

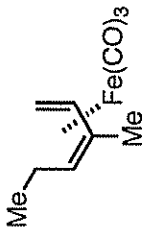
Preparation, Characterization and Reactivity of (3-Methylpentadienyl)iron(1+) Cations

Subhabrata Chaudhury, Shukun Li, Dennis W. Bennett, Tasneem Siddiquee, Daniel T. Haworth,

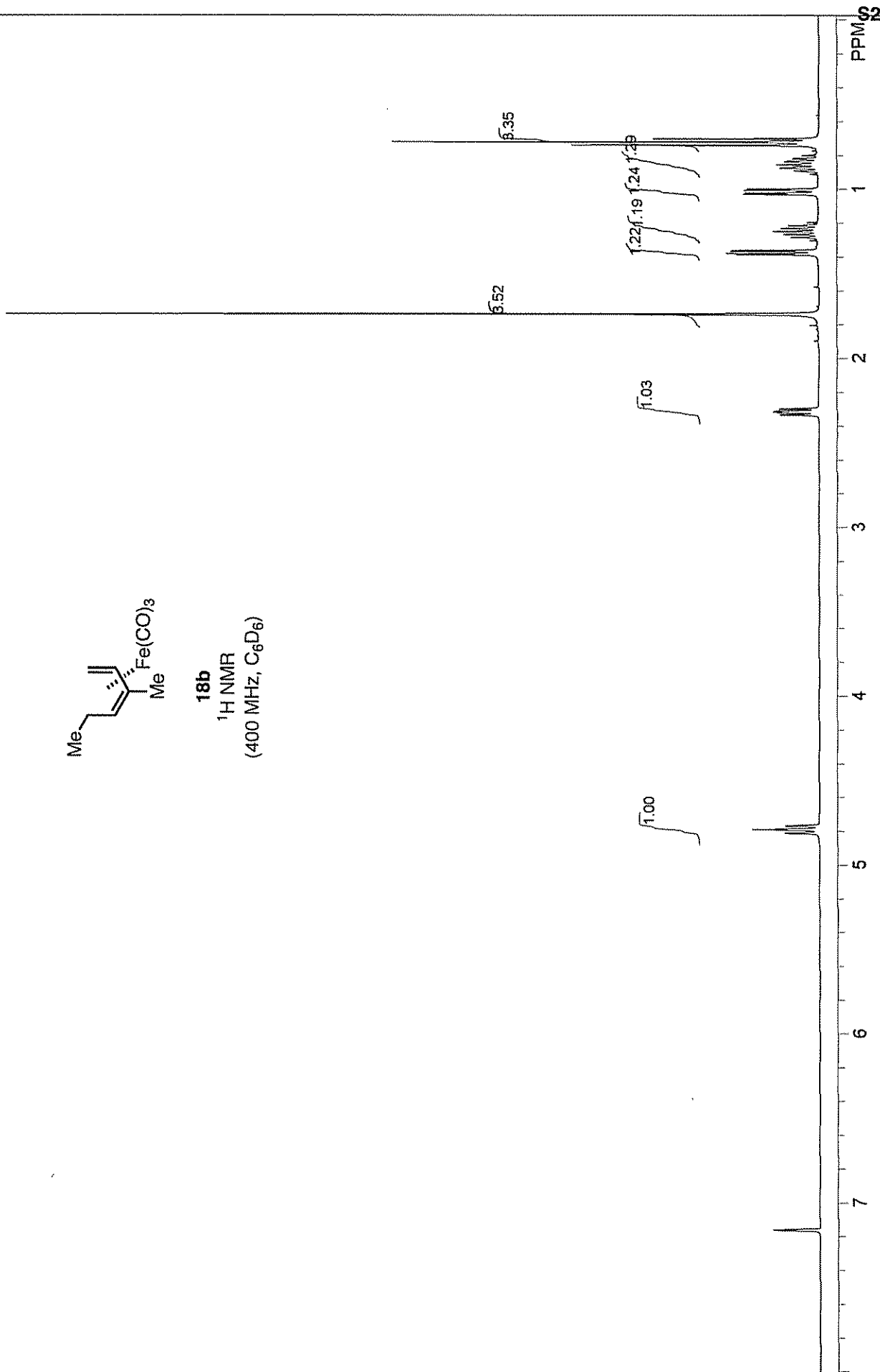
and William A. Donaldson*

Supporting Material

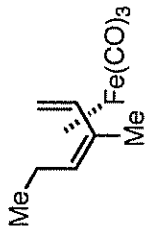
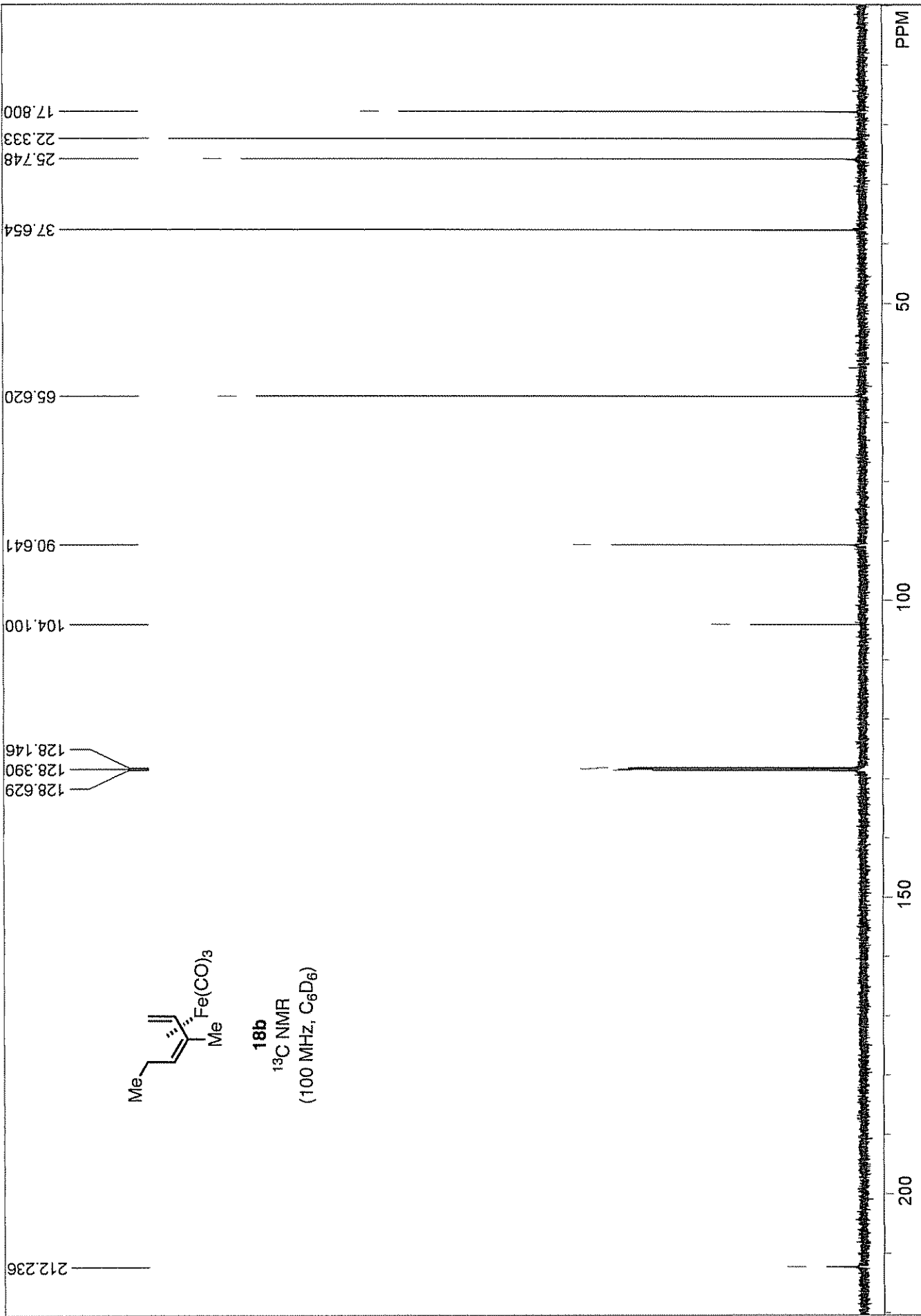
| | |
|--|-----|
| ¹ H NMR spectrum of 18b | S2 |
| ¹³ C NMR spectrum of 18b | S3 |
| ¹ H NMR spectrum of 19d | S4 |
| ¹³ C NMR spectrum of 19d | S5 |
| ¹ H NMR spectrum of 18g | S6 |
| ¹³ C NMR spectrum of 18g | S7 |
| ¹ H NMR spectrum of 18j | S8 |
| ¹³ C NMR spectrum of 18j | S9 |
| ¹ H NMR spectrum of 20f | S10 |
| ¹³ C NMR spectrum of 20f | S11 |
| ¹ H NMR spectrum of 20g | S12 |
| ¹³ C NMR spectrum of 20g | S13 |
| ¹ H NMR spectrum of 20i | S14 |
| ¹³ C NMR spectrum of 20i | S15 |
| ¹ H NMR spectrum of 20j | S16 |
| ¹³ C NMR spectrum of 20j | S17 |
| ¹ H NMR spectrum of 26 | S18 |
| ¹³ C NMR spectrum of 26 | S19 |
| ¹ H NMR spectrum of 28 | S20 |
| ¹³ C NMR spectrum of 28 | S21 |



18b
 $^1\text{H NMR}$
 (400 MHz, C_6D_6)

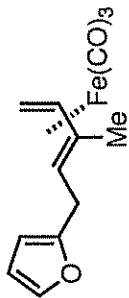


| | | | |
|-------------------------------|-------------|-----------------------------|-----------------------|
| STANDARD 1H OBSERVE - profile | | USER: -- DATE: Dec. 7. 2006 | |
| F1: 399.751 | F2: 100.526 | PTS1d: 13132 | 16384 |
| EX: s2pul | PD: 1.0 sec | LB: 0.0 | Nuts - \$sc707n-1.fid |
| SW1: 6410 | OF1: 2416.1 | | |
| PW: 8.4 us | NA: 8 | | |

