

1-1-2014

# Spectral Data for "Probing the human estrogen receptor-alpha binding requirements for phenolic mono- and di-hydroxyl compounds: A combined synthesis, binding and docking study"

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Jayapal Reddy Gone  
*Marquette University*

Zhengjie He  
*Marquette University*

Julie Lukesh  
*Marquette University*

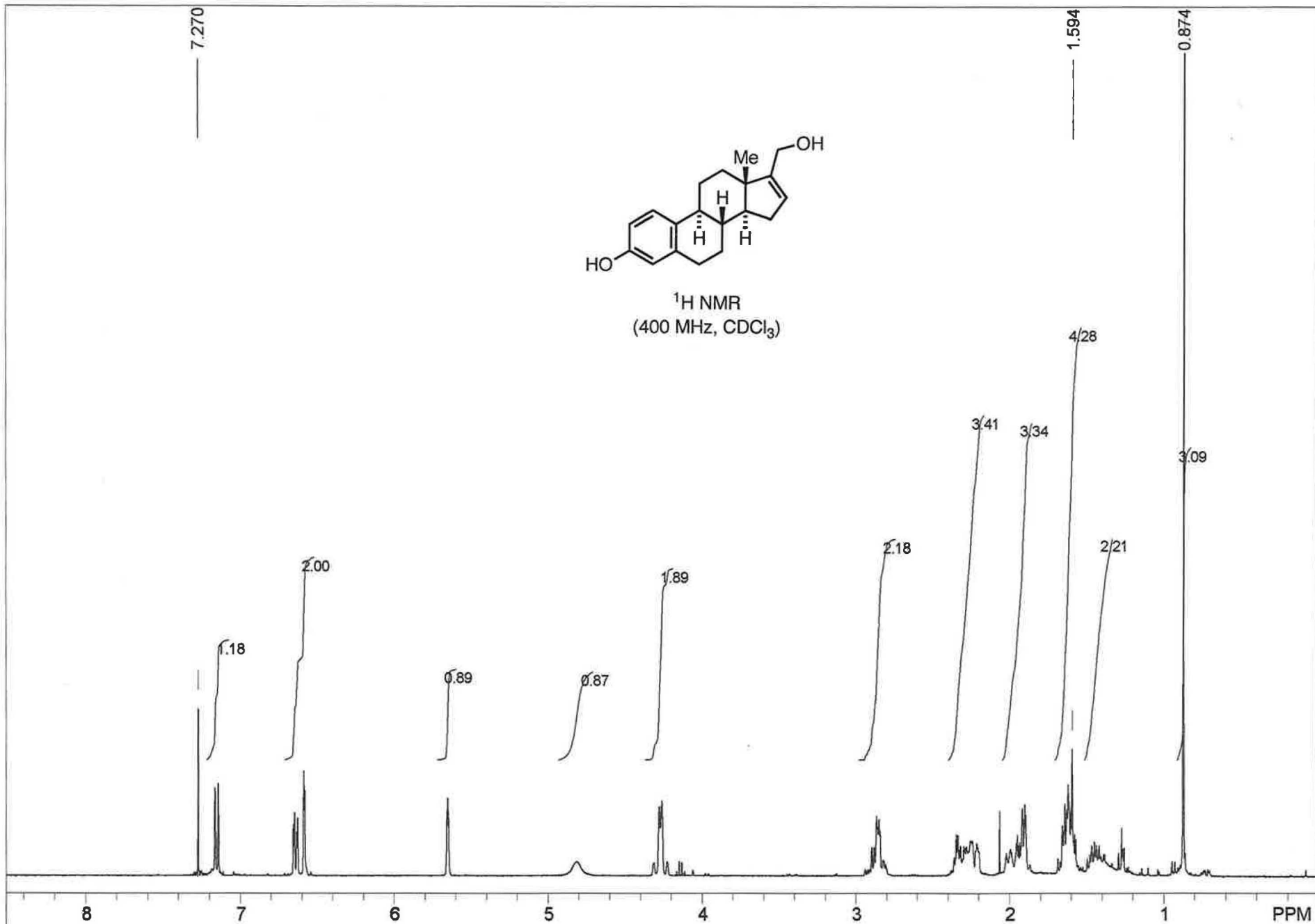
*See next page for additional authors*

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**Authors**

Christopher McCullough, Terrence S. Neumann, Jayapal Reddy Gone, Zhengjie He, Julie Lukesh, Rajesh K. Pandey, William A. Donaldson, and Daniel S. Sem



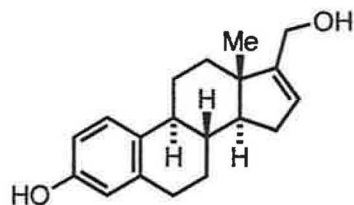
STANDARD 1H OBSERVE - profile

USER: -- DATE: Jan 24 2007

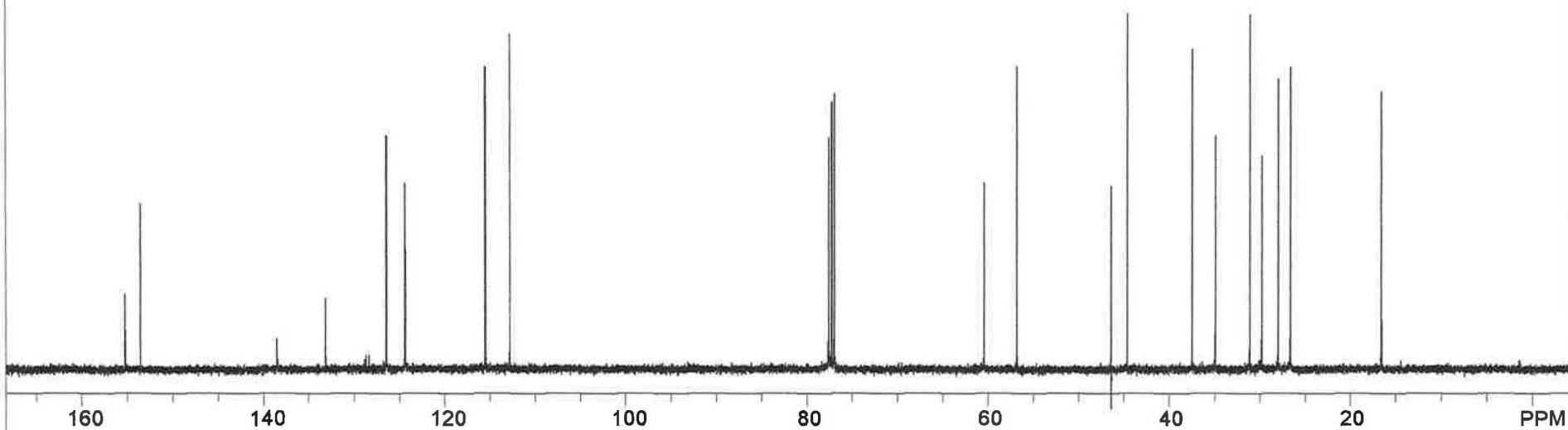
F1: 399.751	F2: 100.526	SW1: 6410	OF1: 2403.1	PTS1d: 13132 , 16384
EX: s2pul	PW: 7.7 us	PD: 1.0 sec	NA: 8	LB: 0.0

Nuts - \$gi-final.fid

155.201  
153.552  
138.503  
133.146  
126.450  
124.355  
115.503  
112.817  
77.559  
77.250  
76.933  
60.403  
56.774  
46.382  
44.570  
37.396  
34.863  
31.078  
29.744  
27.931  
26.605  
16.568



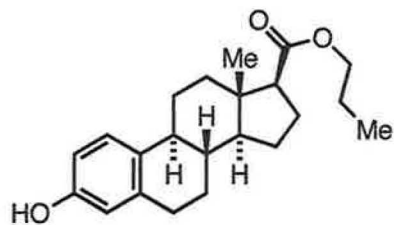
<sup>13</sup>C NMR  
(100 MHz, CDCl<sub>3</sub>)



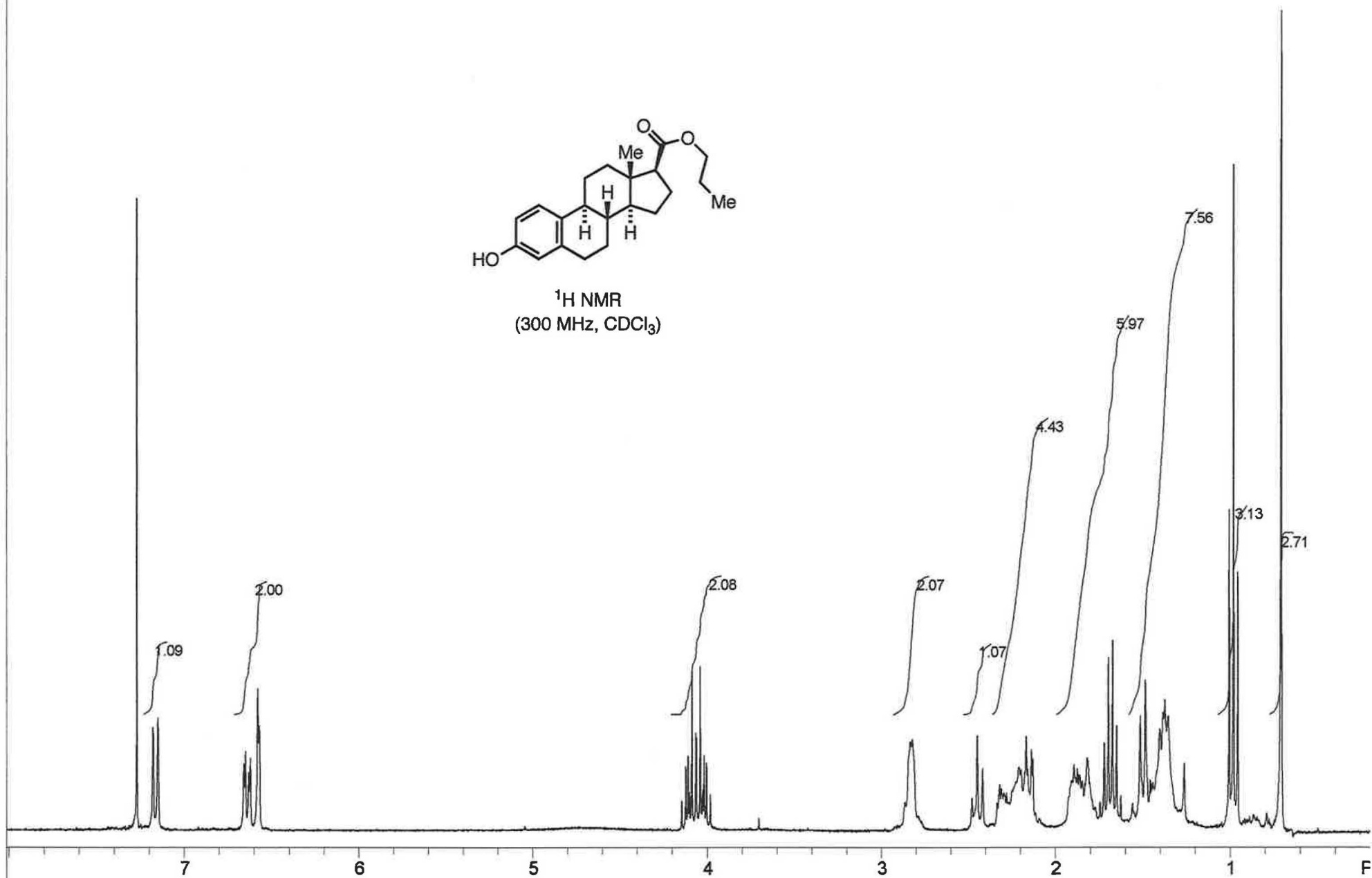
STANDARD 1H OBSERVE - profile

USER: -- DATE: Jan 24 2007

F1: 100.527	F2: 399.751	SW1: 24510	OF1: 10554.2	PTS1d: 31875	32768
EX: s2pul	PW: 7.5 us	PD: 1.0 sec	NA: 16500	LB: 0.0	Nuts - \$gi-overnight.fid



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



STANDARD 1H OBSERVE:blank line

USER: -- DATE: Feb 24 20

F1: 300.142	F2: 75.478	SW1: 4803	OF1: 1803.7	PTS1d: 14409	16384
EX: s2pul	PW: 6.3 us	PD: 1.0 sec	NA: 8	LB: 0.0	Nuts - \$CH-Raney-Nickel-Test

