

Electronic Supplementary Information

Synthesis and configuration of the nonadecenetriol isolated from seeds of *Persea Americana*

Xin Yan,^{a,b} Shao-Min Zhang,^a Yikang Wu*^a and Po Gao*^b

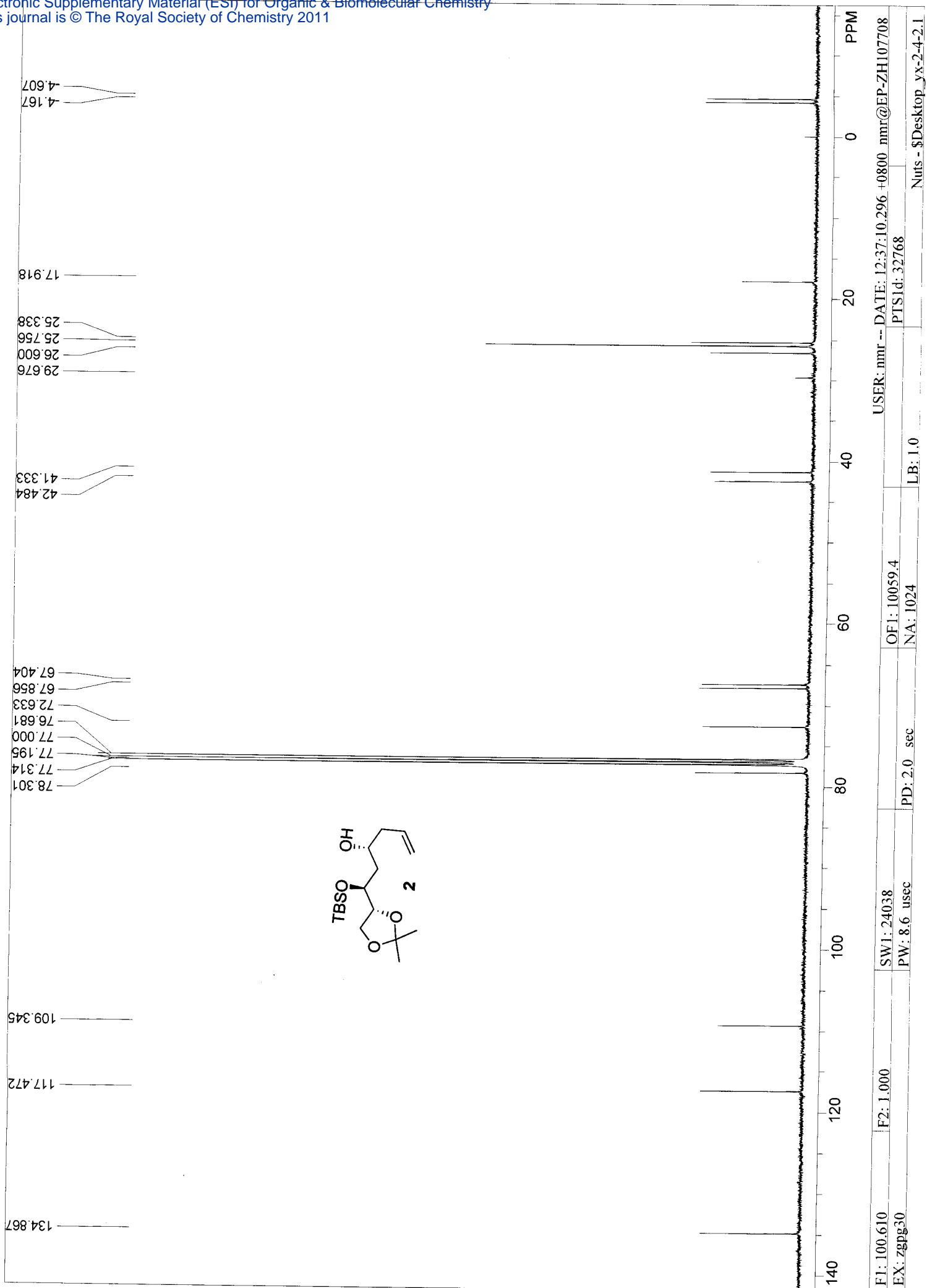
^aState Key Laboratory of Bioorganic and Natural Products Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Road, Shanghai 200032, China

^bSchool of Chemistry and Materials, Heilongjiang University, Harbin 150080, China.

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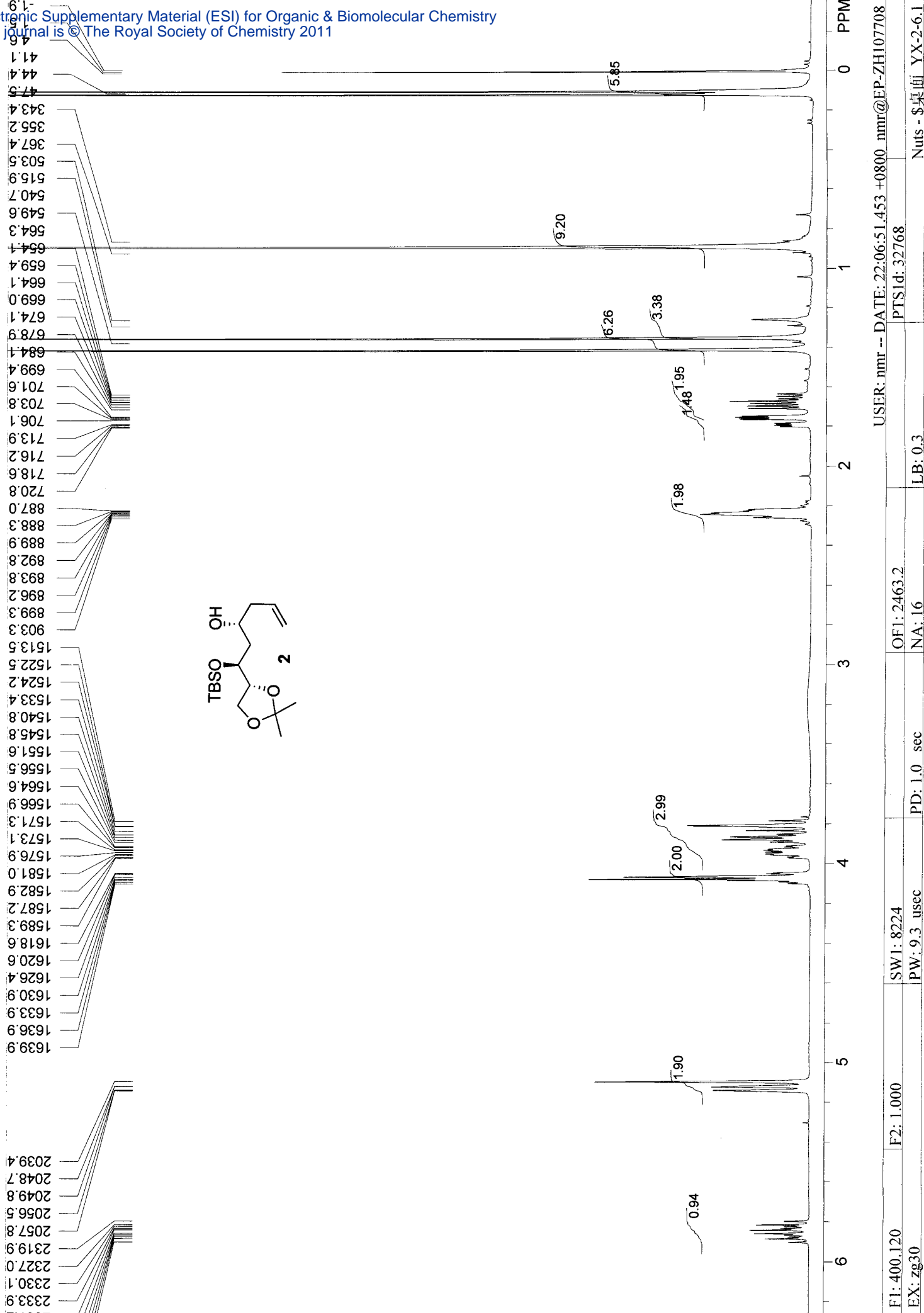
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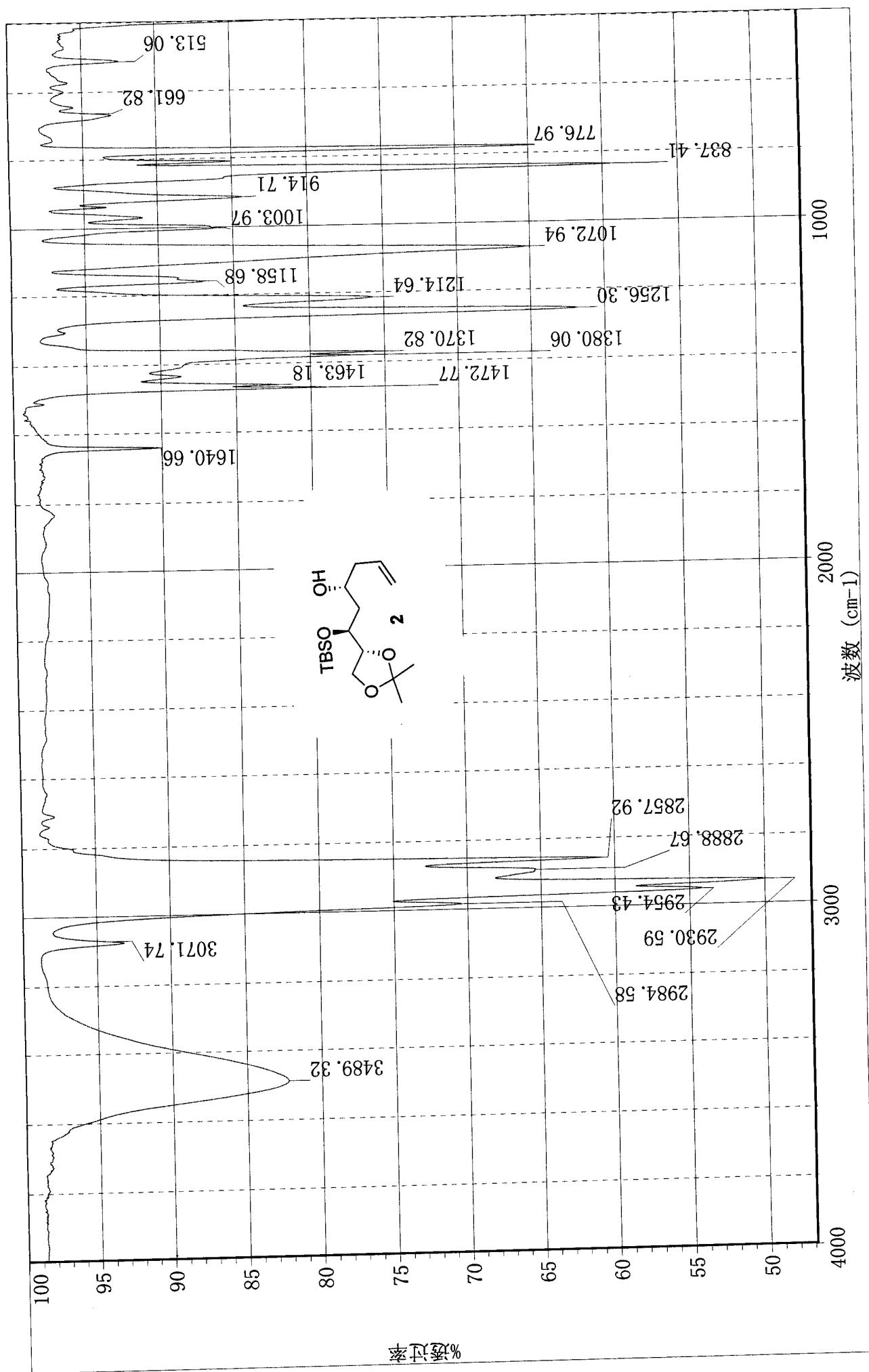


S 2

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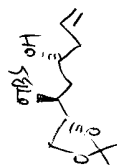
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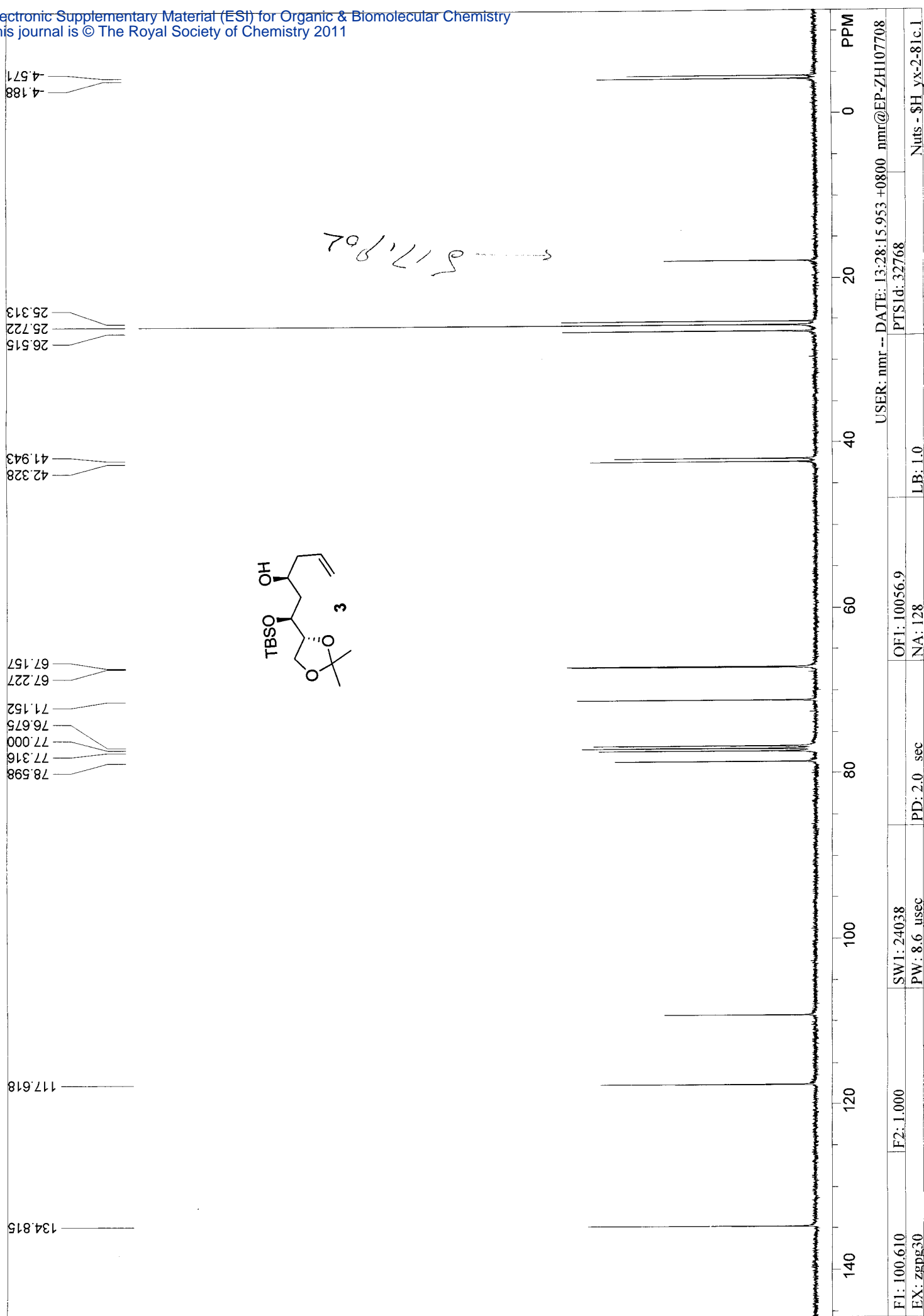


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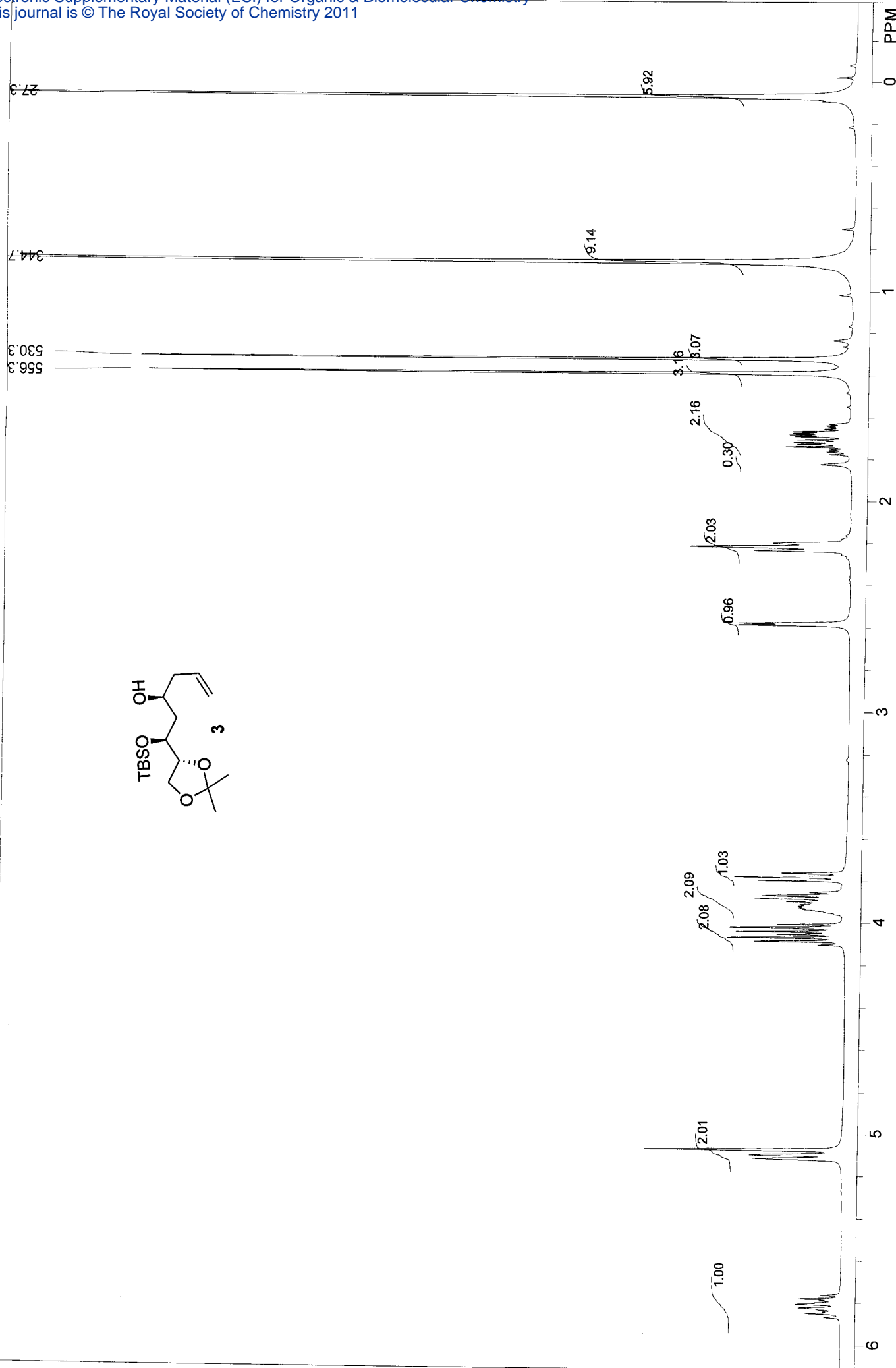
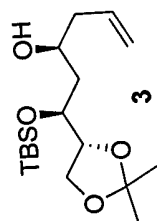


上海有机所生命有机化学国家重点实验室

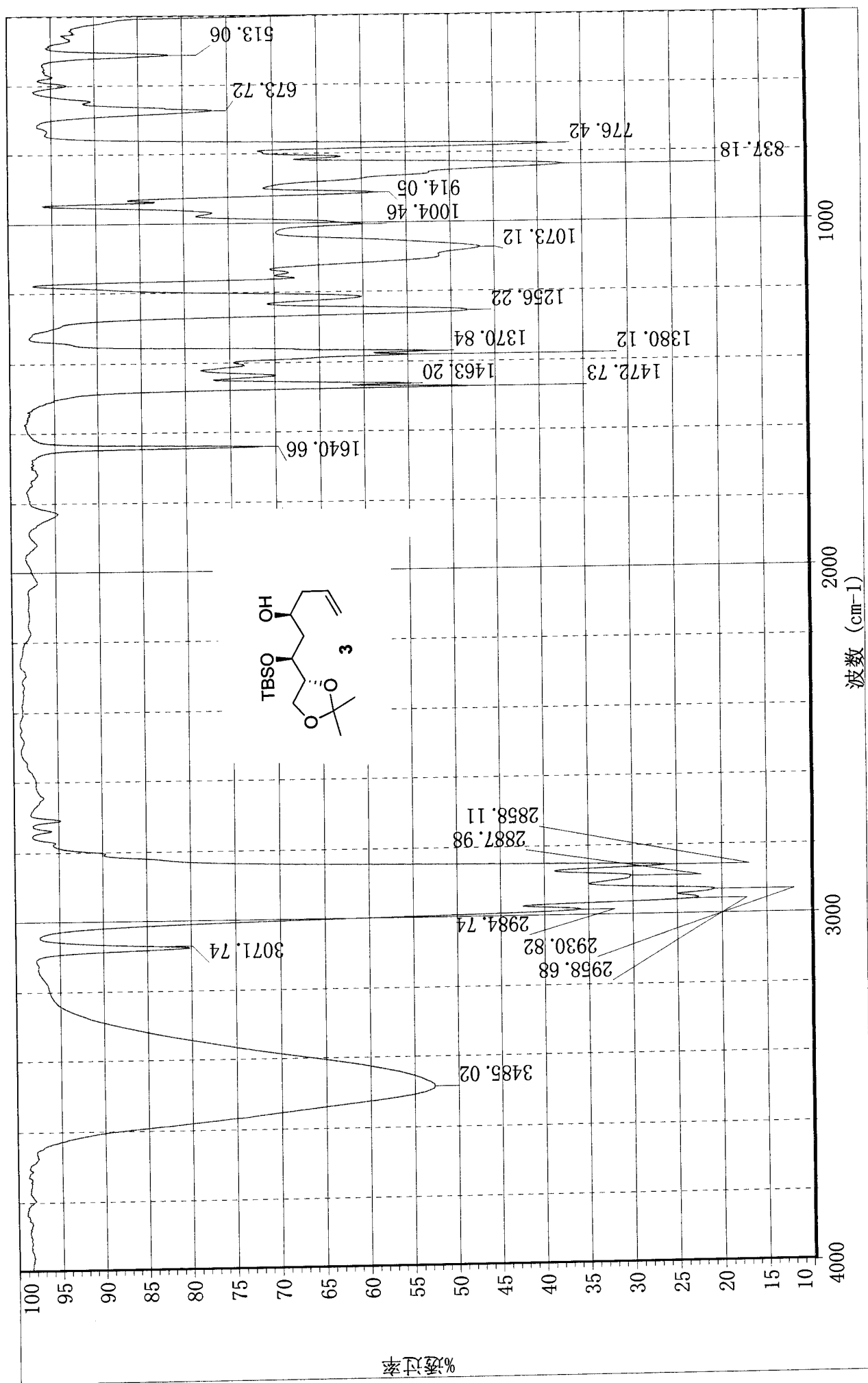


S 5

100 MHz, CDCl₃

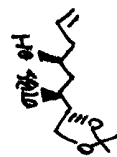


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PW: 9.3 usec
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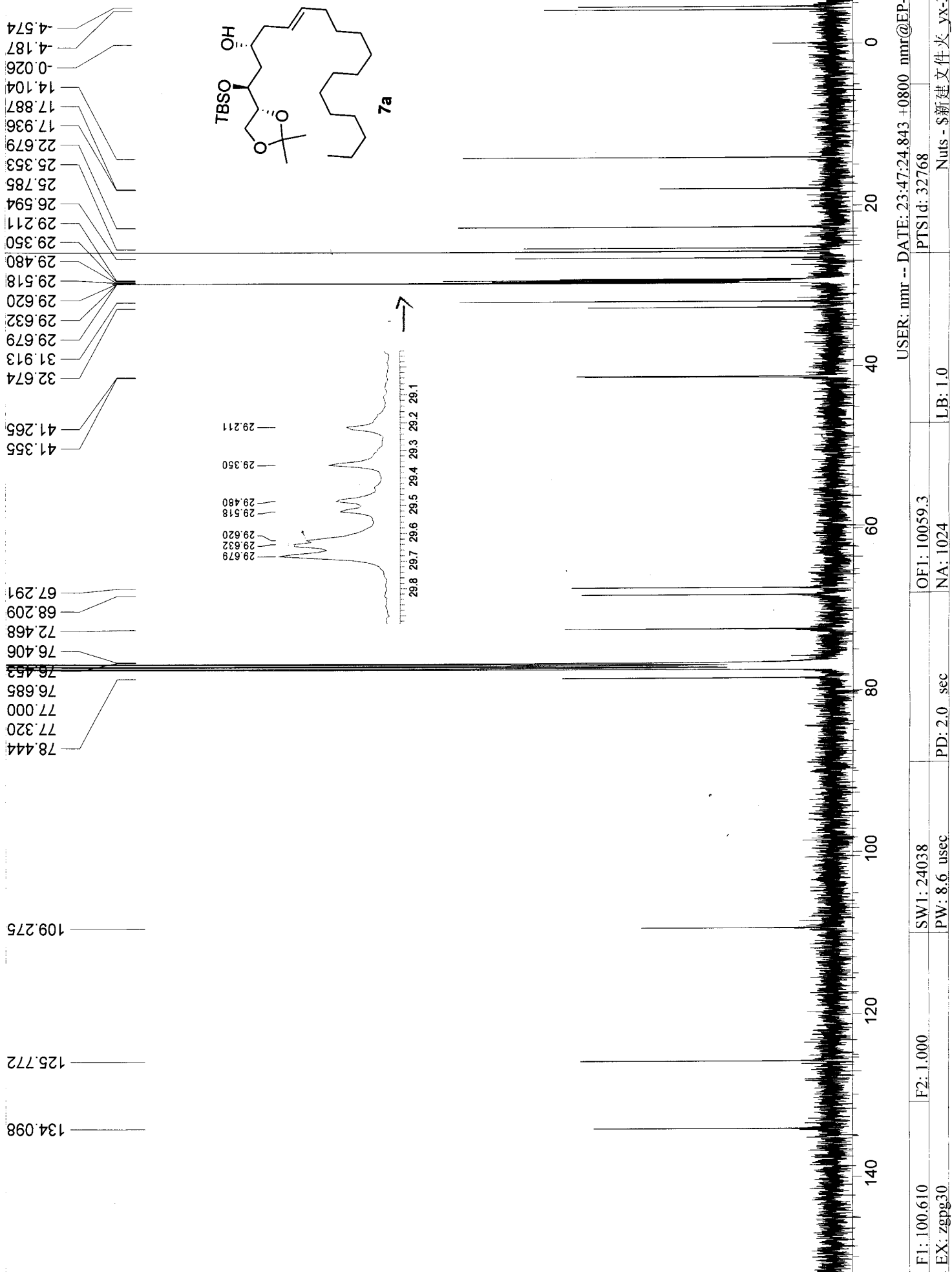


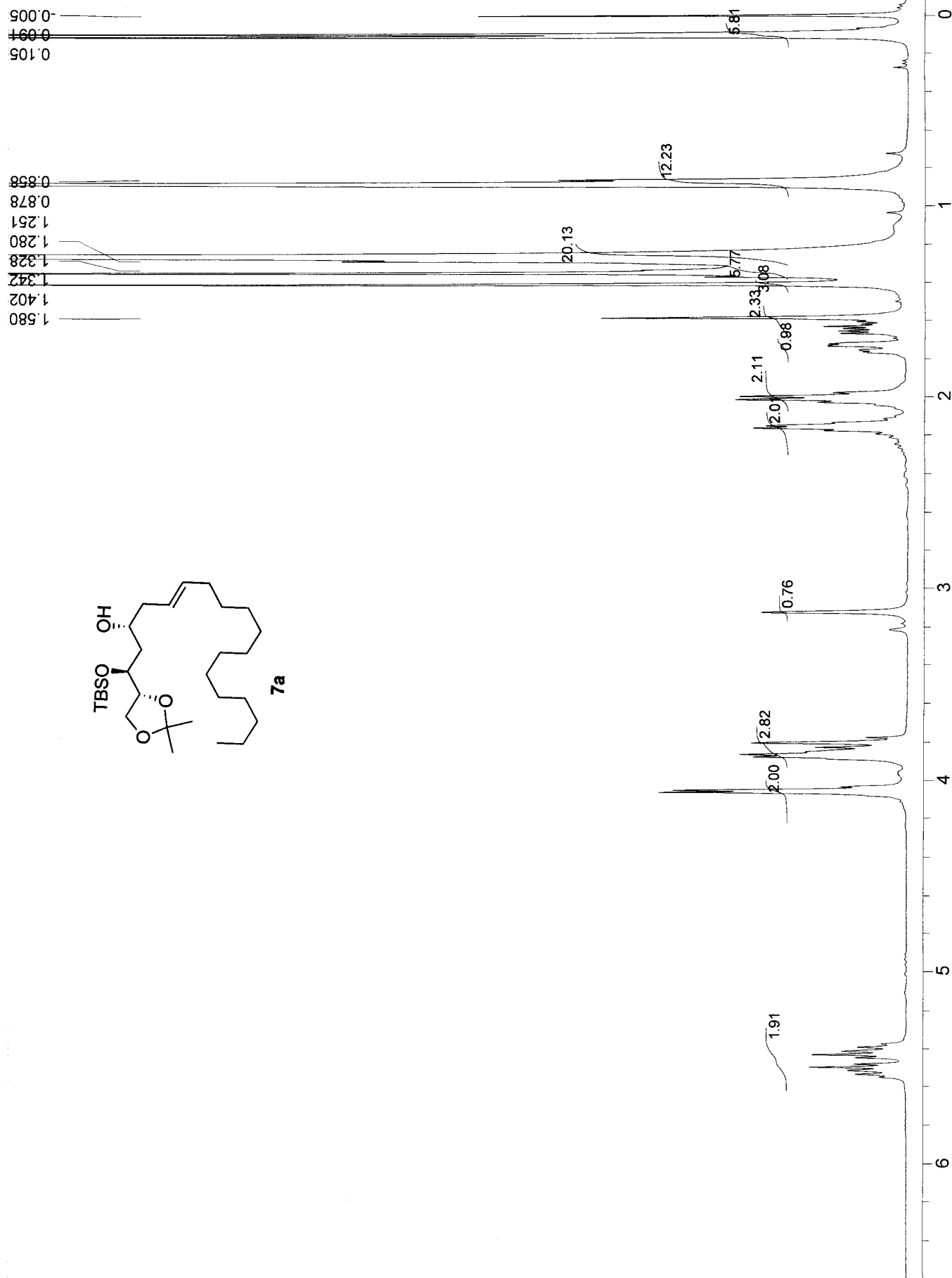
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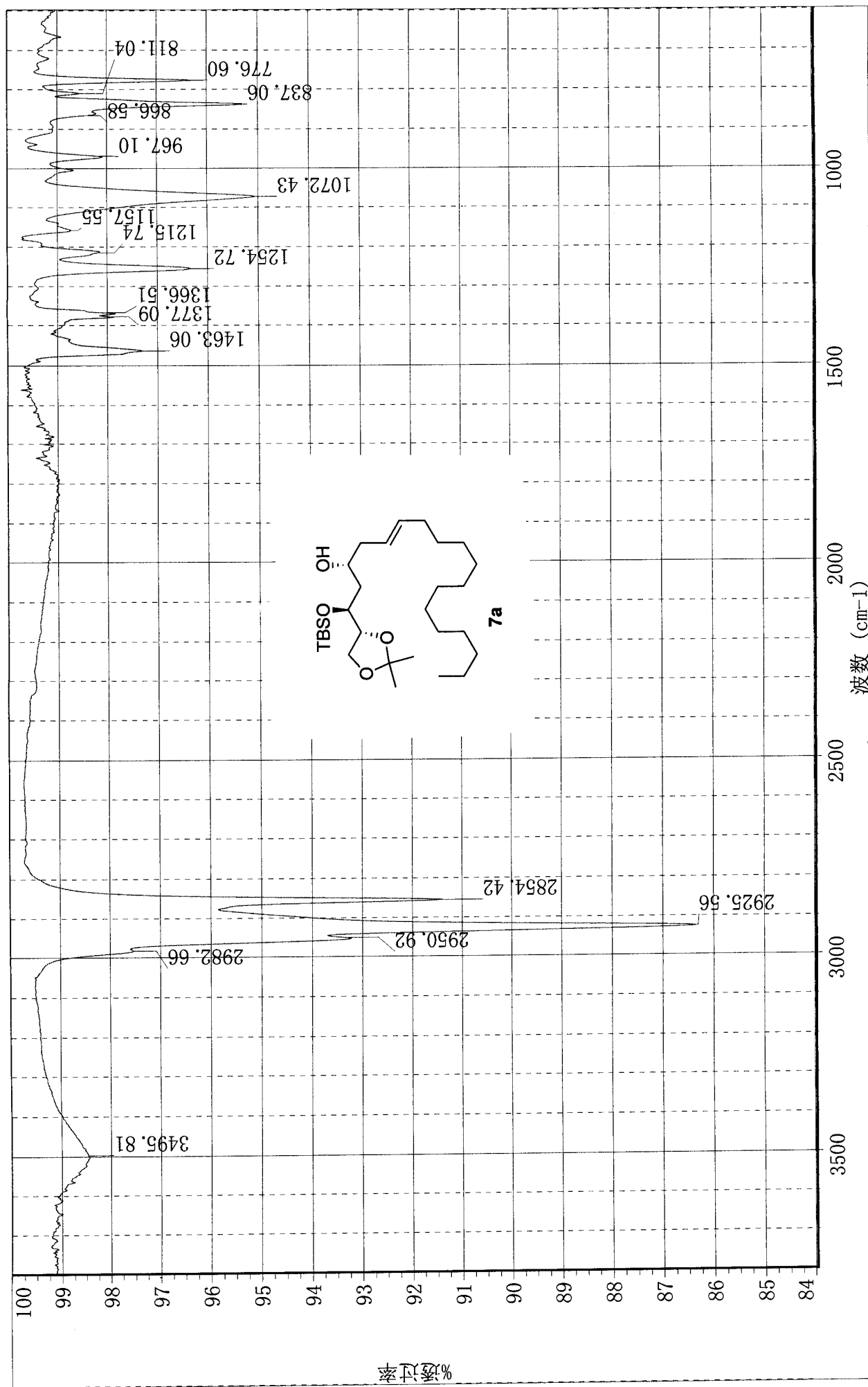


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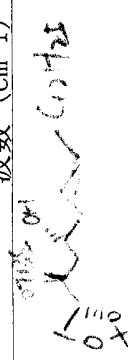


