

SUPPORTING INFORMATION FOR

**Regio- and Stereo-selective Syntheses of the Natural Product  
CCR5 Antagonist Anibamine and its Three Olefin Isomers**

**Feng Zhang, Saheem Zaidi, Kendra M. Haney, Glen E. Kellogg, Yan Zhang\***

*Department of Medicinal Chemistry, Virginia Commonwealth  
University, 800 E. Leigh Street, Richmond, VA 23298, USA*

*Email address: yzhang2@vcu.edu*

**HPLC methods and purity test results:  
Spectra:**

**S2-S10  
S11-S96**

**HPLC methods and purity analysis results:**

HPLC System: Varian Prostar;

Column: Microsorb 100-5 CN (250 × 10 mm);

Injection Volume: 15 -20 µL;

Sample Concentrations: 0.1 – 1.2 mg/0.5 mL in mobile phase;

Single wavelength: 254 nm;

Eluent: acetonitrile (0.5% TFA)/water (60:40) at 4 mL/min over 30 min.

**Table. HPLC purity analysis of target compounds**

<b>Compounds</b>	<b>Compounds code in spectrum</b>	<b>Time (min)</b>	<b>Purity (%)</b>
1	VZAB001	11.438	97.02
2	VZAB002	14.930	96.54
3	VZAB046	11.386	99.39
4	VZAB047	11.770	97.73

vzab001\_fz-1

Title : VZAB001  
Run File : c:\star\data\yy\anibamine analogs final  
result\vzab001-009\redo\vzab001\_fz.run  
Method File : c:\star\data\yy\anibamine analogs final  
result\vzab001-009\redo\vzab001\_fz-1.mth  
Sample ID : Manual Sample

Injection Date: 2011-2-2 11:58 Calculation Date: 2011-2-2 12:34

Operator : Yan Zhang Group Detector Type: 0325  
Workstation: D9288P71 Bus Address : 44  
Instrument : Varian Star #1 Sample Rate : 20.00 Hz  
Channel : 1 = 254 nm Run Time : 30.000 min

\*\* LC Workstation Version 6.41 \*\* 03046-67D0-AE7-0264 \*\*

Run Mode : Analysis  
Peak Measurement: Peak Area  
Calculation Type: Percent

Peak No.	Peak Name	Result (%)	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		2.9828	4.668	0.000	128569	BB	5.5	
2		97.0172	11.438	0.000	4181743	BB	19.6	
Totals:		100.0000		0.000	4310312			

Total Unidentified Counts : 4310312 counts

Detected Peaks: 2 Rejected Peaks: 0 Identified Peaks: 0

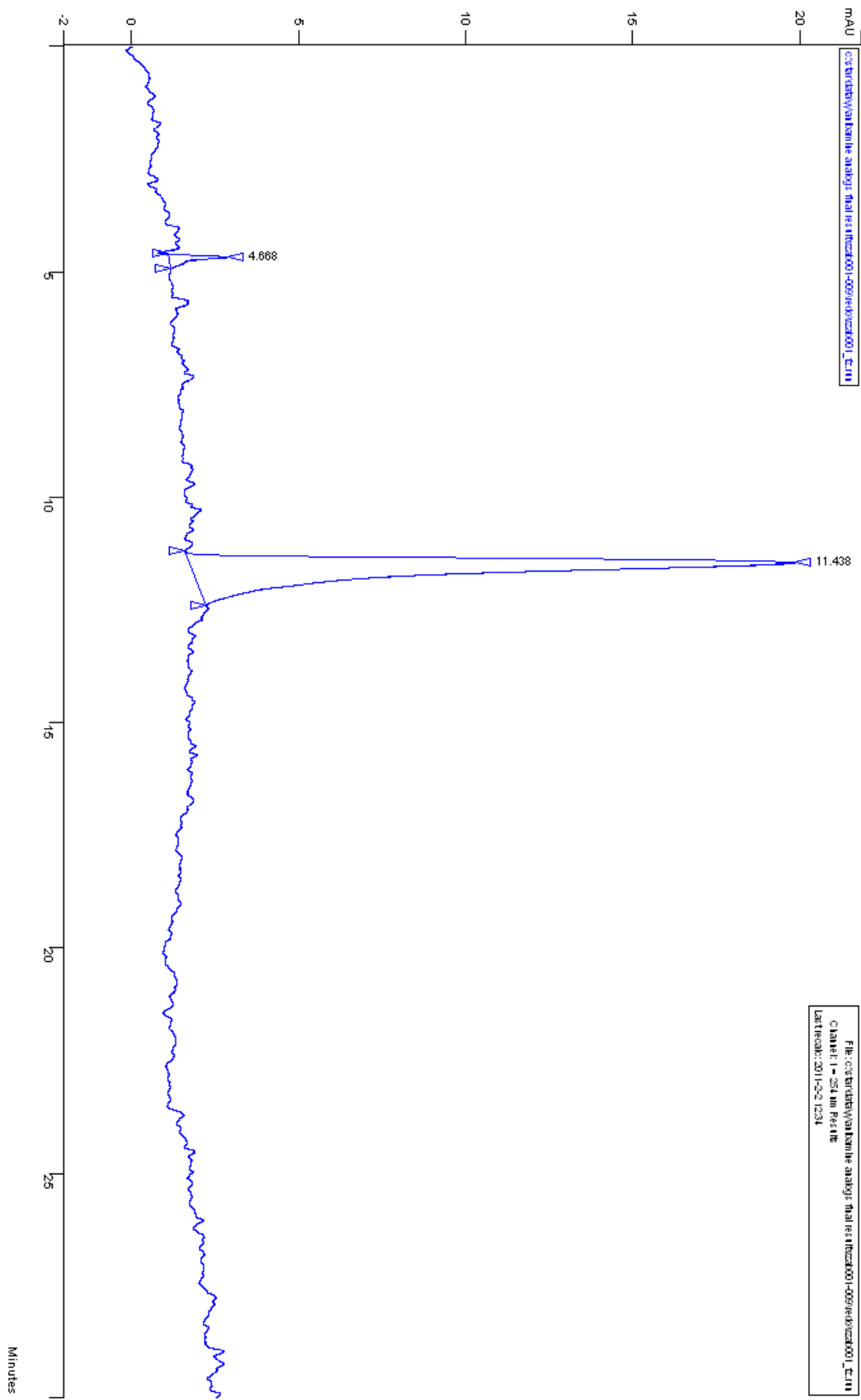
Multiplier: 1 Divisor: 1 Unidentified Peak Factor: 0

Baseline Offset: 0 microAU LSB: 0.1 microAU

Noise (used): 1 microAU - monitored before this run

Manual injection

\*\*\*\*\*



VZAB002\_1\_FZ

File c:\star\data\yy\anibamine analogs final result\vzab002\_1\_fz.run Filetype  
325

WTOASCII Parameters: C:\star\WTOASCII.TXT

1 channels  
 Channel 1 254 nm in AU  
 Base rate 20.0000 Hz Bunch 1 Effective rate 20.00000 Hz. T = 0.000833 min.  
 36000 points from 0.000 to 30.000 minutes  
 Sampling every 4 point(s)  
 Printing points from 0.000 to 30.000 min, point 0 to 35999  
 Channels 1 to 1  
 Results for Channel 1 = 254 nm  
 Title: Report Title  
 Run File: c:\star\data\yy\anibamine analogs final result\vzab002\_1\_fz.run

-----  
 Injection Info  
 -----

Method: C:\star\data\YY\40H2060MeCN4m130MIN.mth  
 Sample: Manual Sample  
 Injection Date: Fri Oct 29 10:53:26 2010  
 Manual injection  
 Operator: Yan Zhang Group  
 Instrument: Varian Star #1  
 Notes:

-----  
 Misc Info  
 -----

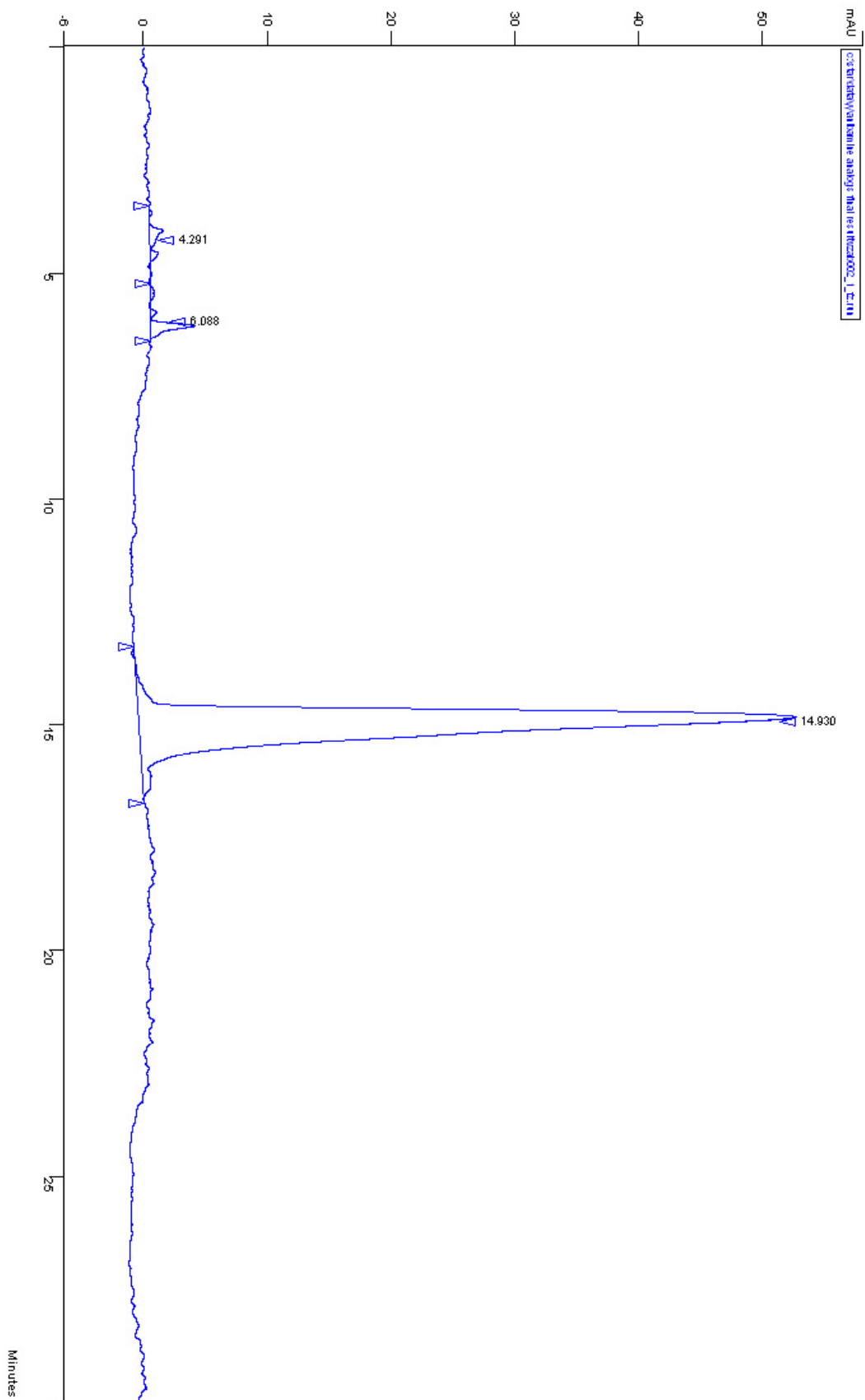
Workstation: D9288P71  
 Bus Address: 44  
 Run Time: 0.000 to 30.000 min.