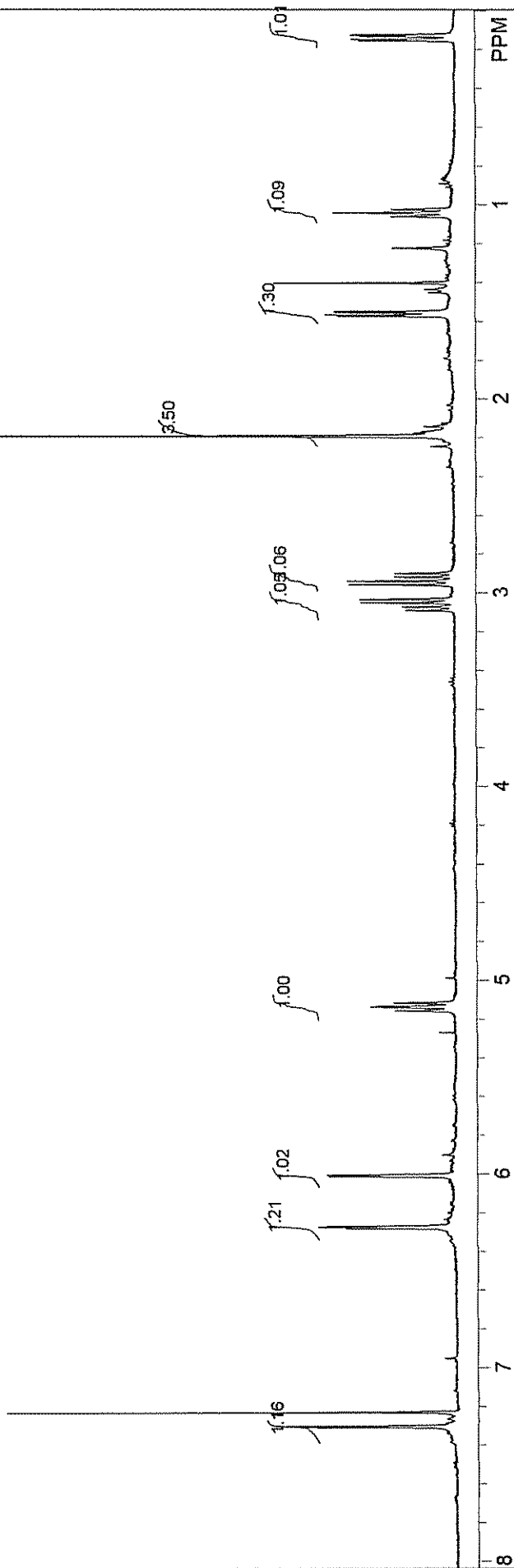


18b
¹³C NMR
 (100 MHz, C₆D₆)

| | | | |
|-------------------------------|-------------|---------------------------|---------------------------|
| STANDARD 1H OBSERVE - profile | | USER: -- DATE: Dec 7 2006 | |
| F1: 100.527 | F2: 399.751 | OF1: 10607.9 | PTS1d: 31875 . 32768 |
| EX: s2pul | PD: 1.0 sec | NA: 256 | LB: 0.0 |
| | SW1: 24510 | | Nuts - \$sc707n-1-13c.fid |
| | PW: 7.5 us | | |



¹H NMR
(400 MHz, CDCl₃)



STANDARD 1H OBSERVE - profile

USER: -- DATE: Dec 5 2006

F1: 399.751 F2: 100.526 PTS1d: 13132 . 16384

OF1: 2387.8

PD: 1.0 sec

SW1: 6410

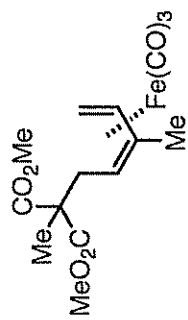
PW: 8.4 us

NA: 8

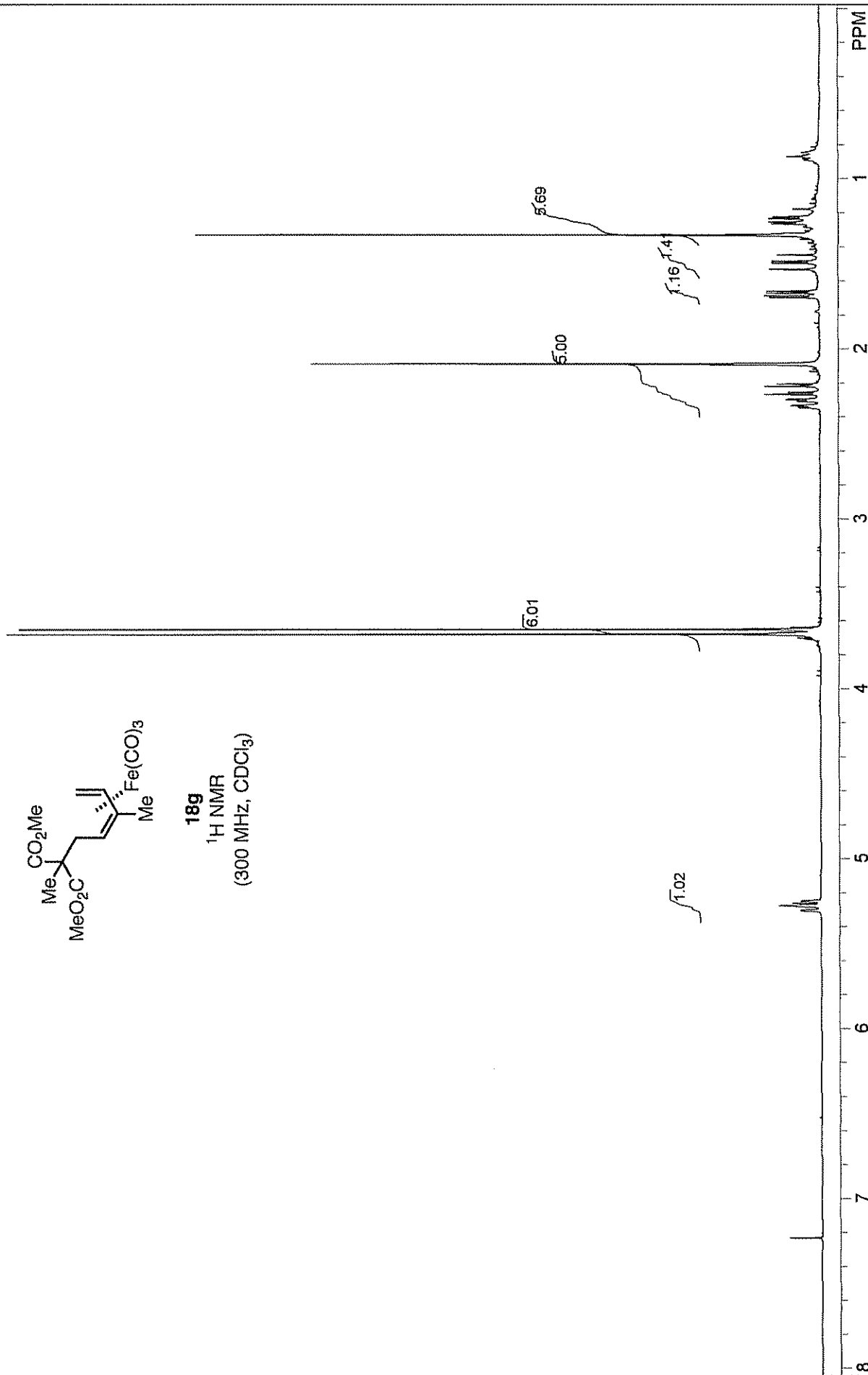
IB: 0.0

EX: s2pul

Nuts - \$sc705n-1.fid



18g
¹H NMR
 (300 MHz, CDCl₃)