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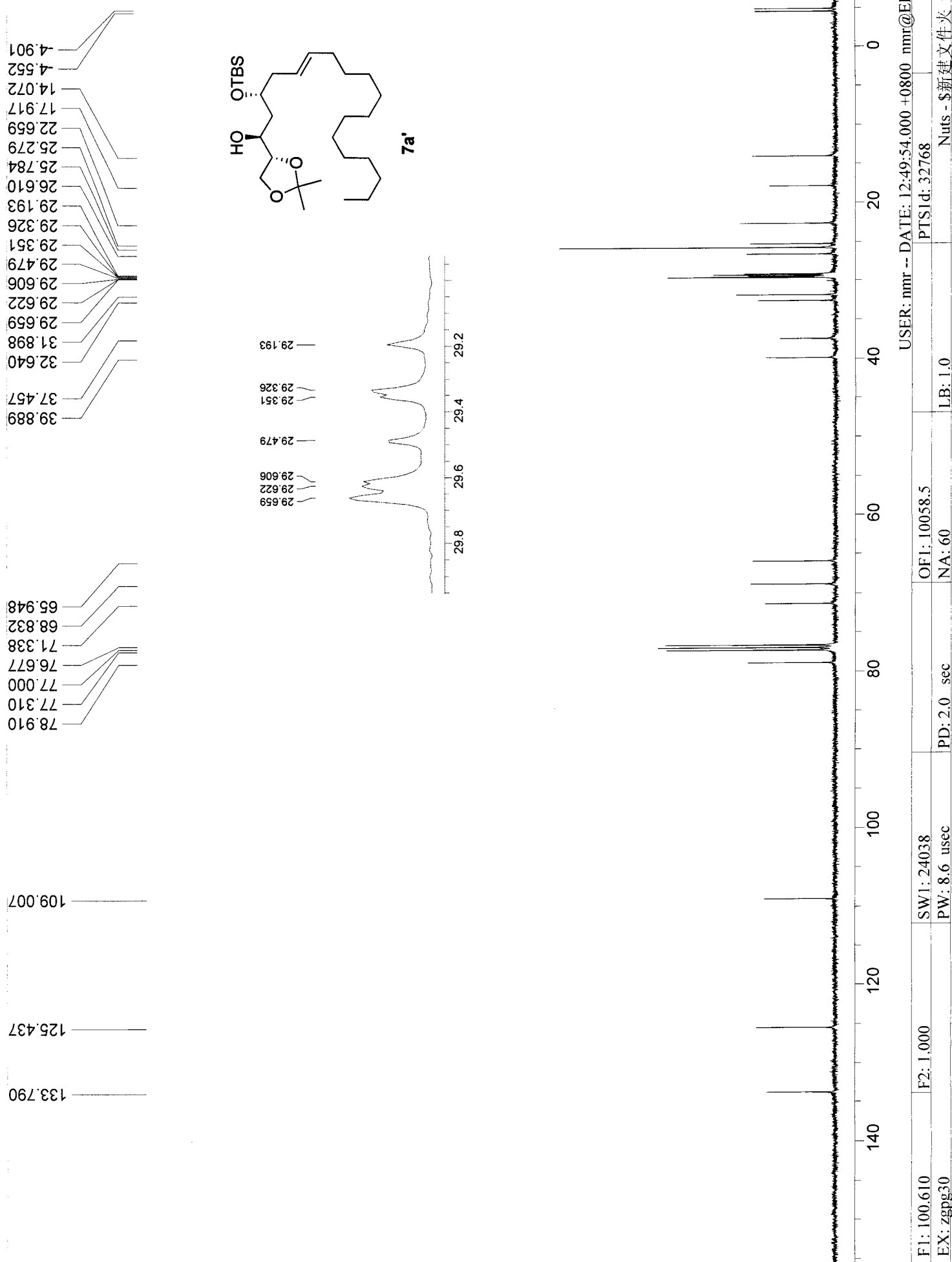


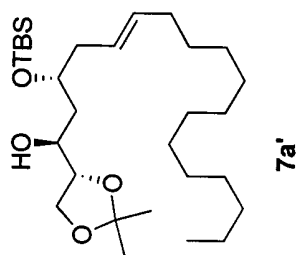
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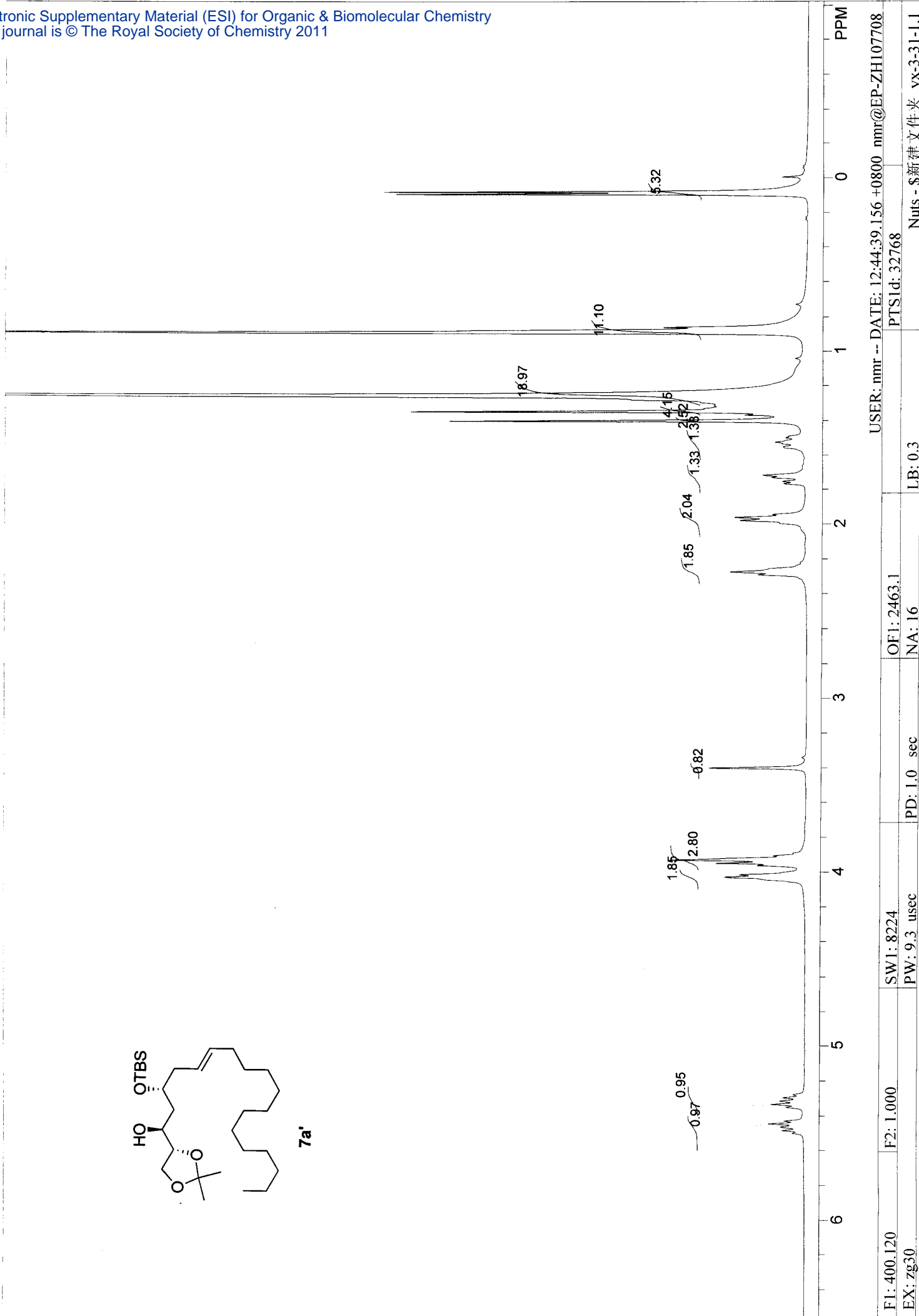


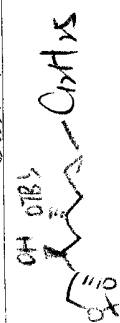
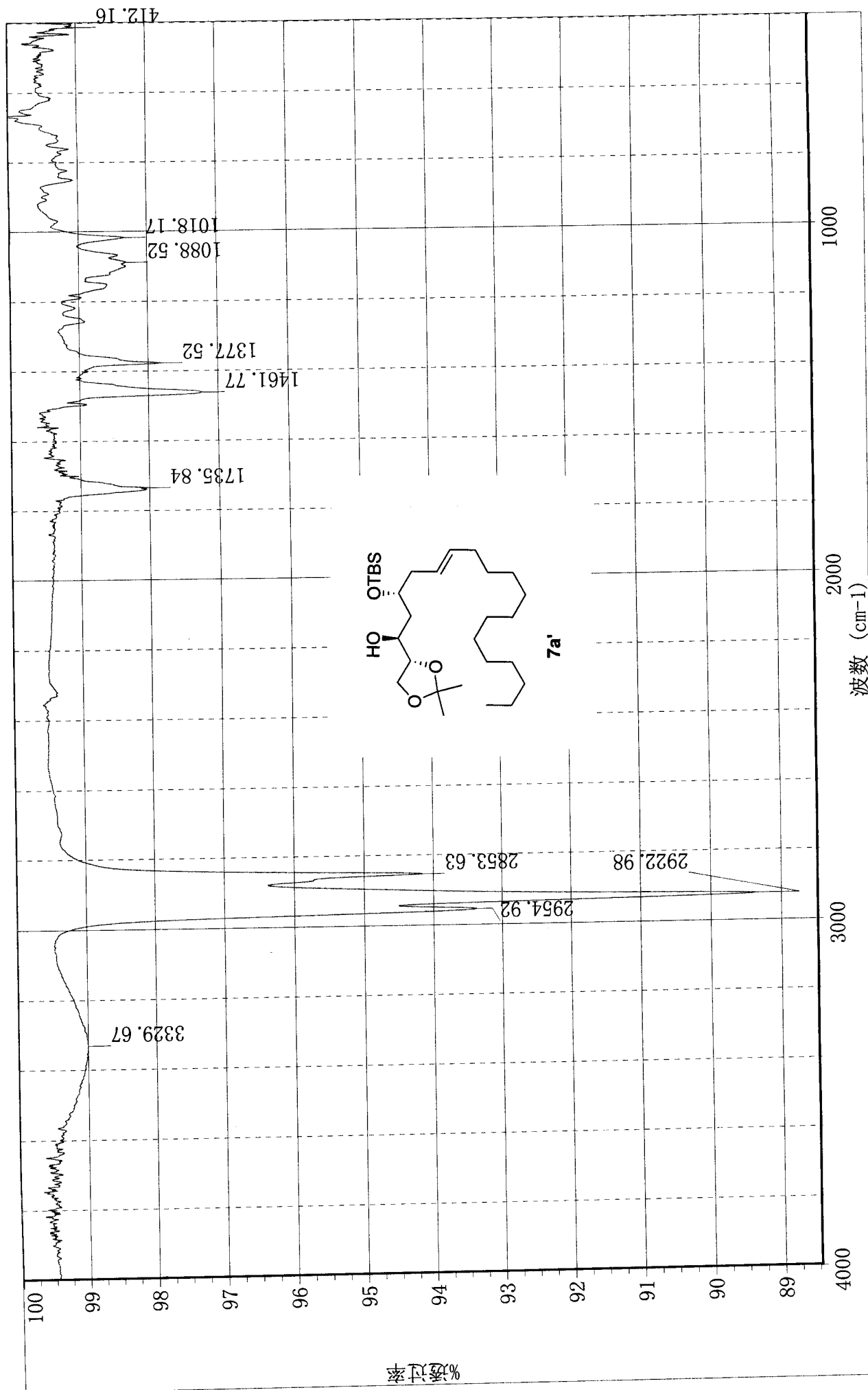
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7a'



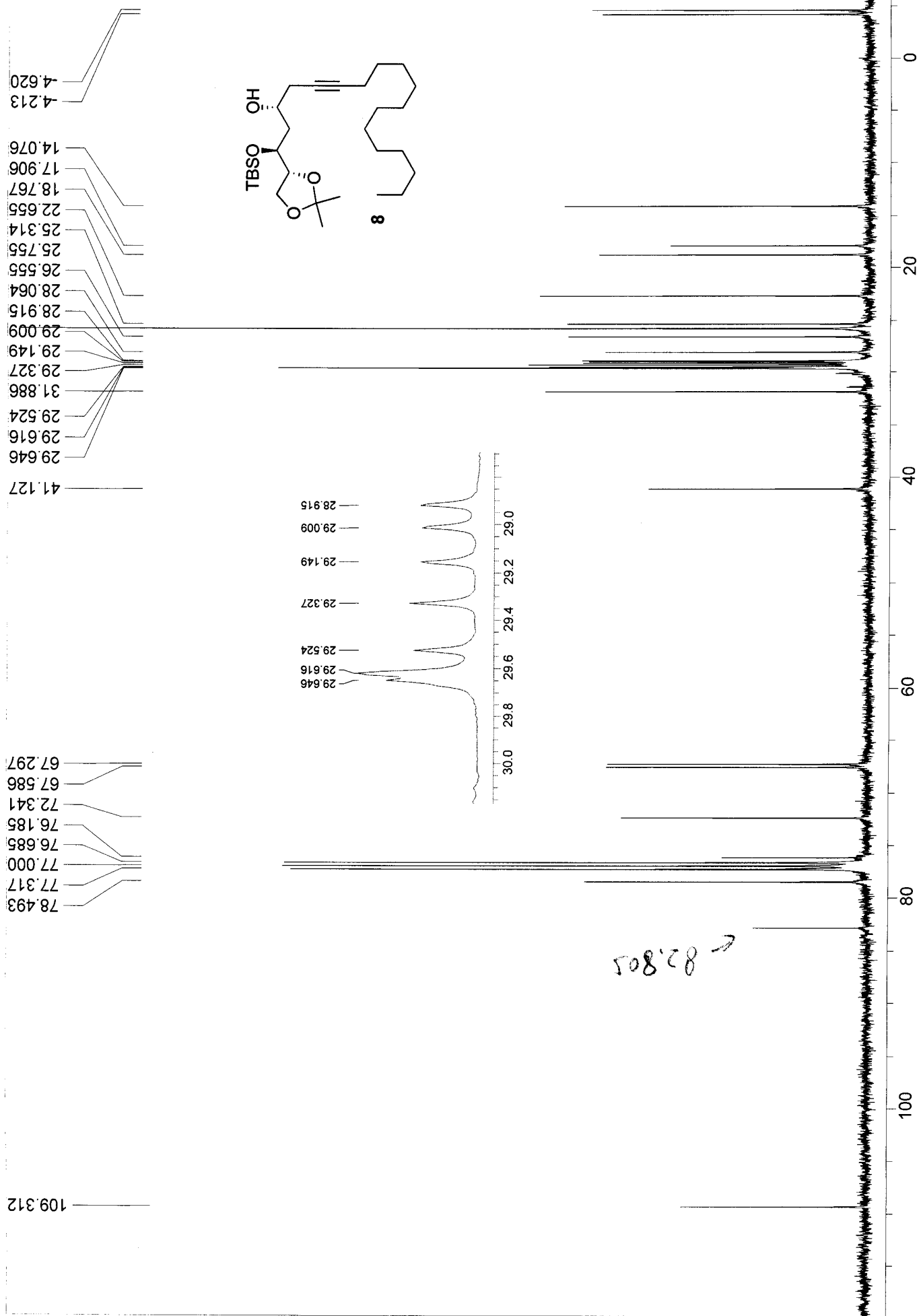


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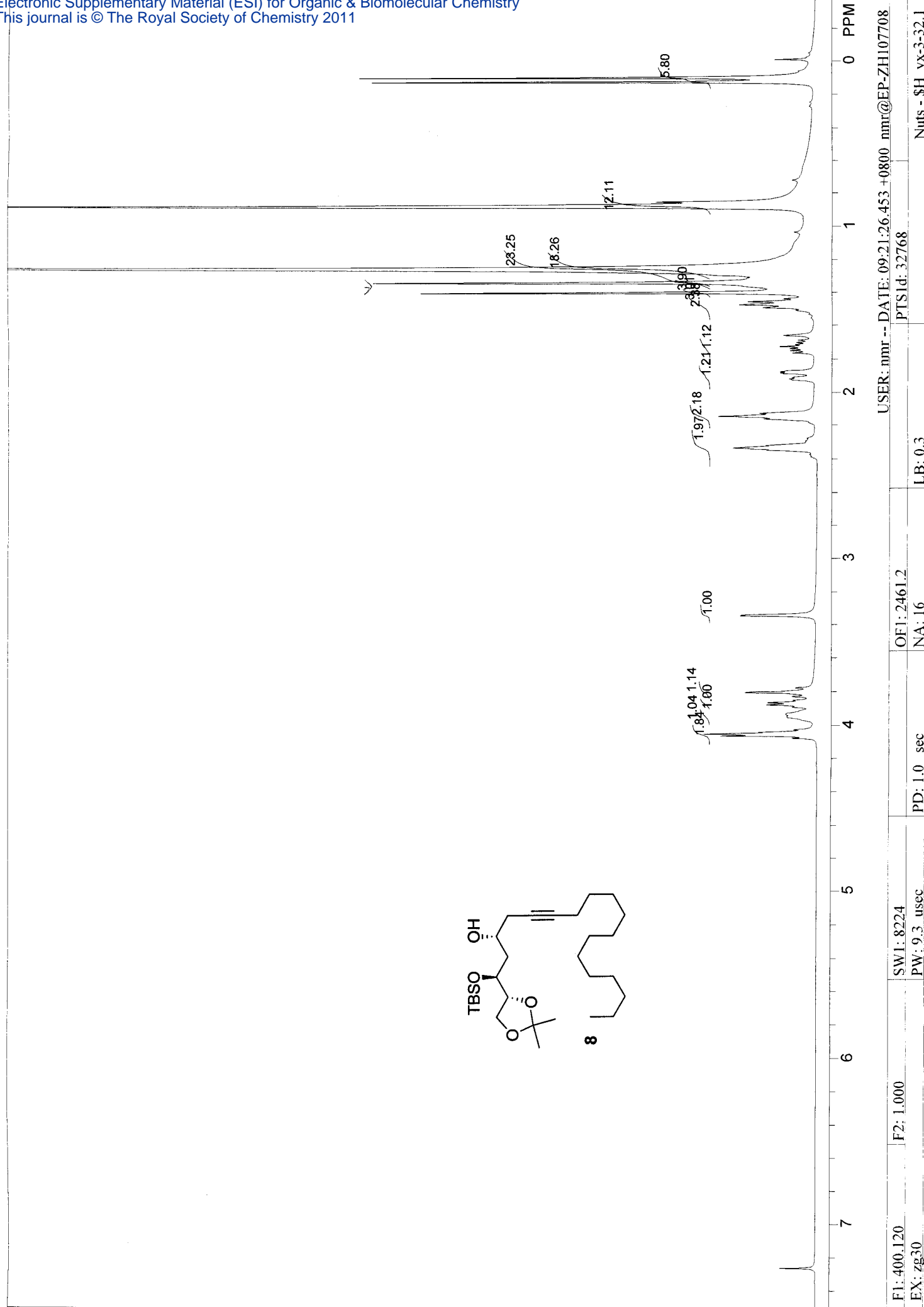
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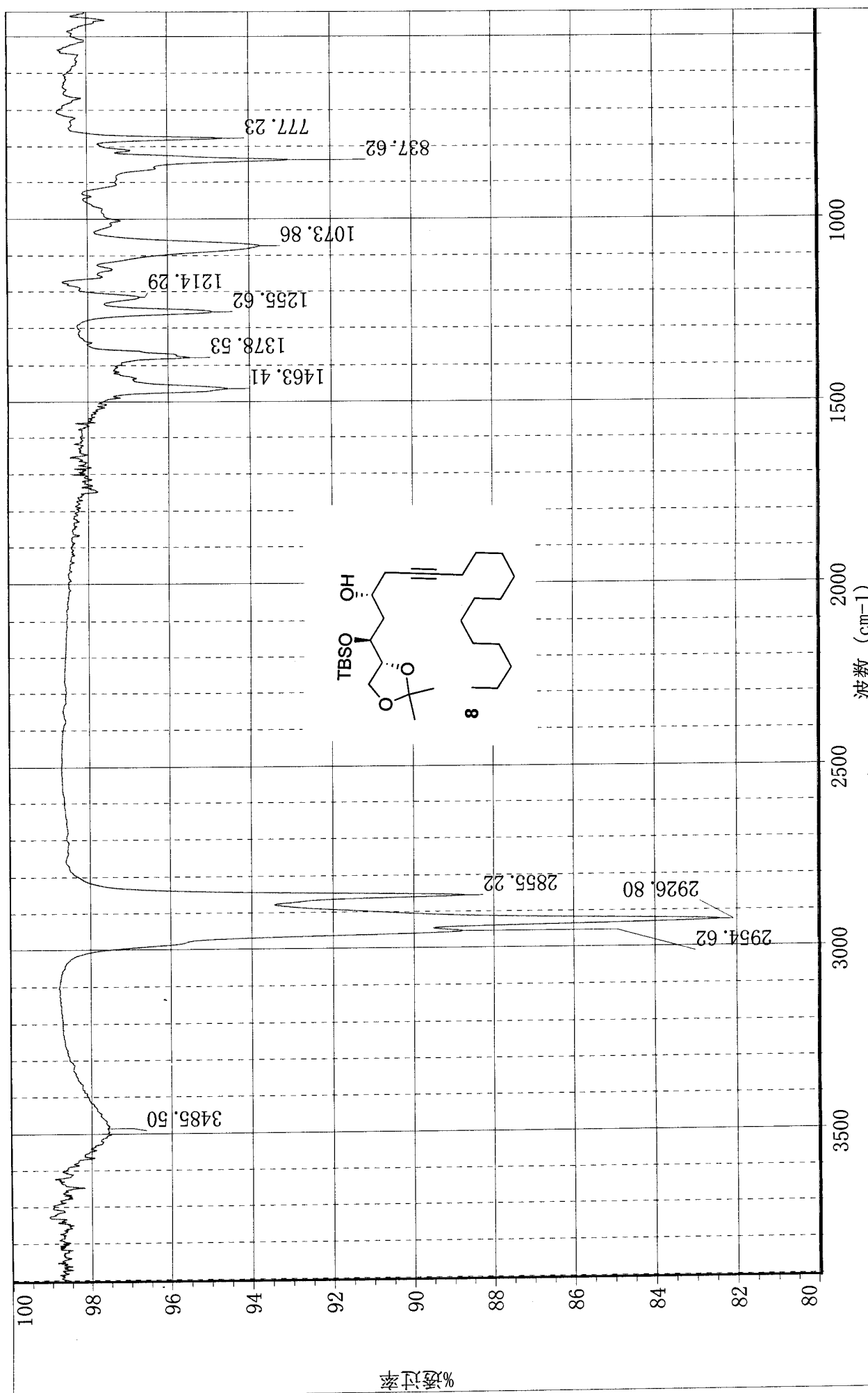
Conflys

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OF1: 10058.1
NA: 256
PD: 2.0 sec
SW1: 24038
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F1: 100.610
F2: 1.000
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LB: 1.0
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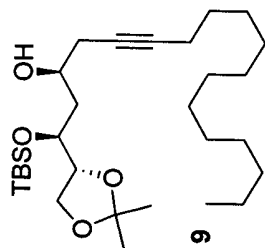


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2010.12.14 15:11:41

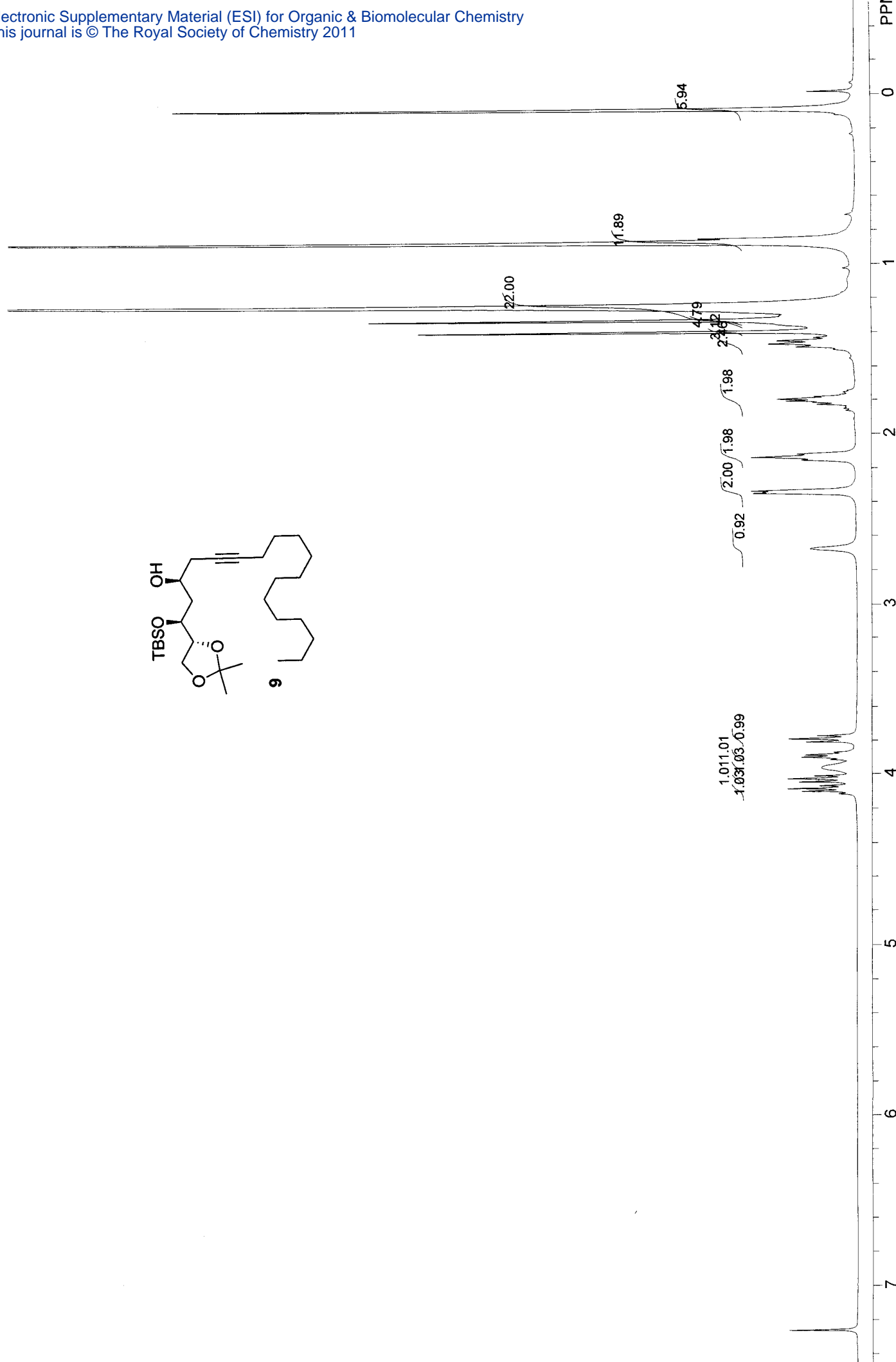
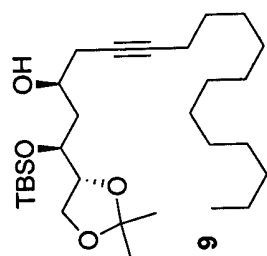
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100 MHz, CDCl₃

S 17

F1: 100.610	F2: 1.000	SWH: 24038	PD: 2.0 sec	OF1: 10053.0	LB: 1.0	USER: mmr -- DATE: 10:47:21.625 +0800_nmr@EP-ZH107708
EX: zgpg30		PW: 8.6 usec	NA: 128	PTSId: 32768		Nuts - \$新建文件火_yx-3-44c.1



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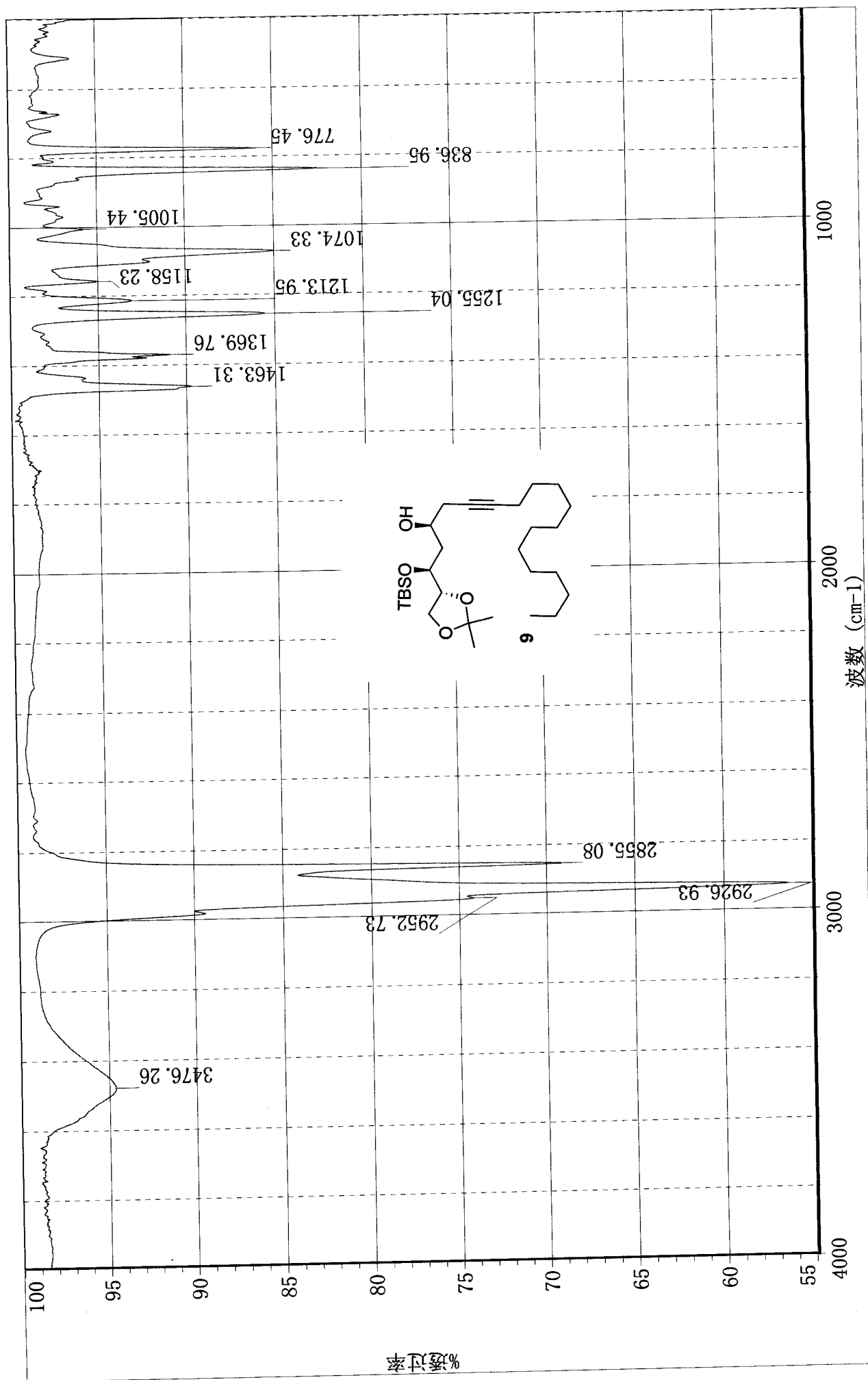
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SW1: 8224

F2: 1.000

I: 400.120

YX-3-644

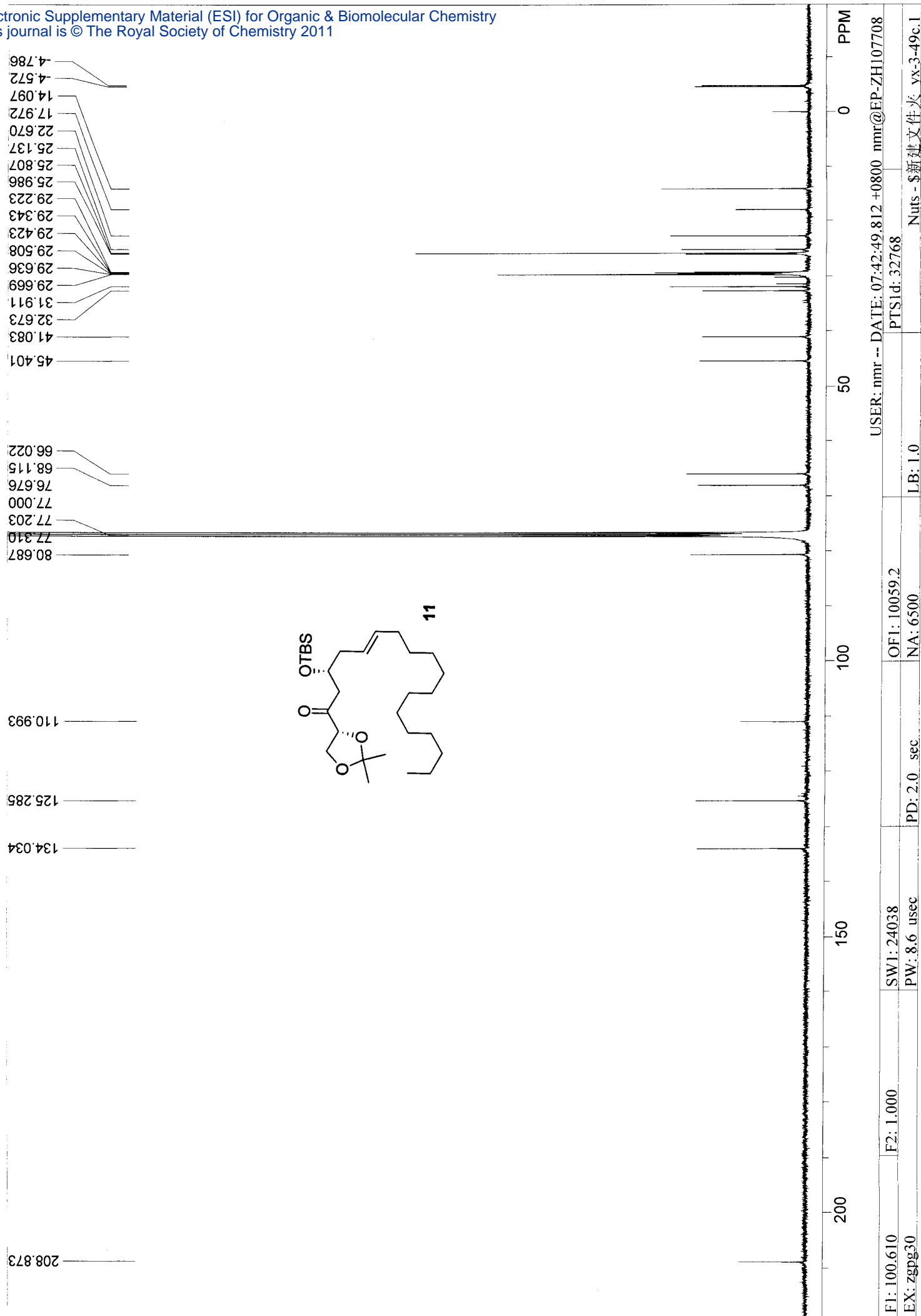


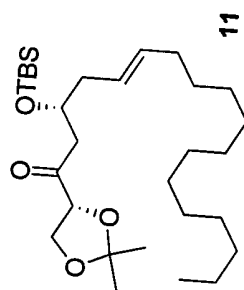
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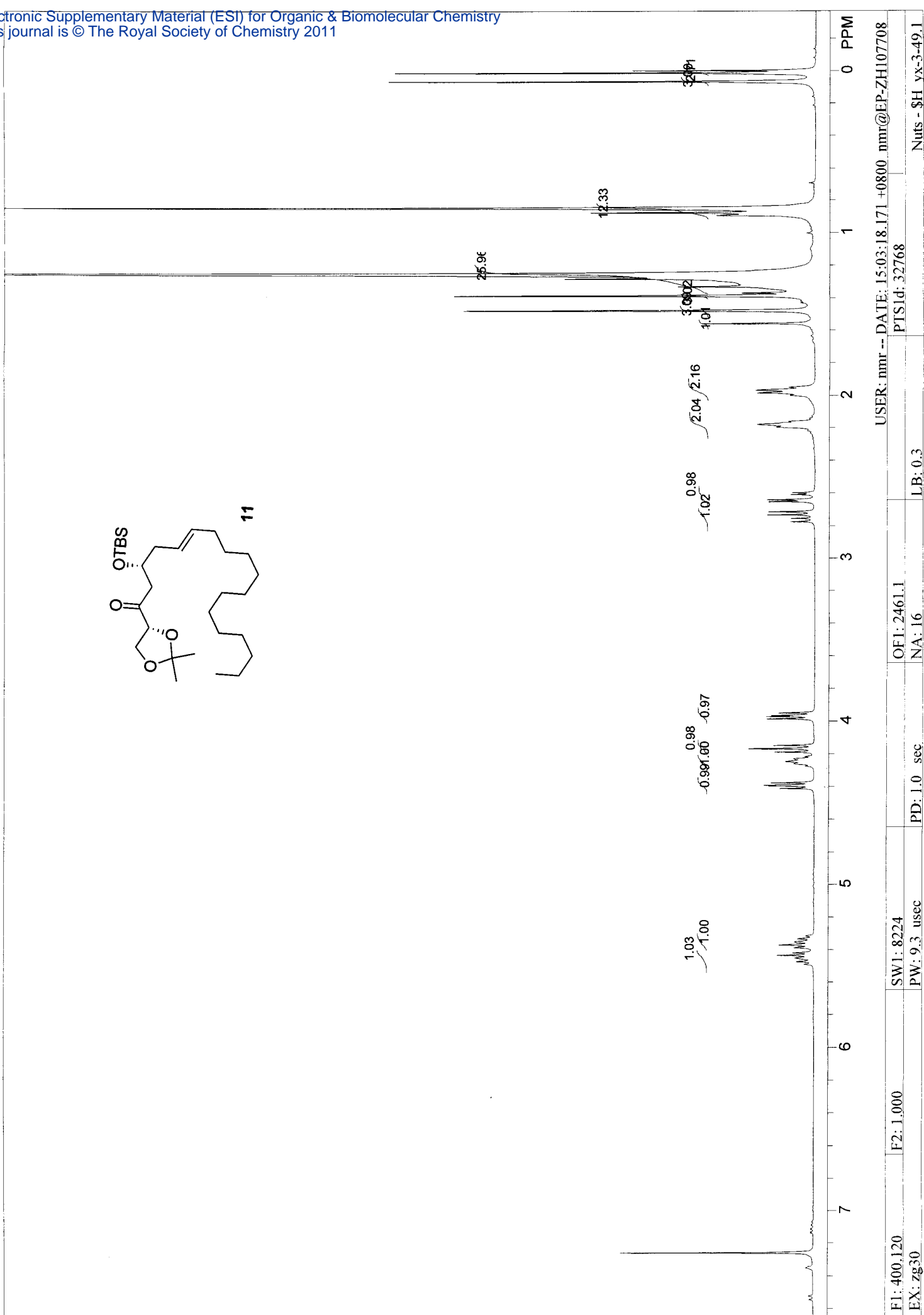
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11



