

Supporting Information

Identification and Characterization of Small Molecules as Potent and Specific EPAC2 Antagonists

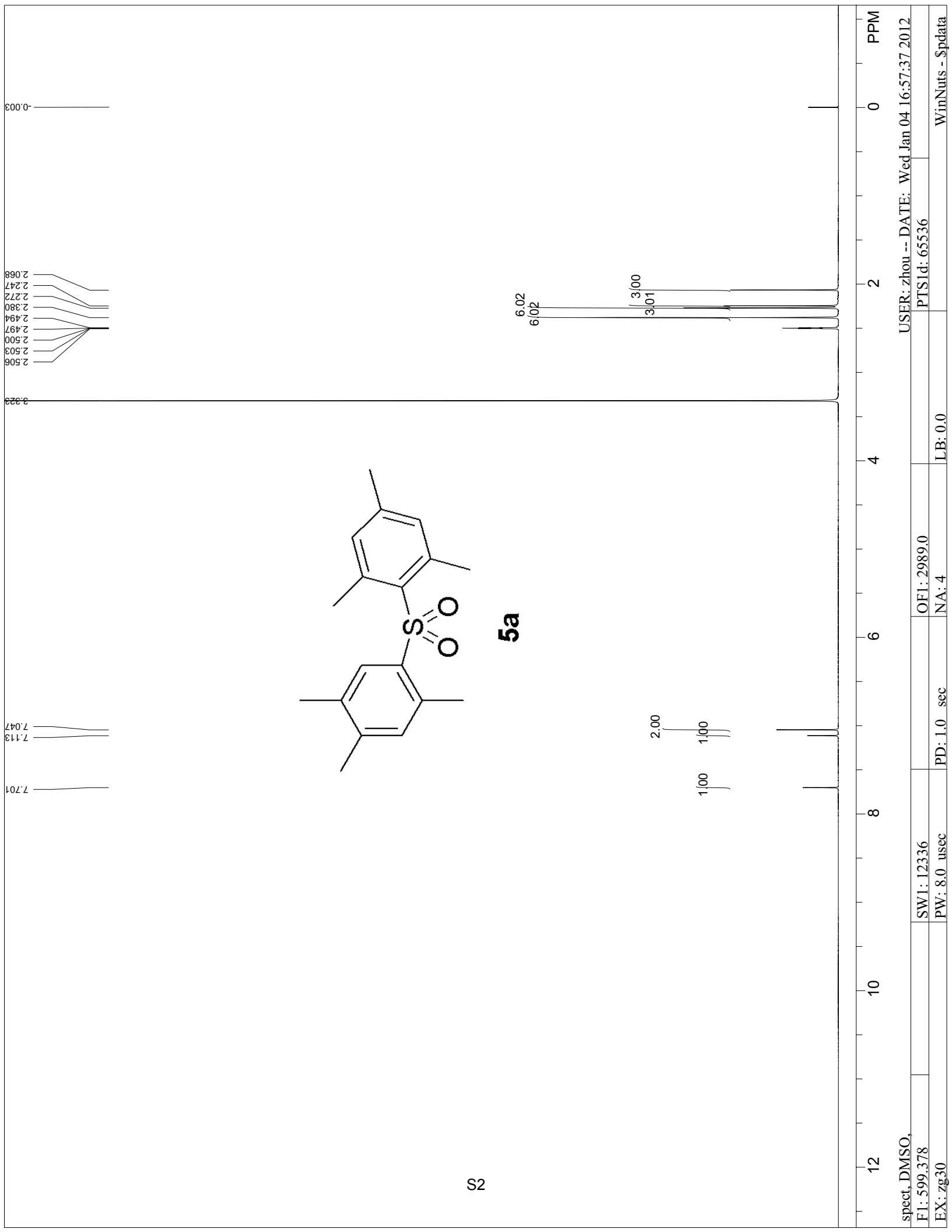
Haijun Chen,[†] Tamara Tsalkova,^{†,‡} Oleg G. Chepurny,[§] Fang C. Mei,^{†,‡} George G. Holz,^{§,ξ}
Xiaodong Cheng,^{†,‡,*} and Jia Zhou^{†,*}

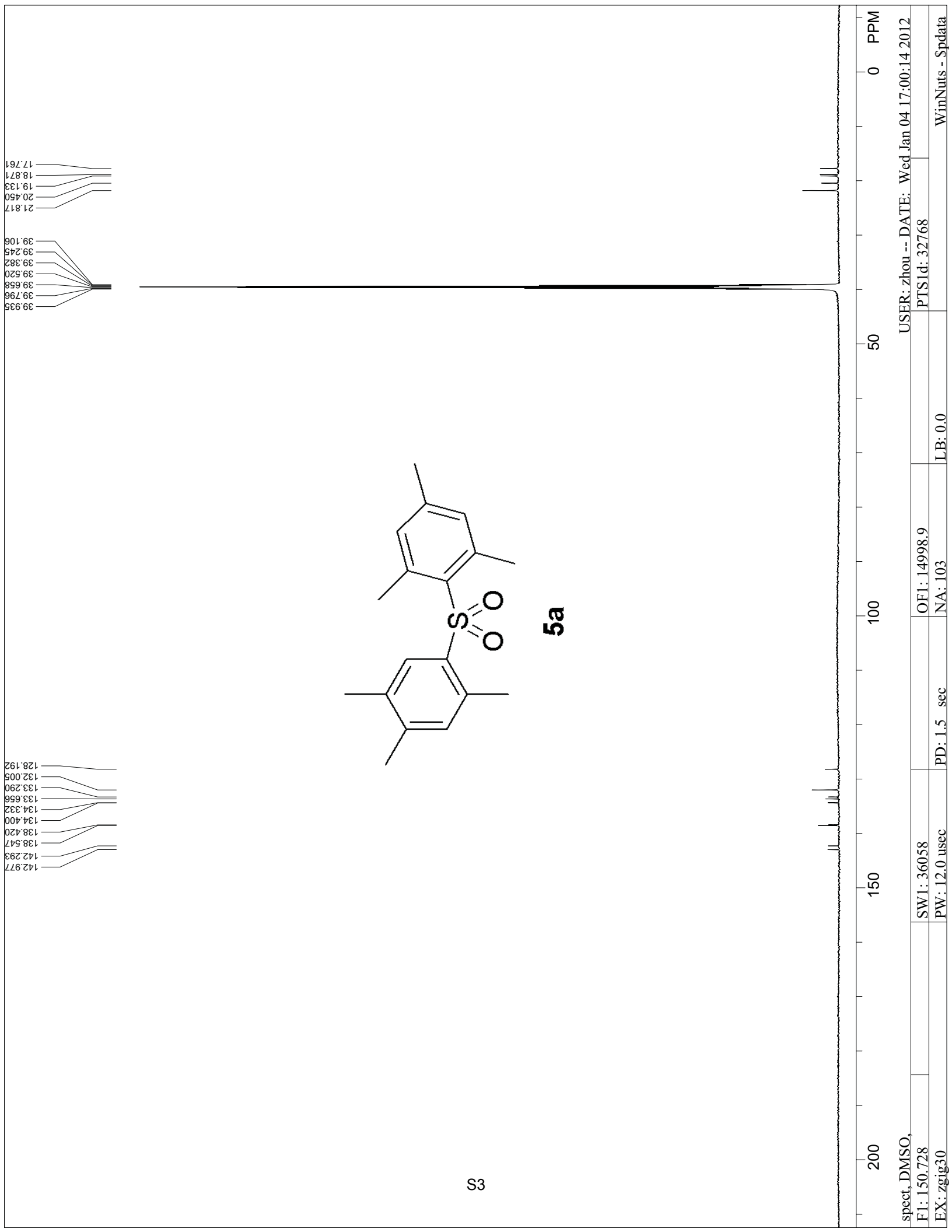
[†]Department of Pharmacology and Toxicology, [‡]Sealy Center for Structural Biology and Molecular
Biophysics, University of Texas Medical Branch, Galveston, Texas 77555, United States

[§]Departments of Medicine and ^ξPharmacology, State University of New York (SUNY), Upstate Medical
University, Syracuse, NY 13210, United States

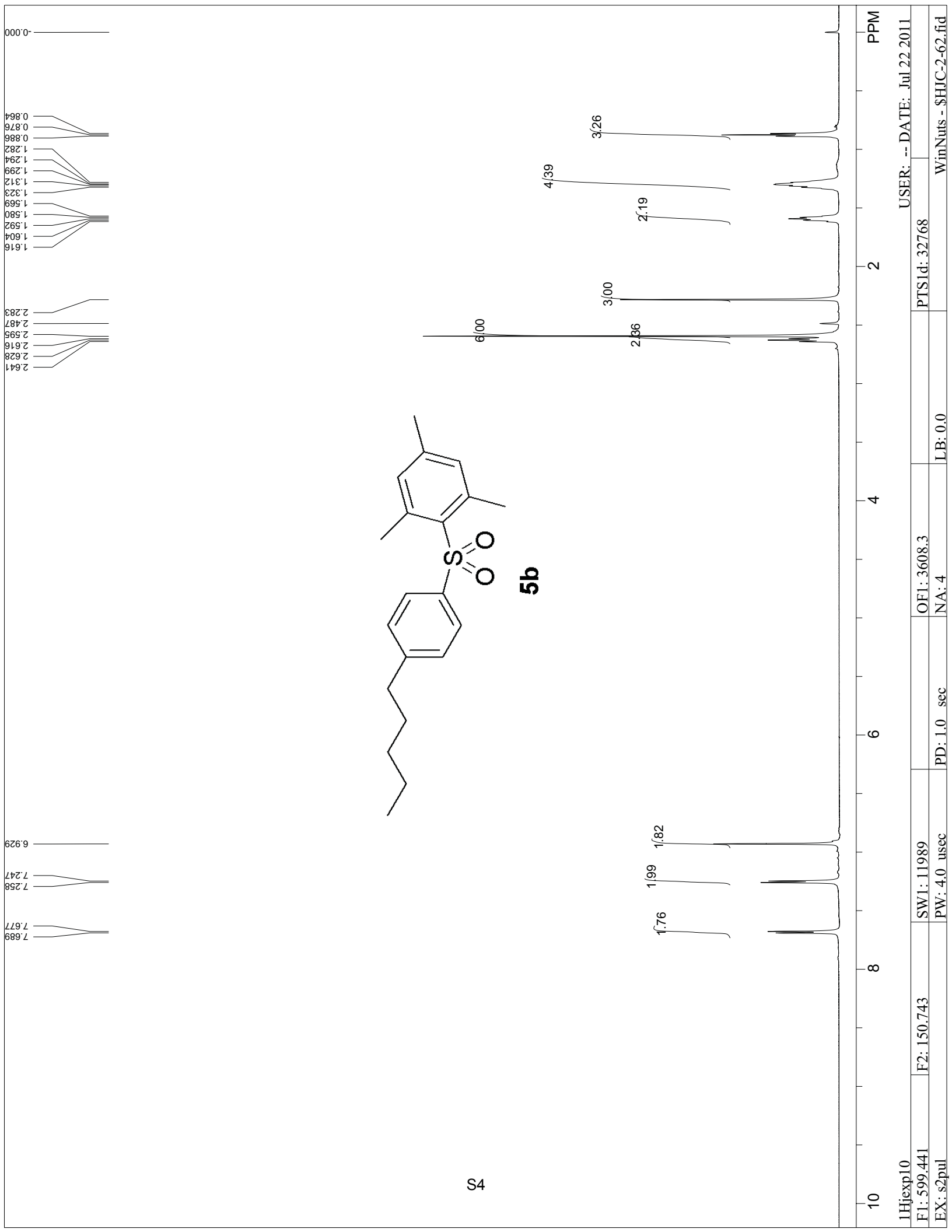
Table of Contents

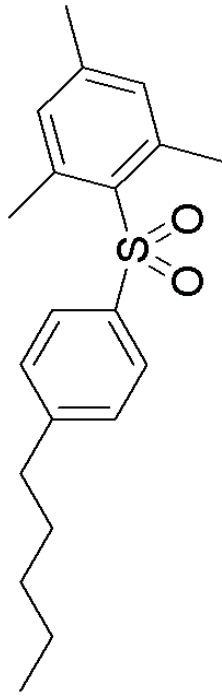
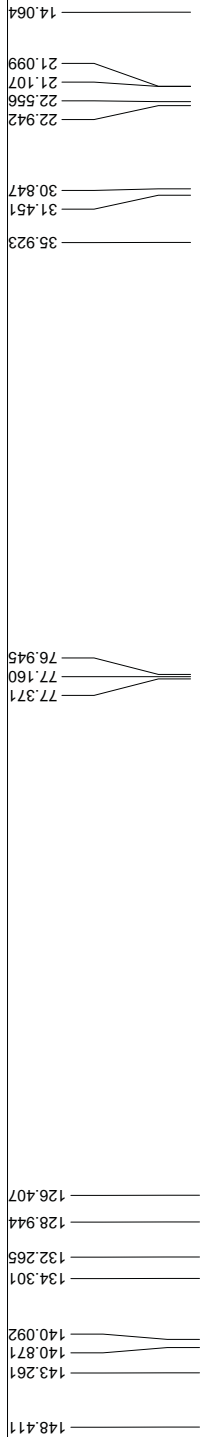
Copies of ¹H and ¹³C NMR spectra S2-S61



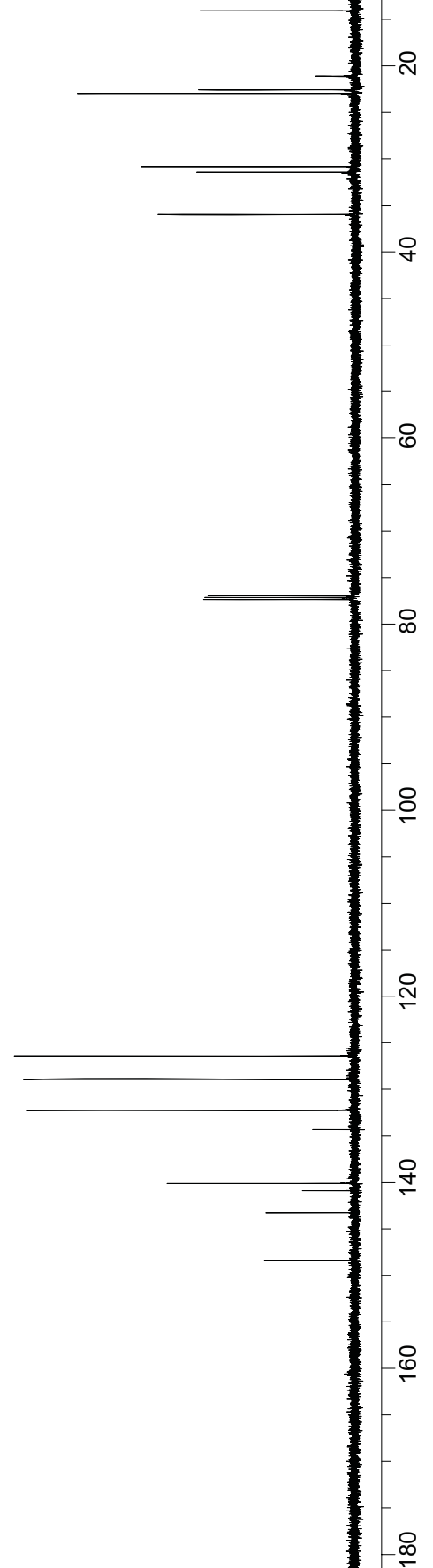


spect, DMSO, F1: 150.728 EX: zgig30 SW1: 36058 PW: 12.0 usec PD: 1.5 sec OF1: 14998.9 NA: 103 LB: 0.0 PTS1d: 32768 WinNuts - \$pdata

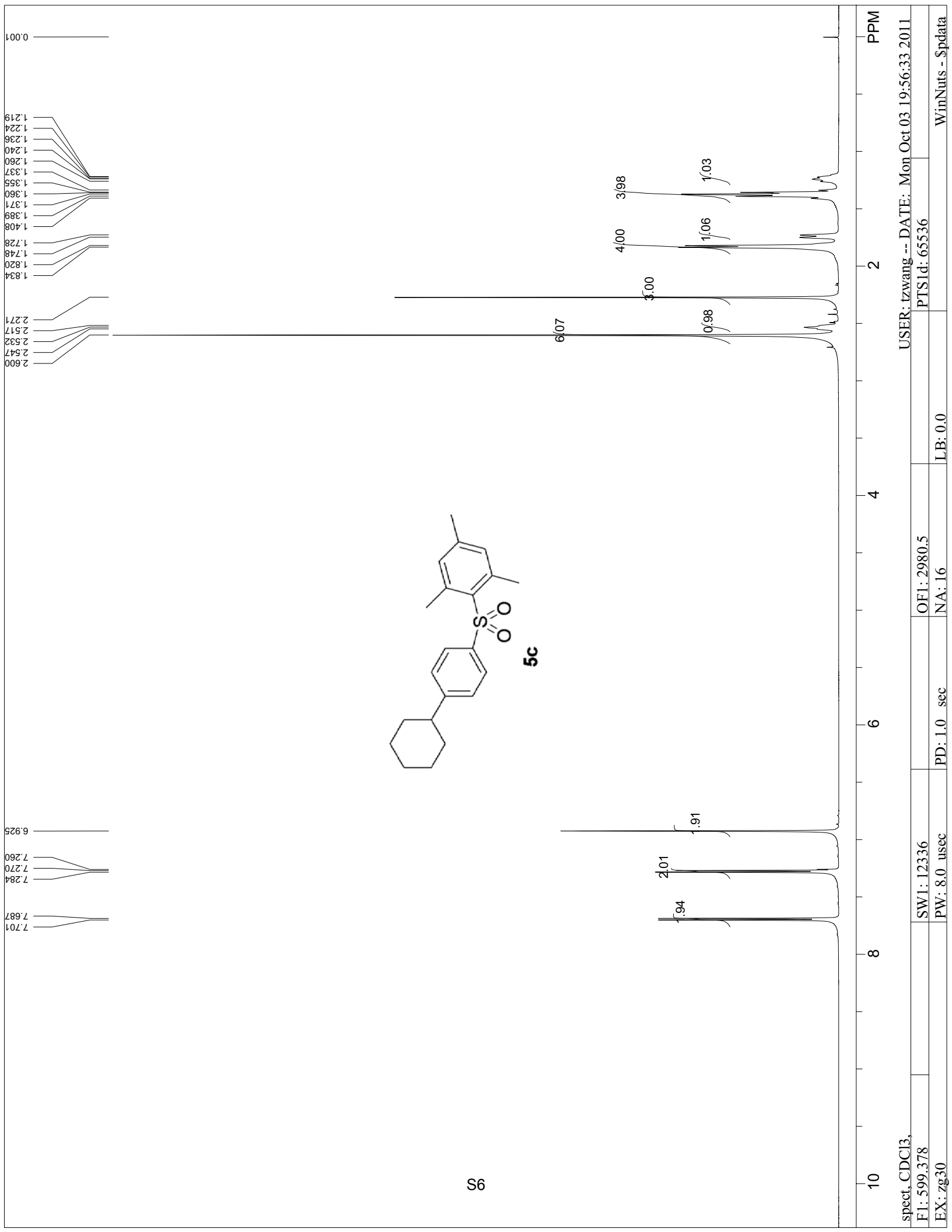


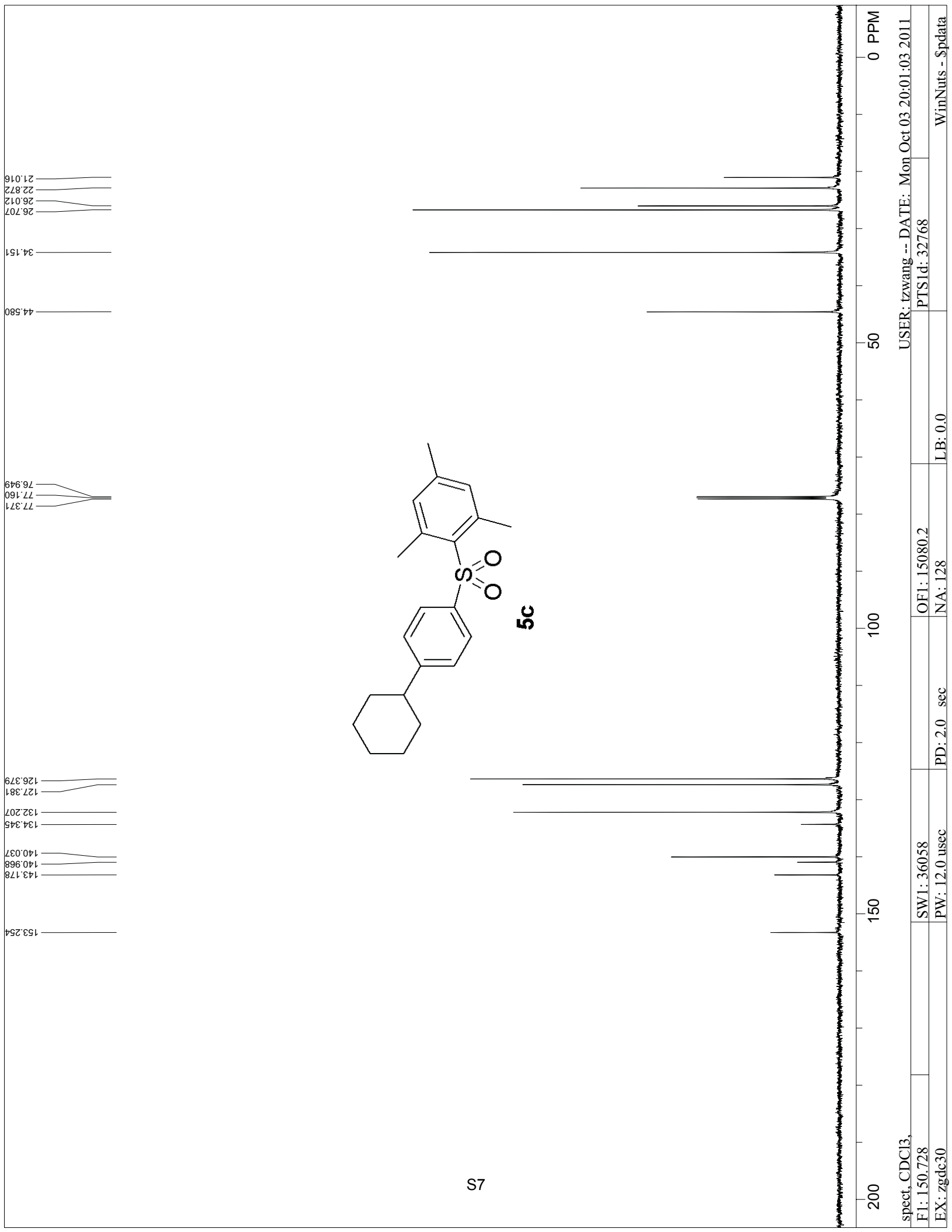


5b

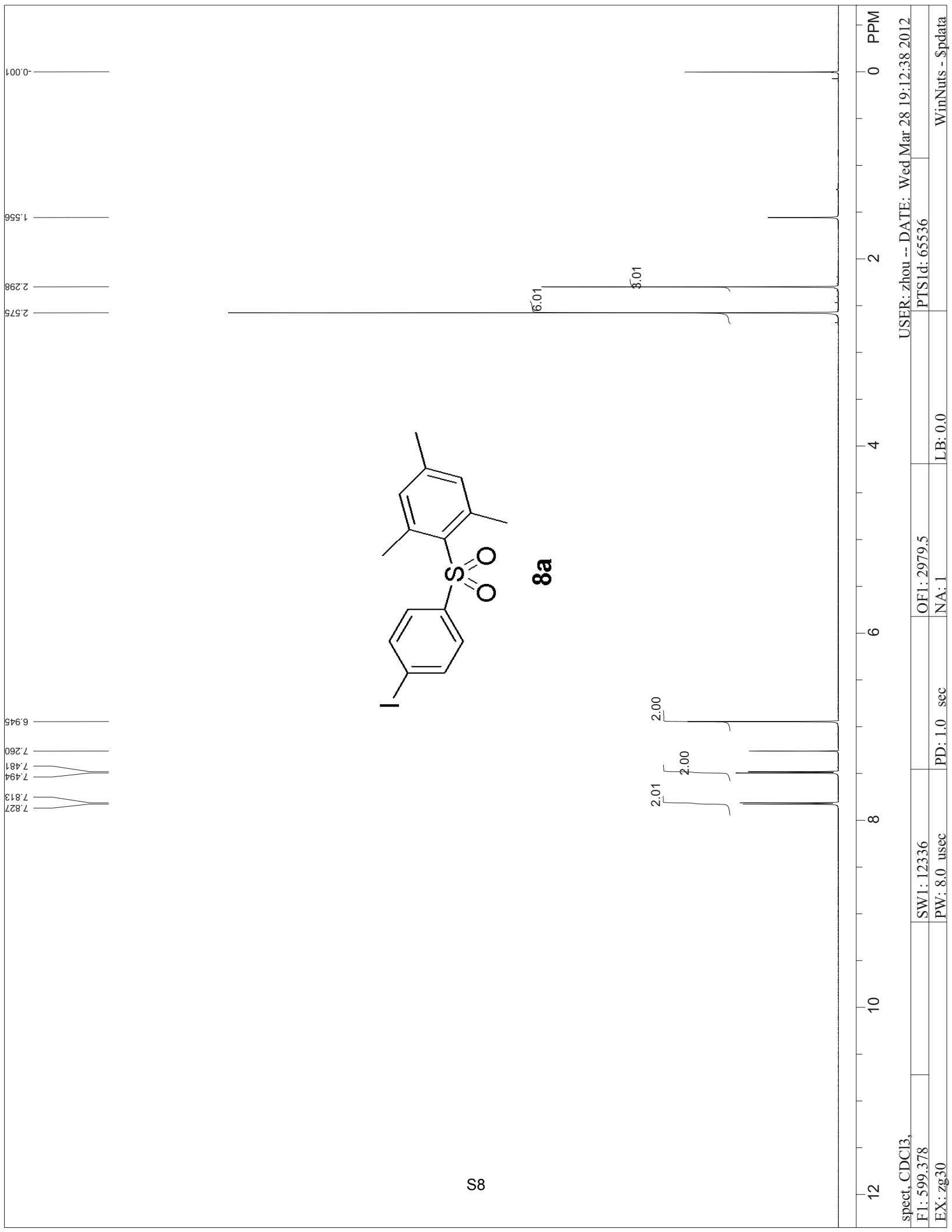


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F2: 599.440	OF1: 13307.9
EX: s2pul	NA: 512
	LB: 0.0
	PD: 1.0 sec
	PW: 8.0 usec
	SW1: 29996
	WinNuts - \$HJC-2-62C-2.fid