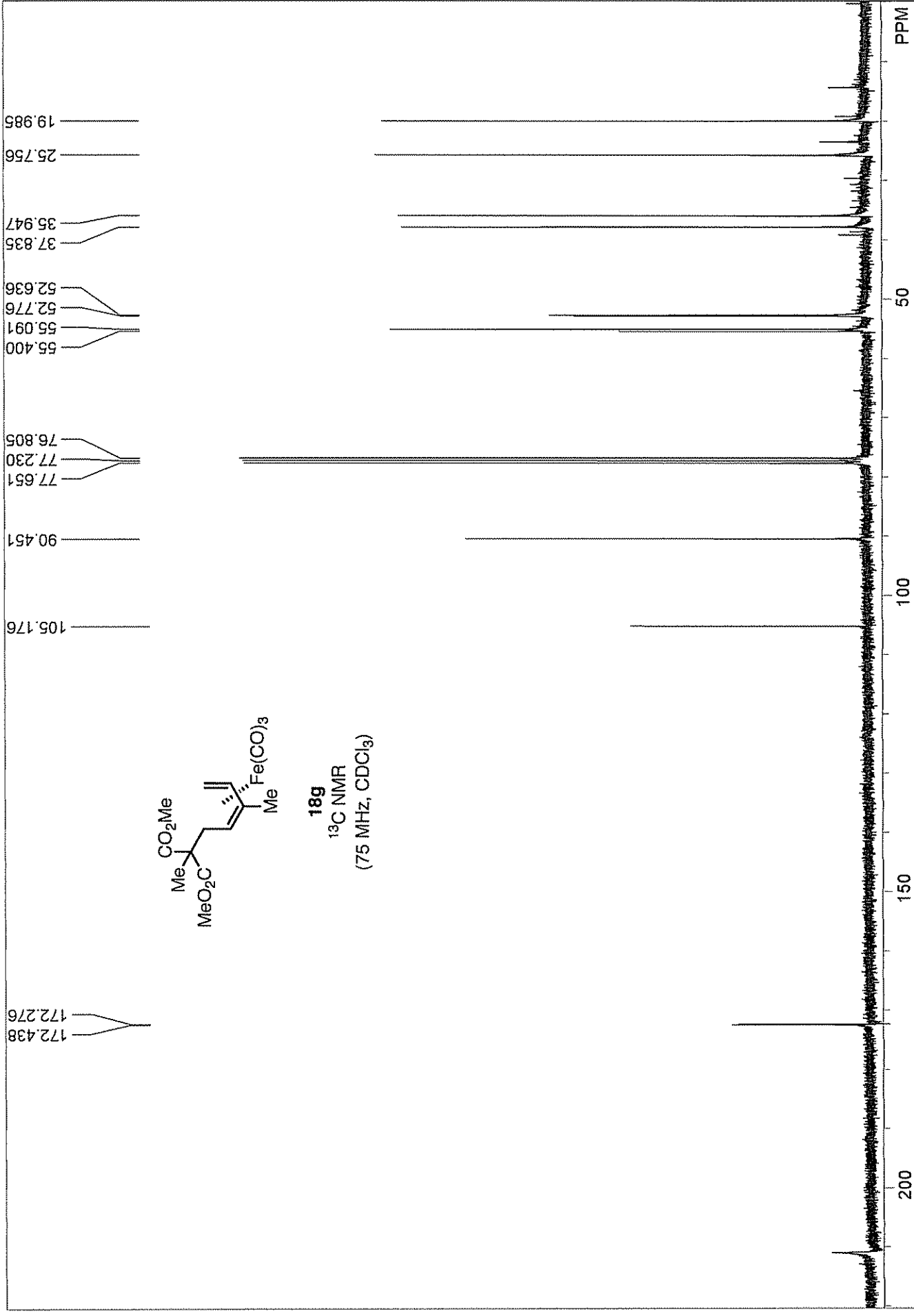


STANDARD 1H OBSERVE: blank line
 F1: 300.142 F2: 75.478
 EX: s2pul

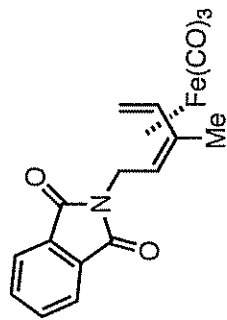
USER: -- DATE: Mar 28 2005
 PTS1d: 14430 16384
 Nuts - \$sc561withdmm.fid

OF1: 1791.4
 NA: 8
 LB: 0.0

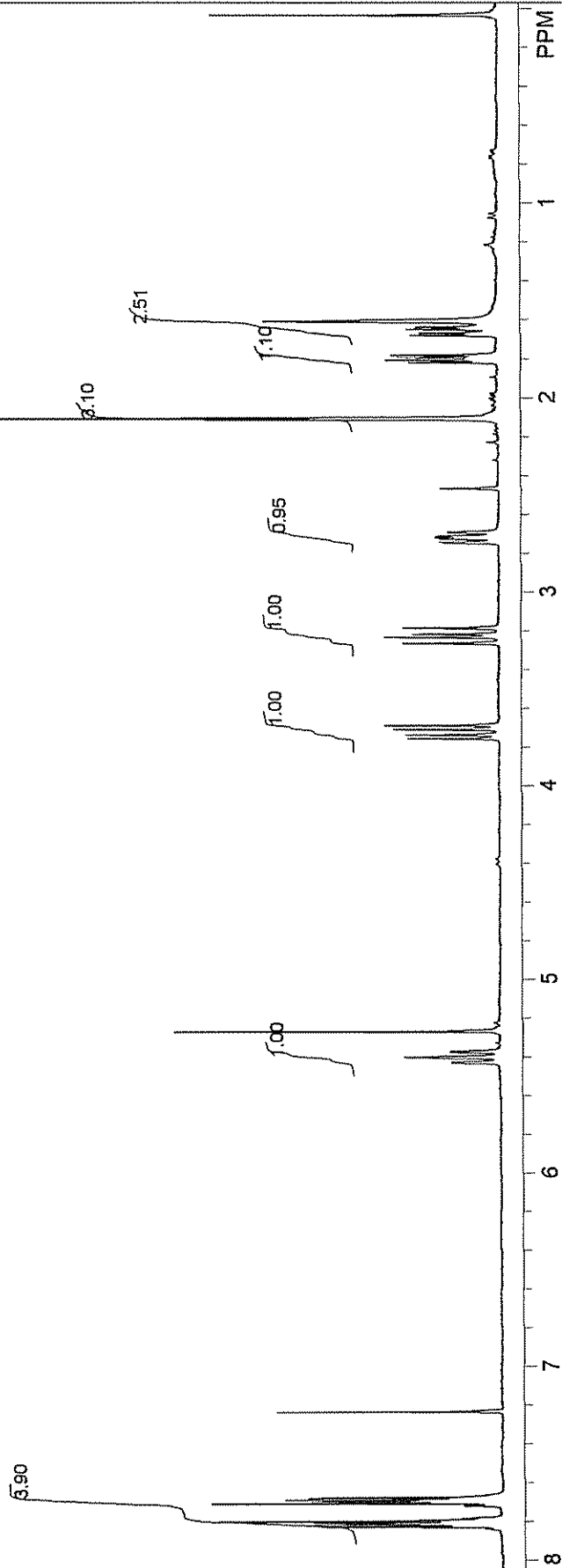
SW1: 4810
 PW: 6.3 us
 PD: 1.0 sec



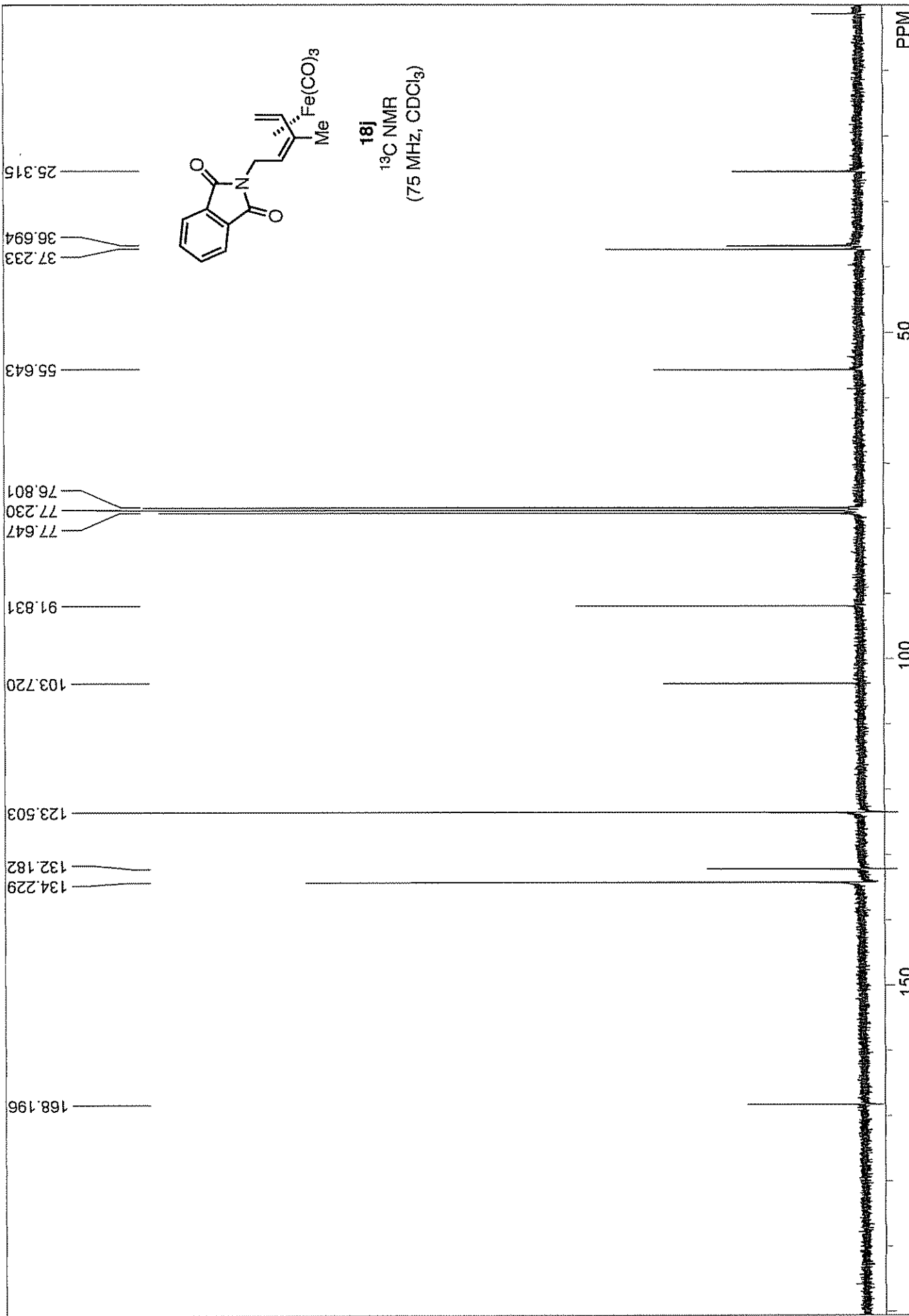
13C OBSERVE: blank line
F1: 75.479 F2: 300.142 SW1: 18868 PD: 1.0 sec
EX: s2pul PW: 7.3 us OF1: 8298.4 NA: LB: 0.0
PTS1d: 18868 32768
USER: -- DATE: Mar 28 2005
Nuts - \$sc361-13c.fid



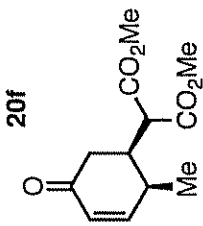
18j
¹H NMR
 (300 MHz, CDCl₃)
 contains CH₂Cl₂ (*)