-----  
 Recalc Info  
 -----

Recalc Method: c:\star\data\yy\anibamine analogs final result\vzab002\_1\_fz-1.mth  
 Recalc Date: Fri Nov 19 09:20:20 2010  
 Operator: Yan Zhang Group  
 Instrument: Varian Star #1  
 Notes:  
 Sample Rate: 20.000 Hz.  
 Measurement Type: 1 = Area  
 Calculation Type: 1 = %  
 Normalize Results: Yes

-----  
 Peak Info for Channel 1  
 -----

3 Peaks (tR	Time offset	RRT	SePCODE	width	Counts	Result)
4.291	0.000	0.0000	BP	21.98	233477	1.197045
6.088	0.000	0.0000	PB	16.92	441300	2.262559
14.930	0.000	0.0000	BB	33.28	18829690	96.540390



vzab046-1

Title : VZAB046  
Run File : c:\star\data\yy\anibamine analogs final  
result\vzab013\_027-029\_040-047\vzab046.run  
Method File : c:\star\data\yy\anibamine analogs final result\vzab046-1.mth  
Sample ID : Manual Sample

Injection Date: 2011-3-2 13:56 Calculation Date: 2011-3-2 15:16

Operator : Yan Zhang Group Detector Type: 0325  
Workstation: D9288P71 Bus Address : 44  
Instrument : Varian Star #1 Sample Rate : 20.00 Hz  
Channel : 1 = 254 nm Run Time : 30.000 min

\*\* LC Workstation Version 6.41 \*\* 03046-67D0-AE7-0264 \*\*

Run Mode : Analysis  
Peak Measurement: Peak Area  
Calculation Type: Percent

Peak No.	Peak Name	Result (%)	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		0.0705	3.716	0.000	67740	BV	10.7	
2		0.0573	3.807	0.000	55093	VV	0.0	
3		0.1759	4.097	0.000	169084	VV	13.0	
4		0.0807	4.513	0.000	77613	VV	12.5	
5		0.0723	4.651	0.000	69519	VV	0.0	
6		0.0866	4.787	0.000	83230	VB	15.6	
7		0.0622	10.510	0.000	59800	BV	13.9	
8		99.3944	11.386	0.000	95533896	VB	45.2	
Totals:		99.9999		0.000	96115975			

Total Unidentified Counts : 96115976 counts

Detected Peaks: 8 Rejected Peaks: 0 Identified Peaks: 0

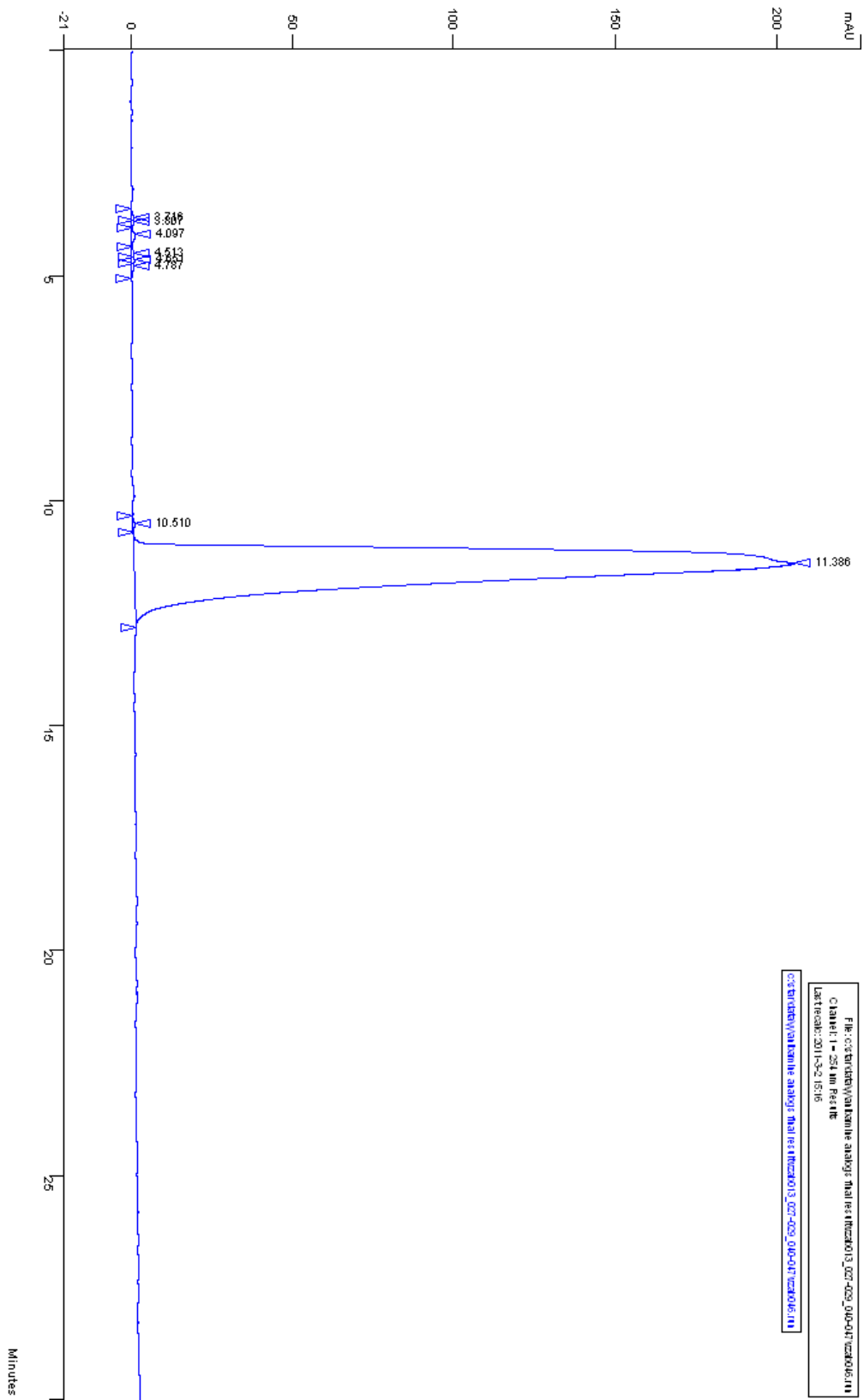
Multiplier: 1 Divisor: 1 Unidentified Peak Factor: 0

Baseline Offset: 0 microAU LSB: 0.1 microAU

Noise (used): 4 microAU - monitored before this run

Manual injection

\*\*\*\*\*



File: c:\tandem\va\kamin\analogs\mal\ref\rt\rt2013\_027-029\_010-017\rt2013\_011  
 Channel: 1 - 254 nm FWHM  
 Last Peak: 2011-02-15 15:16  
 c:\tandem\va\kamin\analogs\mal\ref\rt\rt2013\_027-029\_010-017\rt2013\_011



vzab047-1

Title : VZAB047  
Run File : c:\star\data\yy\anibamine analogs final  
result\vzab013\_027-029\_040-047\vzab047.run  
Method File : c:\star\data\yy\anibamine analogs final result\vzab047-1.mth  
Sample ID : Manual Sample

Injection Date: 2011-3-2 14:28 Calculation Date: 2011-3-2 15:19

Operator : Yan Zhang Group Detector Type: 0325  
Workstation: D9288P71 Bus Address : 44  
Instrument : Varian Star #1 Sample Rate : 20.00 Hz  
Channel : 1 = 254 nm Run Time : 30.000 min

\*\* LC Workstation Version 6.41 \*\* 03046-67D0-AE7-0264 \*\*

Run Mode : Analysis  
Peak Measurement: Peak Area  
Calculation Type: Percent

Peak No.	Peak Name	Result (%)	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		1.7222	11.404	0.000	277011	BV	11.8	
2		97.7347	11.770	0.000	15720707	VB	32.4	
3		0.5431	13.618	0.000	87366	BB	12.9	
Totals:		100.0000		0.000	16085084			

