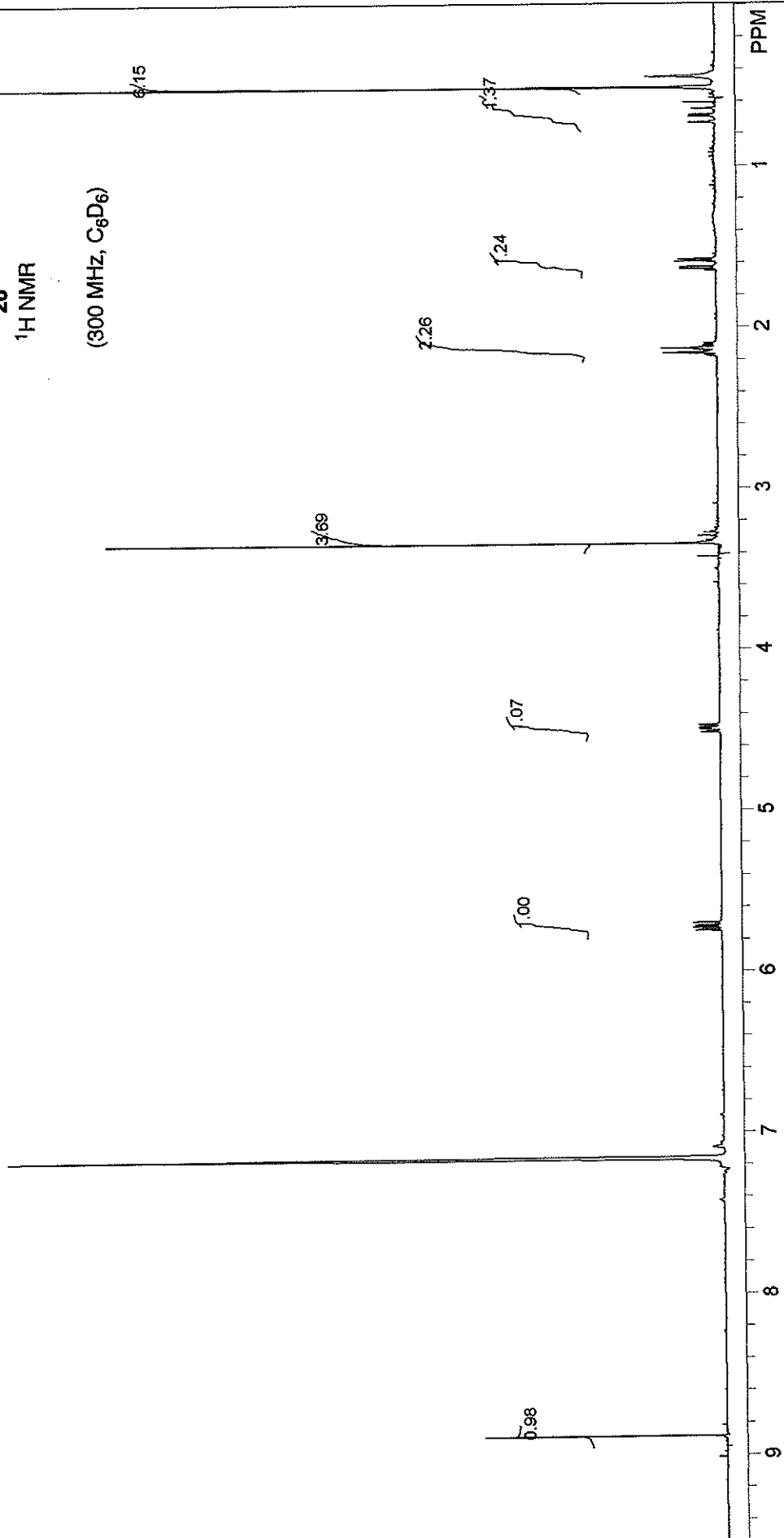


I3C OBSERVE: blank line		USER: -- DATE: Dec 31 2004	
F1: 75.479	F2: 300.142	PTS1d: 18868	32768
EX: s2pul	SW1: 18868	NA: 480	LB: 1.0
	PW: 7.3 us	PD: 1.0 sec	