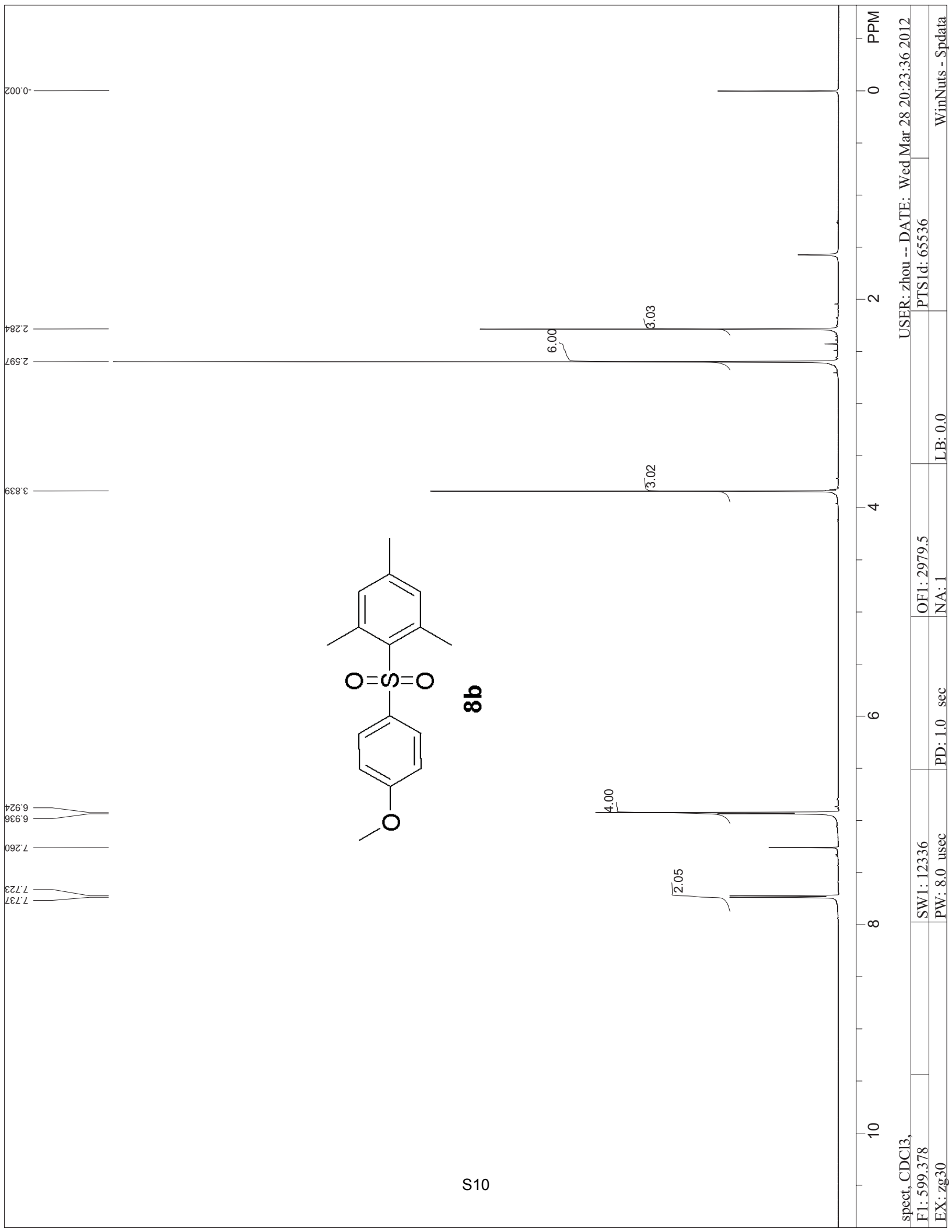




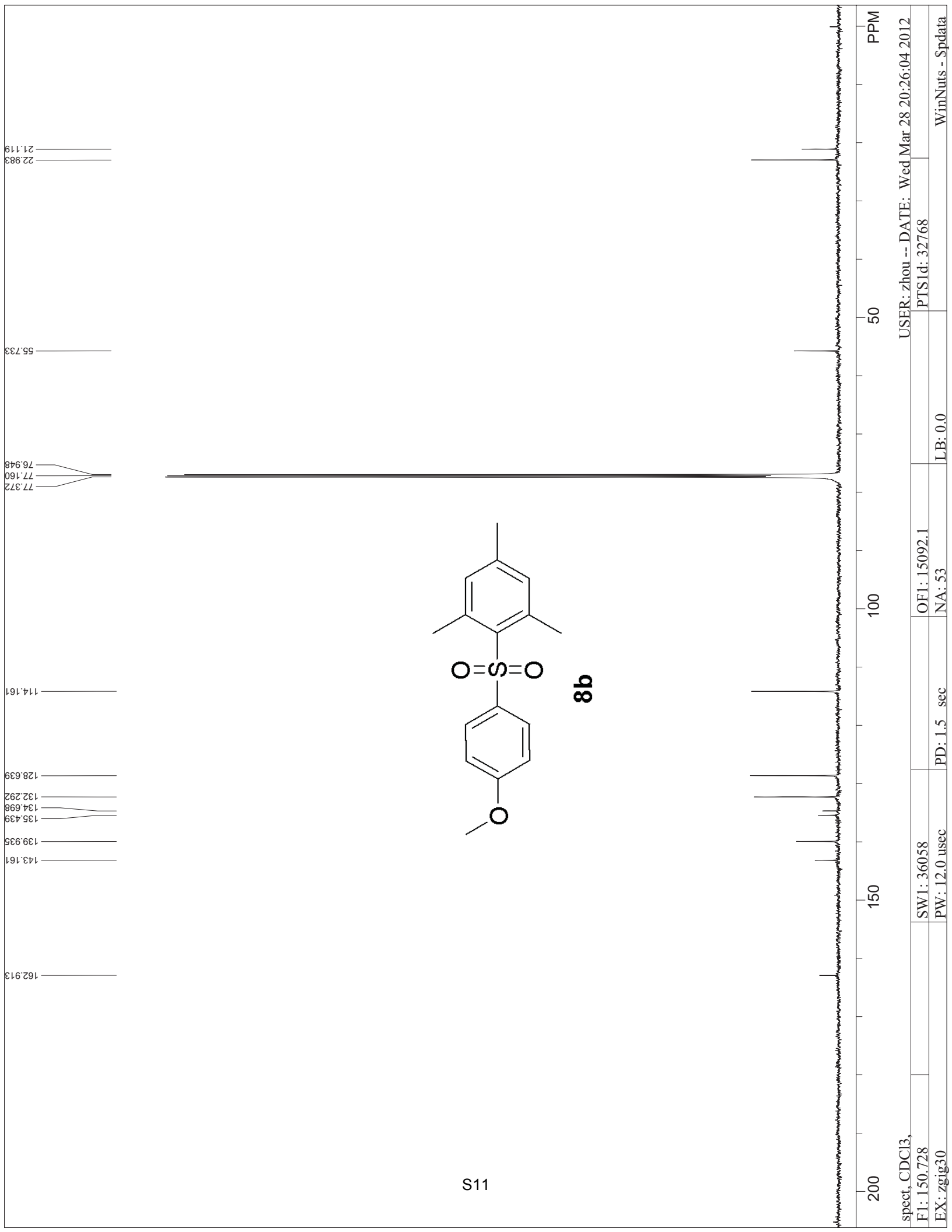
spect, CDCl3, USER: tzwang -- DATE: Mon Oct 03 20:01:03 2011
 F1: 150.728 OF1: 15080.2 PTS1d: 32768
 EX: zgdc30 PD: 2.0 sec LB: 0.0 WinNuts - \$pdata





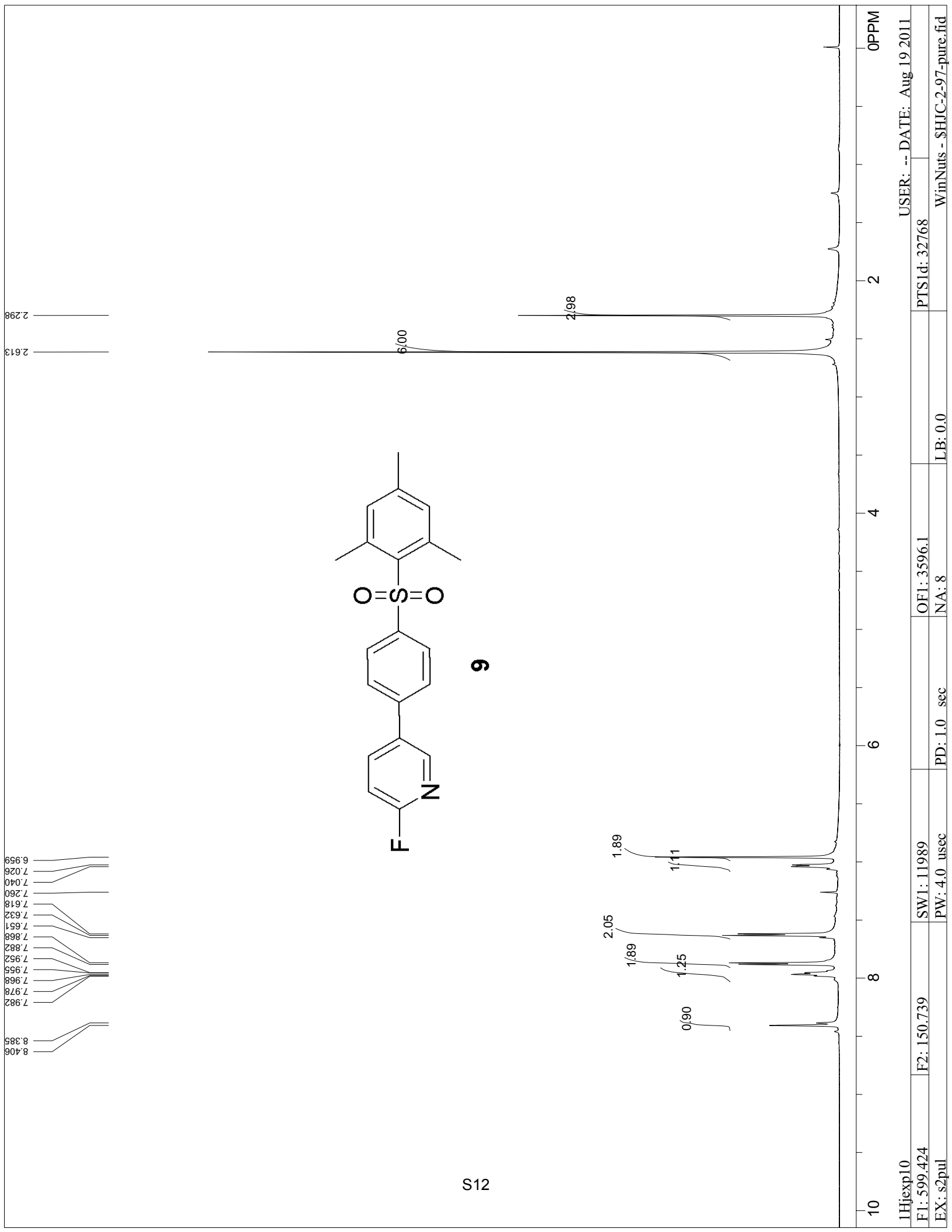


S10

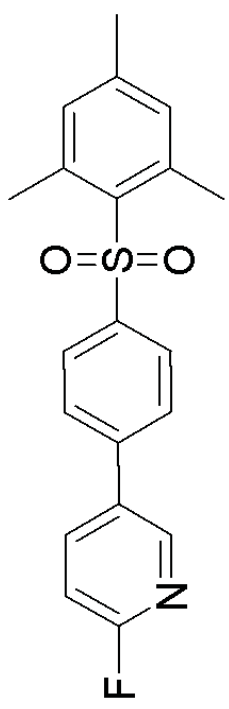


S11

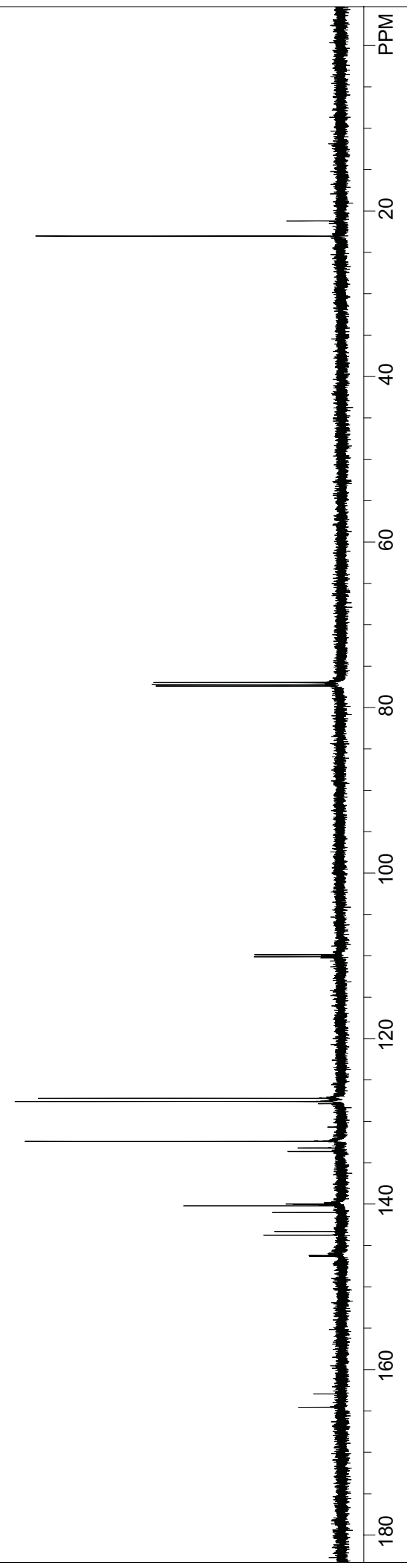
spect, CDCl3, USER: zhou -- DATE: Wed Mar 28 20:26:04 2012
 F1: 150.728 SW1: 36058 OF1: 15092.1 PTS1d: 32768
 EX: zgig30 PW: 12.0 usec PD: 1.5 sec LB: 0.0 WinNuts - \$pdata



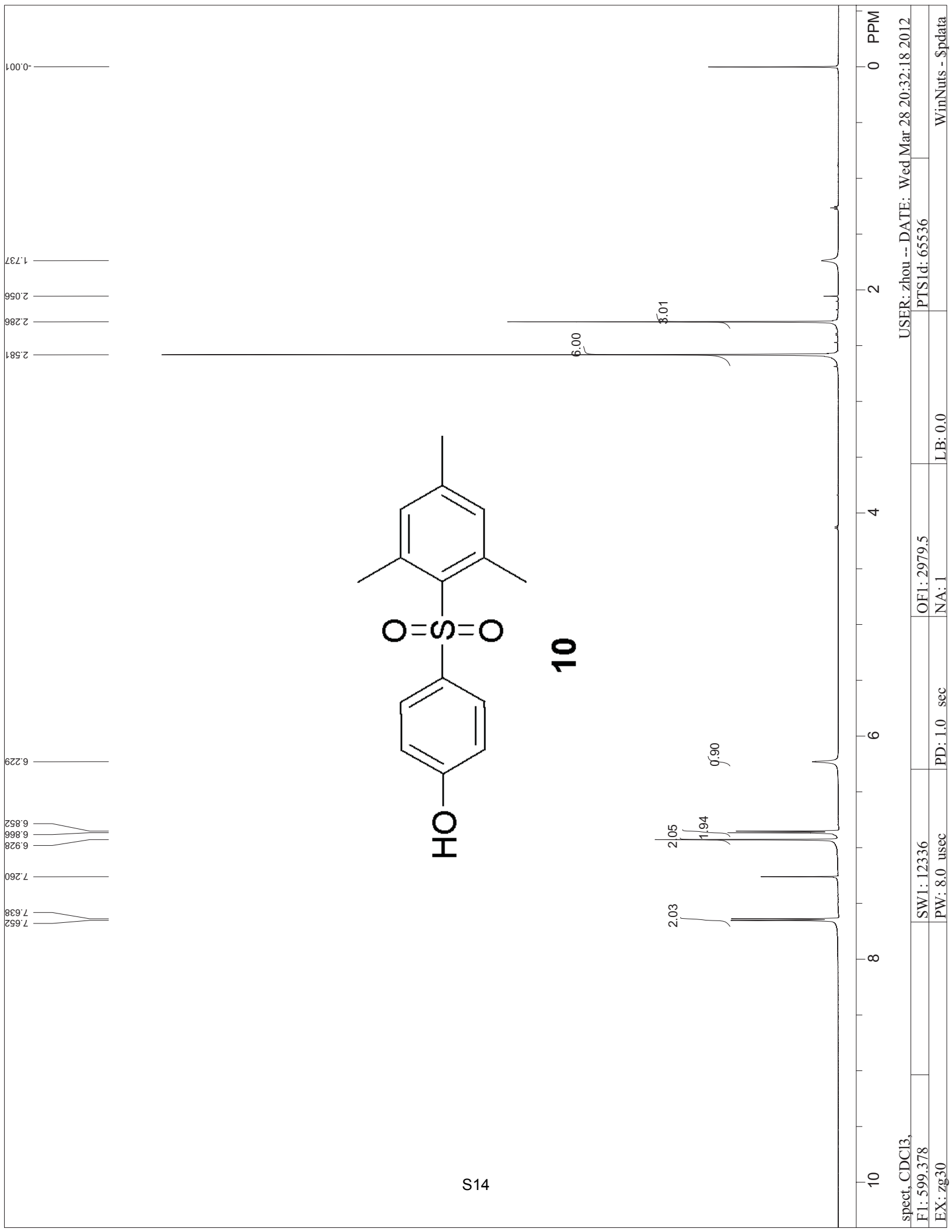
1Hjexp10
 F1: 599.424 F2: 150.739 SW1: 11989 OF1: 3596.1
 EX: s2pul PW: 4.0 usec PD: 1.0 sec NA: 8 LB: 0.0
 USER: -- DATE: Aug 19 2011 PTS1d: 32768
 WinNuts - \$HJC-2-97-pure.fid

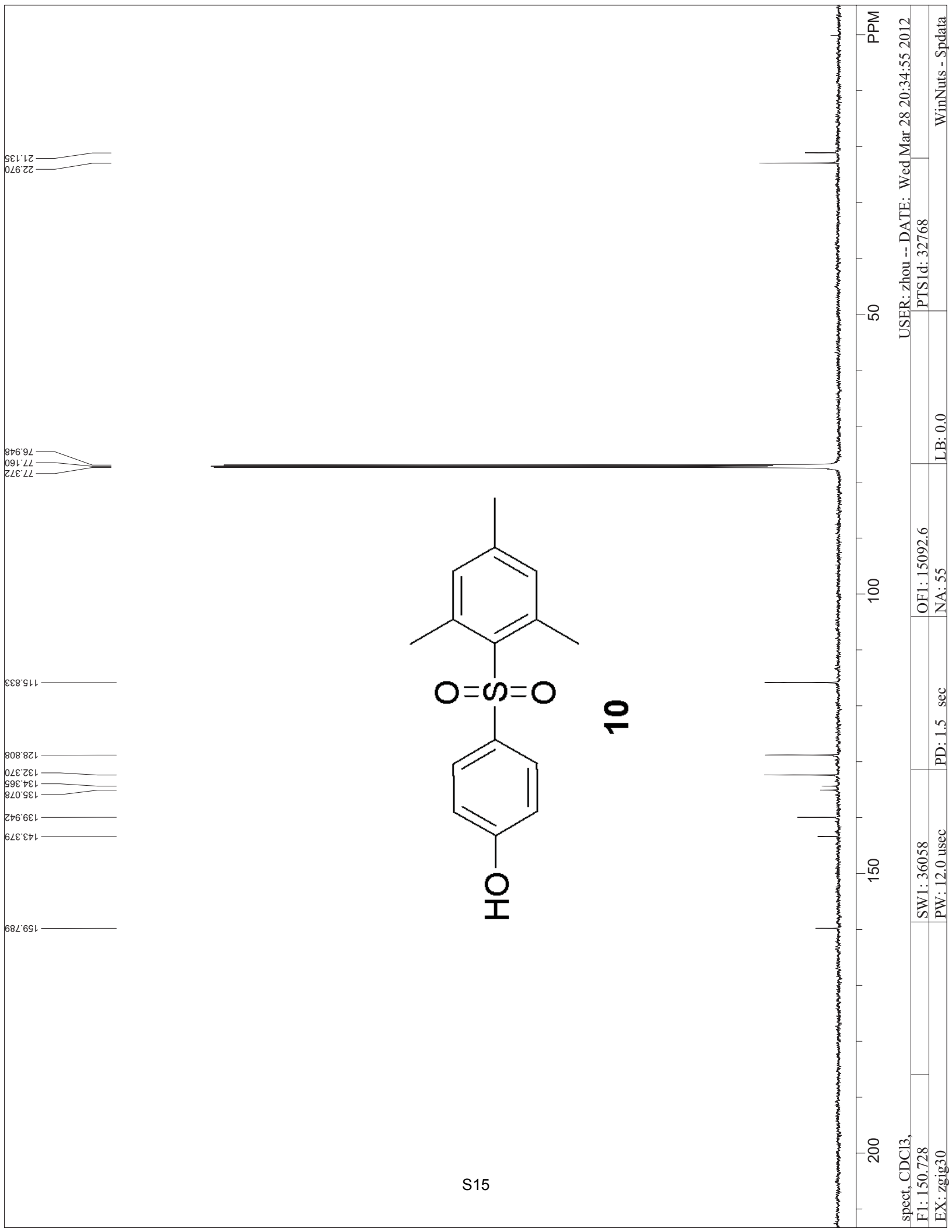


9

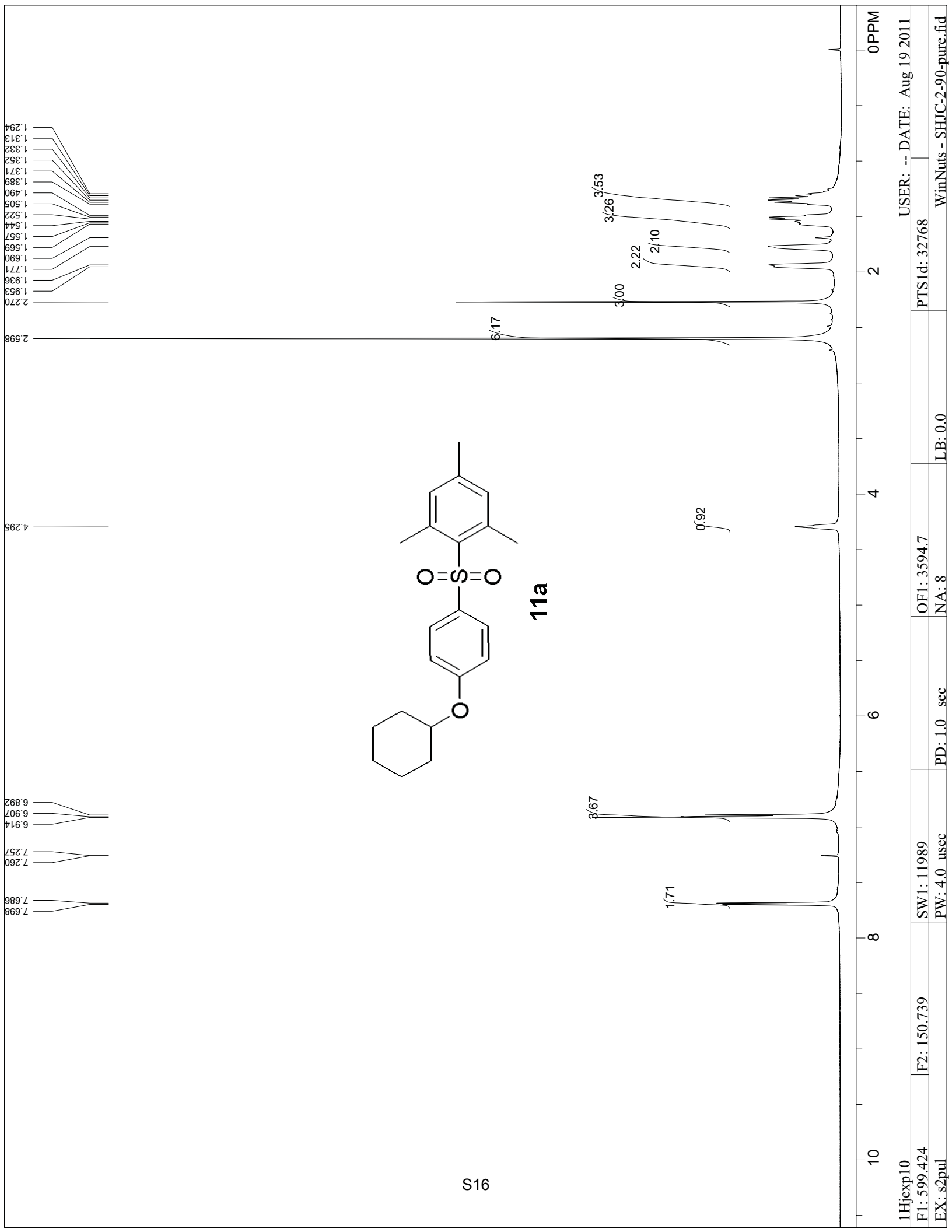


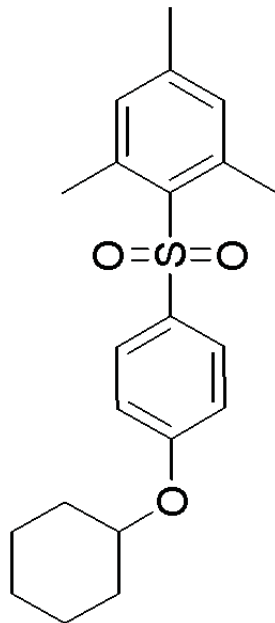
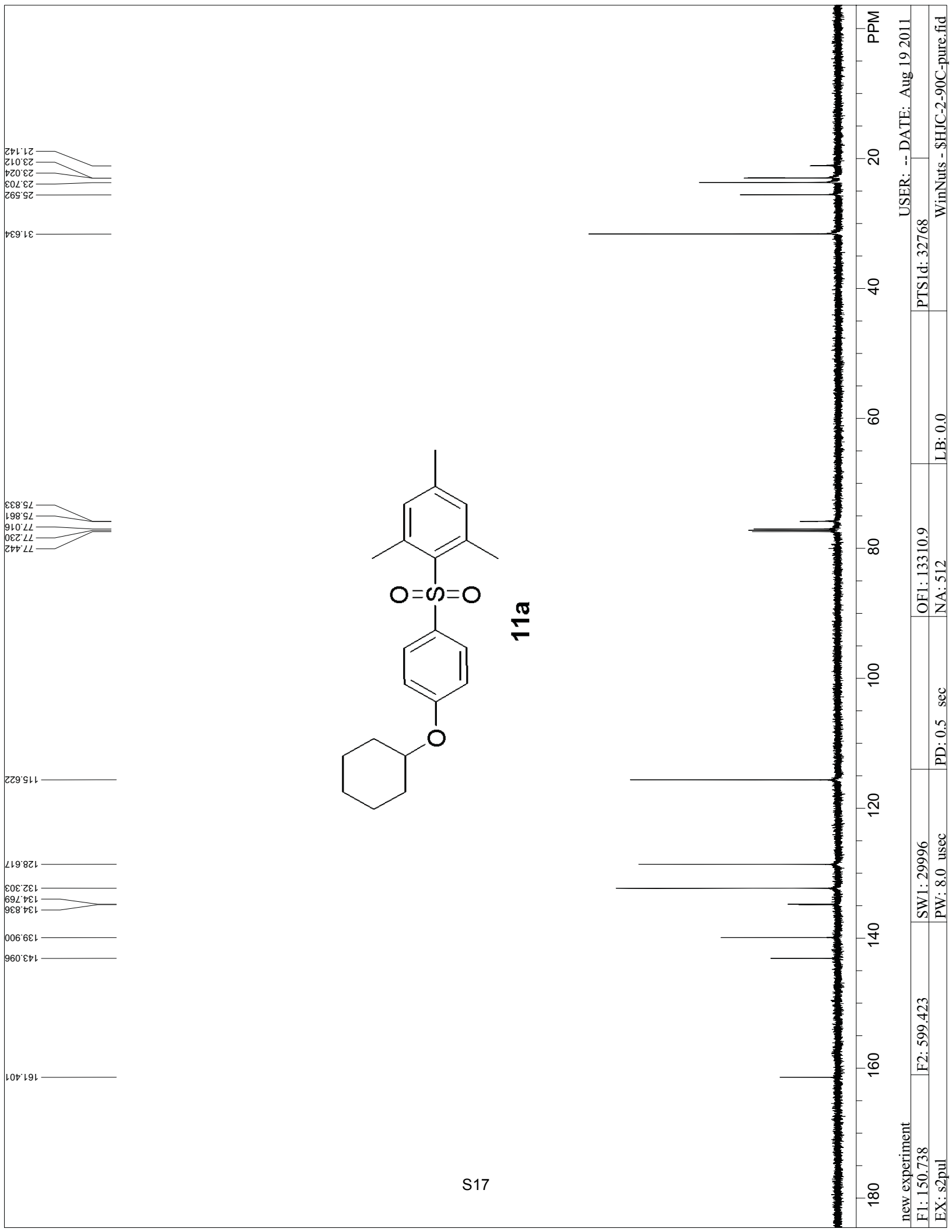
Std carbon	OFI: 13302.6	PTS1d: 32768	USER: -- DATE: Aug 19 2011
F1: 150.738	NA: 1024	LB: 0.0	WinNuts - \$HIC-2-97C-pure-3.fid
EX: s2pul	PD: 1.0 sec		
	SW1: 29996		
	F2: 599.423		
	PW: 8.0 usec		