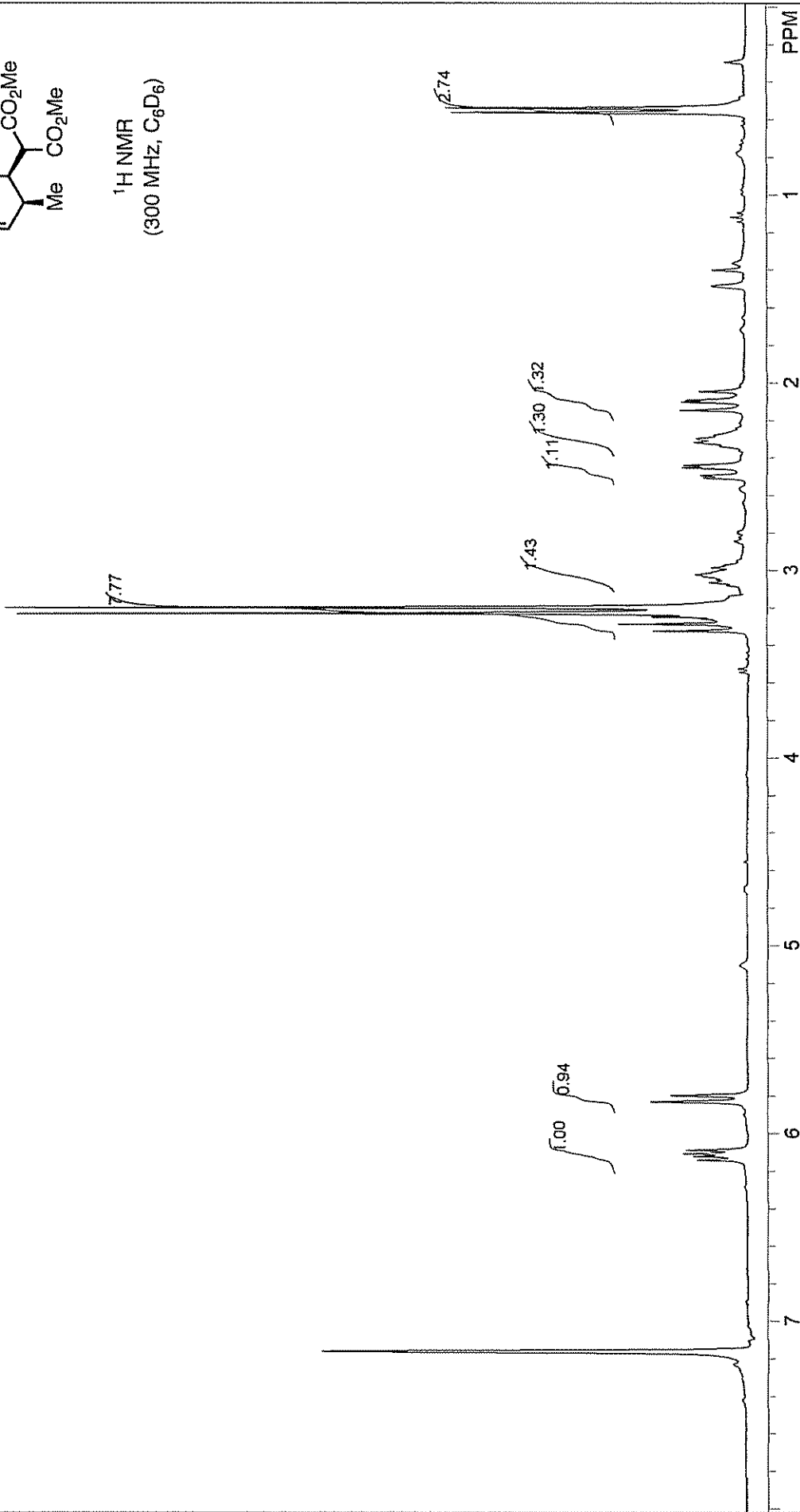
| | | | | |
|---------------------------------|------------|-------------|-------------|----------------------------|
| STANDARD 1H OBSERVE: blank line | SW1: 4810 | OF1: 1792.6 | PTSD: 14430 | USER: -- DATE: Sep 24 2005 |
| F1: 300.145 | F2: 75.479 | NA: 8 | 16384 | |
| EX: s2pul | PW: 6.3 us | PD: 1.0 sec | LB: 0.0 | Nuts - \$sc656re.fid |



13C OBSERVE: blank line
 USER: -- DATE: Sep 24 2005
 F1: 75.479 F2: 300.145 SW1: 18868 OF1: 8298.9 PTS1d: 18868 32768
 EX: sZpul PD: 1.0 sec NA: LB: 0.0
 Nuts - \$sc656-13ere.fid

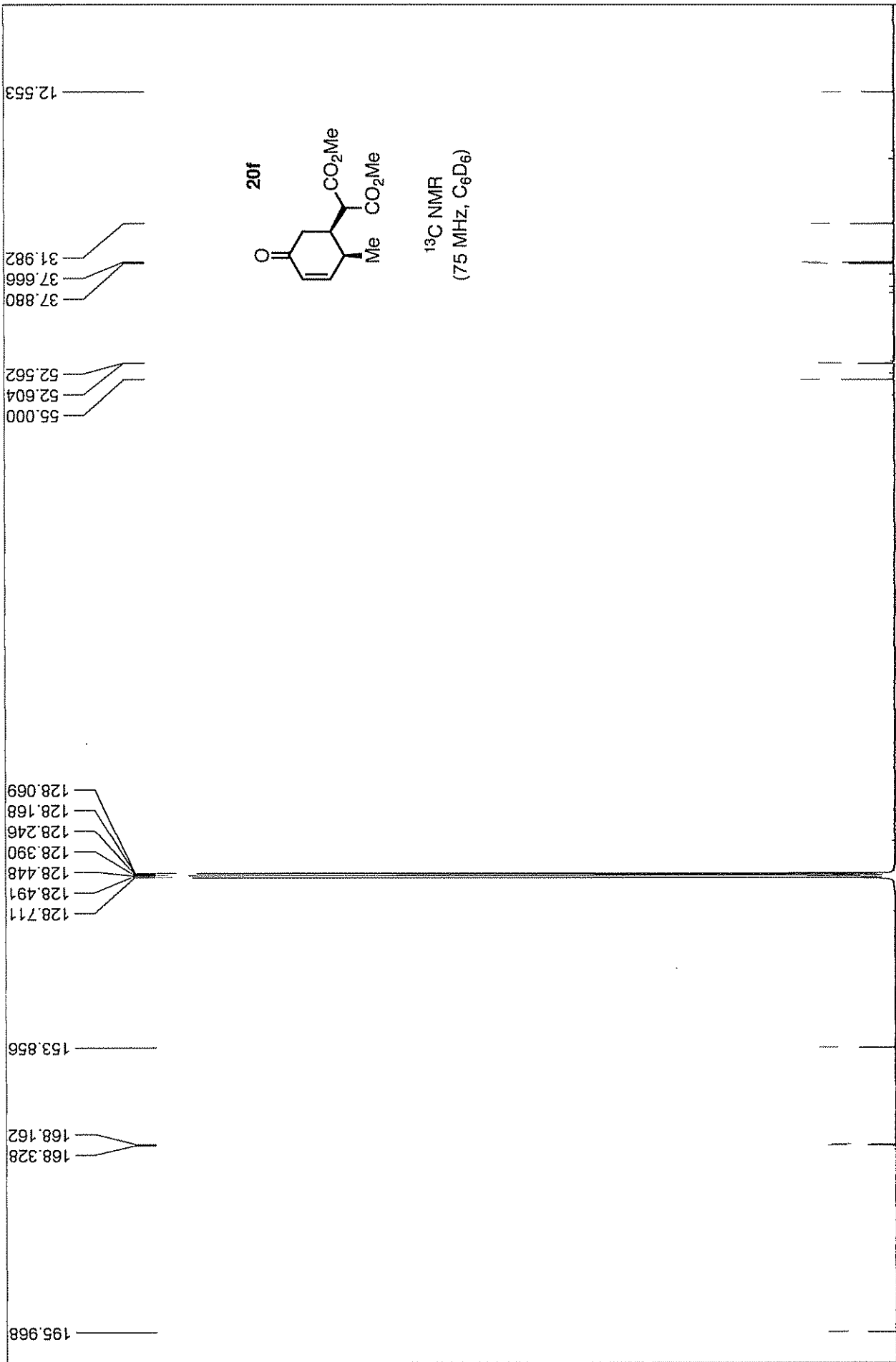


¹H NMR
(300 MHz, C₆D₆)

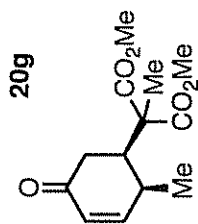


STANDARD 1H OBSERVE:blank line

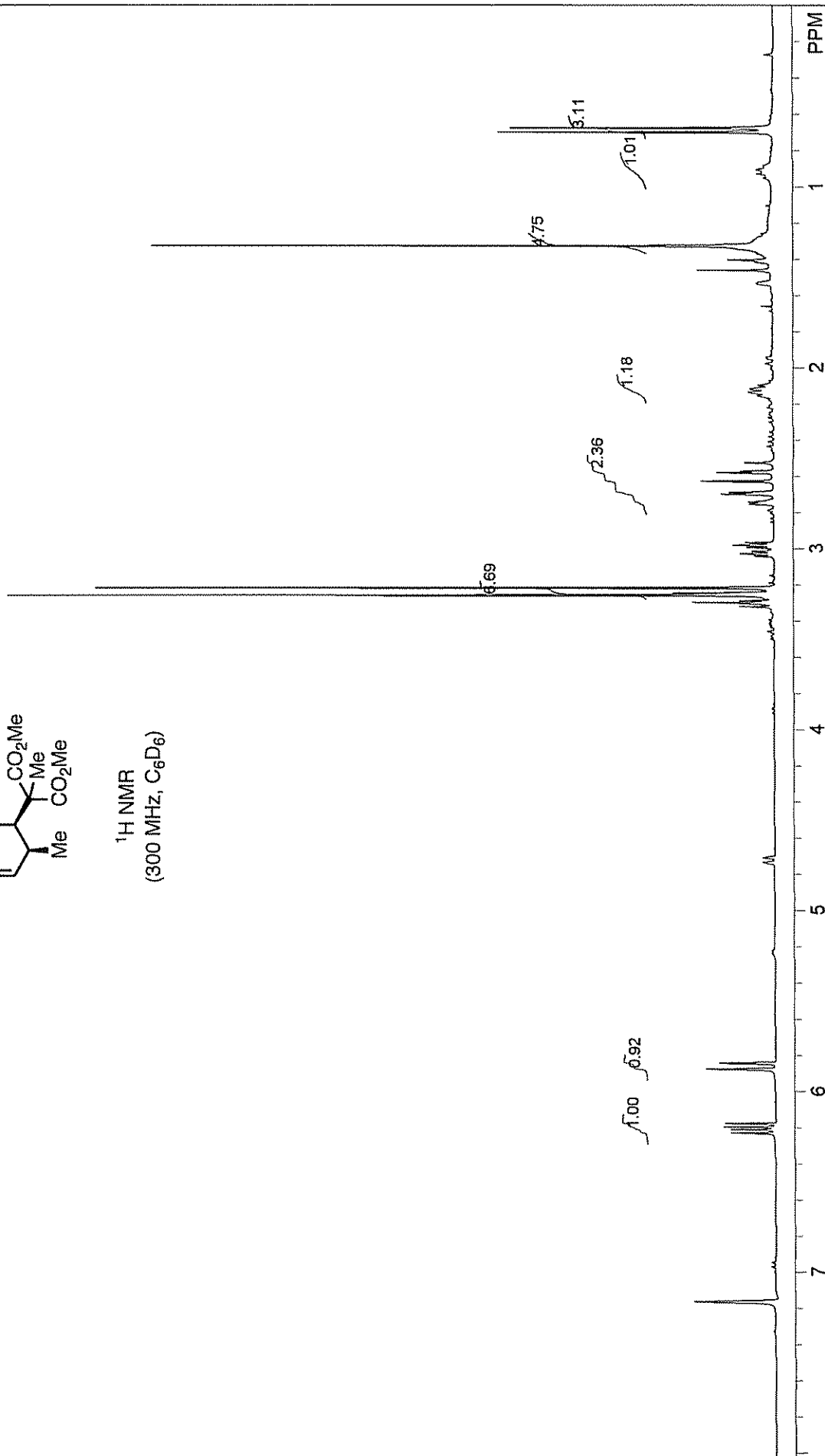
| | | | | | | | |
|-----------|------------|-------------|-------|-------------|--------------|-------|---------------------------|
| EX: s2pul | FW: 6.3 us | PD: 1.0 sec | NA: 8 | OFI: 1811.9 | PTSID: 14409 | 16384 | USER: -- DATE: Jan 6 2005 |
|-----------|------------|-------------|-------|-------------|--------------|-------|---------------------------|