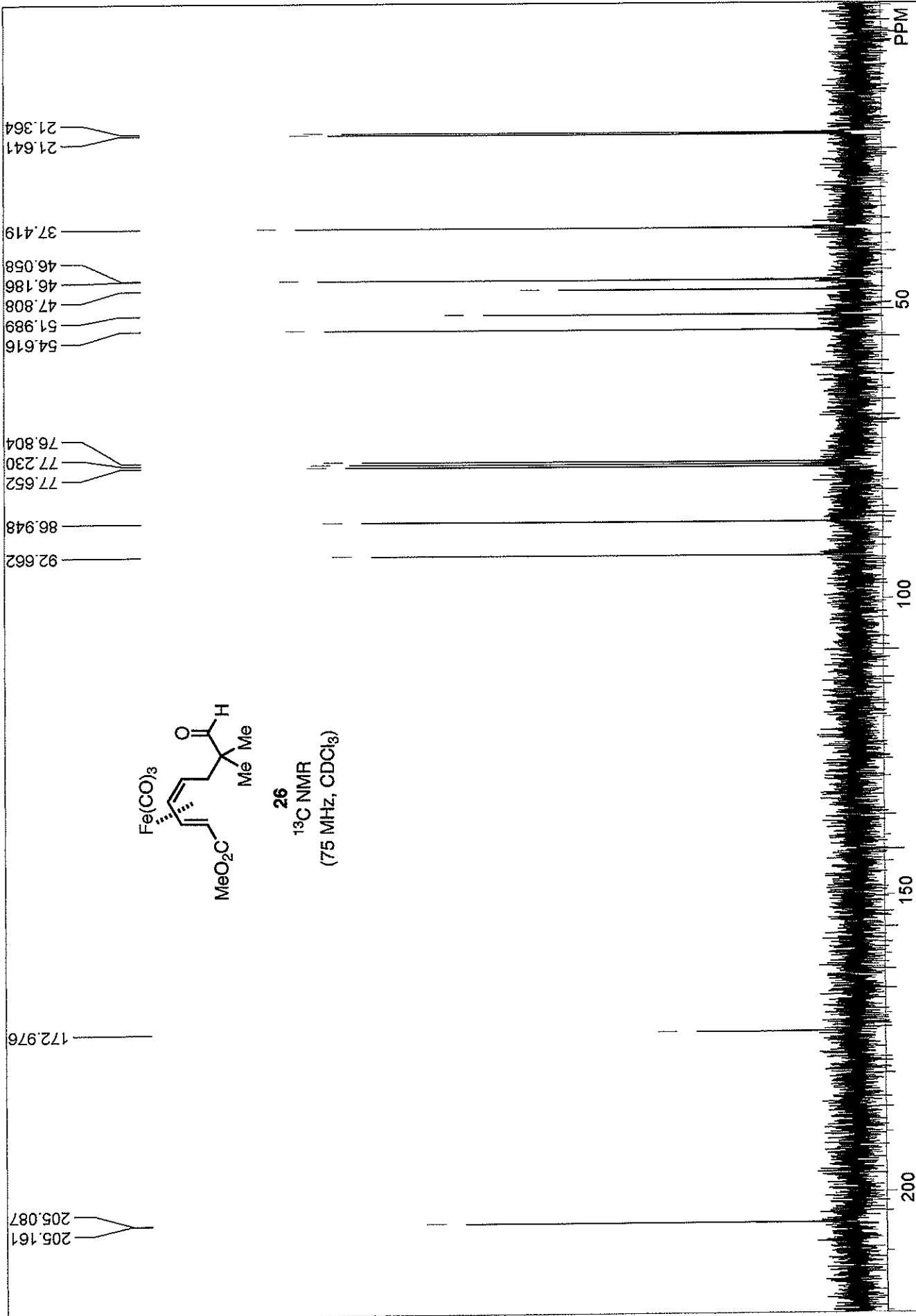


26  
1H NMR

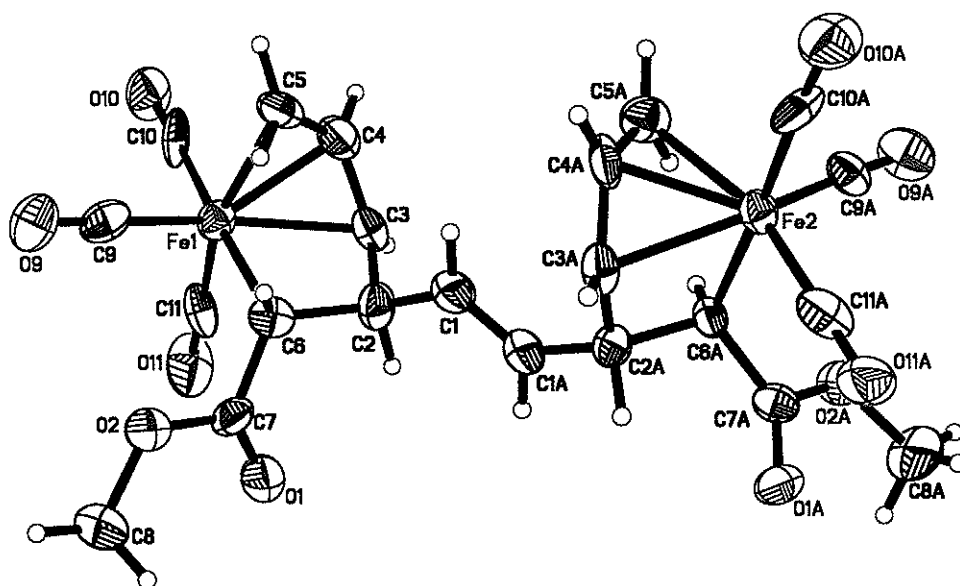
(300 MHz, C6D6)