S15





11a

new experiment

F1: 150.738

F2: 599.423

SW1: 29996

PW: 8.0 usec

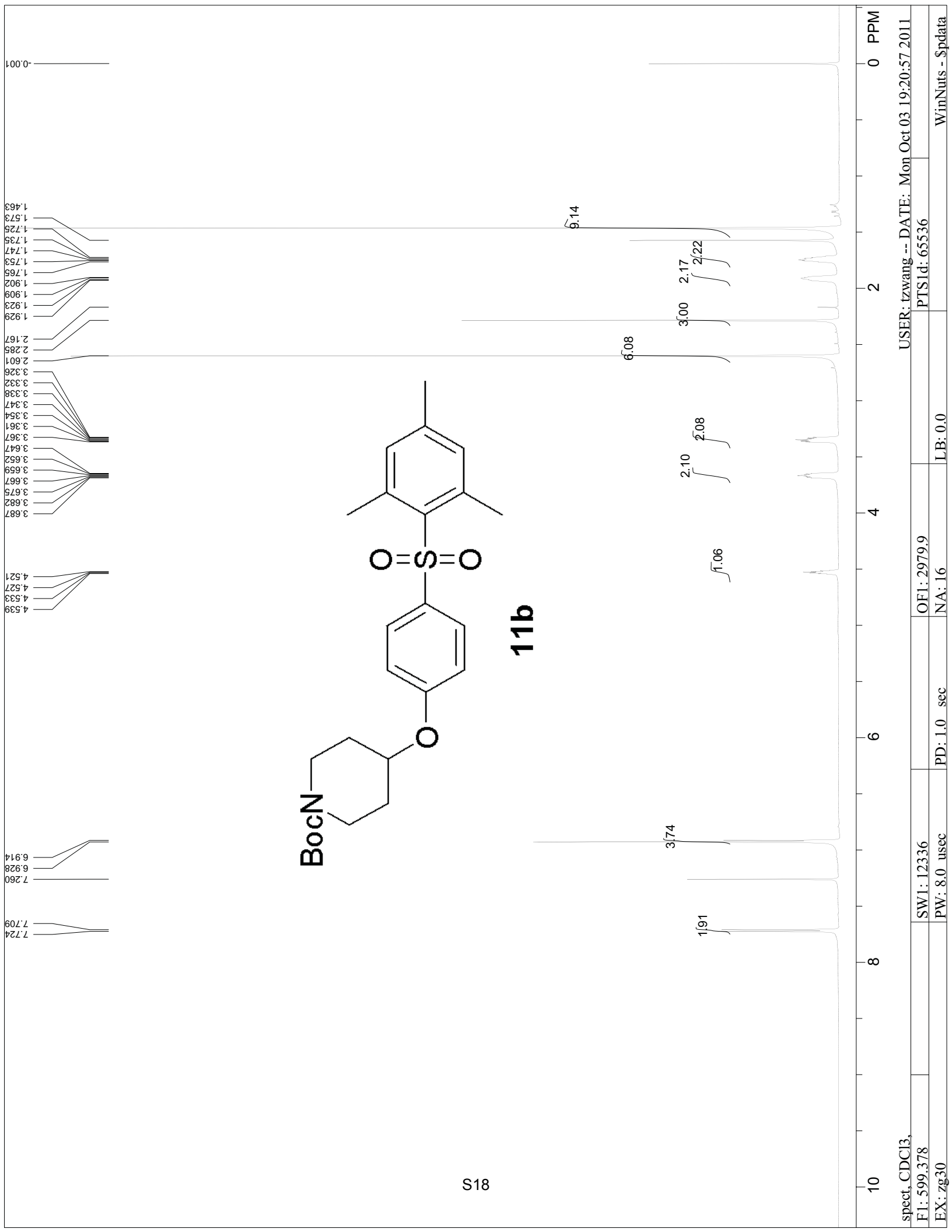
OF1: 13310.9

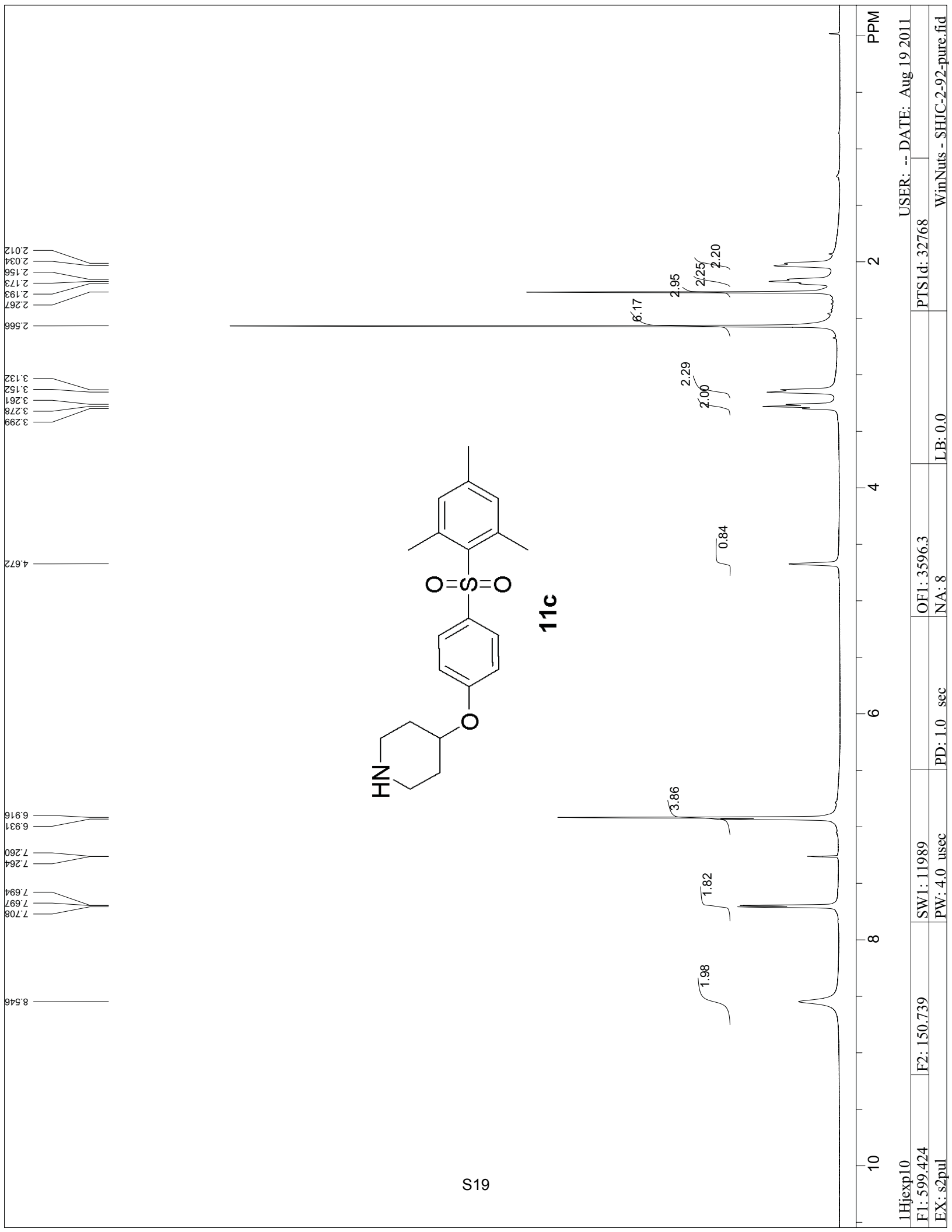
LB: 0.0

PTS1d: 32768

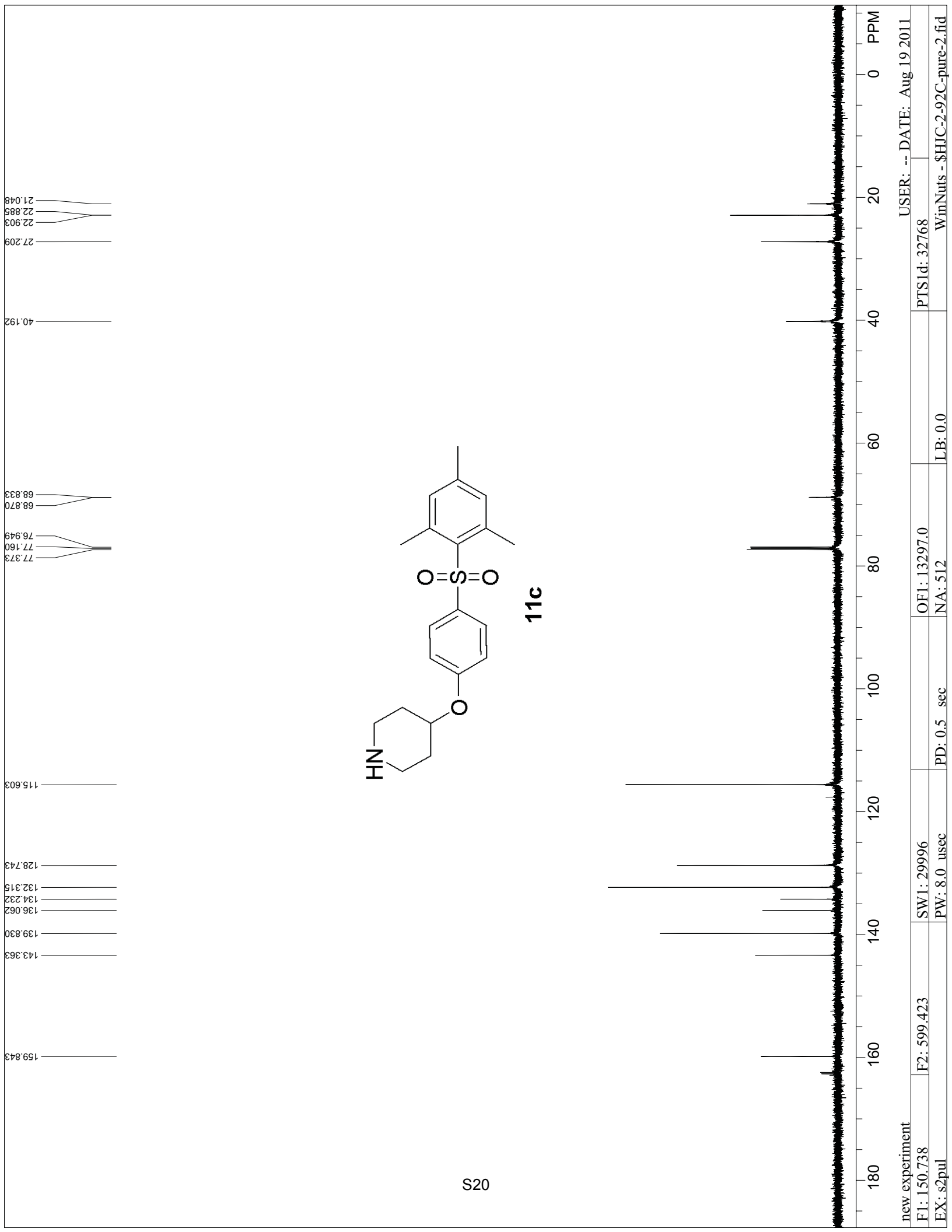
USER: -- DATE: Aug 19 2011

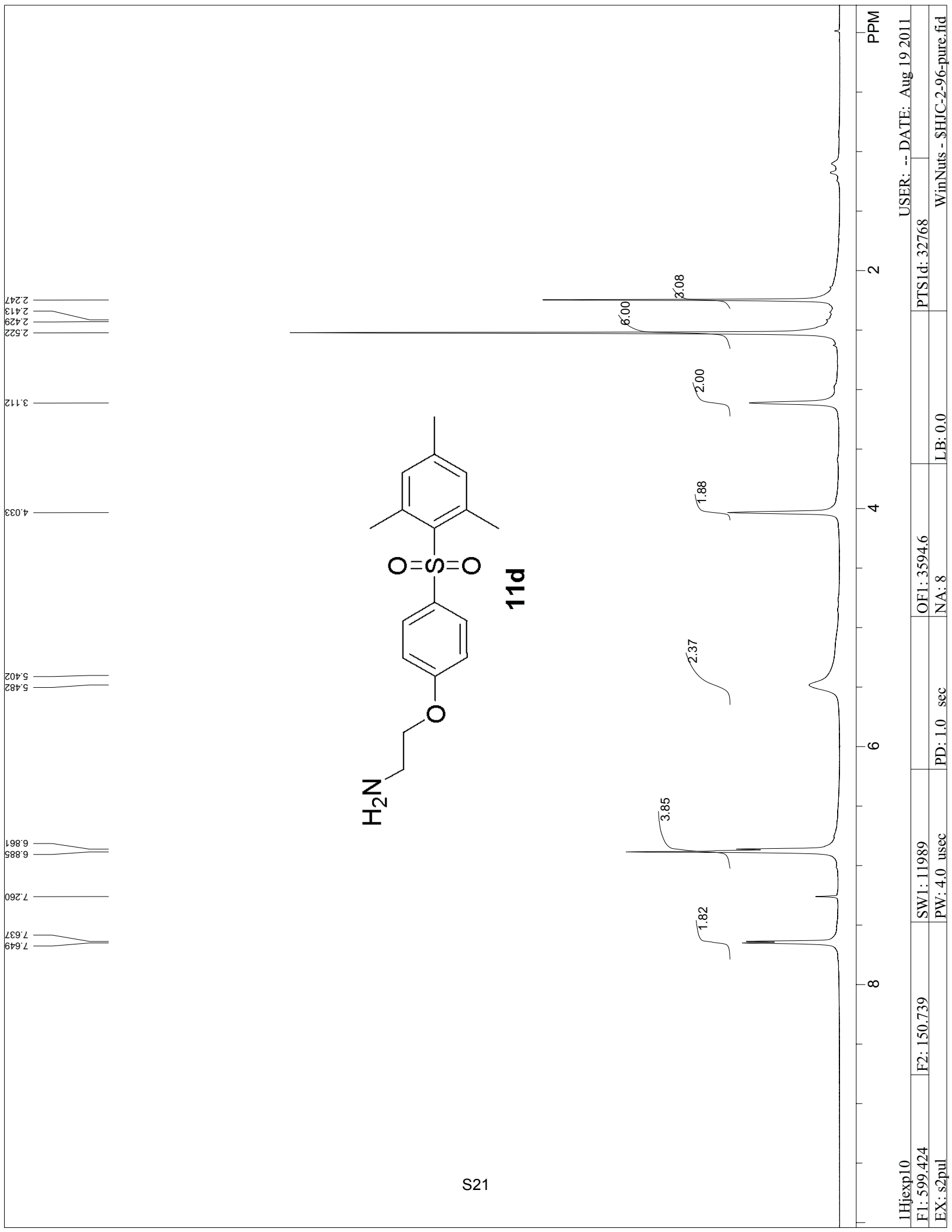
WinNuts - \$HJC-2-90C-pure.fid

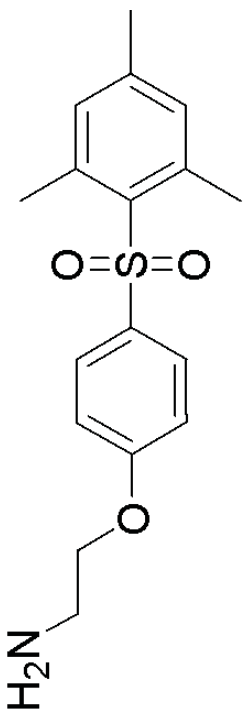




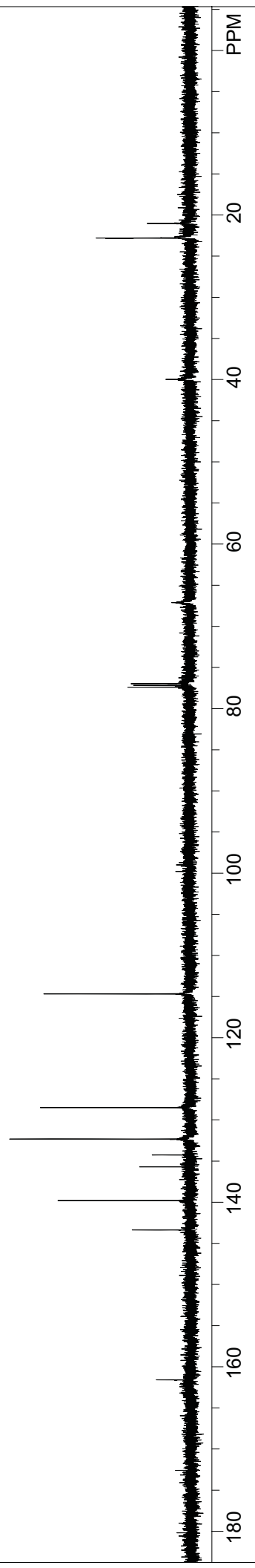
1Hjexp10	SW1: 11989	OF1: 3596.3	PTS1d: 32768	USER: -- DATE: Aug 19 2011
F1: 599.424	F2: 150.739	NA: 8	LB: 0.0	WinNuts - \$HJC-2-92-pure.fid
EX: s2pul	PW: 4.0 usec	PD: 1.0 sec		







11d



new experiment		USER: -- DATE: Aug 19 2011	
F1: 150.738	F2: 599.423	PTS1d: 32768	WinNuts - \$HIC-2-96C-pure-2.fid
EX: s2pul	SW1: 29996	OF1: 13301.1	LB: 0.0
	PW: 8.0 usec	PD: 0.5 sec	NA: 256



1Hjexp10

F1: 599.424

F2: 150.739

SW1: 11989

PD: 1.0 sec

OF1: 3597.1

LB: 0.0

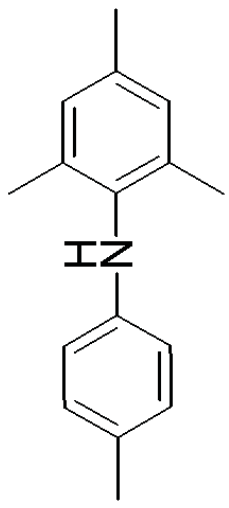
PTS1d: 32768

USER: -- DATE: Aug 19 2011

WinNuts - \$HJC-2-89-pure.fid

20.979
20.519
18.311

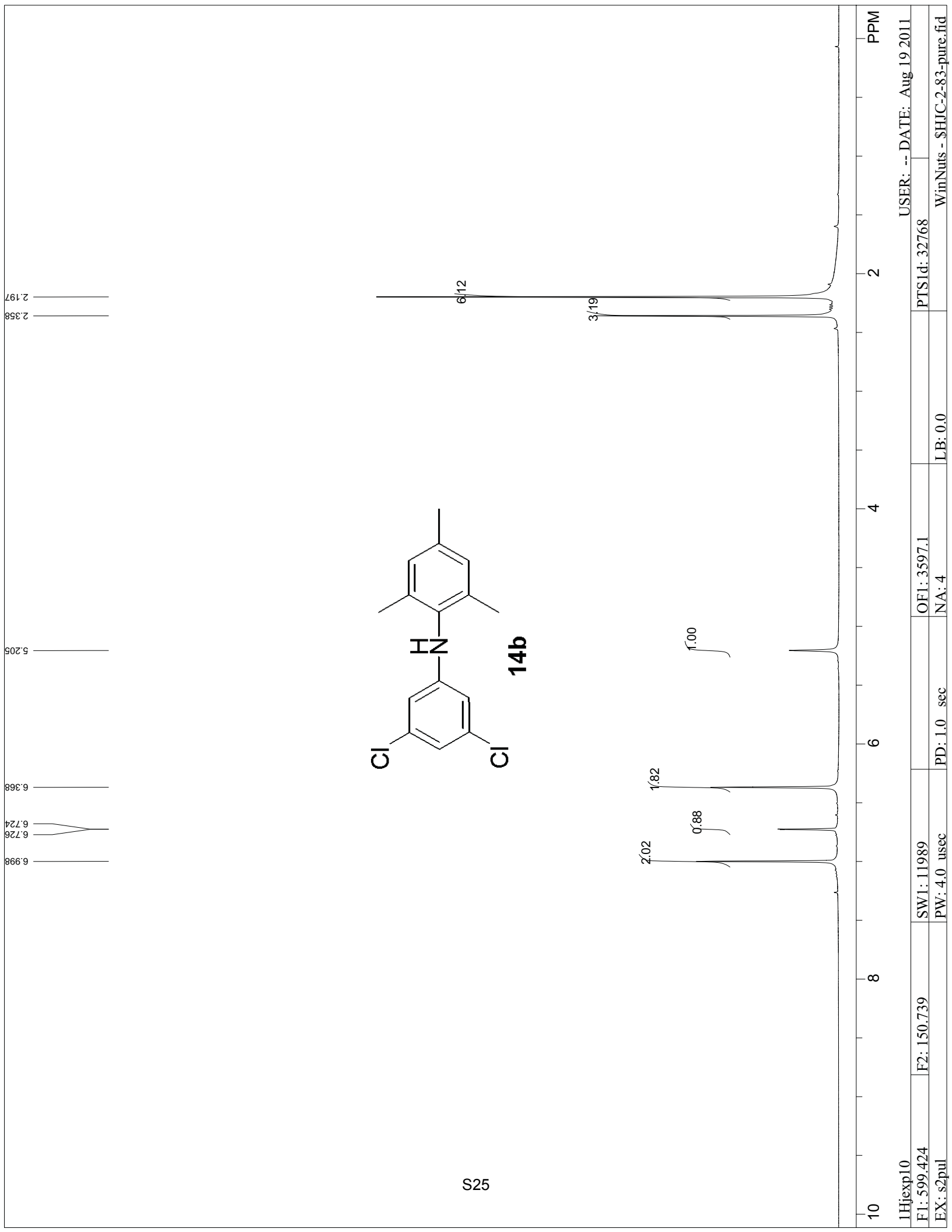
144.370
136.063
135.732
135.099
129.814
129.279
127.112
113.505



14a



Std carbon	USER: -- DATE: Aug 19 2011
F1: 150.738	PTS1d: 32768
F2: 599.423	OF1: 13275.2
EX: s2pul	PD: 1.0 sec
	NA: 256
	LB: 0.0
	WinNuts - \$HJC-2-89C-pure.fid



