

11-1-2012

# Spectral Data for "Reactivity of acyclic (pentadienyl)iron(1+) cations: Synthetic studies directed toward the frondosins"

Do W. Lee  
*Marquette University*

Rajesh K. Pandey  
*Marquette University*

Sergey V. Lindeman  
*Marquette University, sergey.lindeman@marquette.edu*

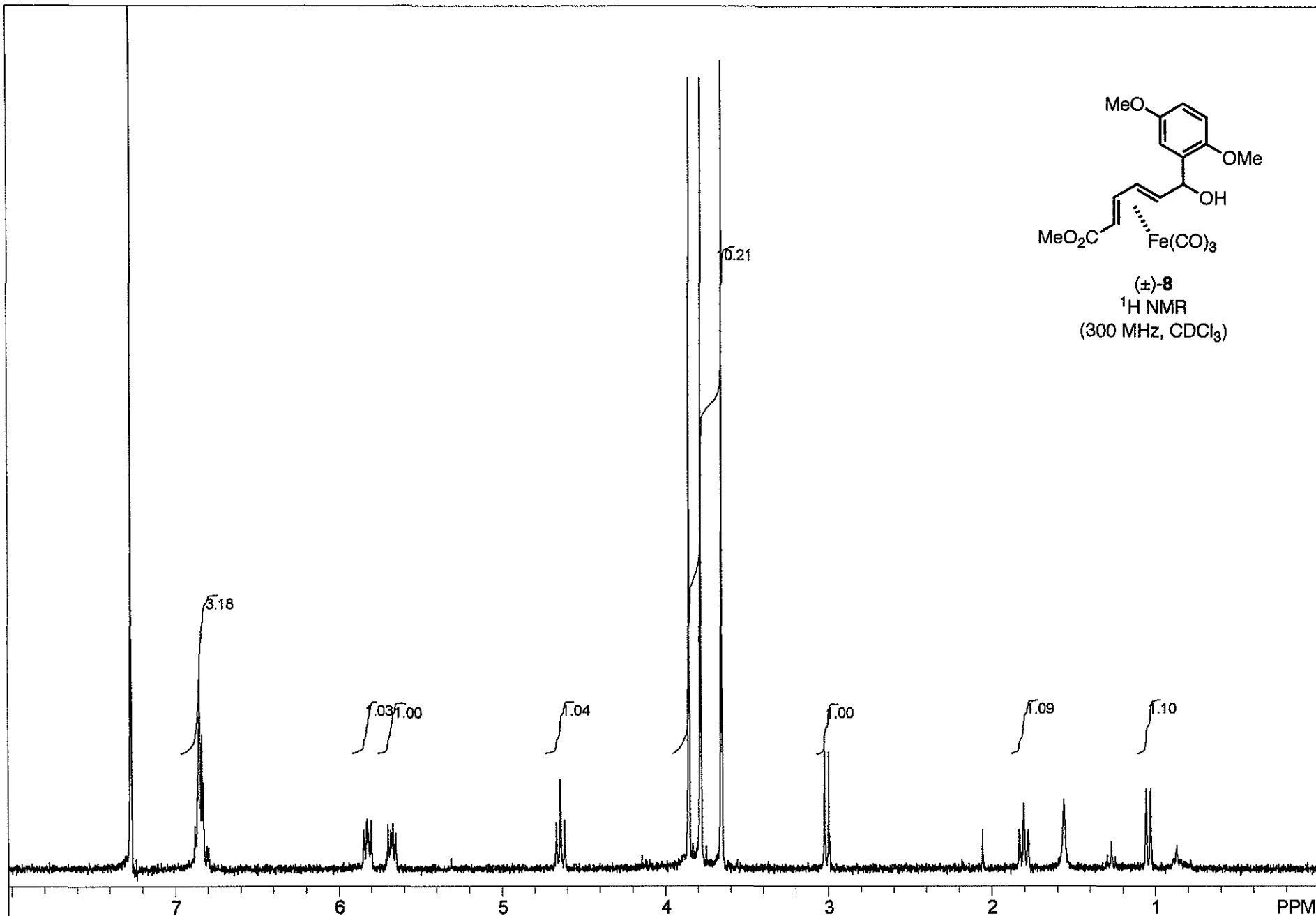
William A. Donaldson  
*Marquette University, william.donaldson@marquette.edu*

---

*Electronic Supporting Information***Reactivity of acyclic (pentadienyl)iron(1+) cations: Synthetic studies directed toward the frondosins**

Do W. Lee, Rajesh K. Pandey, Sergey Lindeman, and William A. Donaldson\*

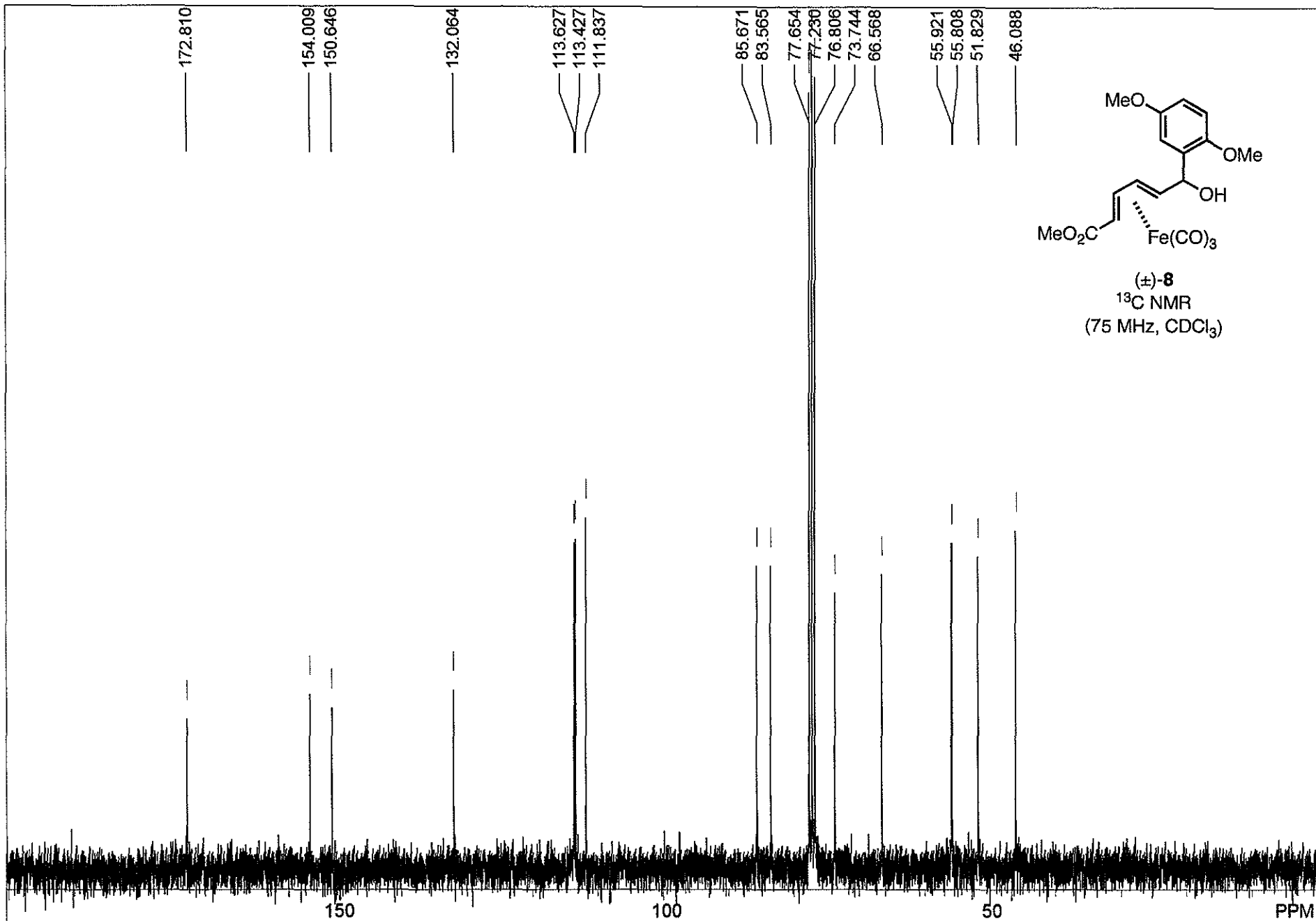
<sup>1</sup> H NMR spectrum of (±)- <b>8</b> (CDCl <sub>3</sub> )	S2
<sup>13</sup> C NMR spectrum of (±)- <b>8</b> (CDCl <sub>3</sub> )	S3
<sup>1</sup> H NMR spectrum of (±)- <b>9a</b> (CD <sub>3</sub> NO <sub>2</sub> )	S4
<sup>13</sup> C NMR spectrum of (±)- <b>9a</b> (CD <sub>3</sub> NO <sub>2</sub> )	S5
<sup>1</sup> H NMR spectrum of (±)- <b>10</b> (CDCl <sub>3</sub> )	S6
<sup>13</sup> C NMR spectrum of (±)- <b>10</b> (CDCl <sub>3</sub> )	S7
<sup>1</sup> H NMR spectrum of (±)- <b>11</b> (CDCl <sub>3</sub> )	S8
<sup>13</sup> C NMR spectrum of (±)- <b>11</b> (CDCl <sub>3</sub> )	S9
<sup>1</sup> H NMR spectrum of (±)- <b>15</b> (CDCl <sub>3</sub> )	S10
<sup>13</sup> C NMR spectrum of (±)- <b>15</b> (CDCl <sub>3</sub> )	S11
<sup>1</sup> H NMR spectrum of (±)- <b>16a</b> (CDCl <sub>3</sub> )	S12
<sup>13</sup> C NMR spectrum of (±)- <b>16a</b> (CDCl <sub>3</sub> )	S13
<sup>1</sup> H NMR spectrum of (±)- <b>17a</b> (CDCl <sub>3</sub> )	S14
<sup>13</sup> C NMR spectrum of (±)- <b>17a</b> (CDCl <sub>3</sub> )	S15
<sup>1</sup> H NMR spectrum of (±)- <b>16b</b> (CDCl <sub>3</sub> )	S16
<sup>13</sup> C NMR spectrum of (±)- <b>16b</b> (CDCl <sub>3</sub> )	S17
<sup>1</sup> H NMR spectrum of (±)- <b>17b</b> (CDCl <sub>3</sub> )	S18
<sup>13</sup> C NMR spectrum of (±)- <b>17b</b> (CDCl <sub>3</sub> )	S19
<sup>1</sup> H NMR spectrum of (±)- <b>12</b> (CDCl <sub>3</sub> )	S20
<sup>13</sup> C NMR spectrum of (±)- <b>12</b> (CDCl <sub>3</sub> )	S21
<sup>1</sup> H NMR spectrum of (±)- <b>18a</b> (CDCl <sub>3</sub> )	S22
<sup>13</sup> C NMR spectrum of (±)- <b>18a</b> (CDCl <sub>3</sub> )	S23
<sup>1</sup> H NMR spectrum of (±)- <b>18b</b> (CDCl <sub>3</sub> )	S24
<sup>13</sup> C NMR spectrum of (±)- <b>18b</b> (CDCl <sub>3</sub> )	S25
ORTEP of (±)- <b>10</b>	S26
ORTEP of (±)- <b>11</b>	S26
ORTEP of (±)- <b>15</b>	S27
ORTEP of (±)- <b>16a</b>	S27



STANDARD 1H OBSERVE:blank line

USER: -- DATE: Feb 20 2008

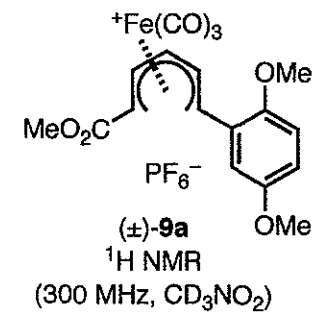
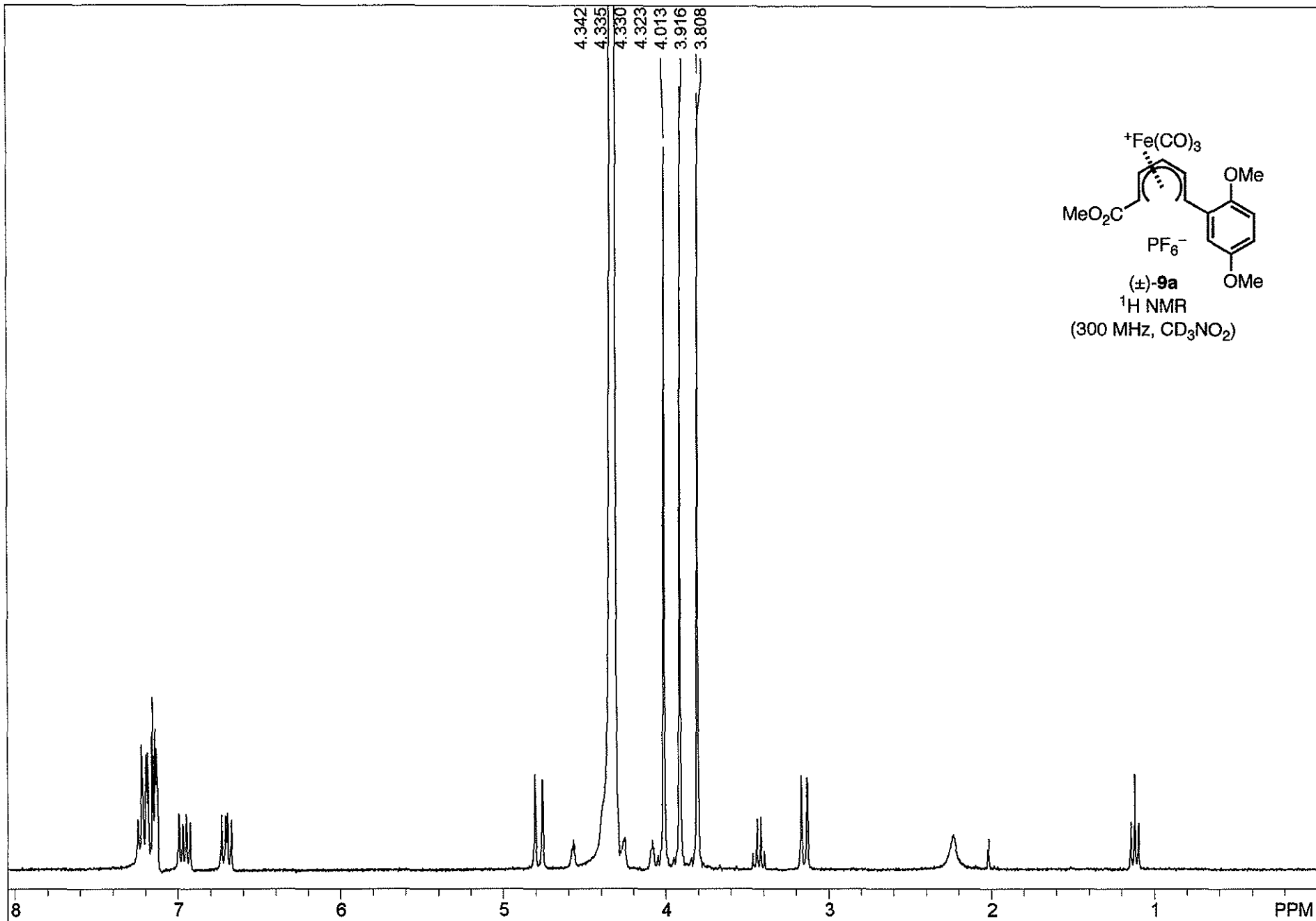
F1: 300.136	F2: 75.476	SW1: 4803		OF1: 1716.6		PTS1d: 9596 , 16384
EX: s2pul	PW: 6.3 us	PD: 1.0 sec	NA: 8	LB: 0.0		Nuts - \$rkp252-HNMR.fid