Total Unidentified Counts : 16085084 counts

Detected Peaks: 3 Rejected Peaks: 0 Identified Peaks: 0

Multiplier: 1 Divisor: 1 Unidentified Peak Factor: 0

Baseline Offset: 0 microAU LSB: 0.1 microAU

Noise (used): 1 microAU - monitored before this run

Manual injection

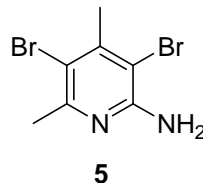
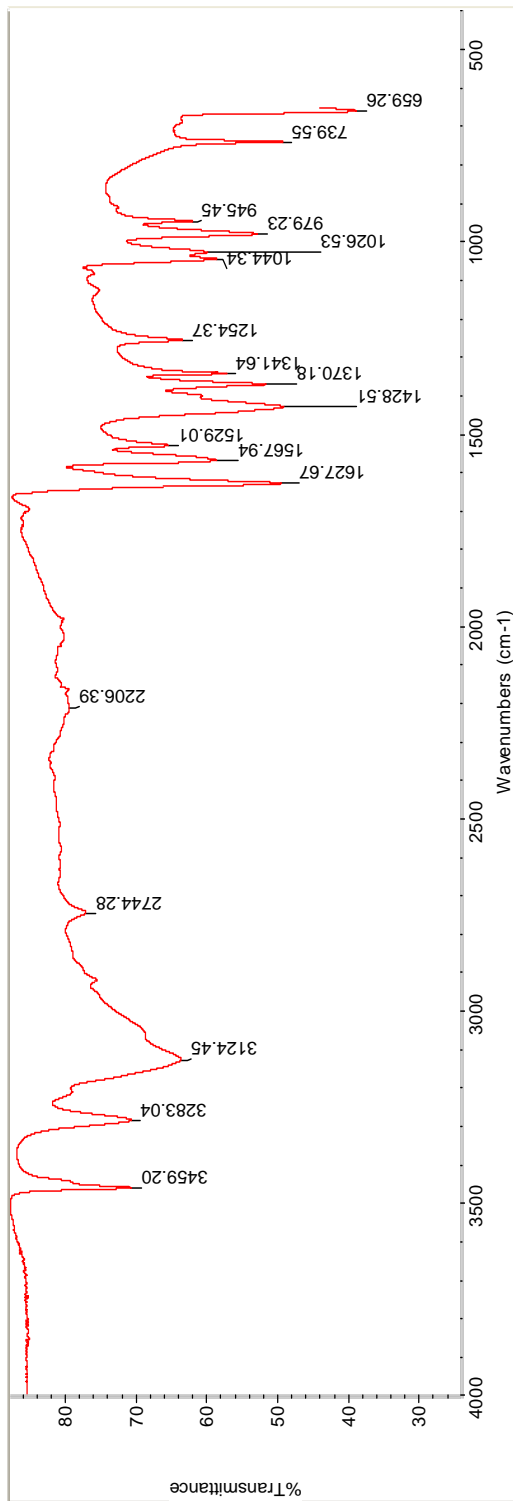
\*\*\*\*\*



Compound 5	-----	Experimnetal code <b>FZ-I-55</b>
Compound 6	-----	Experimnetal code <b>FZ-I-44</b>
Compound 7	-----	Experimnetal code <b>FZ-II-23</b>
Compound 8	-----	Experimnetal code <b>FZ-IV-34</b>
Compound 9	-----	Experimnetal code <b>FZ-I-26</b>
Compound 10	-----	Experimnetal code <b>FZ-IV-47</b>
Compound 11	-----	Experimnetal code <b>FZ-II-33</b>
Compound 12	-----	Experimnetal code <b>FZ-I-83</b>
Compound 13	-----	Experimnetal code <b>FZ-II-70</b>
Compound 14	-----	Experimnetal code <b>FZ-II-72</b>
Compound 1	-----	Experimnetal code <b>FZ-II-74</b>
Compound 15	-----	Experimnetal code <b>FZ-I-32</b>
Compound 16	-----	Experimnetal code <b>FZ-II-67</b>
Compound 17	-----	Experimnetal code <b>FZ-II-68</b>
Compound 2	-----	Experimnetal code <b>FZ-II-21</b>
Compound 18	-----	Experimnetal code <b>FZ-IV-29-1</b>
Compound 19	-----	Experimnetal code <b>FZ-IV-29-2</b>
Compound 20	-----	Experimnetal code <b>FZ-V-03</b>
Compound 21	-----	Experimnetal code <b>FZ-V-04</b>
Compound 3	-----	Experimnetal code <b>FZ-V-05</b>
Compound 22	-----	Experimnetal code <b>FZ-V-06</b>
Compound 23	-----	Experimnetal code <b>FZ-V-07</b>
Compound 4	-----	Experimnetal code <b>FZ-V-08</b>