USER: nmr -- DATE: 15:03:18.171 +0800 nmr@EP-ZH107708

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OF1: 2461.1

NA: 16

PD: 1.0 sec

SW1: 8224

PW: 9.3 usec

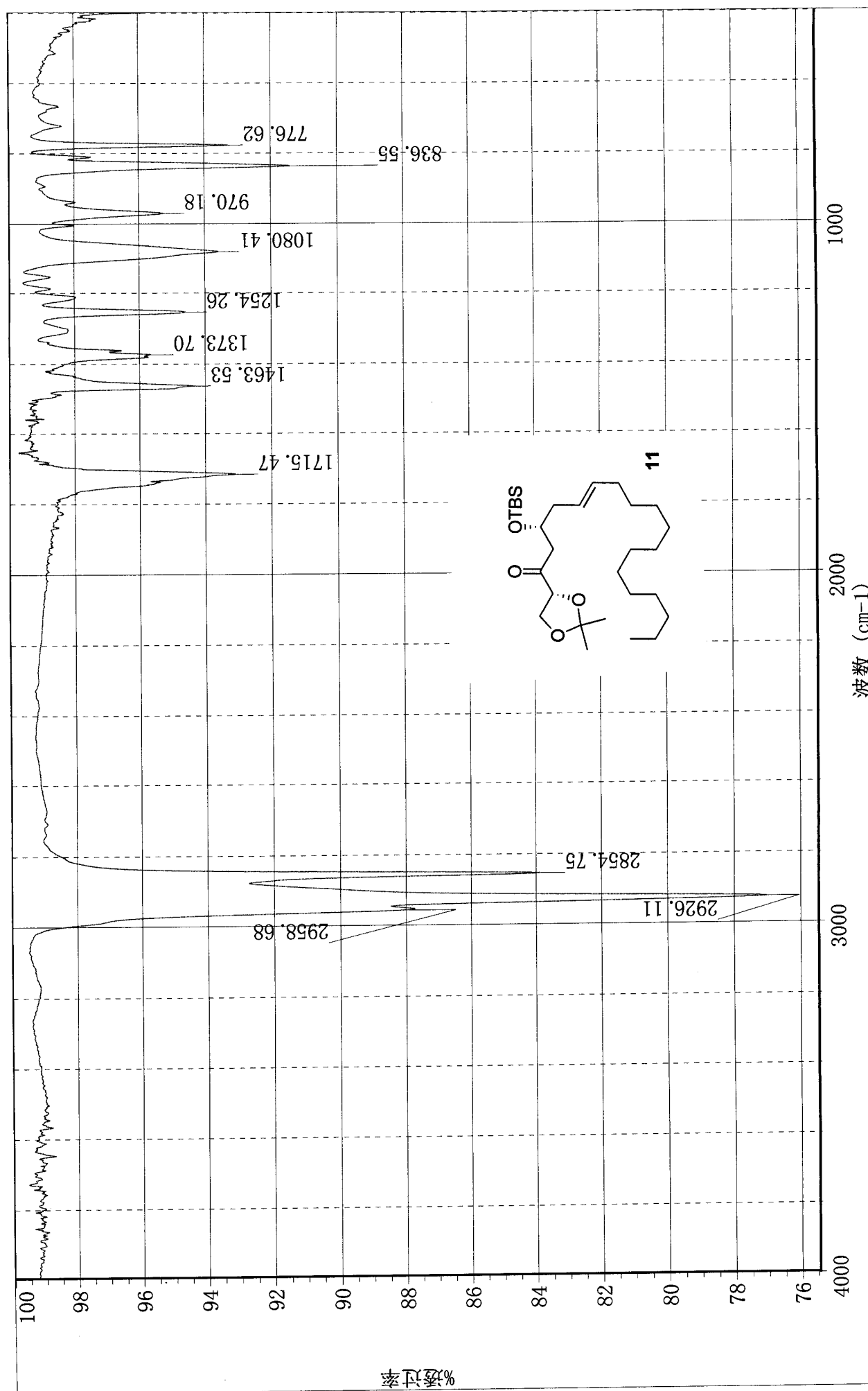
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LB: 0.3

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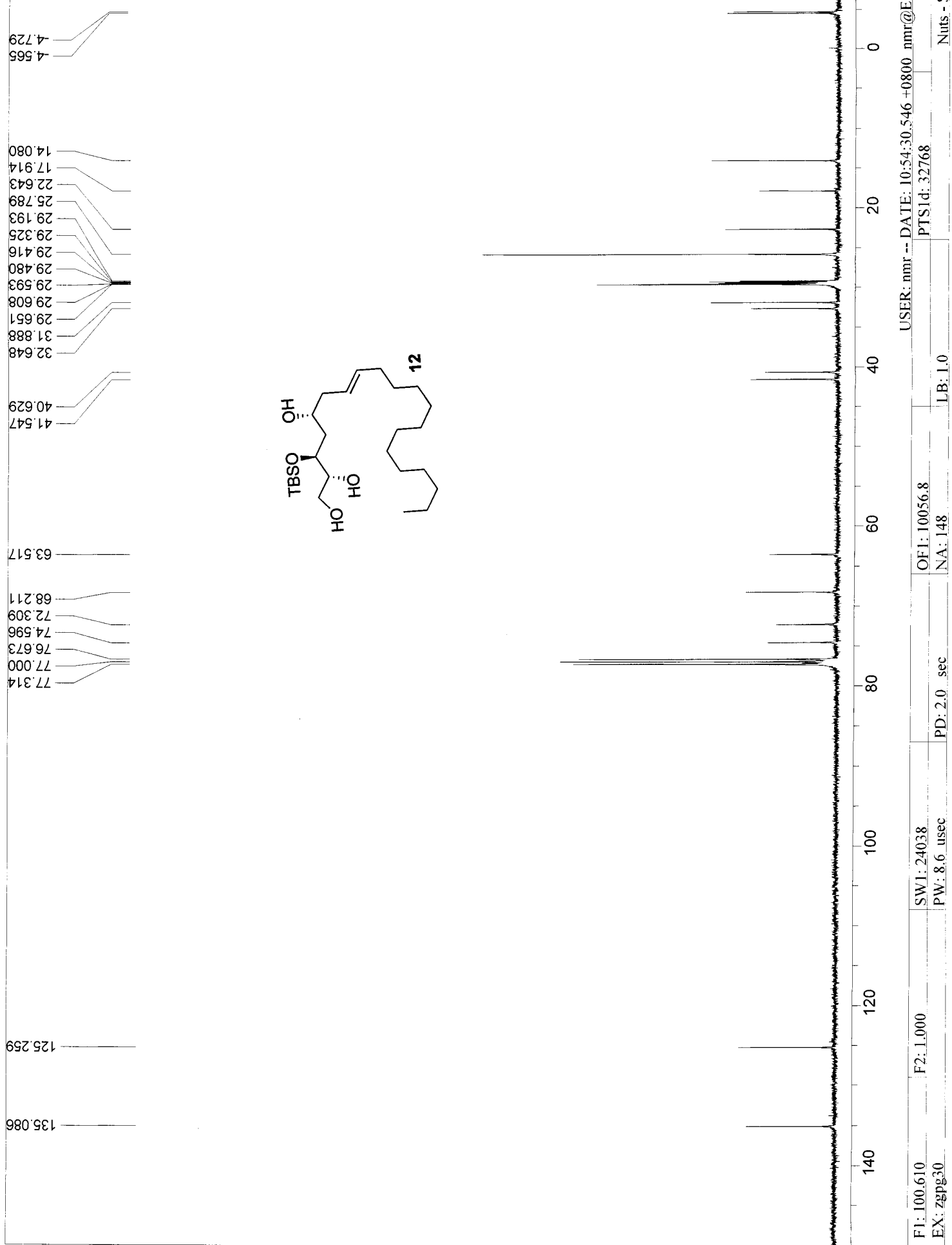


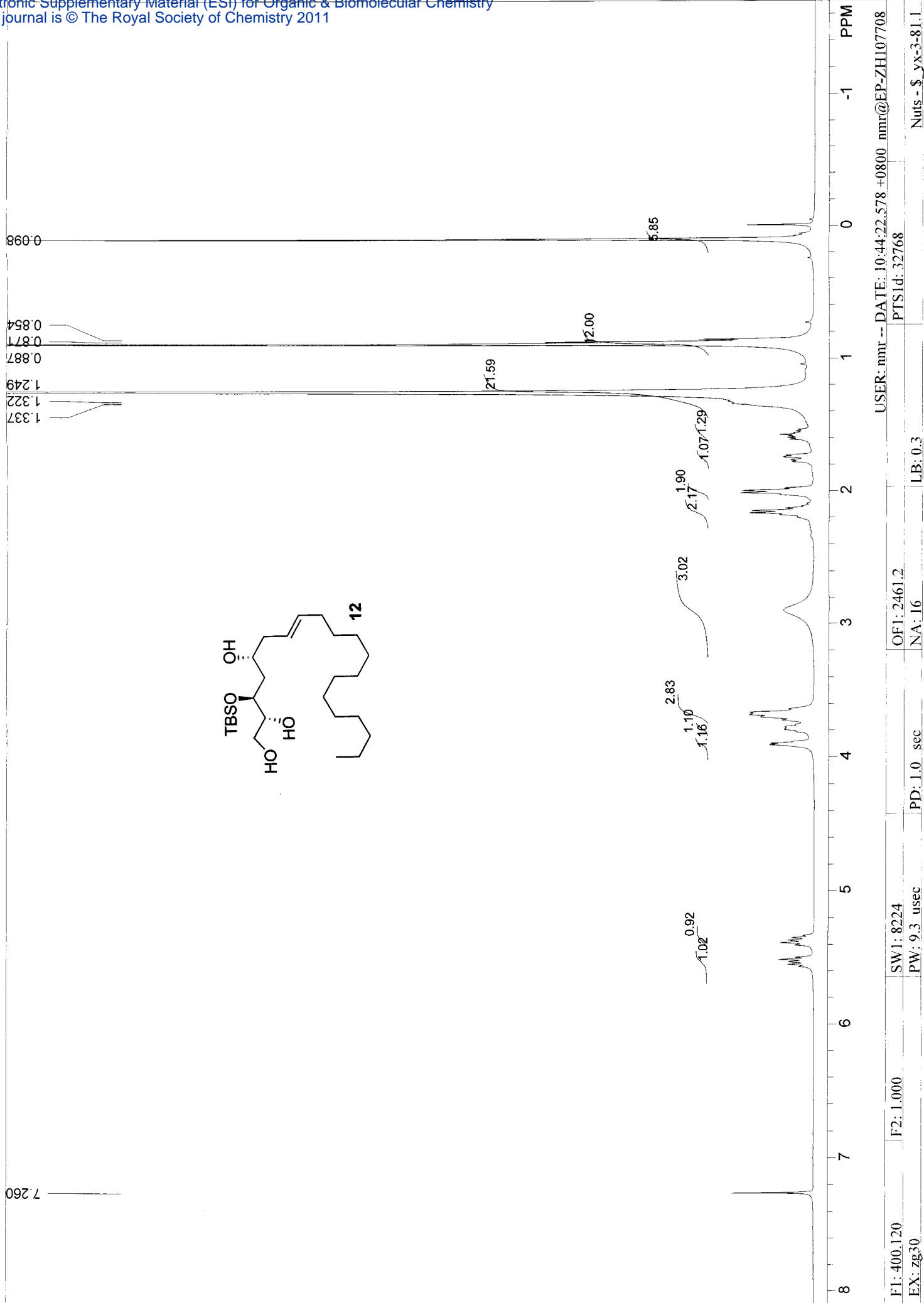
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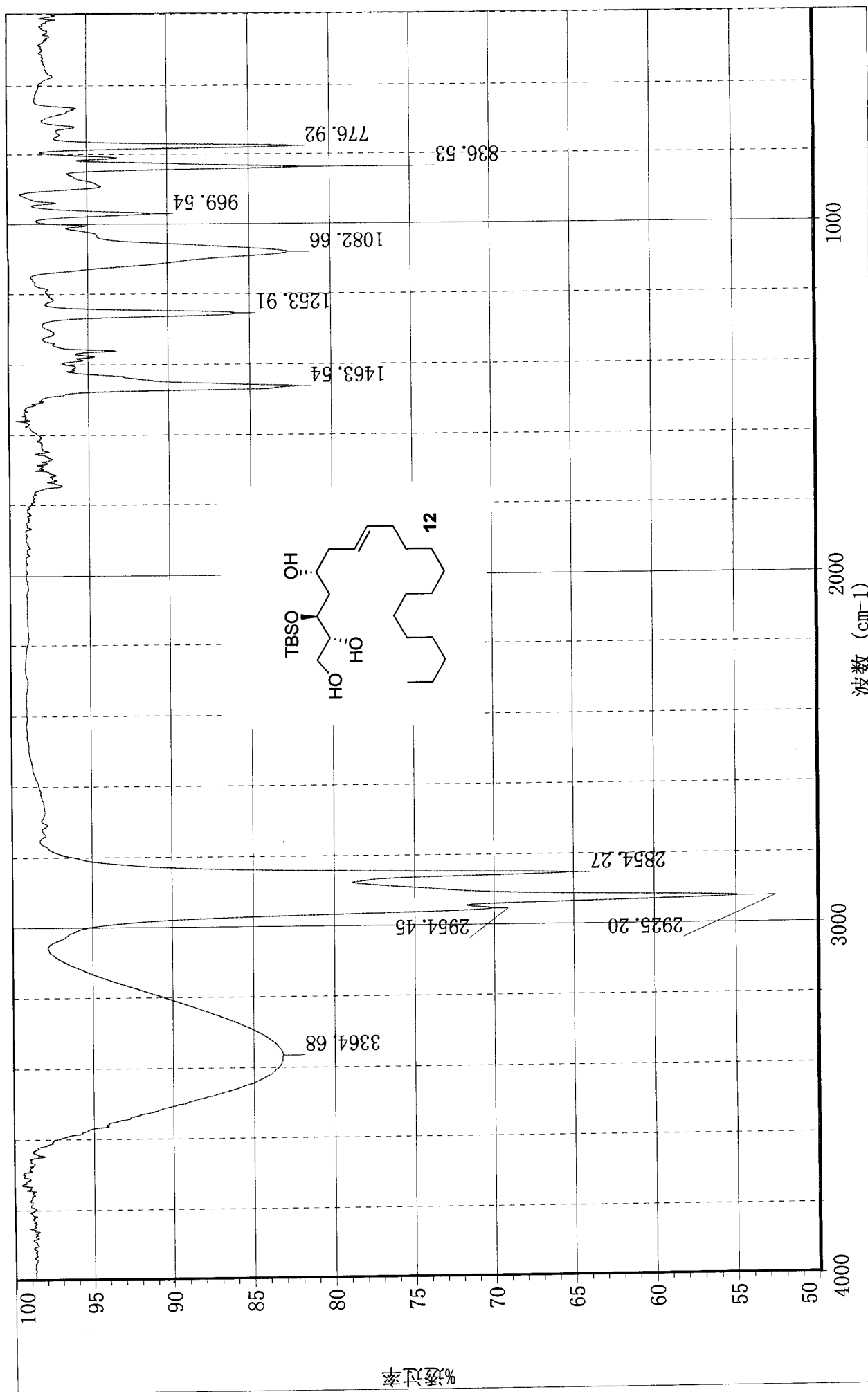
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*yx-3-81

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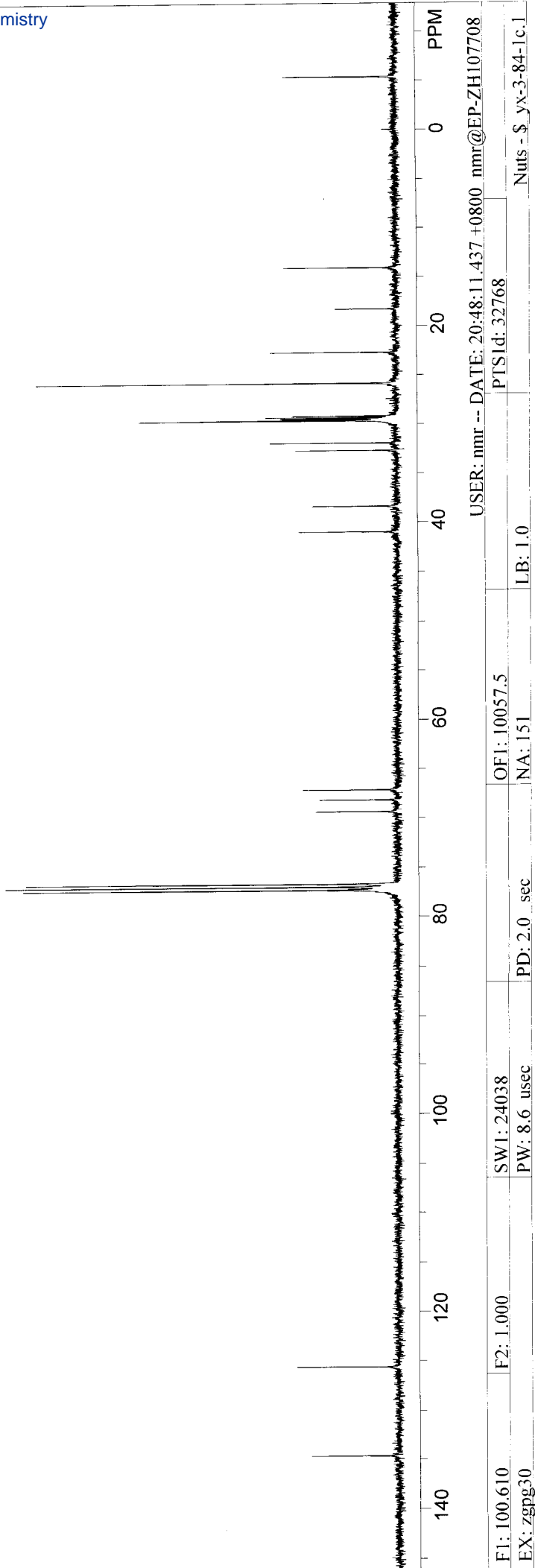
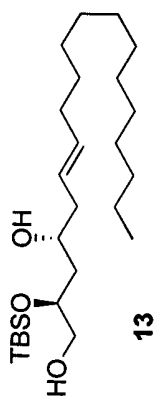
5.431
5.385

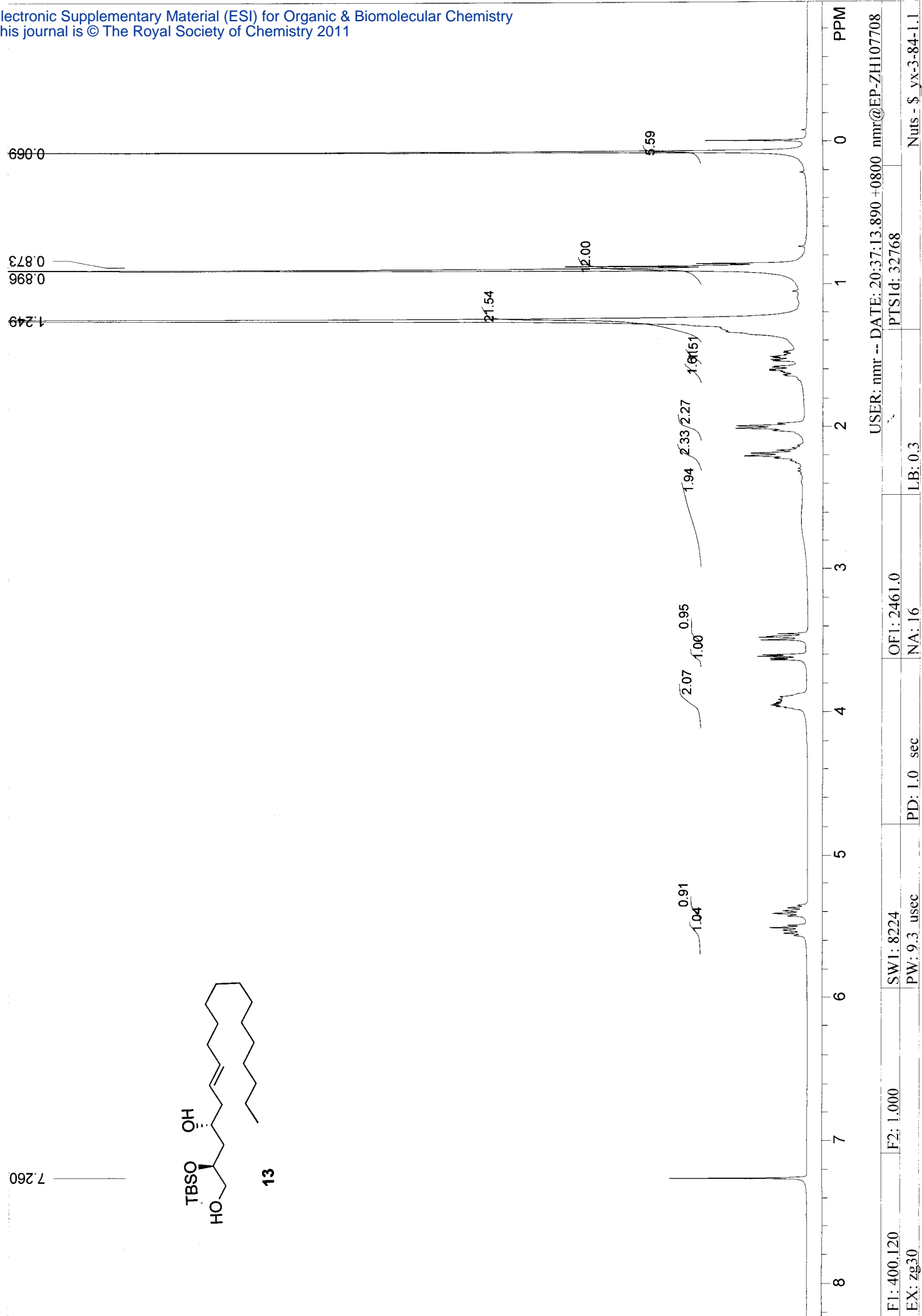
14.083
18.249
22.665
25.847
29.190
29.334
29.444
29.476
29.621
29.658
31.895
32.647
38.379
40.990

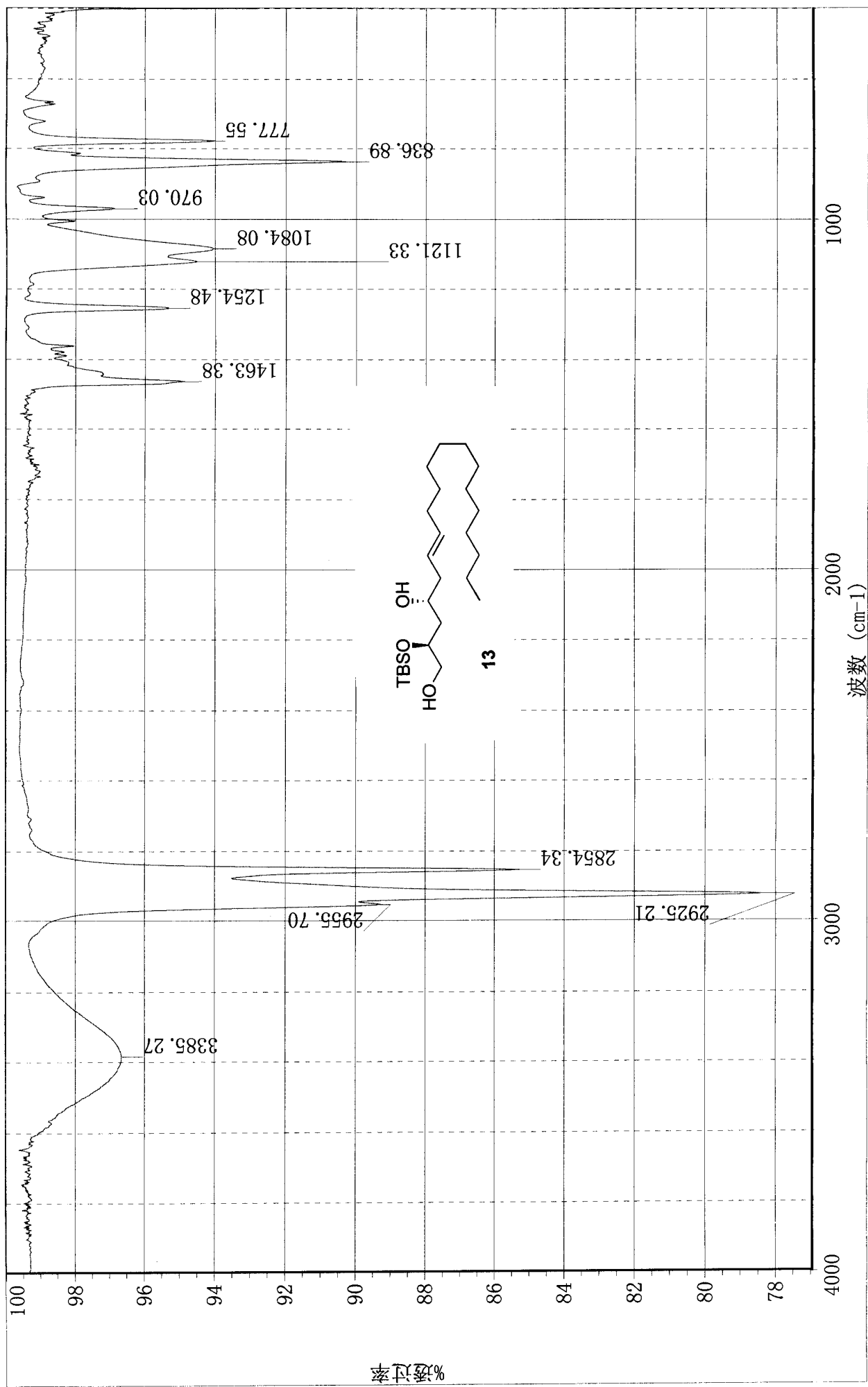
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69.405
76.673
77.000
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125.609