<sup>13</sup>C OBSERVE: blank line

USER: -- DATE: Feb 20 2008

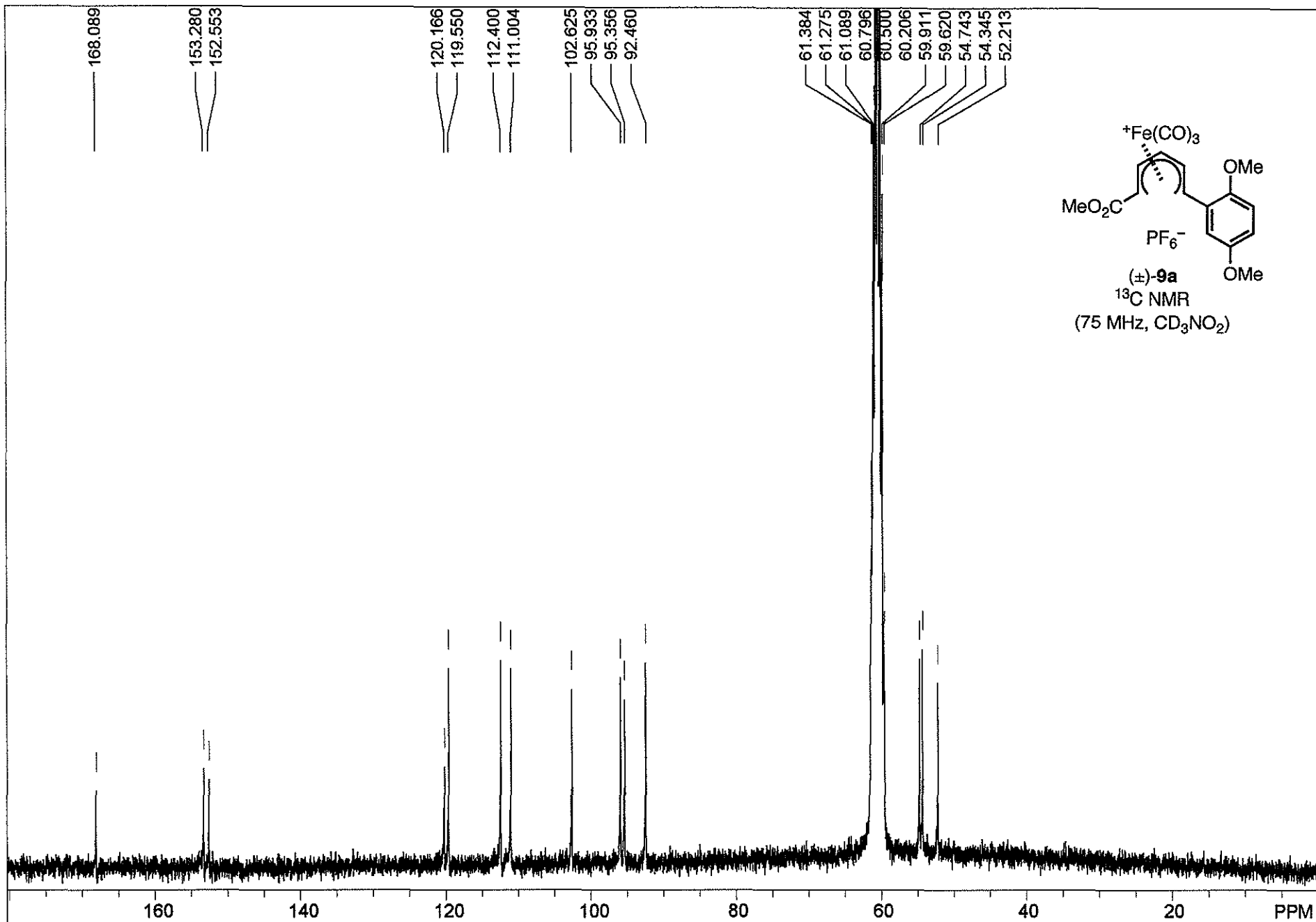
F1: 75.477	F2: 300.135	SW1: 18868	OF1: 8277.9	PTS1d: 34246	65536
EX: s2pul	PW: 7.3 us	PD: 1.0 sec	NA: 320	LB: 1.0	Nuts - \$rpk252-CNMR.fid



STANDARD 1H OBSERVE:blank line

USER: -- DATE: Dec 20 2007

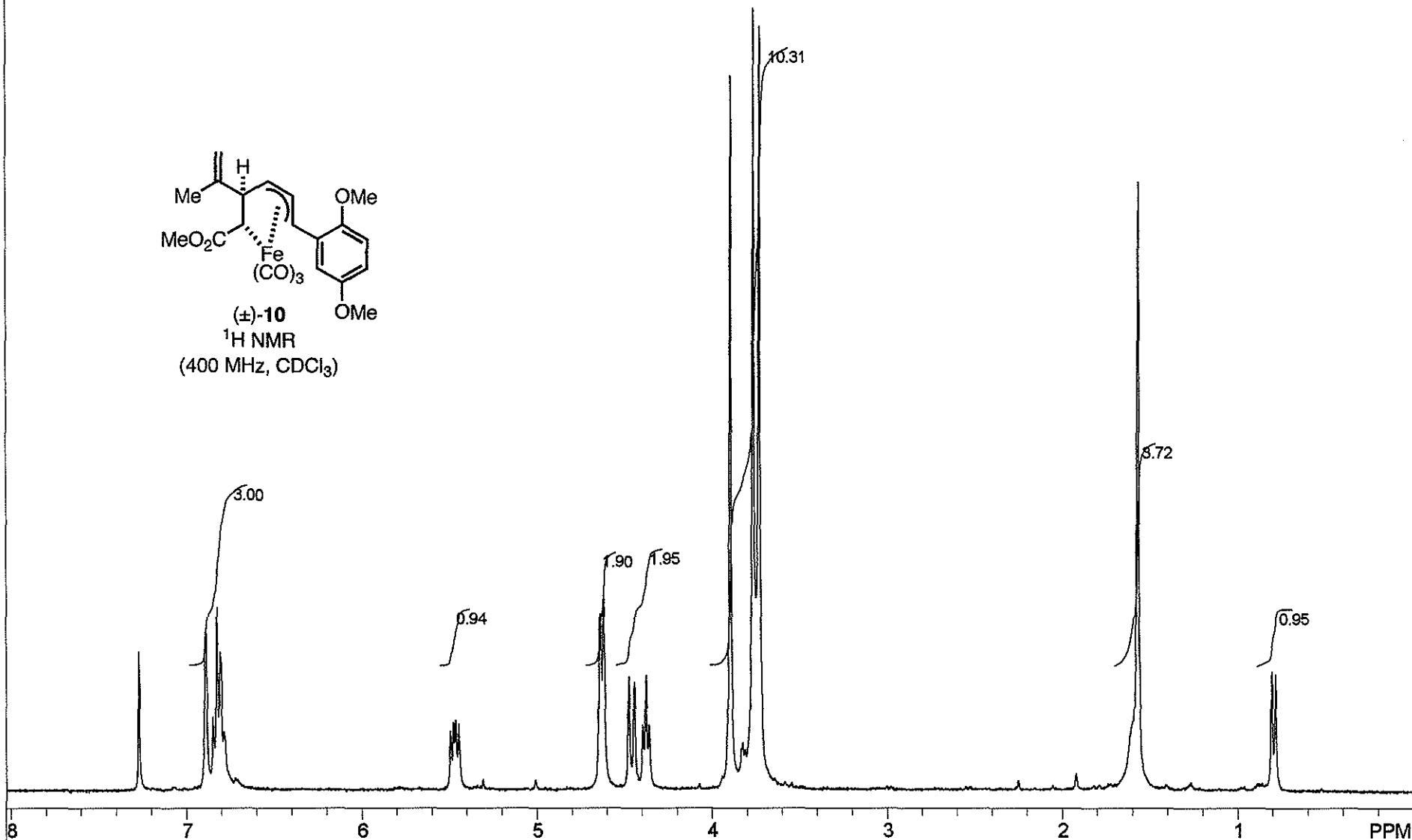
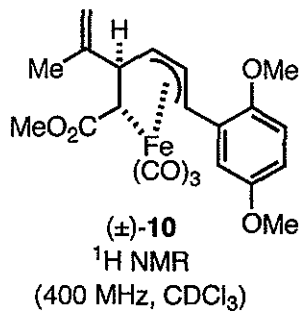
FI: 300.137	F2: 75.477	SW1: 4803	OF1: 2393.0	PTS1d: 9596	16384
EX: s2pul	PW: 6.3 us	PD: 1.0 sec	NA: 64	LB: 0.0	Nuts - \$rkp246.fid



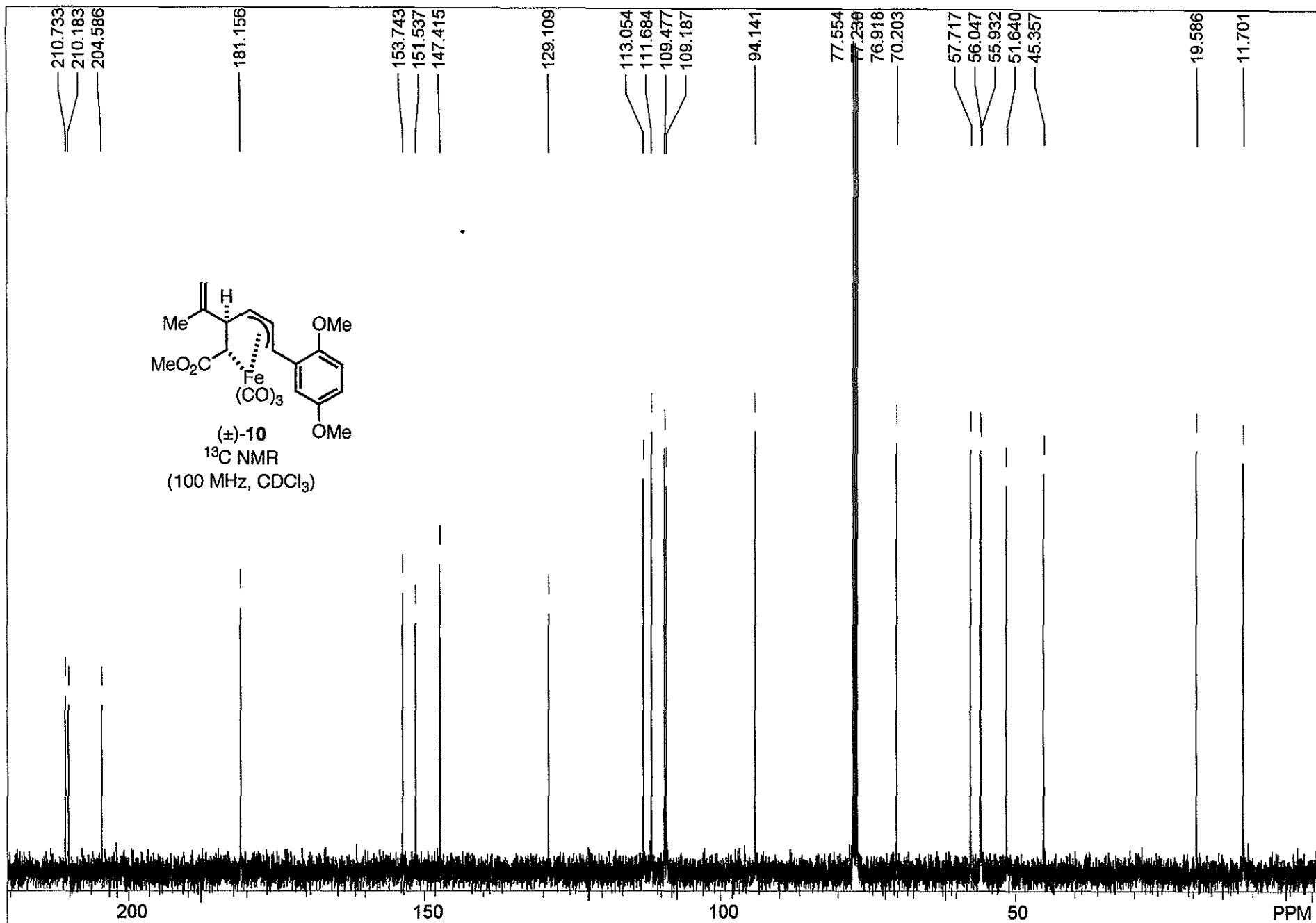
$^{13}\text{C}$  OBSERVE: blank line

USER: -- DATE: Dec 21 2007

F1: 75.477	F2: 300.137	SW1: 18868	OF1: 8274.4	PTS1d: 34246	65536
EX: s2pul	PW: 7.3 us	PD: 1.0 sec	NA: 320	LB: 1.0	Nuts - \$rkp246-CNMR.fid

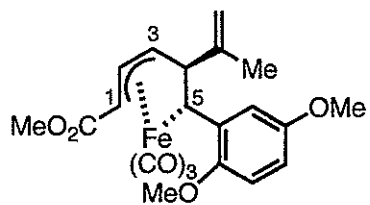


:blank line						USER: -- DATE: Jun 10 2010
F1: 399.746	F2: 100.525	SW1: 6410		OF1: 2403.3		PTS1d: 13132 , 1638#
EX: s2pul	PW: 8.0 us	PD: 1.0 sec	NA: 8	LB: 0.0	Nuts - \$Isopropenylironcomplex-0610-1H.fid	