Thu Apr 14 17:49:37 2011 (G

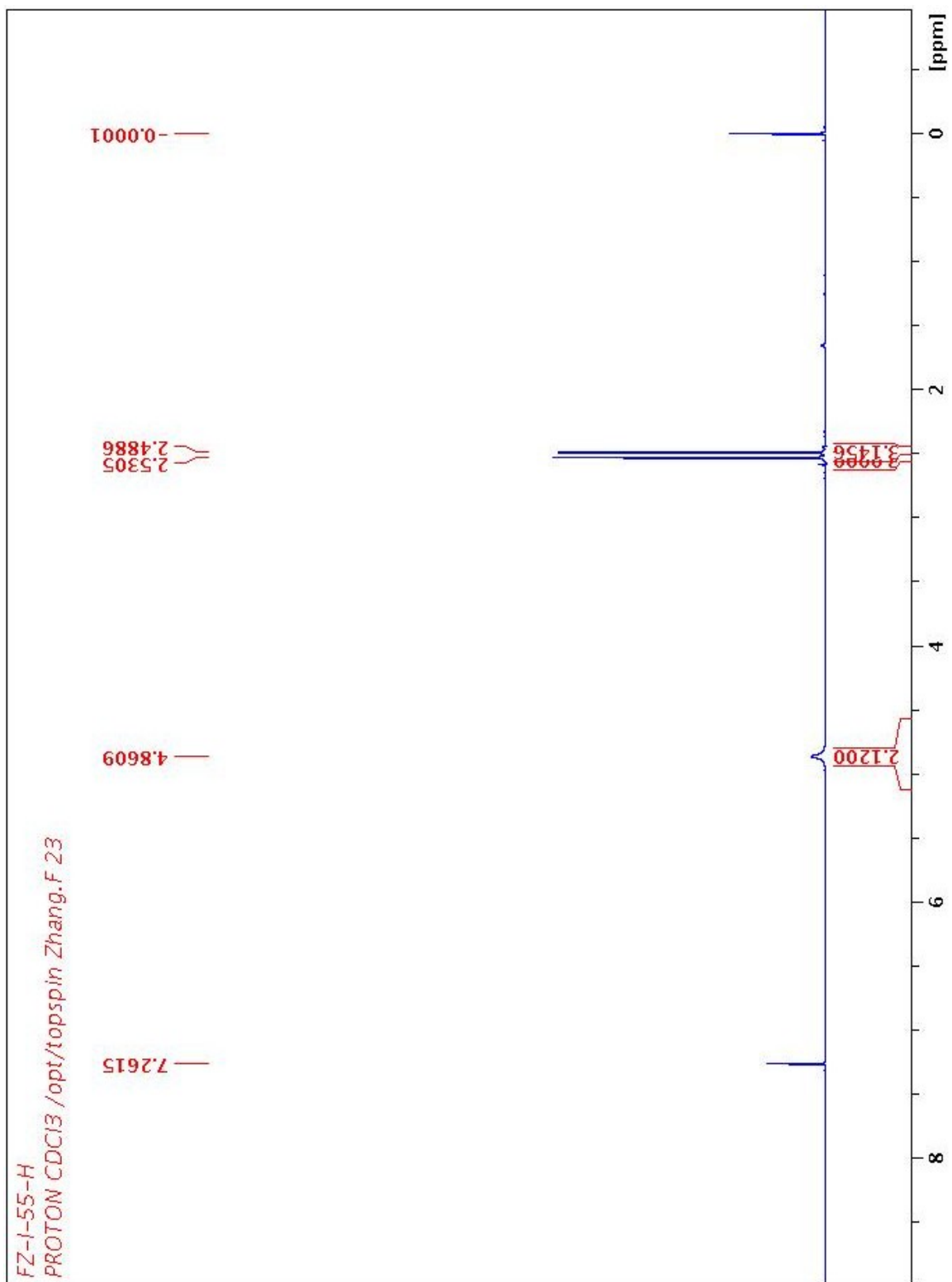
FZ-I-55

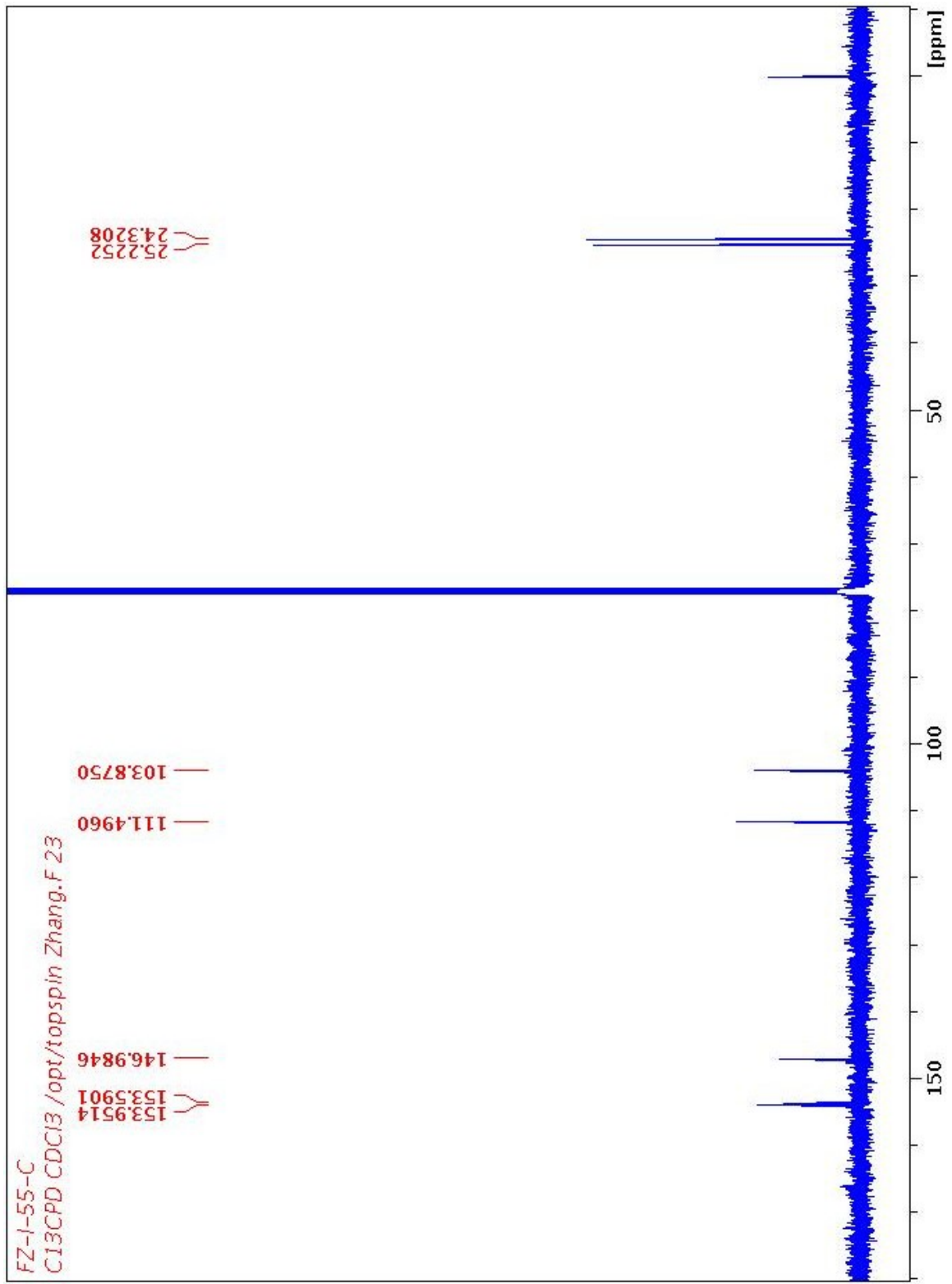


Thu Apr 14 17:49:31 2011 (GMT-04:00)

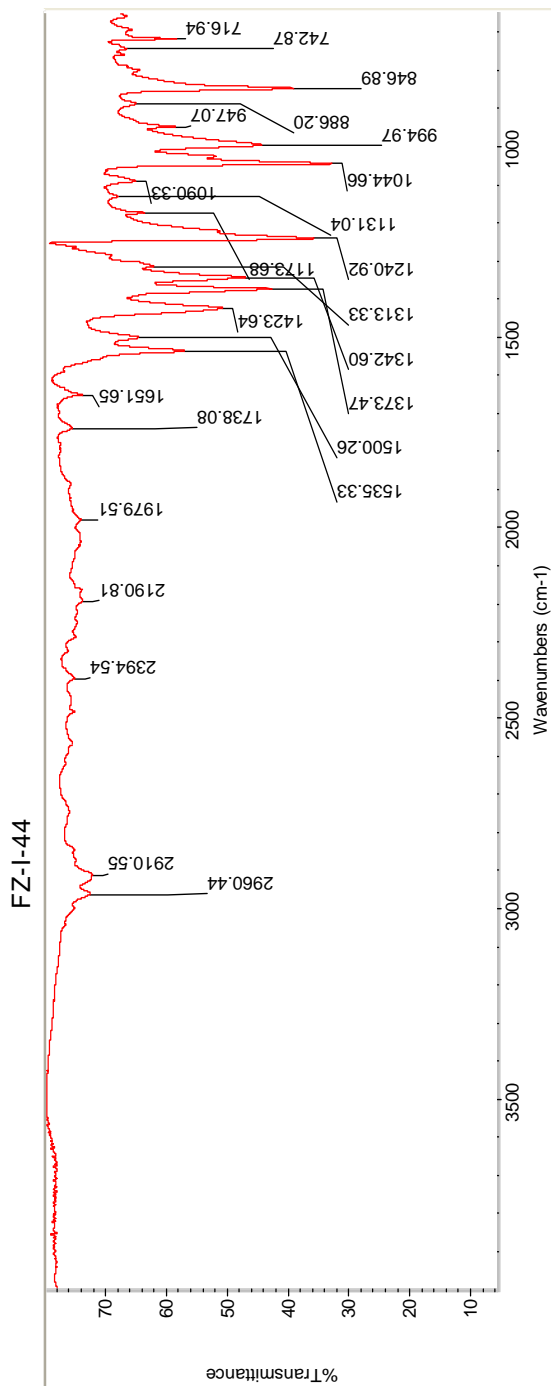
Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 2.0  
Optical velocity: 0.4747  
Aperture: 80.00

Find Peaks:  
Spectrum: FZ-I-55  
Region: 4000.00 400.00  
Absolute threshold: 83.435  
Sensitivity: 50  
Peak list:  
Position: 659.26 Intensity: Intensive  
Position: 739.55 Intensity: Intensive  
Position: 945.45 Intensity: Intensive  
Position: 979.23 Intensity: Intensive  
Position: 1026.53 Intensity: Intensive  
Position: 1044.34 Intensity: Intensive  
Position: 1254.37 Intensity: Intensive





Mon Apr 18 09:14:47 2011 (C)

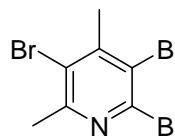


Mon Apr 18 09:14:31 2011 (GMT-04:00)

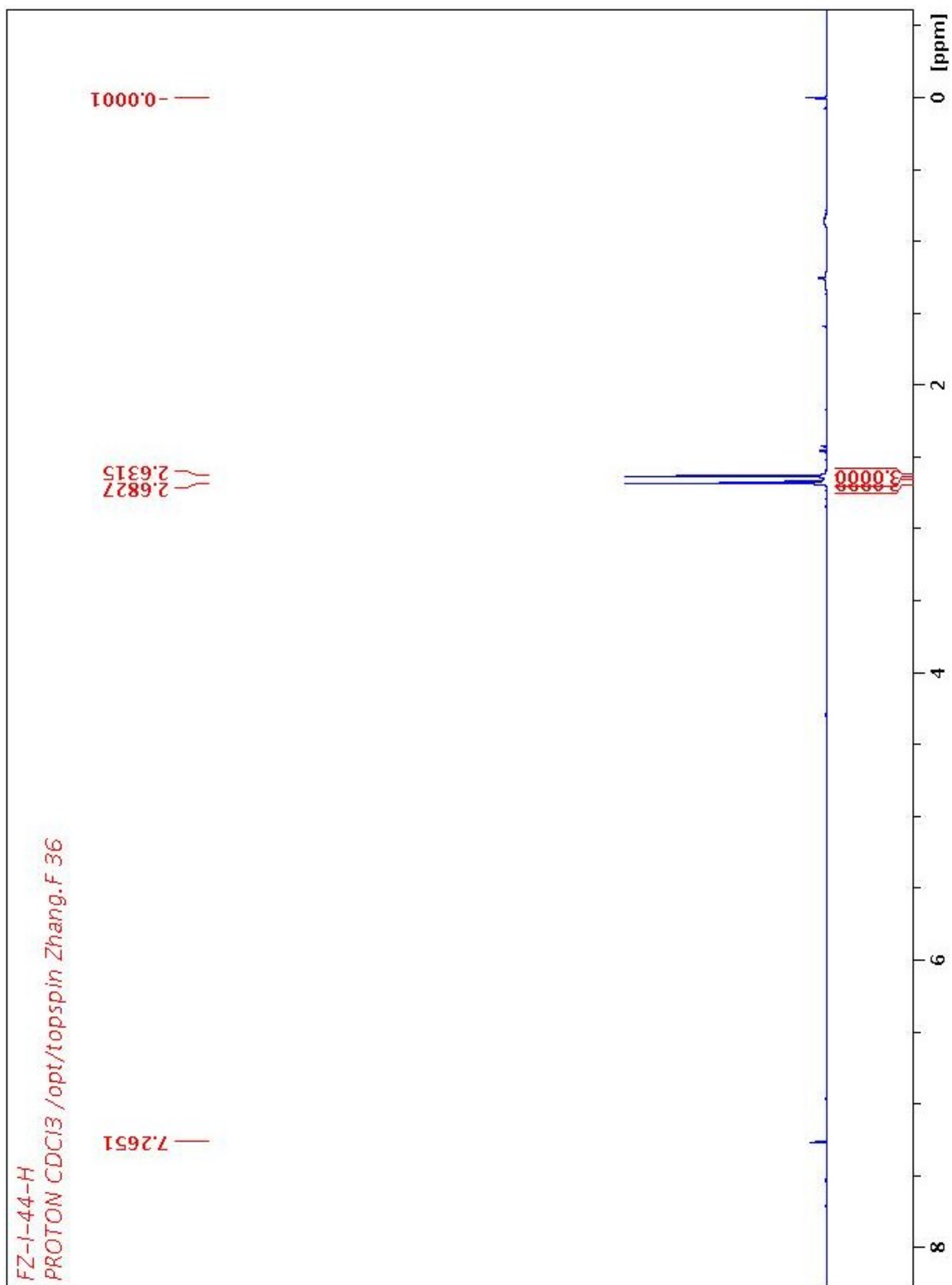
Find Peaks:

Spectrum:	FZ-I-44
Region:	4000.00 400.00
Absolute threshold:	75.745
Sensitivity:	50
Peak list:	
Position:	716.94 Intensity:
Position:	742.87 Intensity:
Position:	846.89 Intensity:
Position:	886.20 Intensity:
Position:	947.07 Intensity:
Position:	994.97 Intensity:
Position:	1044.66 Intensity:

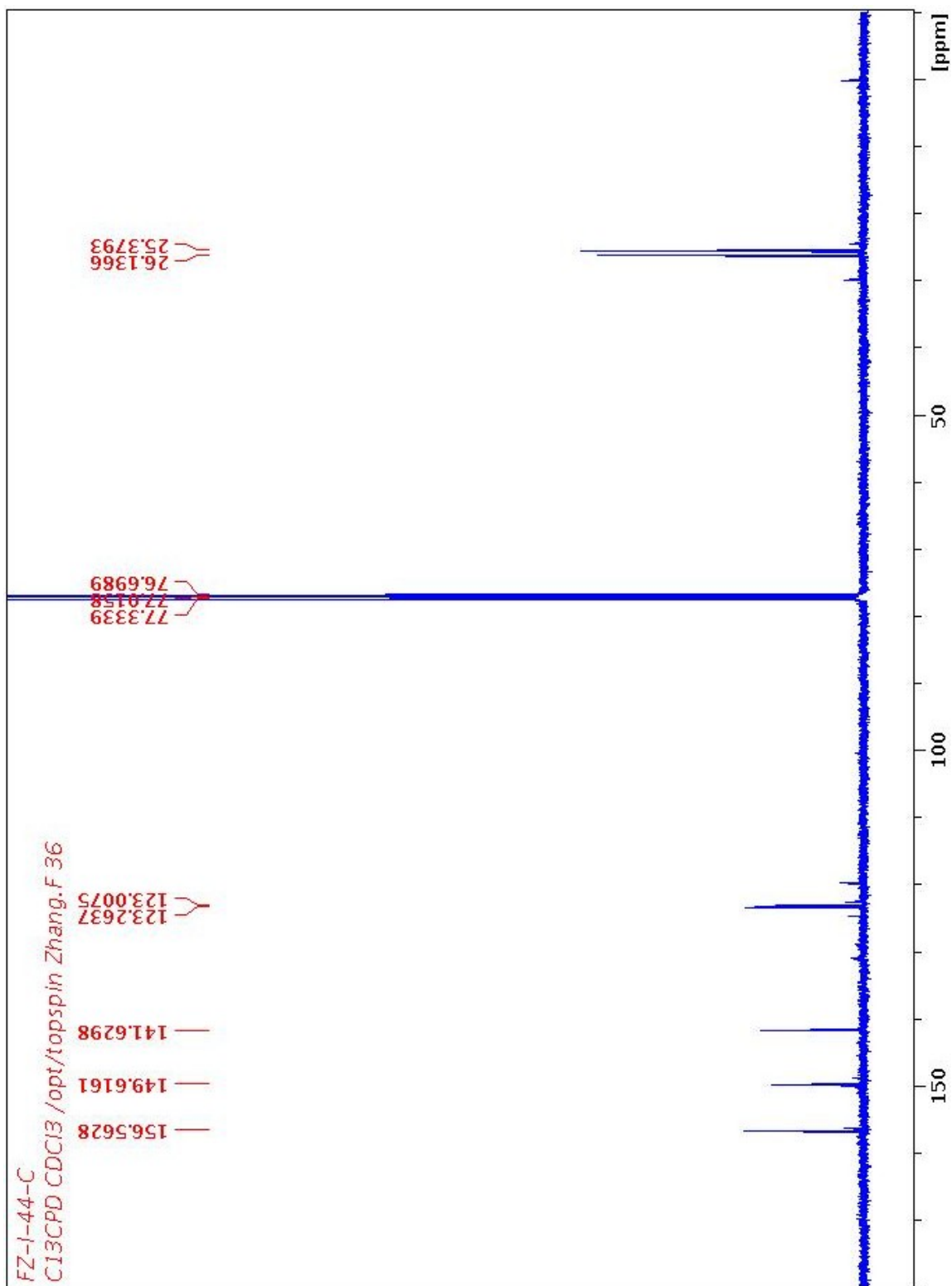
Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 2.0  
Optical velocity: 0.4747  
Aperture: 80.00



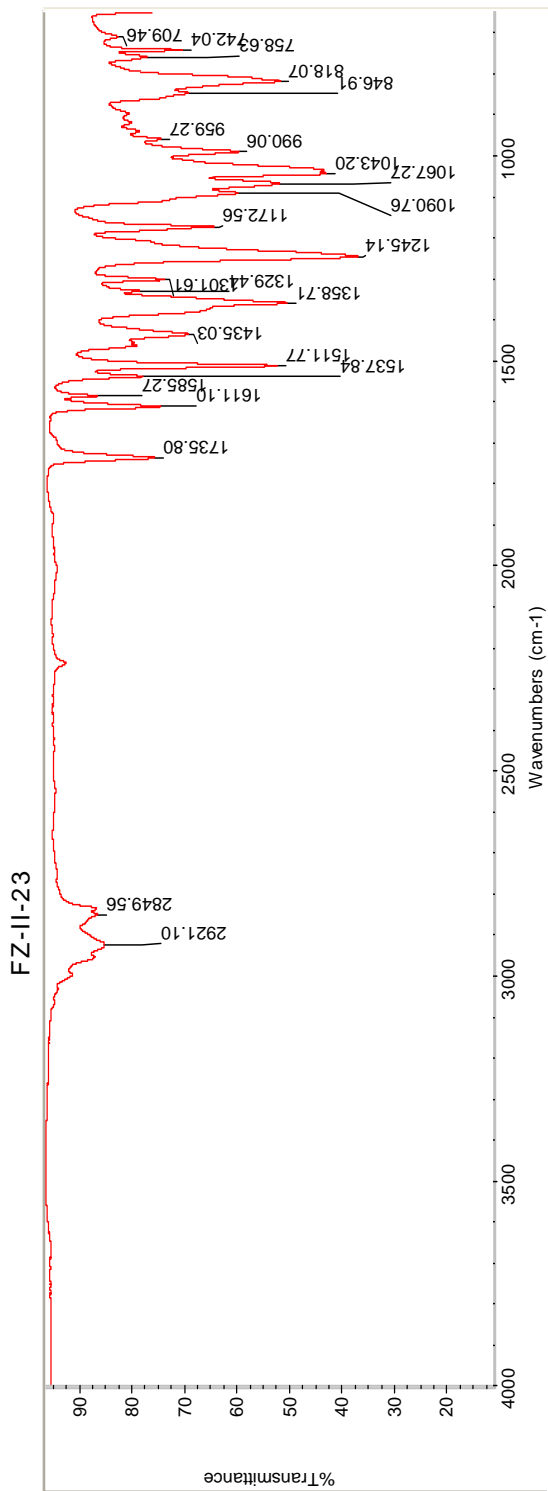
9







Thu Apr 14 17:57:47 2011 (G

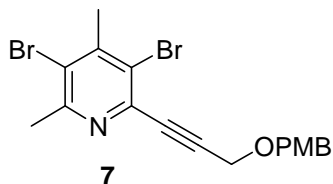


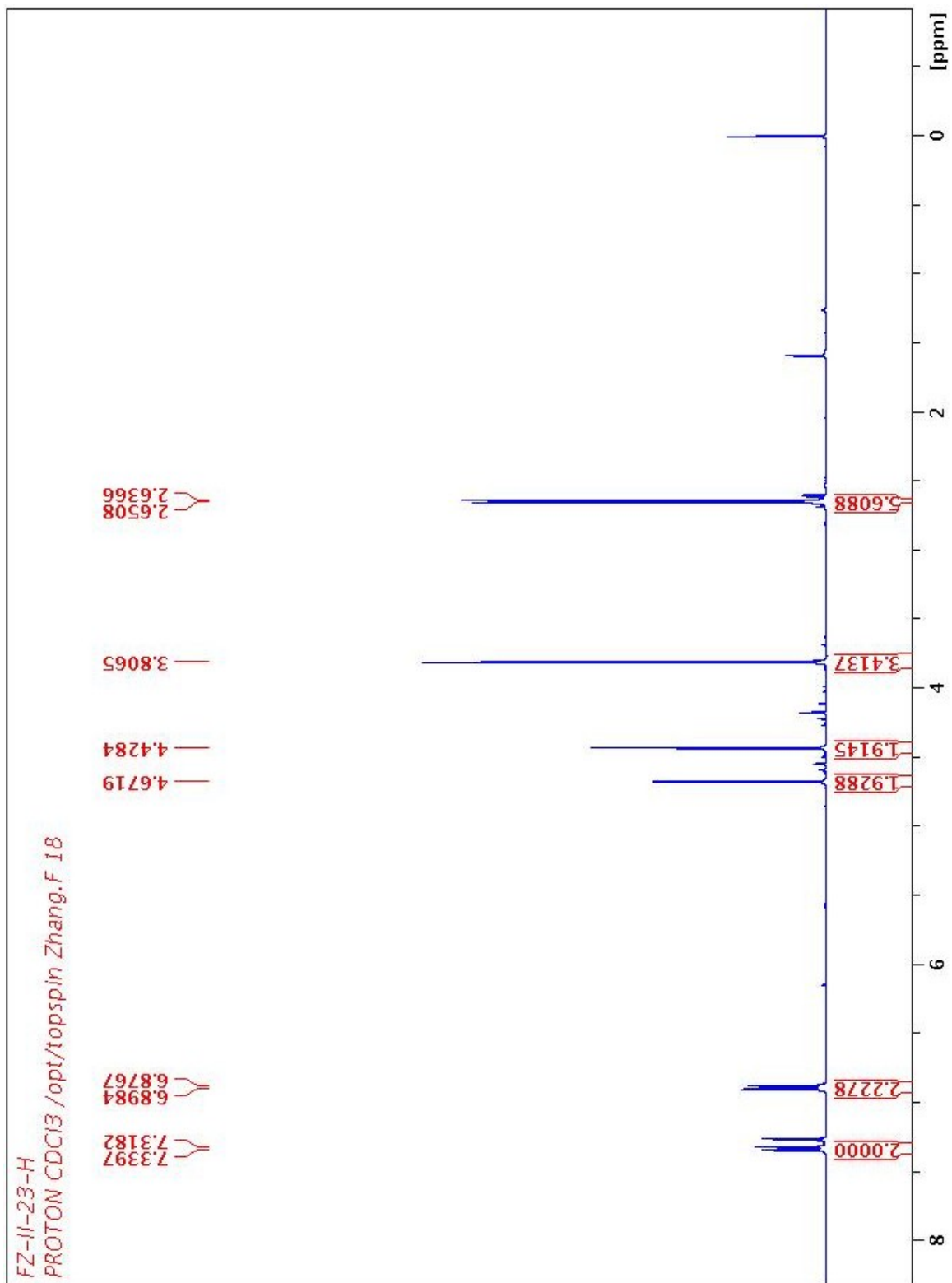
Thu Apr 14 17:57:42 2011 (GMT-04:00)