174.568  
174.514

153.525

138.427

132.808

126.703

115.427

112.835

77.647

77.230

76.800

66.052

55.626

55.117

44.548

43.923

39.015

38.567

29.831

27.842

26.734

24.376

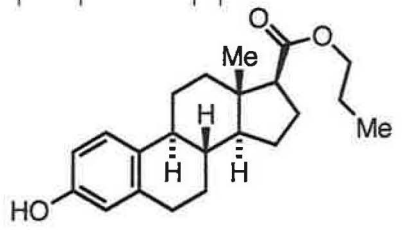
23.769

22.327

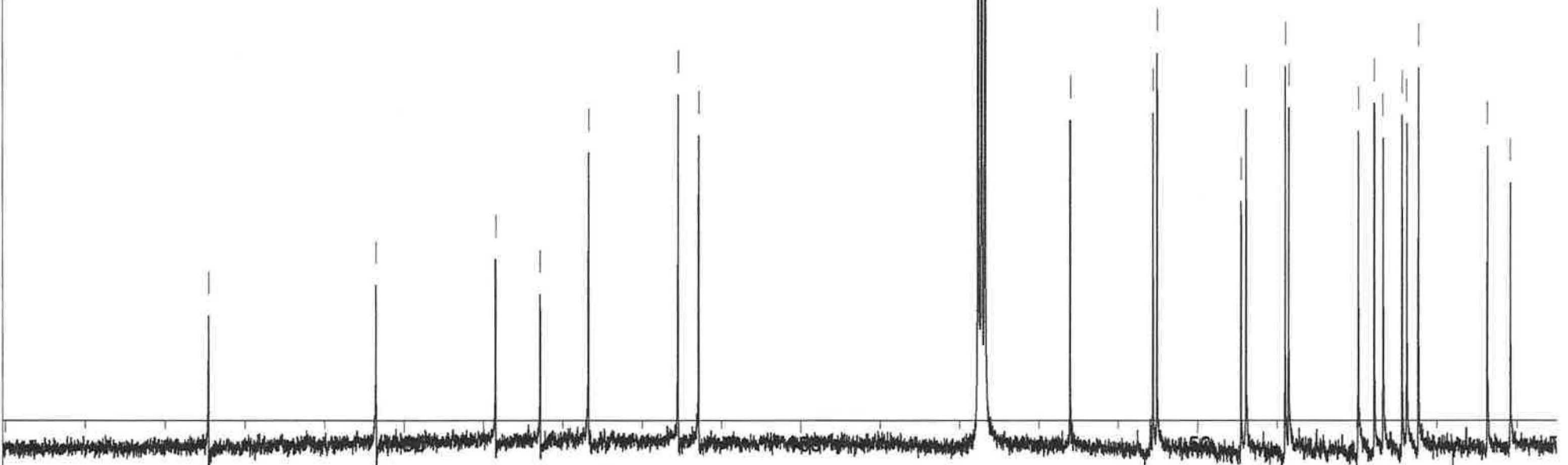
18.021

13.716

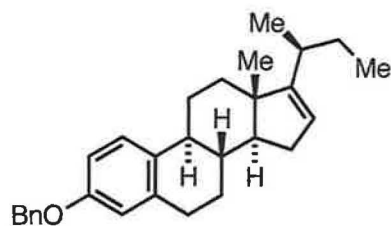
10.856



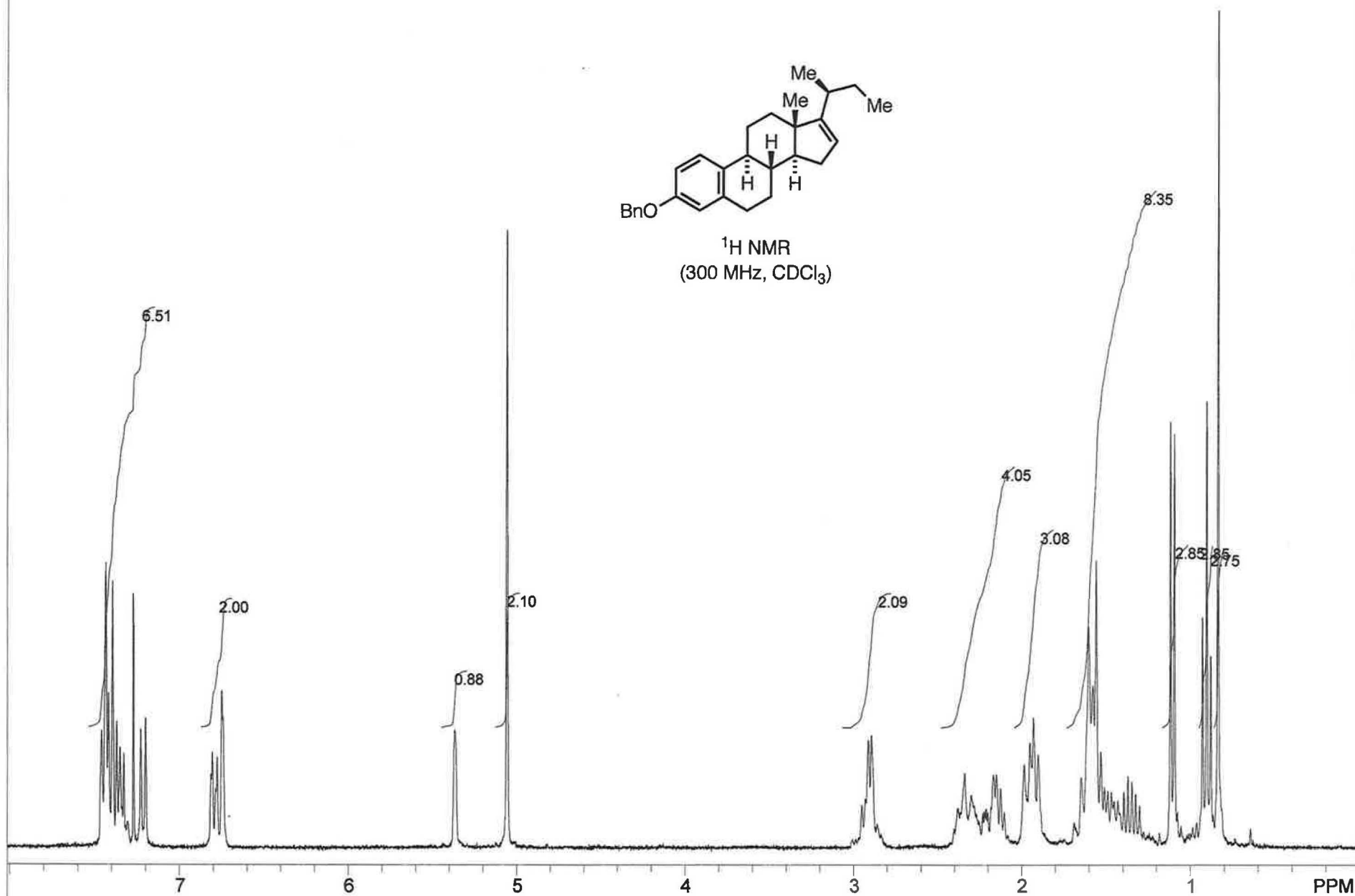
<sup>13</sup>C NMR  
(75 MHz, CDCl<sub>3</sub>)



13C OBSERVE: blank line				USER: -- DATE: Feb 1 20		
F1: 75.479	F2: 300.142	SW1: 18868	OF1: 8291.9	PTS1d: 18868	32768	
EX: s2pul	PW: 7.3 us	PD: 1.0 sec	NA:	LB: 1.5		Nuts - Sch-r-13c-2



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

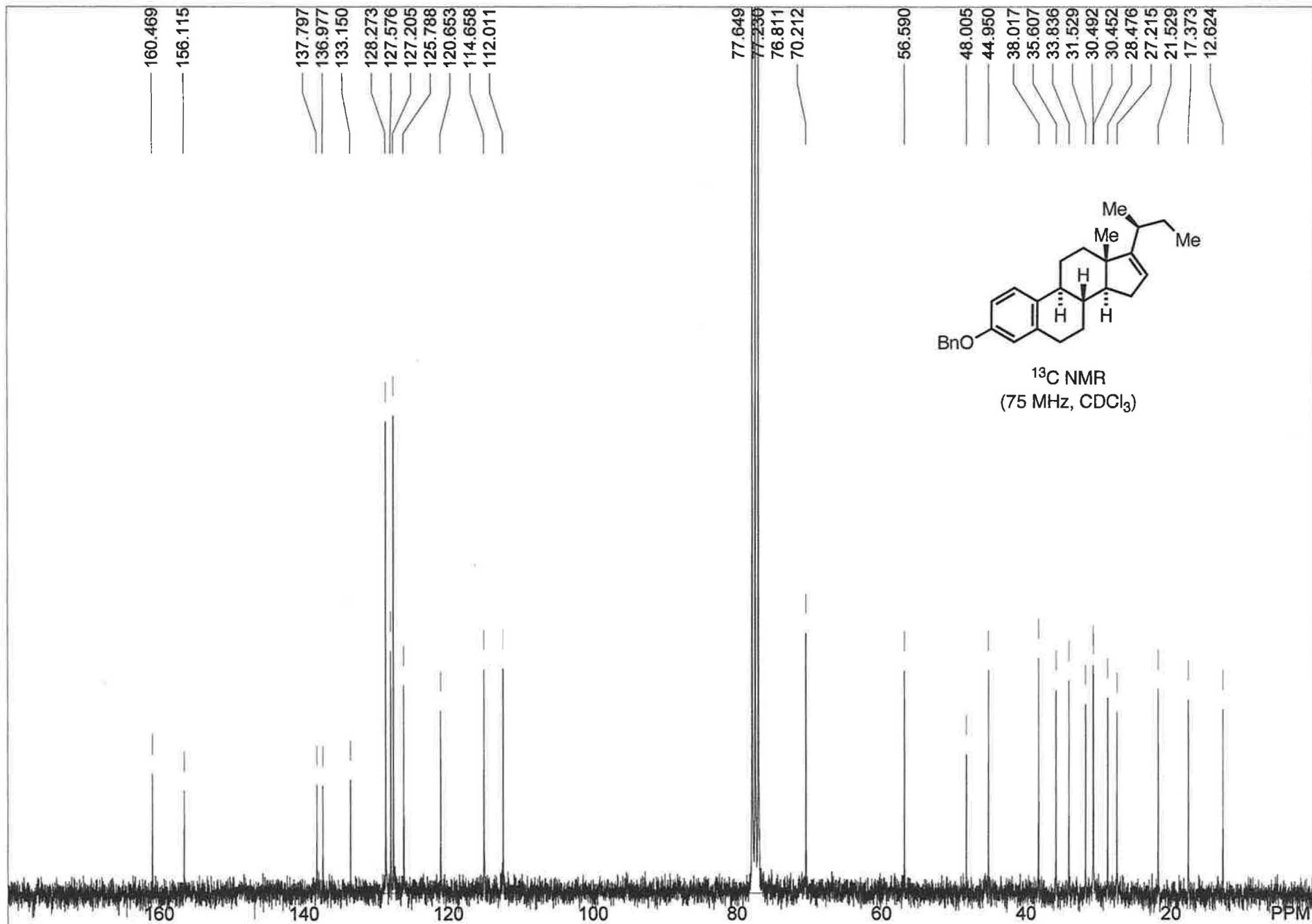


STANDARD 1H OBSERVE:blank line

USER: -- DATE: Oct 3 2002

F1: 300.151	F2: 75.480	SW1: 4810	OF1: 1806.5	PTS1d: 14430 , 16384
EX: s2pul	PW: 6.0 us	PD: 1.0 sec	NA: 8	LB: 0.0

Nuts - \$zhep217.fid



:blank line

USER: -- DATE: Oct 3 2002

F1: 75.481

F2: 300.150

SW1: 18868

OF1: 8277.1

PTS1d: 18868 , 32768

EX: s2pul

PW: 7.3 us

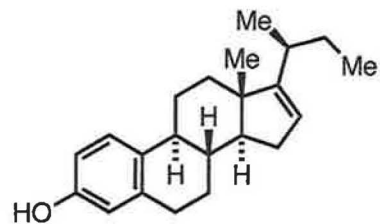
PD: 1.0 sec

NA: 5000

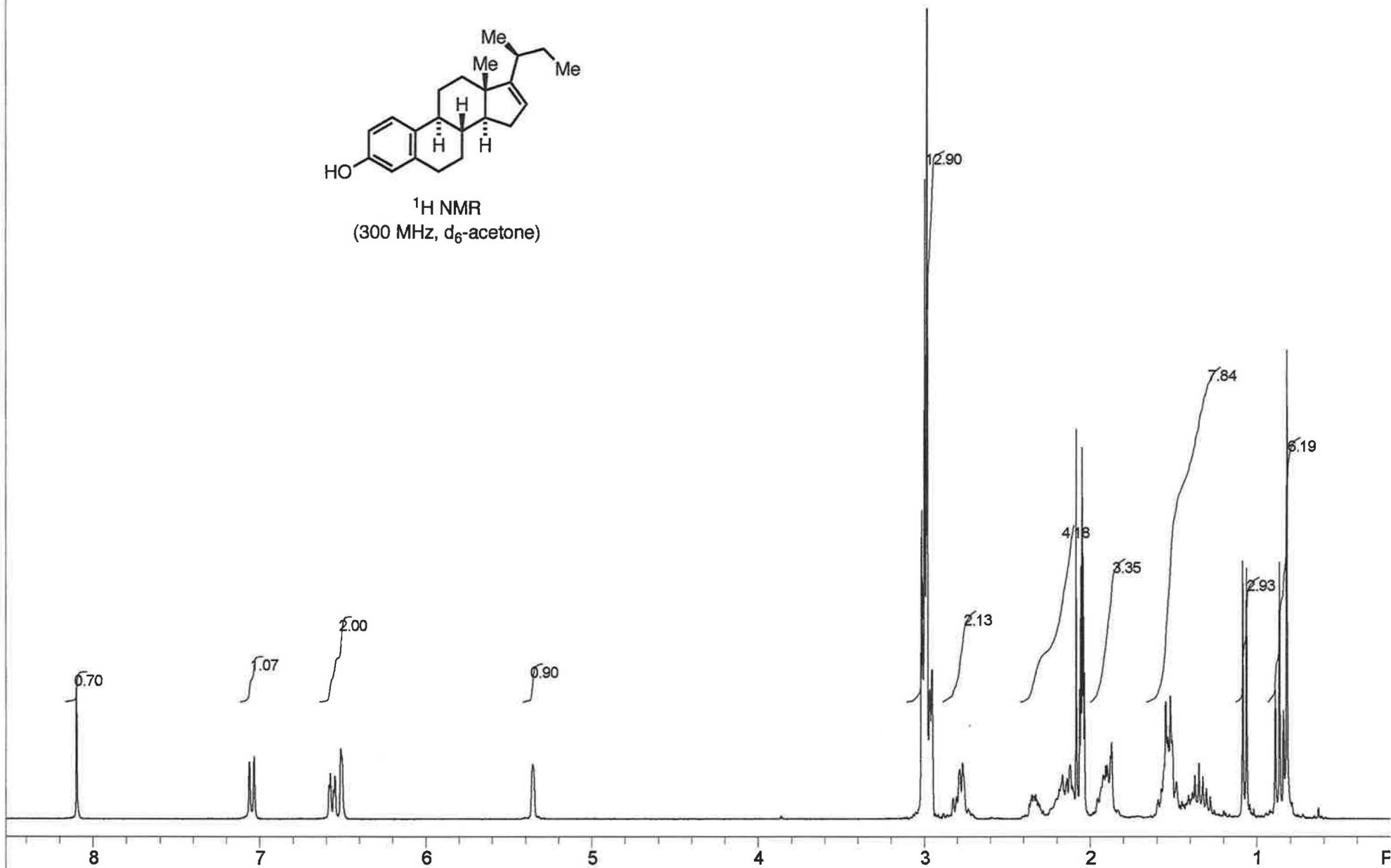
LB: 1.0

Nuts - \$CARBON.fid





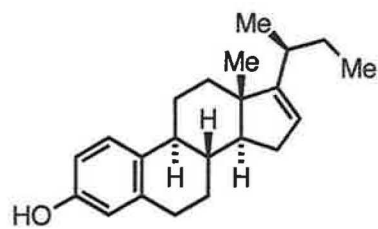
<sup>1</sup>H NMR  
(300 MHz, d<sub>6</sub>-acetone)