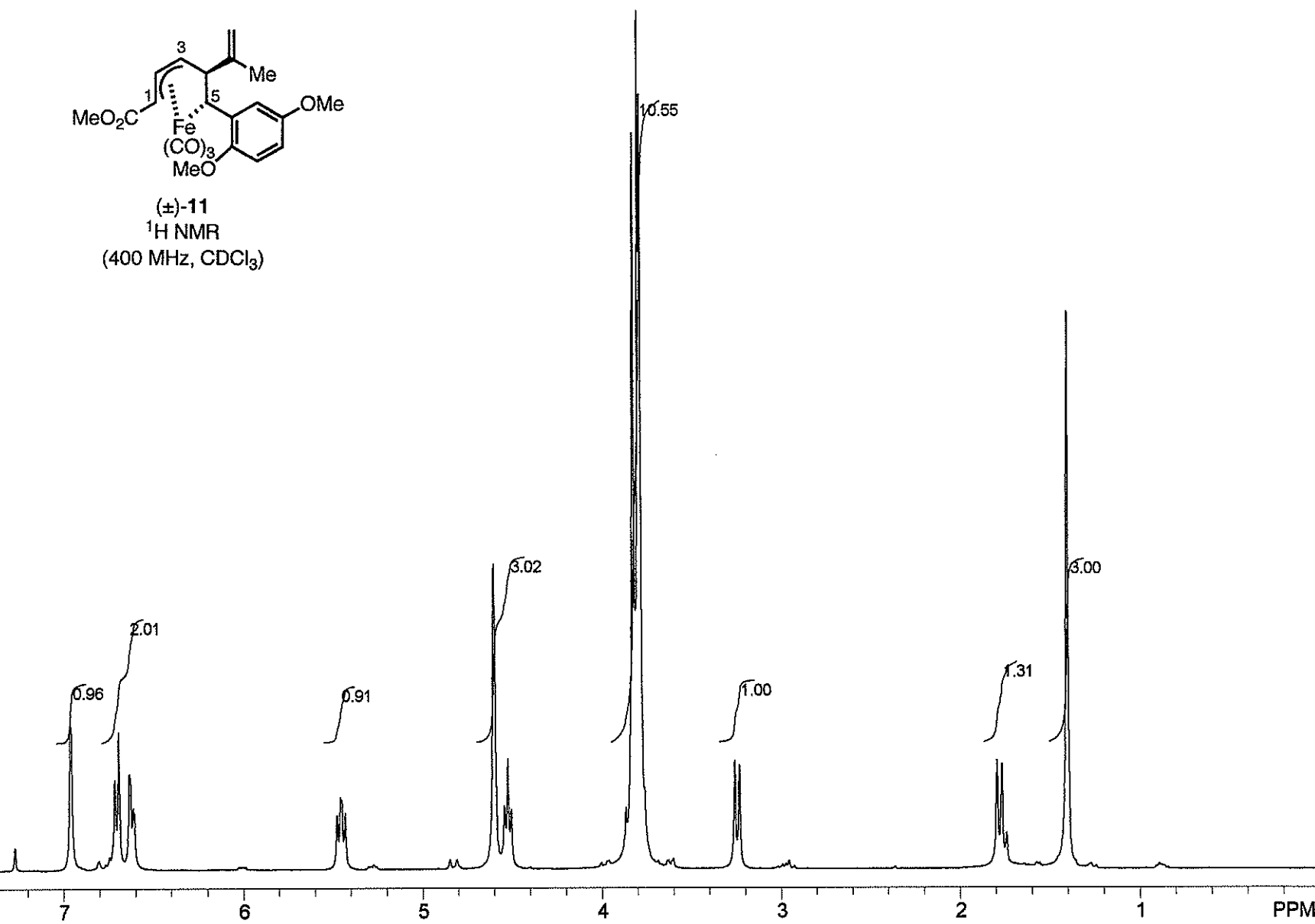


:blank line			USER: -- DATE: Jun 10 2010			
F1: 100.526	F2: 399.745	SW1: 24510		OF1: 10574.1		PTS1d: 31875 , 32768
EX: s2pul	PW: 5.8 us	PD: 1.0 sec	NA: 1024	LB: 1.0	Nuts - \$Isopropenylironcomplex-0610-13C.fid	

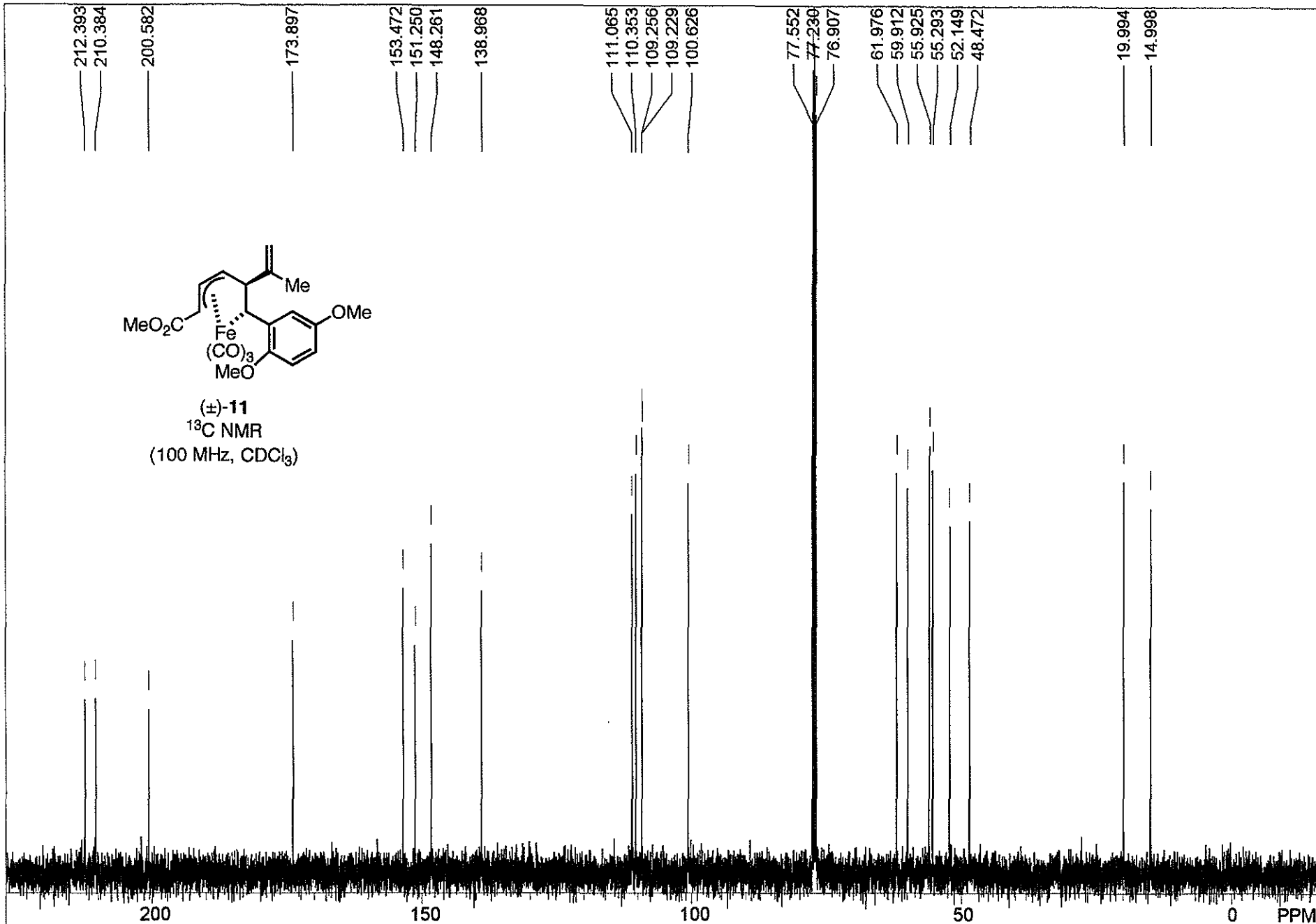




(±)-11  
<sup>1</sup>H NMR  
 (400 MHz, CDCl<sub>3</sub>)



.blank line				USER: -- DATE: Jun 18 2010			
F1: 399.746	F2: 100.525	SW1: 6410		OF1: 2403.5		PTS1d: 13132 , 16384	
EX: s2pul	PW: 8.0 us	PD: 1.0 sec	NA: 8	LB: 0.0	Nuts - \$Isopropenylironcomplex-1stband-0618-1H.fid		



:blank line

USER: -- DATE: Jun 18 2010

F1: 100.526

F2: 399.745

SW1: 24510

OF1: 10573.8

PTS1d: 31875 . 32768

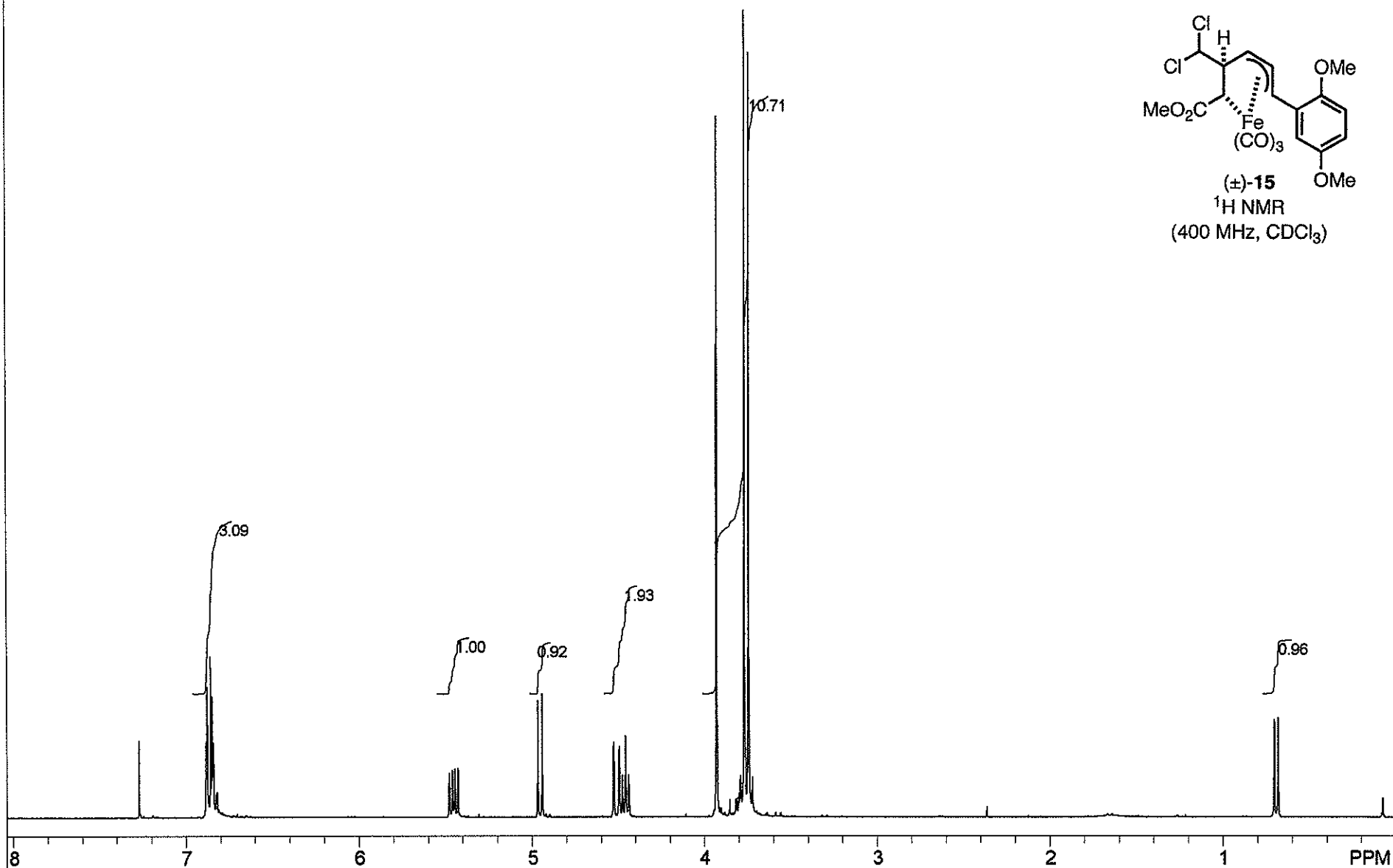
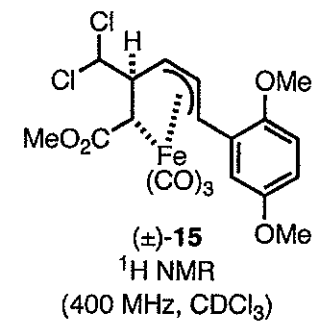
EX: s2pul