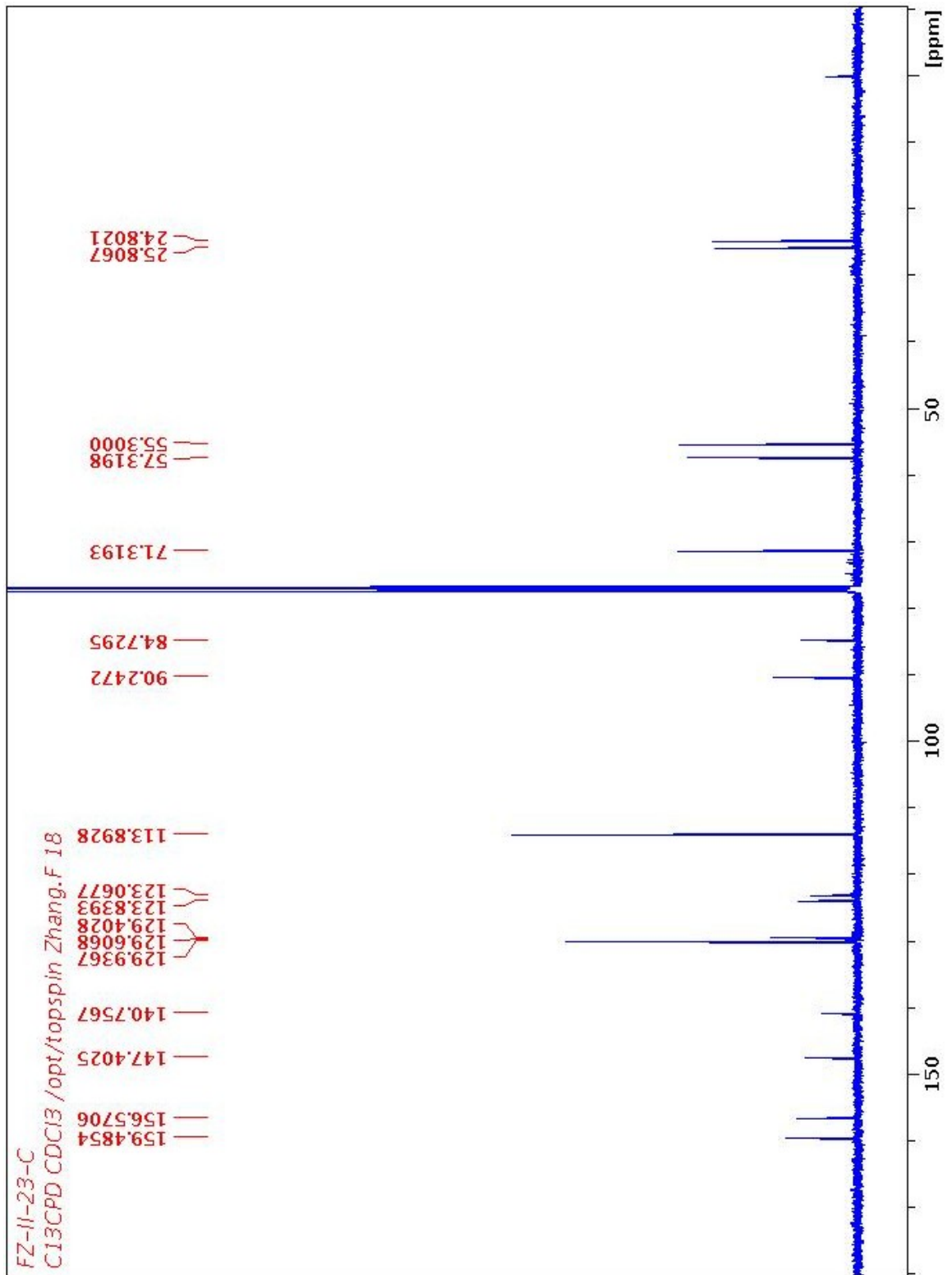
FIND PEAKS:

Spectrum:	FZ-II-23	Intensity:
Region:	4000.12	649.89
Absolute threshold:	91.560	
Sensitivity:	50	
Peak list:		
Position:	709.46	Intensity:
Position:	742.04	Intensity:
Position:	758.63	Intensity:
Position:	818.07	Intensity:
Position:	846.91	Intensity:
Position:	959.27	Intensity:
Position:	990.06	Intensity:

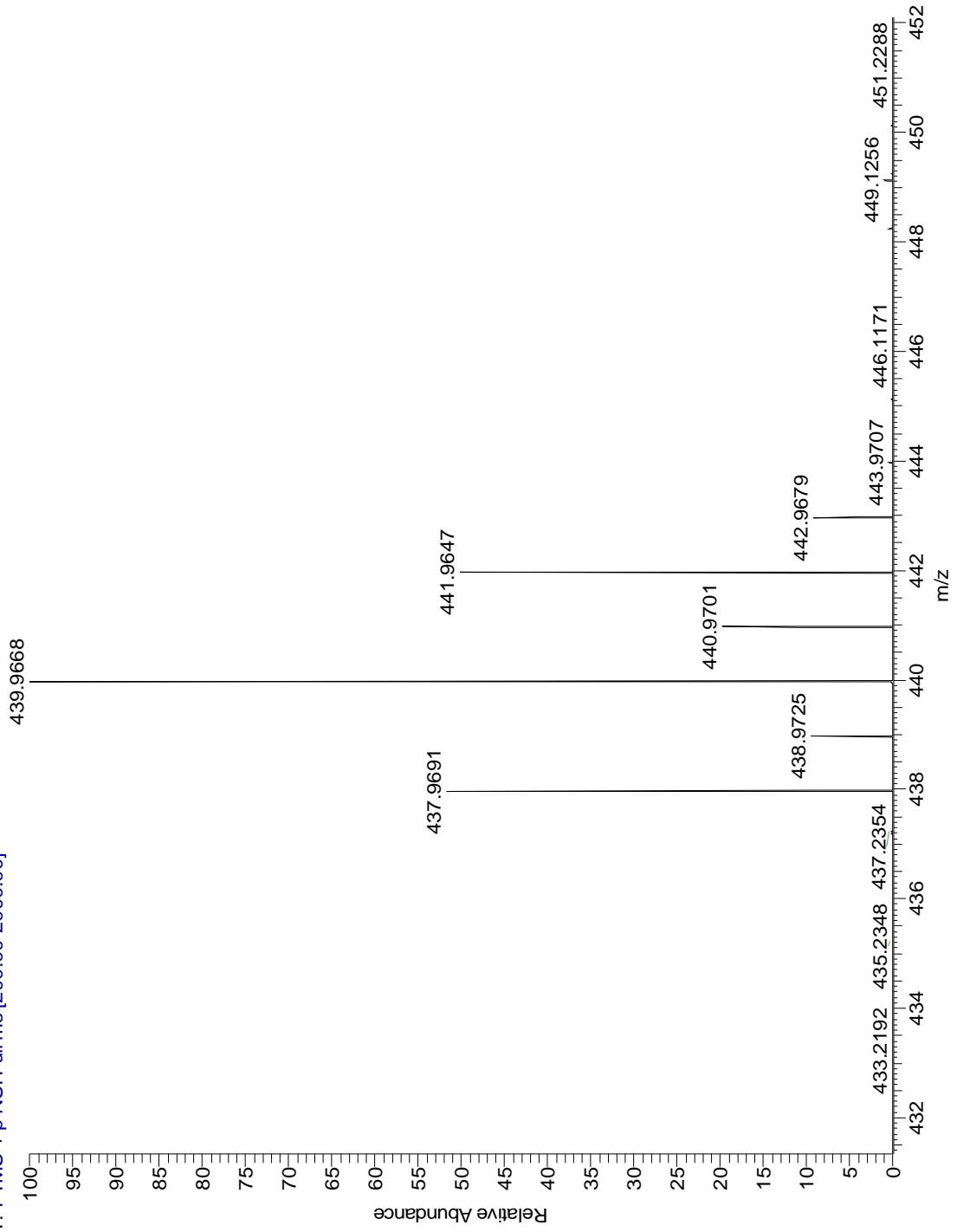
Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00





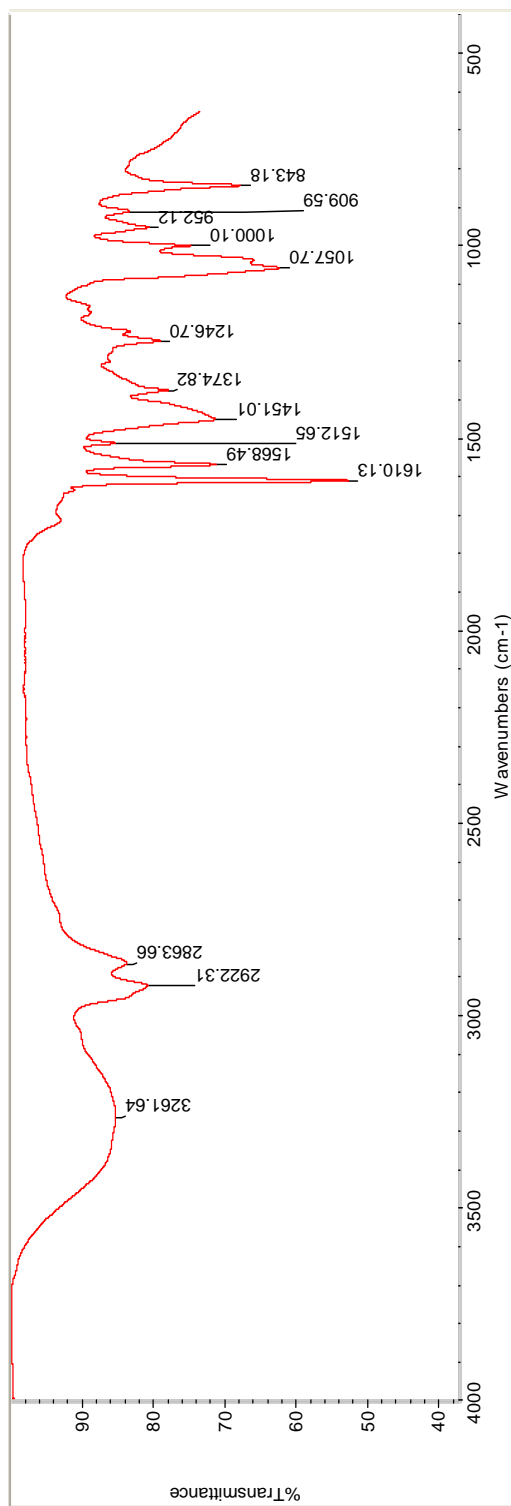


r110809r01 #4-49 RT: 0.04-0.66 AV: 46 NL: 3.96E7  
T: FTMS + p NSI Full ms [200.00-2000.00]