USER: -- DATE: Aug 19 2011

PTS1d: 32768

OF1: 3597.1

NA: 4

PD: 1.0 sec

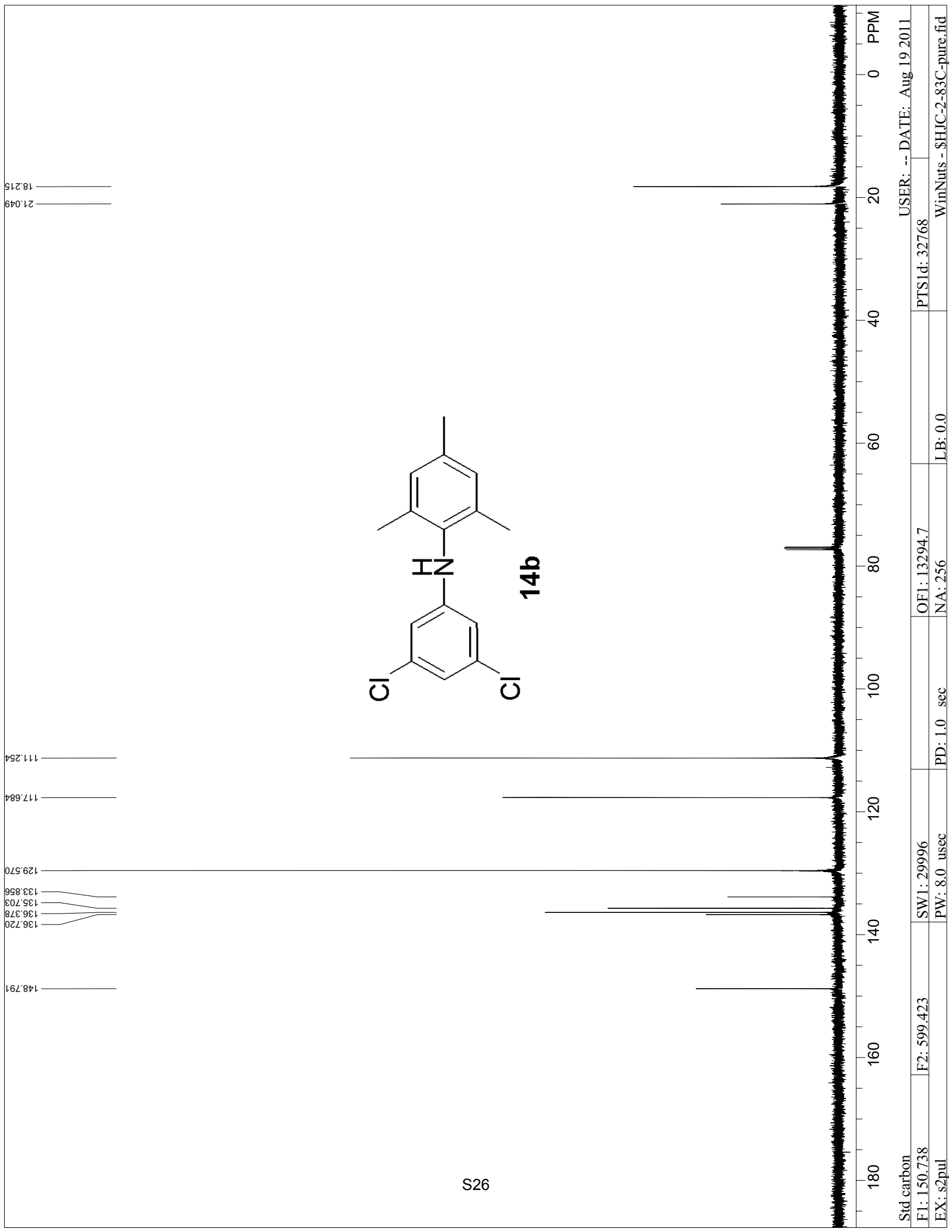
SW1: 11989

F2: 150.739

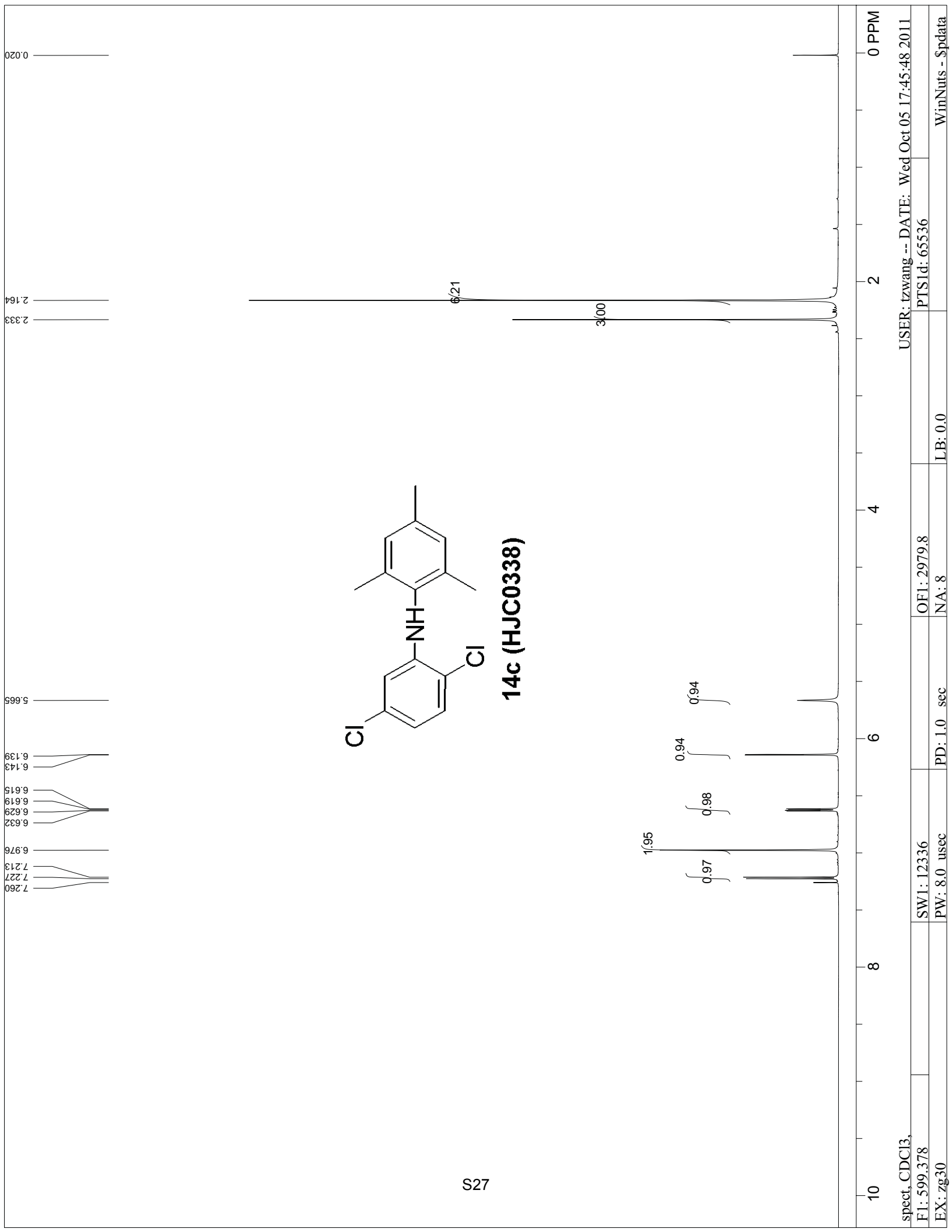
EX: s2pul

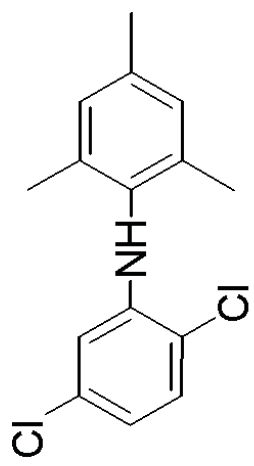
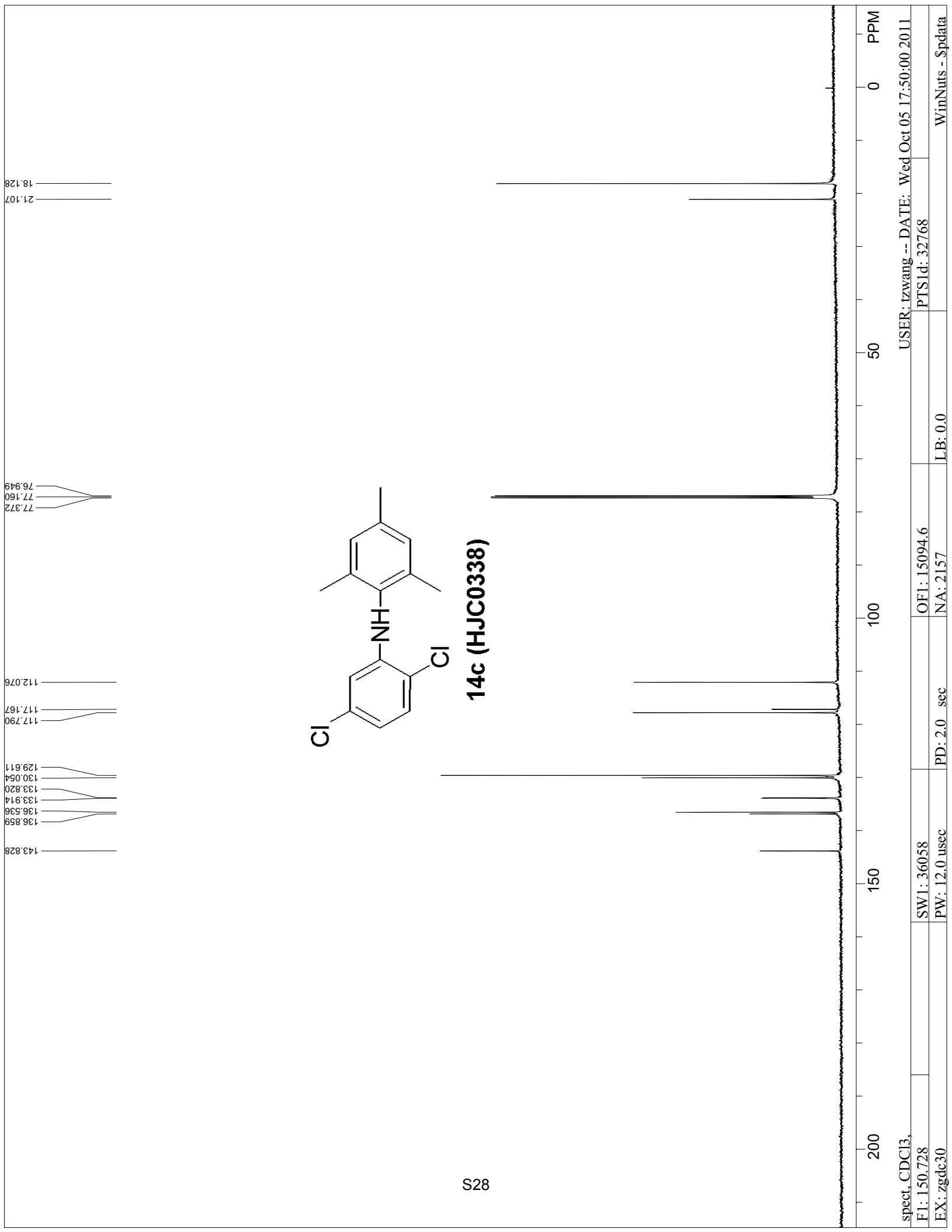
LB: 0.0

WinNuts - \$HJC-2-83-pure.fid



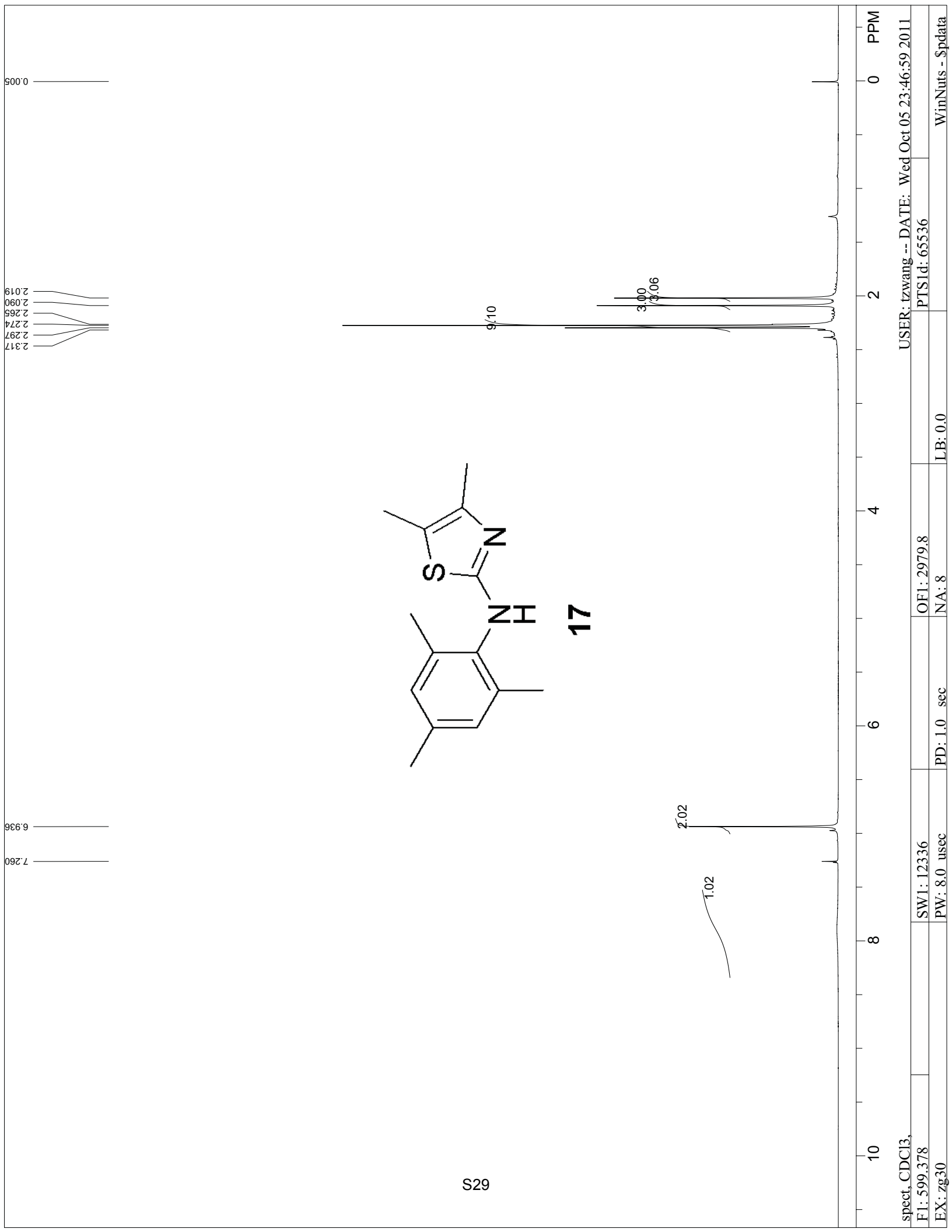
Std carbon
 F1: 150.738
 EX: s2pul
 F2: 599.423
 SW1: 29996
 PW: 8.0 usec
 OF1: 13294.7
 PD: 1.0 sec
 NA: 256
 PTS1d: 32768
 LB: 0.0
 USER: -- DATE: Aug 19 2011
 WinNuts - \$HJC-2-83C-pure.fid



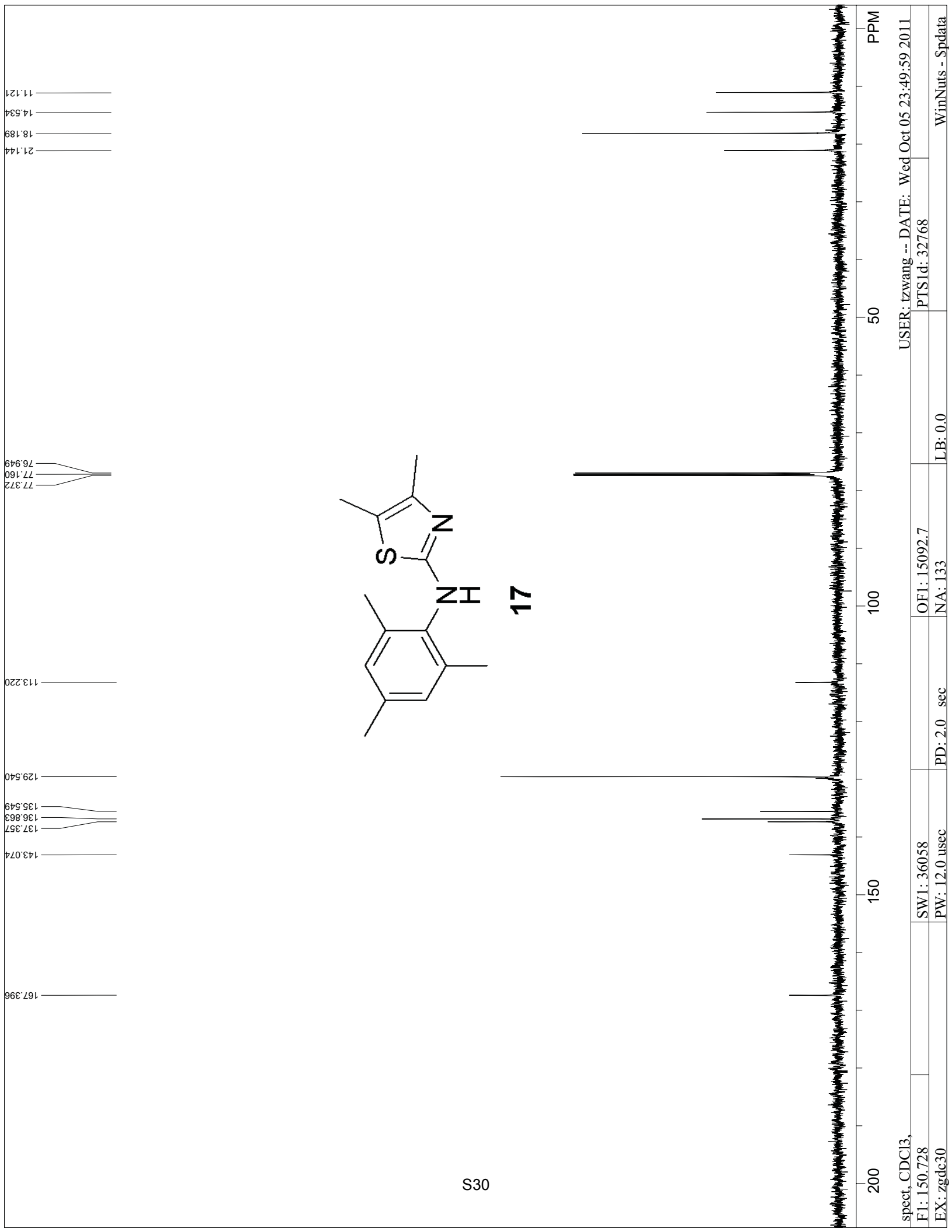


14c (HJC0338)

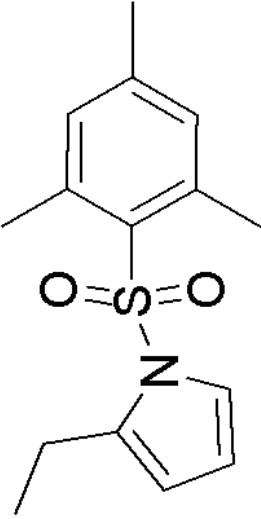
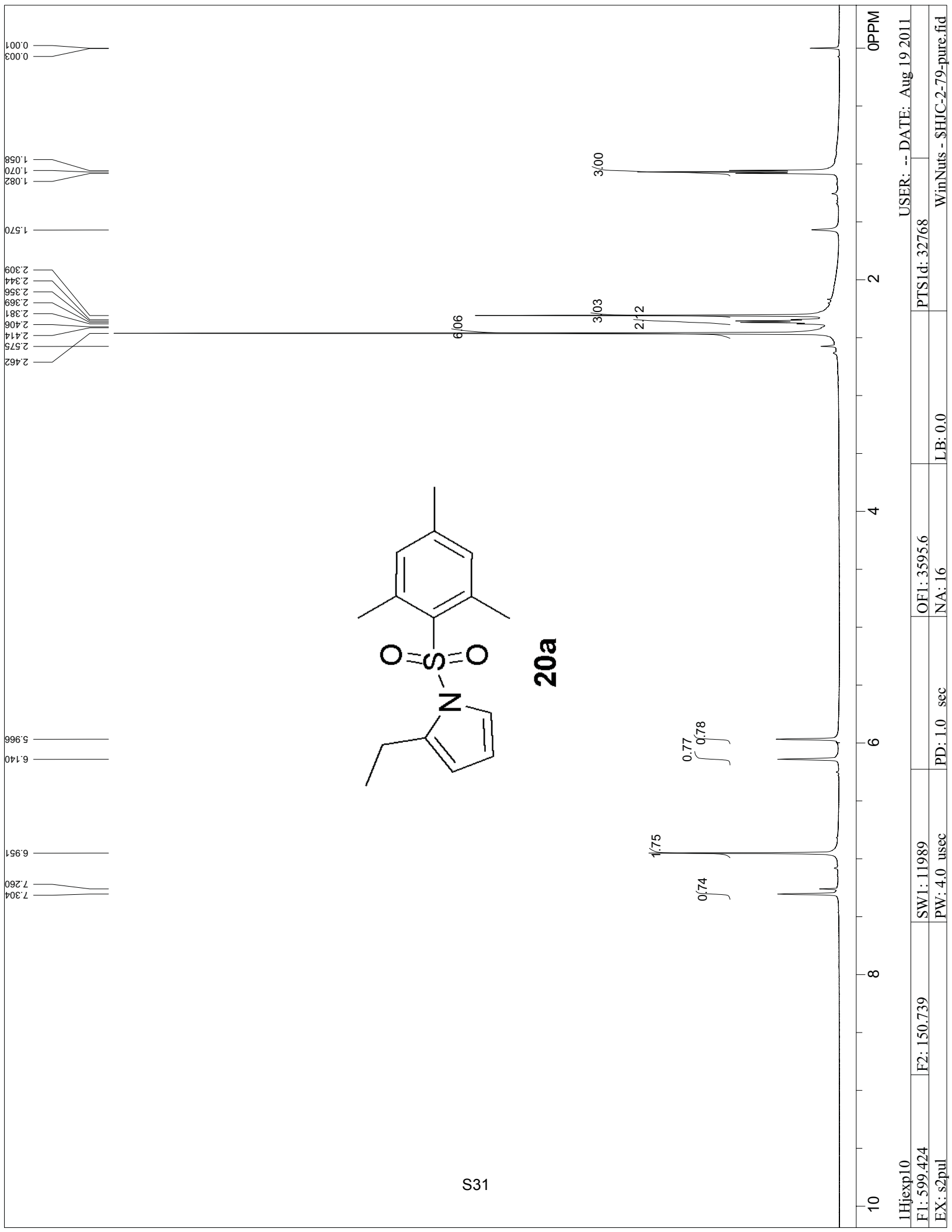
spect, CDCI3,	USER: tzwang -- DATE: Wed Oct 05 17:50:00 2011
F1: 150.728	PTS1d: 32768
EX: zgdc30	LB: 0.0
SW1: 36058	OF1: 15094.6
PW: 12.0 usec	NA: 2157
PD: 2.0 sec	
	WinNuts - \$pdata



spect, CDCl3, USER: tzwang --- DATE: Wed Oct 05 23:46:59 2011
 F1: 599.378 SW1: 12336 OF1: 2979.8 PTS1d: 65536
 EX: zg30 PW: 8.0 usec PD: 1.0 sec NA: 8 LB: 0.0 WinNuts - \$pdata

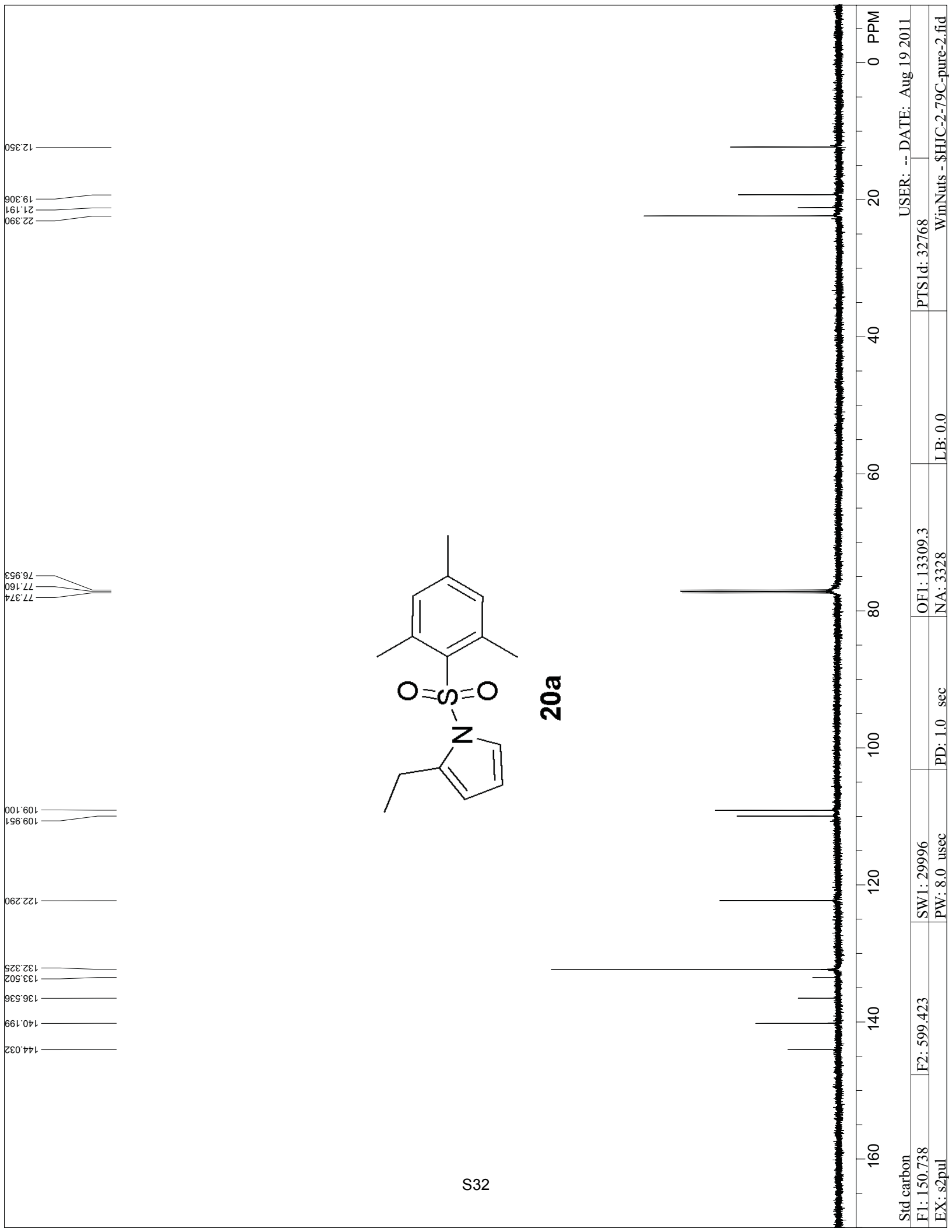


spect, CDCI3, USER: tzwang -- DATE: Wed Oct 05 23:49:59 2011
 F1: 150.728 OF1: 15092.7 PTS1d: 32768
 EX: zgdc30 SW1: 36058 NA: 133 LB: 0.0 WinNuts - \$pdata
 PD: 2.0 sec