PW: 5.8 us

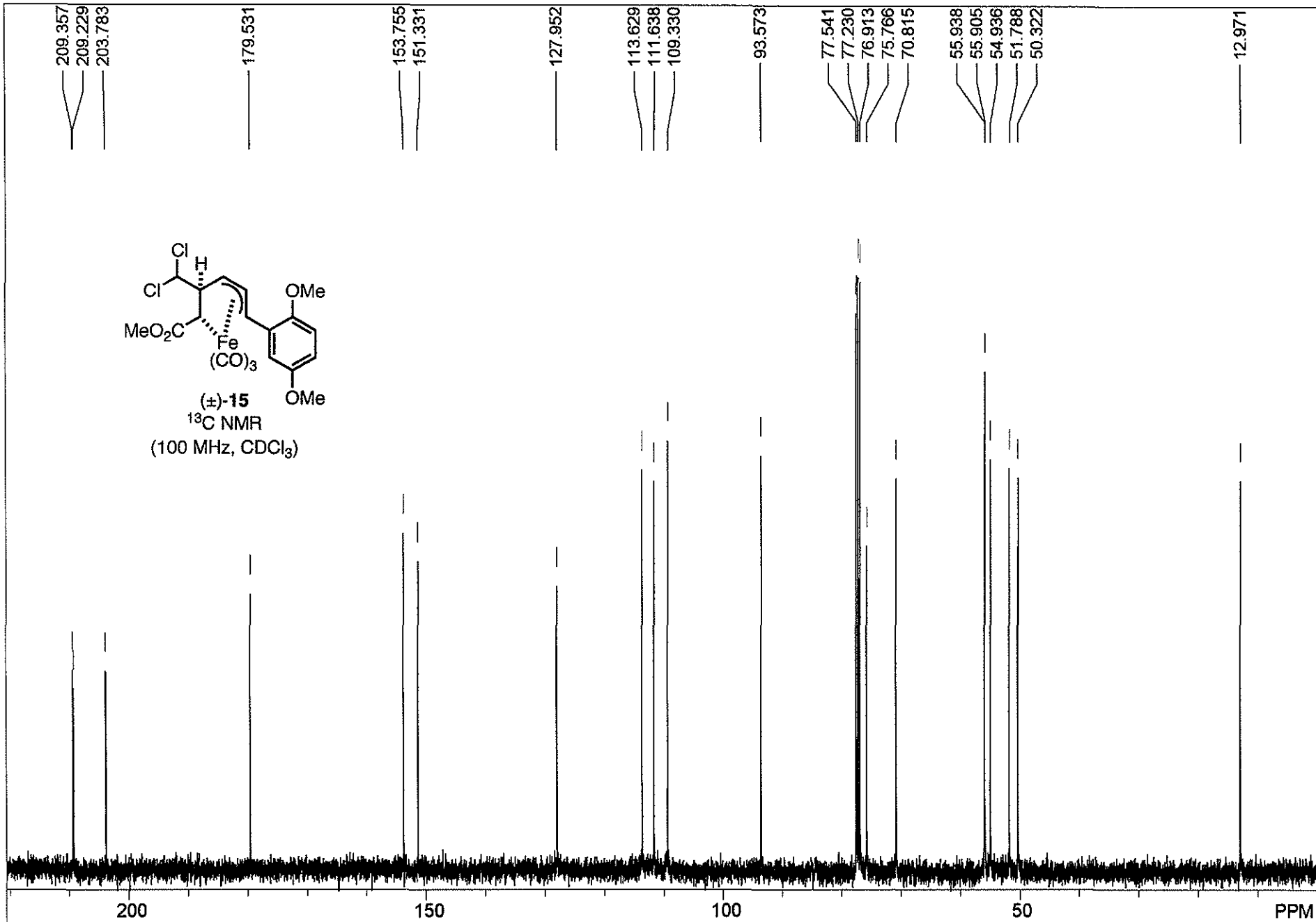
PD: 1.0 sec

NA: 512

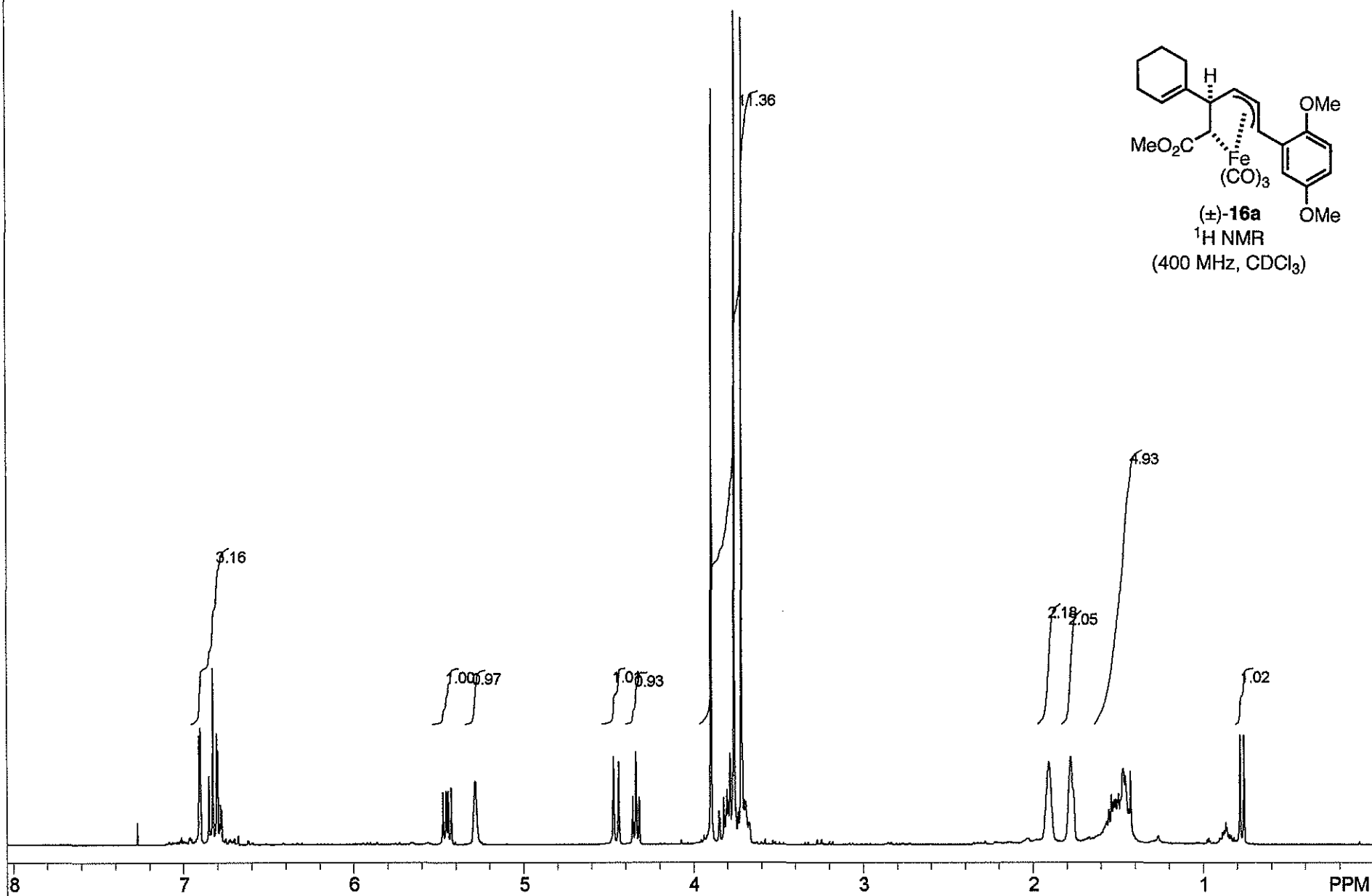
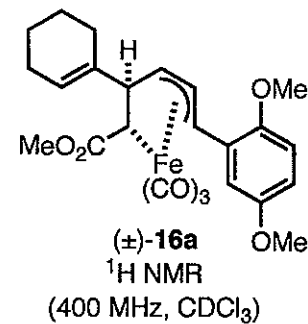
LB: 1.0 Nuts - \$Isopropenylironcomplex-1stband-0618-13C.fid



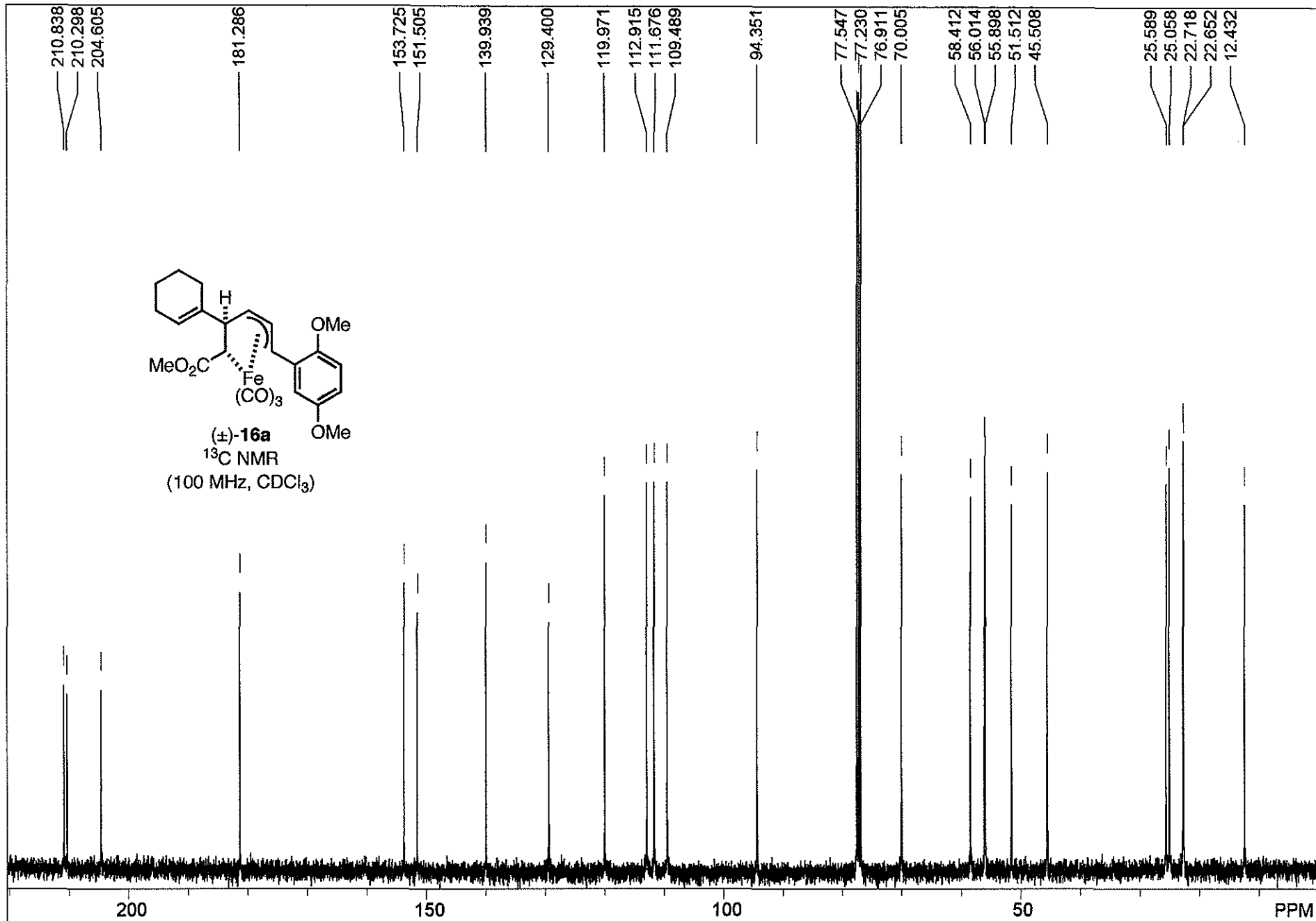
:blank line						USER: -- DATE: Aug 10 2010
F1: 399.746	F2: 100.525	SW1: 6410		OF1: 2403.5		PTS1d: 13132 . 16384
EX: s2pul	PW: 8.0 us	PD: 1.0 sec	NA: 8	LB: 0.0		Nuts - \$dlee0810-1-1H.fid



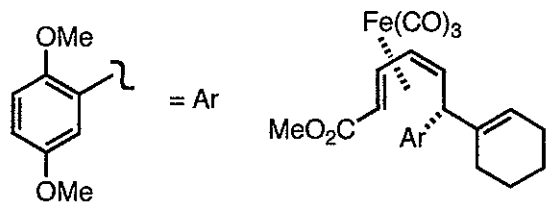
:blank line						USER: -- DATE: Aug 10 2010
F1: 100.526	F2: 399.745	SW1: 24510		OF1: 10568.7		PTS1d: 31875 , 32768
EX: s2pul		PW: 5.8 us	PD: 1.0 sec	NA: 628	LB: 1.0	Nuts - \$dlee0810-1-13C.fid



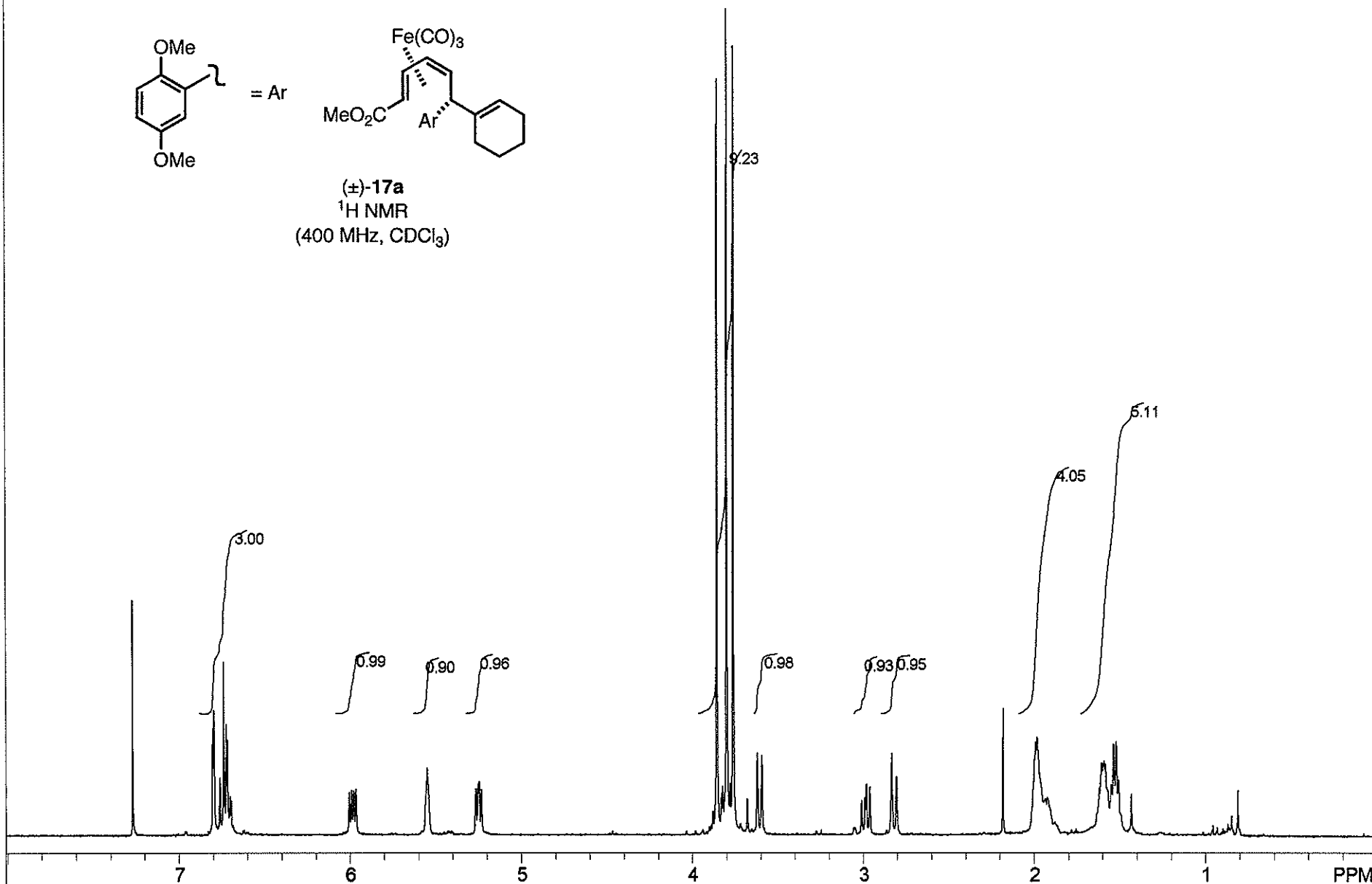
.blank line						USER: -- DATE: Sep 1 2010
F1: 399.746	F2: 100.525	SW1: 6410		OF1: 2403.2		PTS1d: 13132 , 16384
EX: s2pul	PW: 8.0 us	PD: 1.0 sec	NA: 8	LB: 0.0		Nuts - \$dlee090110-2-1H.fid