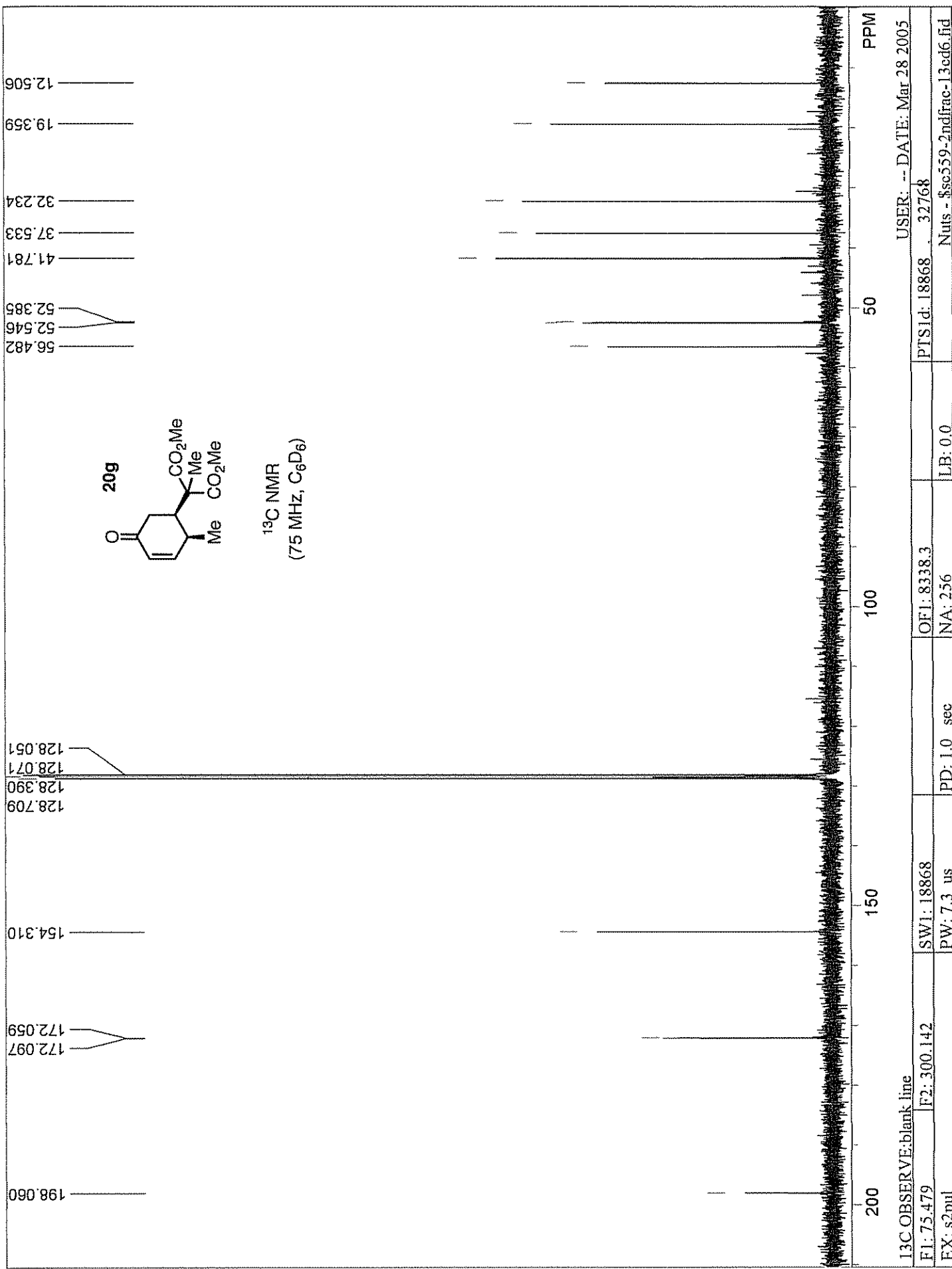
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|-------------------------|-------------|---------------------------|--------------------------------|
| 13C OBSERVE: blank_line | | USER: -- DATE: Jan 6 2005 | |
| F1: 75.479 | F2: 300.142 | PTSID: 18868 | 32768 |
| EX: s2pul | SW1: 18868 | OF1: 8339.9 | |
| | PW: 7.3 us | NA: | LB: 0.0 |
| | PD: 1.0 sec | | Nuts - fssc518mbenzene-13c.fid |

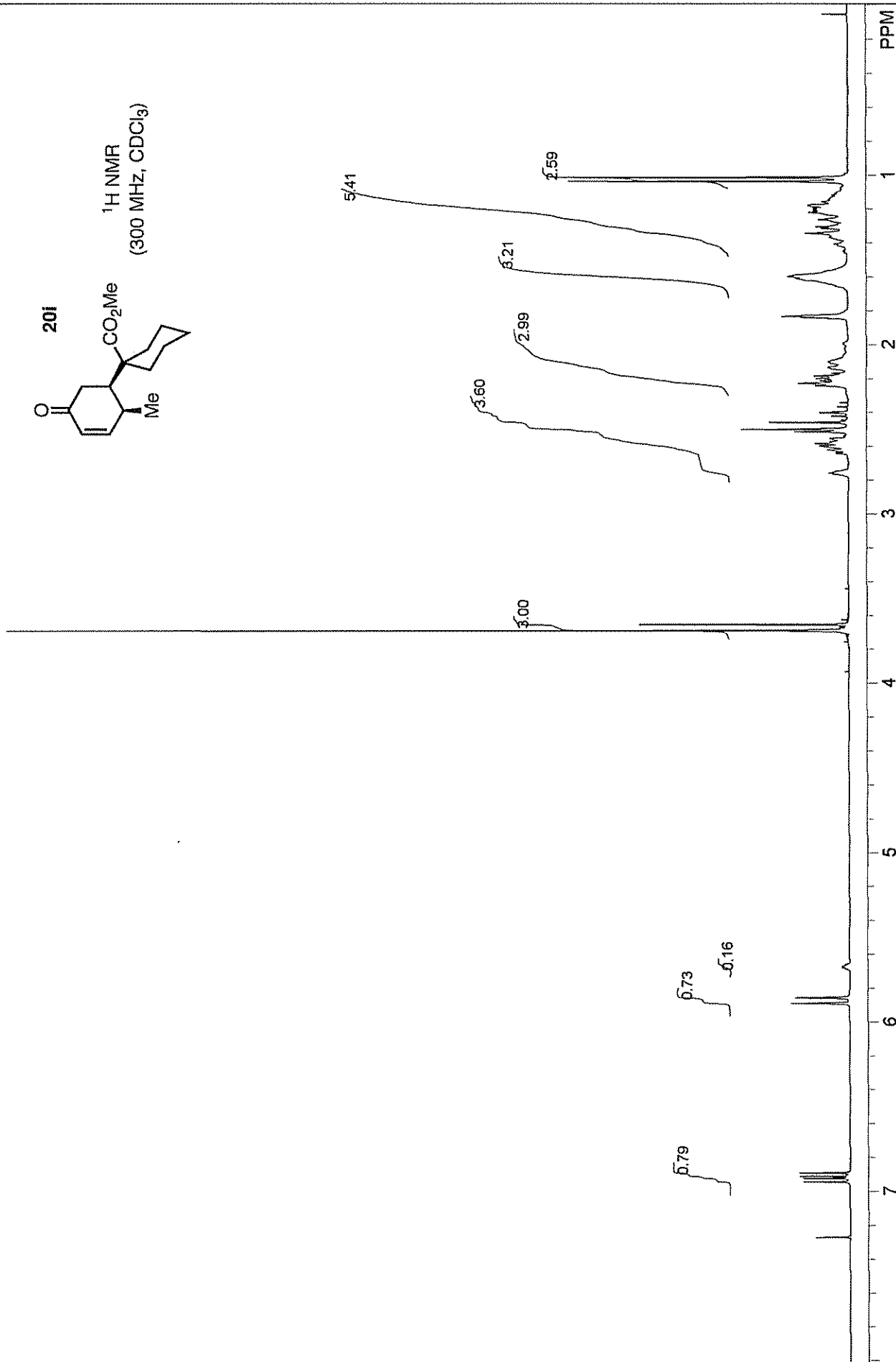
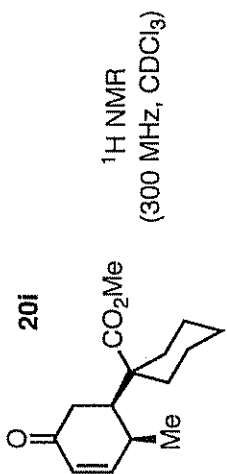


¹H NMR
(300 MHz, C₆D₆)