STANDARD 1H OBSERVE:blank line

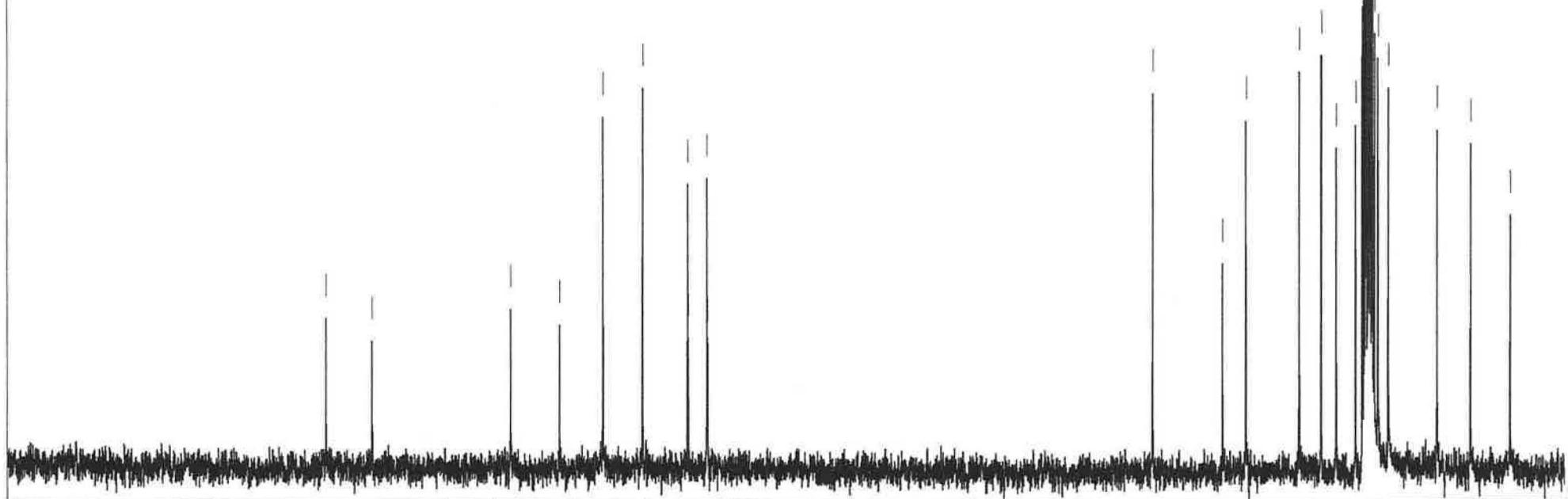
USER: -- DATE: Oct 8 20

F1: 300.152	F2: 75.480	SW1: 4810	OF1: 1795.3	PTS1d: 14430	16384
EX: s2pul	PW: 6.0 us	PD: 1.0 sec	NA: 8	LB: 0.0	Nuts - \$zhep218



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

160.649  
154.891  
137.445  
131.309  
125.854  
120.891  
115.258  
115.167  
112.829  
112.745  
56.922  
35.822  
48.170  
45.247  
33.946  
31.538  
30.687  
30.628  
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30.300  
30.181  
29.920  
29.673  
29.419  
29.156  
28.737  
27.450



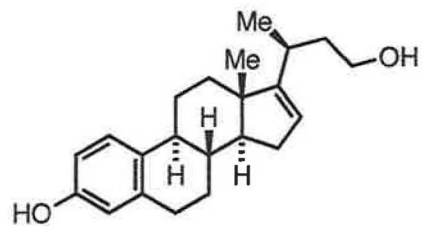
150

100

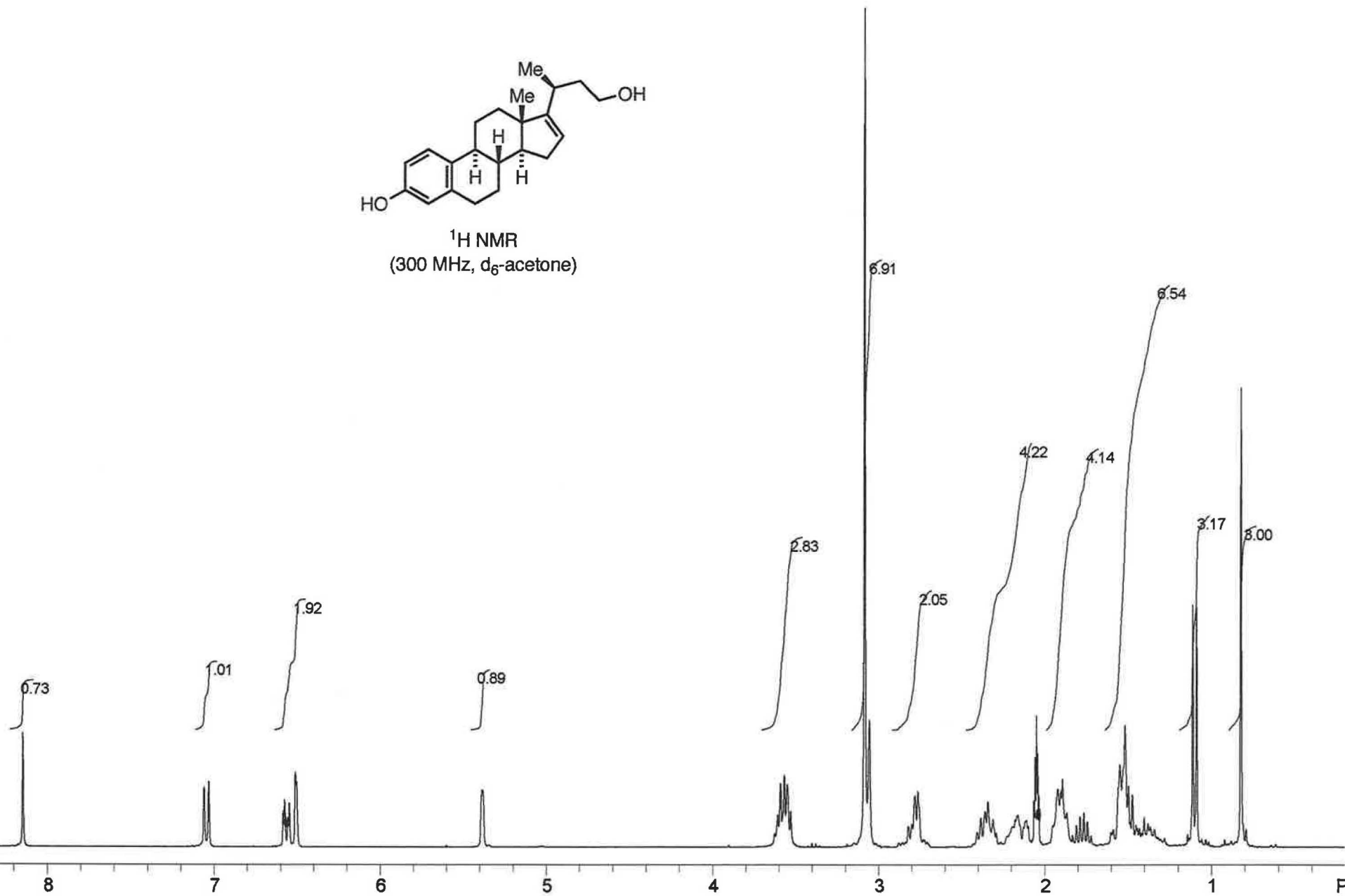
50

F

:blank line			USER: -- DATE: Oct 8 20			
F1: 75.481	F2: 300.152	SW1: 18868	OF1: 8299.9	PTS1d: 18868	32768	
EX: s2pul	PW: 7.3 us	PD: 1.0 sec	NA: 2000	LB: 1.5	Nuts - \$CARBON	



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

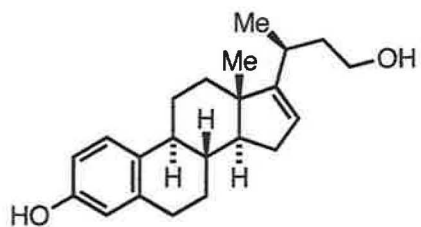


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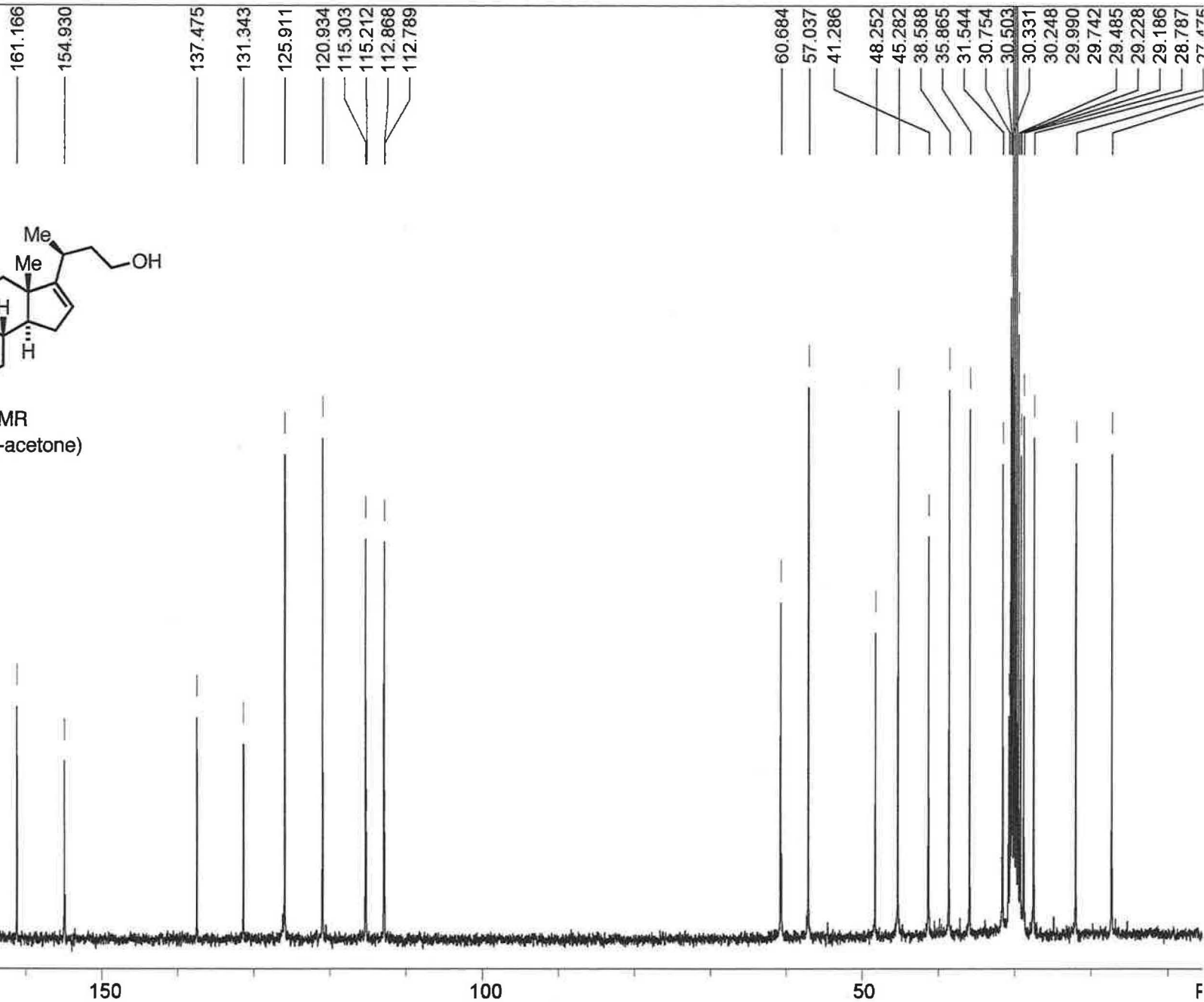
USER: -- DATE: Sep 23 20

F1: 300.152	F2: 75.480	SW1: 4810	OF1: 1795.3	PTS1d: 14430 , 16384
EX: s2pul	PW: 6.0 us	PD: 1.0 sec	NA: 8	LB: 0.0

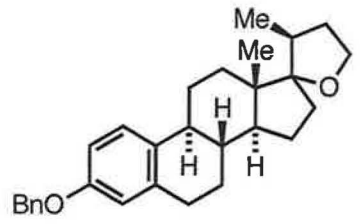
Nuts - Szhep212



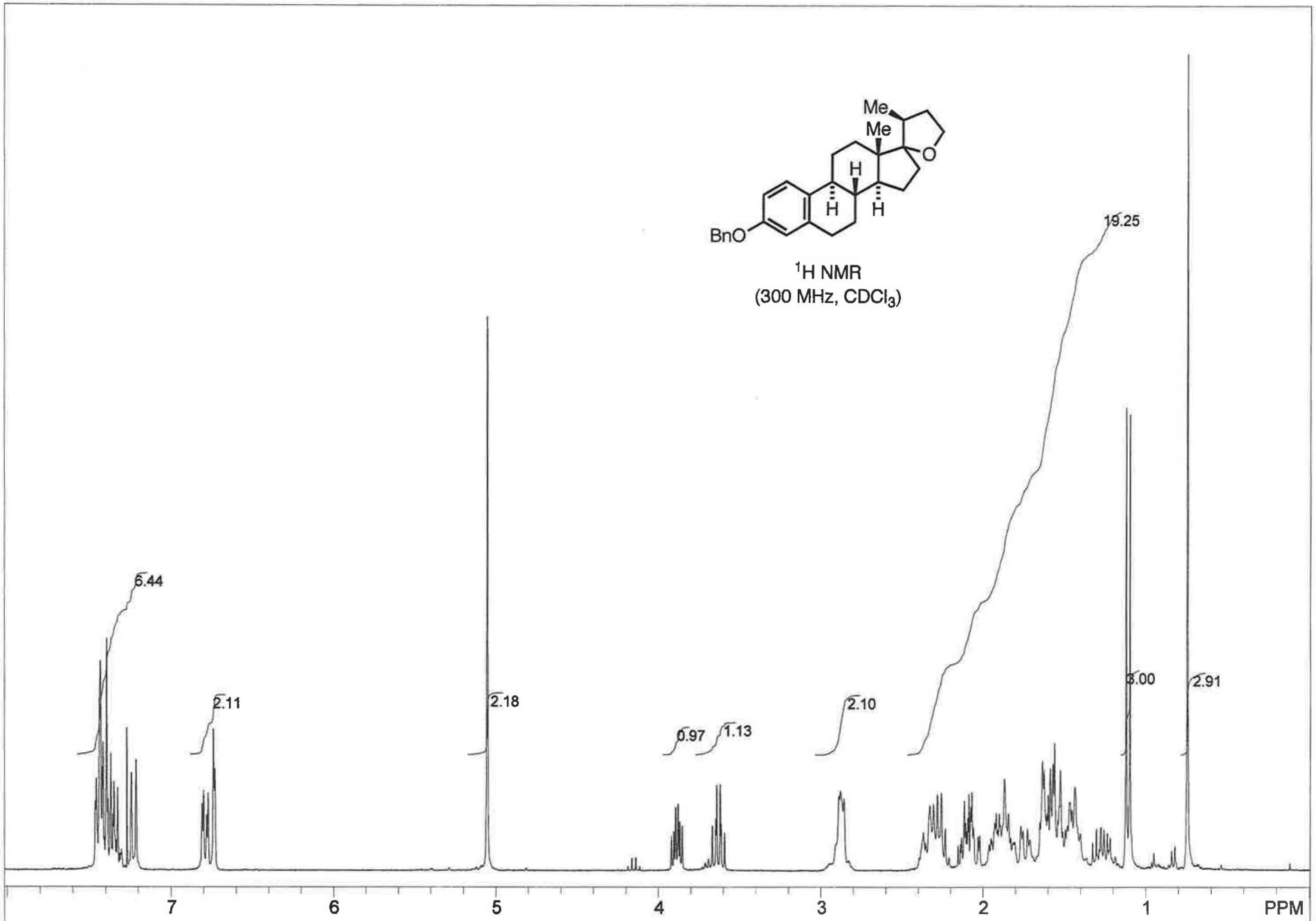
<sup>13</sup>C NMR  
(75 MHz, d<sub>6</sub>-acetone)