:blank line			USER: -- DATE: Sep 13 2010			
F1: 100.526	F2: 399.745	SW1: 24510		OF1: 10570.0		PTS1d: 31875 . 32768
EX: s2pul	PW: 5.8 us	PD: 1.0 sec	NA: 1500	LB: 1.0	Nuts - \$dlee0913-2-13C.fid	

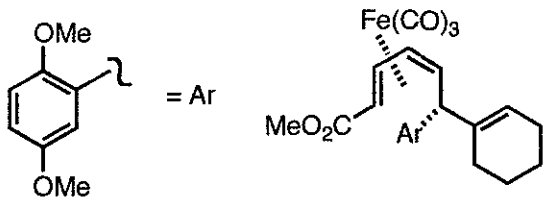


(±)-17a  
<sup>1</sup>H NMR  
 (400 MHz, CDCl<sub>3</sub>)

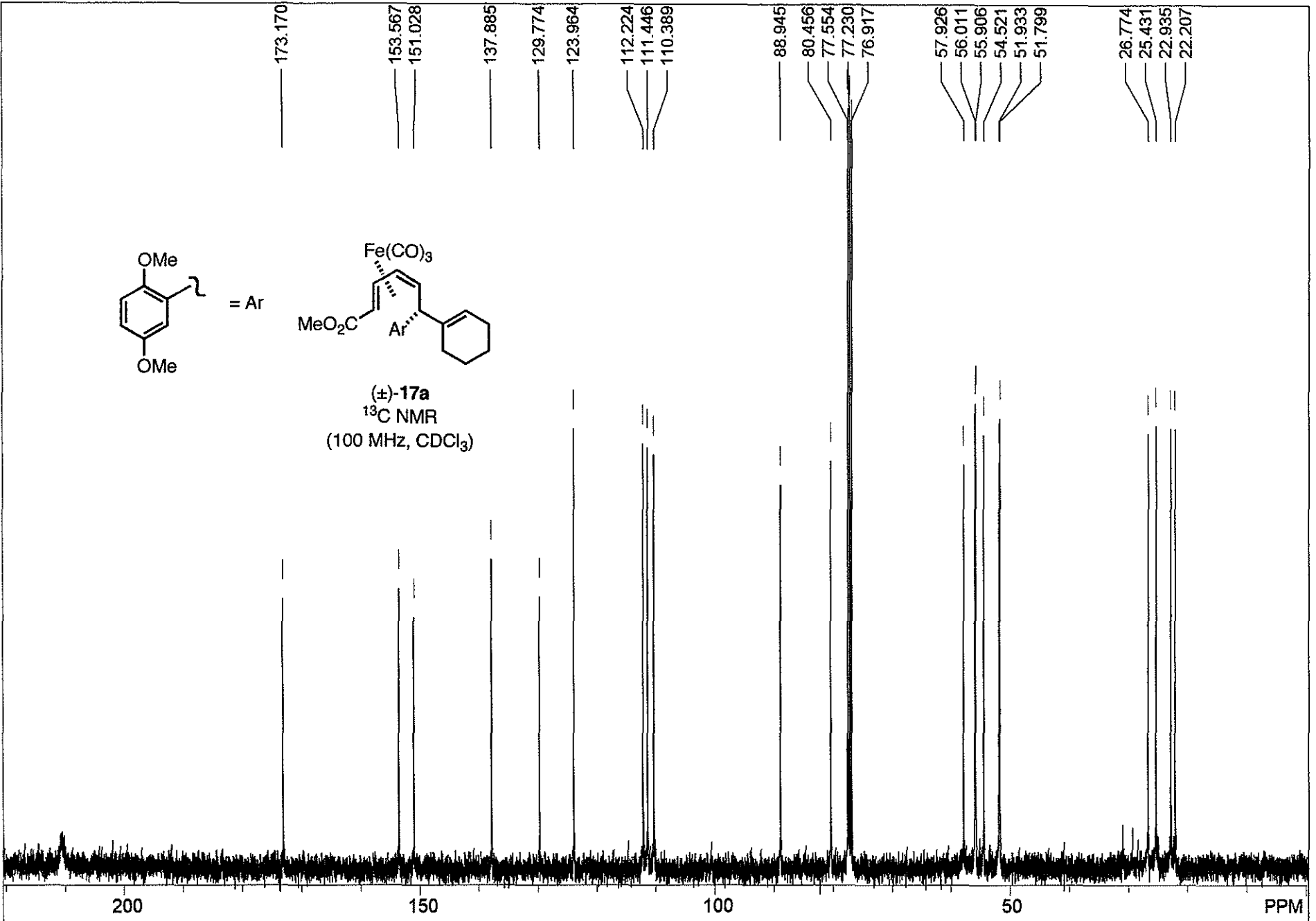


:blank line				USER: -- DATE: Sep 13 2010		
F1: 399.746	F2: 100.525	SW1: 6410		OF1: 2402.9		PTS1d: 13132 , 16384
EX: s2pul		PW: 8.0 us	PD: 1.0 sec	NA: 8	LB: 0.0	Nuts - \$dlee0913-1-1H.fid

173.170  
 153.567  
 151.028  
 137.885  
 129.774  
 123.964  
 112.224  
 111.446  
 110.389  
 88.945  
 80.456  
 77.554  
 77.230  
 76.917  
 57.926  
 56.011  
 55.906  
 54.521  
 51.933  
 51.799  
 26.774  
 25.431  
 22.935  
 22.207

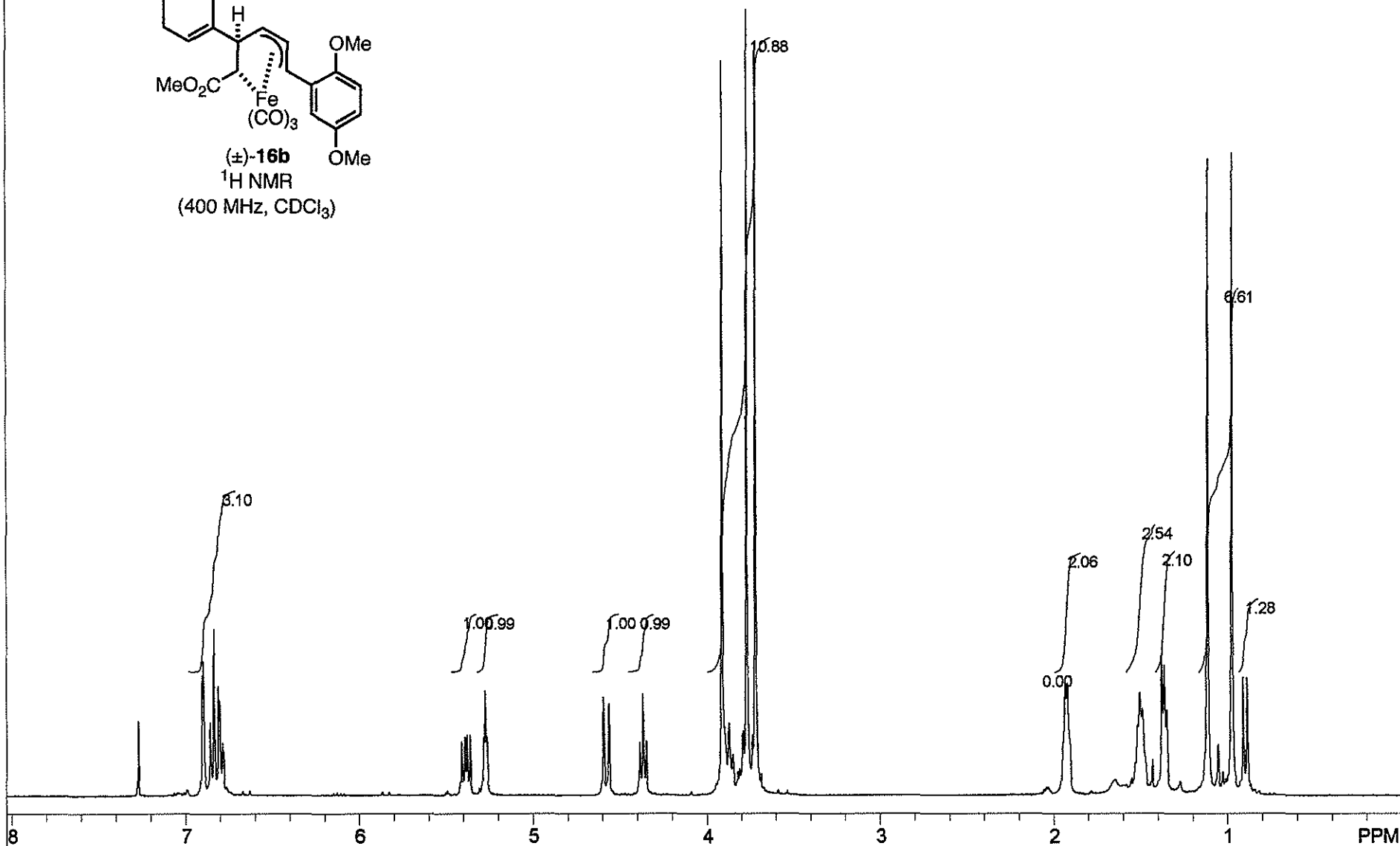
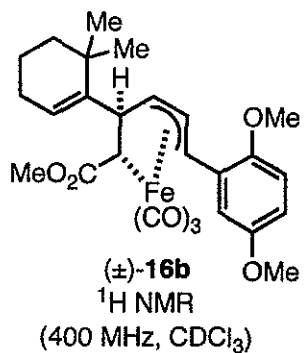


(±)-17a  
<sup>13</sup>C NMR  
 (100 MHz, CDCl<sub>3</sub>)

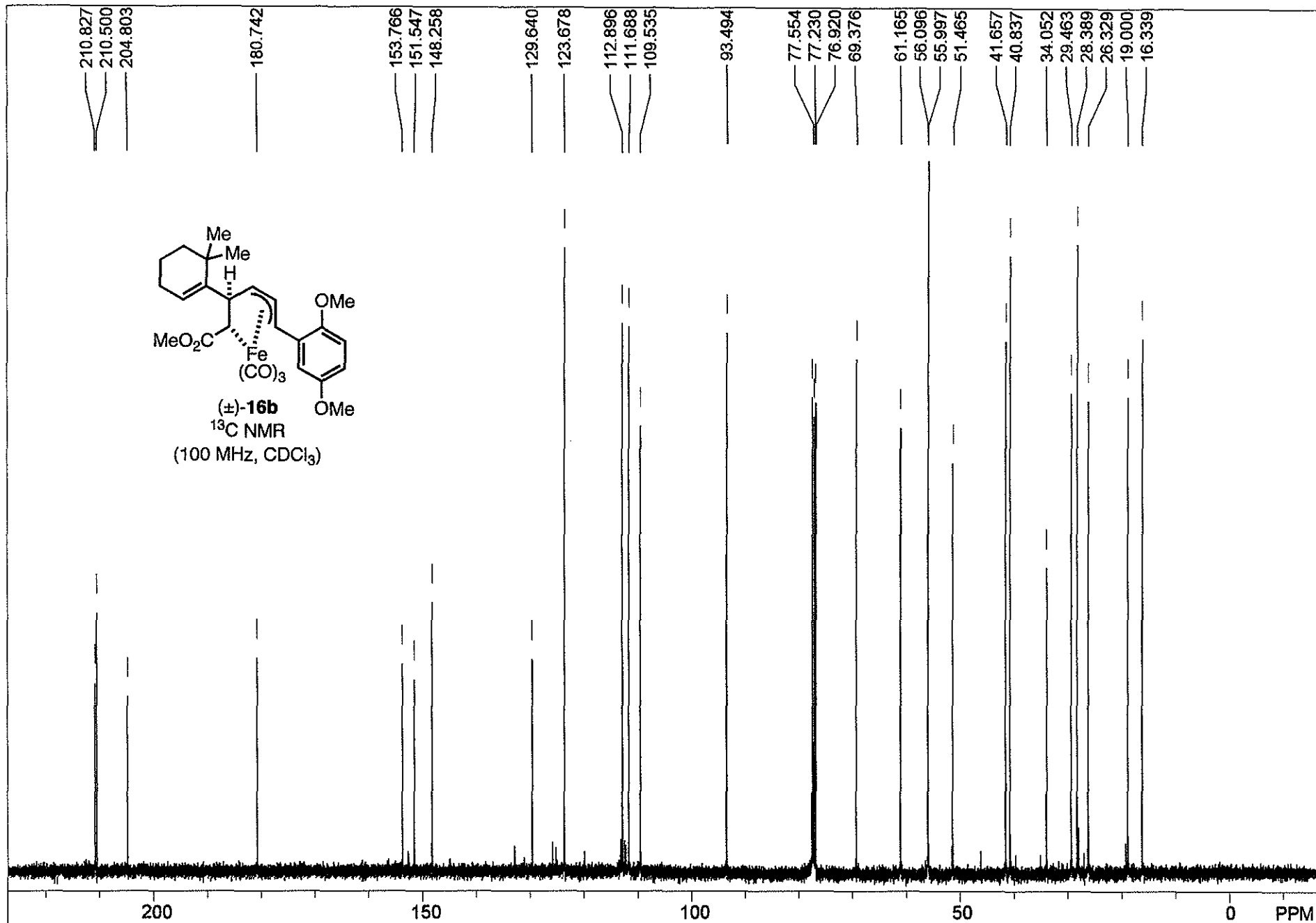


:blank line				USER: -- DATE: Sep 13 2010		
F1: 100.526	F2: 399.745	SW1: 24510		OF1: 10571.1		PTSId: 31875 . 32768
EX: s2pul	PW: 5.8 us	PD: 1.0 sec	NA: 1500	LB: 1.0		Nuts - \$dlee0913-1-13C.fid