134.651





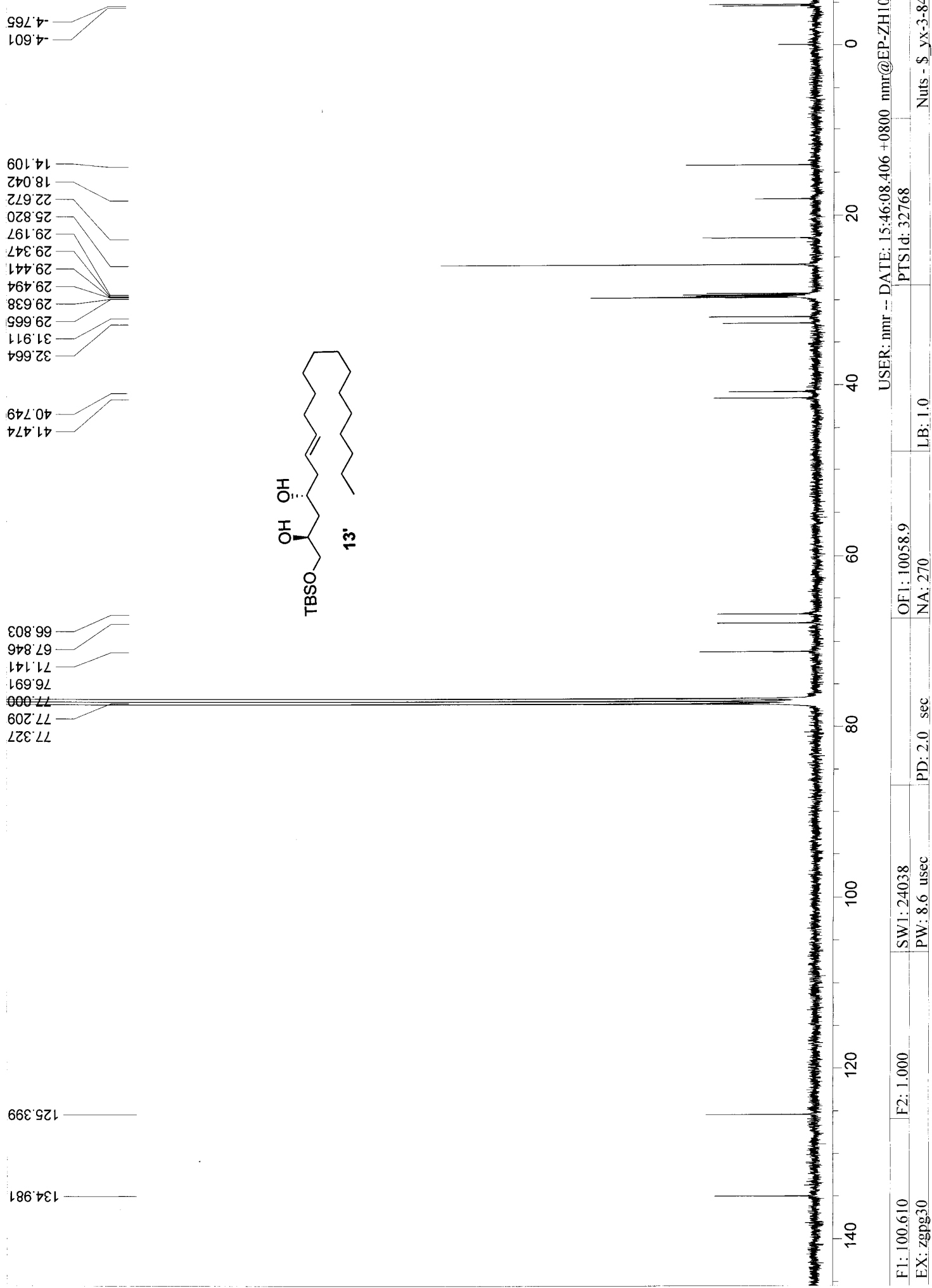


82 S

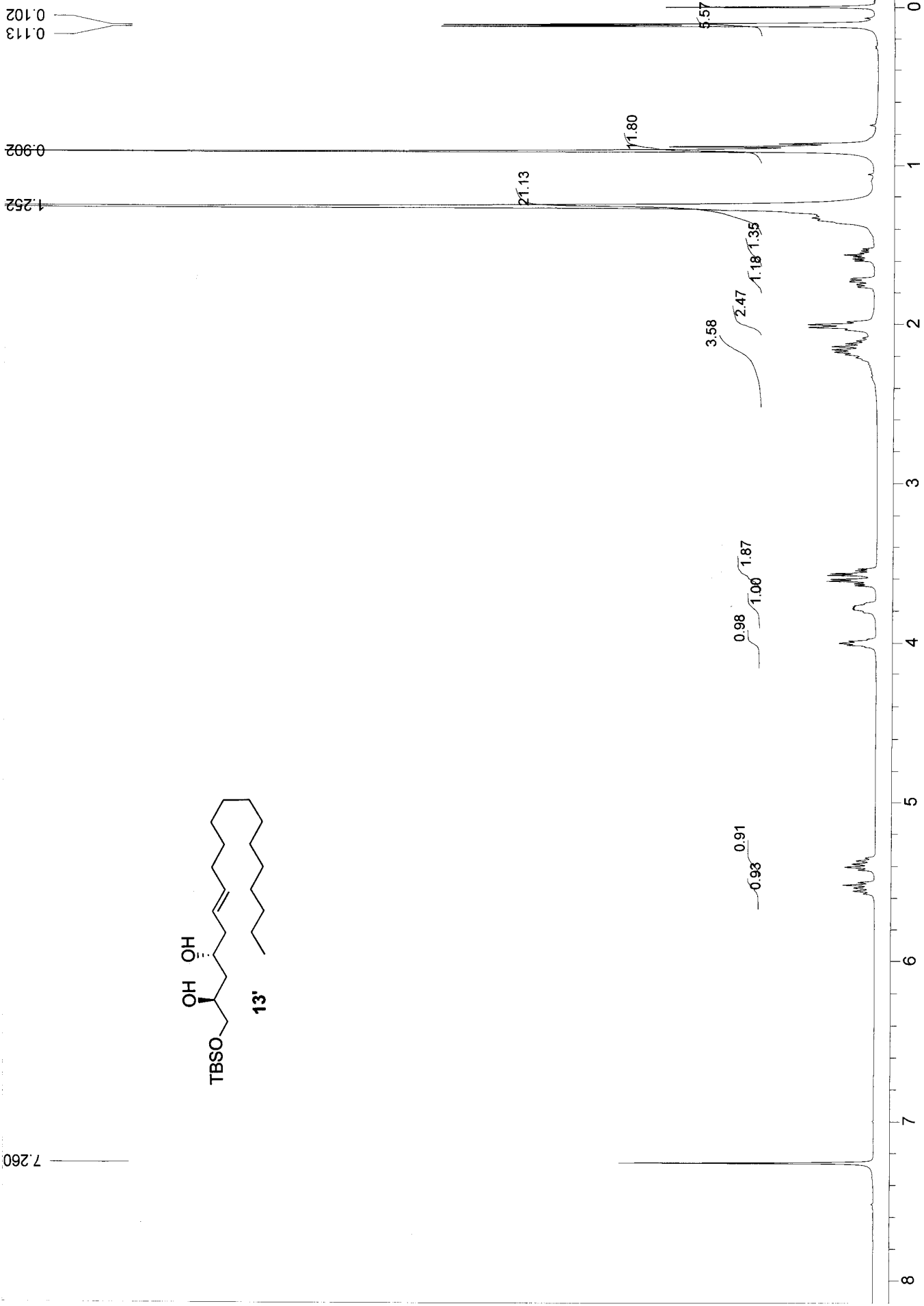
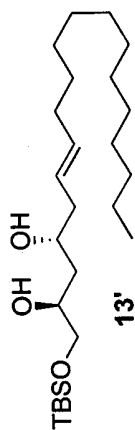
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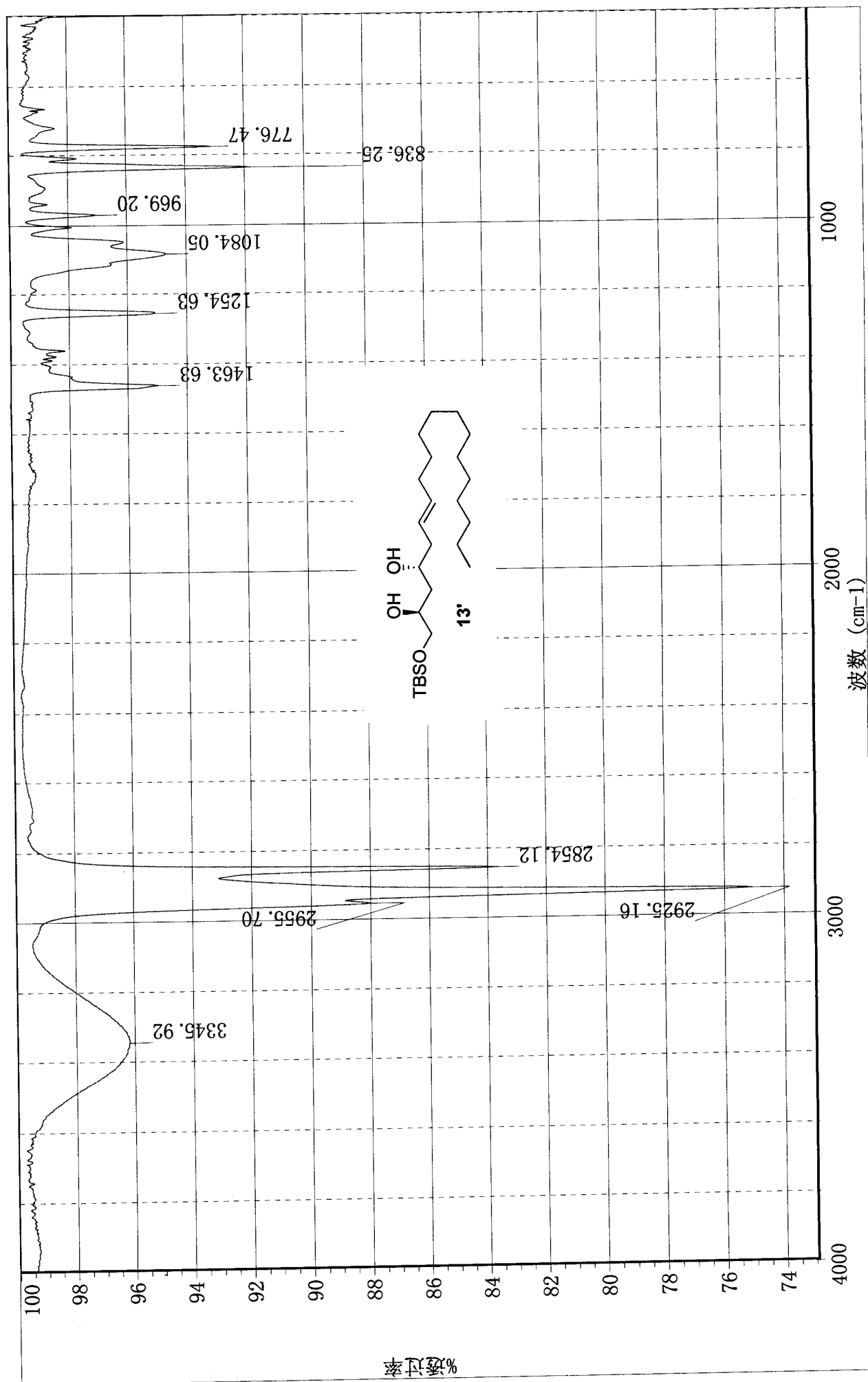
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 USER: nmr -- DATE: 15:46:08.406 +0800 nmr@EP-ZH107708
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F2: 1.000
SW1: 8224
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PD: 1.0 sec
OF1: 2461.1
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LB: 0.3
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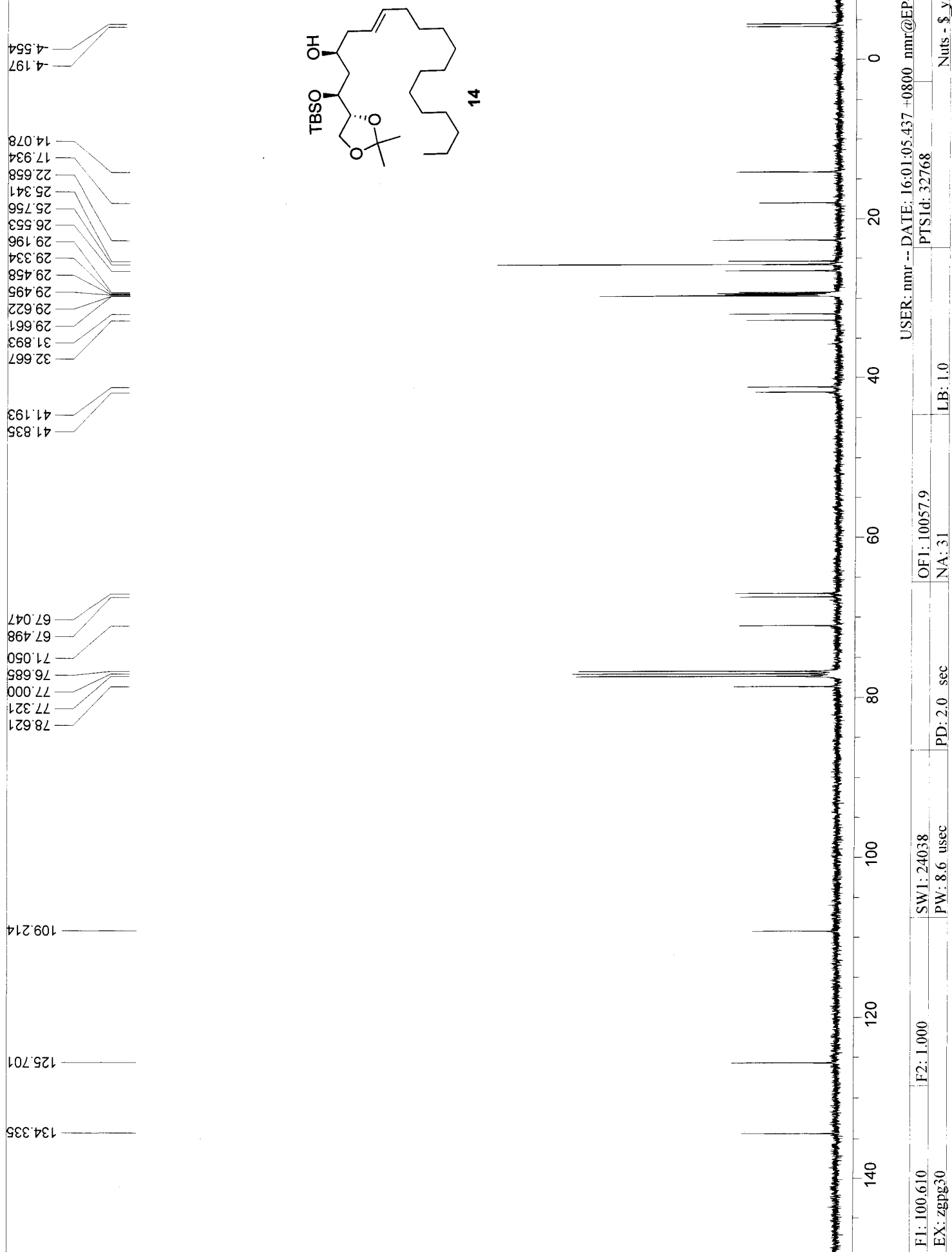


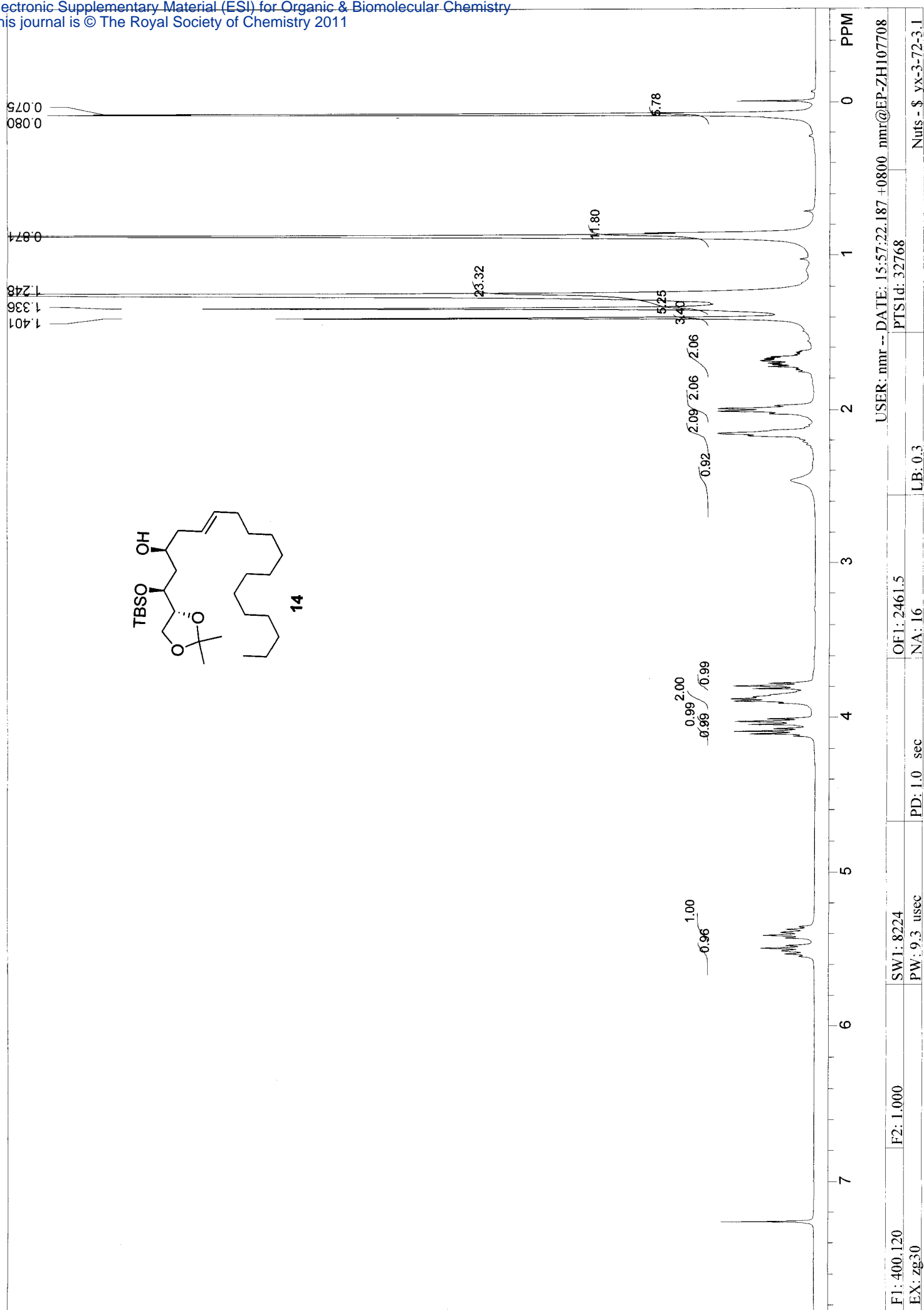
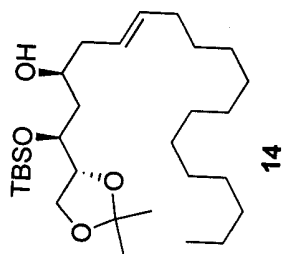
13 S

**yx-3-84-2

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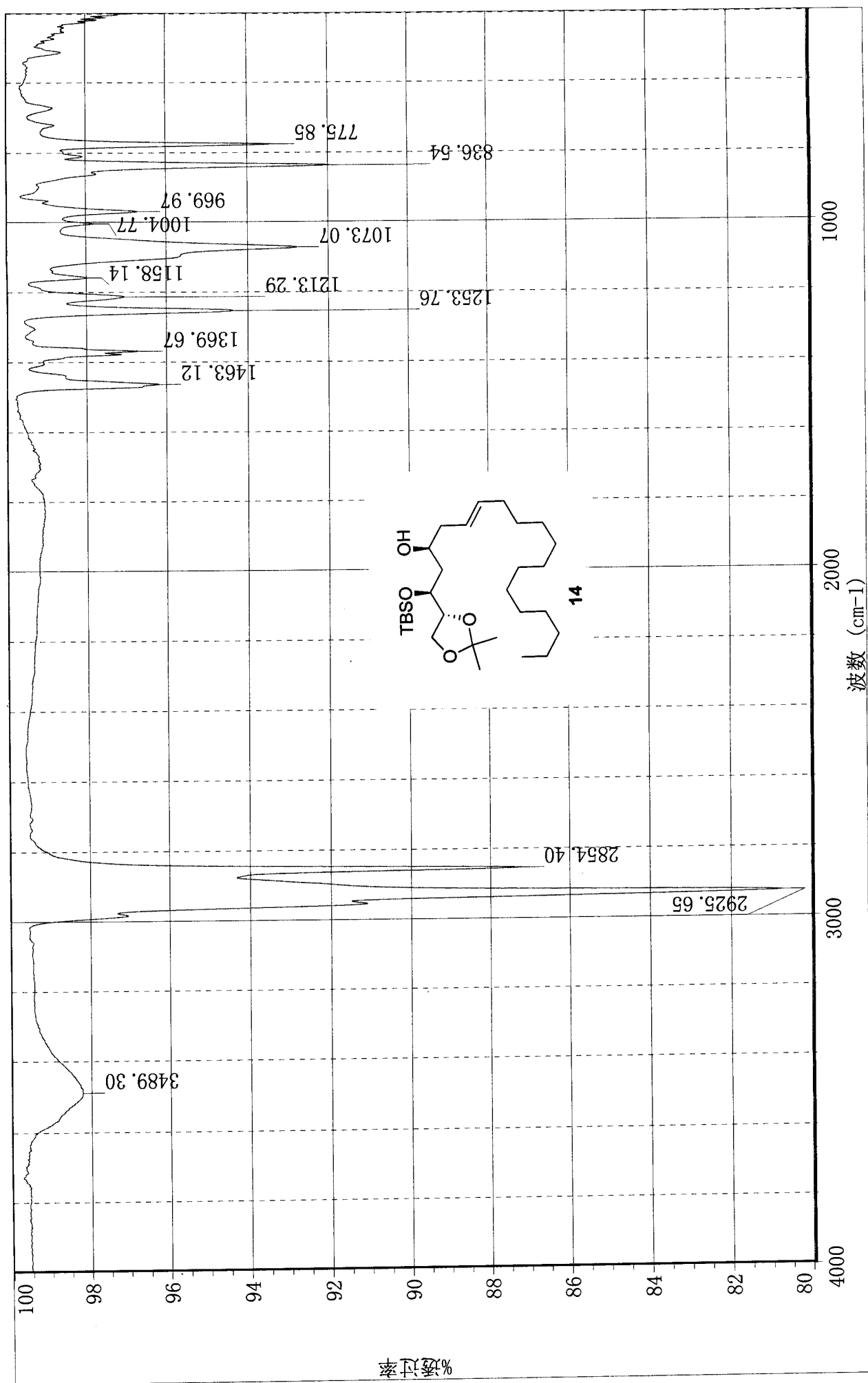
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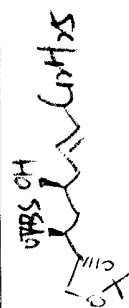
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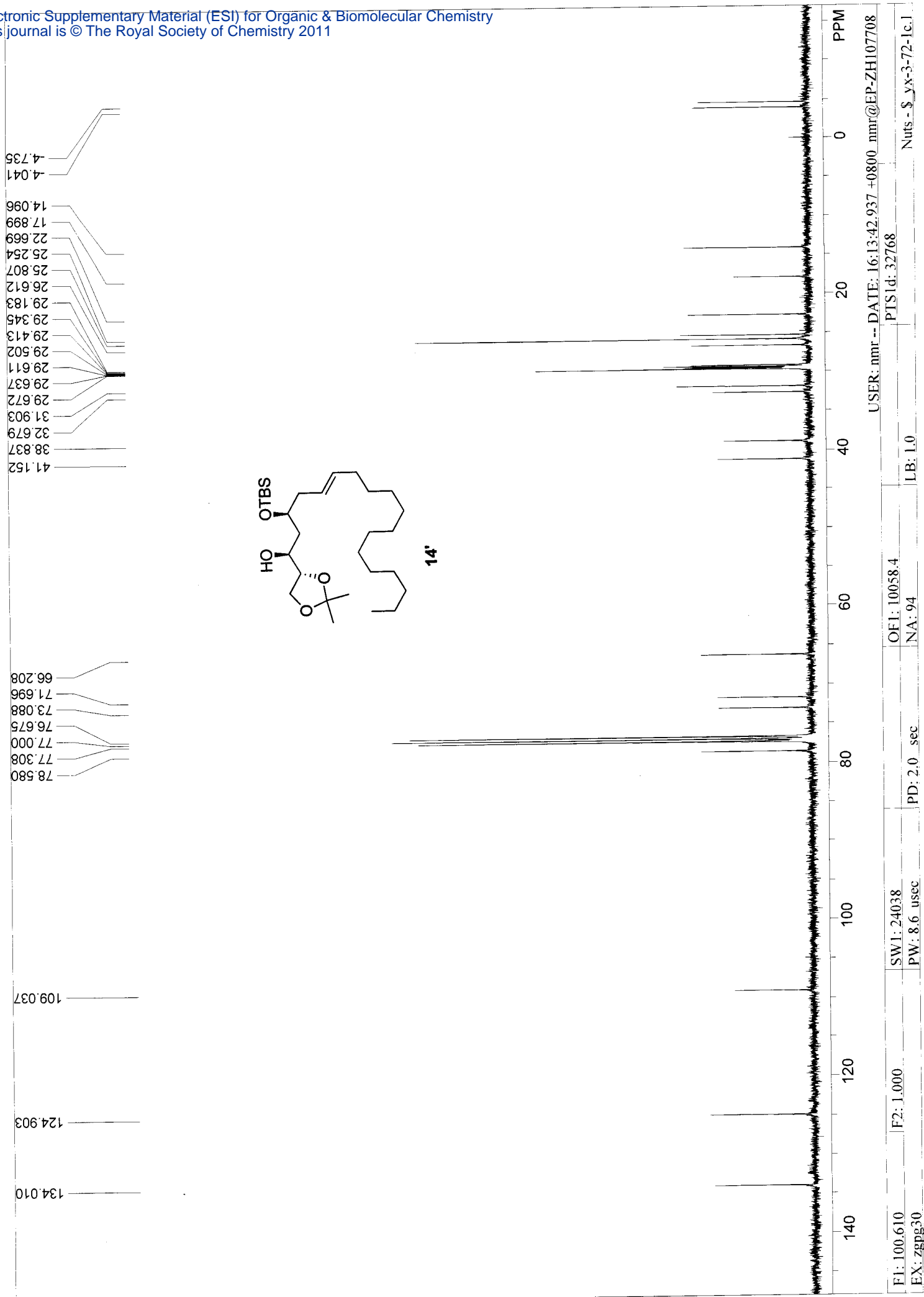
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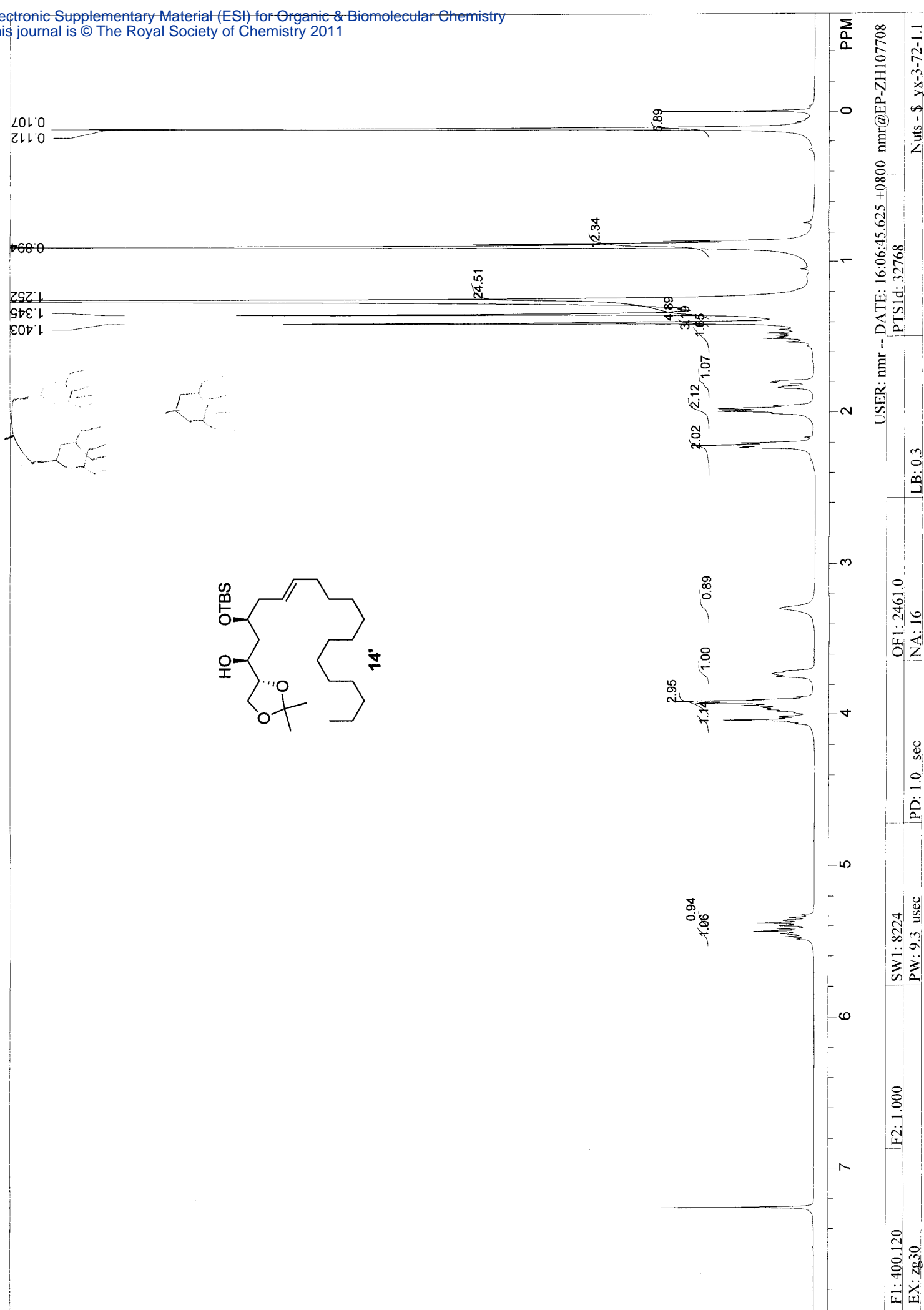


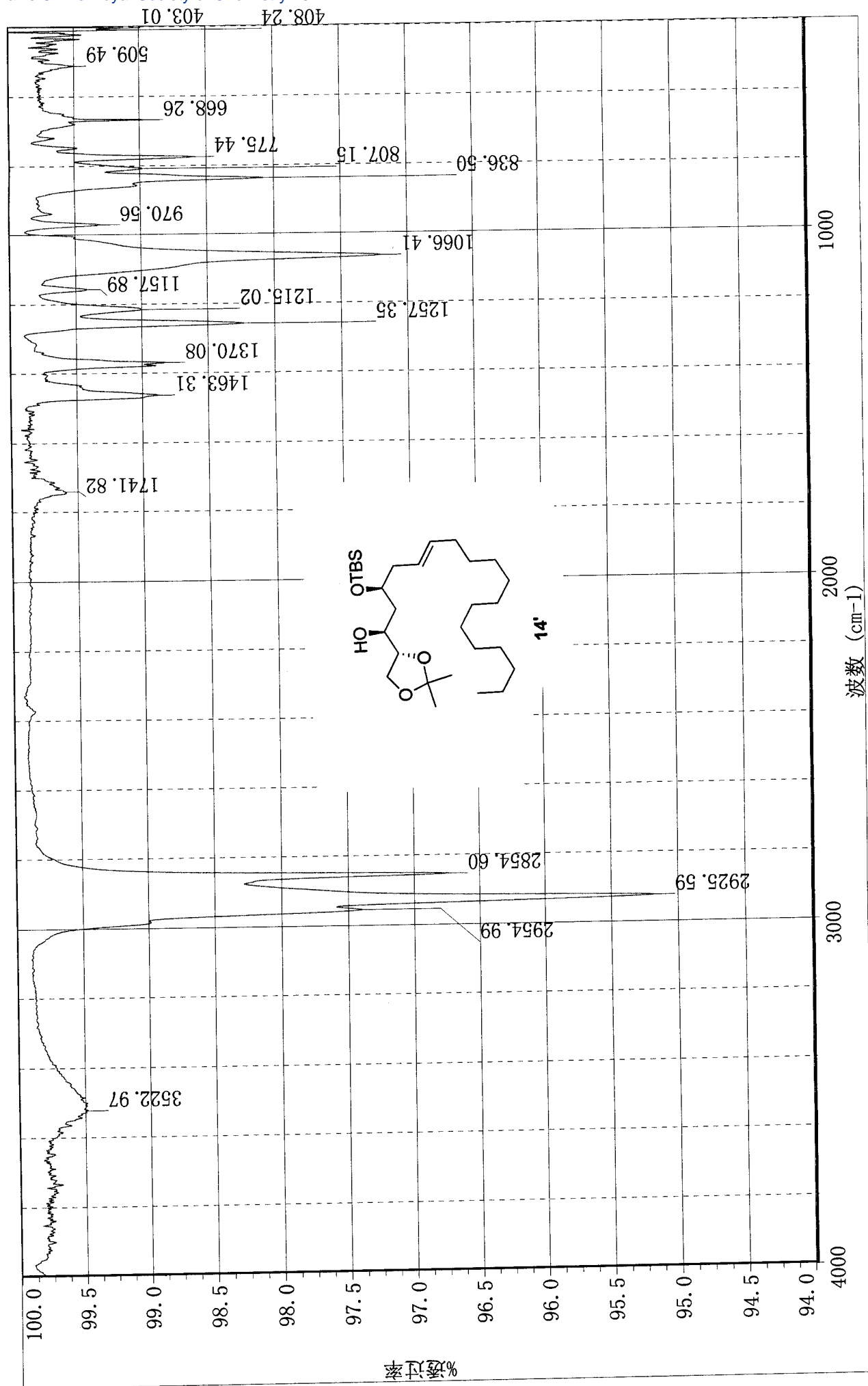
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采集时间: 星期一 3月 28 20:19:10 2011 (GMT+08:00)



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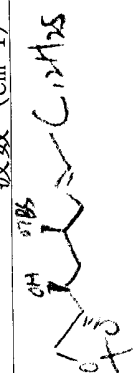




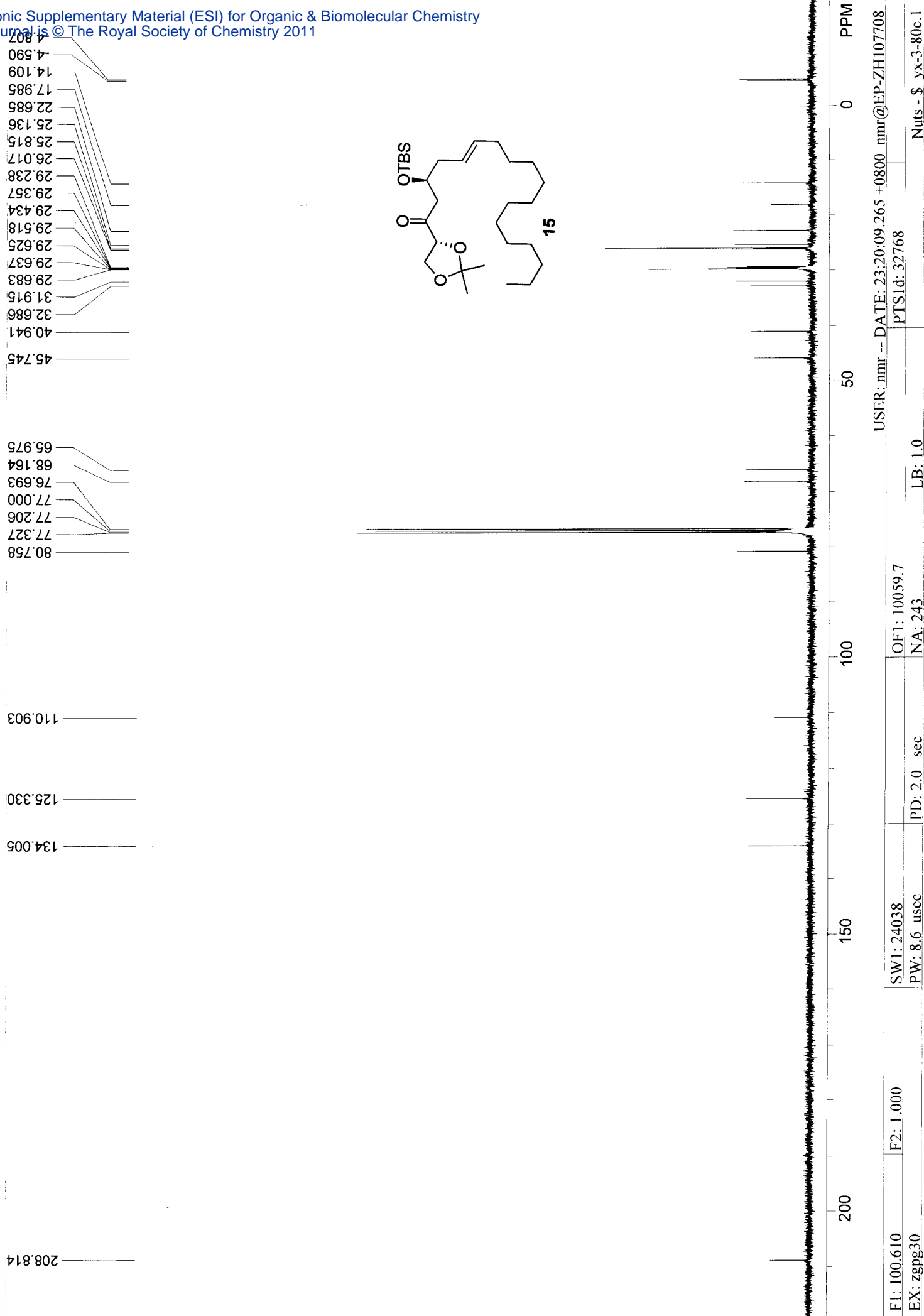


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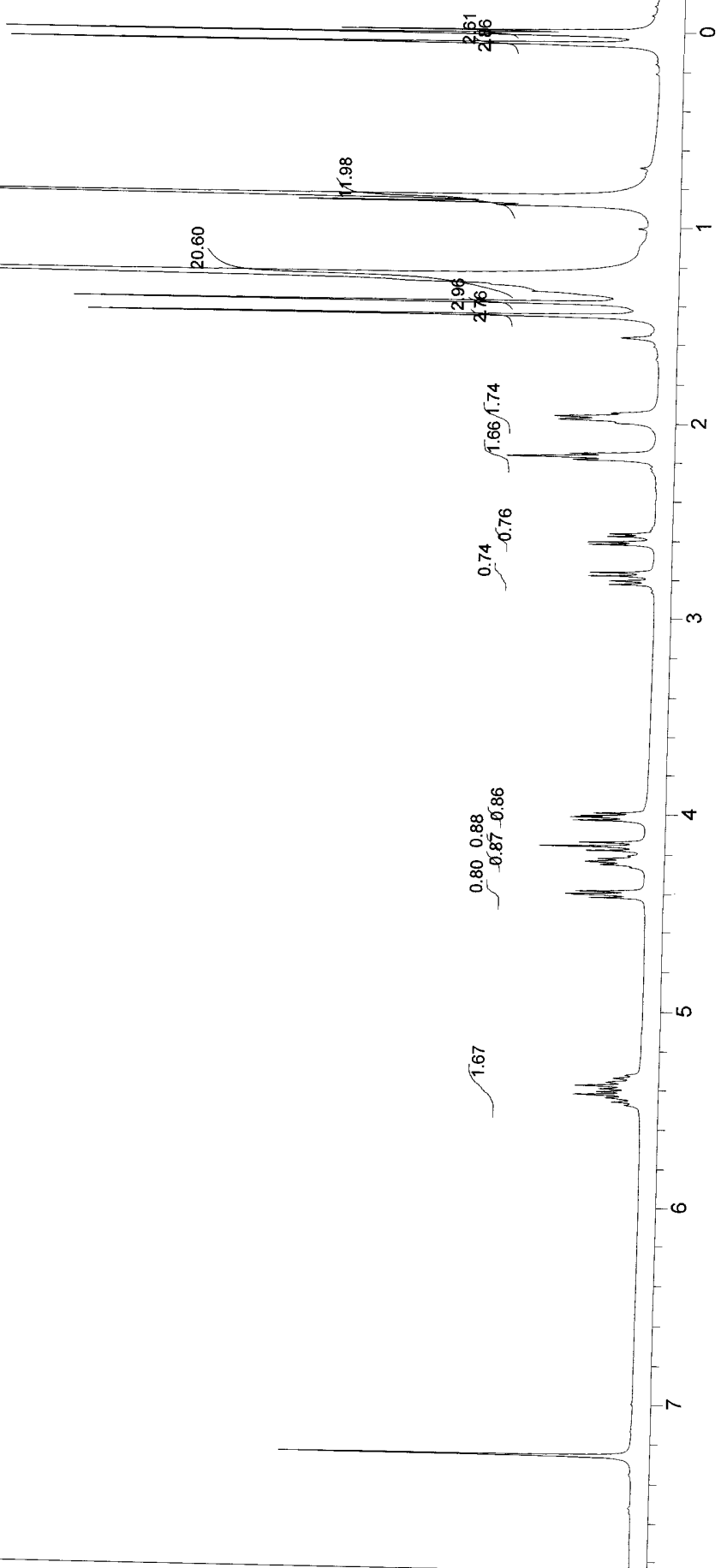
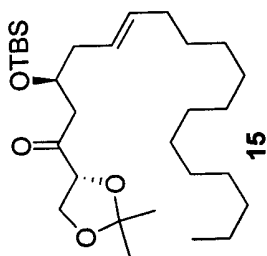
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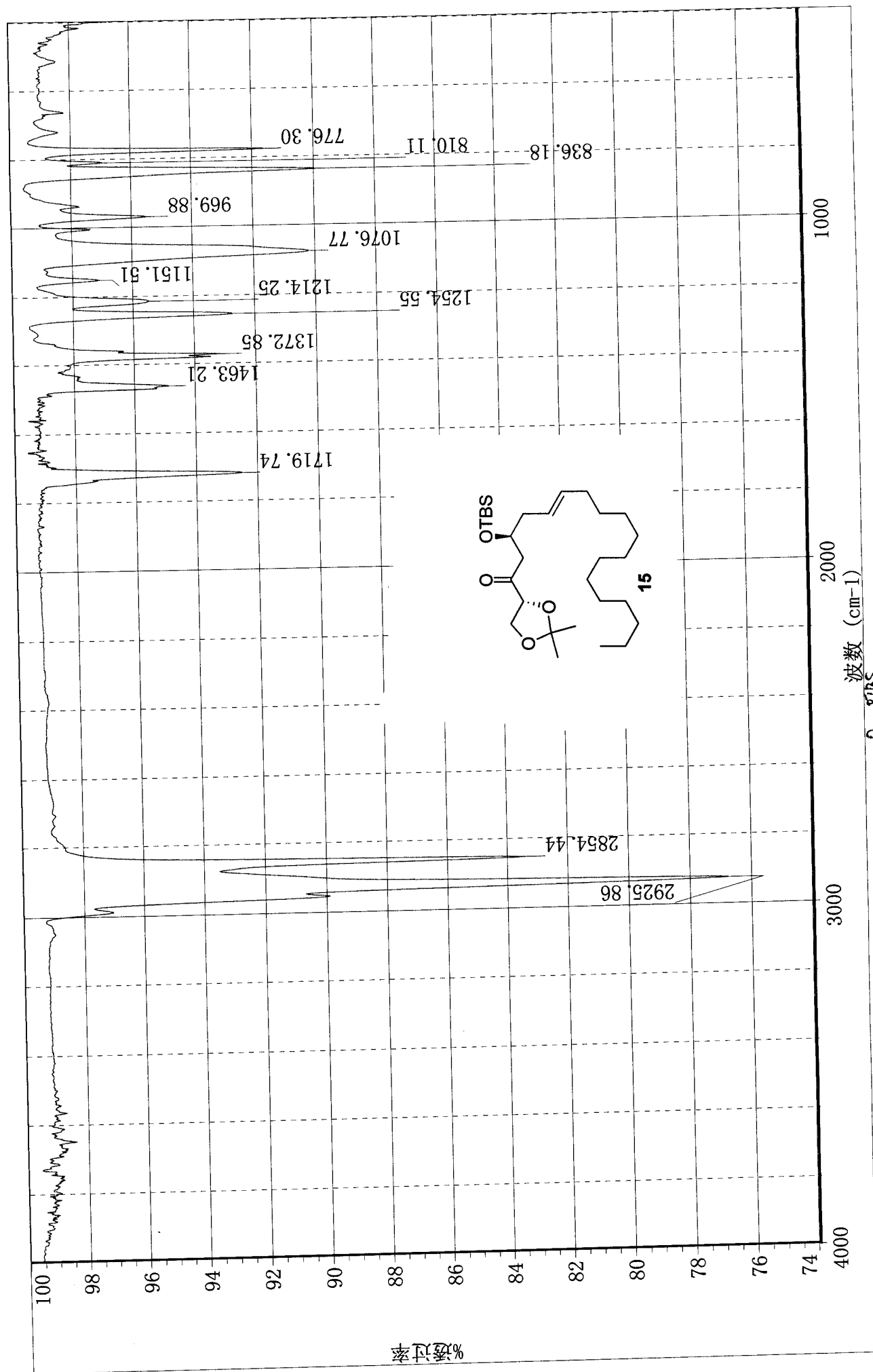
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0.063
0.014
0.952
1.253
1.386
1.455