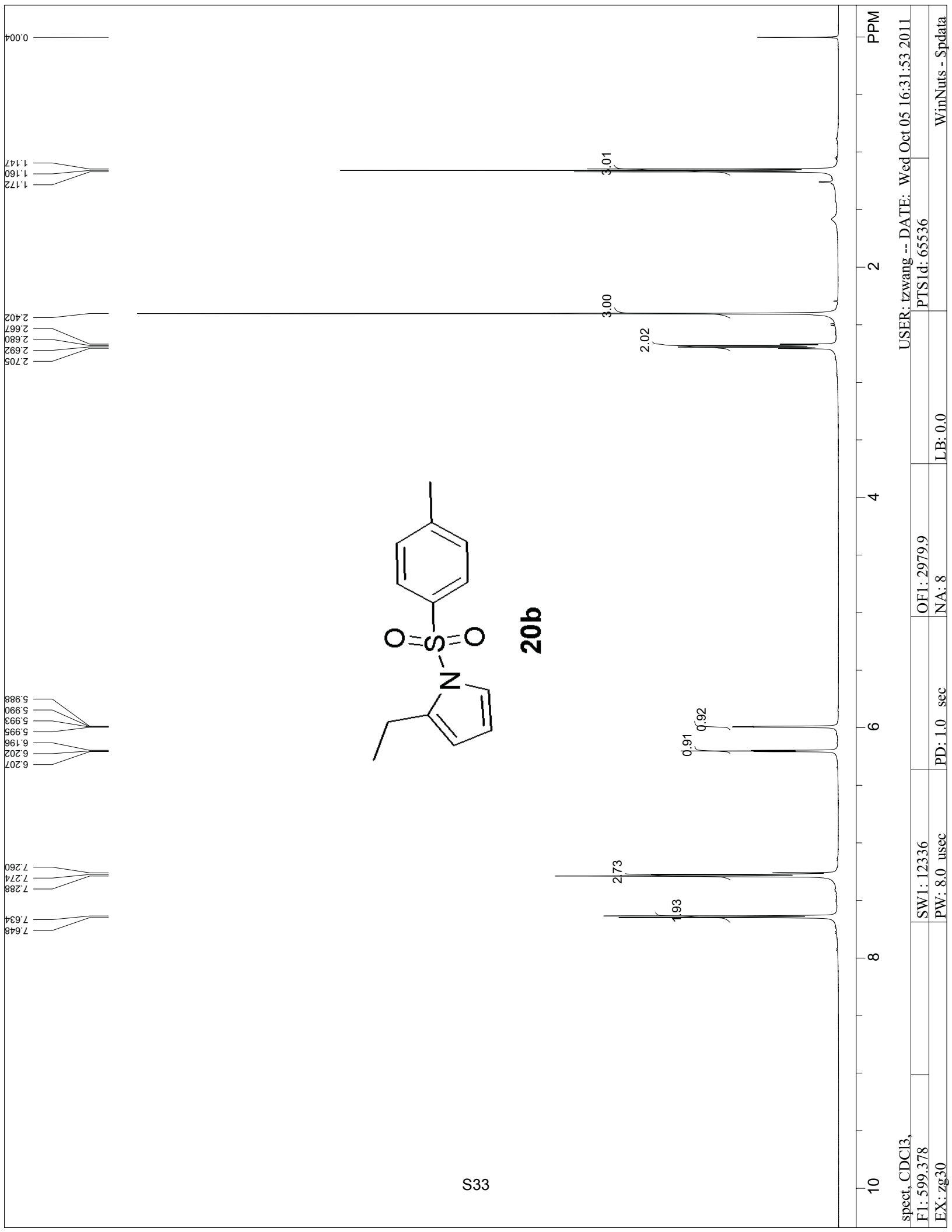


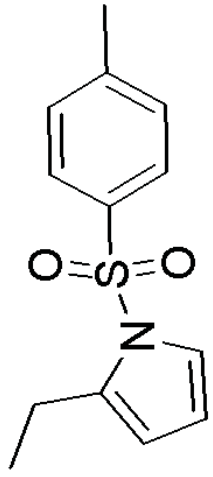
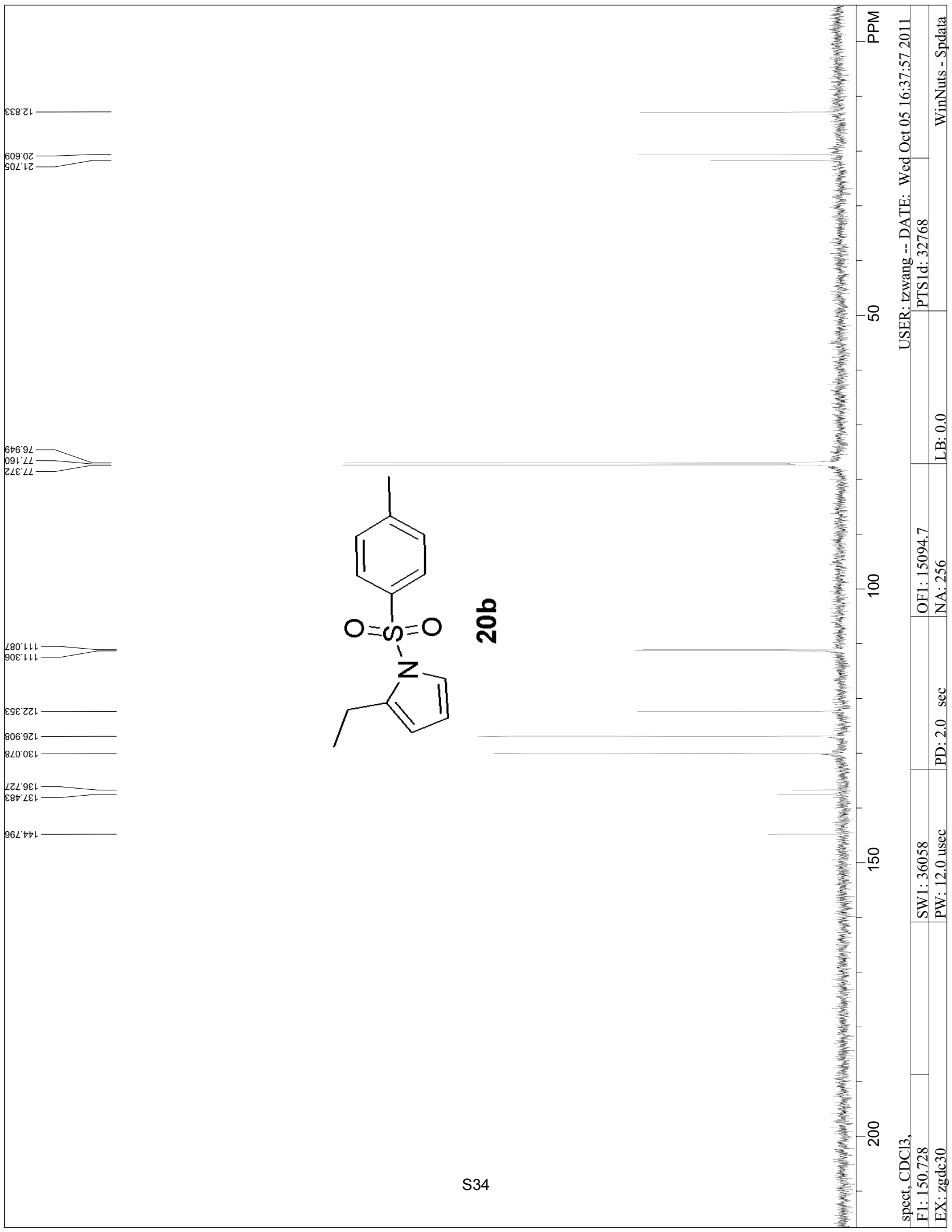
20a

1Hjexp10	USER: --	DATE: Aug 19 2011
F1: 599.424	PTS1d: 32768	
F2: 150.739	OF1: 3595.6	
EX: s2pul	NA: 16	LB: 0.0
	PD: 1.0 sec	



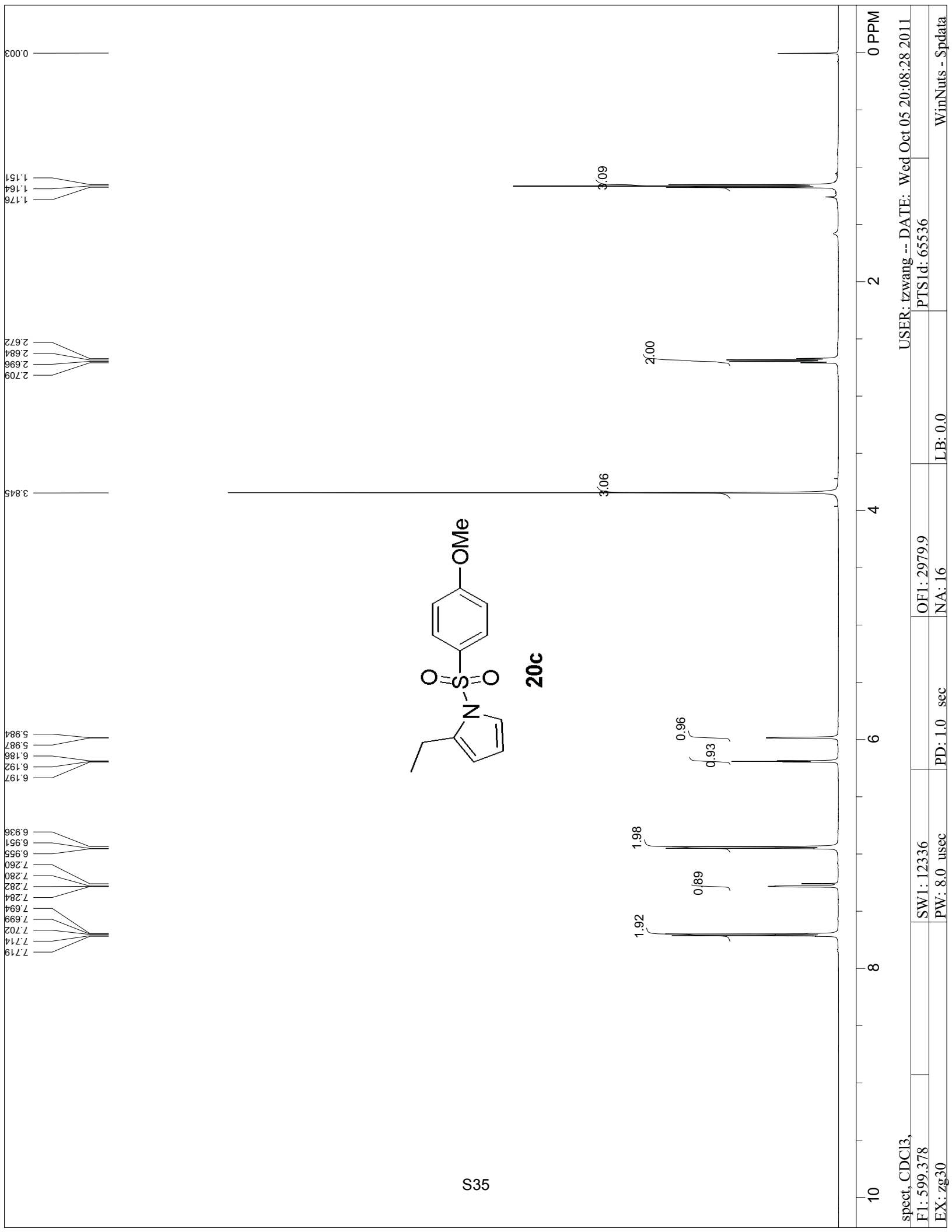
Std carbon
 F1: 150.738 F2: 599.423 SW1: 29996 OF1: 13309.3
 EX: s2pul PW: 8.0 usec PD: 1.0 sec NA: 3328 LB: 0.0
 USER: -- DATE: Aug 19 2011 PTS1d: 32768
 WinNuts - \$HIC-2-79C-pure-2.fid



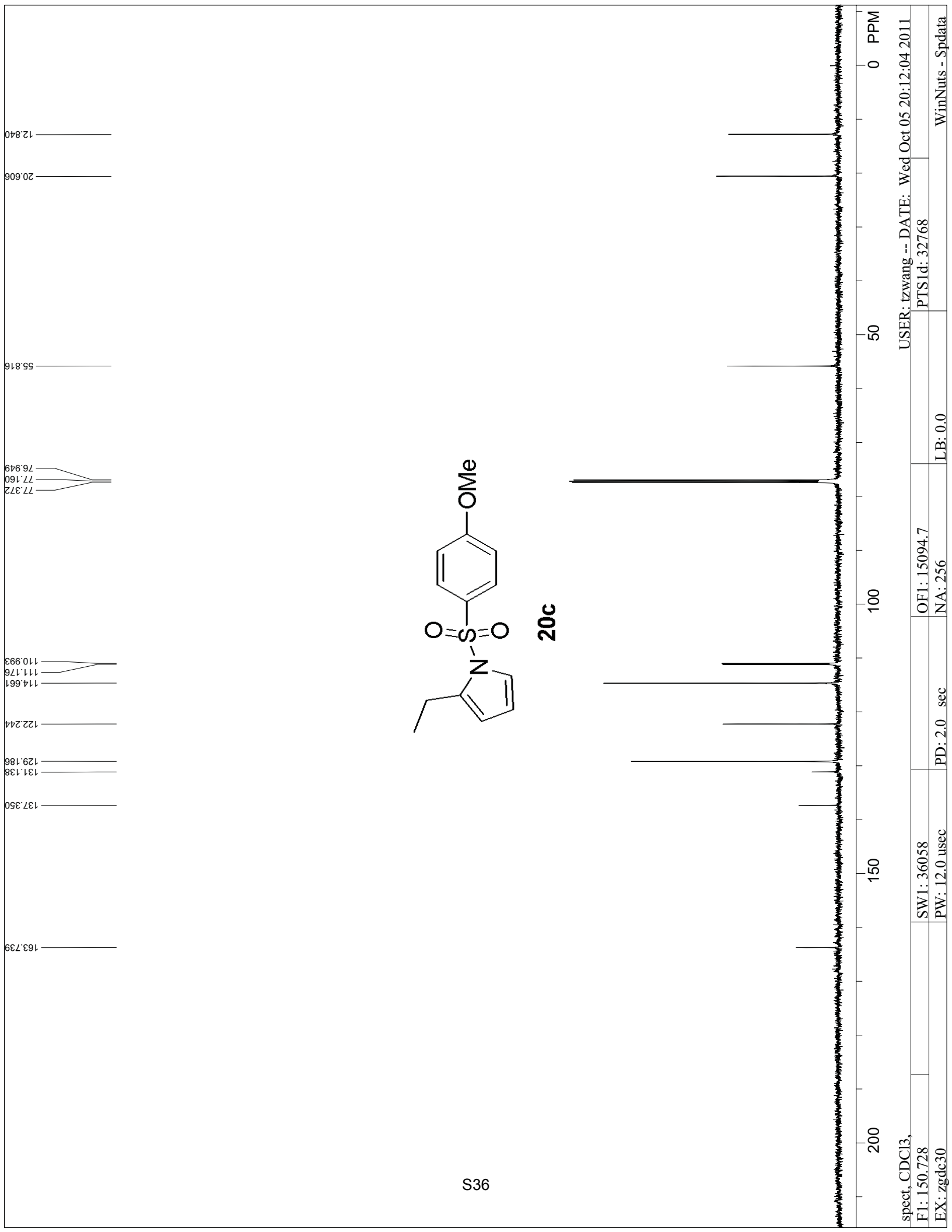


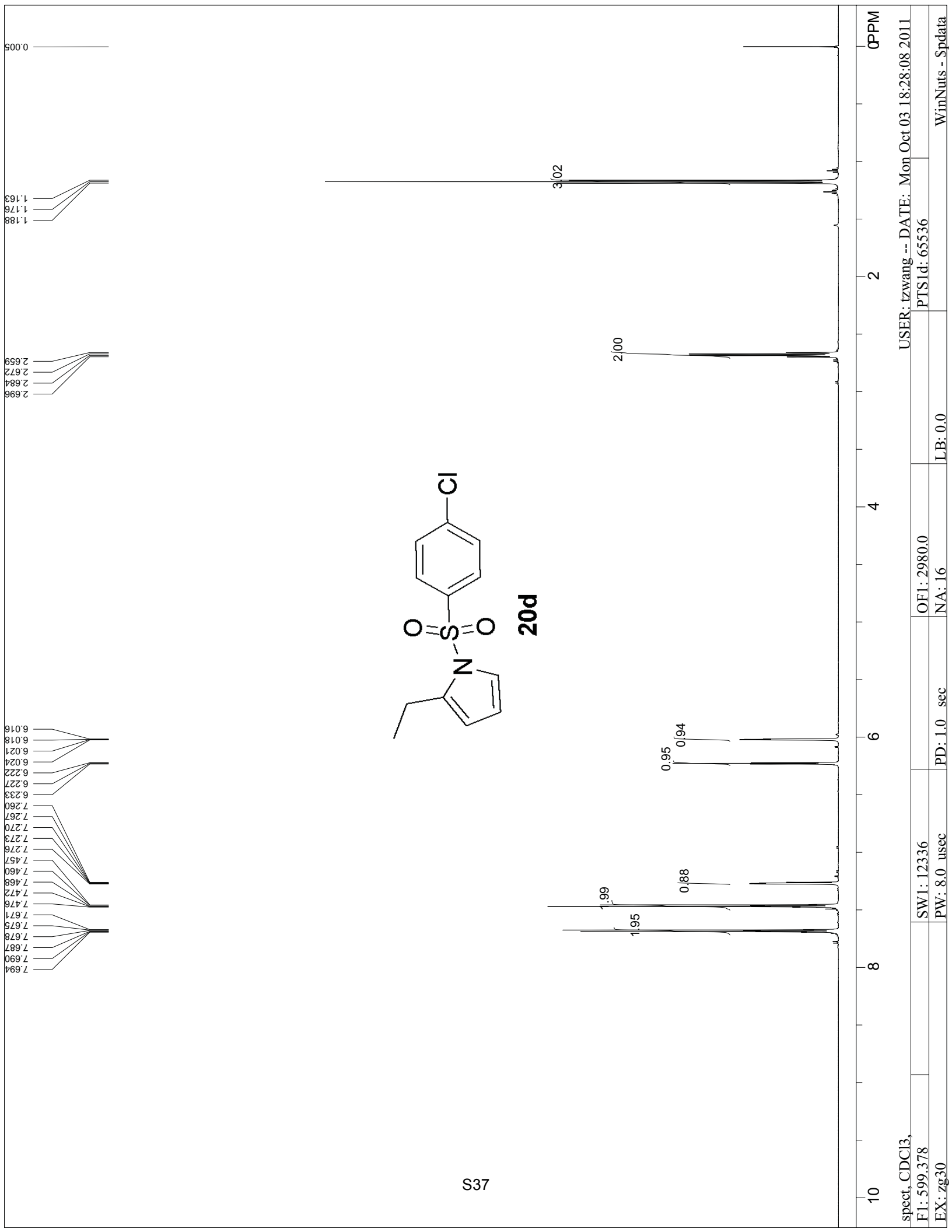
20b

spect, CDCI3,	USER: tzwang -- DATE: Wed Oct 05 16:37:57 2011
F1: 150.728	PTS1d: 32768
EX: zgdc30	LB: 0.0
SW1: 36058	OF1: 15094.7
PW: 12.0 usec	NA: 256
PD: 2.0 sec	
	WinNuts - \$pdata