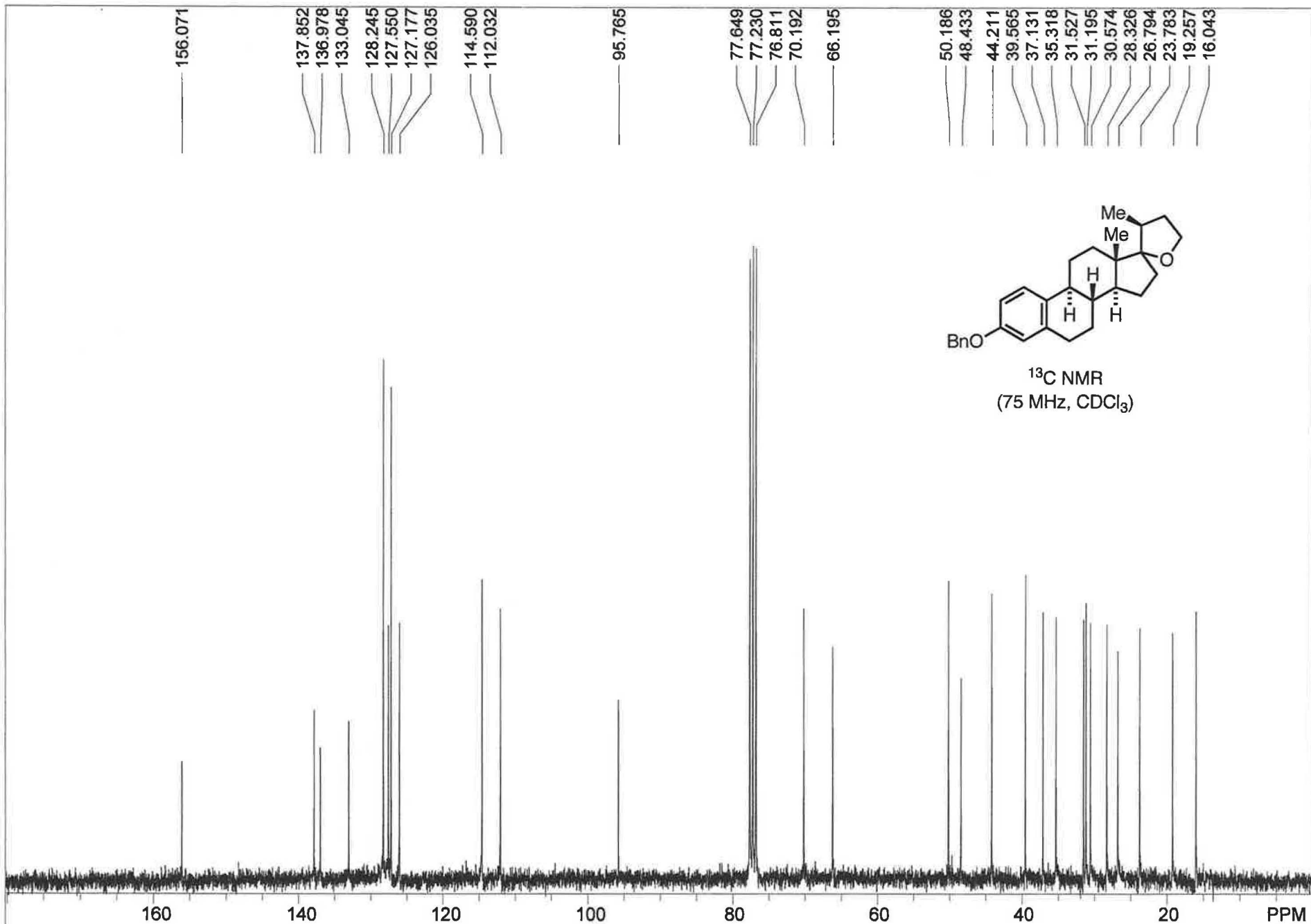
:blank line			USER: -- DATE: Sep 23 20			
F1: 75.481	F2: 300.152	SW1: 18868	OF1: 8302.7	PTS1d: 18868	32768	
EX: s2pul	PW: 7.3 us	PD: 1.0 sec	NA: 5000	LB: 1.5	Nuts - \$CARBON	



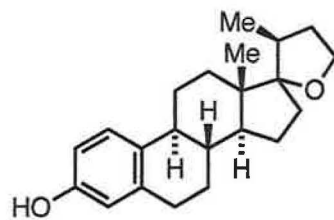
<sup>1</sup>H NMR  
(300 MHz, CDCl<sub>3</sub>)



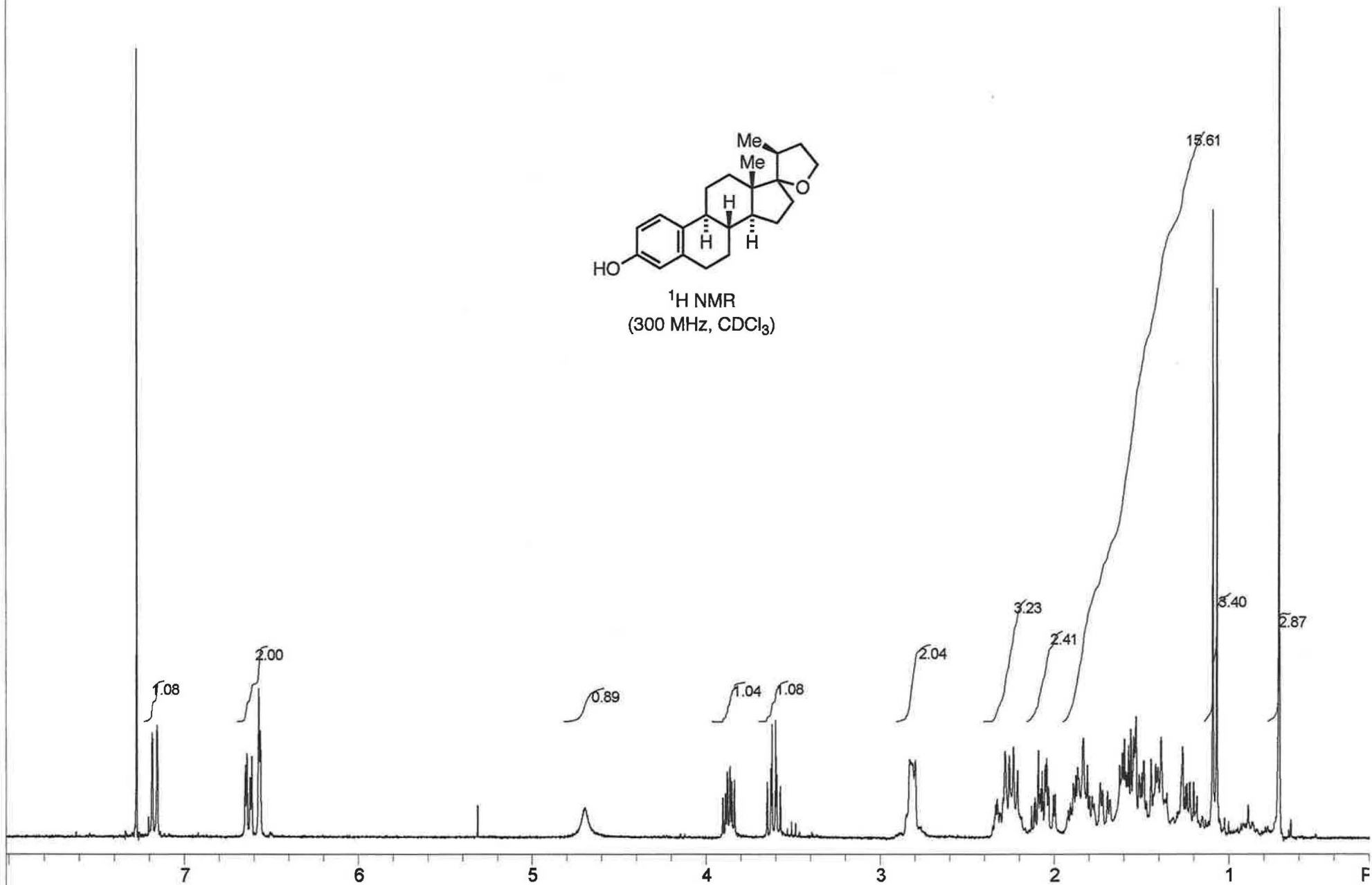
STANDARD 1H OBSERVE;blank line				USER: -- DATE: Aug 7 2002			
F1: 300.151	F2: 75.480	SW1: 4810		OF1: 1806.9		PTS1d: 14430 , 16384	
EX: s2pul		PW: 6.0 us	PD: 1.0 sec	NA: 8	LB: 0.0	Nuts - \$zhep194d.fid	



:blank line				USER: -- DATE: Aug 7 2002		
F1: 75.481	F2: 300.150	SW1: 18868		OF1: 8275.9		PTS1d: 18868 , 32768
EX: s2pul		PW: 7.3 us	PD: 1.0 sec	NA: 2000	LB: 1.0	Nuts - \$CARBON.fid



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

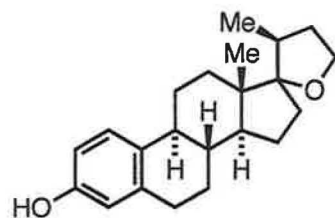


STANDARD 1H OBSERVE:blank line

USER: -- DATE: Feb 29 20

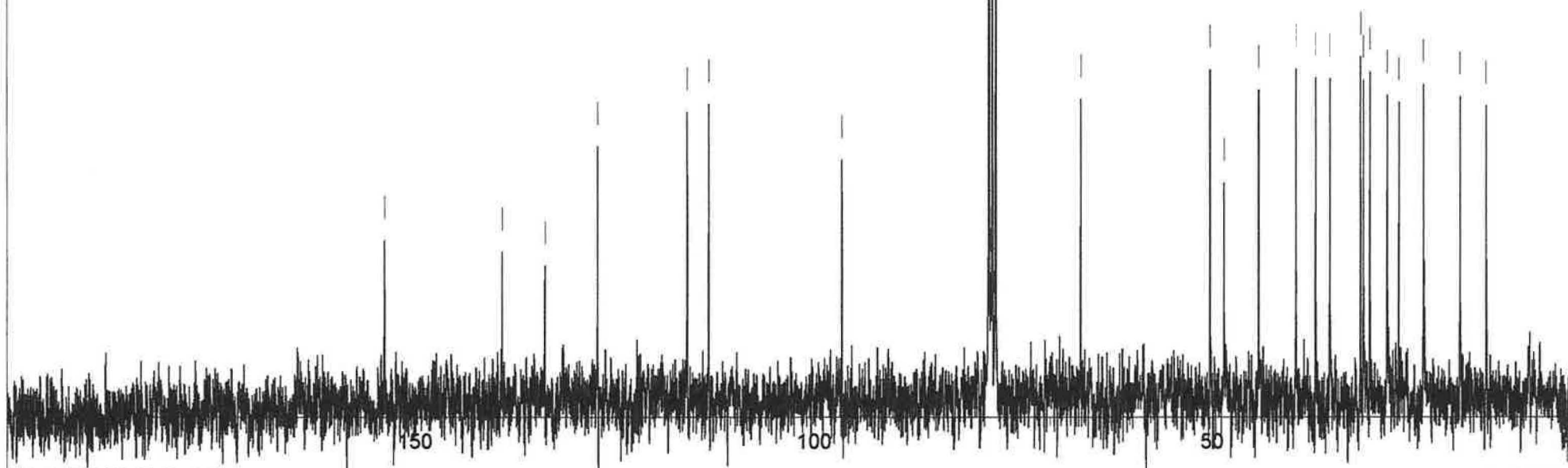
F1: 300.142	F2: 75.478	SW1: 4803	OF1: 1803.0	PTS1d: 14409 , 16384
EX: s2pul	PW: 6.0 us	PD: 1.0 sec	NA: 8	LB: 0.0

Nuts - \$j1528a



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

- 153.308
- 138.566
- 133.223
- 126.598
- 126.507
- 115.374
- 112.679
- 96.057
- 77.661
- 77.439
- 77.236
- 77.043
- 76.816
- 66.152
- 57.937
- 49.969
- 48.231
- 43.896
- 39.248
- 39.190
- 36.798
- 35.020
- 31.198
- 30.844
- 30.028
- 27.873
- 26.421
- 23.367
- 23.215
- 18.822
- 15.575



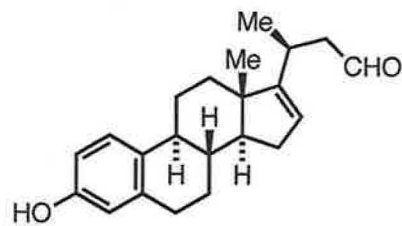
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USER: -- DATE: Feb 29 20