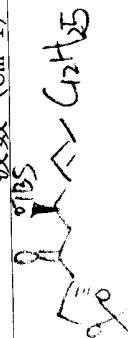


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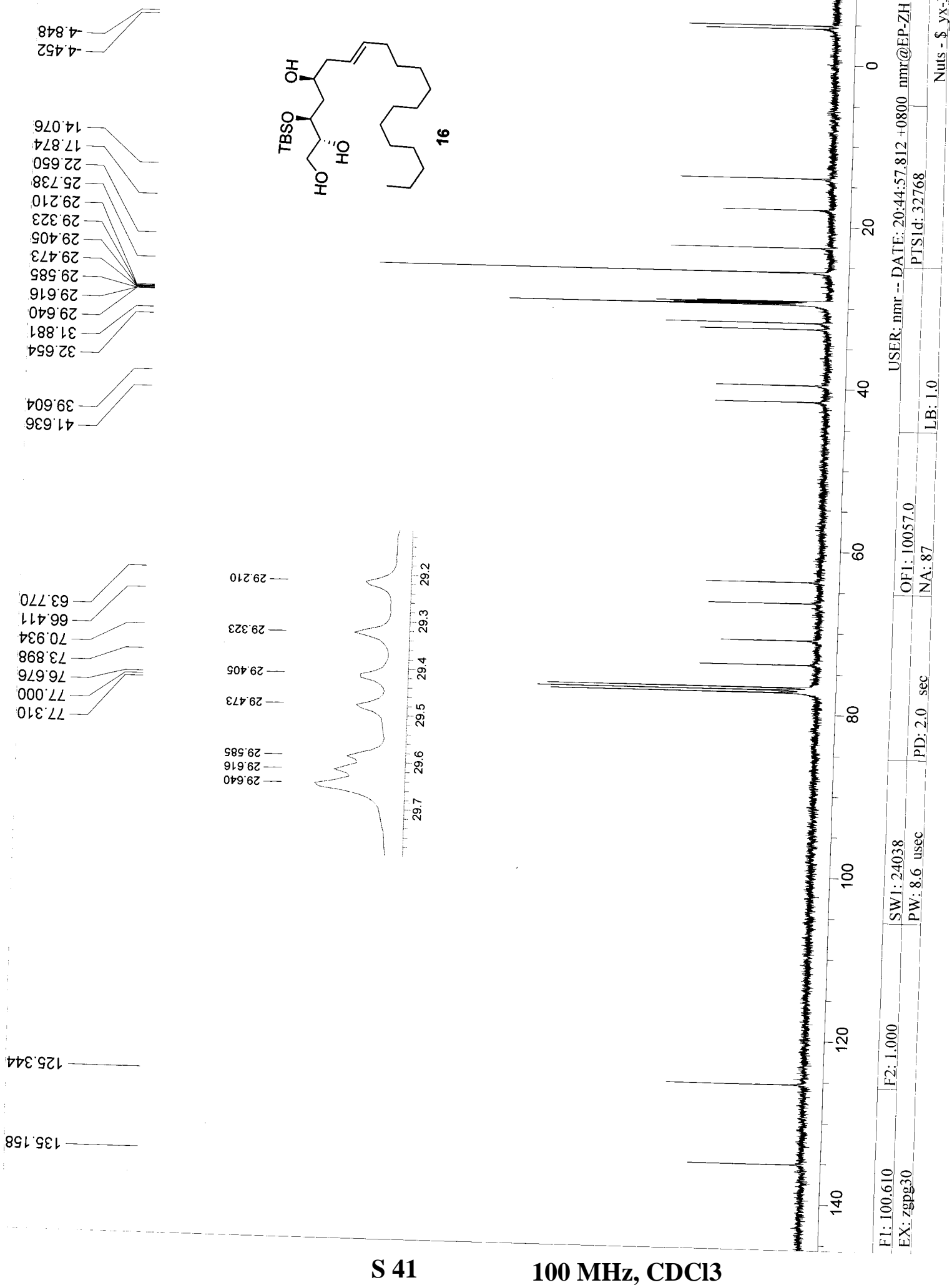


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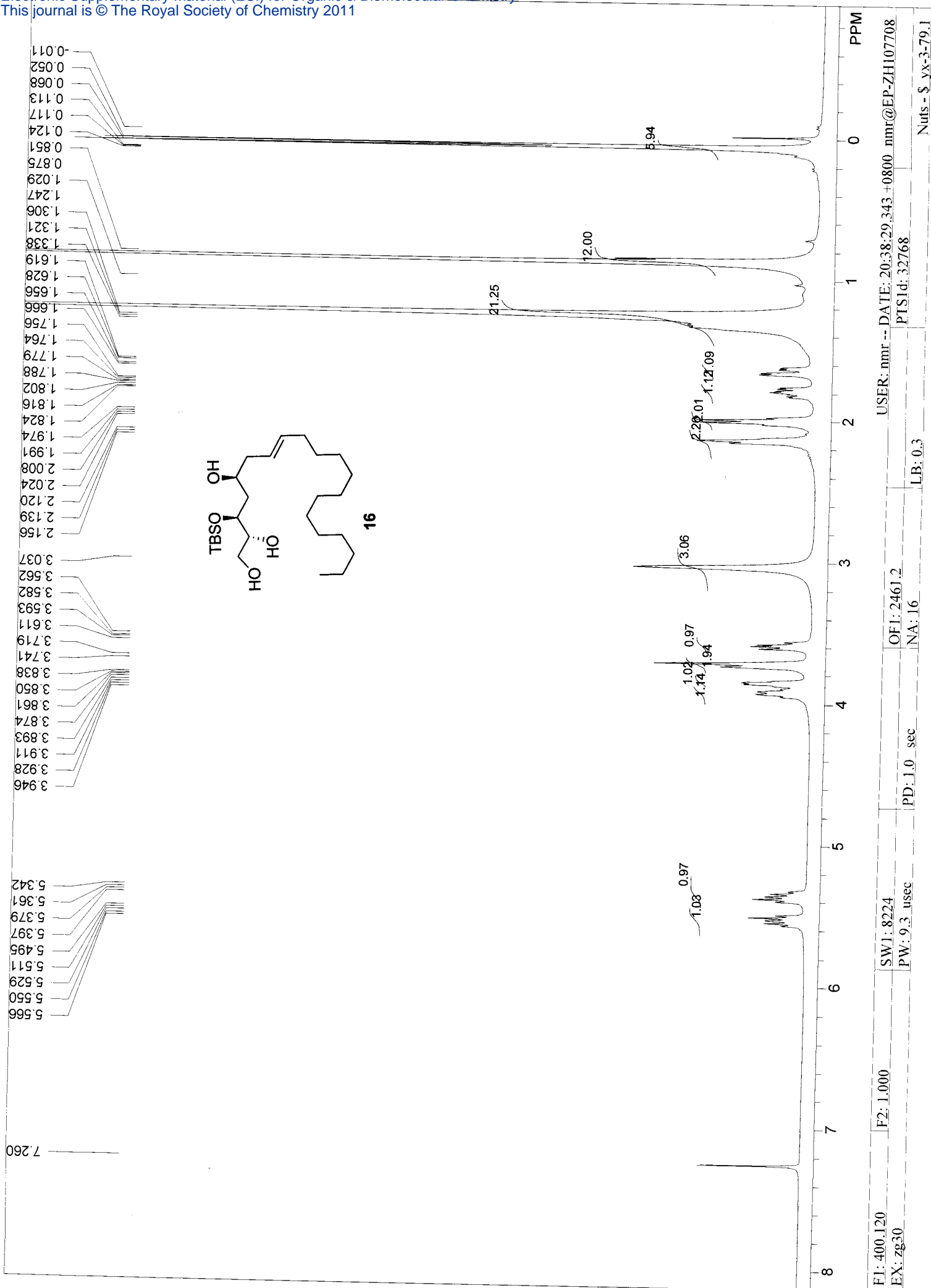


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S 41

100 MHz, CDCl₃



F1: 400.120
EX: zg30

F2: 1.000

SW1: 8224
PW: 9.3 usec

PD: 1.0 sec

NA: 16

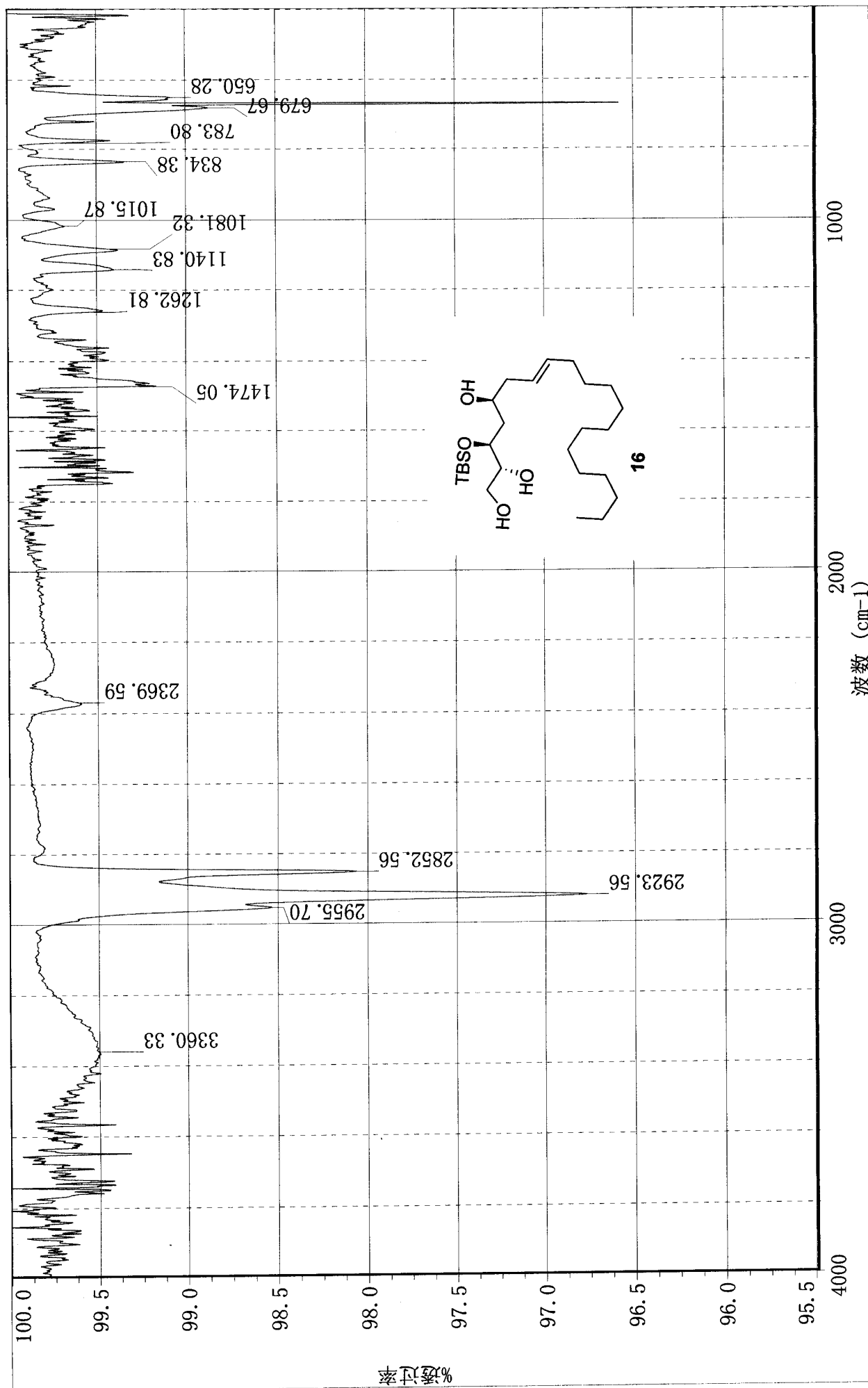
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PTSId: 32768

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LB: 0.3

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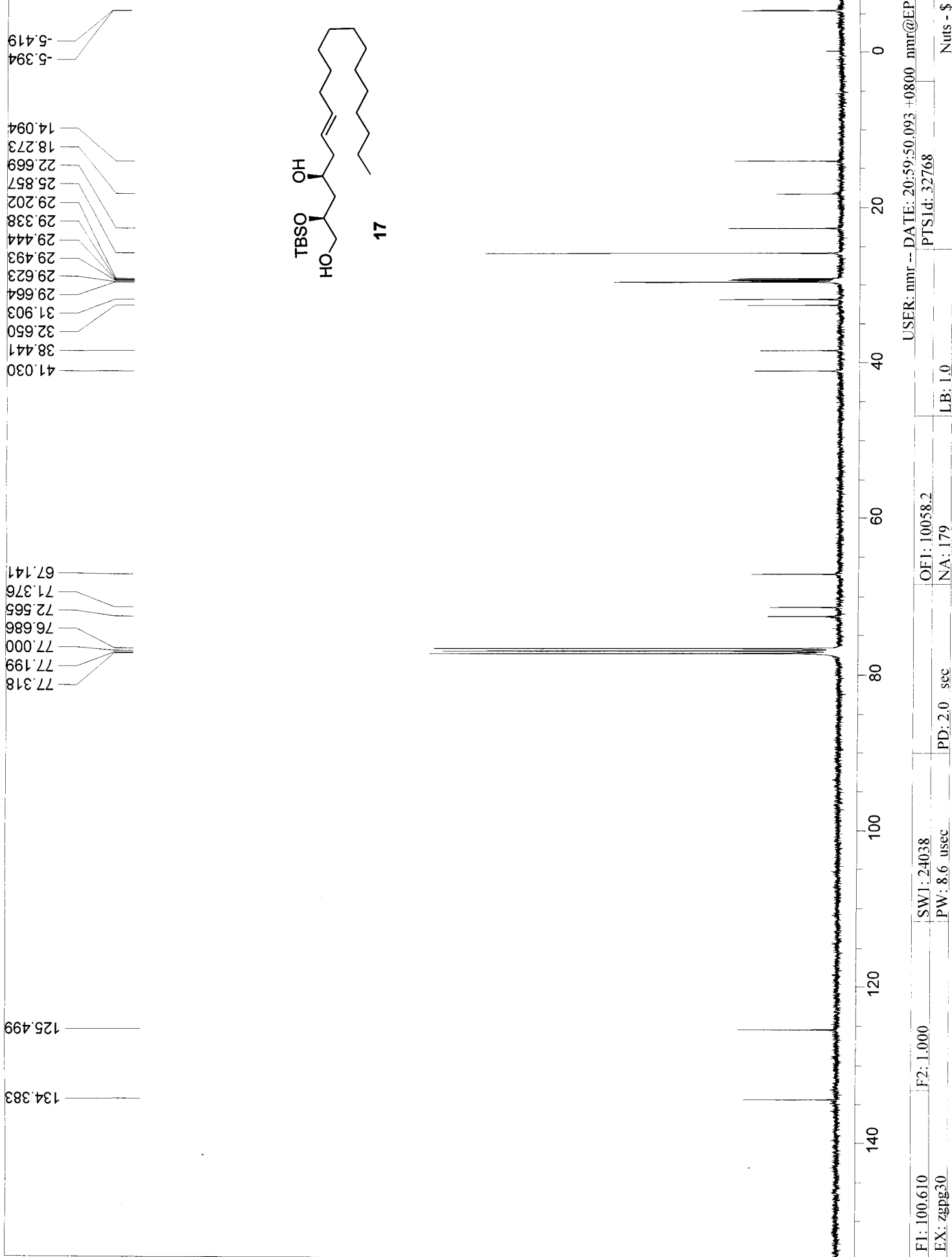


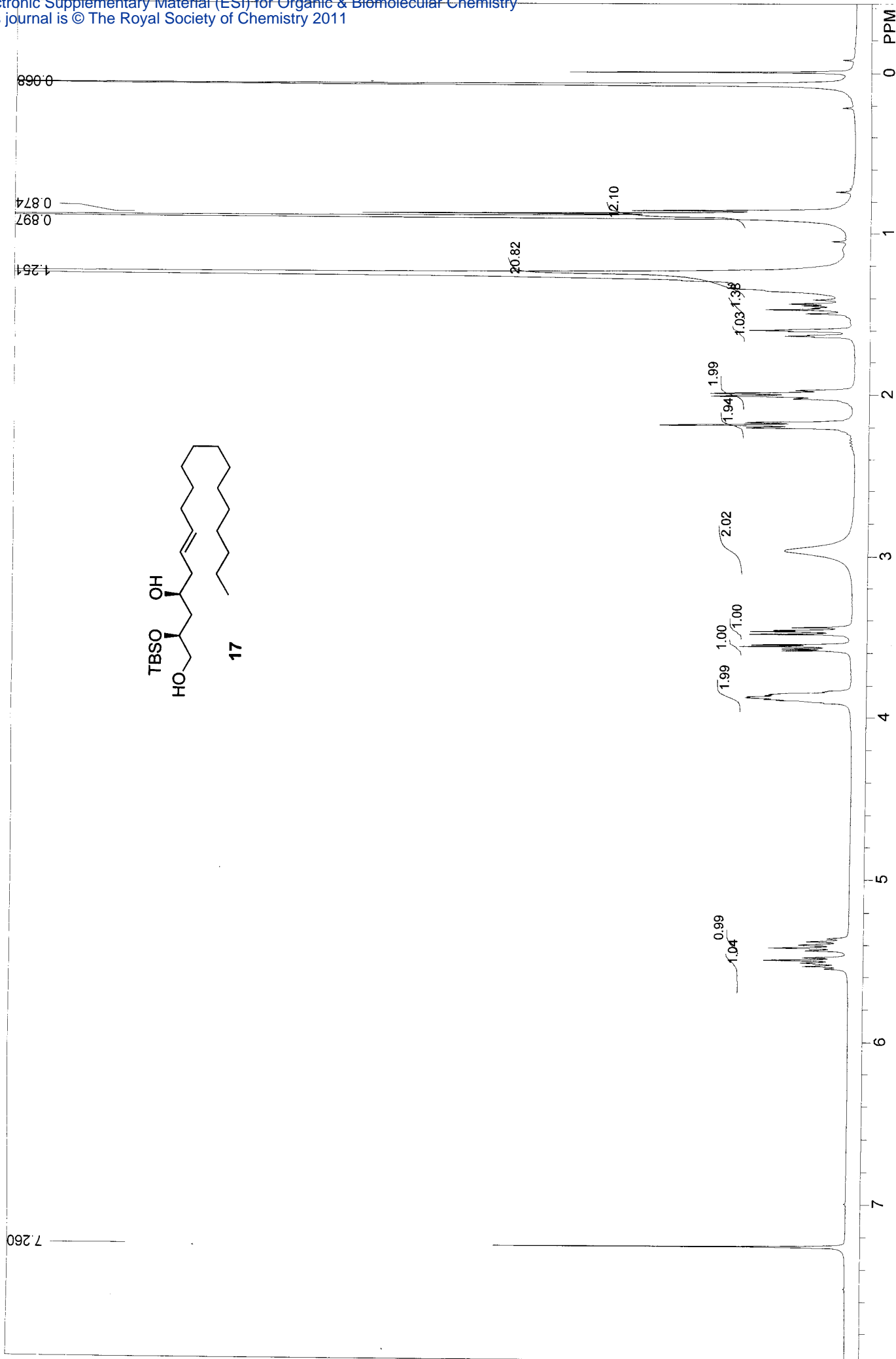
**yx-3-79

采集时间: 星期一 5月 09 10:44:51 2011 (GMT+08:00)

Handwritten signature and initials.

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USER: nmr -- DATE: 21-02-2011 08:00 nmr@EP-ZHI07708

PTS1d: 32768

LB: 0.3

OF1: 2461.0

NA: 16

PD: 1.0 sec

SW1: 8224

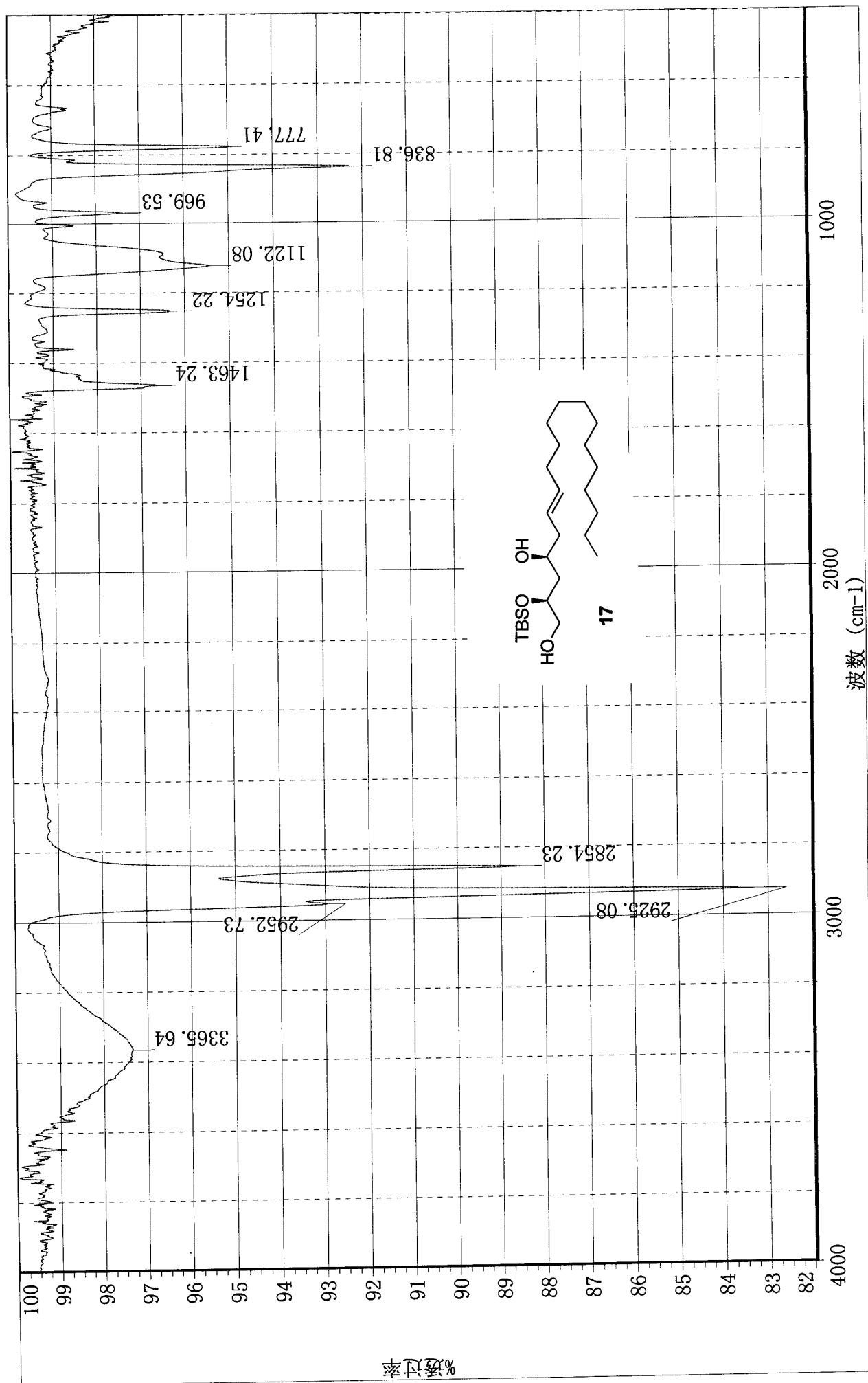
PW: 9.3 usec

F2: 1.000

F1: 400.120

EX: zg30

Nuts - \$ yx-3-83.1

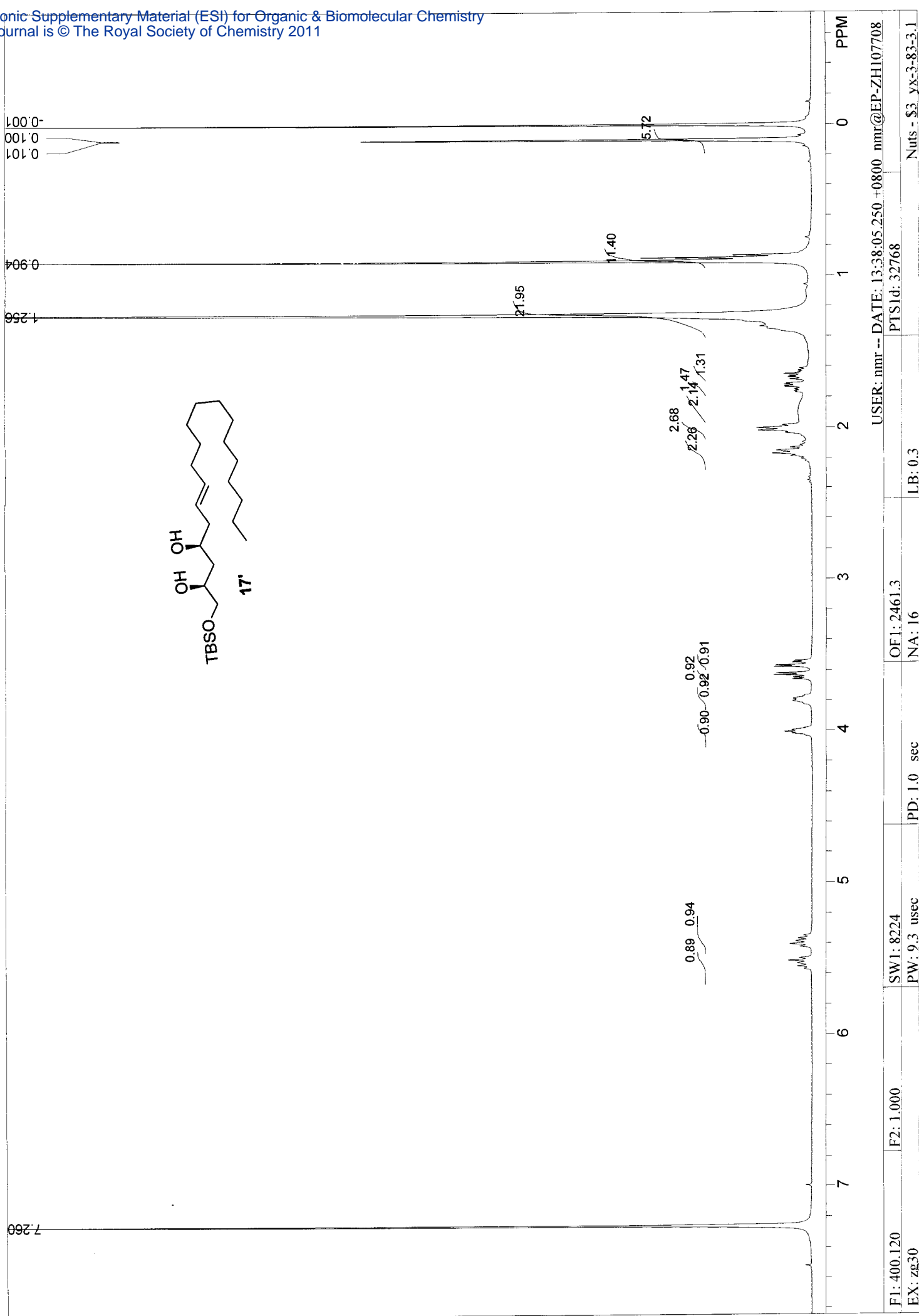


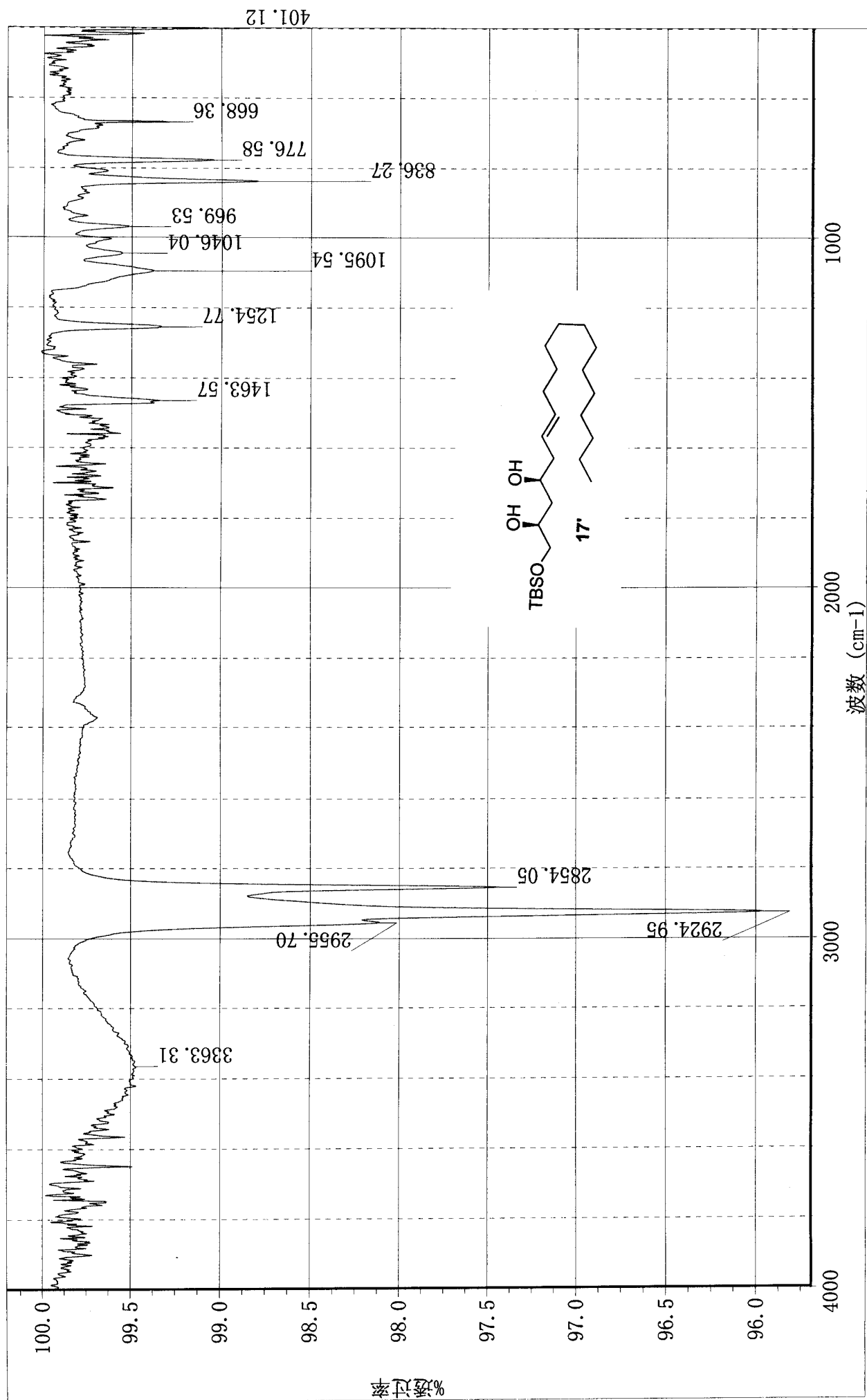
*yx-3-83

采集时间: 星期五 4月 01 18:59:16 2011 (GMT+08:00)



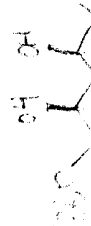
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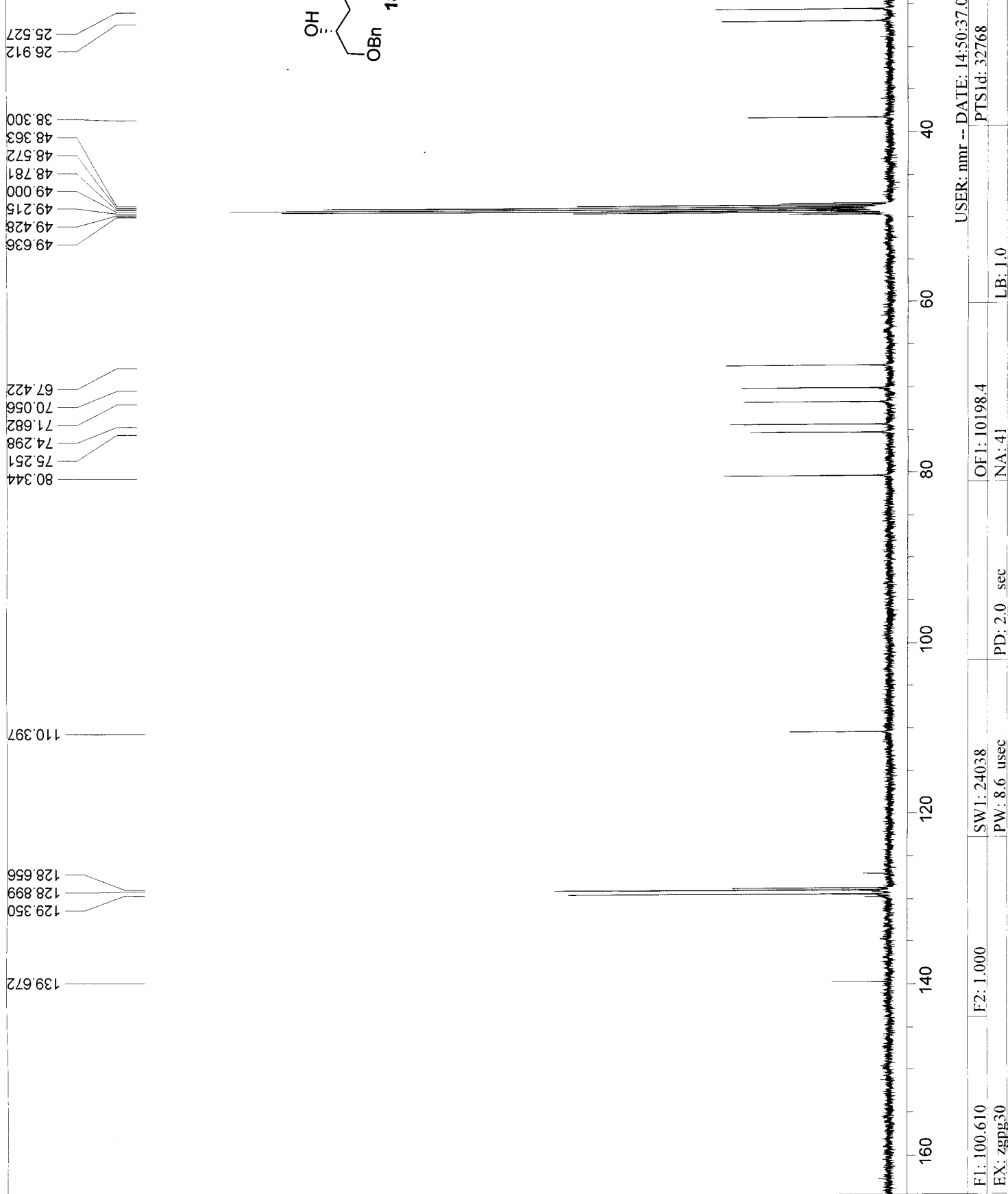
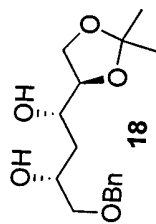