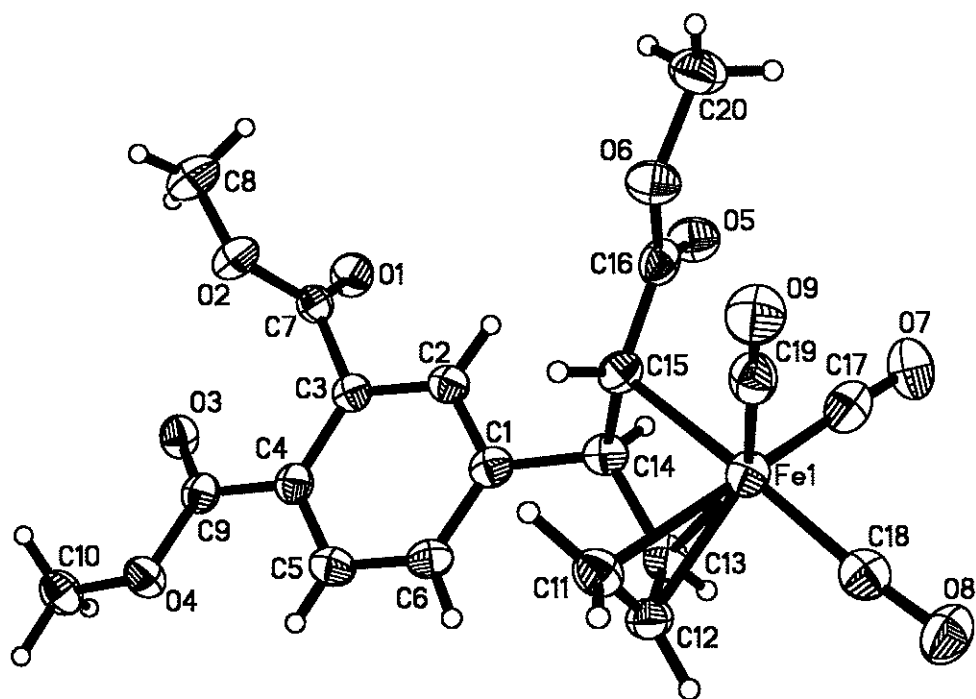
STANDARD 1H OBSERVE; blank line		USER: -- DATE: Jan 2 2005	
F1: 300.142	F2: 75.478	PTSId: 14409	16384
EX: s2pul	SW1: 4803	OF1: 1812.8	Nuts - \$nw8chrom-C6D6.fid
	PW: 6.3 us	NA: 8	LB: 0.0
	PD: 1.0 sec		



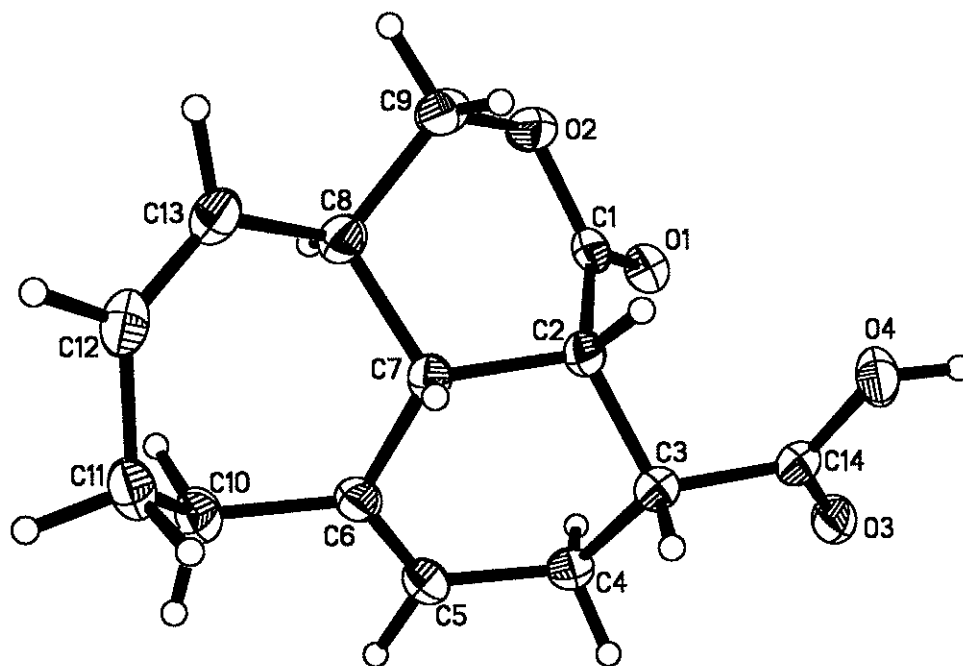
13C OBSERVE: blank line		USER: -- DATE: Sep 27 2004	
F1: 75.479	F2: 300.142	PTSID: 18868	32768
EX: s2pul	PW: 7.3 us	OF1: 8292.6	LB: 1.0
	PD: 1.0 sec	NA: 128	Nuts - \$nw8chromC13.frd

ORTEP of bimetallic complex *dl-7*





ORTEP of 3-pentene-1,5-diyl complex 15



ORTEP of product (21) from cycloaddition of 4i with maleic anhydride