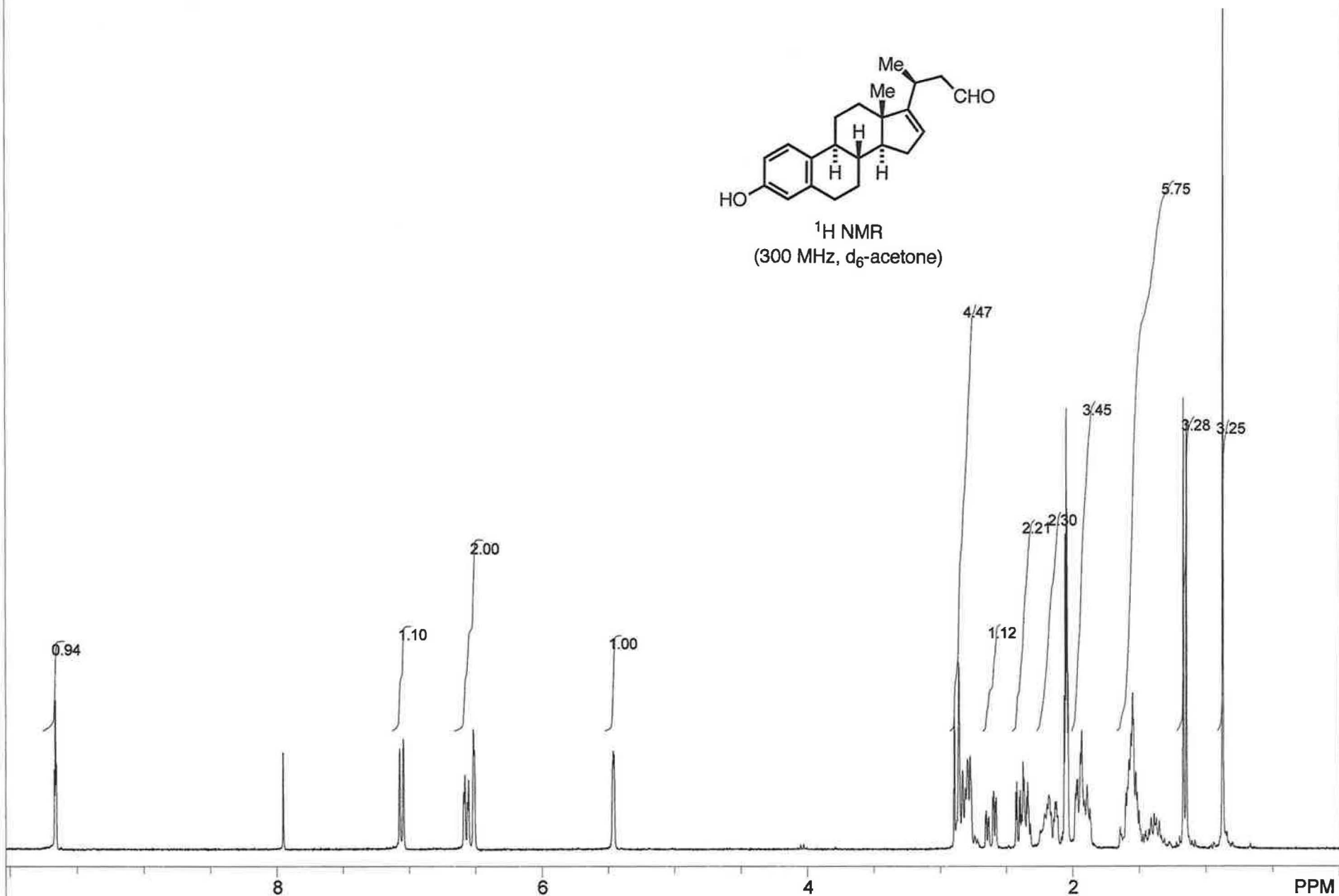
F1: 75.479	F2: 300.142	SW1: 18868	OF1: 8295.6	PTS1d: 18868 , 32768
EX: s2pul	PW: 7.3 us	PD: 1.0 sec	NA: 256	LB: 2.0

Nuts - \$il528carbon





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



STANDARD 1H OBSERVE:blank line

USER: -- DATE: Oct 31 2002

F1: 300.152

F2: 75.480

SW1: 4810

OF1: 1795.4

PTS1d: 14430 , 16384

EX: s2pul

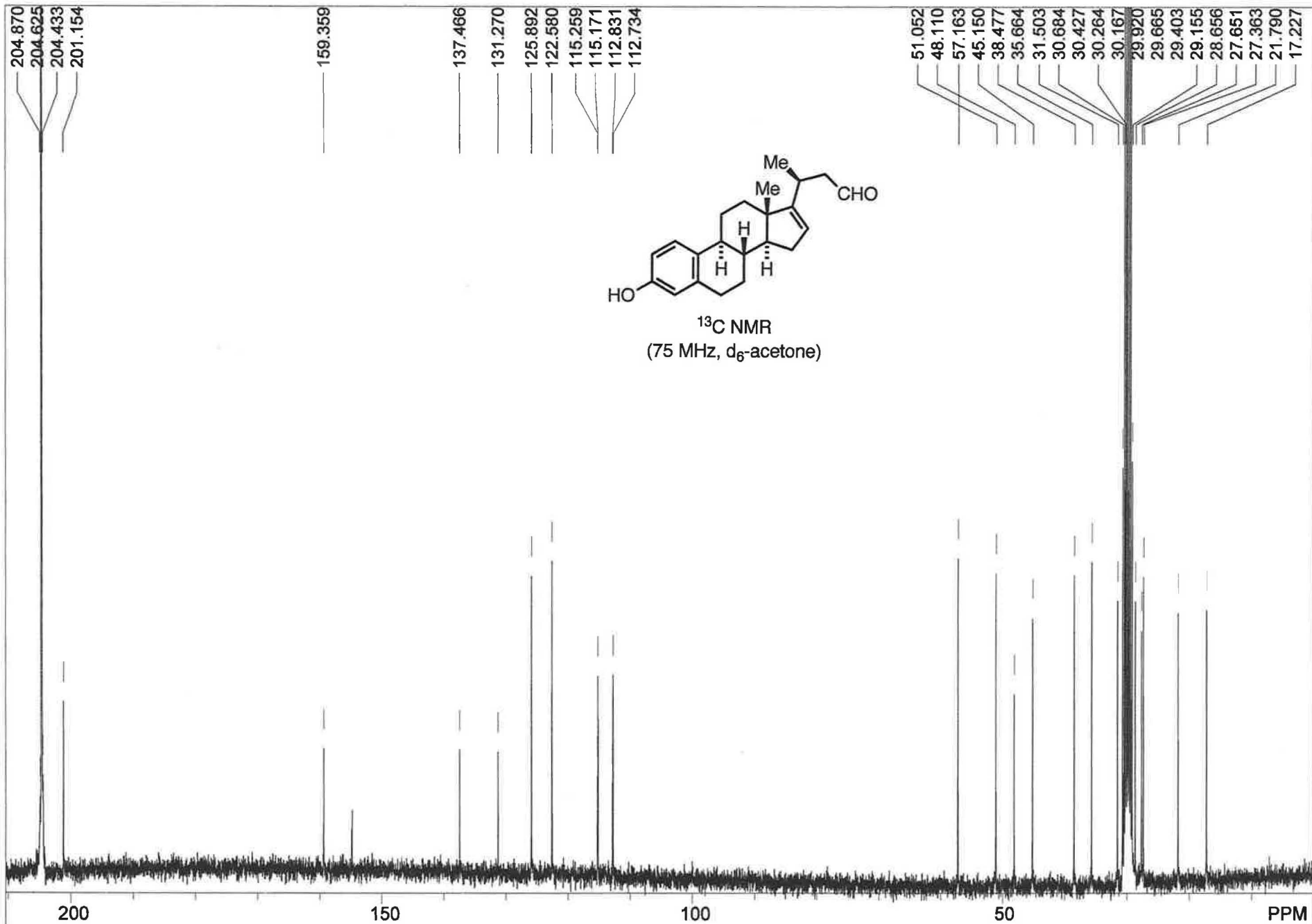
PW: 6.0 us

PD: 1.0 sec

NA: 8

LB: 0.0

Nuts - \$zhep235.fid



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USER: -- DATE: Oct 31 2002

F1: 75.481

F2: 300.152

SW1: 18868

OF1: 8300.1

PTS1d: 18868 , 32768

EX: s2pul

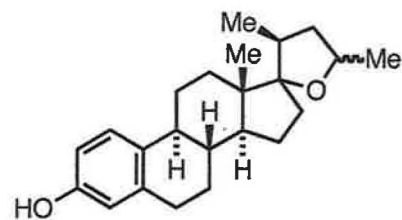
PW: 7.3 us

PD: 1.0 sec

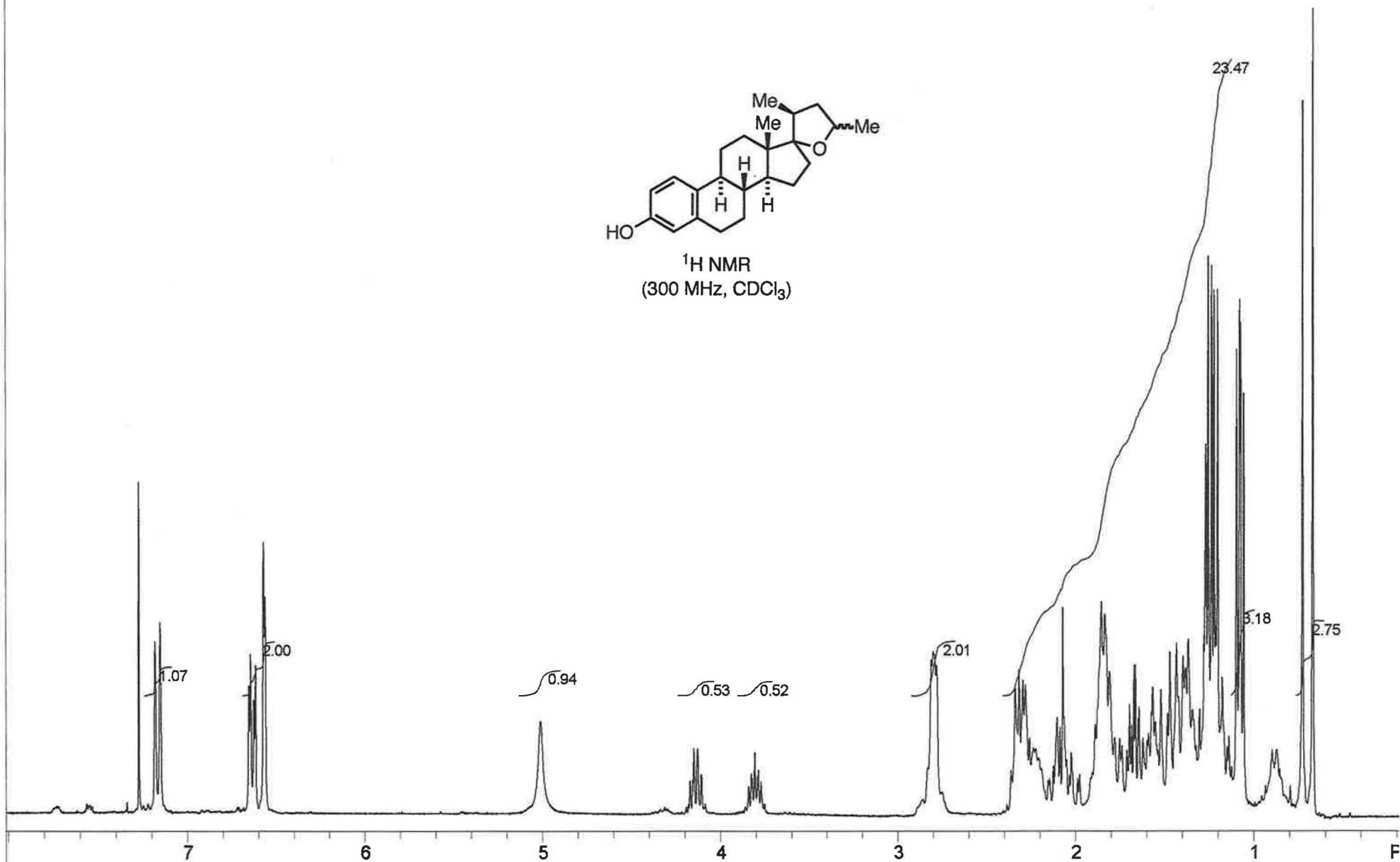
NA: 5000

LB: 1.0

Nuts - \$CARBON.fid



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

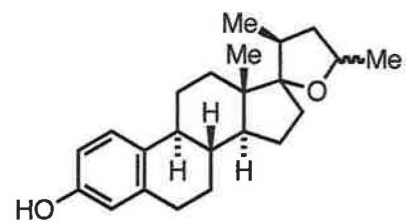


STANDARD 1H OBSERVE:blank line

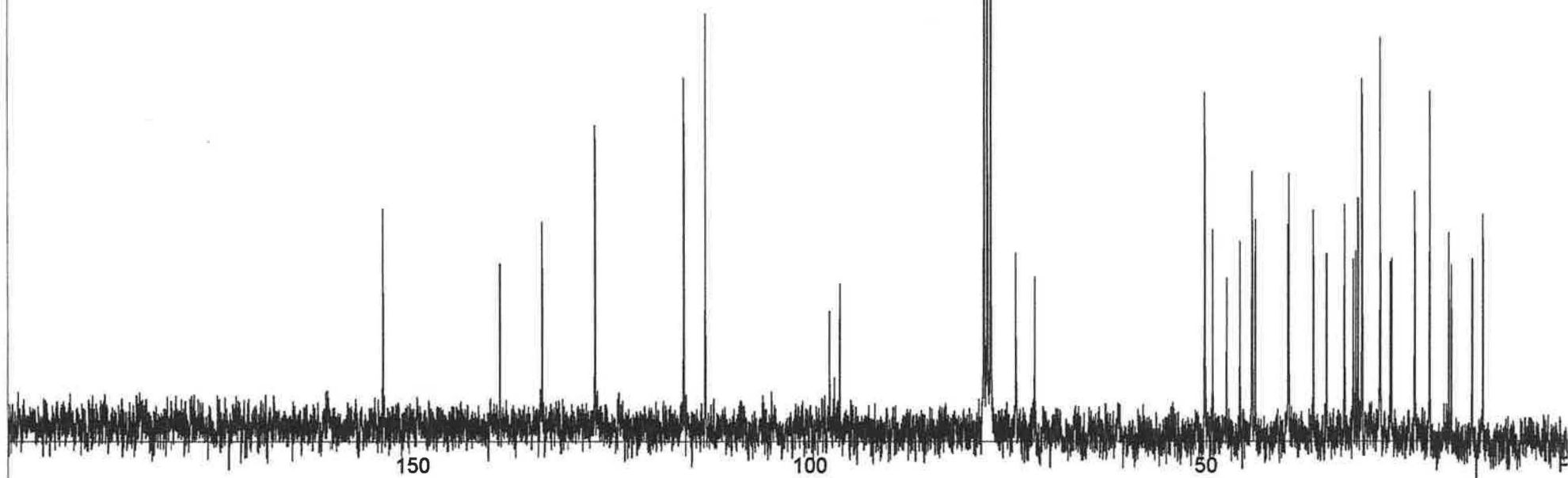
USER: -- DATE: Mar 3 20

F1: 300.142	F2: 75.478	SW1: 4803	OF1: 1802.7	PTS1d: 14409 , 16384
EX: s2pul	PW: 6.0 us	PD: 1.0 sec	NA: 8	LB: 0.0