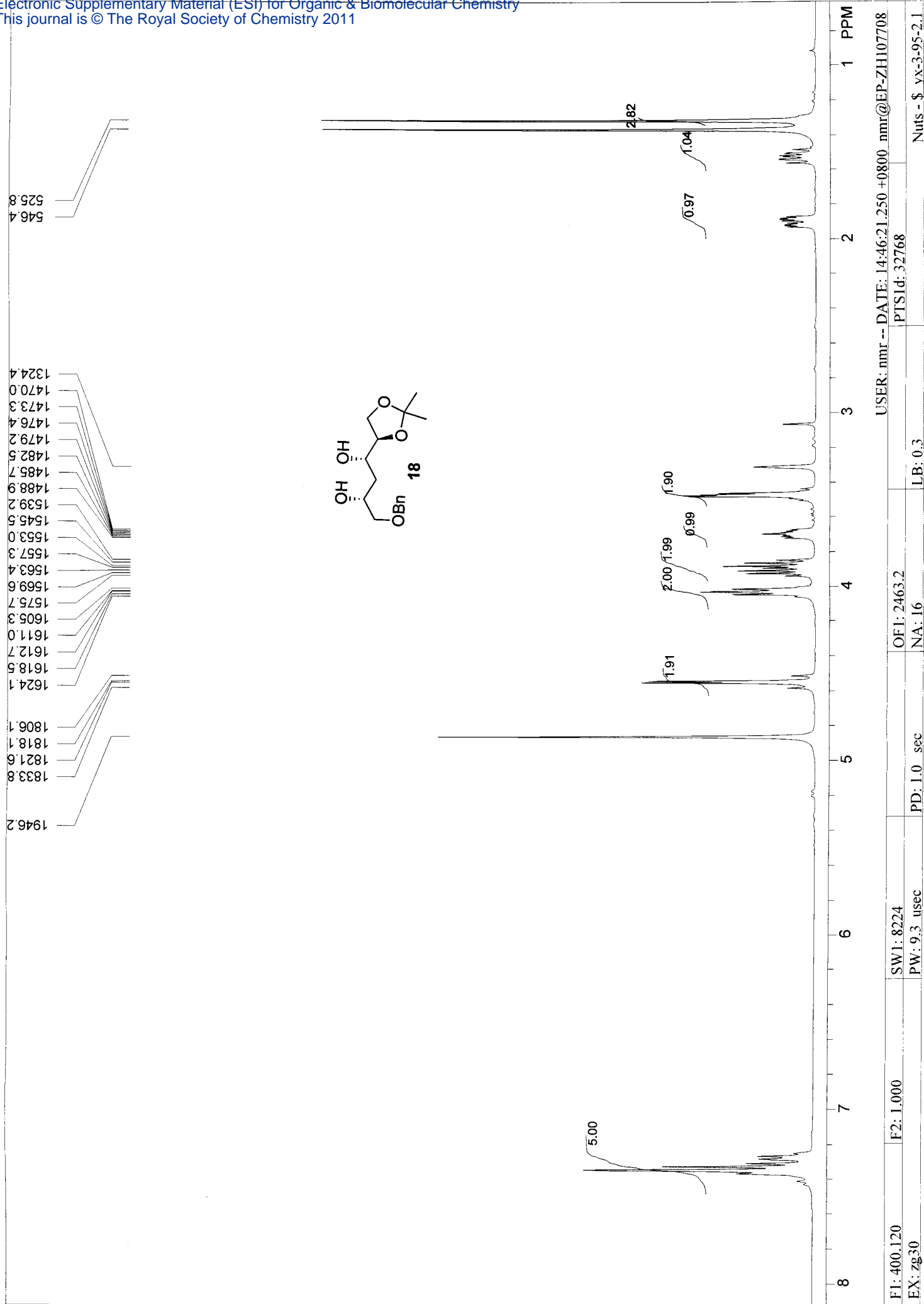
**yx-3-83-3

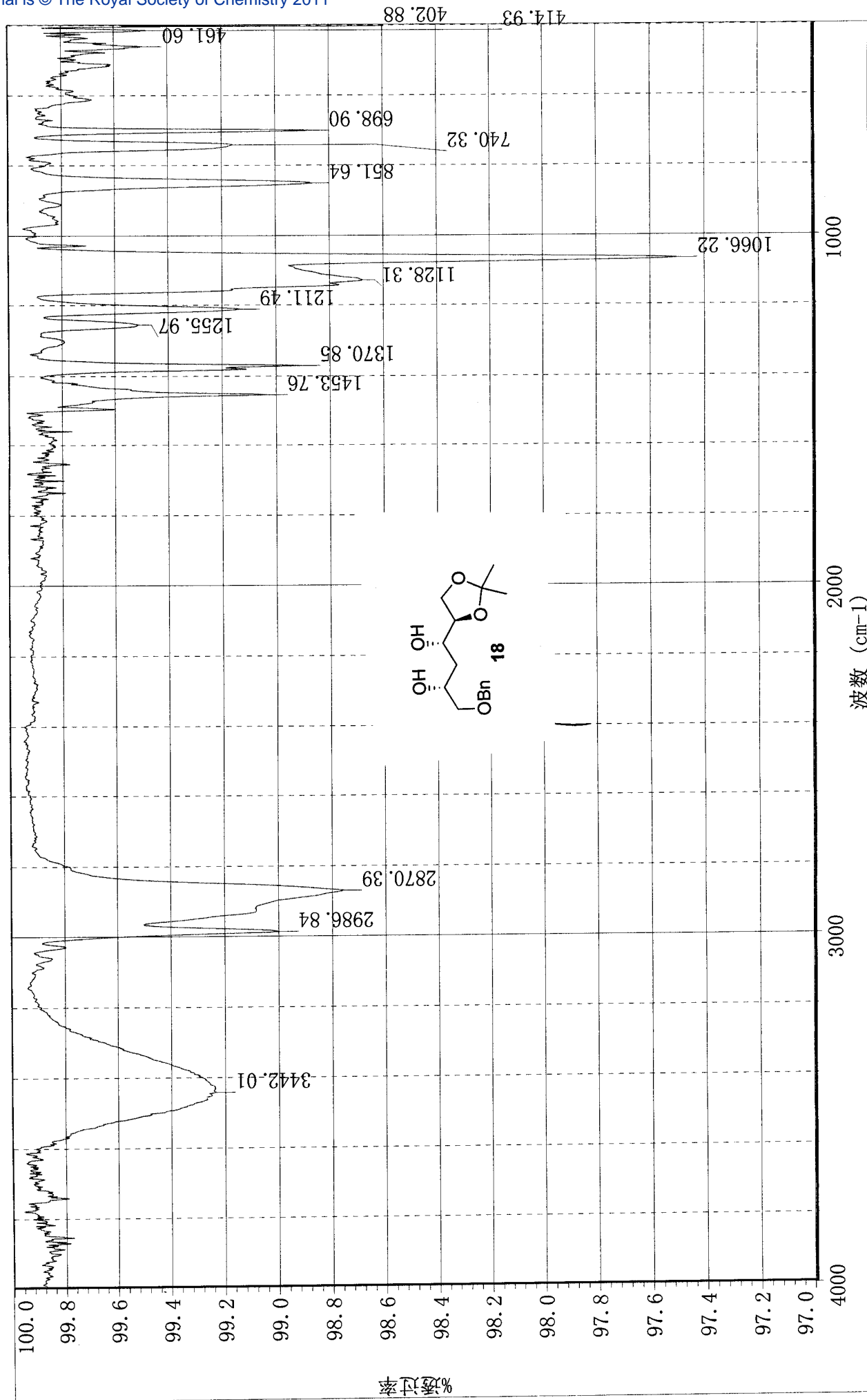
采集时间: 星期一 5月 09 10:32:43 2011 (GMT+08:00)



Gr 175 上海有机所生命有机化学国家重点实验室







**星期五 5月 13 15:52:51 2011

采集时间: 星期五 5月 13 15:53:32 2011 (GMT+08:00)



上海有机所生命有机化学国家重点实验室

20.932
21.058
25.011
26.188
31.554

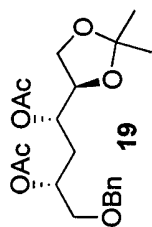
65.825
69.880
70.208
70.552
73.067
76.626
76.683
77.000
77.318

109.650

127.540
127.612
128.285

137.786

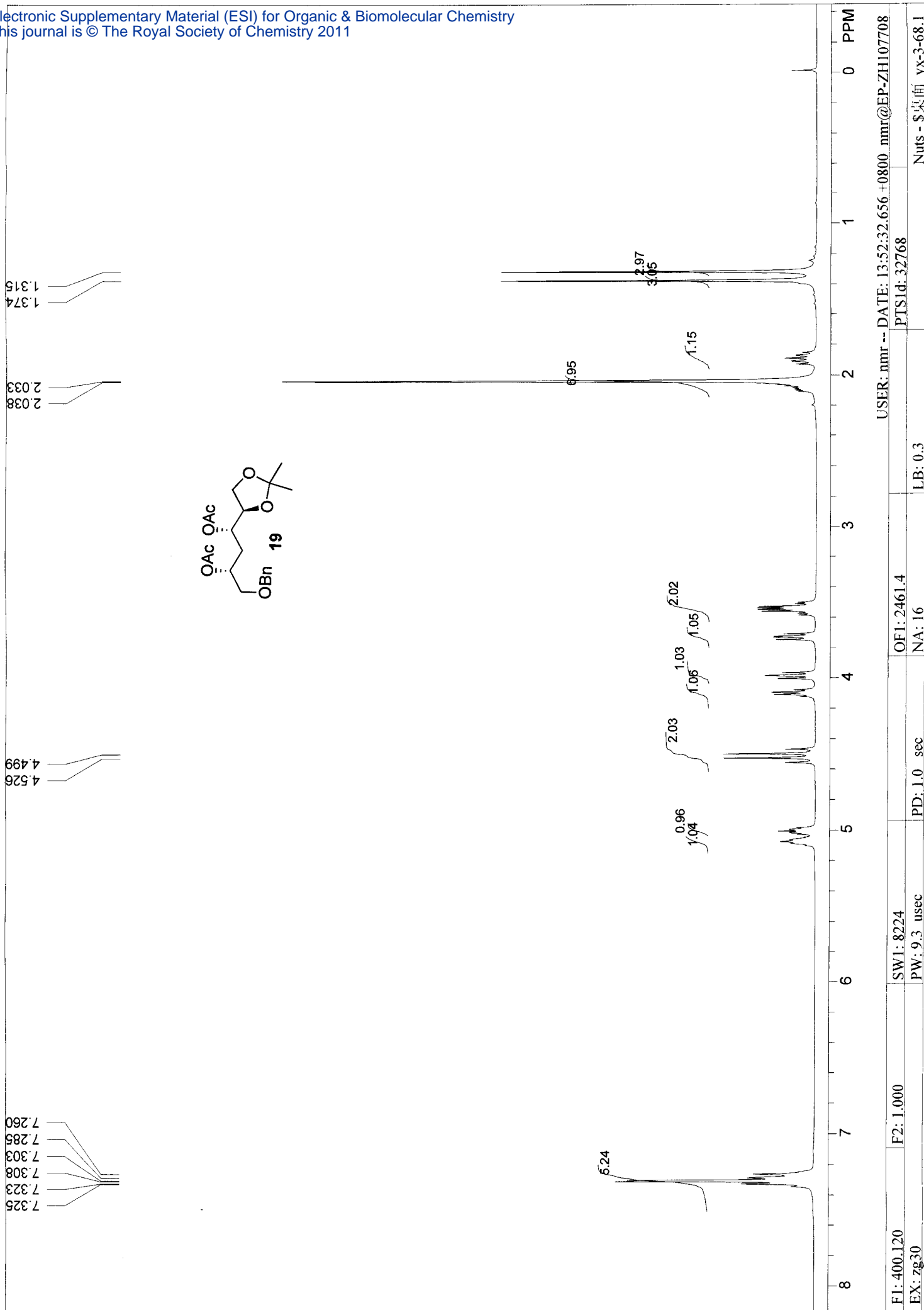
170.182
170.195

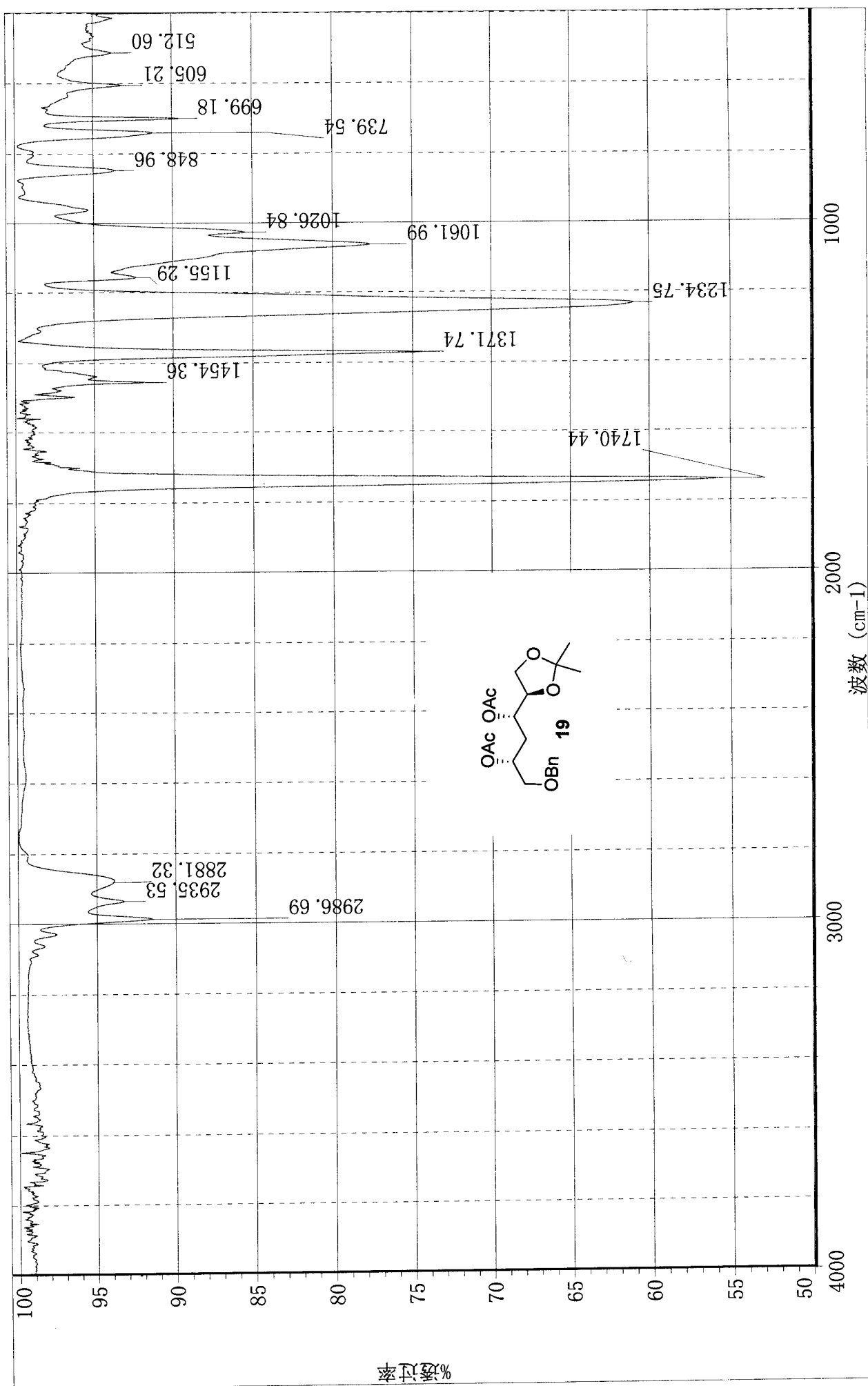


S 52

100 MHz, CDCl₃



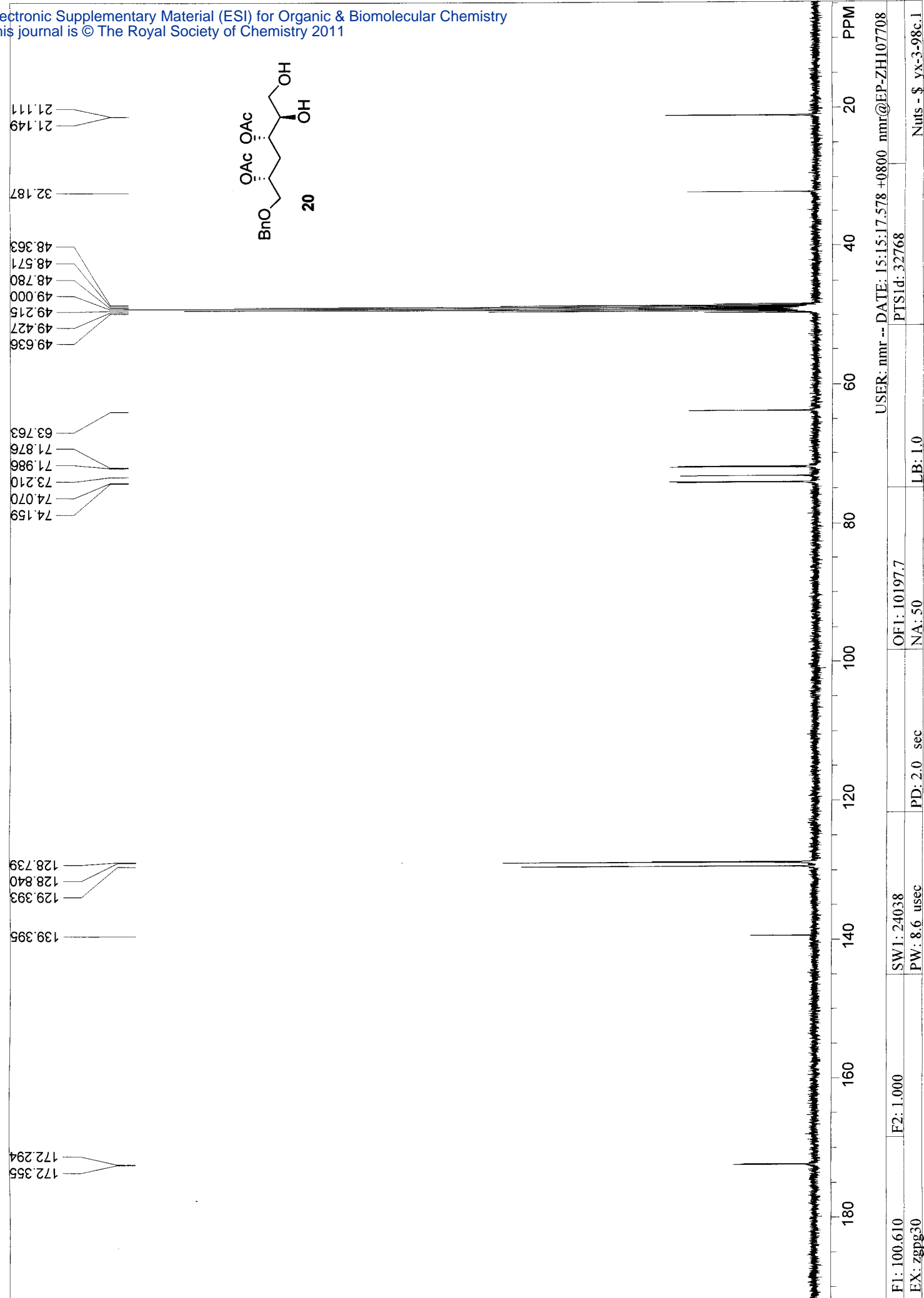


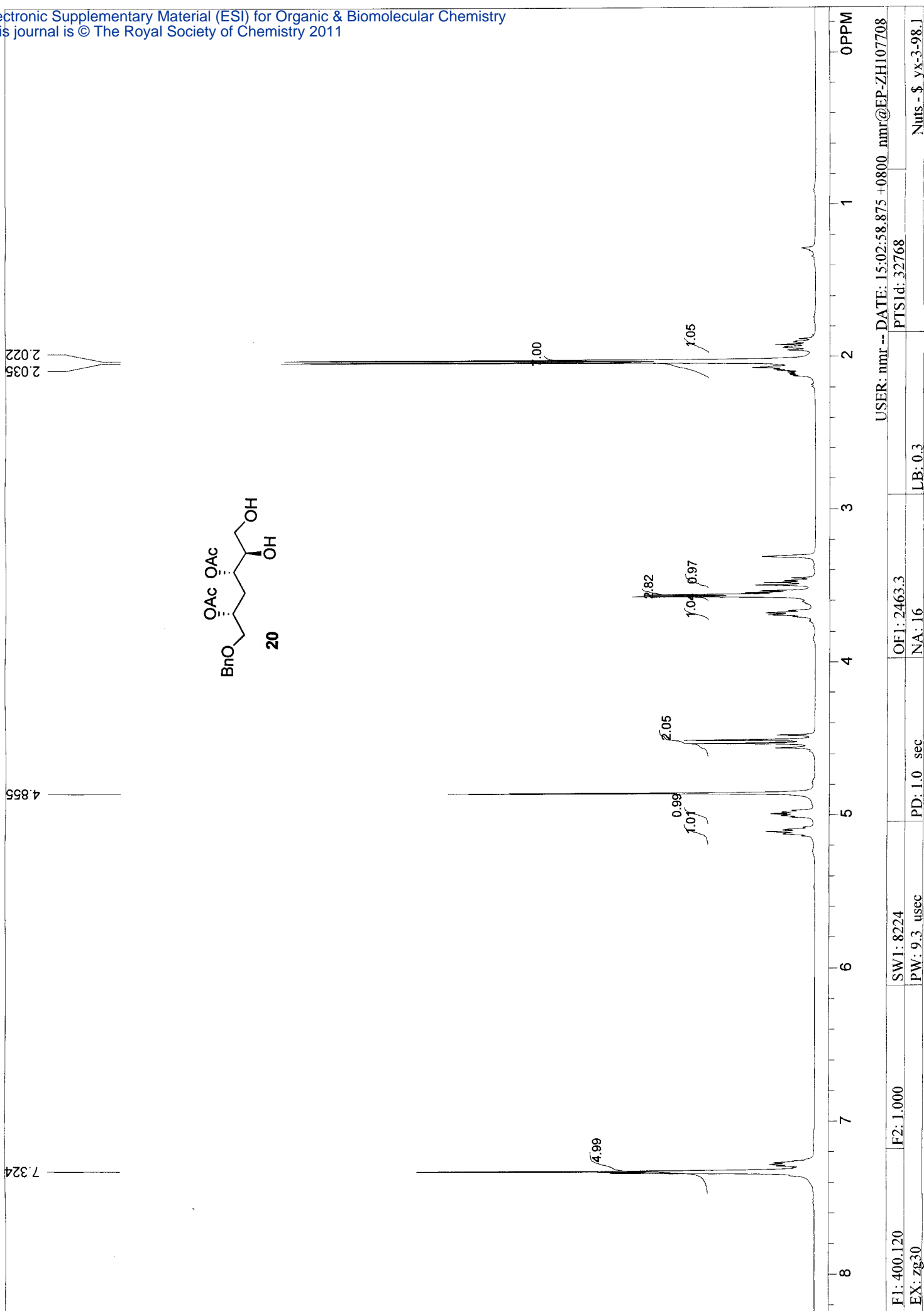


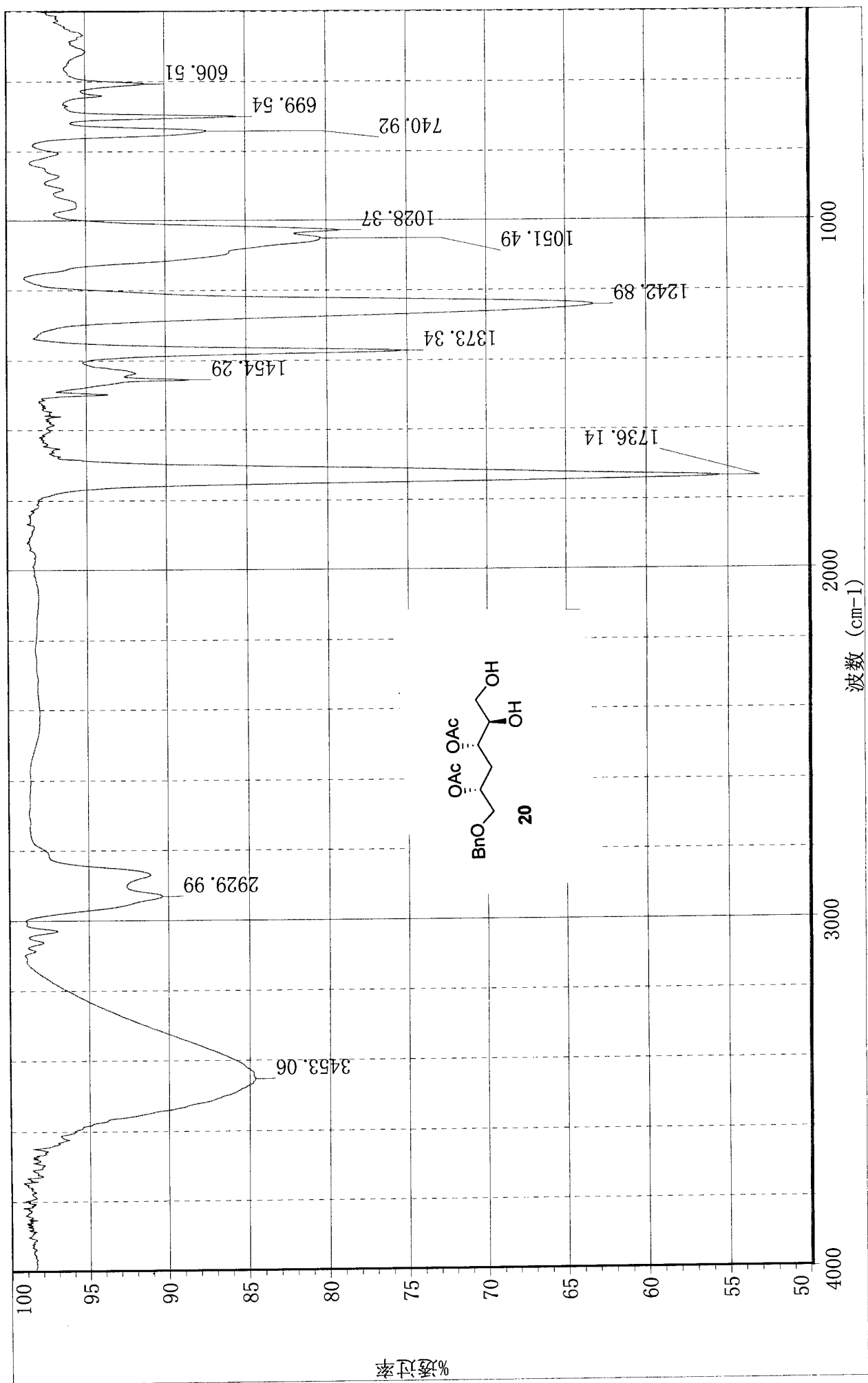
**yx-4-7

采集时间: 星期五 5月 13 16:02:27 2011 (GMT+08:00)



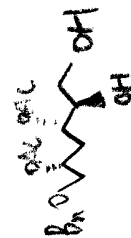




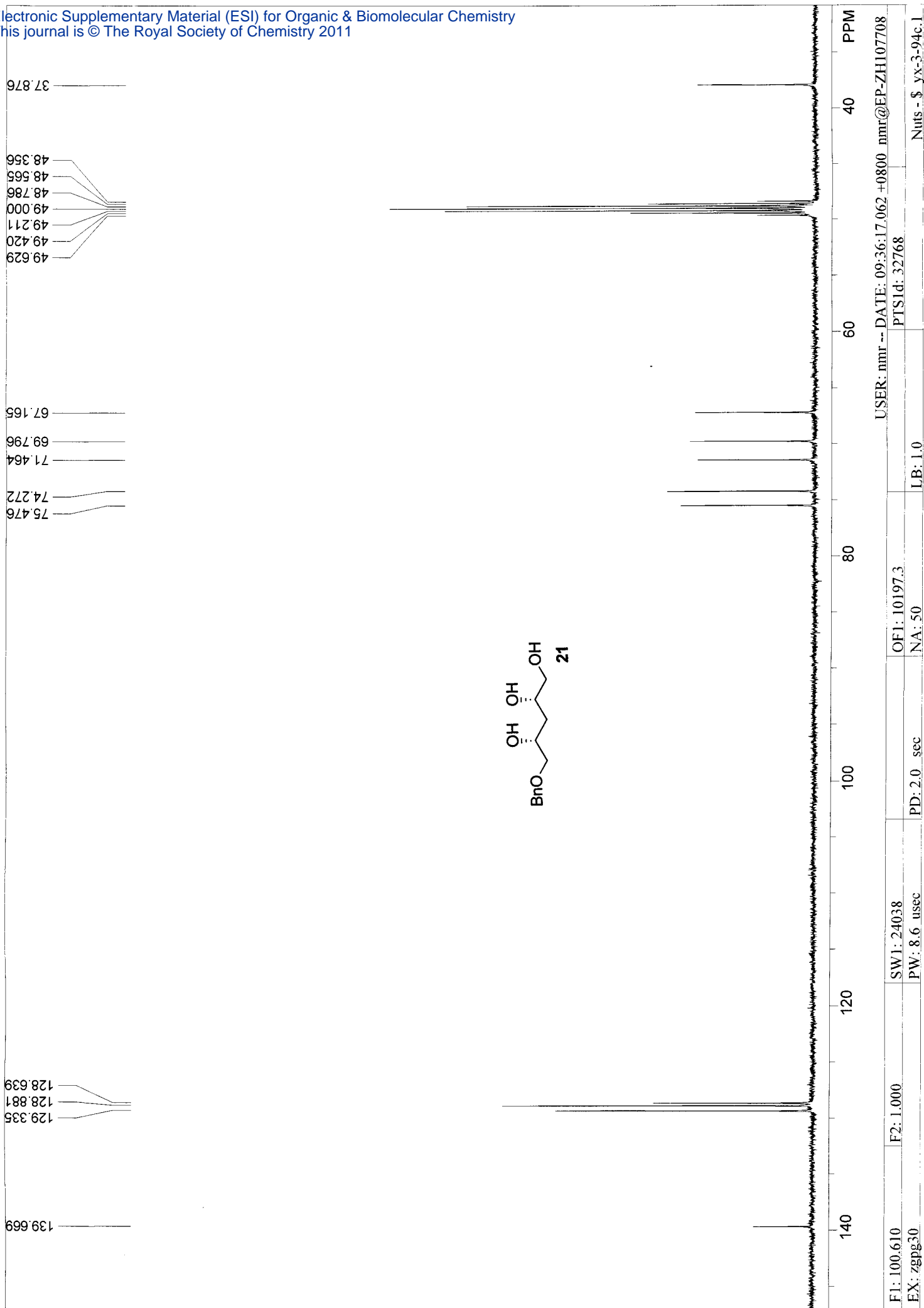


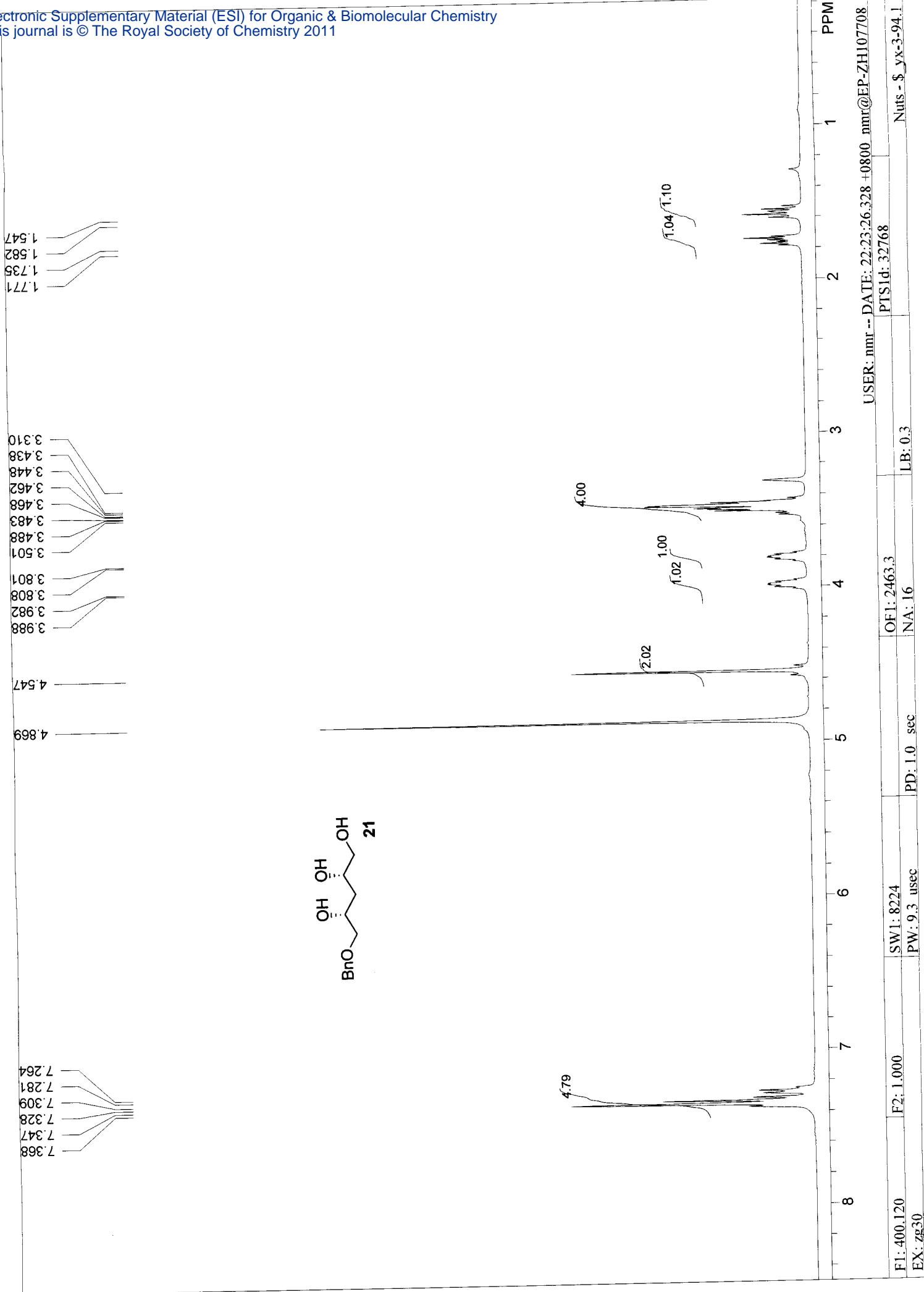
*yx-3-98

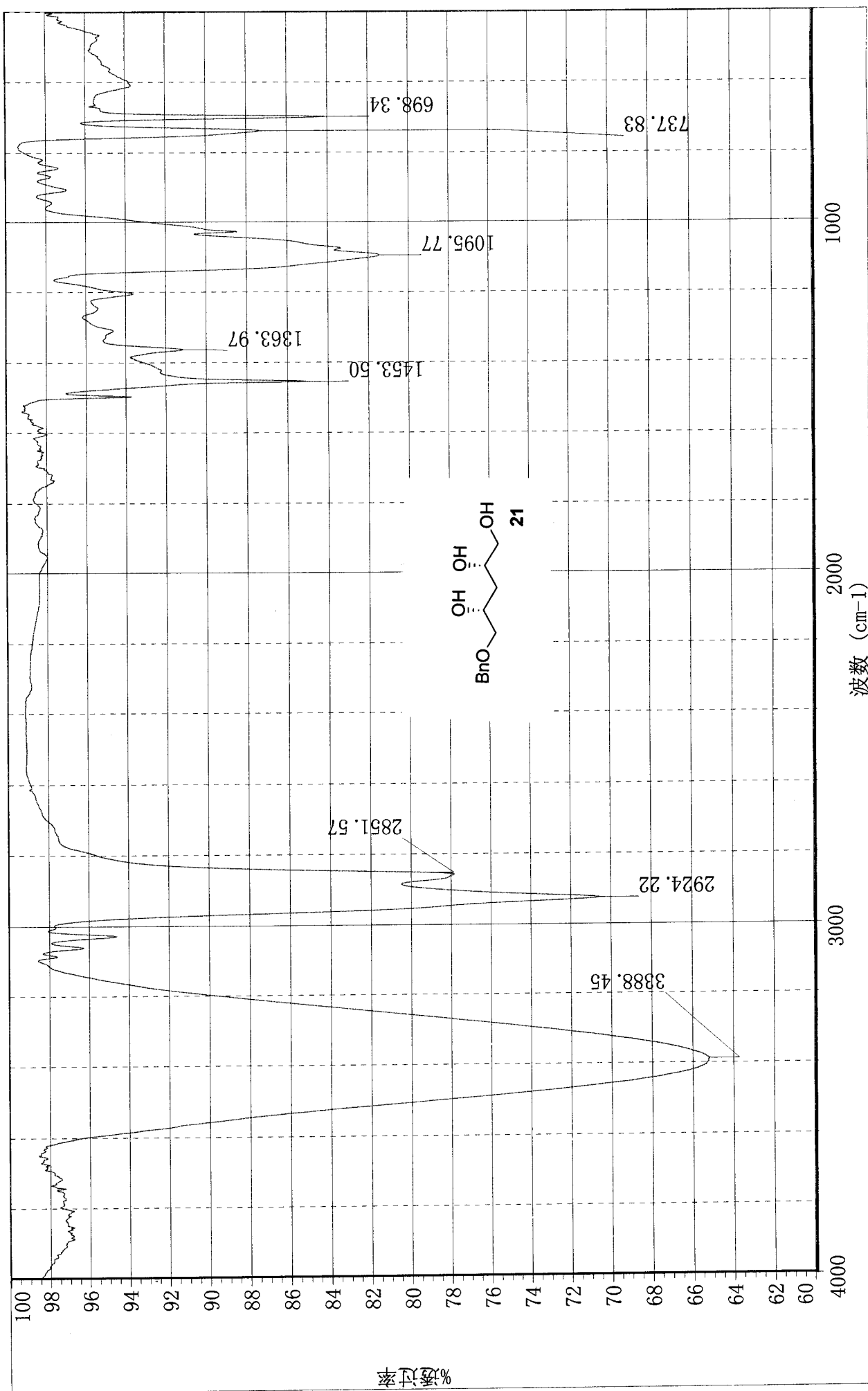
采集时间: 星期五 5月 13 16:11:38 2011 (GMT+08:00)