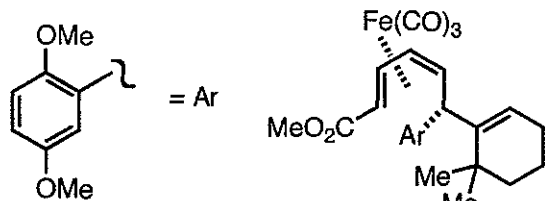




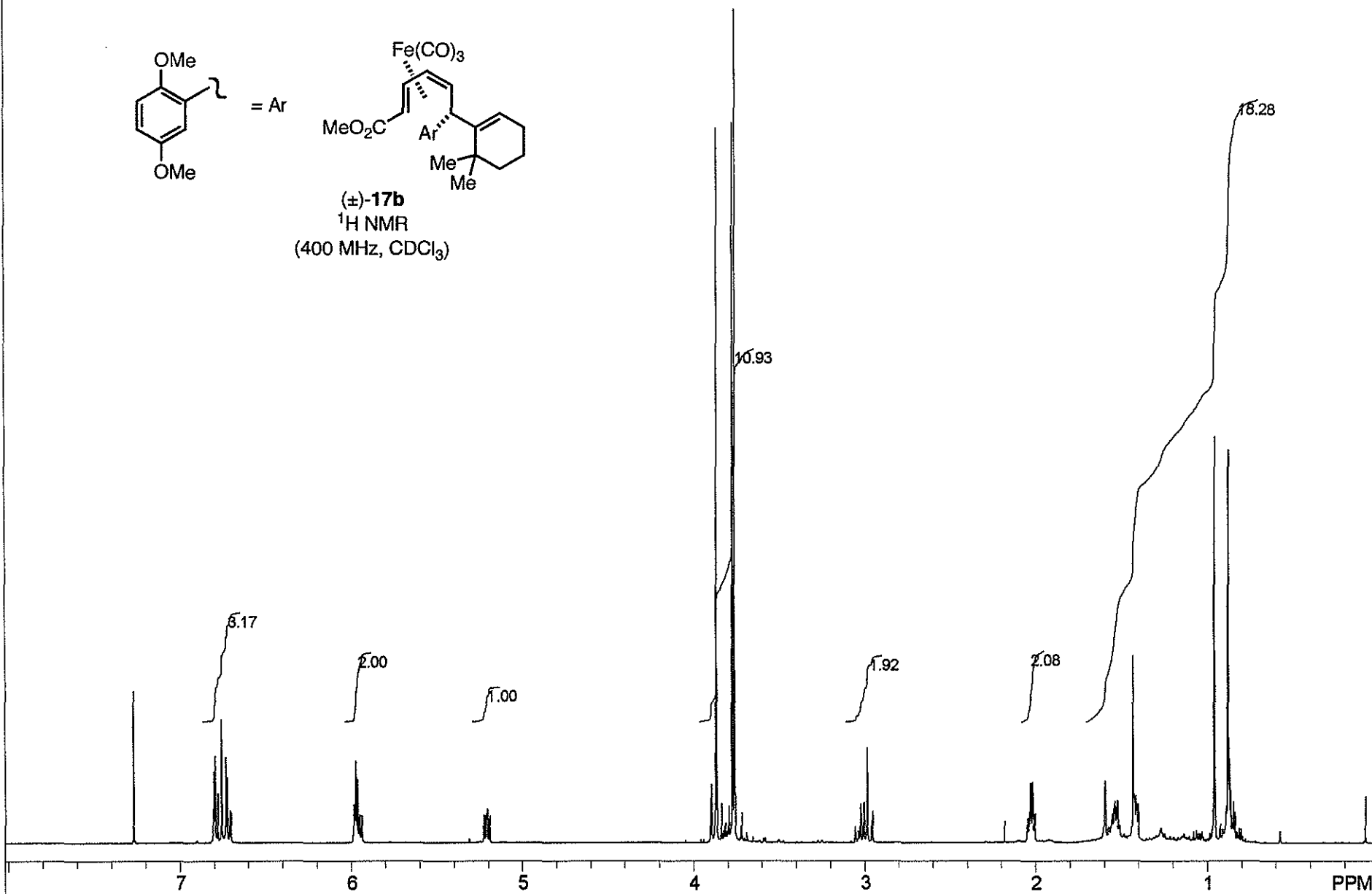
:blank line						USER: -- DATE: Nov 8 2010
F1: 399.746	F2: 100.525	SW1: 6410		OF1: 2403.5		PTS1d: 13132 . 16384
EX: s2pul		PW: 8.0 us	PD: 1.0 sec	NA: 8	LB: 0.0	Nuts - \$dlee110810-2-1H.fid



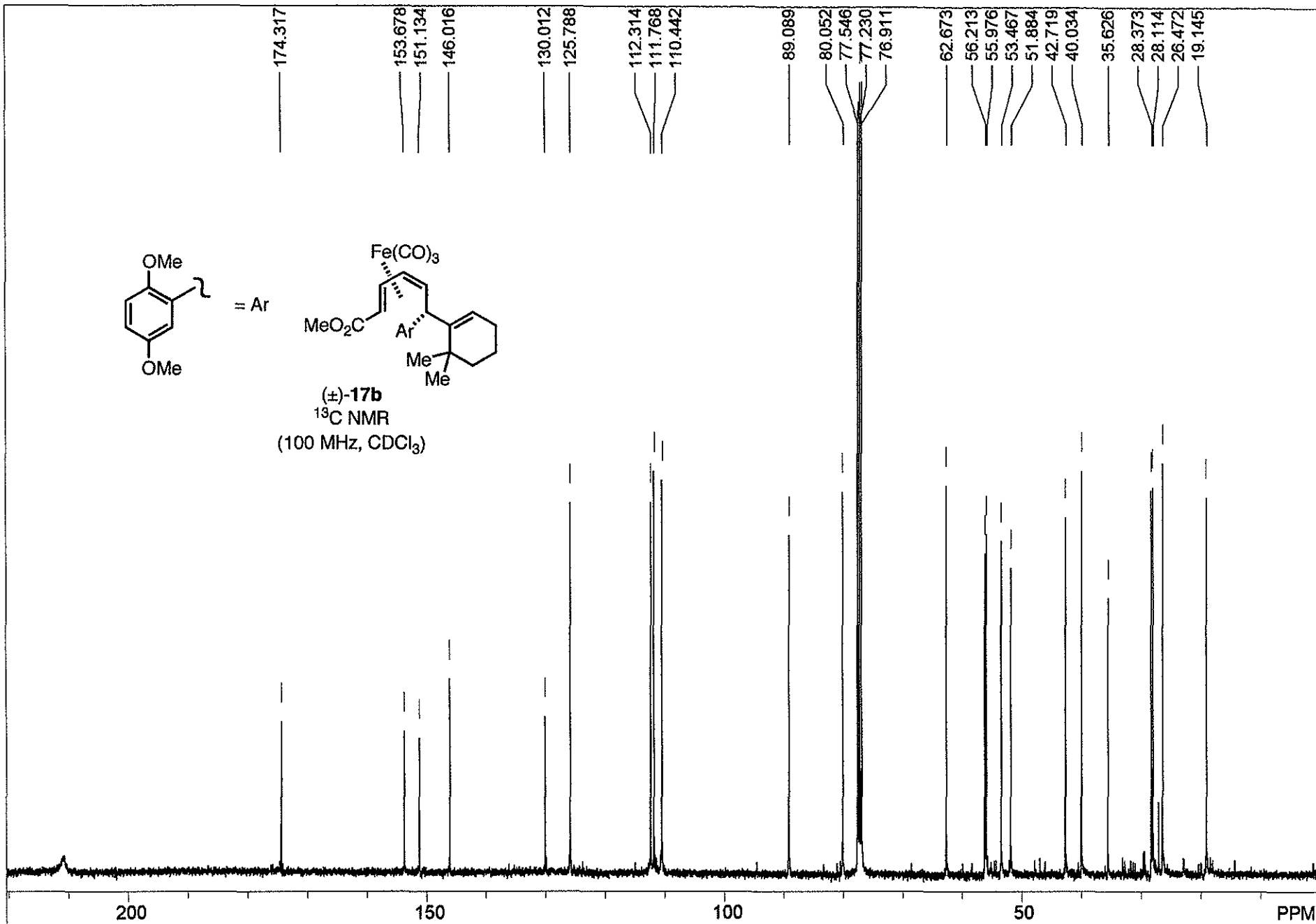
:blank line				USER: -- DATE: Nov 8 2010		
F1: 100.526	F2: 399.745	SW1: 24510	OF1: 10576.4	PTS1d: 31875 , 32768		
EX: s2pul	PW: 5.8 us	PD: 1.0 sec	NA: 15000	LB: 0.0	Nuts - \$dlee110810-2-13C.fid	



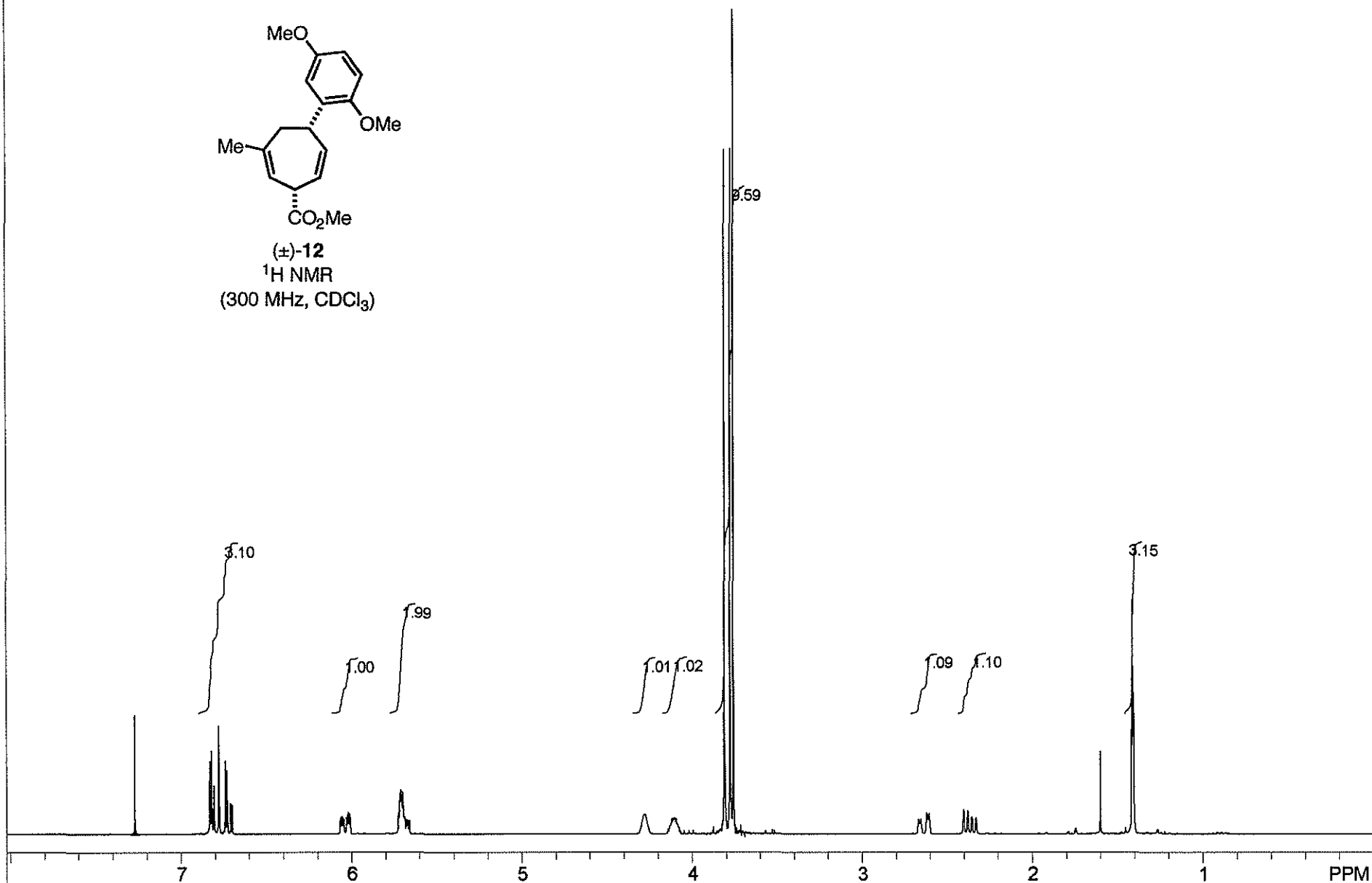
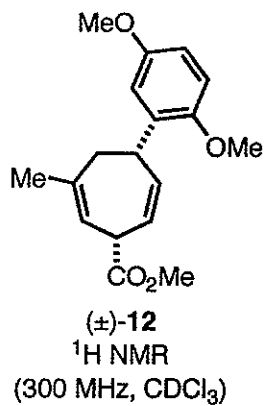
**(±)-17b**  
<sup>1</sup>H NMR  
 (400 MHz, CDCl<sub>3</sub>)



:blank line			USER: -- DATE: Nov 10 2010			
F1: 399.746	F2: 100.525	SW1: 6410	OF1: 2402.9	PTS1d: 13132	16384	
EX: s2pul	PW: 8.0 us	PD: 1.0 sec	NA: 8	LB: 0.0	Nuts - \$dlee111010-1-1H.fid	



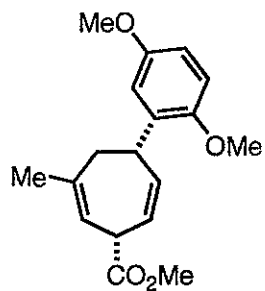
:blank line			USER: -- DATE: Nov 9 2010			
F1: 100.526	F2: 399.745	SW1: 24510		OF1: 10576.0		PTS1d: 31875 . 32768
EX: s2pul	PW: 5.8 us	PD: 1.0 sec	NA: 20000	LB: 1.0	Nuts - \$dlee111010-1-13C.fid	