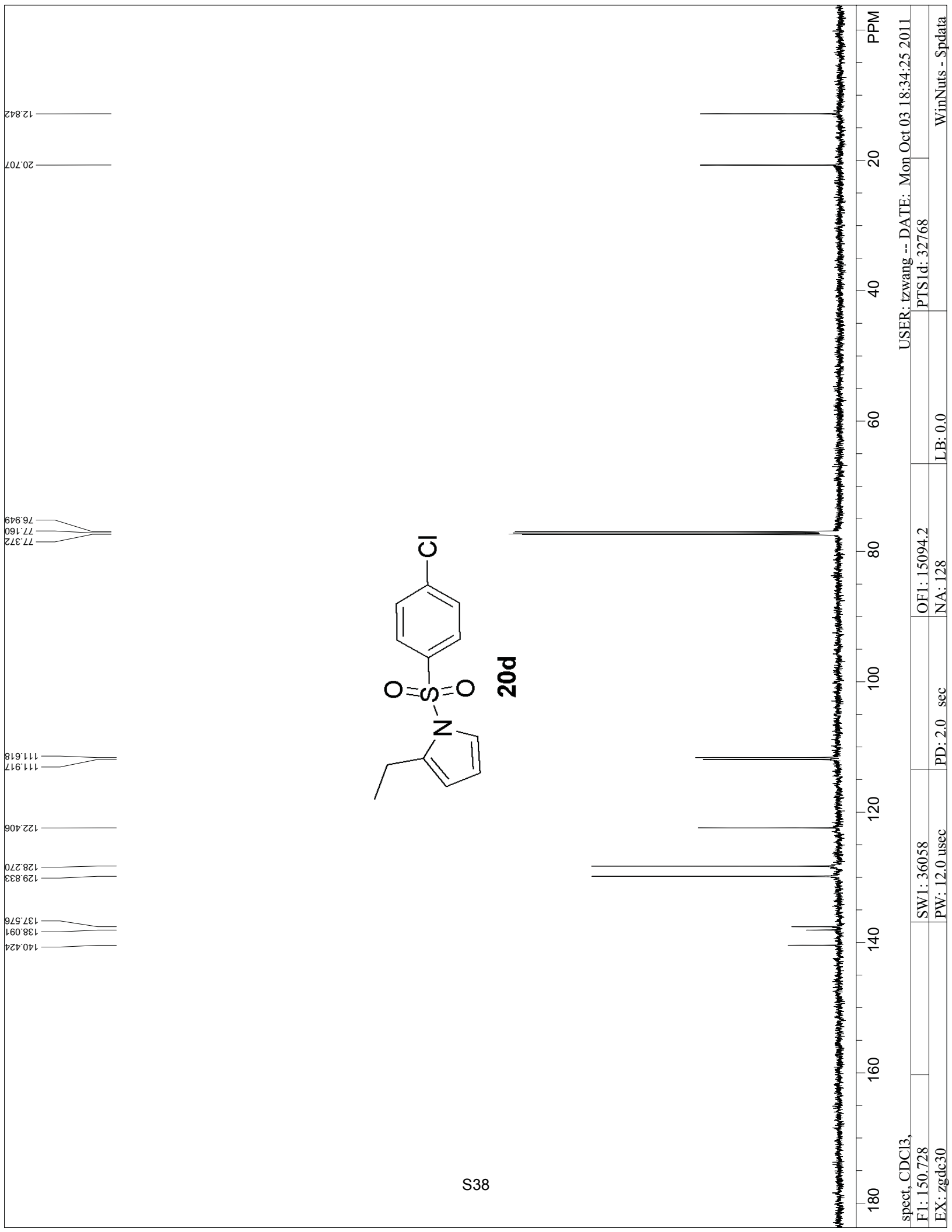


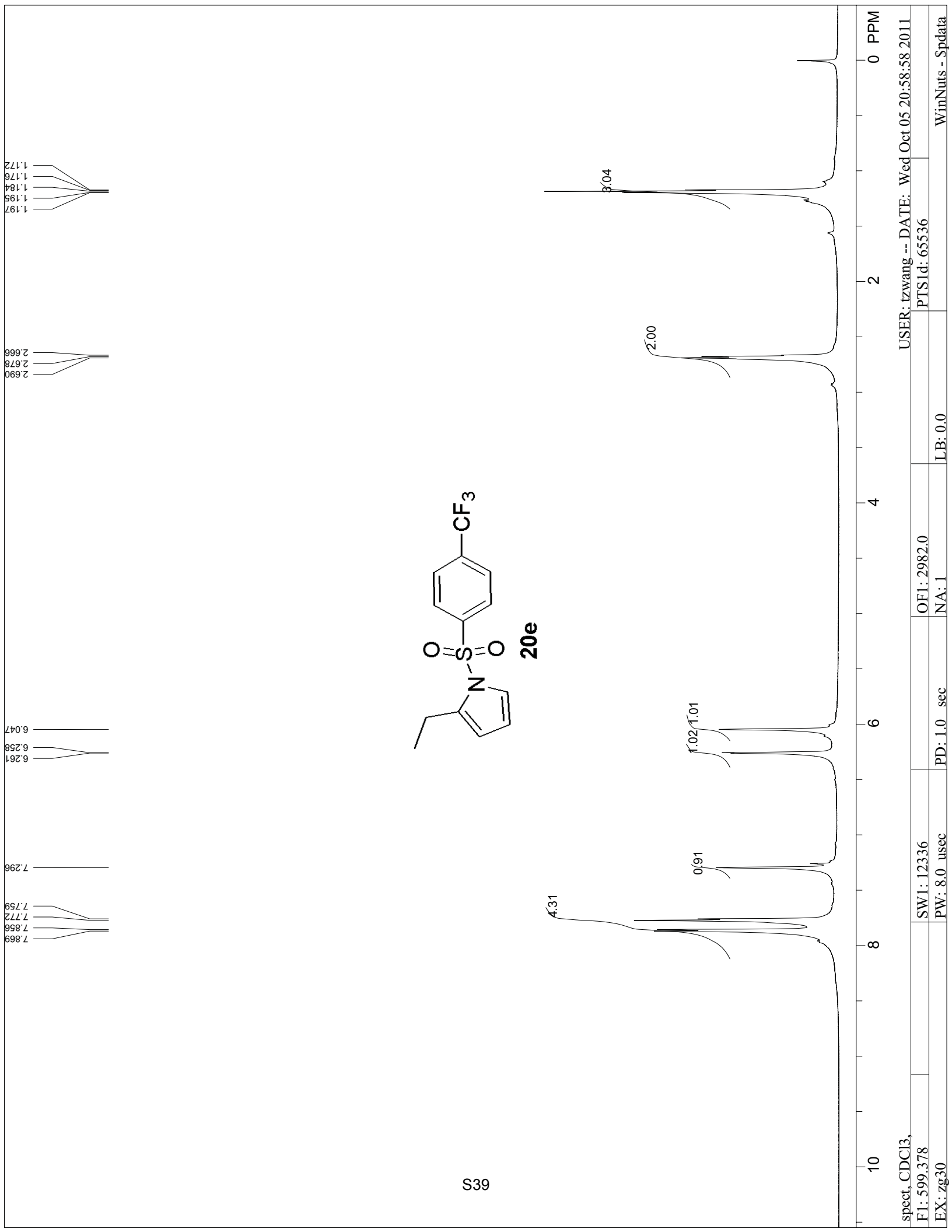
S35



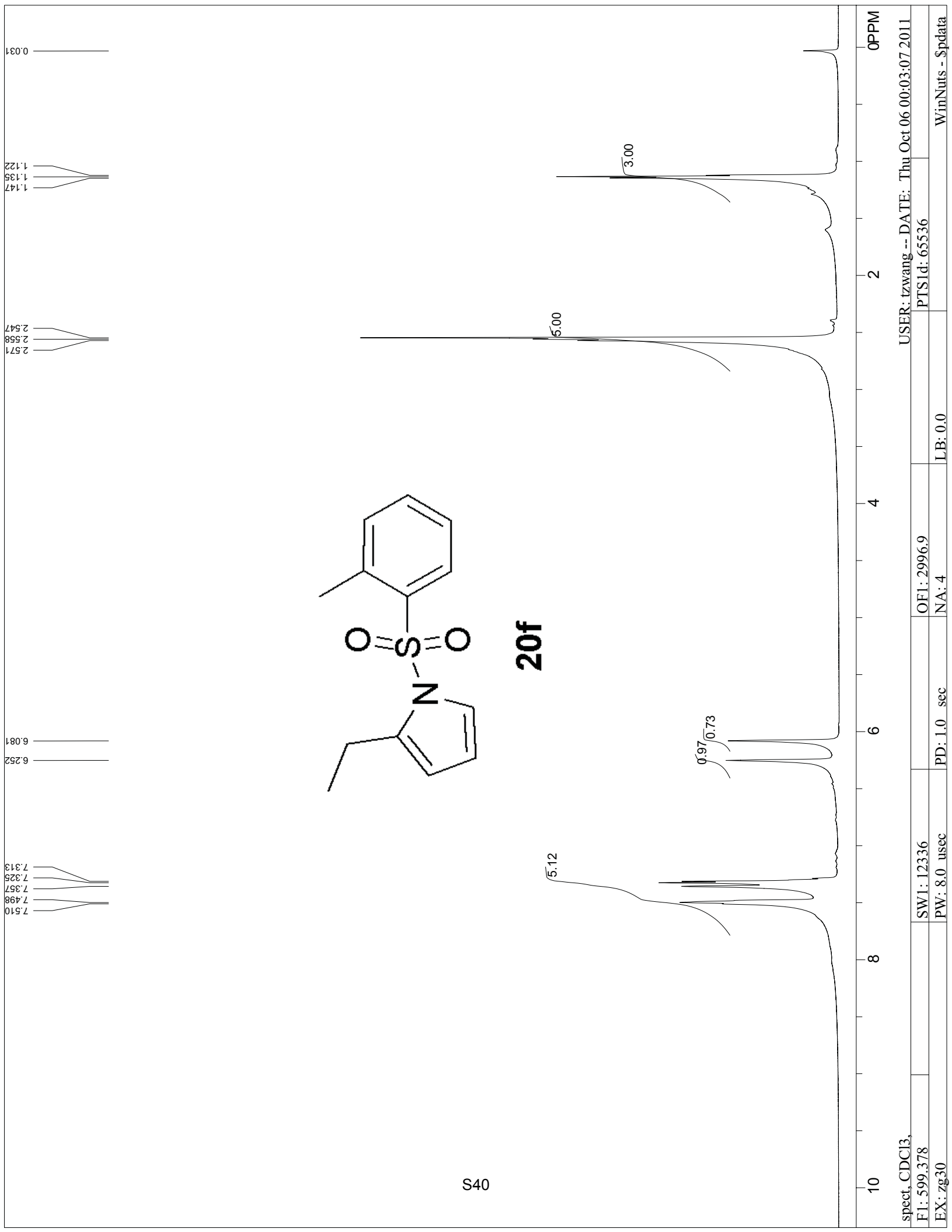


spect, CDCl3, USER: tzwang -- DATE: Mon Oct 03 18:28:08 2011
 F1: 599.378 OF1: 2980.0 PTS1d: 65536
 EX: zg30 PW: 8.0 usec PD: 1.0 sec LB: 0.0 WinNuts - \$pdata

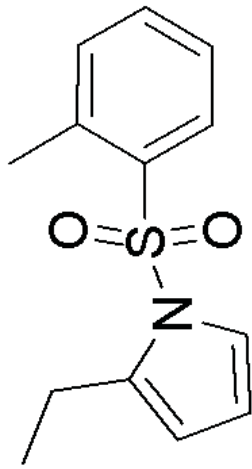
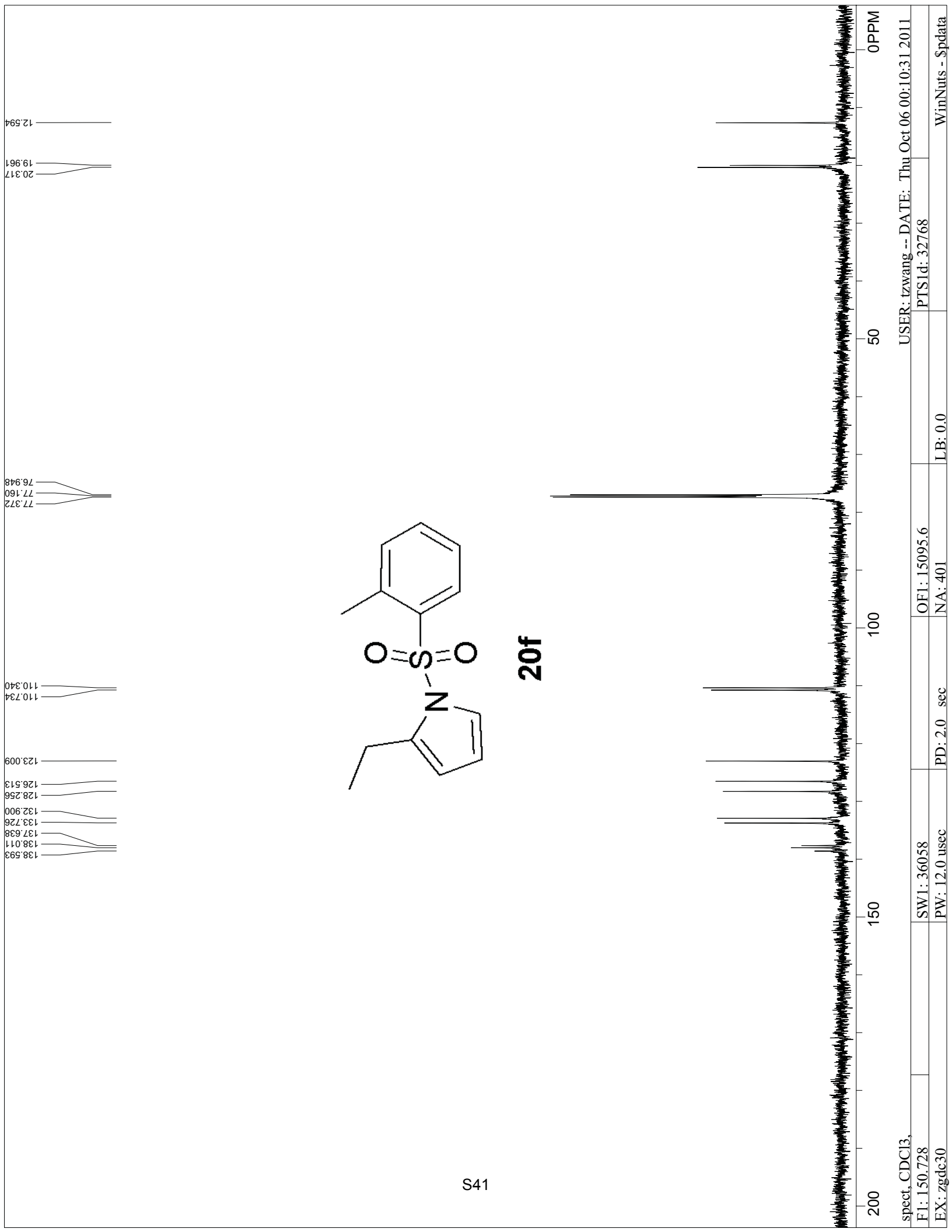




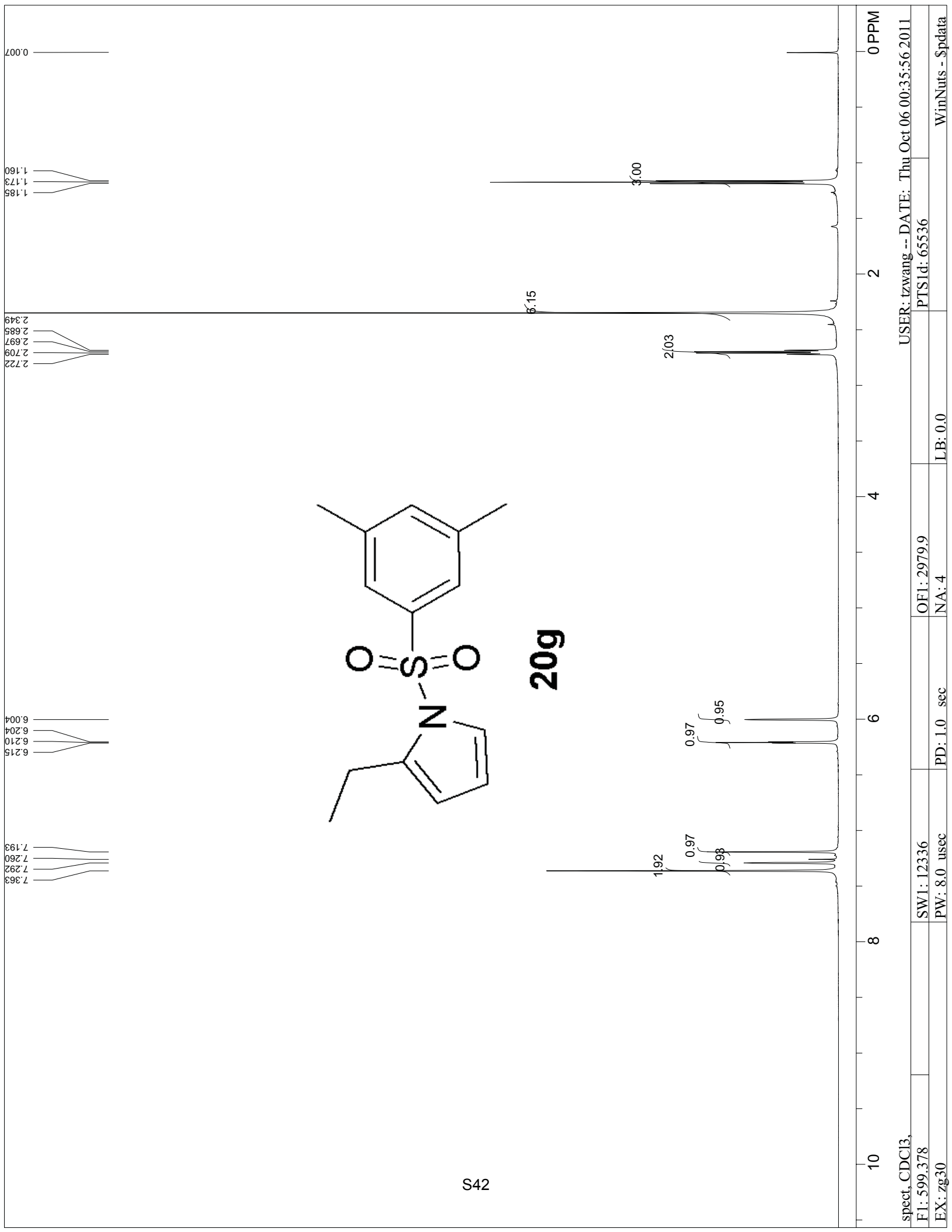
spect, CDCl3, USER: tzwang --- DATE: Wed Oct 05 20:58:58 2011
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 EX: zg30 PW: 8.0 usec PD: 1.0 sec NA: 1 LB: 0.0 WinNuts - \$pdata

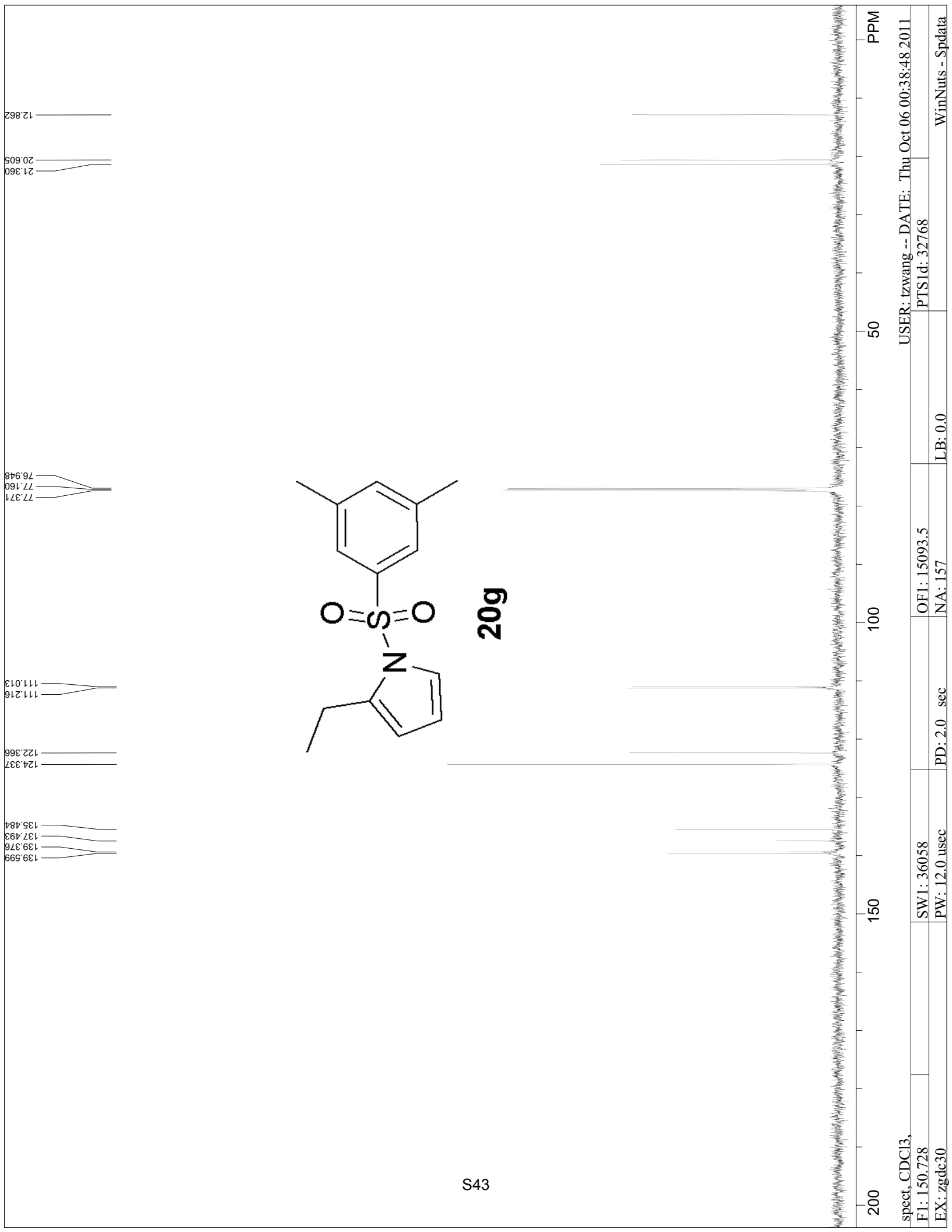


spect. CDCl3, F1: 599.378, EX: zg30, SW1: 12336, PW: 8.0 usec, OF1: 2996.9, NA: 4, PD: 1.0 sec, LB: 0.0, PTS1d: 65536, WinNuts - \$pdata, USER: tzwang -- DATE: Thu Oct 06 00:03:07 2011



20f





PPM

50

100

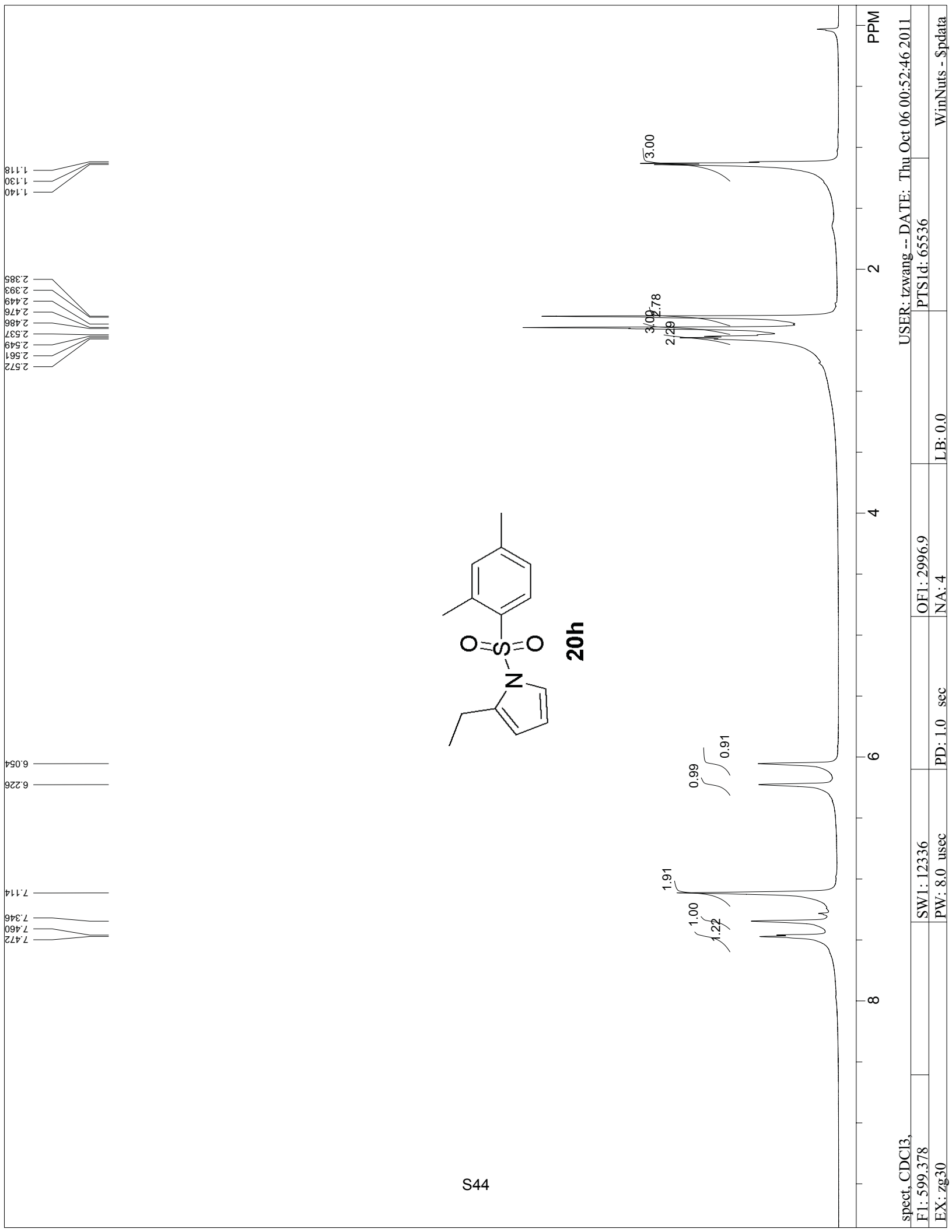
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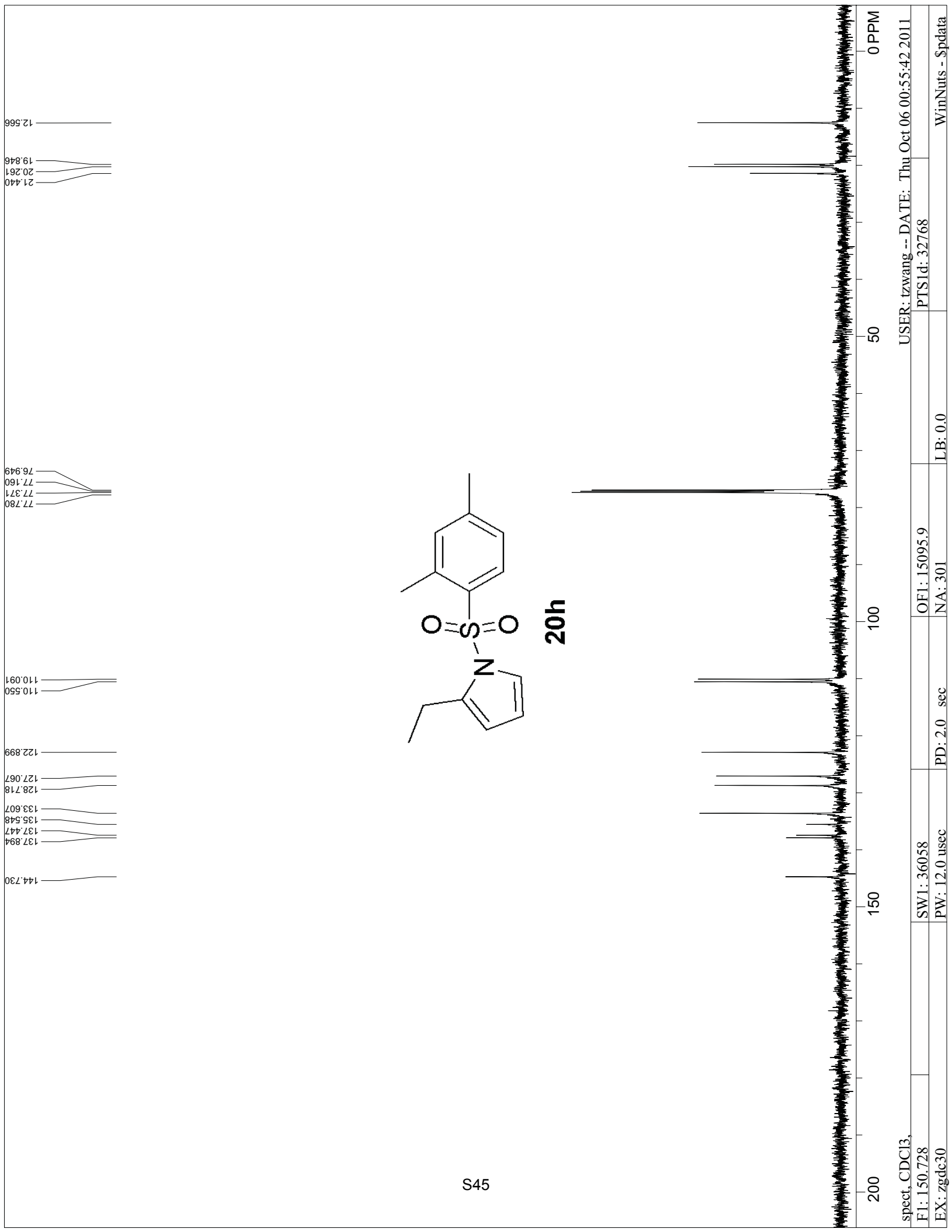
200