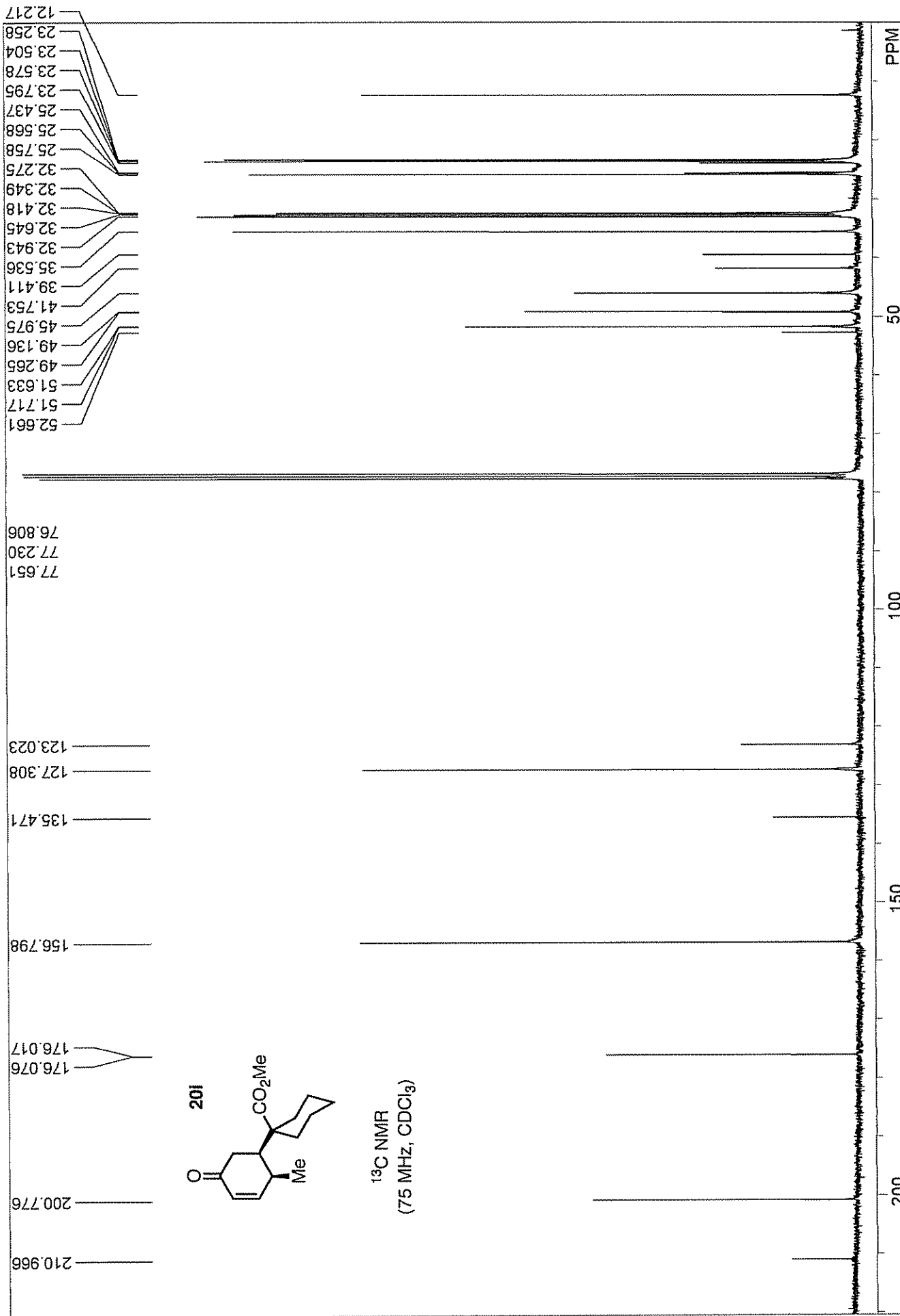
| | | | |
|--------------------------------|-------------|----------------------------|--------------------------|
| STANDARD 1H OBSERVE:blank line | | USER: -- DATE: Mar 28 2005 | |
| F1: 300.142 | F2: 75.478 | PTSD: 1.4430 | 16384 |
| EX: s2pul | | LB: 0.0 | Nuts - \$sc592ndfrac.fid |
| SW1: 4810 | OF1: 1813.2 | | |
| PW: 6.3 us | NA: 8 | | |
| PD: 1.0 sec | | | |





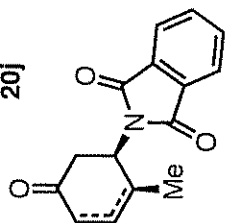
STANDARD 1H OBSERVE:blank line

| | | | | | | |
|-------------|------------|------------|-------------|-------------|---------|----------------------------|
| F1: 300.145 | F2: 75.479 | SW1: 4810 | OF1: 1805.1 | PTSD: 14430 | 16384 | USER: -- DATE: Oct 27 2005 |
| EX: s2pul | | PW: 6.3 us | PD: 1.0 sec | NA: 8 | LB: 0.0 | Nuts - \$sc677-1.fid |

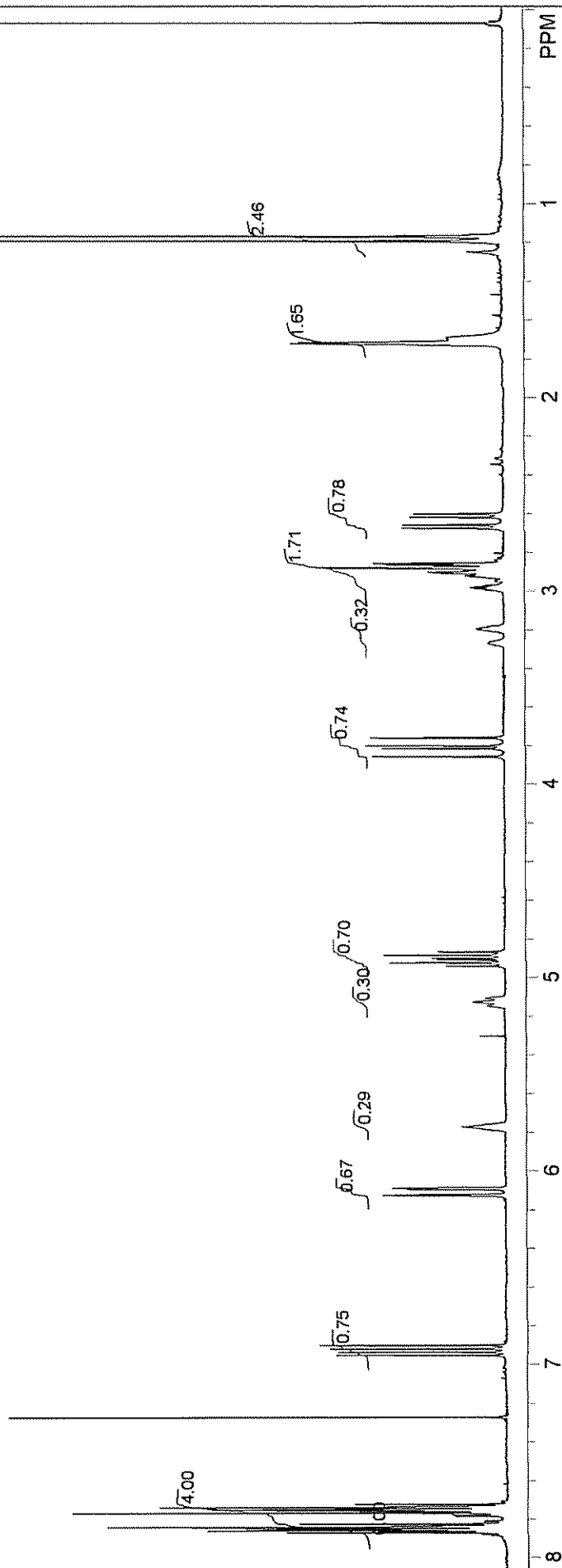


| | | | |
|-------------------------|-------------|----------------------------|--------------------------|
| I3C OBSERVE: blank line | | USER: -- DATE: Oct.27.2005 | |
| F1: 75.479 | F2: 300.145 | PTS1d: 18868 | 32768 |
| EX: s2pul | SW1: 18868 | OF1: 8297.3 | NA: |
| | PW: 7.3 us | PD: 1.0 sec | NA: |
| | | LB: 1.0 | Nuts - \$sc677-1-13C.fid |

20j



¹H NMR
(300 MHz, CDCl₃)