STANDARD 1H OBSERVE:blank line

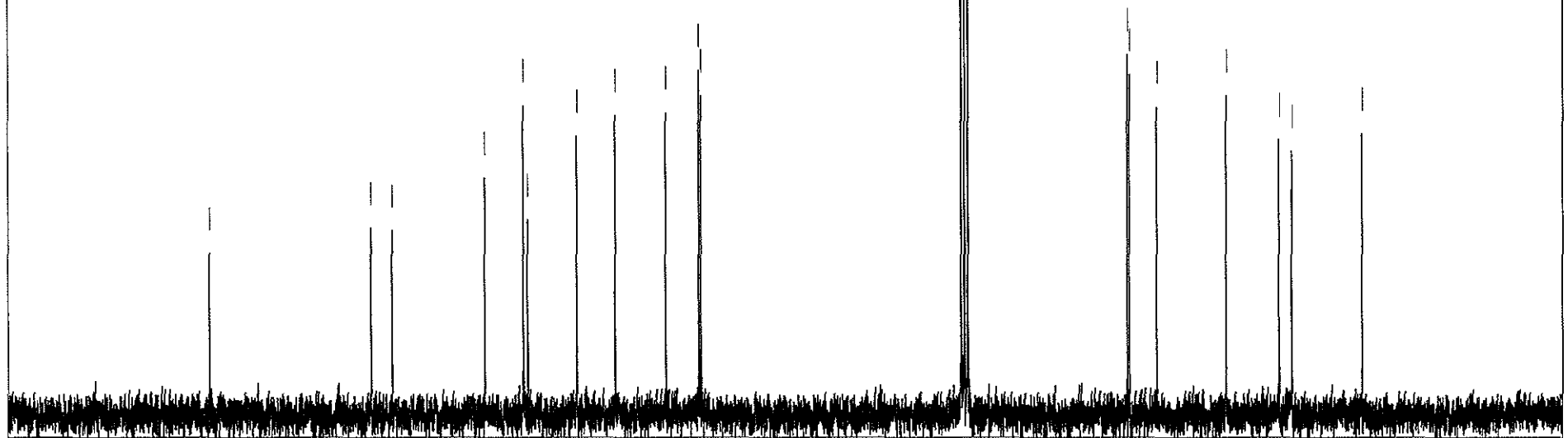
USER: -- DATE: May 29 2008

F1: 300.136	F2: 75.476	SW1: 4803		OF1: 1803.8		PTS1d: 9596 . 16384
EX: s2pul		PW: 6.3 us	PD: 1.0 sec	NA: 8	LB: 0.0	Nuts - \$gj-229.fid



(±)-12  
<sup>13</sup>C NMR  
 (75 MHz, CDCl<sub>3</sub>)

174.540  
 153.725  
 151.011  
 139.123  
 134.173  
 133.604  
 127.266  
 122.332  
 115.806  
 111.539  
 111.270  
 77.653  
 77.250  
 76.807  
 56.215  
 55.944  
 52.431  
 43.508  
 36.729  
 35.083  
 26.063



150

100

50

PPM

<sup>13</sup>C OBSERVE: blank line

USER: -- DATE: May 29 2008

F1: 75.477

F2: 300.135

SW1: 18868

OF1: 8300.2

PTS1d: 34246 , 65536

EX: s2pul

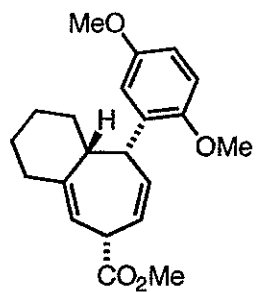
PW: 7.3 us

PD: 1.0 sec

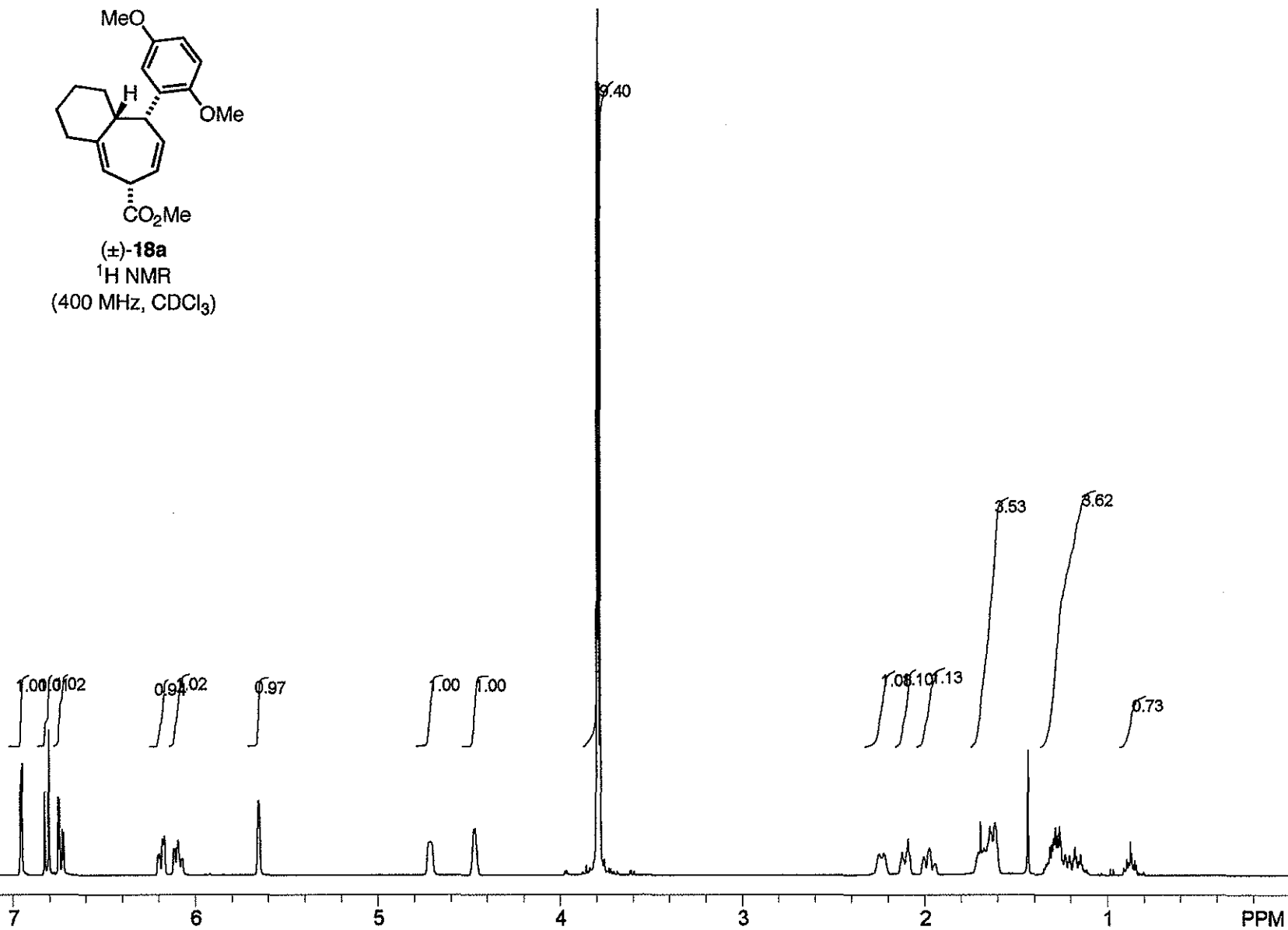
NA: 600

LB: 1.0

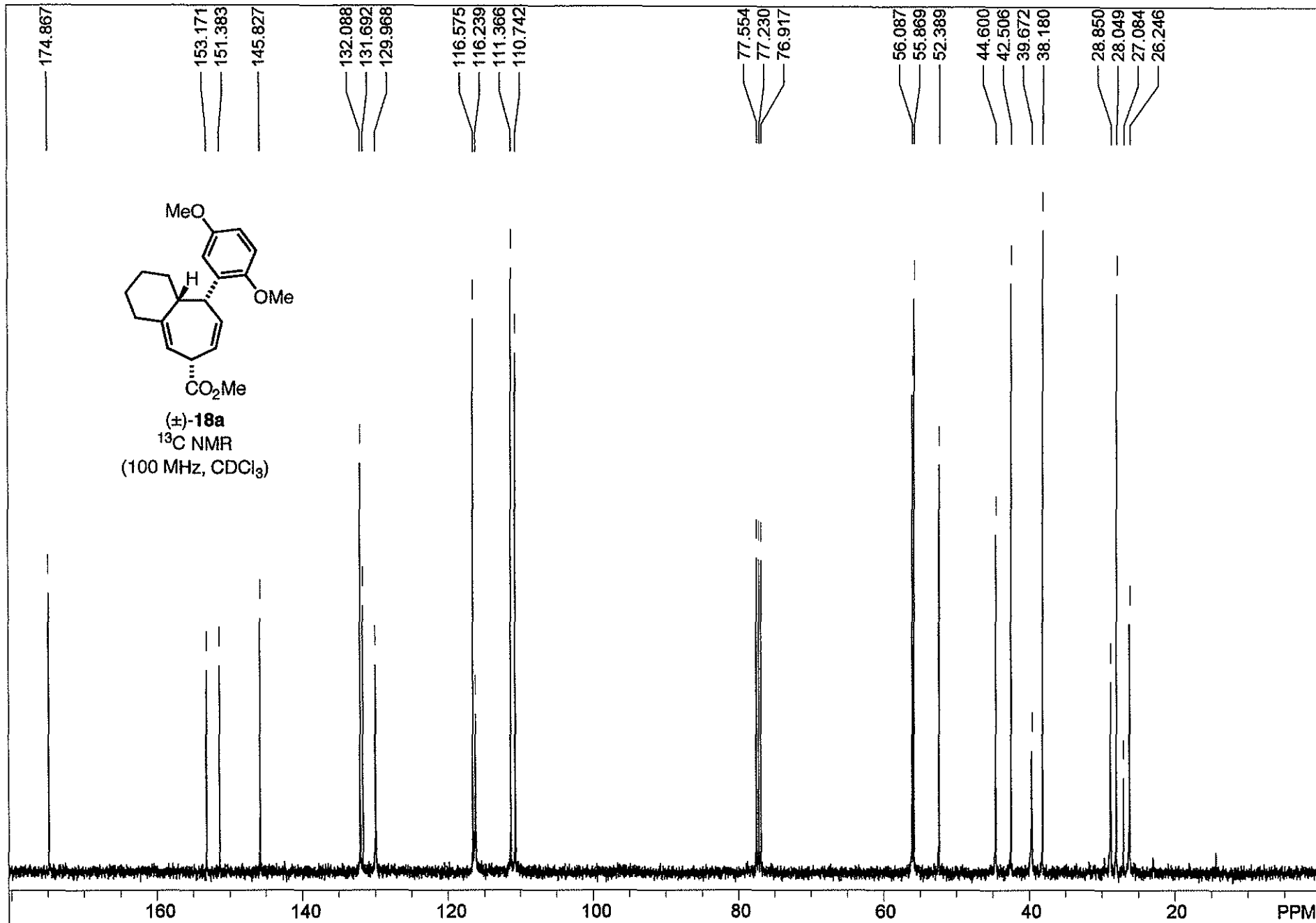
Nuts - \$gj-229-c13.fid



(±)-**18a**  
<sup>1</sup>H NMR  
 (400 MHz, CDCl<sub>3</sub>)

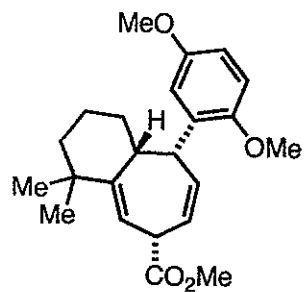


:blank line						USER: -- DATE: Nov 10 2010	
F1: 399.746	F2: 100.525	SW1: 6410		OF1: 2403.4		PTS1d: 13132 . 16384	
EX: s2pul	PW: 8.0 us	PD: 1.0 sec	NA: 8	LB: 0.0	Nuts - \$dlee111110-1-1H.fid		

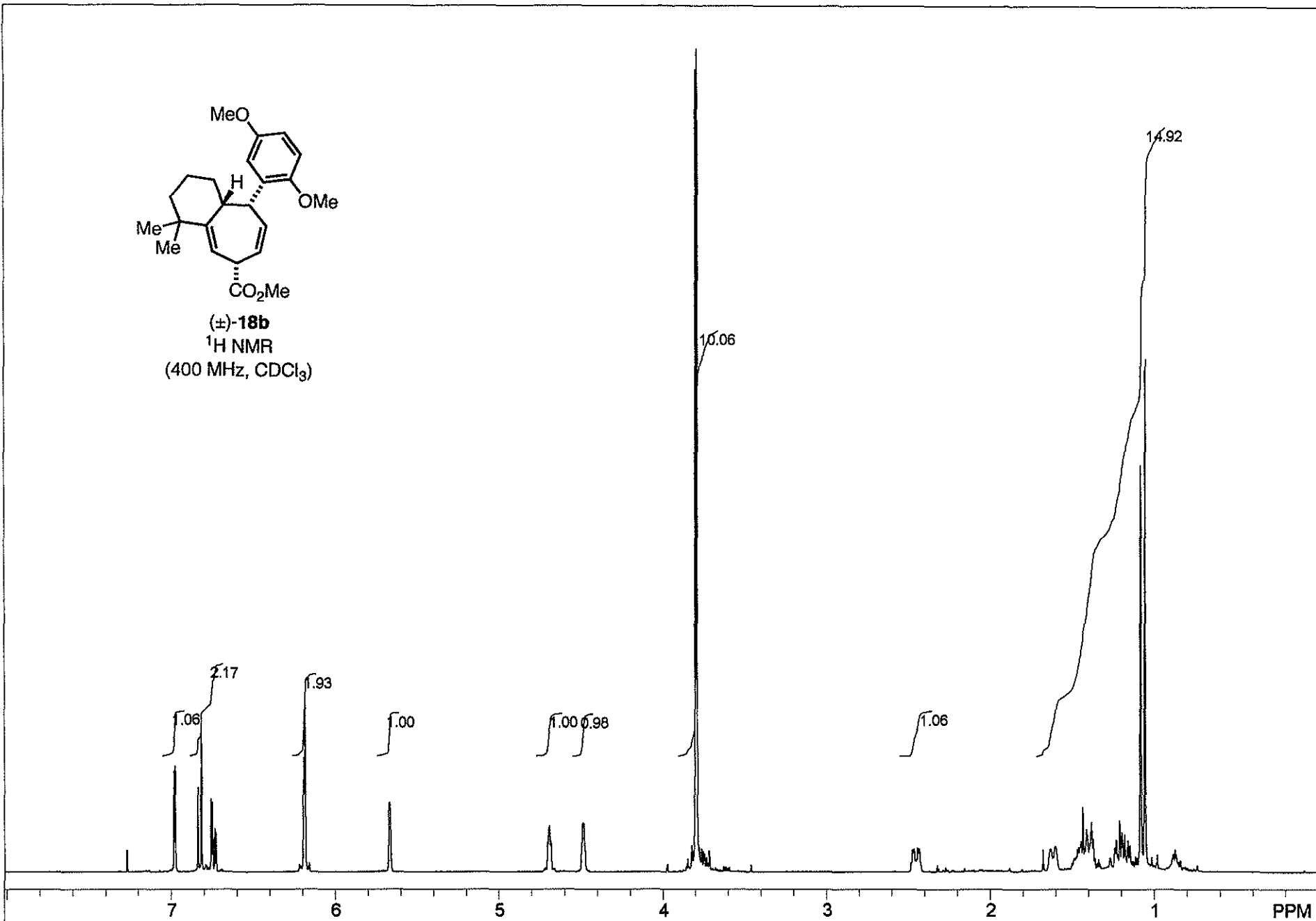


:blank line			USER: -- DATE: Nov 10 2010			
F1: 100.526	F2: 399.745	SW1: 24510	OF1: 10573.2	PTS1d: 31875 . 32768		
EX: s2pul	PW: 5.8 us	PD: 1.0 sec	NA: 660	LB: 1.0	Nuts - \$dlee111110-1-13C.fid	