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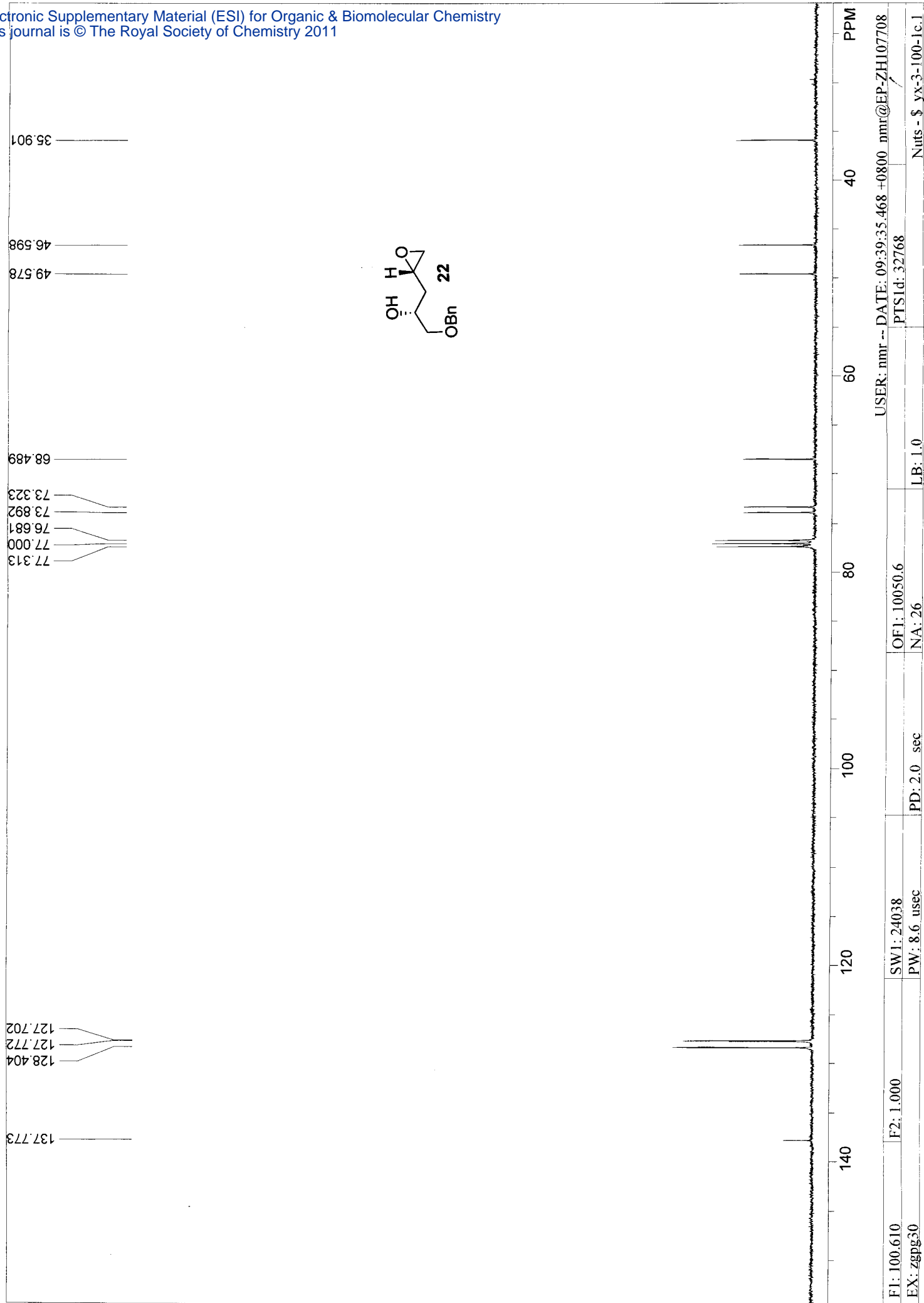




**星期五 5月 13 16:48:48 2011
采集时间: 星期五 5月 13 16:49:29 2011 (GMT+08:00)



上海有机所生命有机化学国家重点实验室

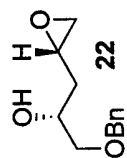


S 61

100 MHz, CDCl₃

4.561

7.338



4.85

1.89

0.94

1.95

0.90

0.98

0.86

0.91

1.11

1.00

7

6

5

4

3

2

1

0

PPM

F1: 400.120

F2: 1.000

SW1: 8224

PW: 9.3 usec

PD: 1.0 sec

OF1: 2461.2

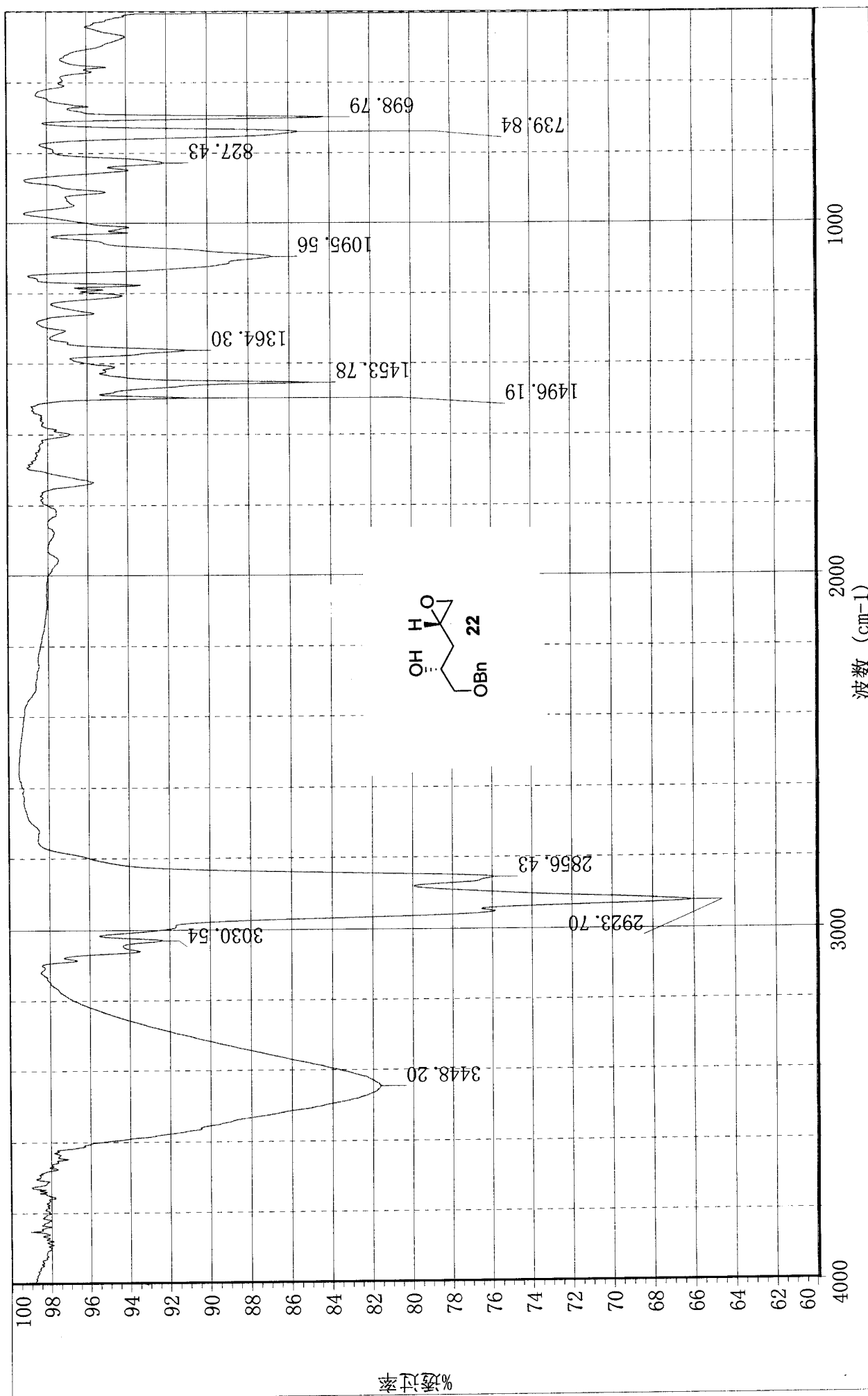
NA: 16

LB: 0.3

PTSID: 32768

USER: nmr -- DATE: 14:38:45.437 +0800 nmr@EP-ZH107708

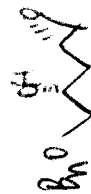
Nuts - \$ _yx-3-100-In.1



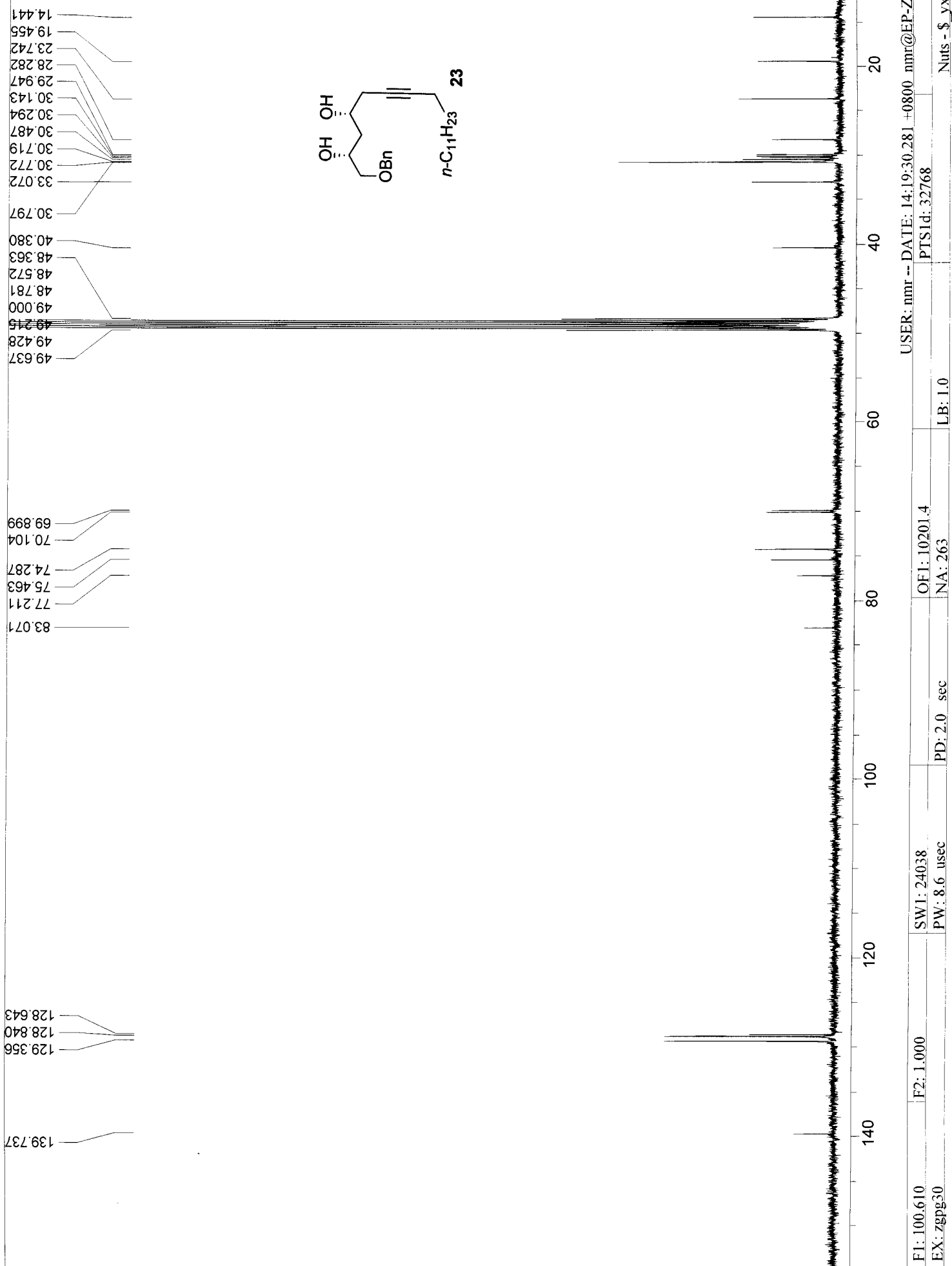
S 93

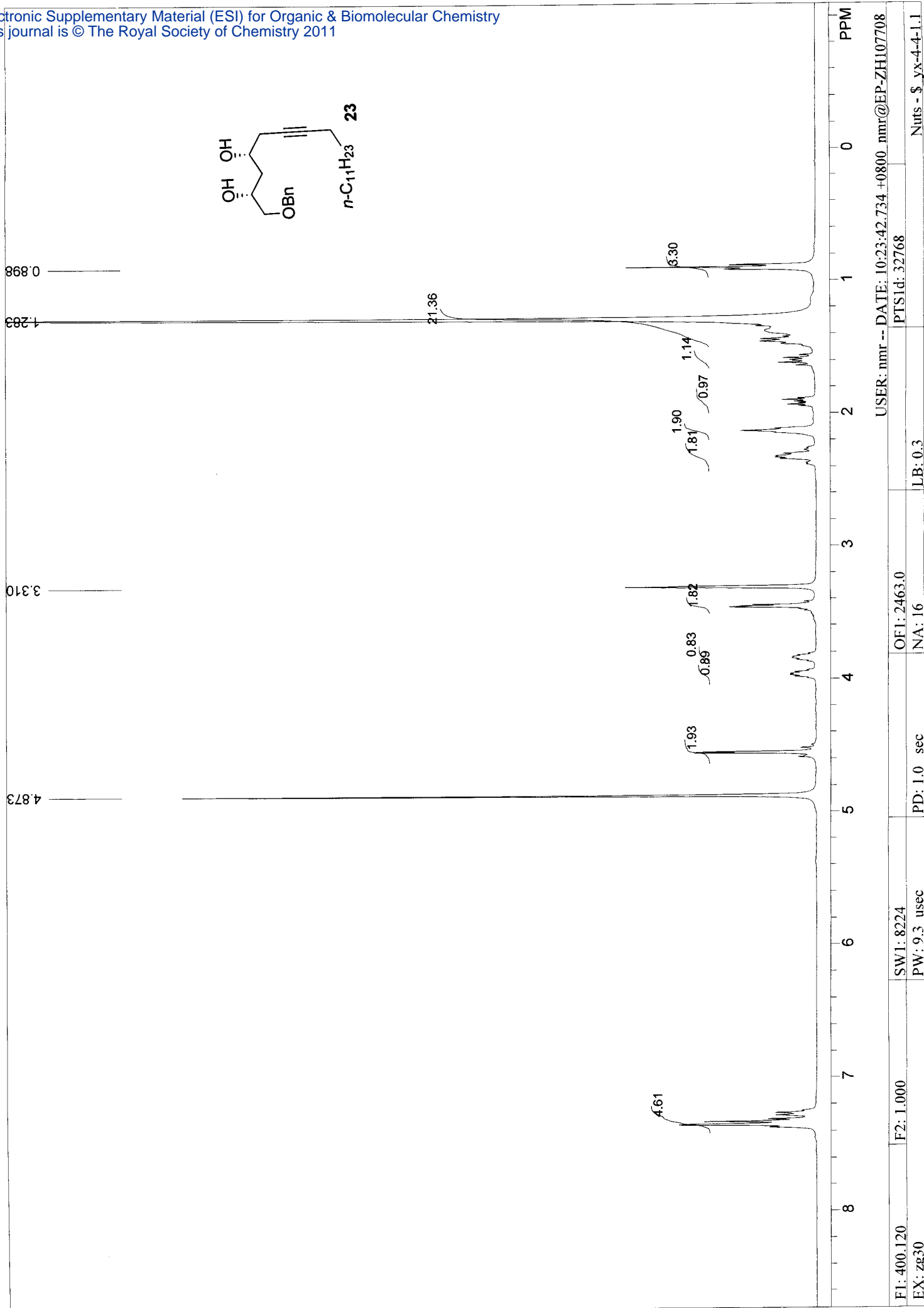
**星期五 5月 13 16:33:28 2011

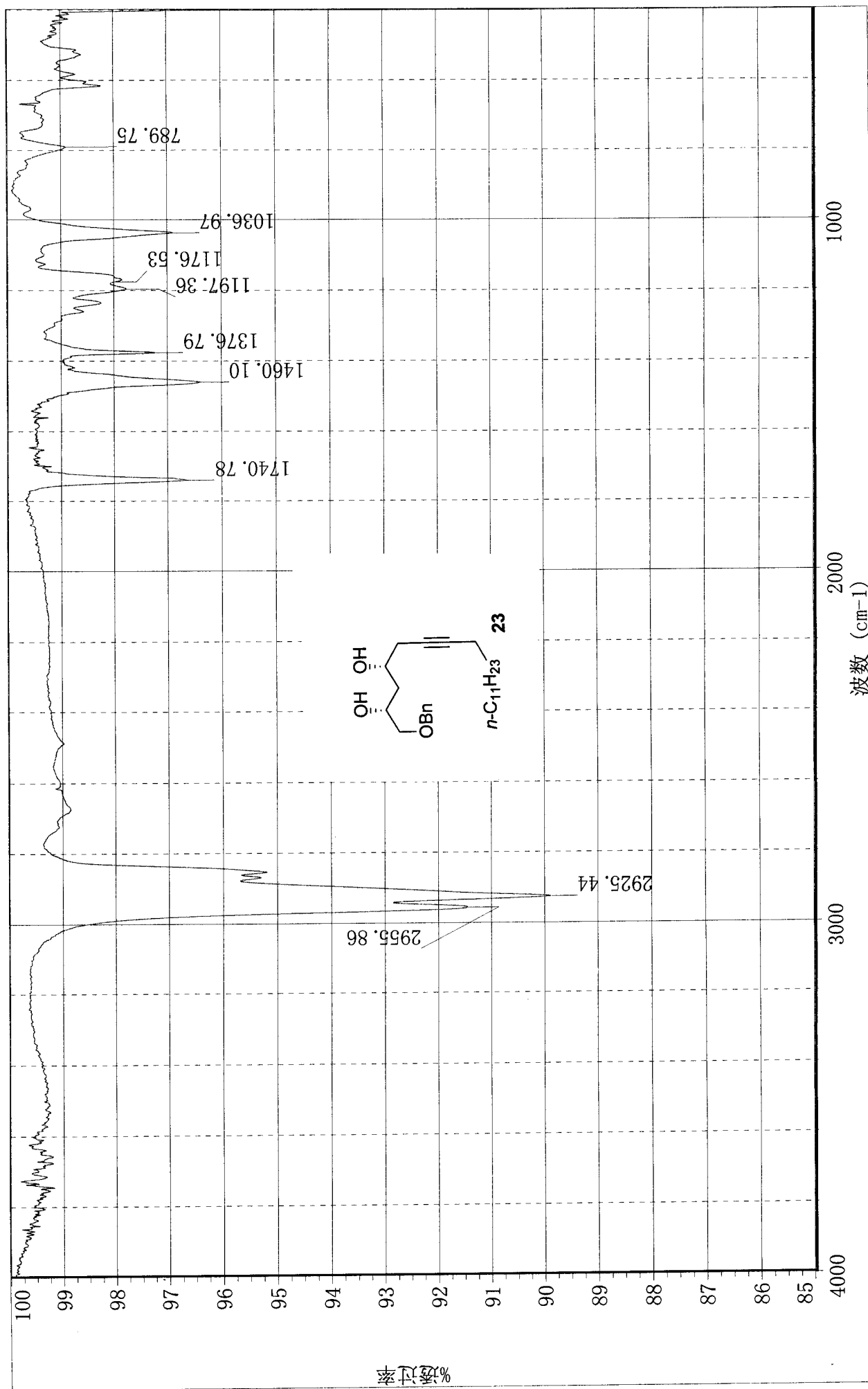
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上海有机所生命有机化学国家重点实验室





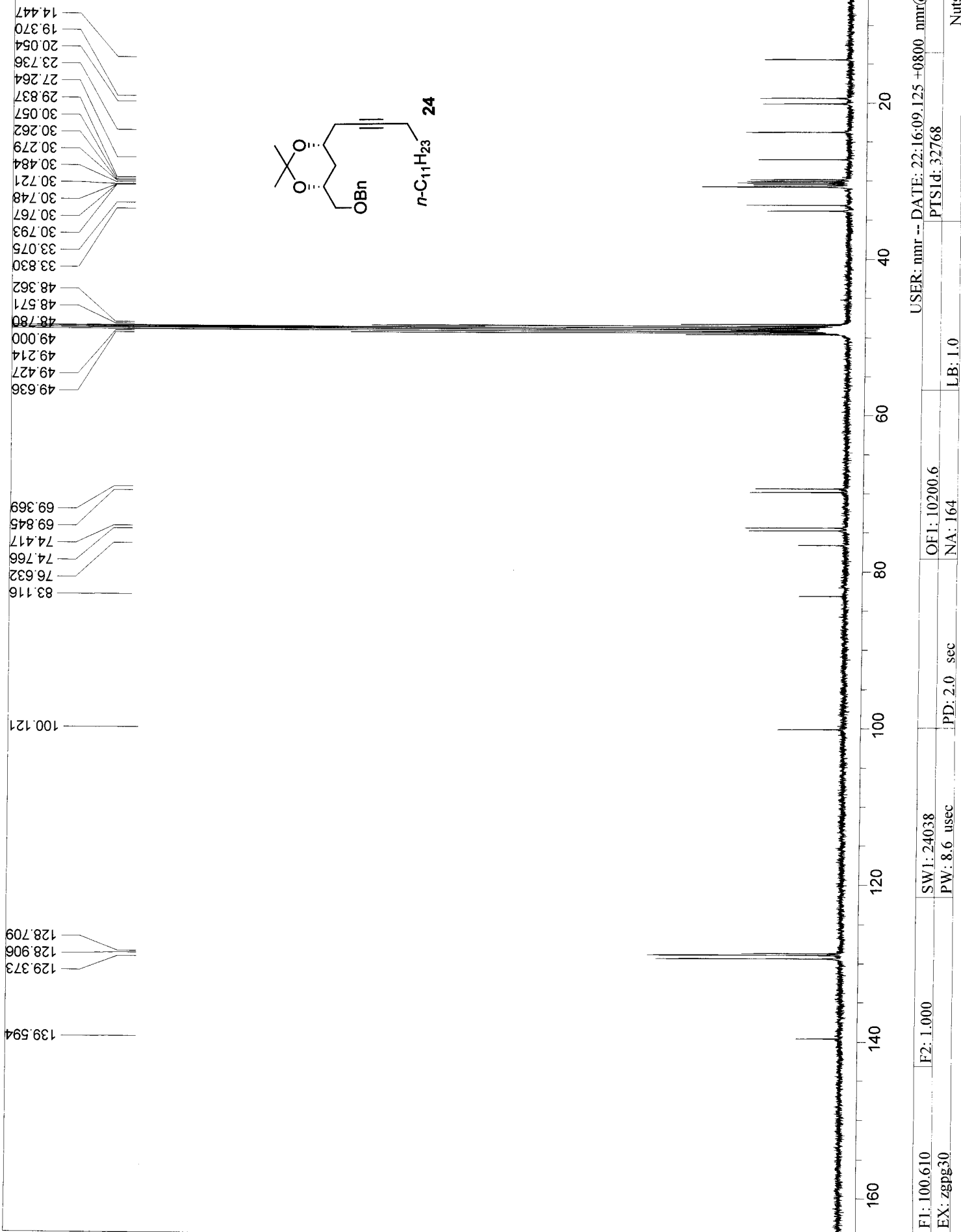


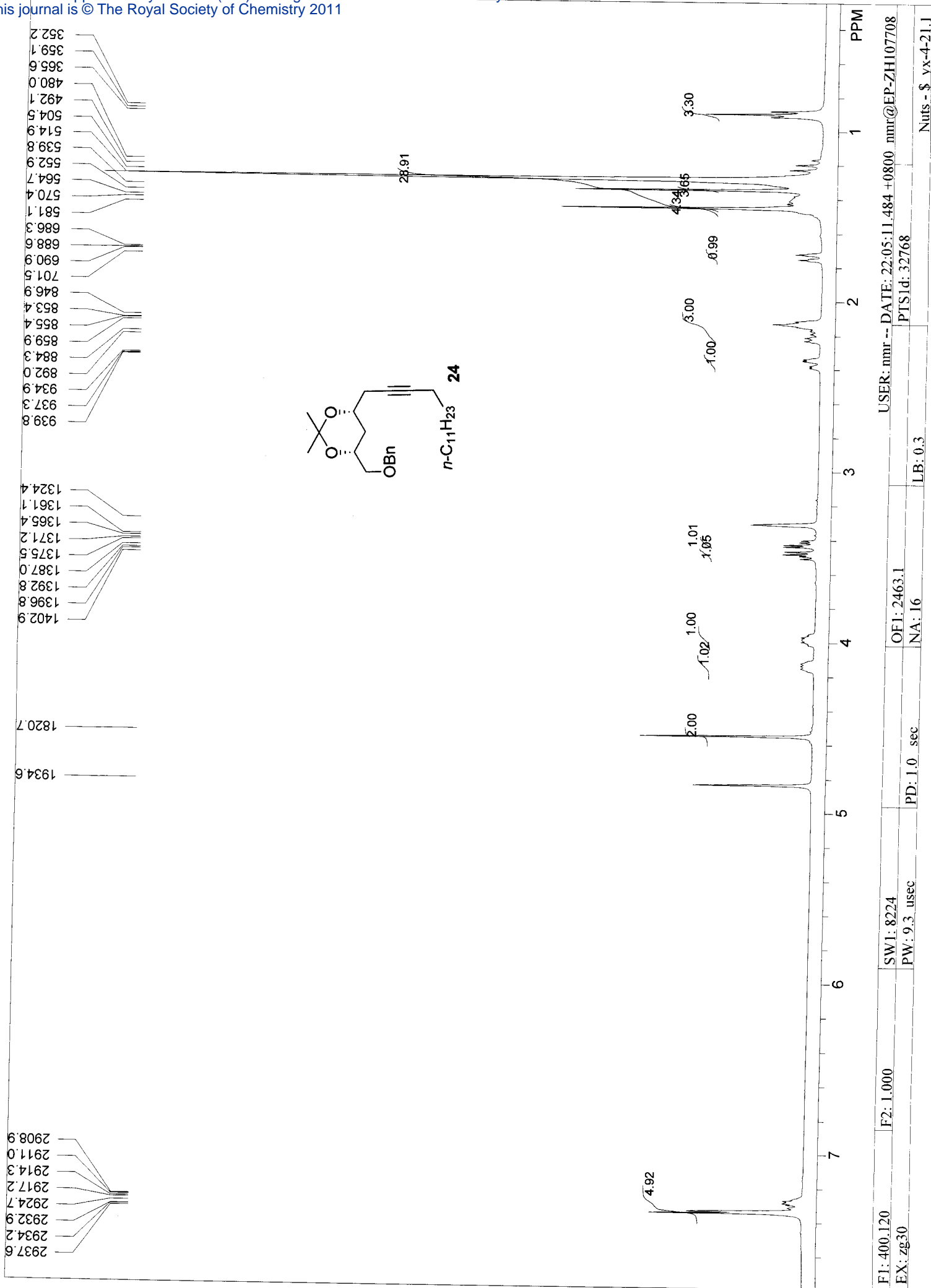
**星期五 5月 13 16:57:50 2011

采集时间: 星期五 5月 13 16:58:31 2011 (GMT+08:00)

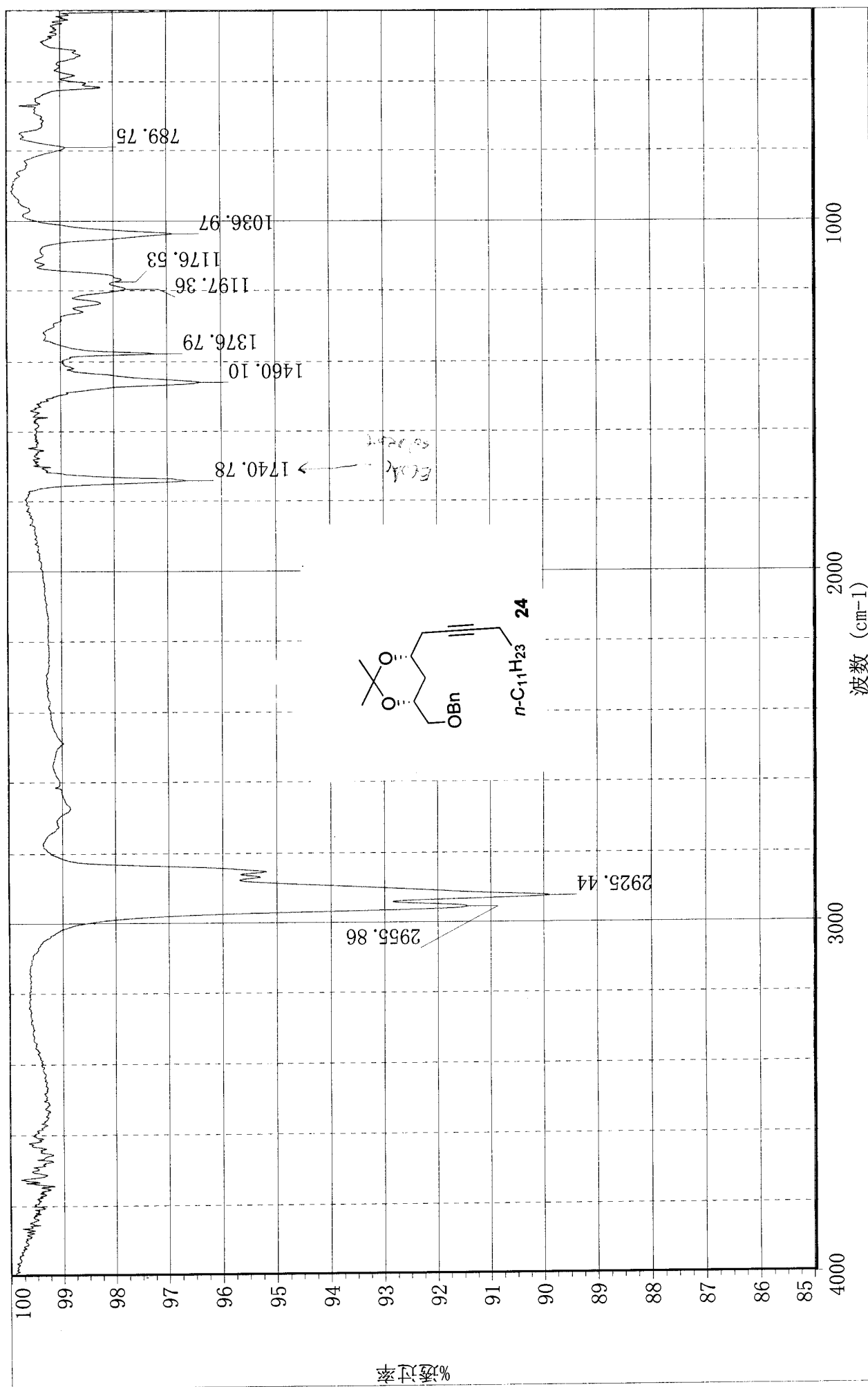


上海有机所生命有机化学国家重点实验室





F1: 400.120 F2: 1.000 SW1: 8224
 EX: zg30 PD: 1.0 sec OF1: 2463.1 NA: 16
 USER: mmr -- DATE: 22:05:11.484 +0800 nmr@EP-ZH107708
 PTS1d: 32768 LB: 0.3
 Nuts - \$ _yx-4-21.1