Nuts - \$1529



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

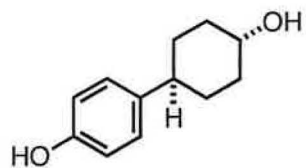


<sup>13</sup>C OBSERVE: blank line

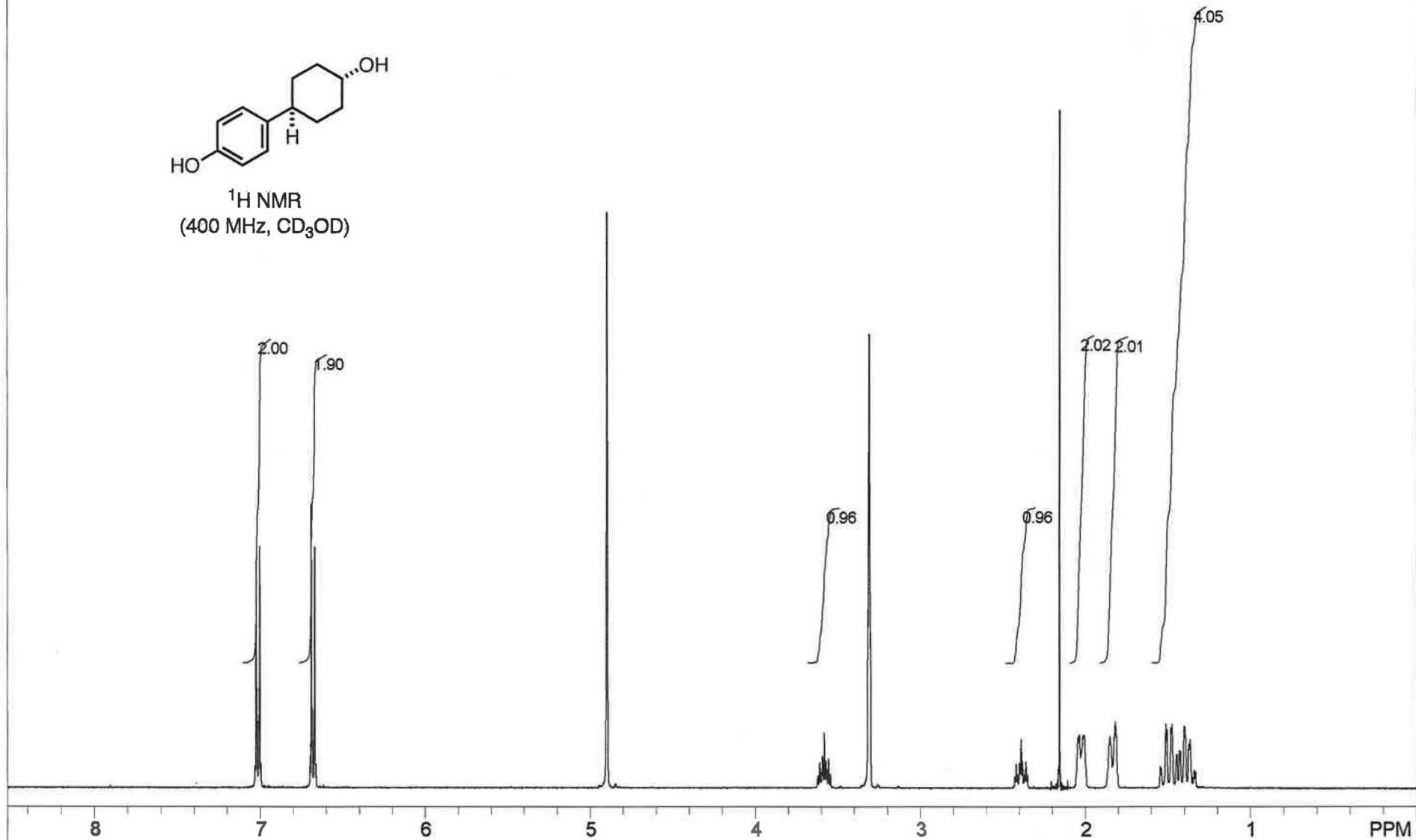
USER: -- DATE: Mar 3 20

F1: 75.479	F2: 300.142	SW1: 18868	OF1: 8293.9	PTS1d: 18868 , 32768
EX: s2pul	PW: 7.3 us	PD: 1.0 sec	NA: 256	LB: 2.0

Nuts - \$j1529carbon



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

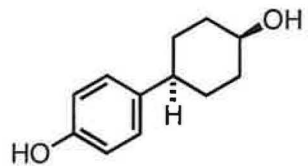


STANDARD 1H OBSERVE - profile

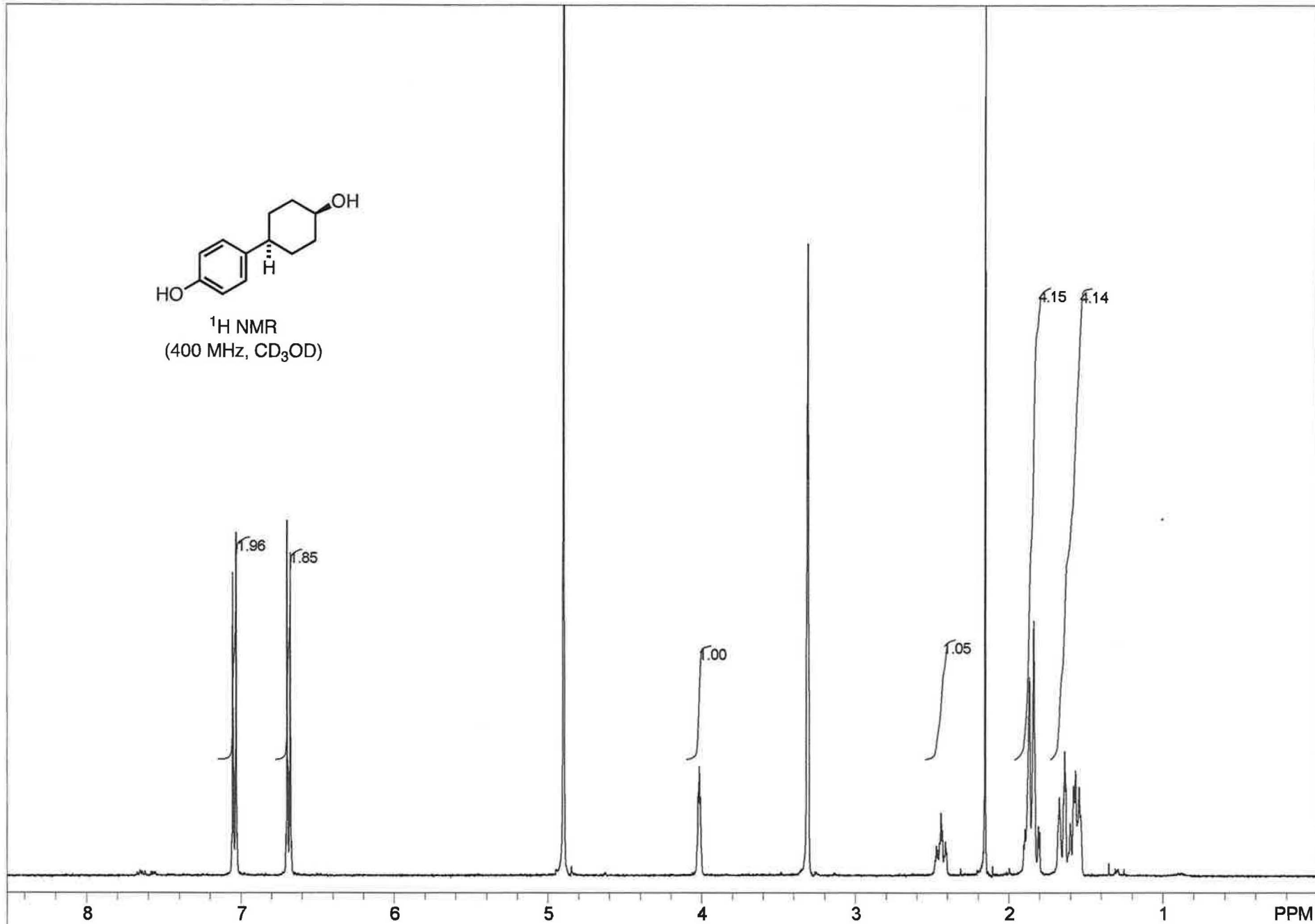
USER: -- DATE: Feb 19 2007

F1: 399.753	F2: 100.527	SW1: 6410	OF1: 2402.0	PTS1d: 13132 , 16384
EX: s2pul	PW: 7.7 us	PD: 1.0 sec	NA: 8	LB: 0.0

Nuts - \$rkp130-II-F-major.fid



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

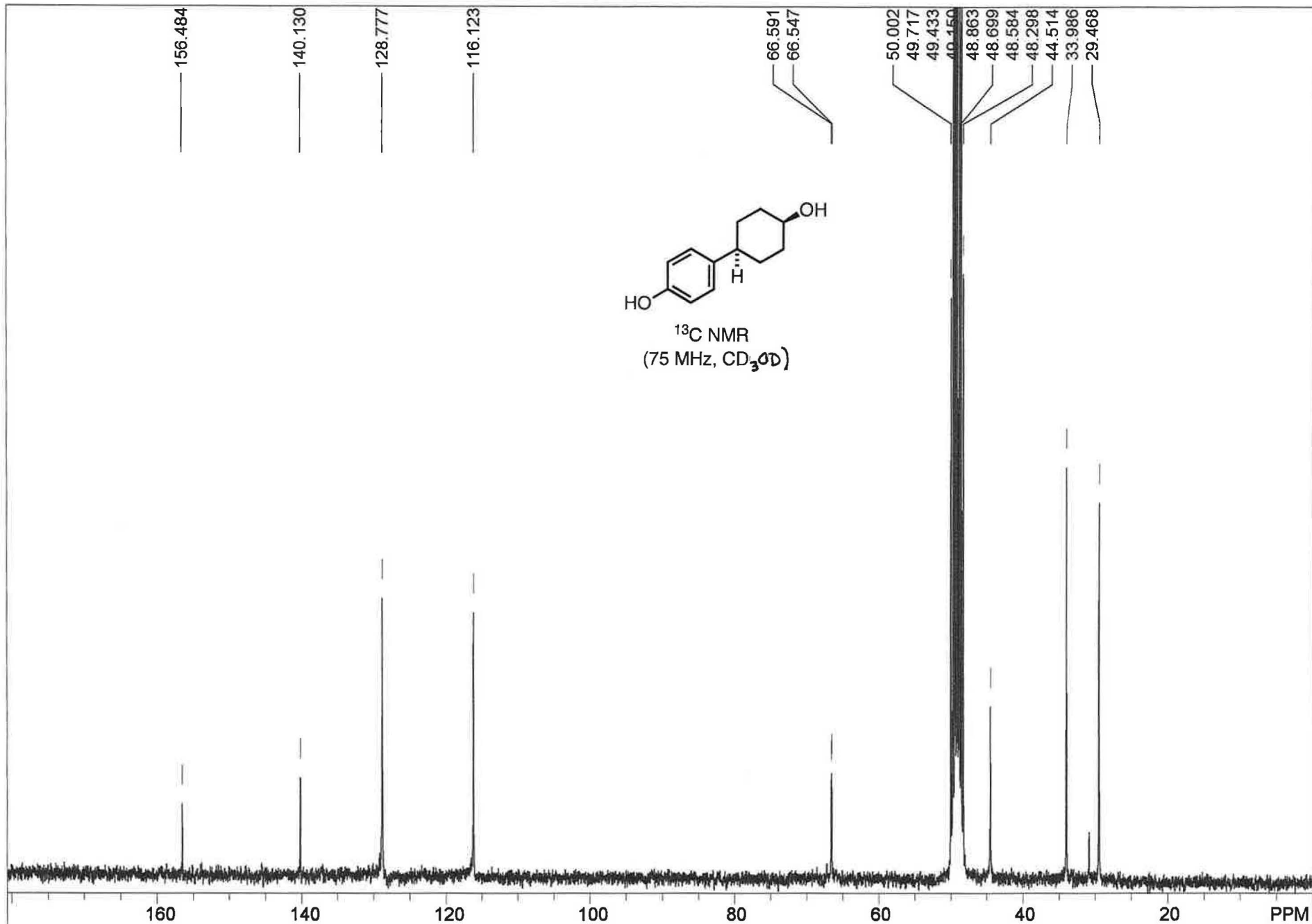


STANDARD 1H OBSERVE - profile

USER: -- DATE: Feb 19 2007

F1: 399.751	F2: 100.526	SW1: 6410	OF1: 827.0	PTS1d: 13132 , 16384
EX: s2pul	PW: 7.7 us	PD: 1.0 sec	NA: 8	LB: 0.0