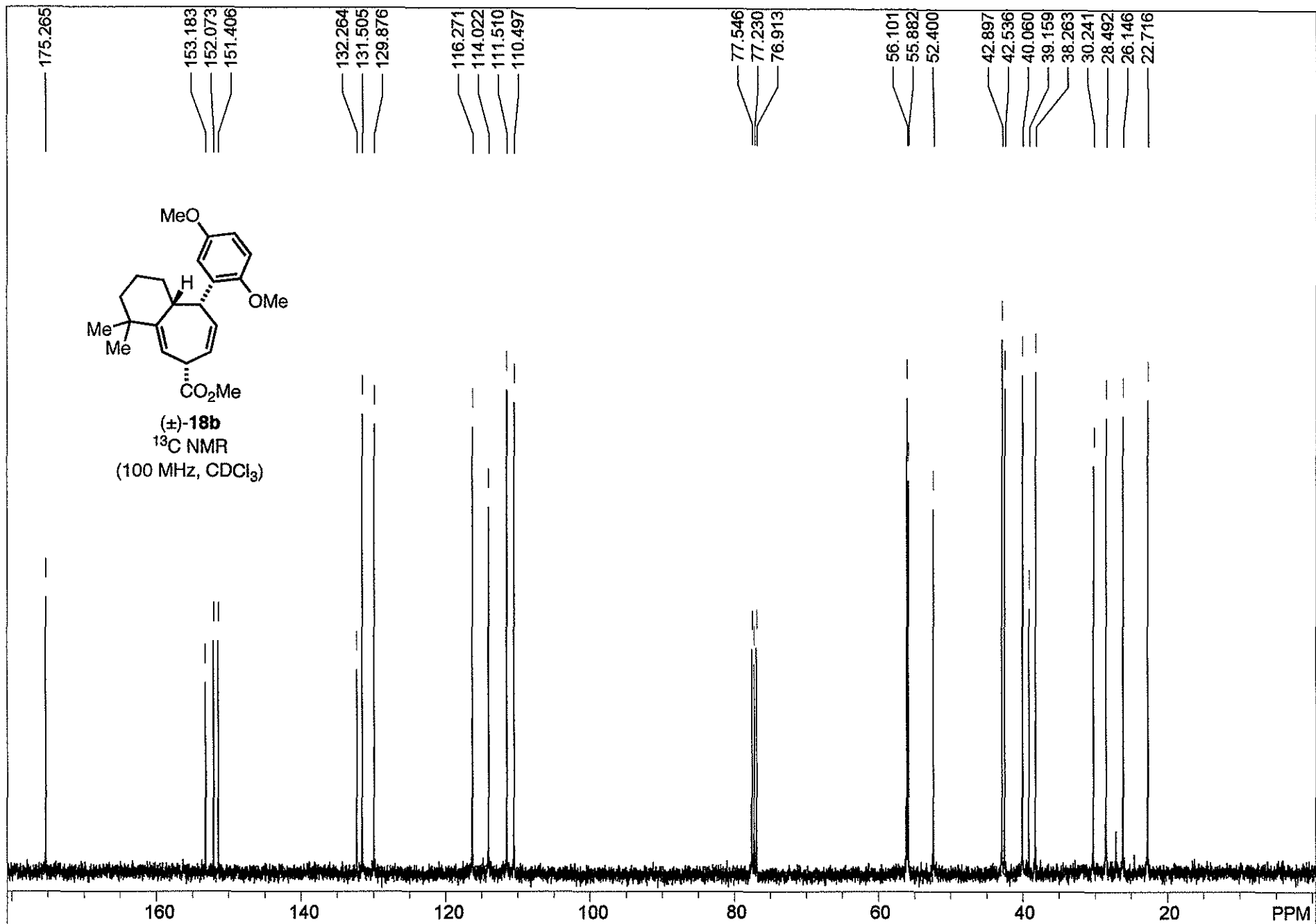




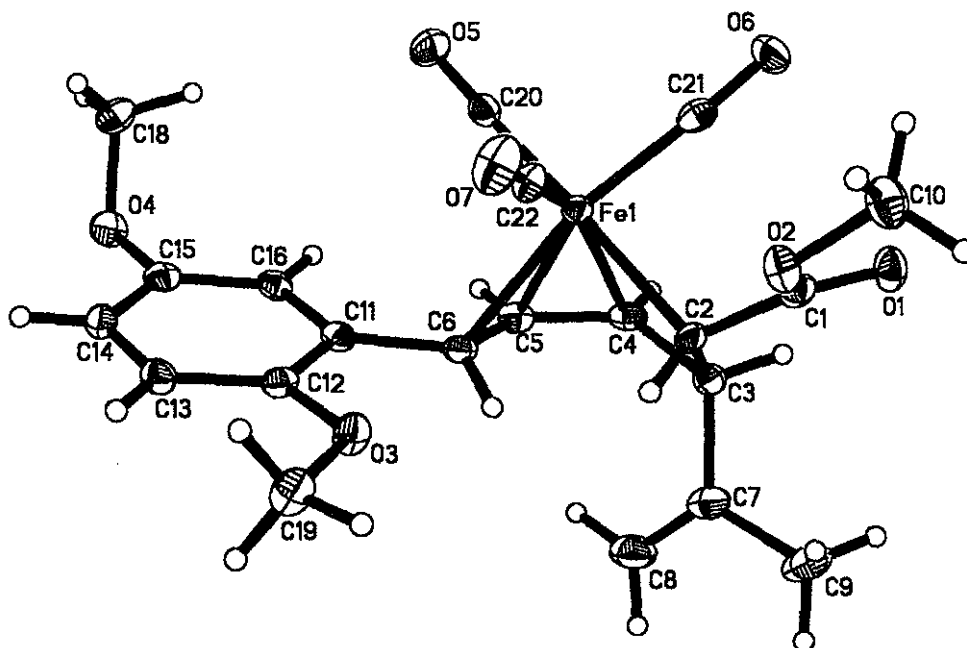
(±)-**18b**  
<sup>1</sup>H NMR  
 (400 MHz, CDCl<sub>3</sub>)



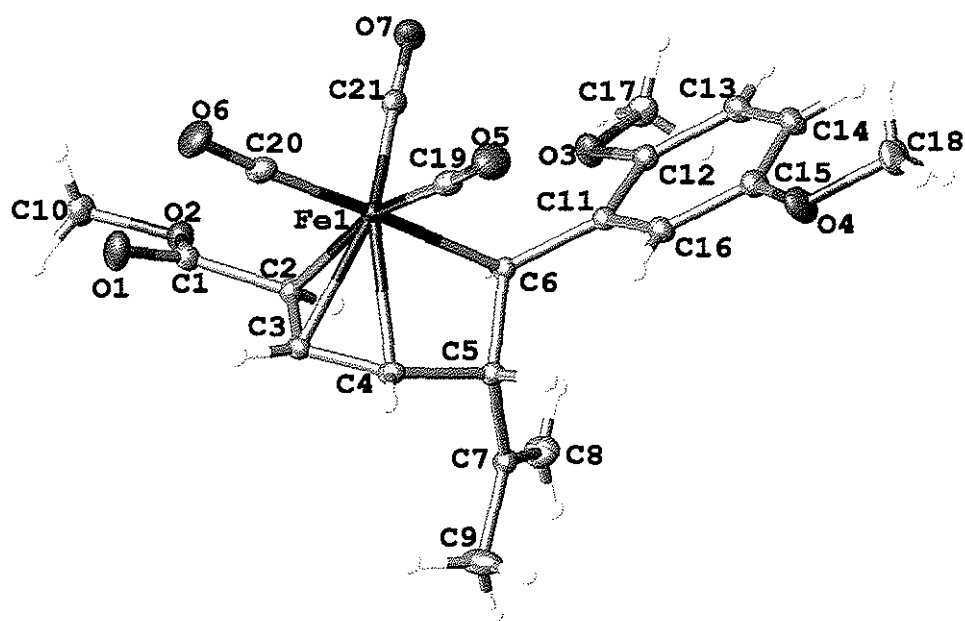
:blank line				USER: -- DATE: Jan 21 2011		
F1: 399.746	F2: 100.525	SW1: 6410		OF1: 2403.5		PTSId: 13132 . 1638#
EX: s2pul	PW: 8.0 us	PD: 1.0 sec	NA: 8	LB: 0.0		Nuts - \$dlee012111-2-1H.fid



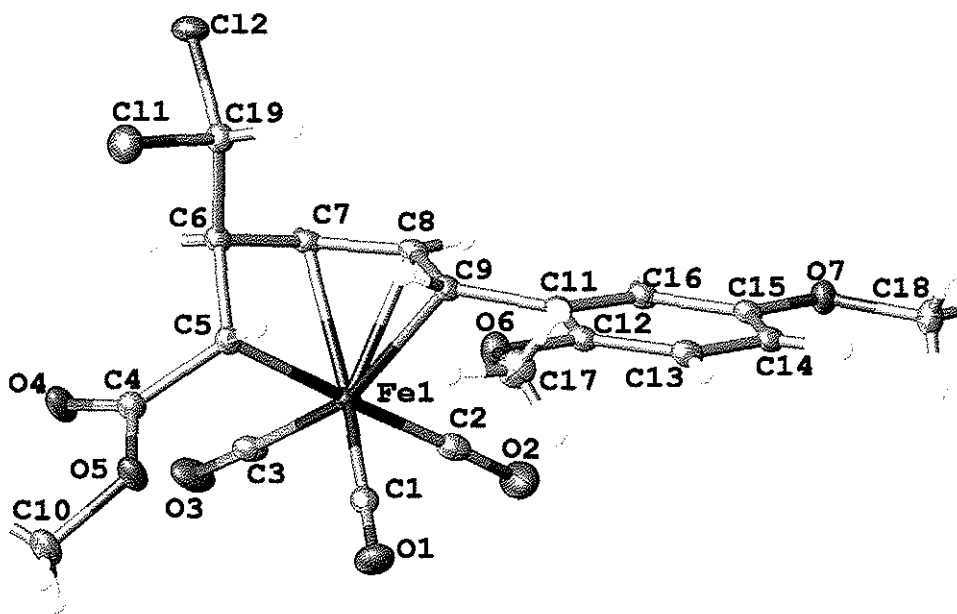
:blank line			USER: -- DATE: Jan 21 2011			
F1: 100.526	F2: 399.745	SW1: 24510	OF1: 10572.7	PTS1d: 31875 , 32768		
EX: s2pul	PW: 5.8 us	PD: 1.0 sec	NA: 300	LB: 1.0	Nuts - \$dlee012111-2-13C.fid	



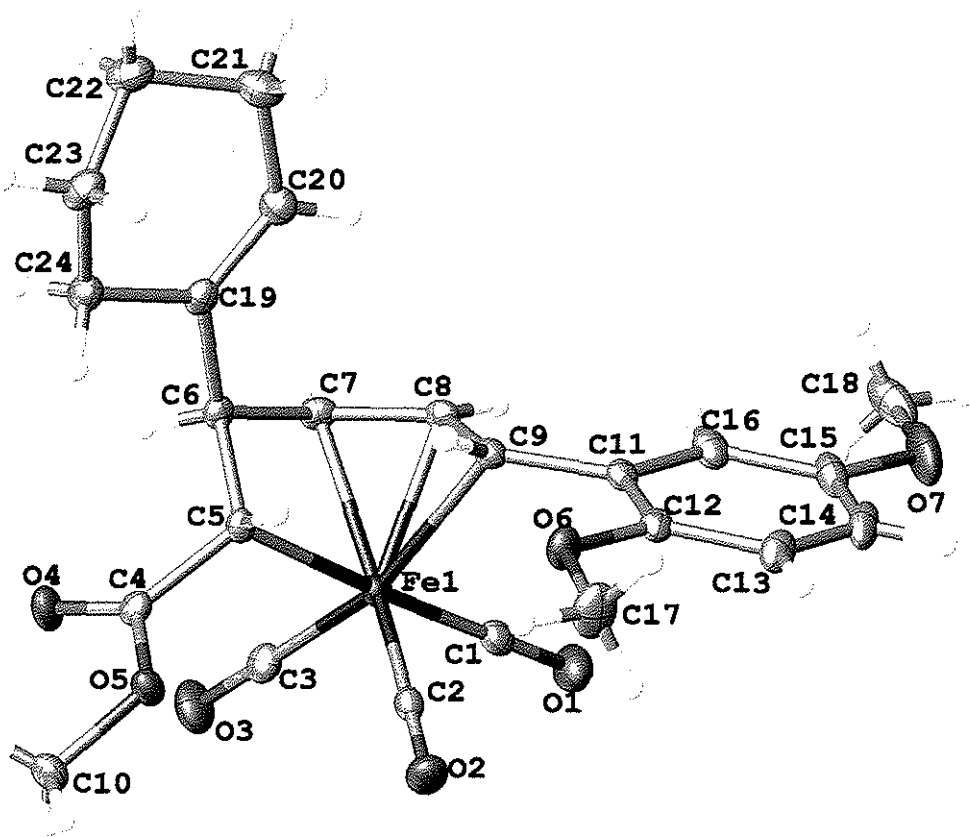
ORTEP of (±)-10



ORTEP of (±)-11



ORTEP of (±)-15



ORTEP of (±)-16a