spect, CDCI3, USER: tzwang -- DATE: Thu Oct 06 00:38:48 2011

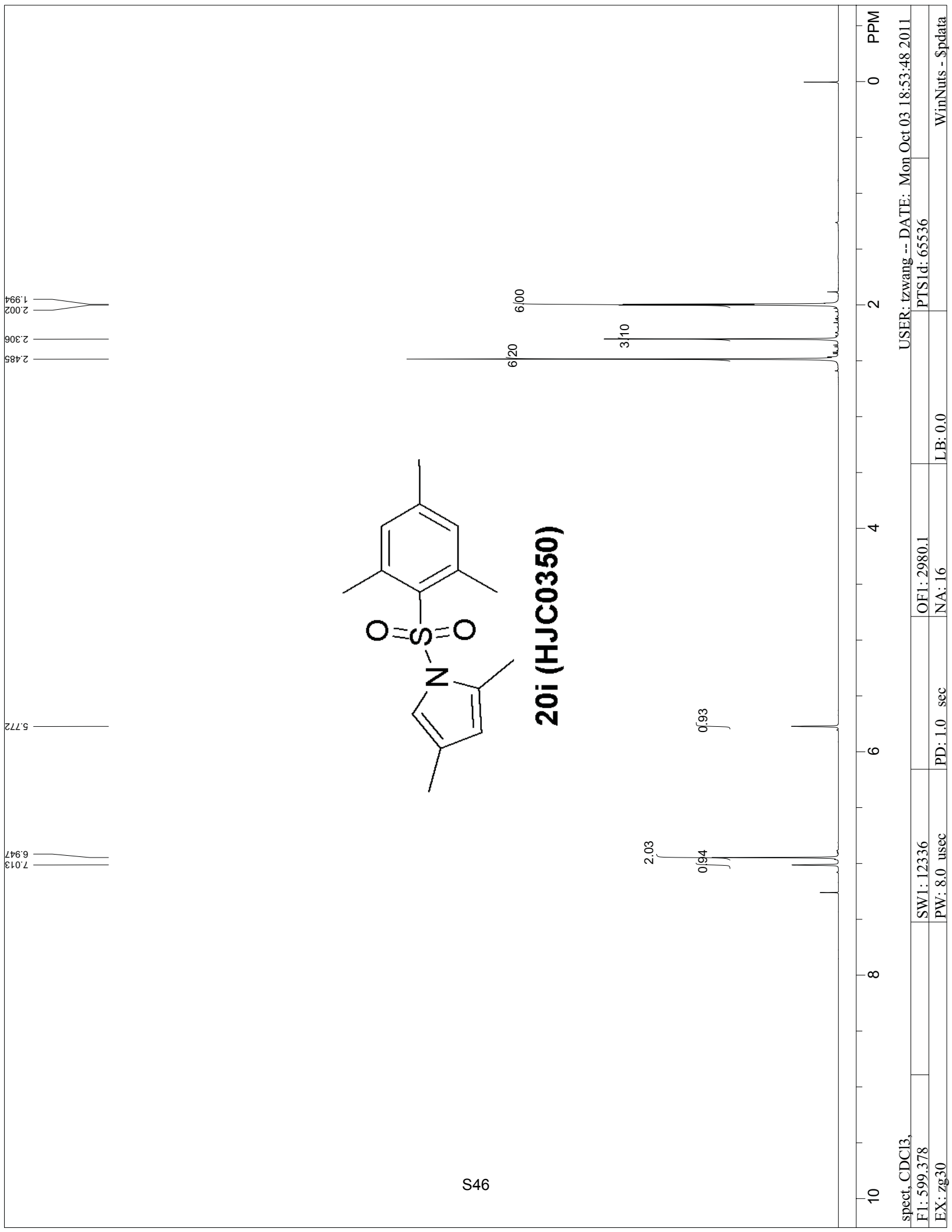
F1: 150.728 OF1: 15093.5 PTS1d: 32768

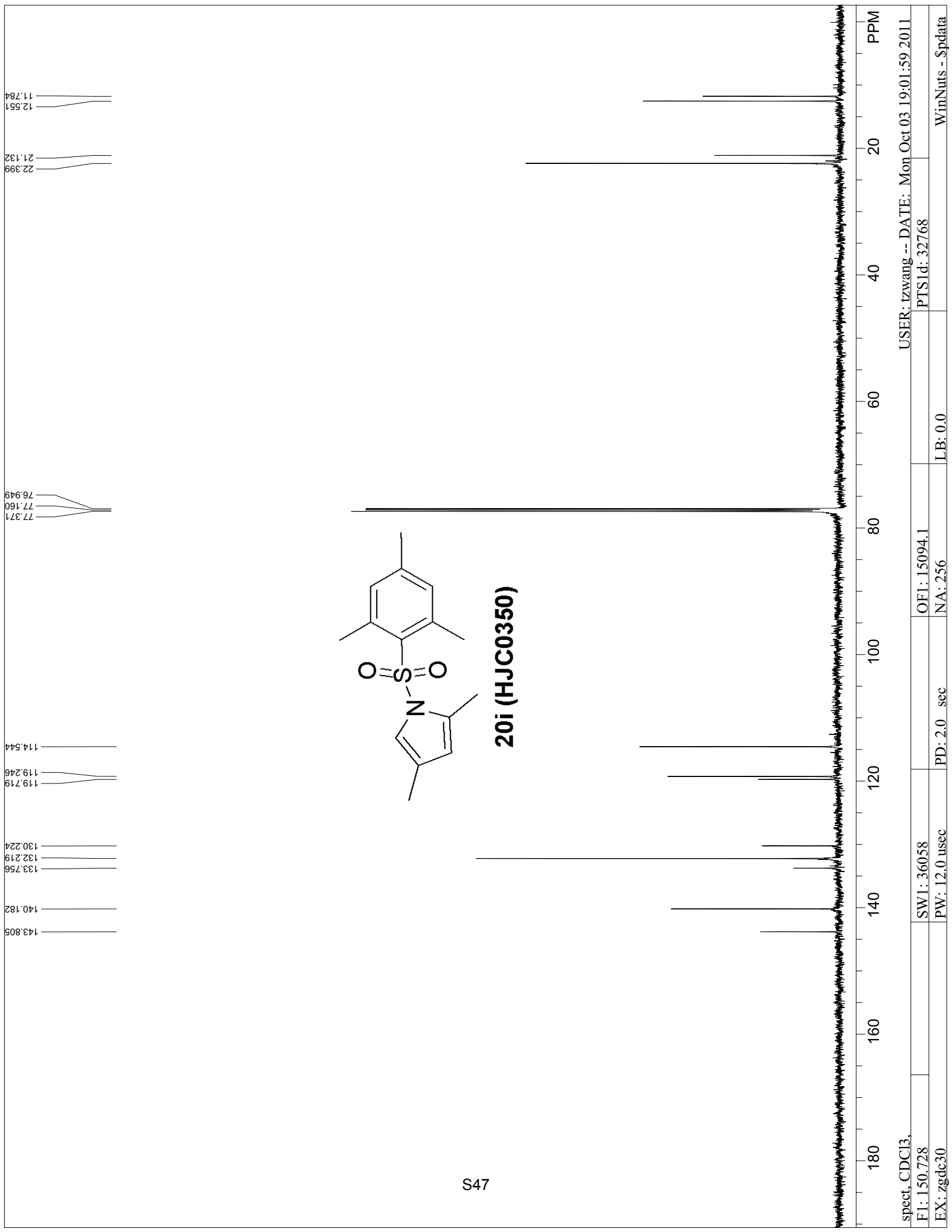
EX: zgdc30 PD: 2.0 sec LB: 0.0 WinNuts - \$pdata



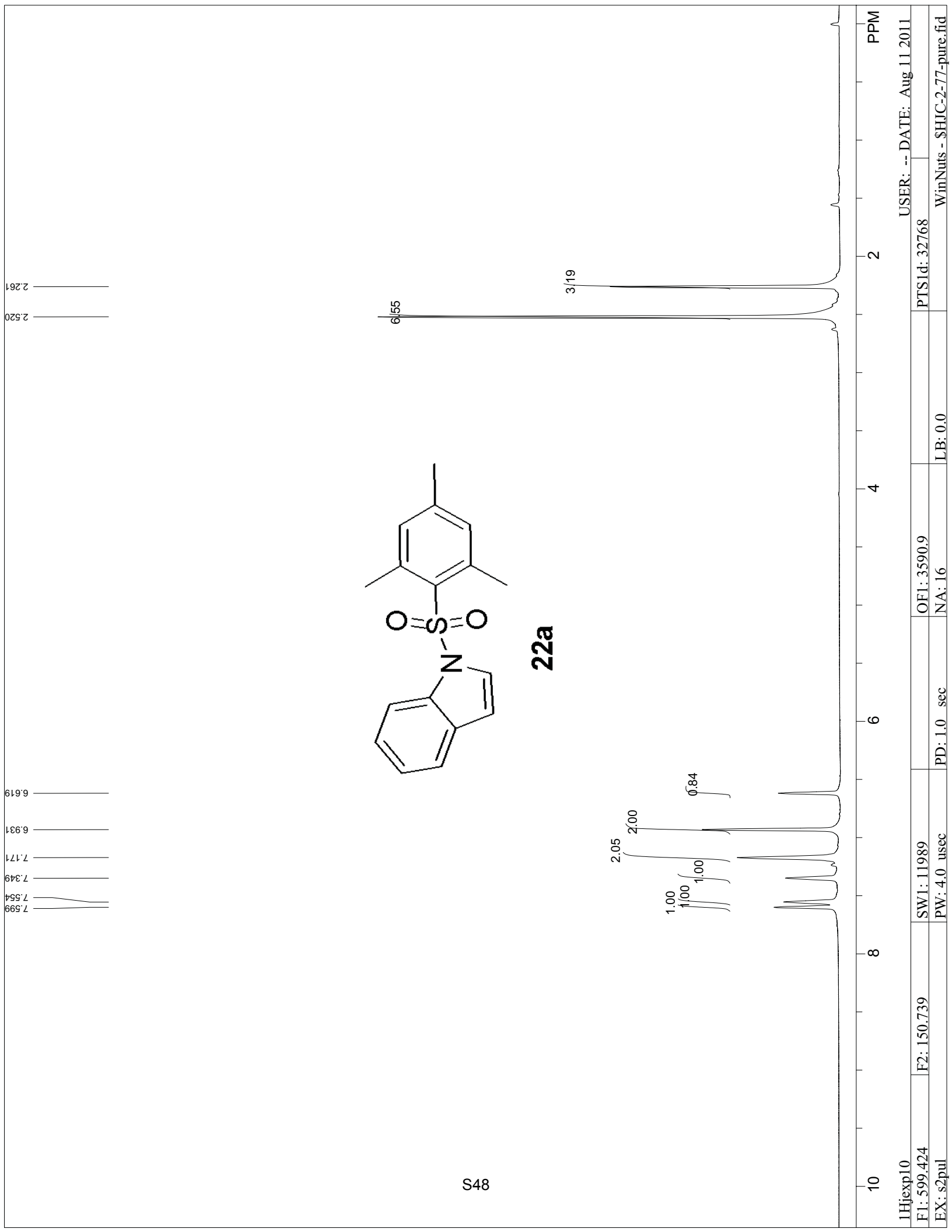


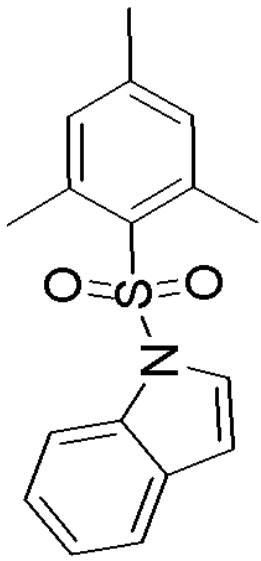
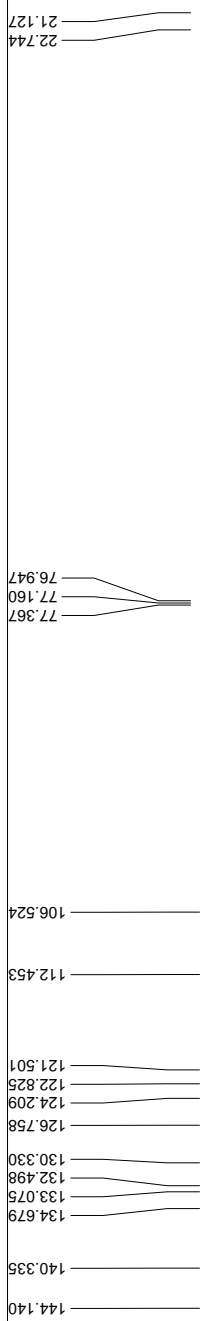
spect, CDCI3, USER: tzvwang -- DATE: Thu Oct 06 00:55:42 2011
 F1: 150.728 OF1: 15095.9 PTS1d: 32768
 EX: zgdc30 PD: 2.0 sec NA: 301 LB: 0.0 WinNuts - \$pdata



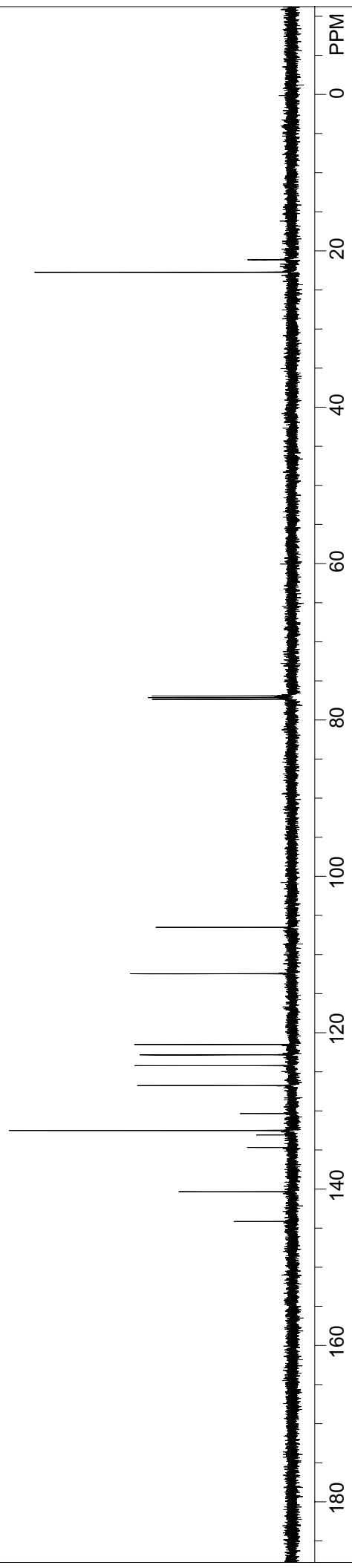


spect, CDCI3, USER: tzwang -- DATE: Mon Oct 03 19:01:59 2011
 F1: 150.728 OF1: 15094.1 PTS1d: 32768
 EX: zgdc30 PW: 12.0 usec PD: 2.0 sec LB: 0.0 WinNuts - \$pdata

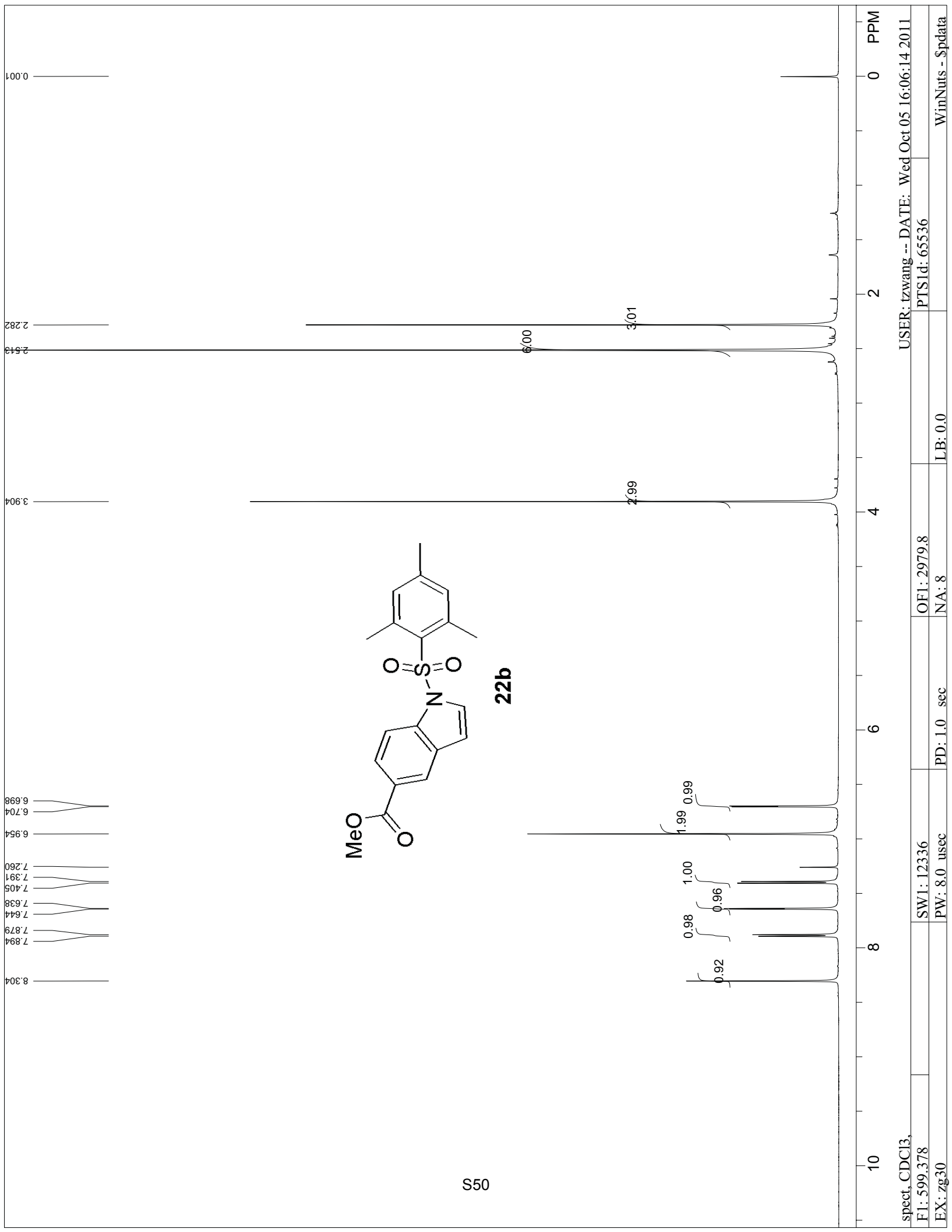




22a



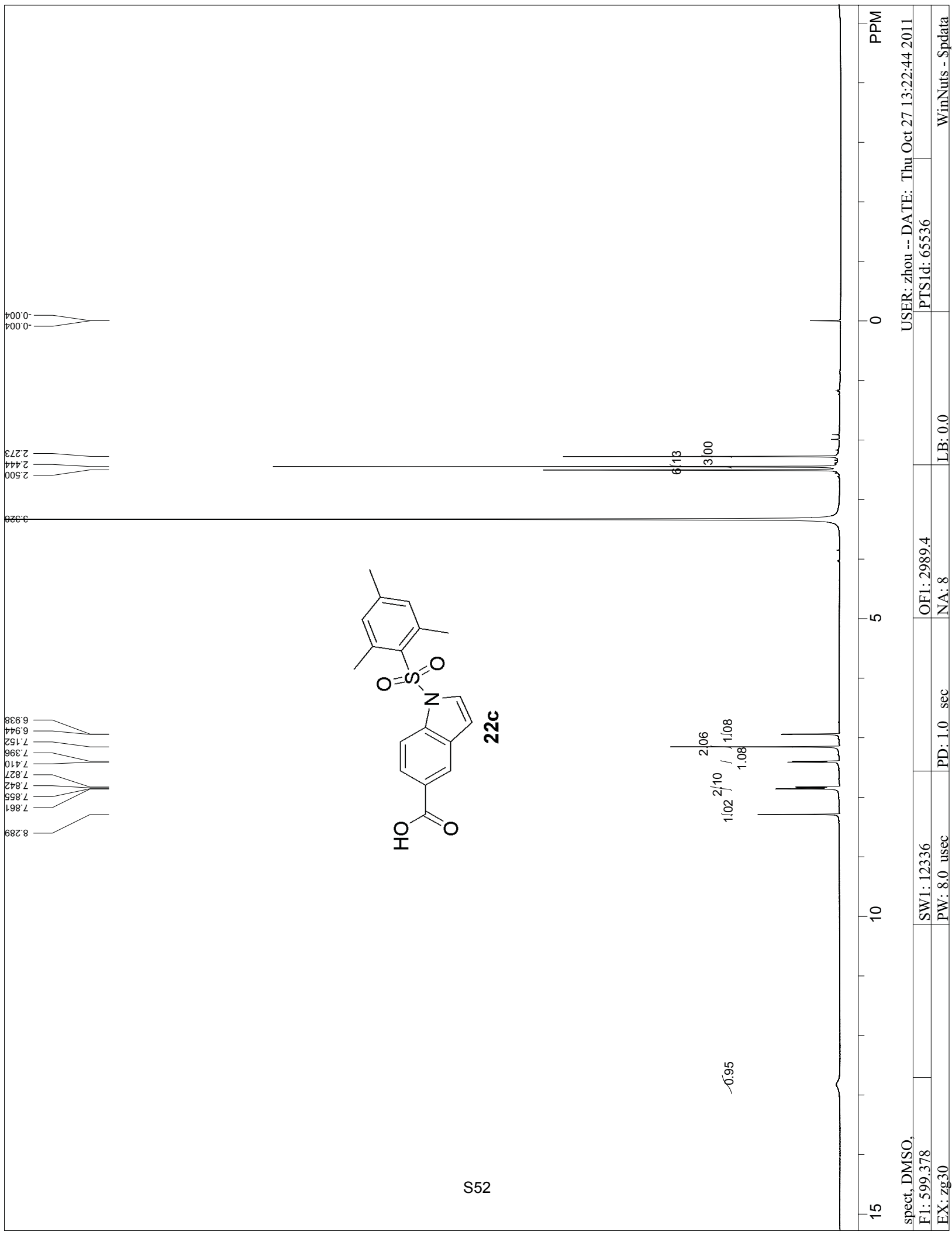
Std carbon	USER: -- DATE: Aug 11 2011
F1: 150.738	PTS1d: 32768
F2: 599.423	OF1: 13303.8
EX: s2pul	NA: 512
	LB: 0.0
	PD: 1.0 sec
	PW: 8.0 usec
	SW1: 29996
	WinNuts - \$HIC-2-77C-pure-2.fid



S50

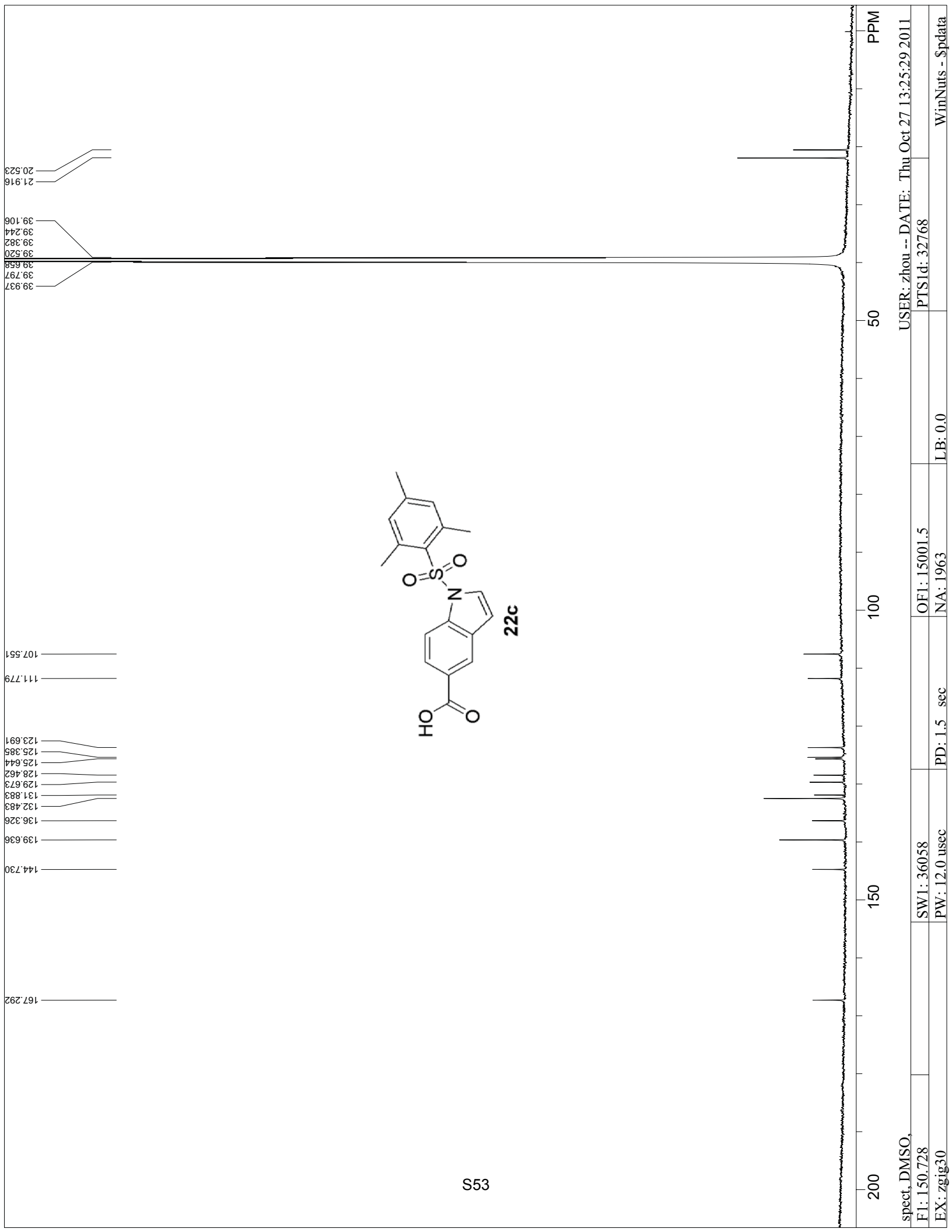


spect, CDCI3, USER: tzwang -- DATE: Wed Oct 05 16:09:53 2011
 F1: 150.728 PTS1d: 32768
 EX: zgdc30 LB: 0.0 OF1: 15092.0 NA: 256
 PD: 2.0 sec SW1: 36058 PW: 12.0 usec
 WinNuts - \$pdata



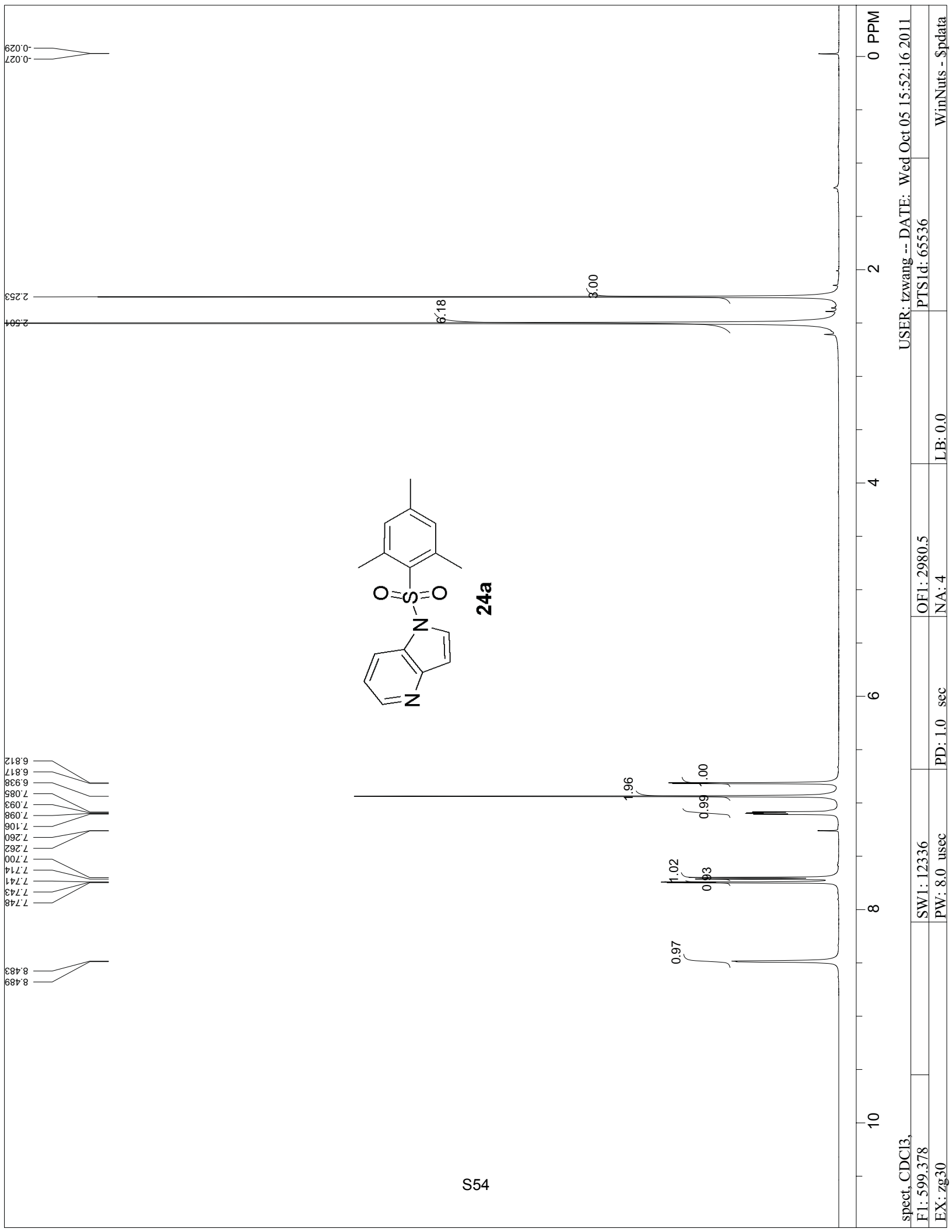
S52

spect, DMSO, USER: zhou -- DATE: Thu Oct 27 13:22:44 2011
 F1: 599.378 OF1: 2989.4 PTS1d: 65536
 EX: zg30 PW: 8.0 usec PD: 1.0 sec NA: 8 LB: 0.0 WinNuts - \$pdata