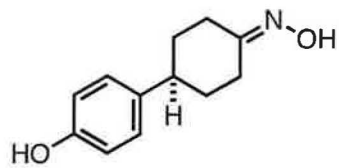
Nuts - \$rkp130-I-F-minor.fid



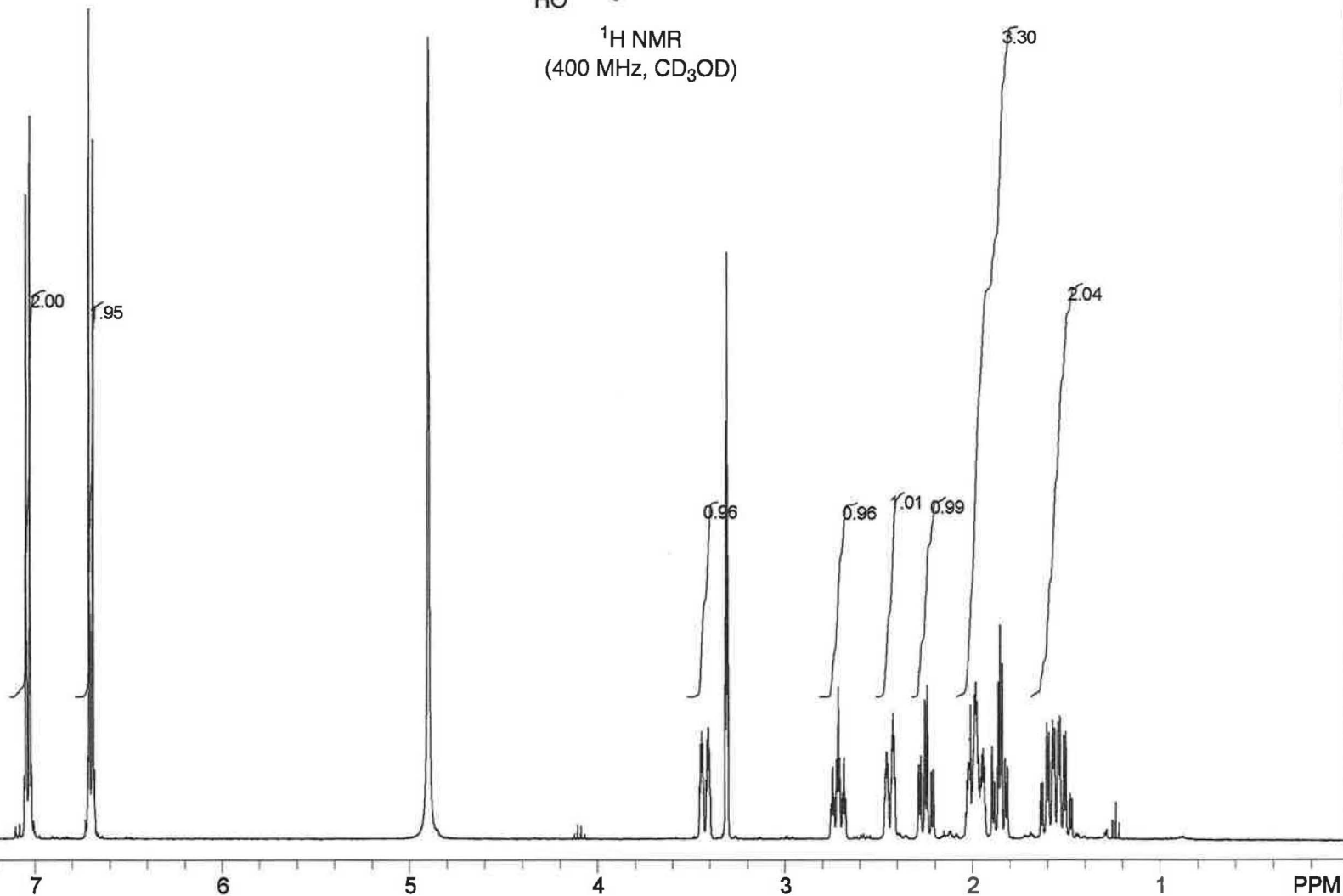
13C OBSERVE:blank line

USER: -- DATE: Feb 19 2007

F1: 75.477	F2: 300.137	SW1: 18868	OF1: 8402.5	PTS1d: 34246	65536
EX: s2pul	PW: 7.3 us	PD: 1.0 sec	NA: 64	LB: 1.5	Nuts - \$rkp130-I-F-CNMR.fid



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

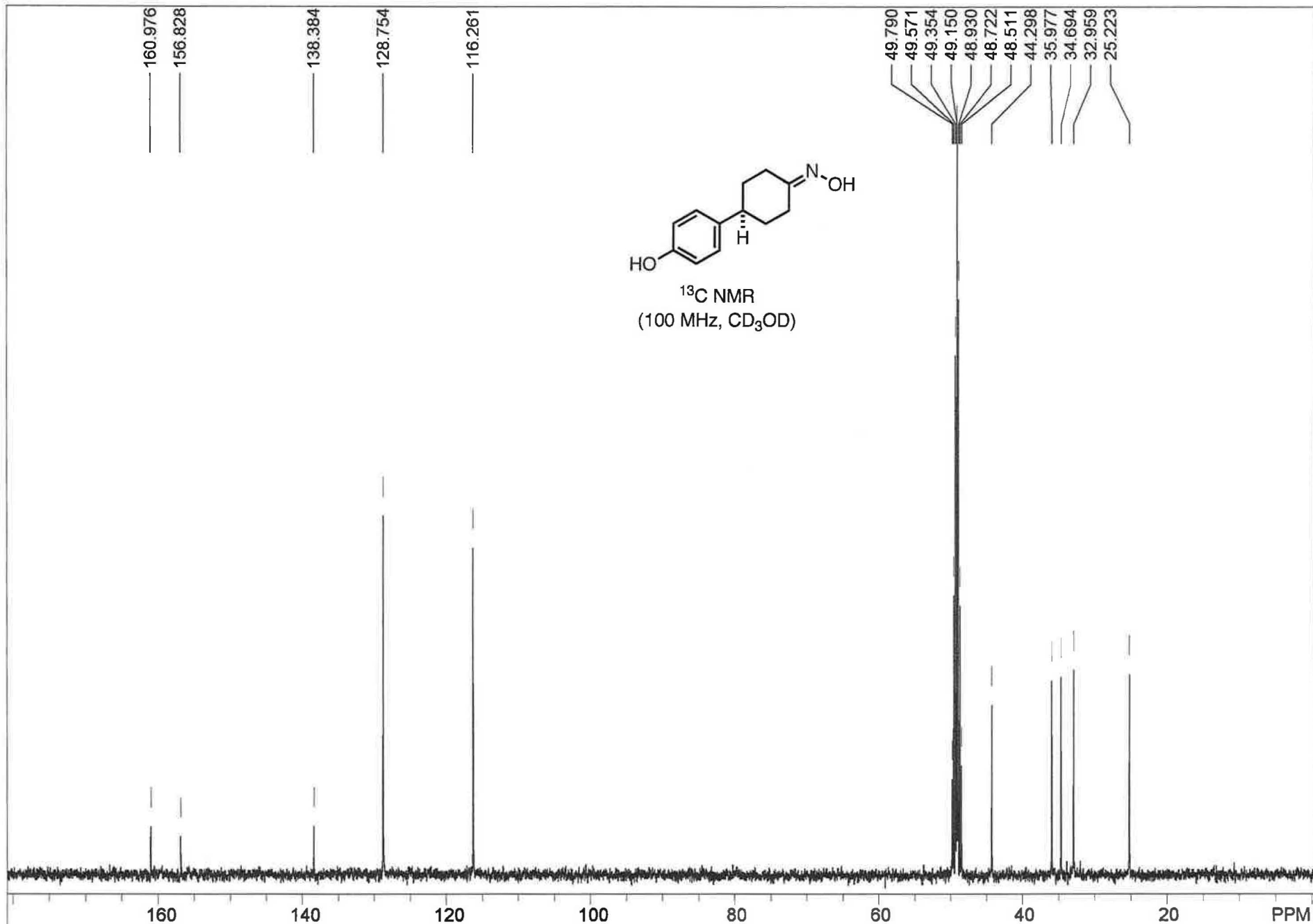


STANDARD 1H OBSERVE - profile

USER: -- DATE: Feb 15 2007

F1: 399.753	F2: 100.527	SW1: 6410		OF1: 2901.8		PTS1d: 13132 , 16384
EX: s2pul		PW: 7.7 us	PD: 1.0 sec	NA: 8	LB: 0.0	Nuts - \$rpk134-crude.fid

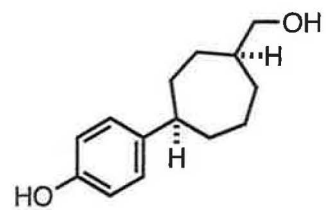




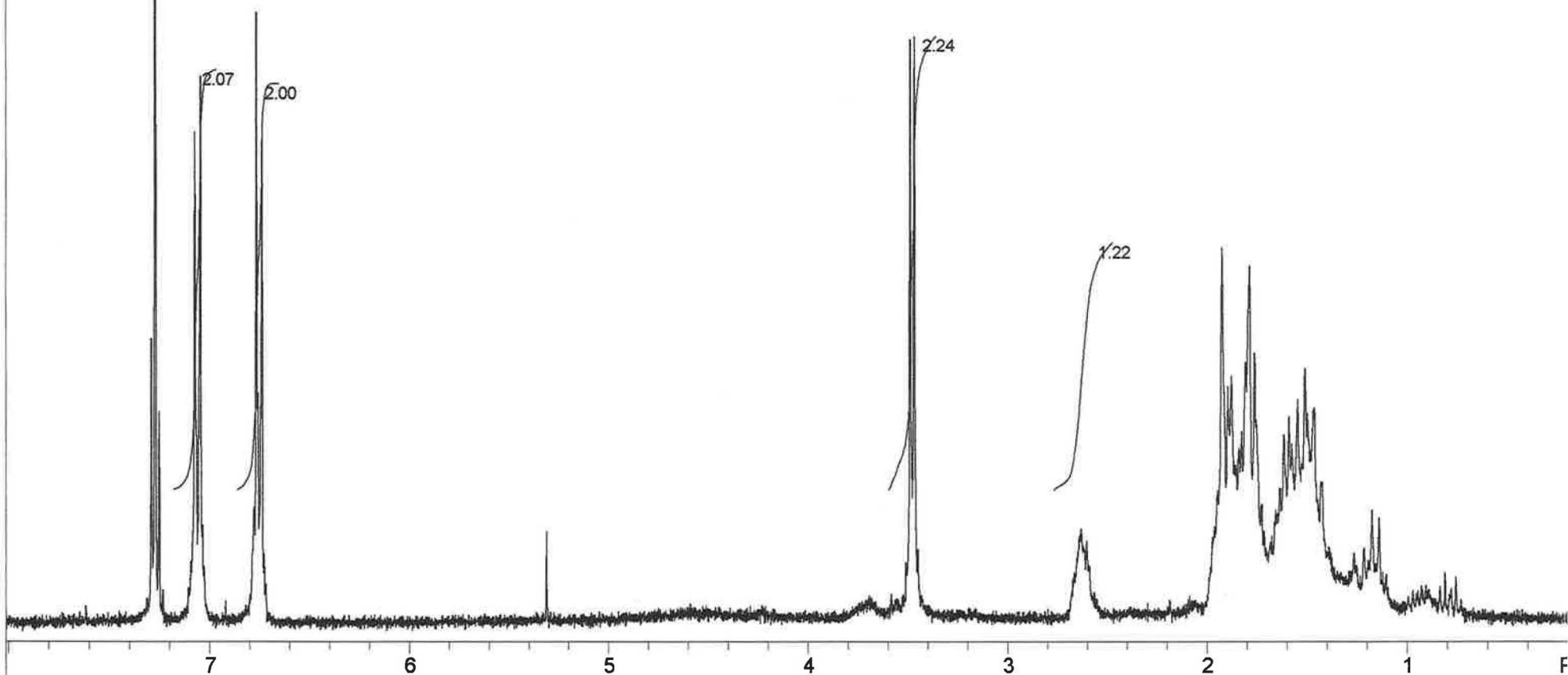
STANDARD 1H OBSERVE - profile

USER: -- DATE: Feb 15 2007

F1: 100.528	F2: 399.753	SW1: 24510	OF1: 10813.6	PTS1d: 31875	32768
EX: s2pul	PW: 7.5 us	PD: 1.0 sec	NA: 256	LB: 2.0	Nuts - \$rkp134-CNMR.fid



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

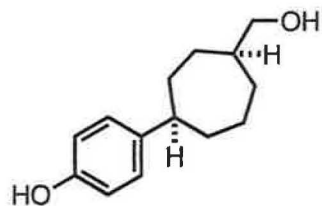


STANDARD 1H OBSERVE:blank line

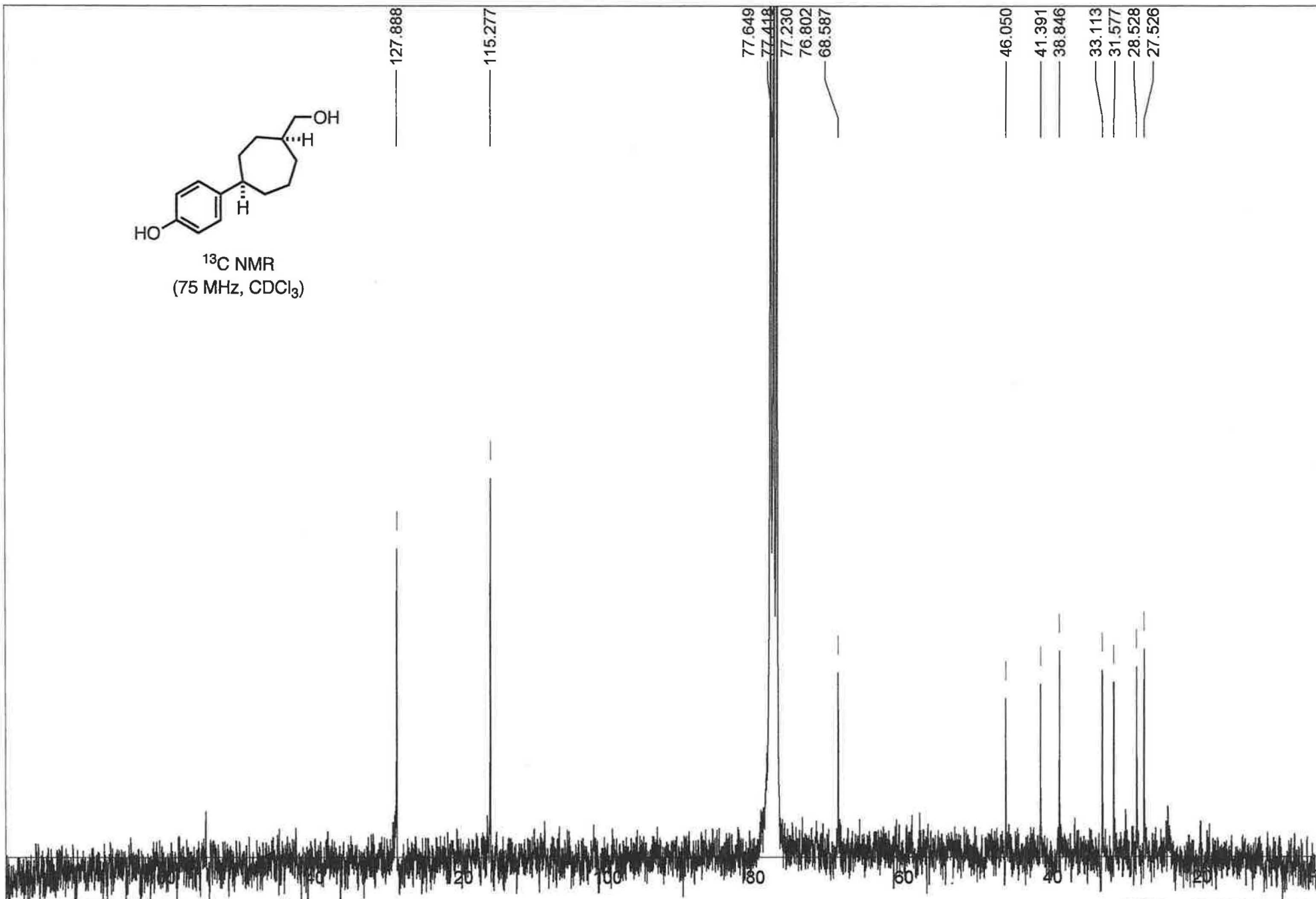
USER: -- DATE: Oct 11 20

F1: 300.145	F2: 75.479	SW1: 4810	OF1: 1804.1	PTS1d: 14430 , 16384
EX: s2pul	PW: 6.3 us	PD: 1.0 sec	NA: 64	LB: 0.0