STANDARD 1H OBSERVE: blank line

F1: 300.145

F2: 75.479

SW1: 4810

PW: 6.3 us

PD: 1.0 sec

OF1: 1805.2

NA: 8

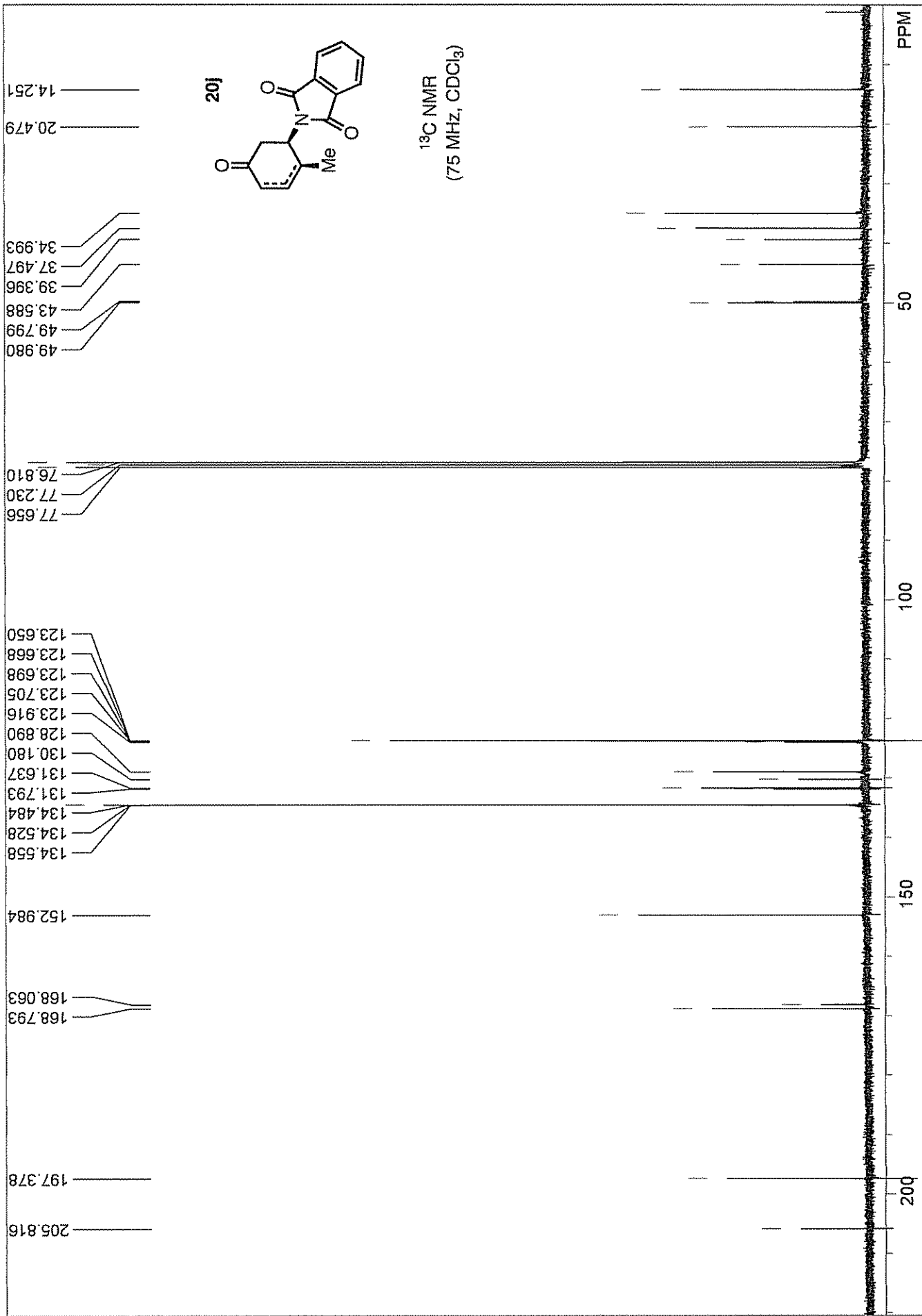
LR: 0.0

PTS1d: 14430

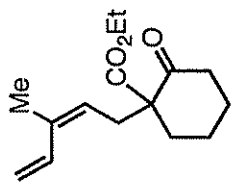
16384

USER: -- DATE: Oct.29.2005

Nuts - \$sec674fmal.fid

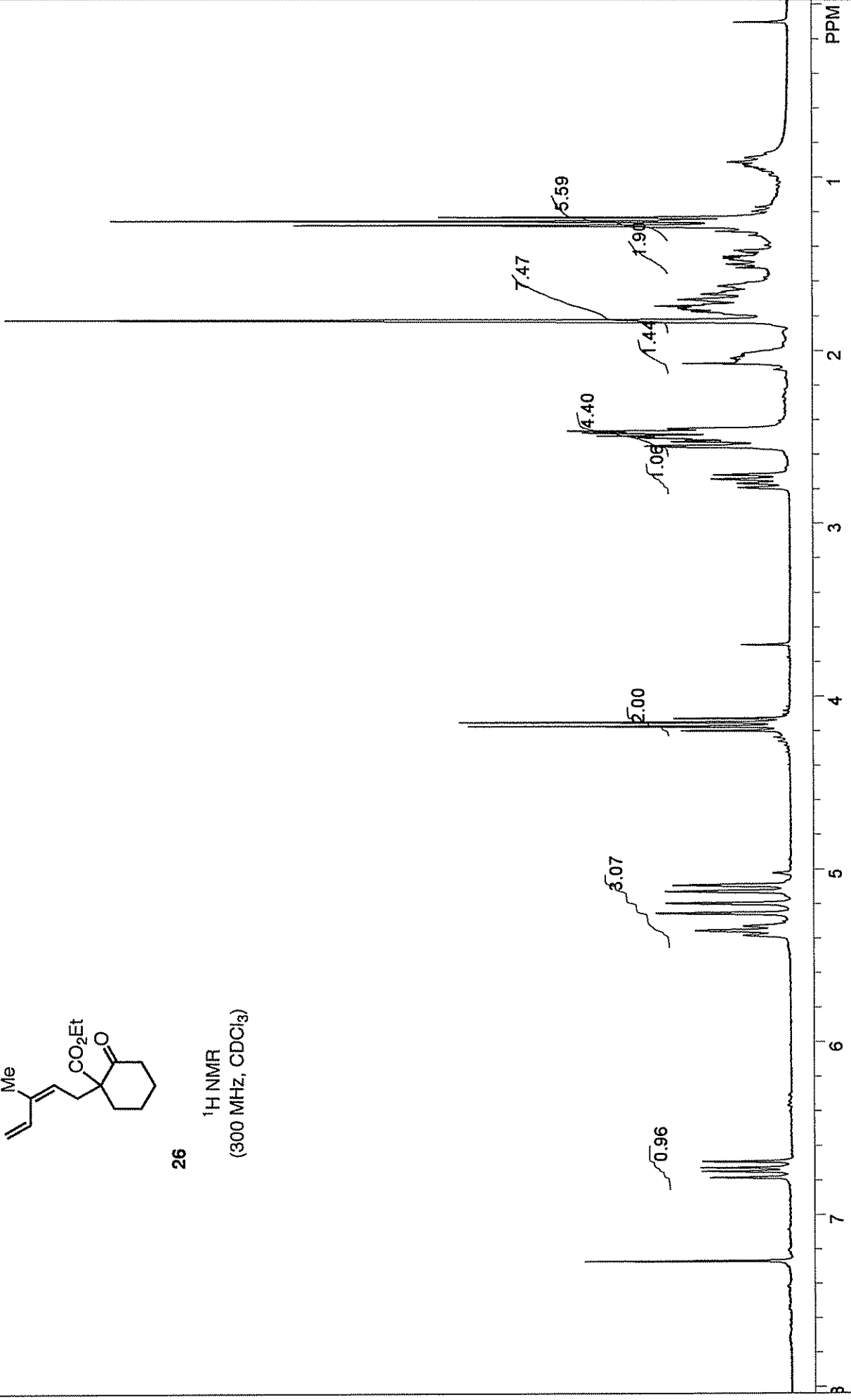


13C OBSERVE: blank line
 USER: -- DATE: Oct 29 2005
 F1: 75.479 F2: 300.145 SW1: 18868 OF1: 8299.2 PTS1d: 18868 32768
 EX: s2pul PD: 1.0 sec NA: LB: 0.0
 Nuts - \$sc674final-13c.fid

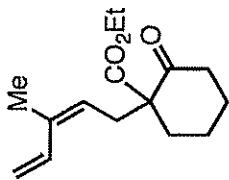


26

¹H NMR
(300 MHz, CDCl₃)

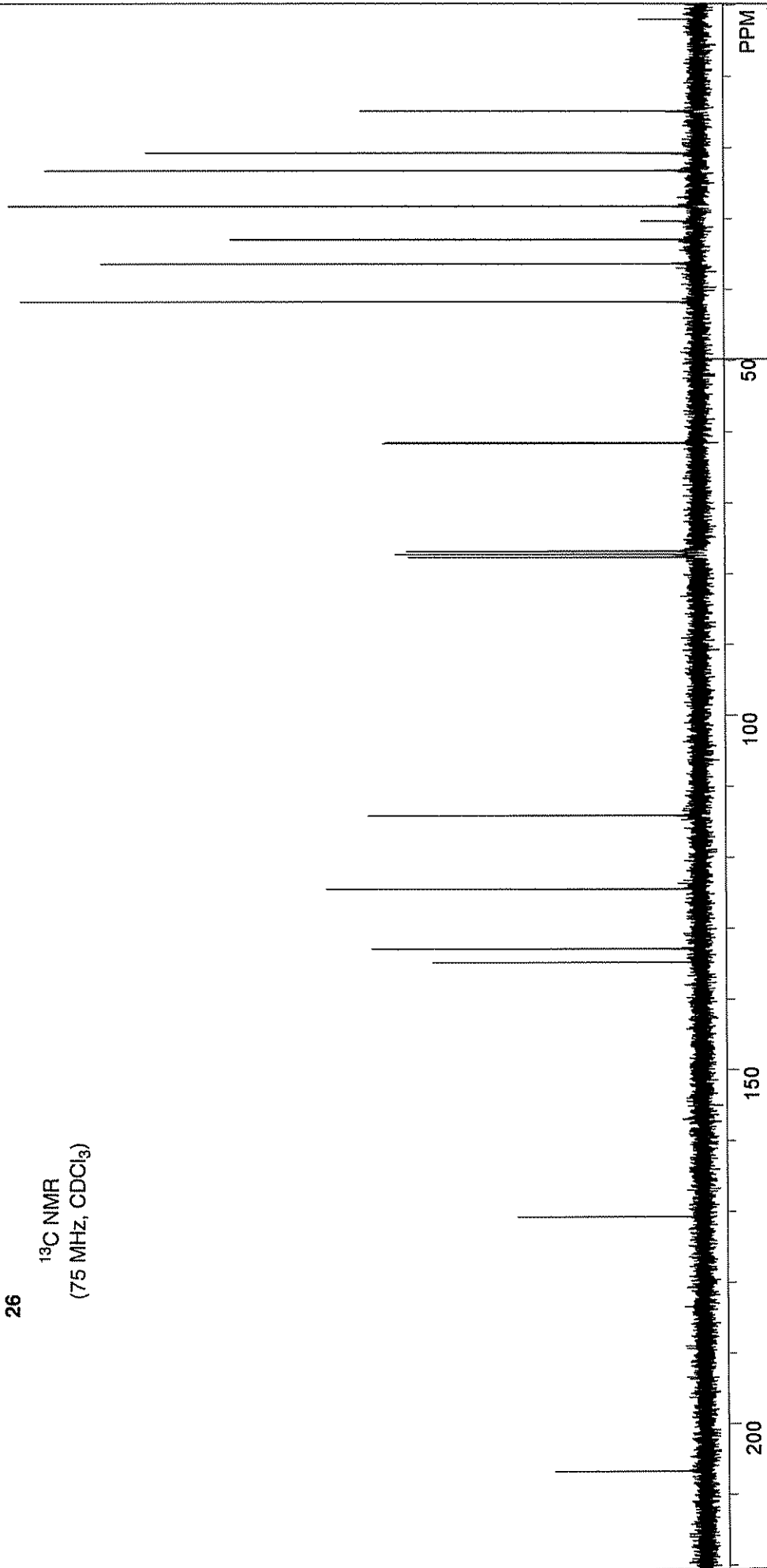


| | | | |
|--------------------------------|--------------|----------------------------|------------------------|
| STANDARD 1H OBSERVE blank line | | USER: -- DATE: Sep 16 2002 | |
| F1: 300.151 | F2: 75.480 | OF1: 1805.8 | PTS1d: 16384 |
| EX: s2pul | PD: 1.0 sec | NA: 8 | WinNuts - \$lsk373.fid |
| | PW: 6.0 usec | LB: 0.0 | |