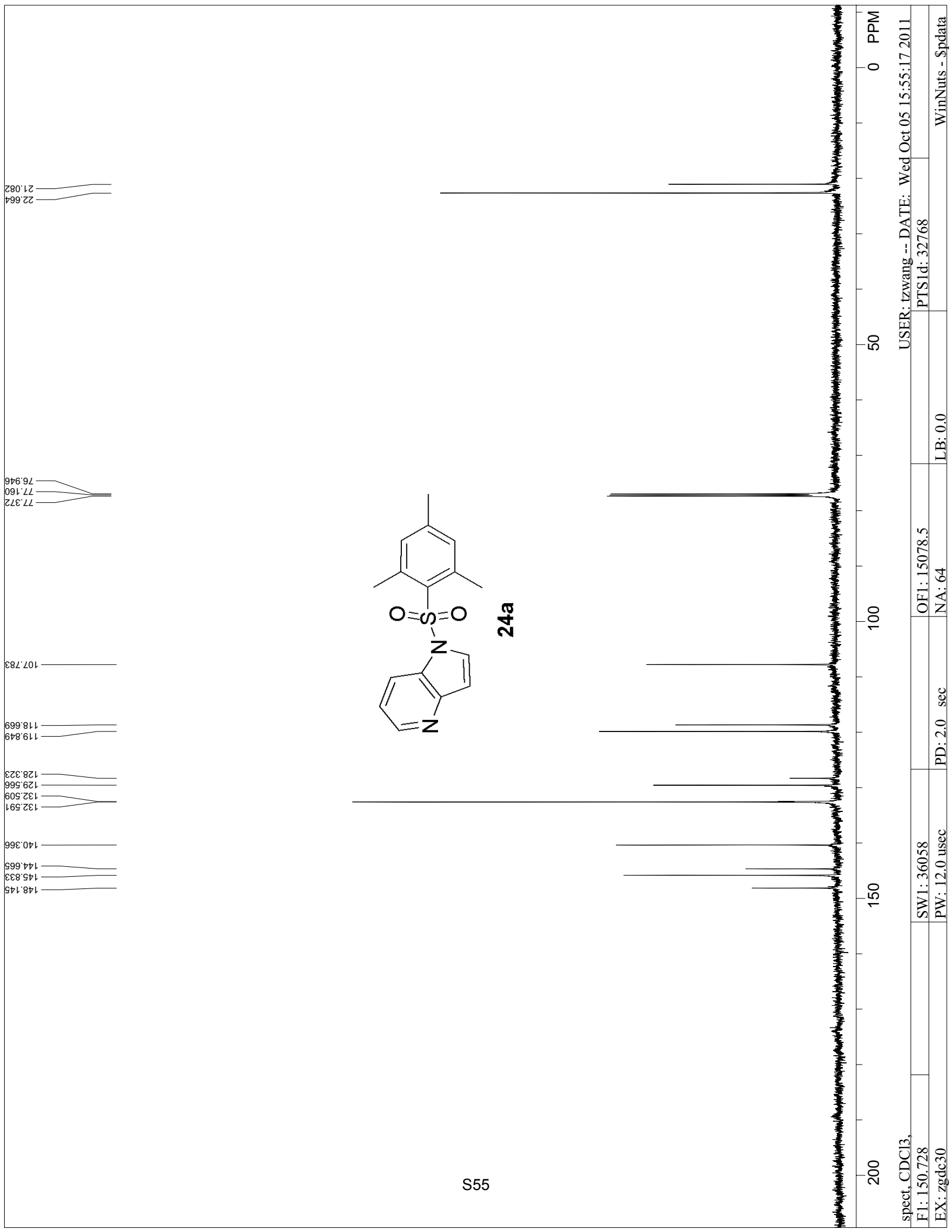


S53

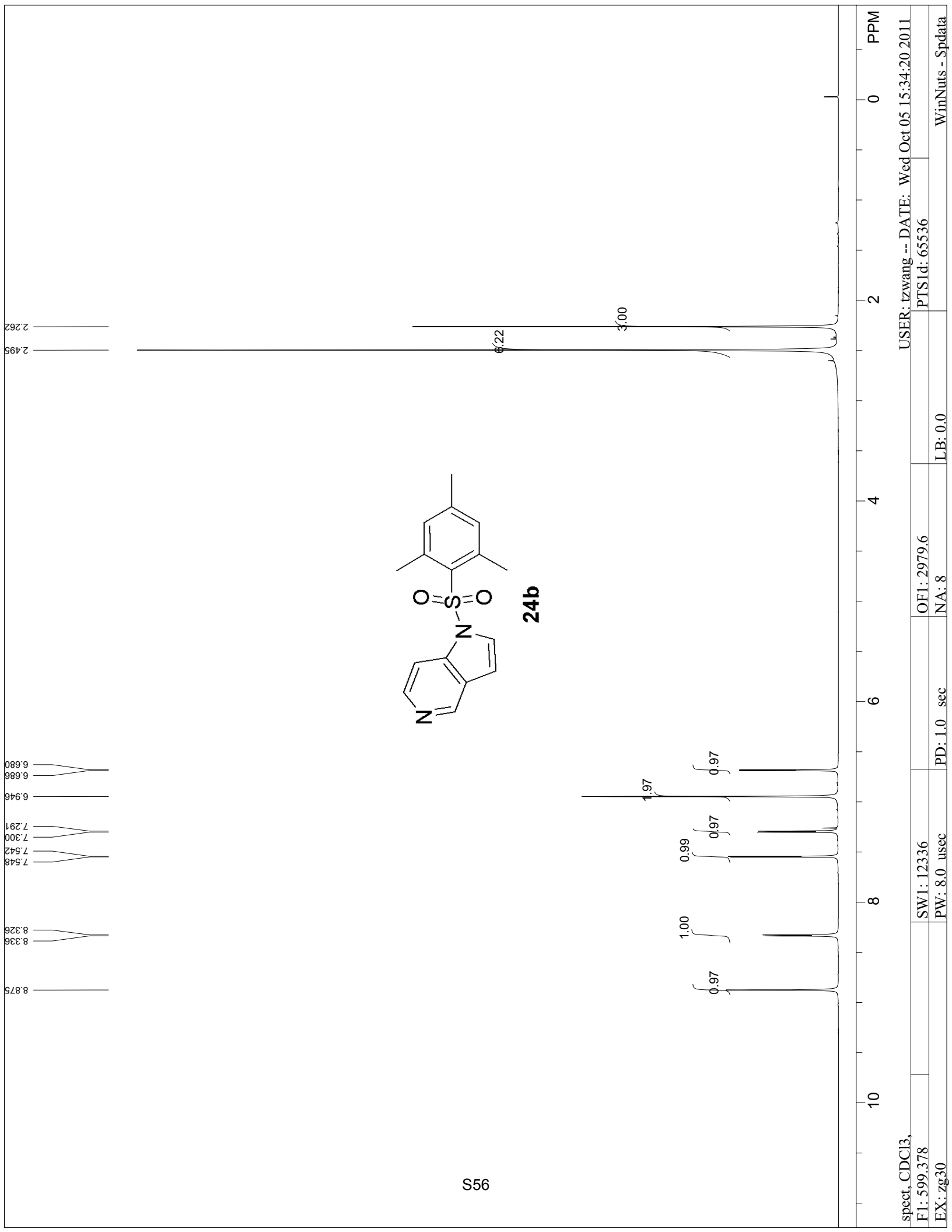
spect, DMSO,	USER: zhou -- DATE: Thu Oct 27 13:25:29 2011
F1: 150.728	PTS1d: 32768
EX: zgig30	LB: 0.0
SW1: 36058	OF1: 15001.5
PW: 12.0 usec	NA: 1963
PD: 1.5 sec	
	WinNuts - \$pdata

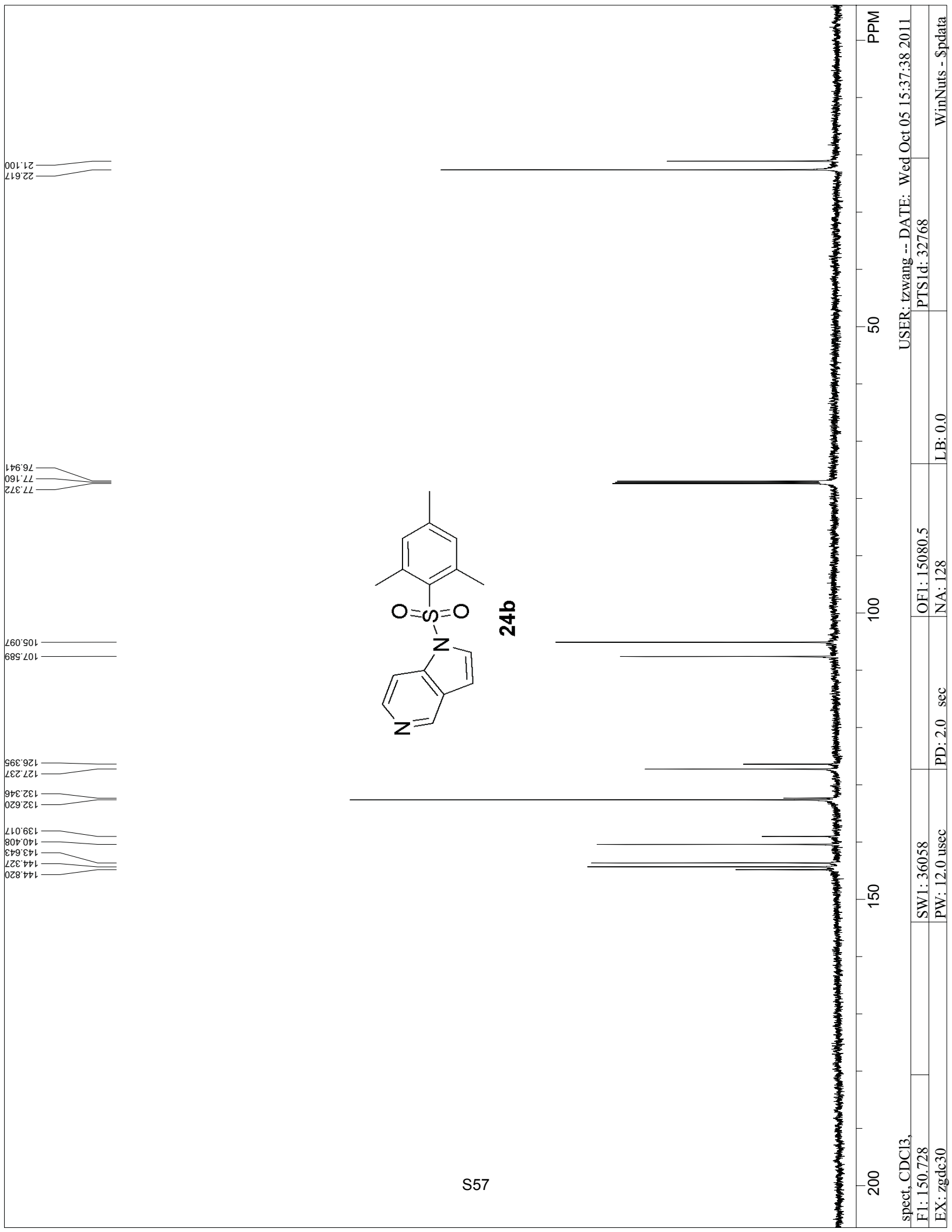


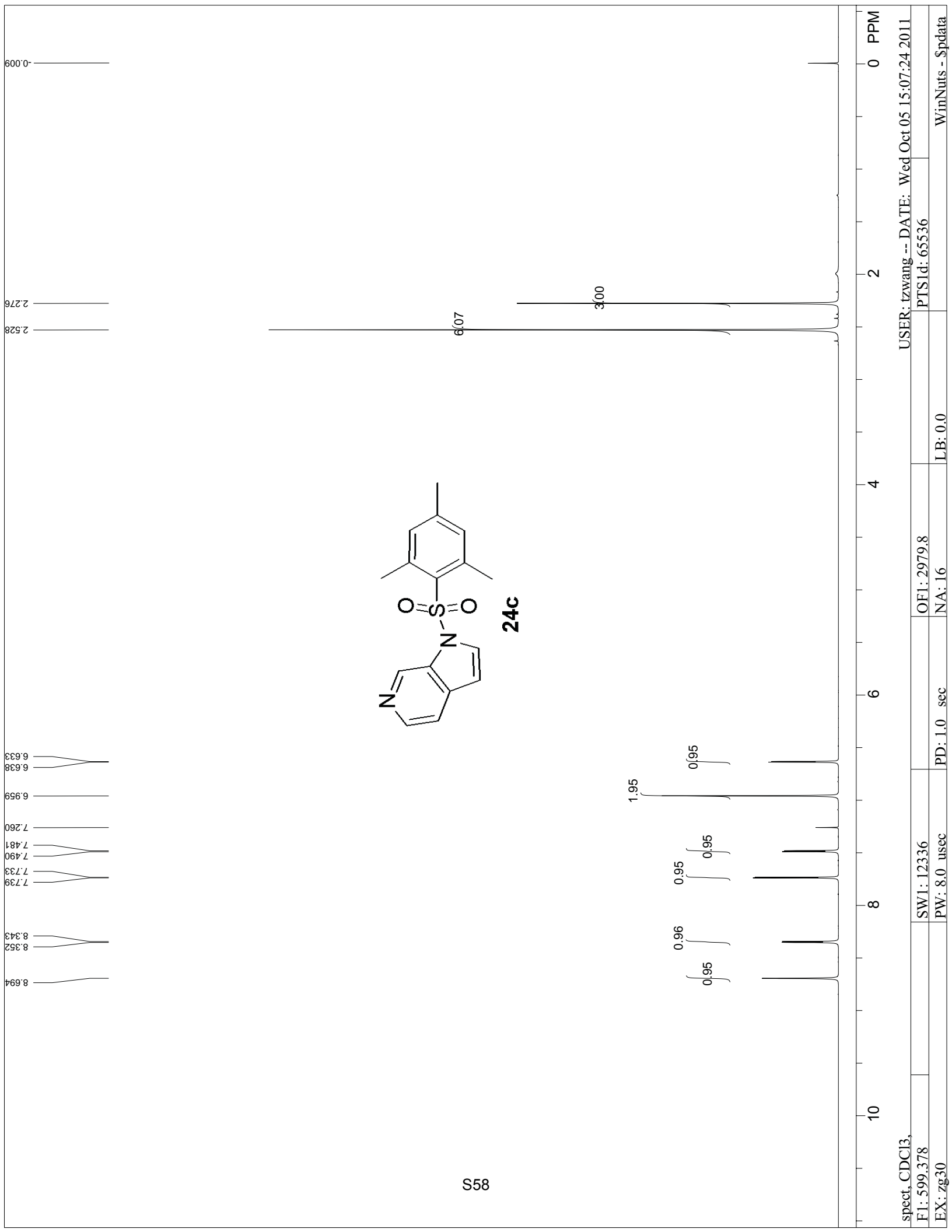
S54



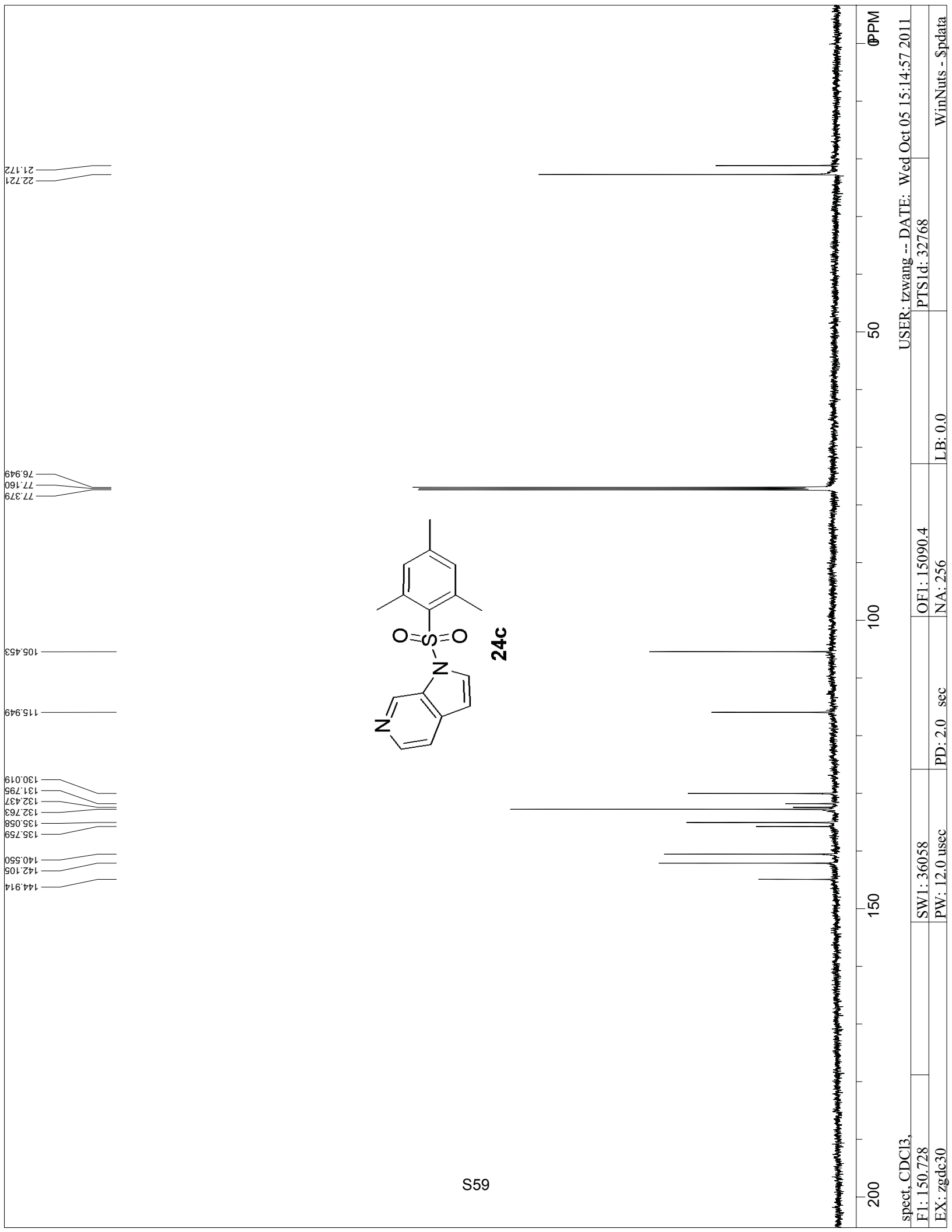
spect, CDCl3, USER: tzwang -- DATE: Wed Oct 05 15:55:17 2011
 F1: 150.728 OF1: 15078.5 PTS1d: 32768
 EX: zgdc30 PD: 2.0 sec NA: 64 LB: 0.0 WinNuts - \$pdata





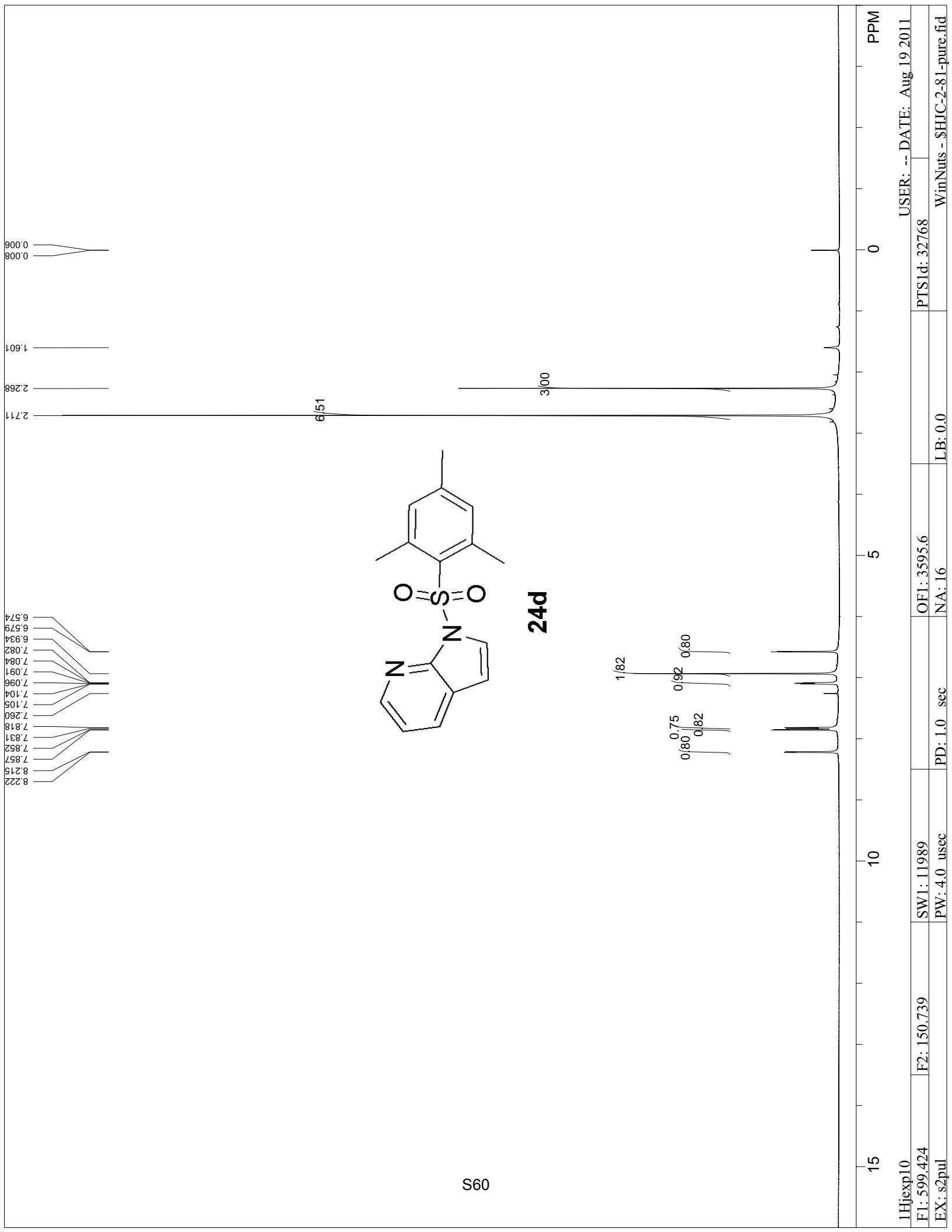


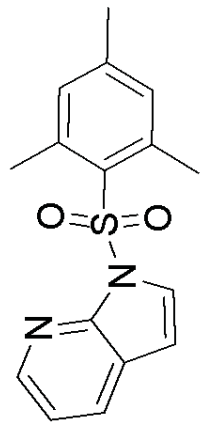
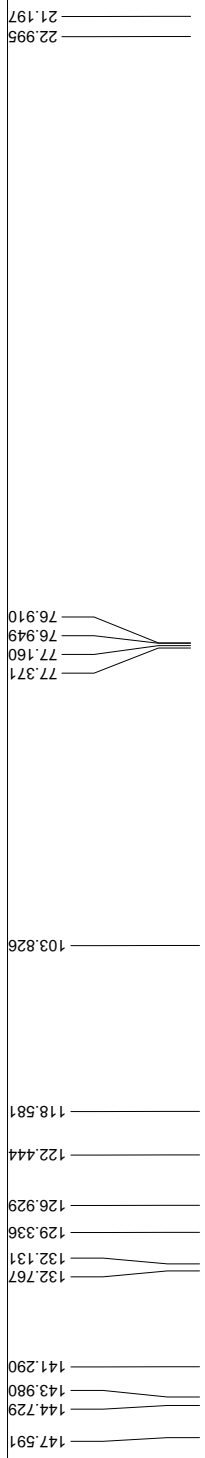
S58



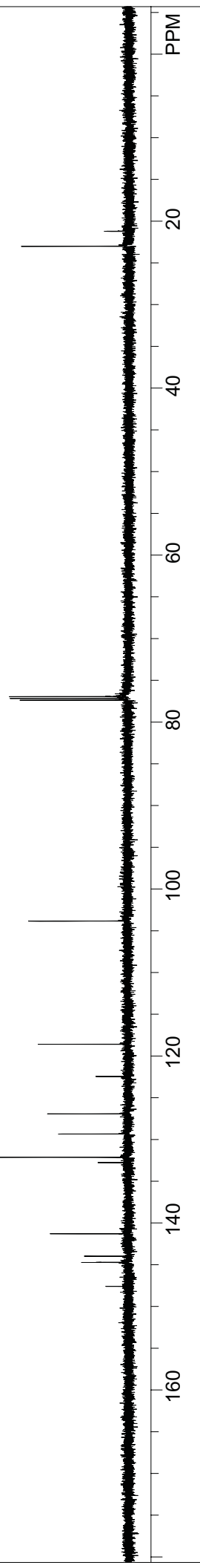
S59

200	150	100	50	0 PPM
spect, CDCI3,				USER: tzwang -- DATE: Wed Oct 05 15:14:57 2011
F1: 150.728	SW1: 36058	OF1: 15090.4	PTS1d: 32768	
EX: zgdc30	PW: 12.0 usec	PD: 2.0 sec	NA: 256	LB: 0.0
				WinNuts - \$pdata





24d



Std carbon	USER: --	DATE: Aug 19 2011
F1: 150.738	PTS1d: 32768	
EX: s2pul	LB: 0.0	WinNuts - \$HIC-2-81C-pure-2.fid
	OF1: 13306.0	
	NA: 512	
	PD: 1.0 sec	
	SW1: 29996	
	PW: 8.0 usec	