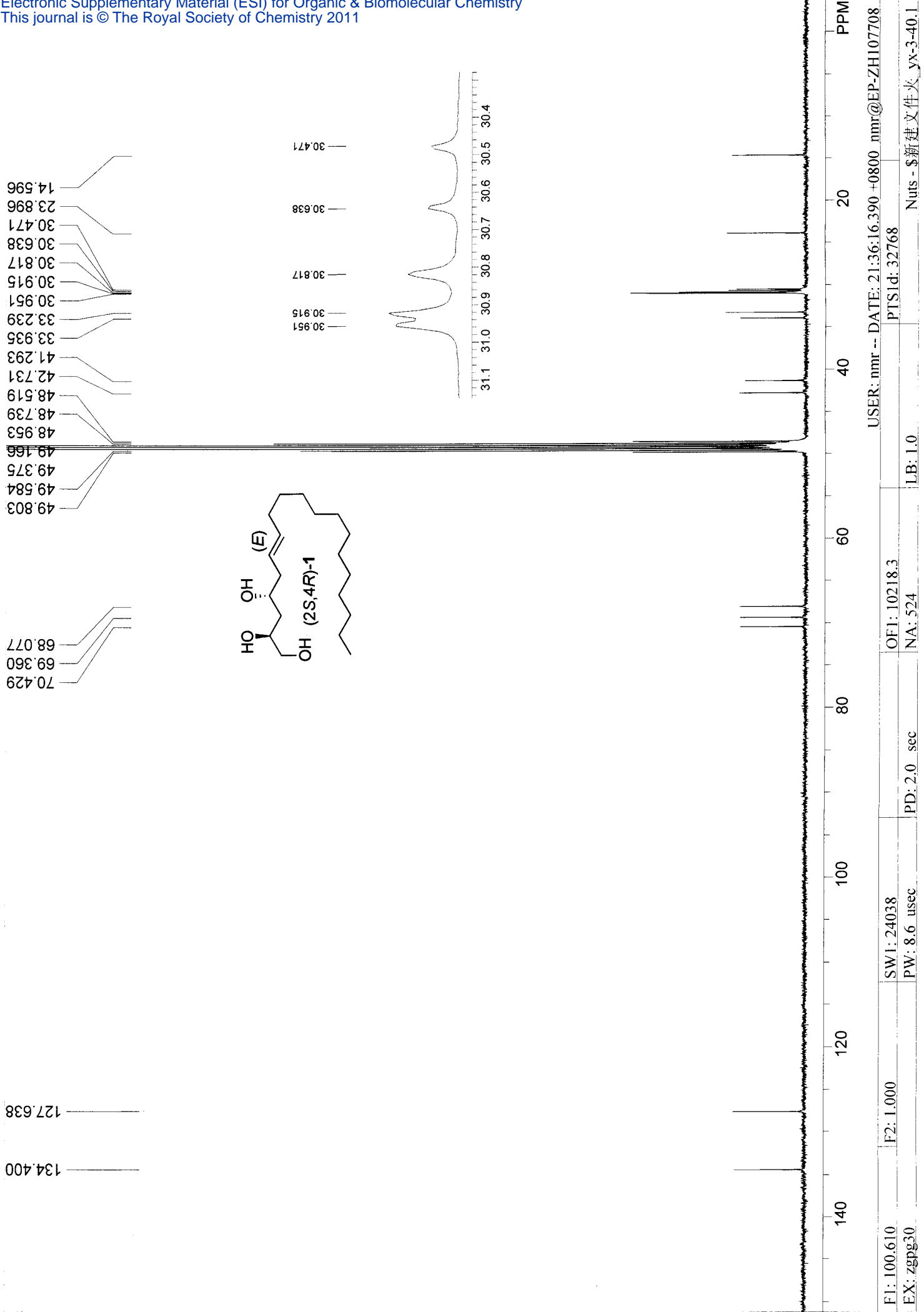
S 69

**星期五 5月 13 16:57:50 2011

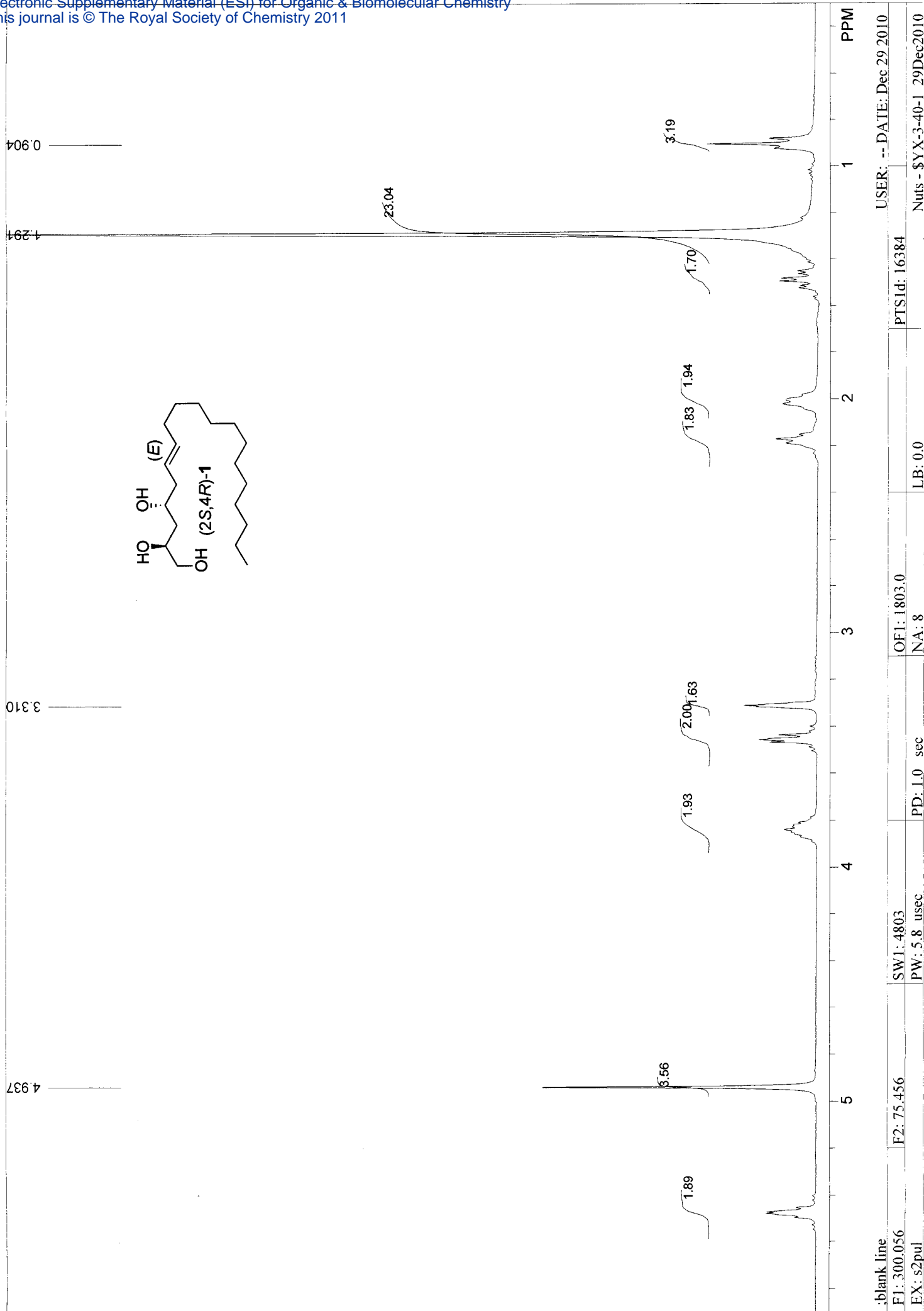
采集时间: 星期五 5月 13 16:58:31 2011 (GMT+08:00)

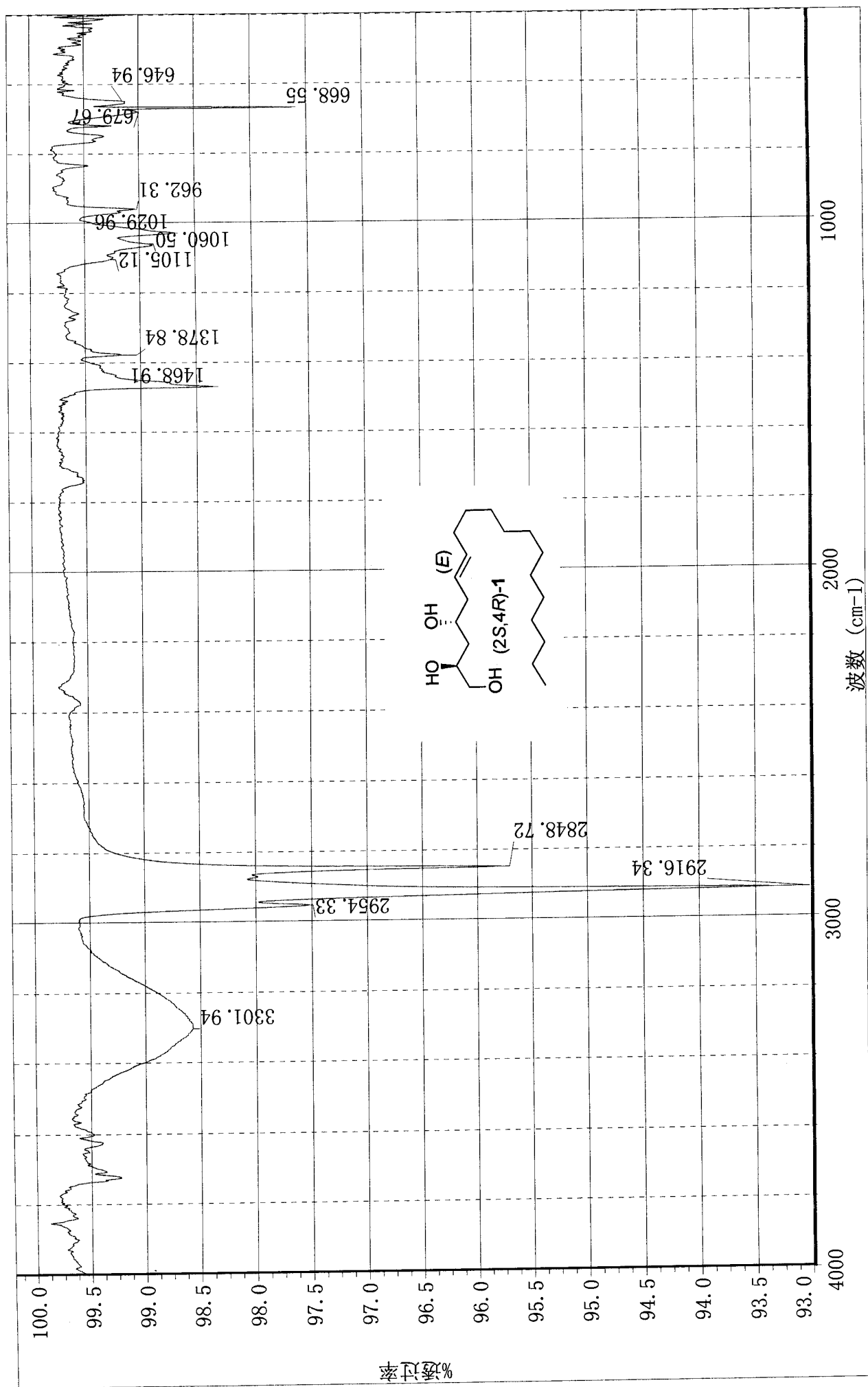


上海有机所生命有机化学国家重点实验室



F1: 100.610 F2: 1.000 SW1: 24038 OF1: 10218.3
 EX: zgpg30 PD: 2.0 sec NA: 524 LB: 1.0
 USER: nmr -- DATE: 21:36:16.390 +0800 nmr@EP-ZHI07708
 P1SId: 32768 Nuts - \$新建文件夹_yx-3-40.1





****yx-3-40

采集时间: 星期三 2月 16 09:53:30 2011 (GMT+08:00)

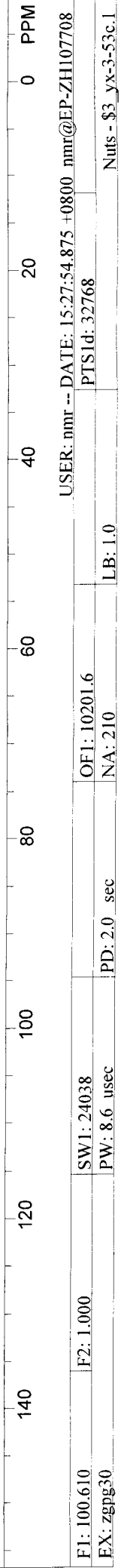
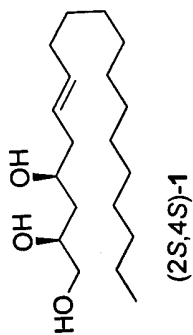


上海有机所生命有机化学国家重点实验室

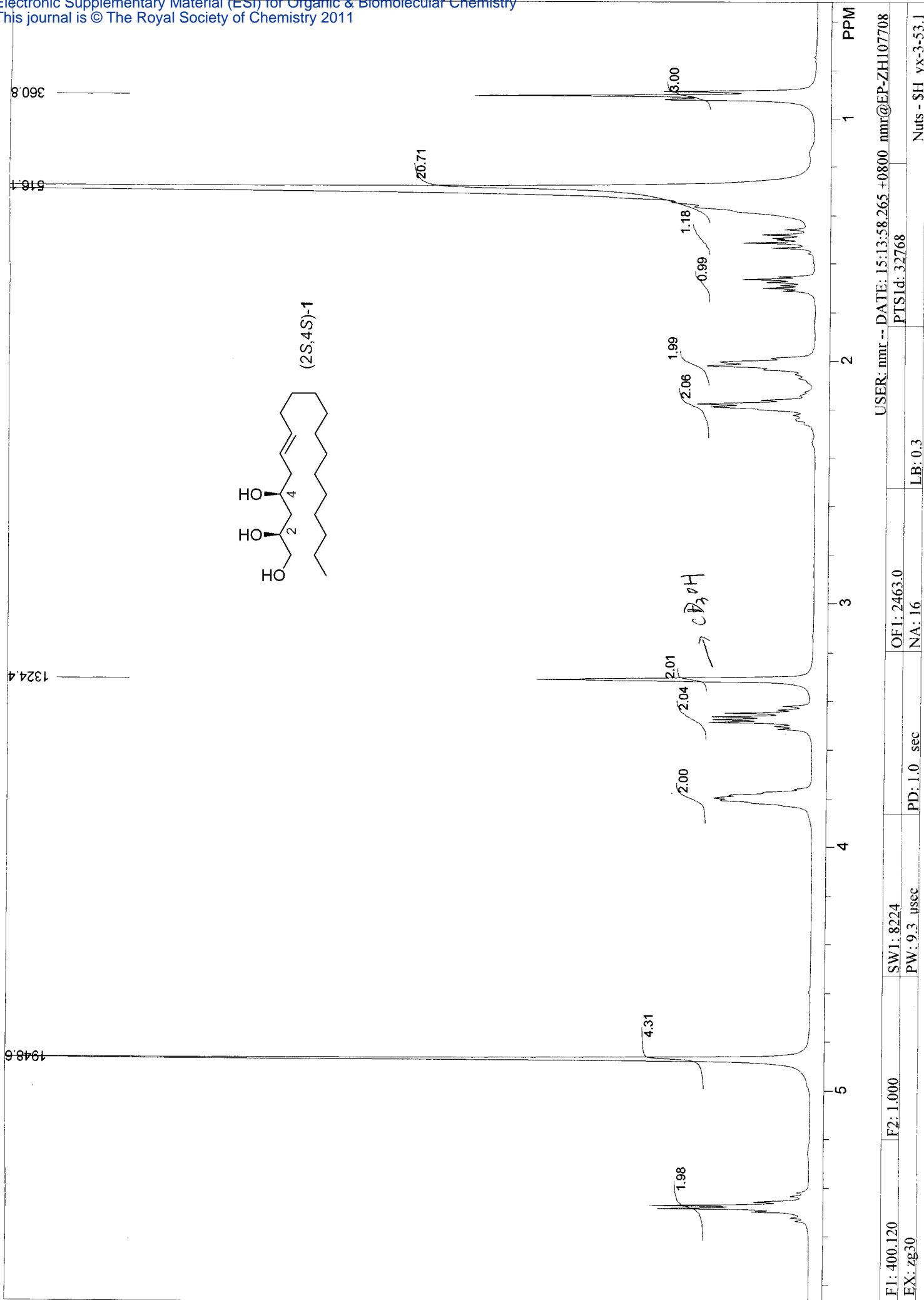
14.428
23.733
30.290
30.472
30.638
30.759
30.790
33.074
33.755
40.459
41.841
48.353
48.571
48.786
49.000
49.209
49.418
49.635

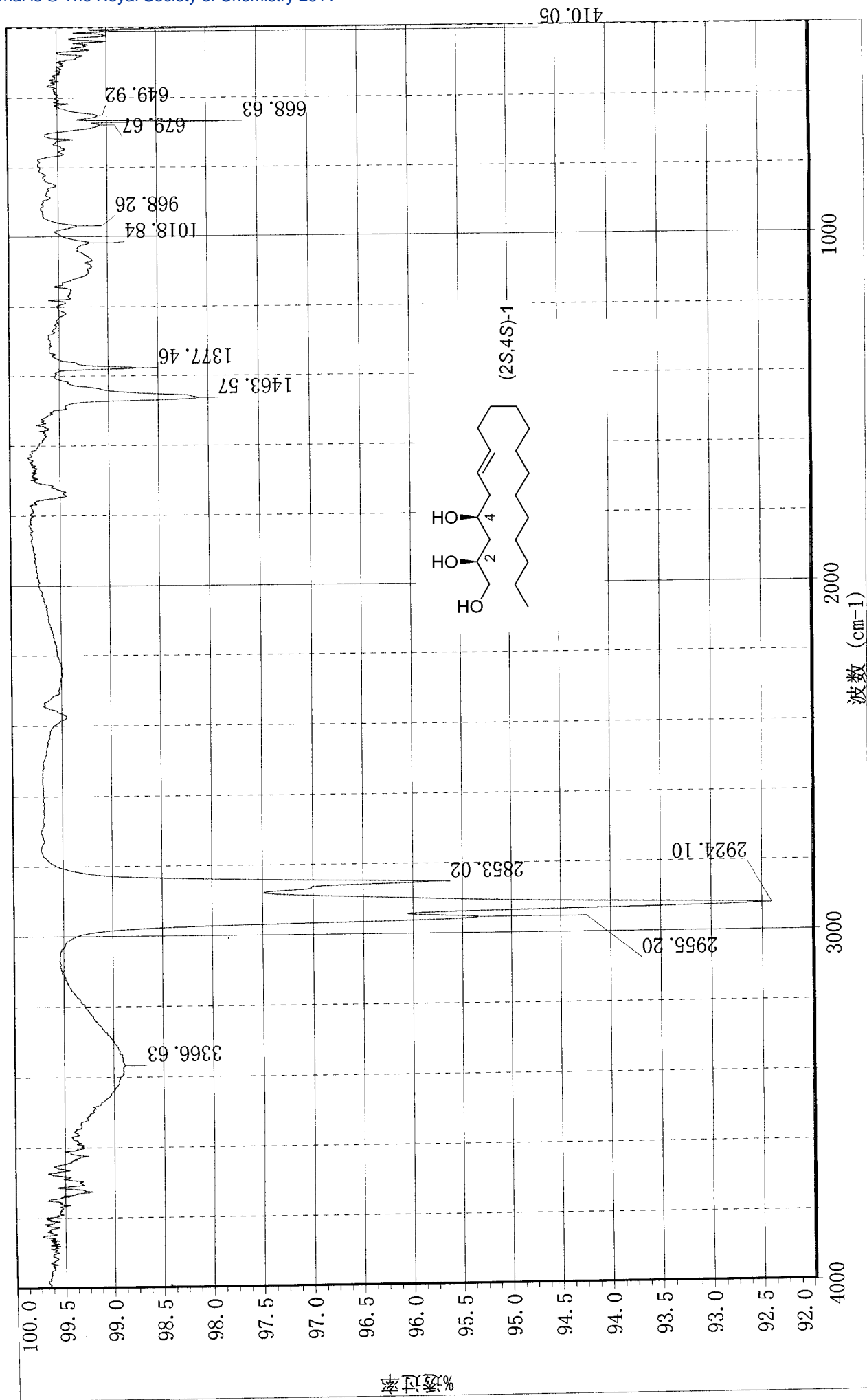
67.240
71.200
72.090

127.211
134.404



F1: 100.610 F2: 1.000 SW1: 24038
EX: zgpg30 PD: 2.0 sec NA: 210 OF1: 10201.6 LB: 1.0
USER: nmr -- DATE: 15:27:54.875 +0800 nmr@EP-ZH1107708
PTSID: 32768 Nuts - \$3_yx-3-53c.1





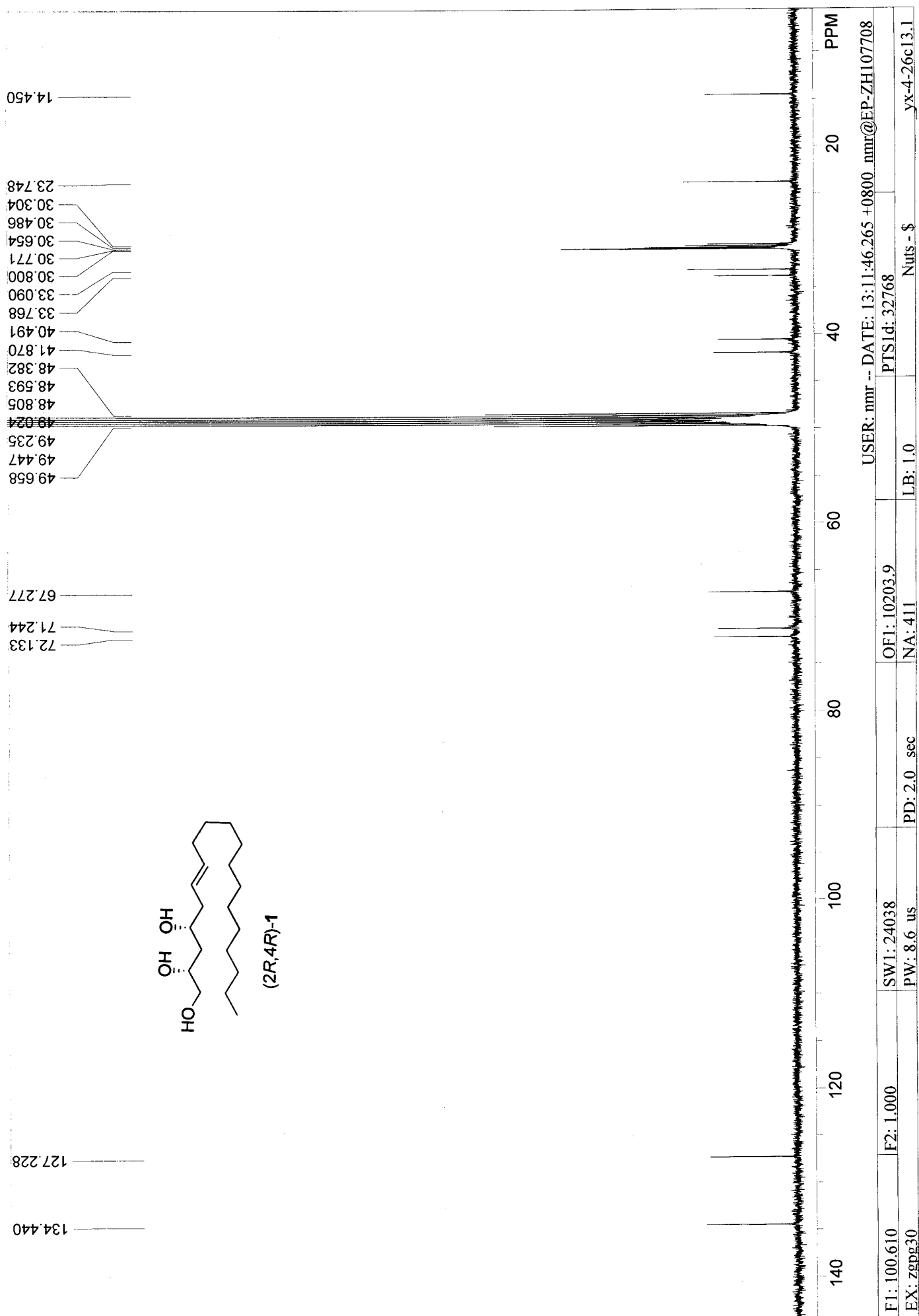
S 75

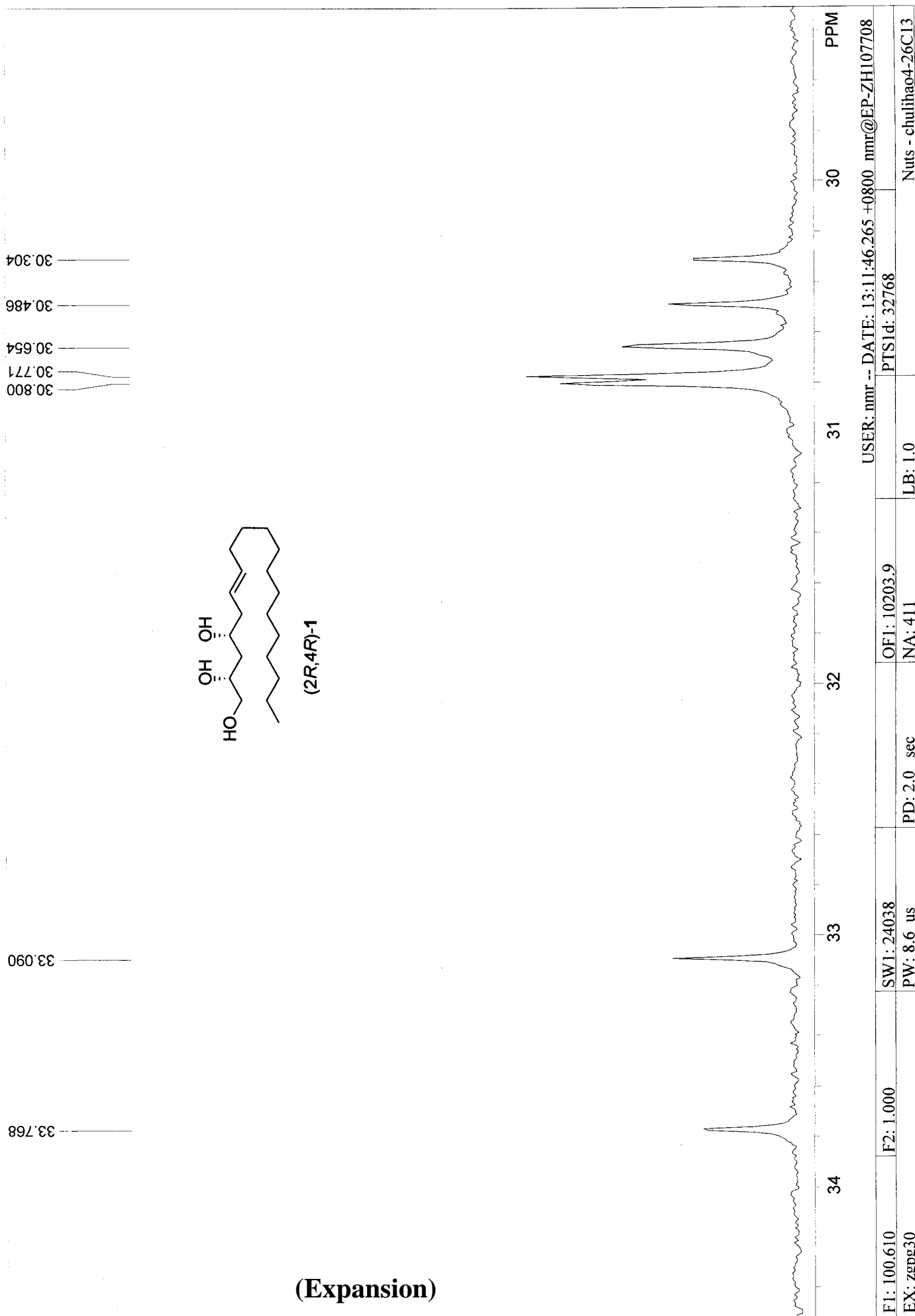
*yx-3-53

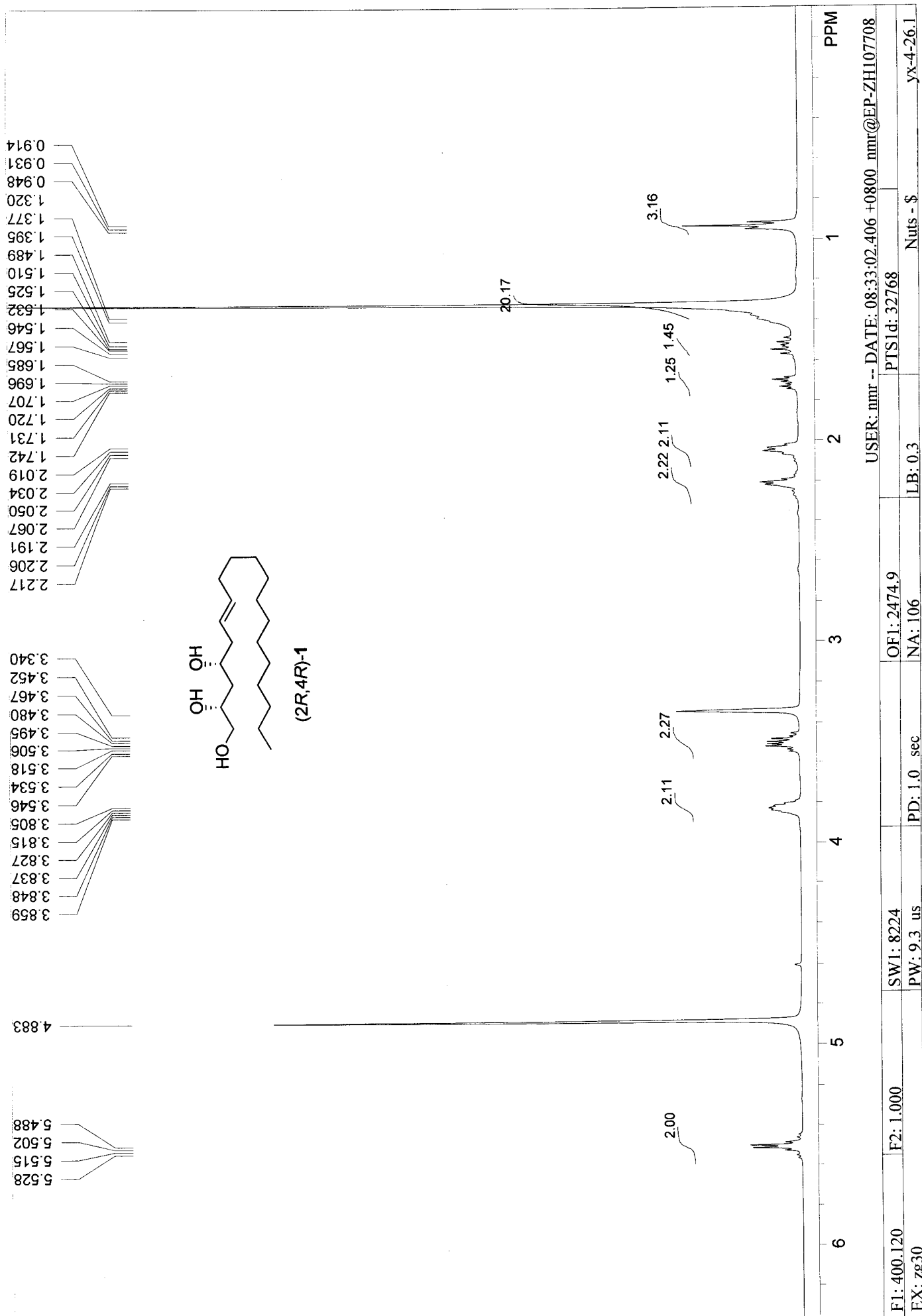
采集时间: 星期三 2月 16 10:11:36 2011 (GMT+08:00)

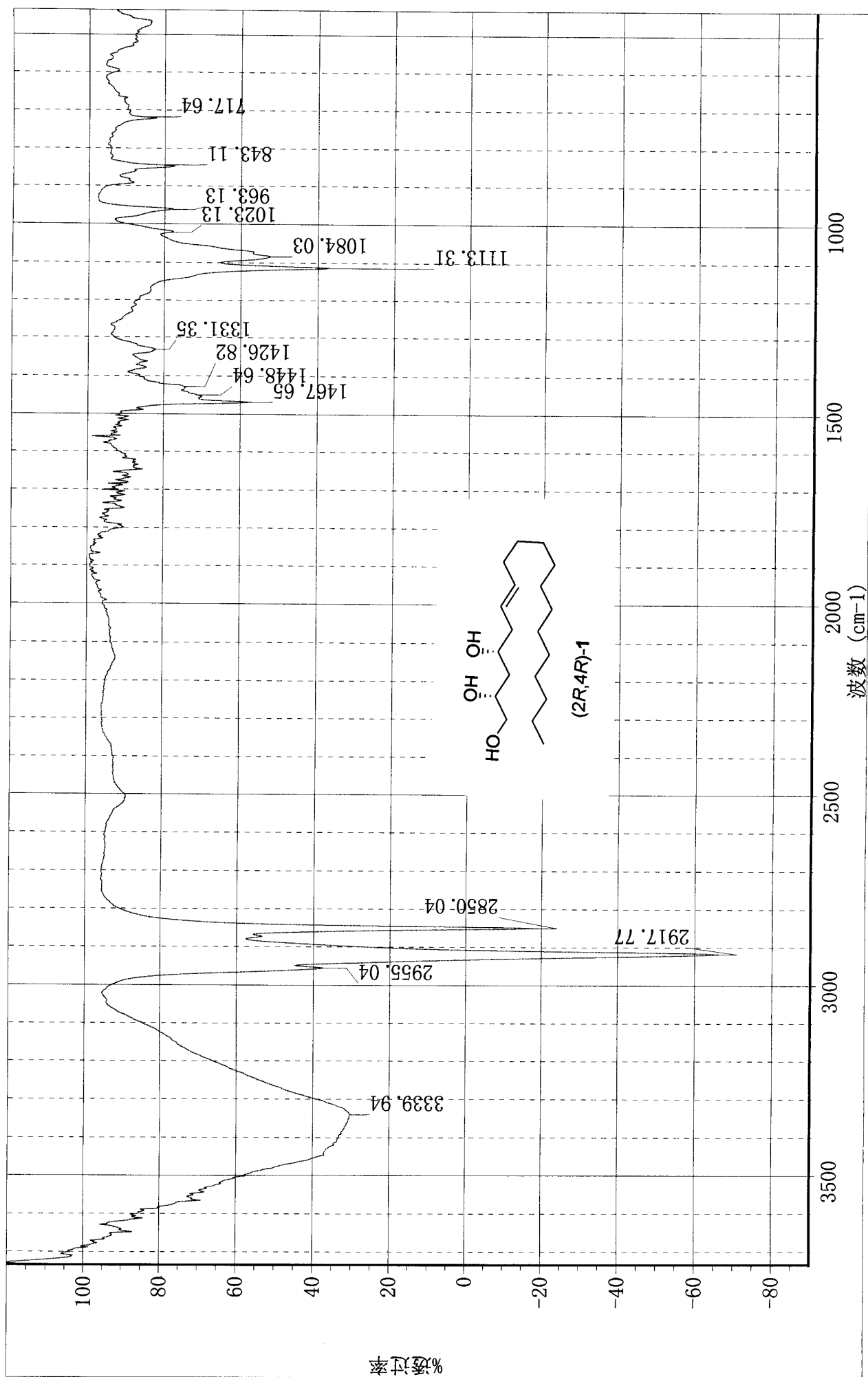


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yx-4-26KBr

采集时间: 星期二 5月 31 21:56:37 2011 (GMT+08:00)

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Tabular data comparison between the natural **-1** and synthetic (2*R*,4*R*)-**1**

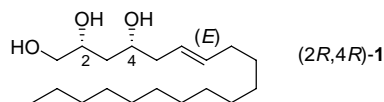


Table S-1. ¹H NMR data comparison

Natural 1 (CD ₃ OD, 500 MHz) ^a	(2 <i>R</i> ,4 <i>R</i>)- 1 (400 MHz, CD ₃ OD)
5.50 (dt, <i>J</i> = 15, 6 Hz, 1H, H-7)	5.52 (dt, <i>J</i> = 15.4, 6.8 Hz, 1H)
5.45 (dt, <i>J</i> = 15, 6 Hz, 1H, H-6)	5.49 (dt, <i>J</i> = 15.3, 6.0 Hz, 1H)
3.80 (m, 1H, H-2)	3.86-3.81 (m, 2H)
3.78 (m, 1H, H-4)	
3.49 (dd, <i>J</i> = 11, 5 Hz, 1H, H-1b)	3.55-3.45 (m, 2H)
3.44 (dd, <i>J</i> = 11, 6Hz, 1H, H-1a)	
2.17 (m, 2H, H-5)	2.22-2.19 (m, 2H)
2.01 (m, 2H, H-8)	2.07-2.02 (m, 2H)
1.68 (dt, <i>J</i> = 14, 4 Hz, 1H, H-3b)	1.71 (dt, <i>J</i> = 14.0, 4.4 Hz, 1H)
1.50 (dt, <i>J</i> = 14, 8 Hz, 1H, H-3a)	1.53 (dt, <i>J</i> = 14.3, 6.5 Hz, 1H)
(not given)	1.38-1.30 (m, 20H)
0.9 (t, <i>J</i> = 7 Hz, 3H, H-19)	0.93 (t, <i>J</i> = 6.8 Hz, 3H)

^aTaken from: F. Abe, S. Nagafuji, M. Okawa, J. Kinjo, H. Akahane, T. Ogura, M. A. Martinez-Alfaro and R. Reys-Chilpa, *Biol. Parm. Bull.*, 2005, **28**, 1314. ^bThis work.

Table S-2. ¹³C NMR data comparison

Natural -1 (CD ₃ OD, 500 MHz) ^a	(2 <i>R</i> ,4 <i>R</i>)- 1 (400 MHz, CD ₃ OD) ^b
134.4 (C-6)	134.4
127.2 (C-7)	127.2
72.2 (C-2)	72.1
71.3 (C-4)	71.2
67.3 (C-1)	67.3
41.9 (C-5)	41.9
40.5 (C-3)	40.5
33.7 (C-8)	33.8
33.0 (C-17)	33.1
30.3~30.8 (C-9 to C-16)	30.80, 30.77, 30.6, 30.5, 30.3
23.3 (C-18)	23.7
14.4 (C-19)	14.4

^aTaken from: F. Abe, S. Nagafuji, M. Okawa, J. Kinjo, H. Akahane, T. Ogura, M. A. Martinez-Alfaro and R. Reys-Chilpa, *Biol. Parm. Bull.*, 2005, **28**, 1314. ^bThis work.