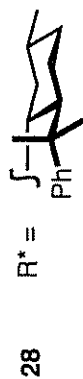
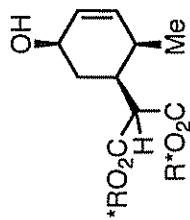


26

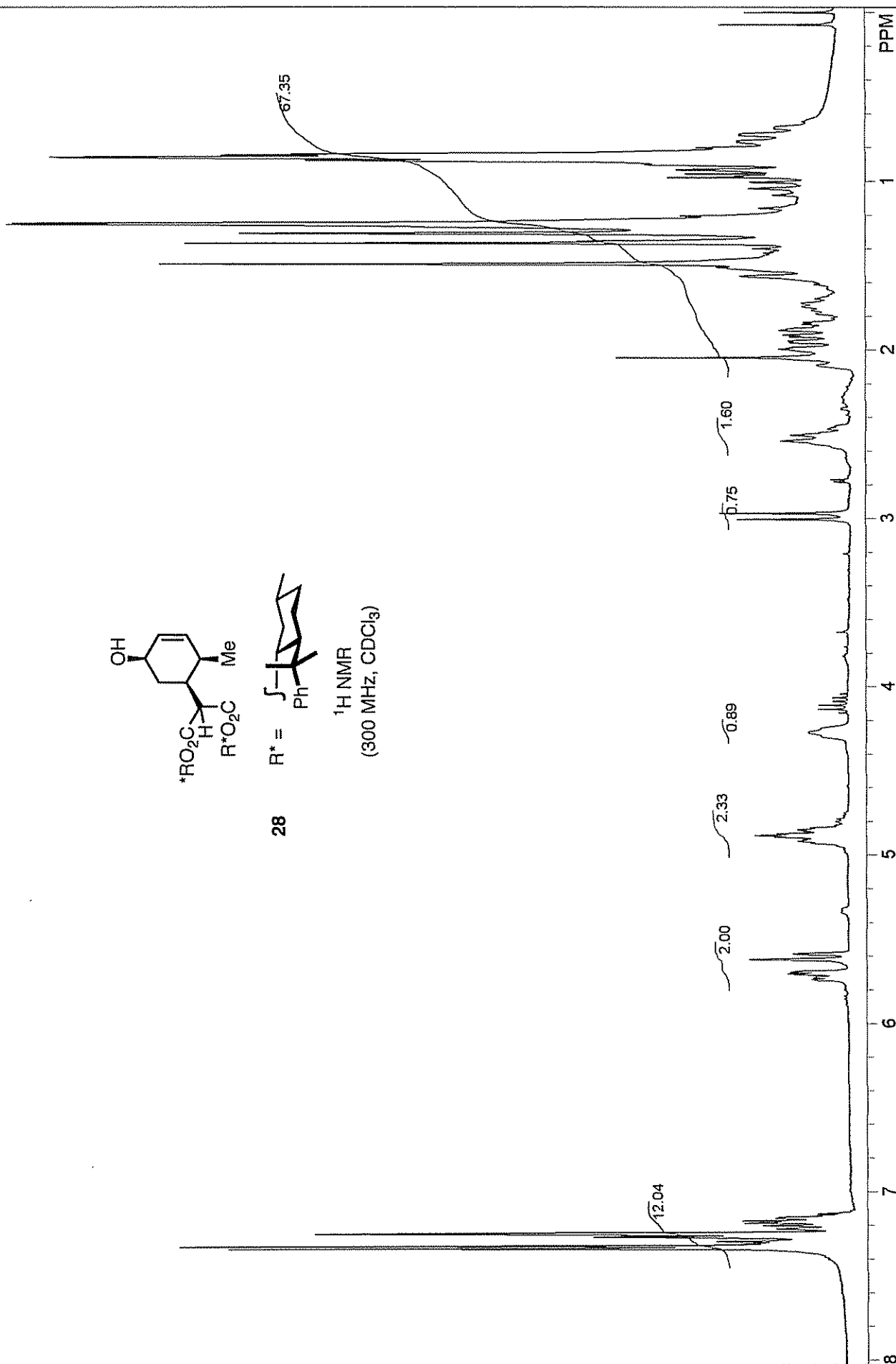
¹³C NMR
(75 MHz, CDCl₃)



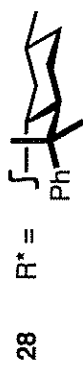
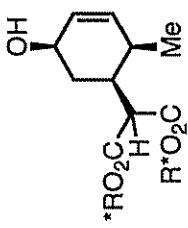
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|------------------------|--------------|----------------------------|----------------------------|
| 13C OBSERVE blank line | | USER: -- DATE: Sep 16 2007 | |
| F1: 75.481 | F2: 300.150 | PTSI d: 32768 | WinNuts - \$lsk373-13c.fid |
| EX: s2pul | PD: 1.0 sec | LB: 0.0 | |
| | SW1: 18868 | OF1: 8279.6 | |
| | PW: 7.3 usec | NA: 448 | |



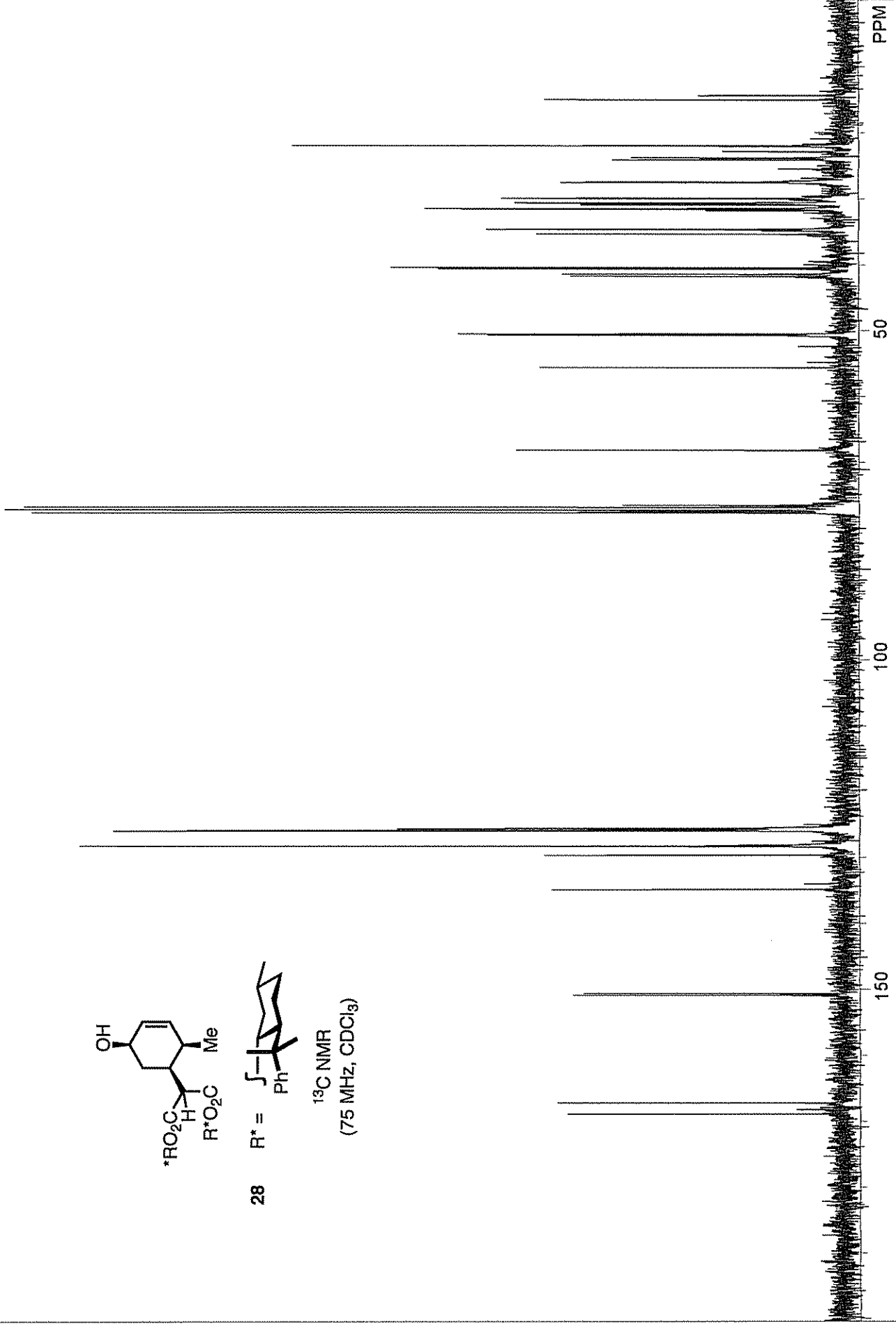
¹H NMR
(300 MHz, CDCl₃)



| | | | |
|--------------------------------|-------------|---------------------------|--------------------|
| STANDARD 1H OBSERVE:blank line | | USER: --DATE: Apr 11 2005 | |
| F1: 300.142 | F2: 75.478 | PTS1d: 14430 | 16384 |
| EX: s2pul | SW1: 4810 | OF1: 1798.3 | |
| | PW: 6.3 us | NA: 8 | |
| | PD: 1.0 sec | LB: 0.0 | |
| | | | Nuts - \$sc569.fid |



¹³C NMR
(75 MHz, CDCl₃)



| | |
|------------------------|----------------------------|
| 13C.OBSERVE:blank line | USER: -- DATE: Apr 11 2005 |
| F1: 75.479 | PTSId: 18868 |
| F2: 300.142 | 32768 |
| EX: s2pul | IB: 1.0 |
| | NA: |
| | PD: 1.0 sec |
| | OF1: 8296.5 |
| | Nuts - \$se369-13c.fid |