Nuts - \$rkp086-II-F-H1NMR



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

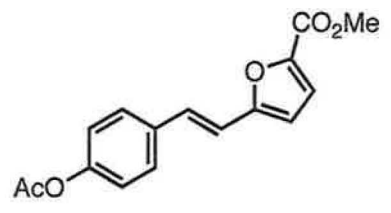


<sup>13</sup>C OBSERVE: blank line

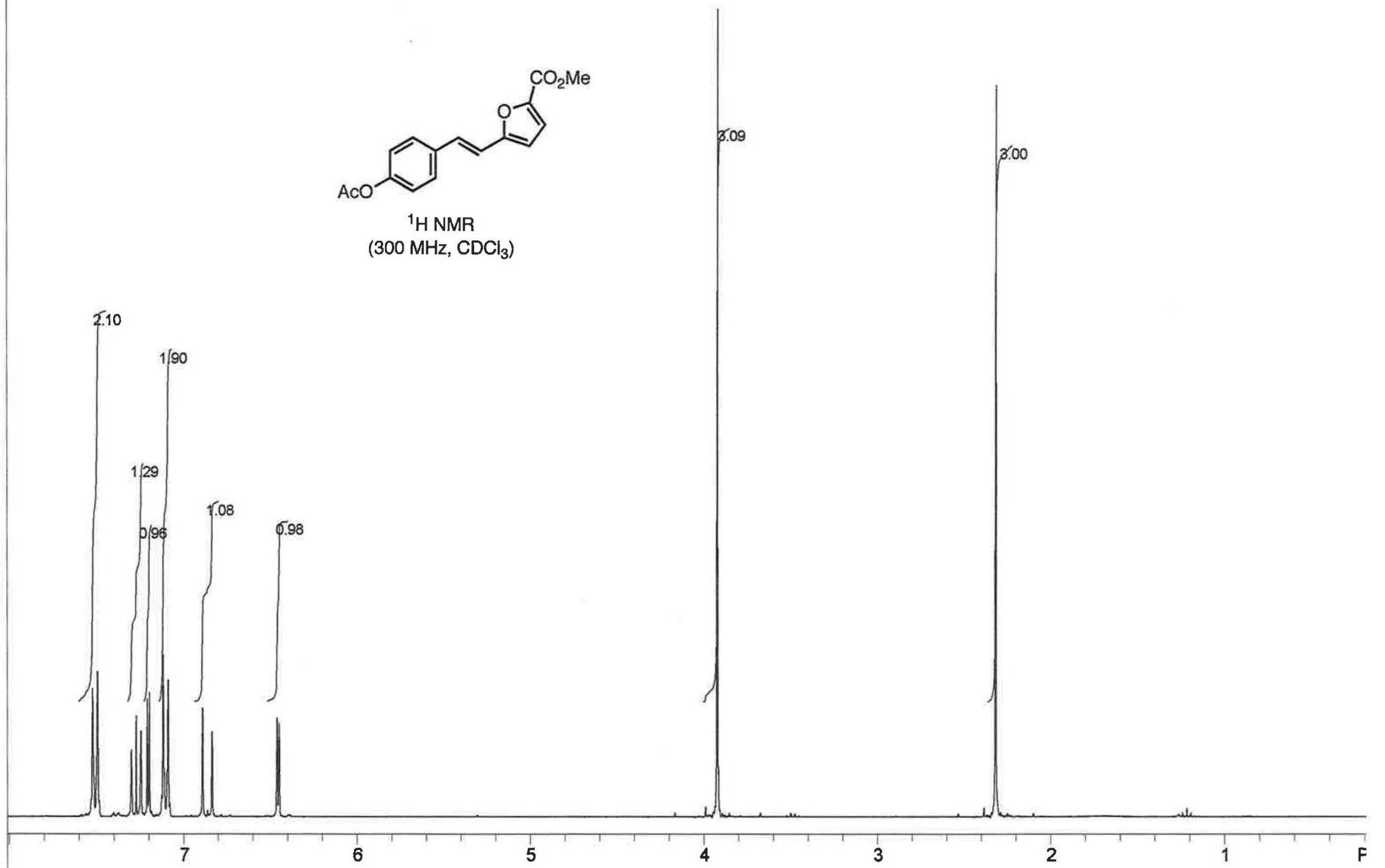
USER: -- DATE: Oct 14 20

F1: 75.479	F2: 300.145	SW1: 18868	OF1: 8300.1	PTS1d: 18868 , 32768
EX: s2pul	PW: 7.3 us	PD: 1.0 sec	NA: 24000	LB: 2.0

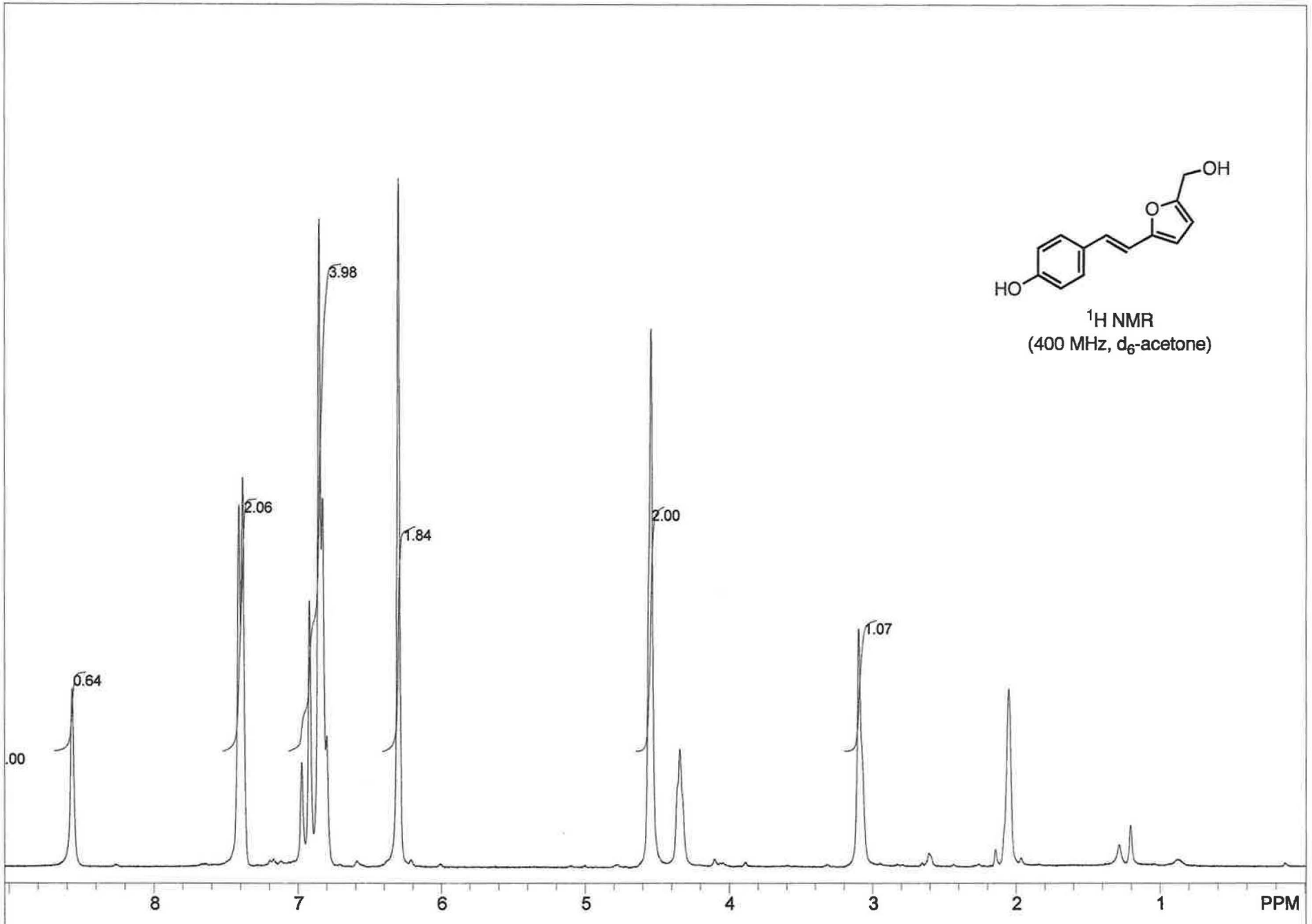
Nuts - \$rkp086-II-F-CNMR



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



STANDARD 1H OBSERVE:blank line					USER: -- DATE: Sep 21 20	
F1: 300.145	F2: 75.479	SW1: 4810	OF1: 1804.3	PTS1d: 14409	16384	
EX: s2pul	PW: 6.3 us	PD: 1.0 sec	NA: 8	LB: 0.0	Nuts - \$rqp-HH-sample	



STANDARD 1H OBSERVE:blank line				USER: -- DATE: Sep 30 2006		
F1: 300.147	F2: 75.479	SW1: 4810		OF1: 1800.9		PTS1d: 14409 , 16384
EX: s2pul		PW: 6.3 us	PD: 1.0 sec	NA: 8	LB: 0.0	Nuts - Srkp084-HNMR

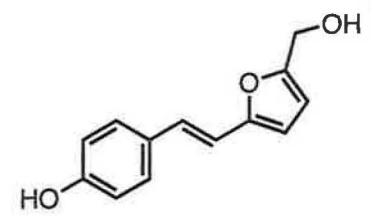
158.244  
155.860  
154.067

129.654  
128.582  
127.410

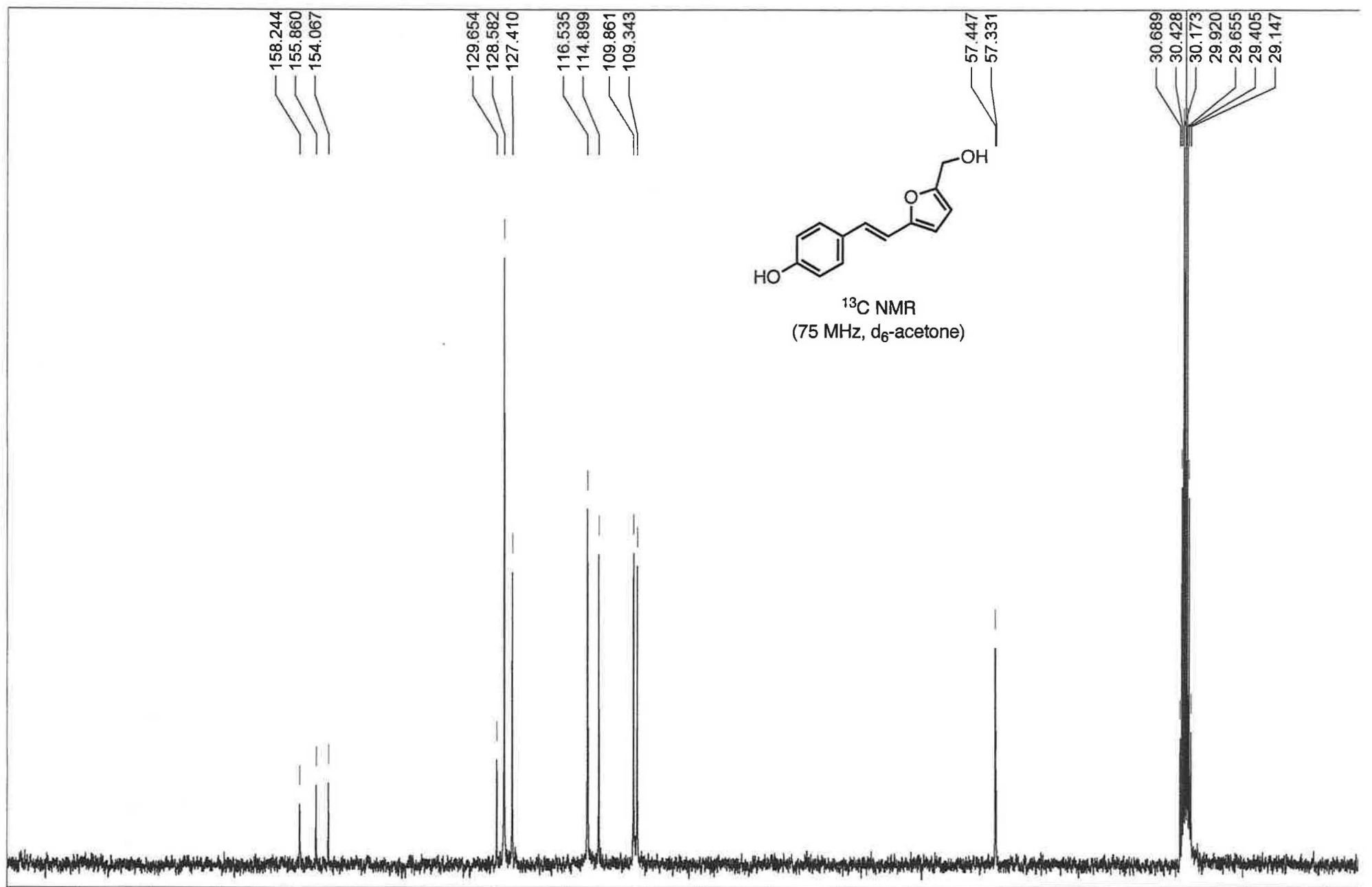
116.535  
114.899  
109.861  
109.343

57.447  
57.331

30.689  
30.428  
30.173  
29.920  
29.655  
29.405  
29.147



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



150 100 50 F

13C OBSERVE:blank line			USER: -- DATE: Sep 30 20			
F1: 75.480	F2: 300.147	SW1: 18868	OF1: 8355.2	PTS1d: 18868	32768	
EX: s2pul	PW: 7.3 us	PD: 1.0 sec	NA:	LB: 2.0	Nuts - \$rkp084-CNMR	