Thu Apr 14 17:55:52 2011 (G

FZ-IV-34



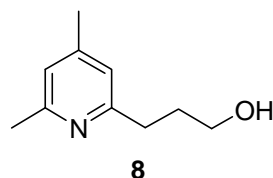
Thu Apr 14 17:55:46 2011 (GMT-04:00)

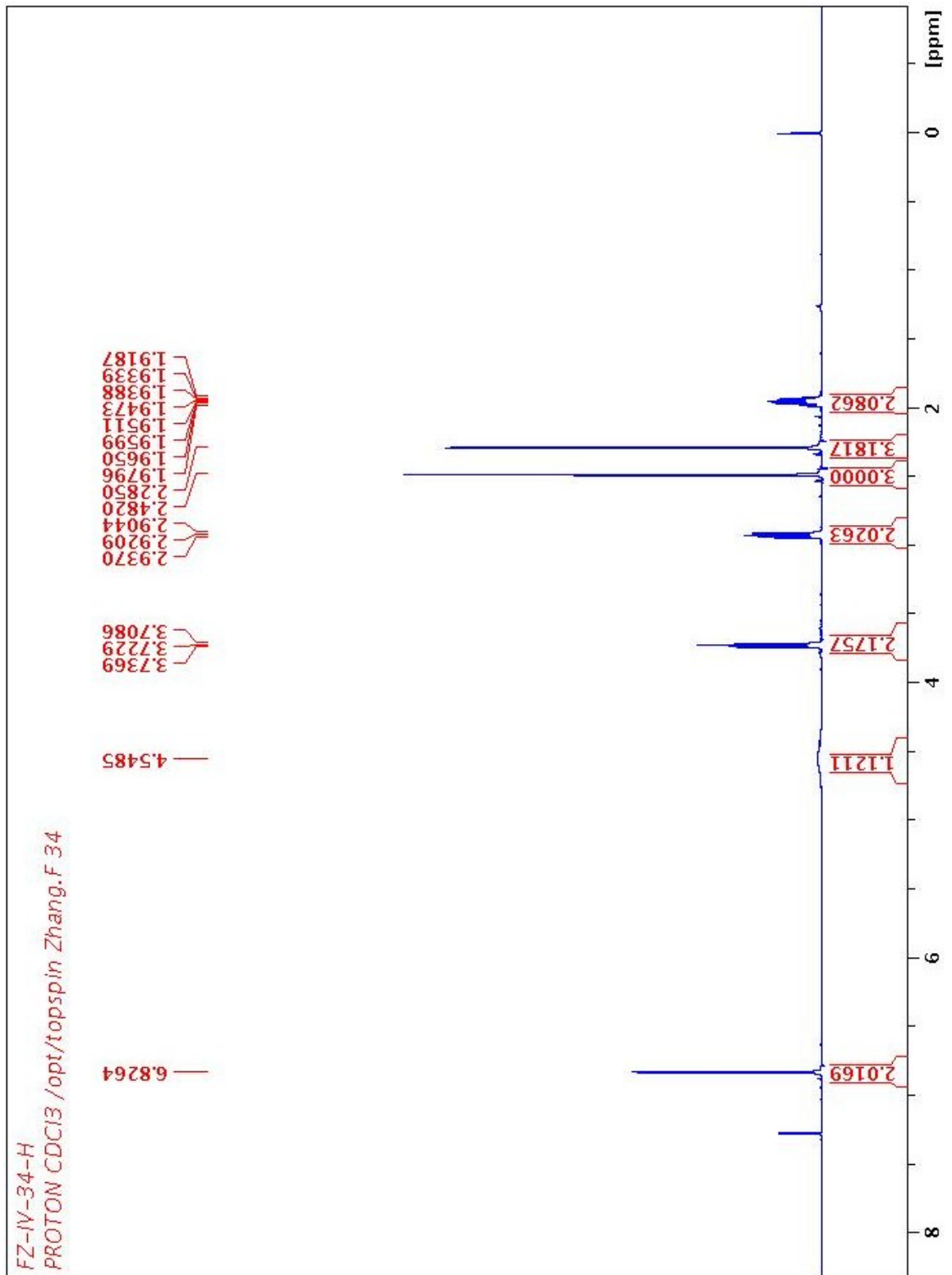
Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 2.0  
Optical velocity: 0.4747  
Aperture: 80.00

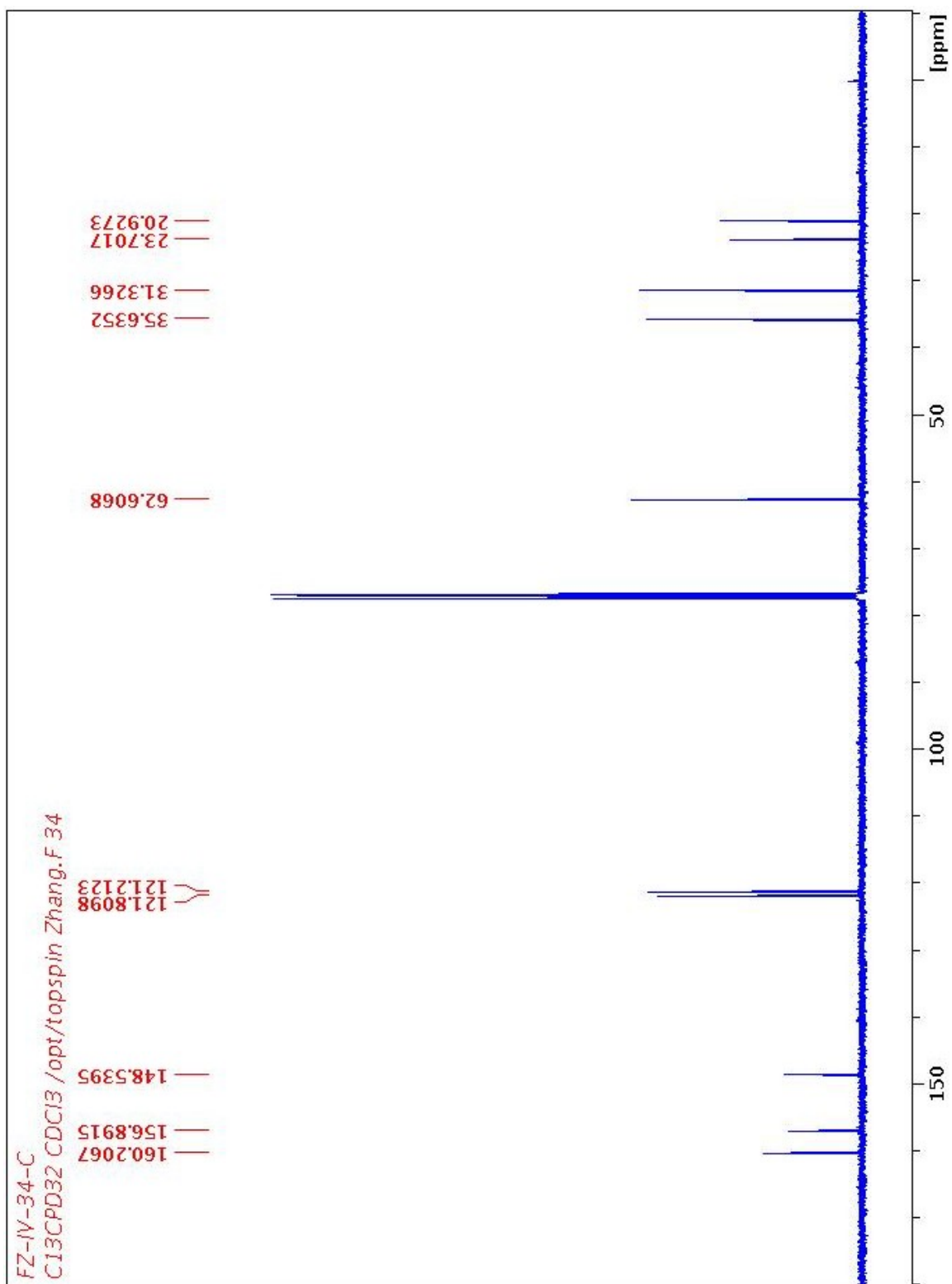
FIND PEAKS:

Spectrum: FZ-IV-34  
Region: 4000.00 400.00  
Absolute threshold: 95.750  
Sensitivity: 50

Peak list:	Position:	Intensity:
	843.18	Intensity:
	909.59	Intensity:
	952.12	Intensity:
	1000.10	Intensity:
	1057.70	Intensity:
	1246.70	Intensity:
	1374.82	Intensity:

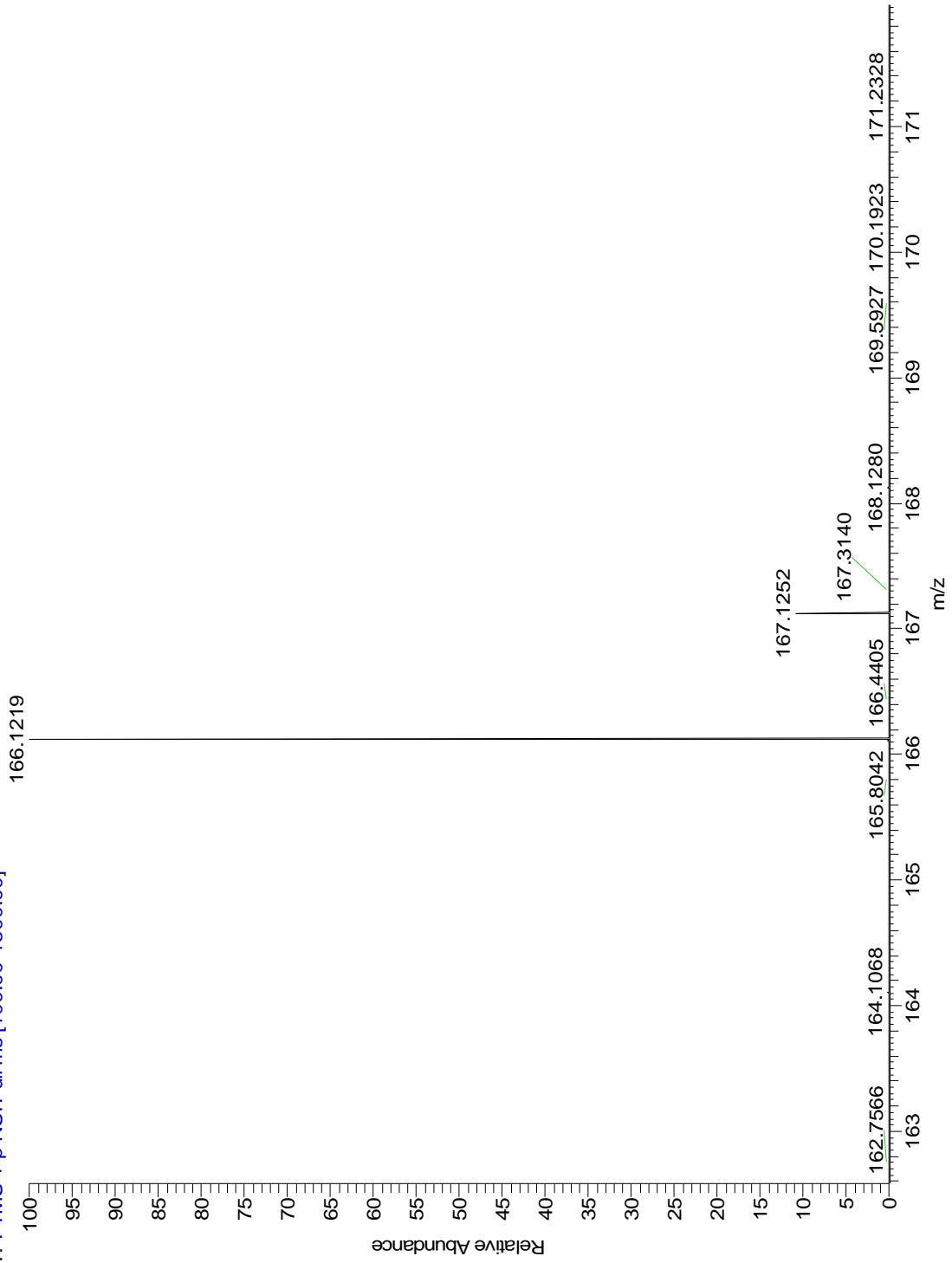




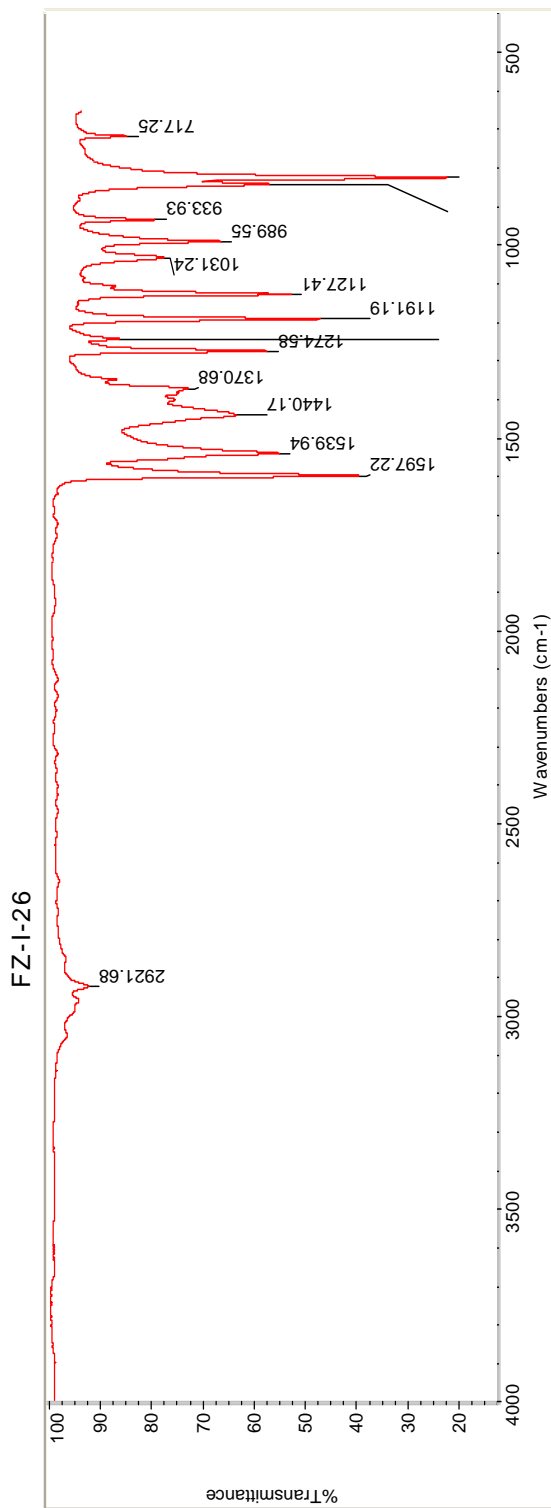




r110809r02 #1-49 RT: 0.00-0.67 AV: 49 NL: 1.26E9  
T: FTMS + p NSIFull ms [100.00-1500.00]



Thu Apr 14 17:46:47 2011 (G

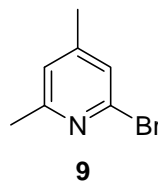


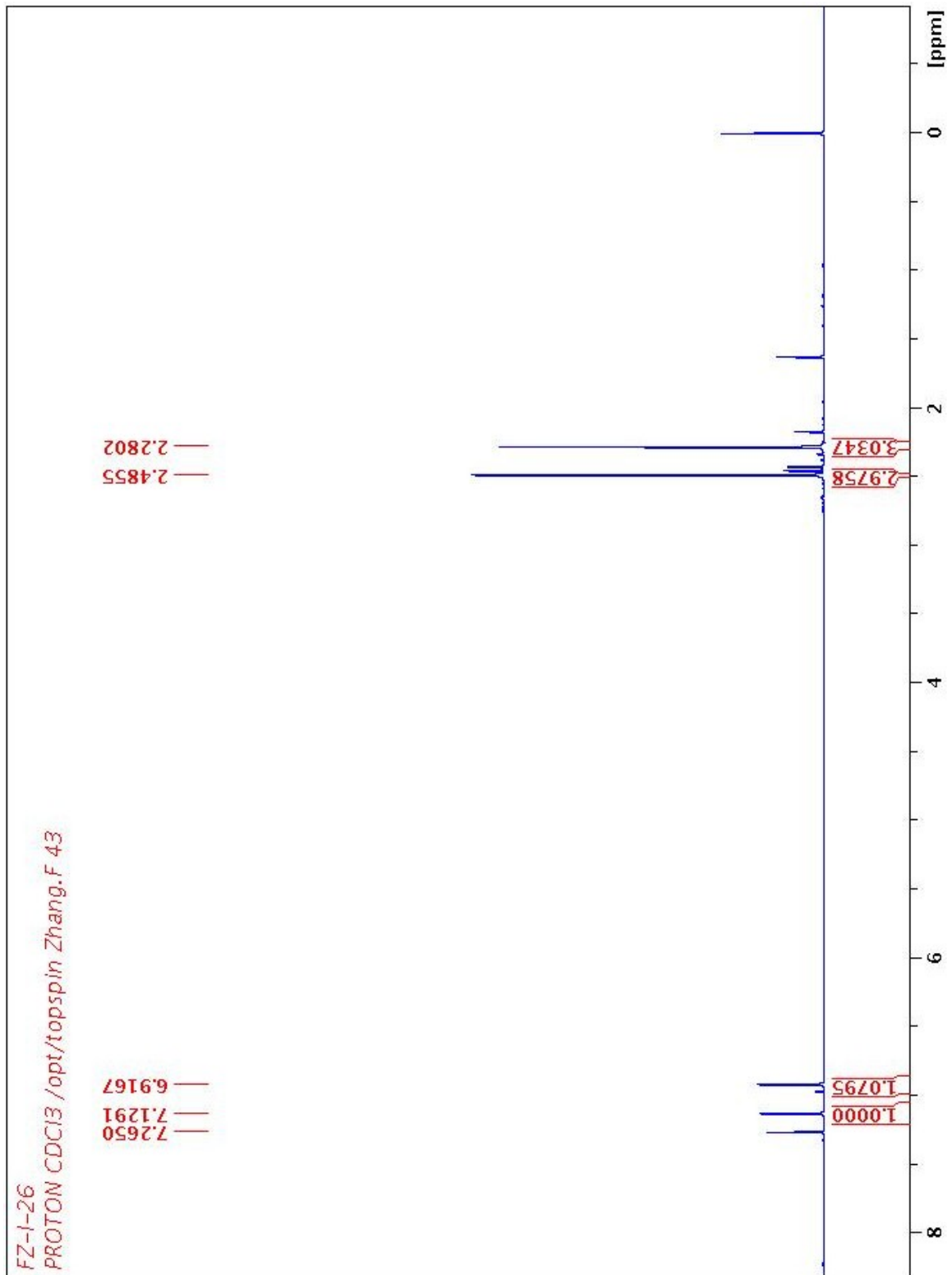
Thu Apr 14 17:46:46 2011 (GMT-04:00)

Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 2.0  
Optical velocity: 0.4747  
Aperture: 80.00

FIND PEAKS:

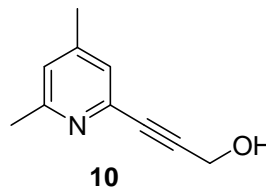
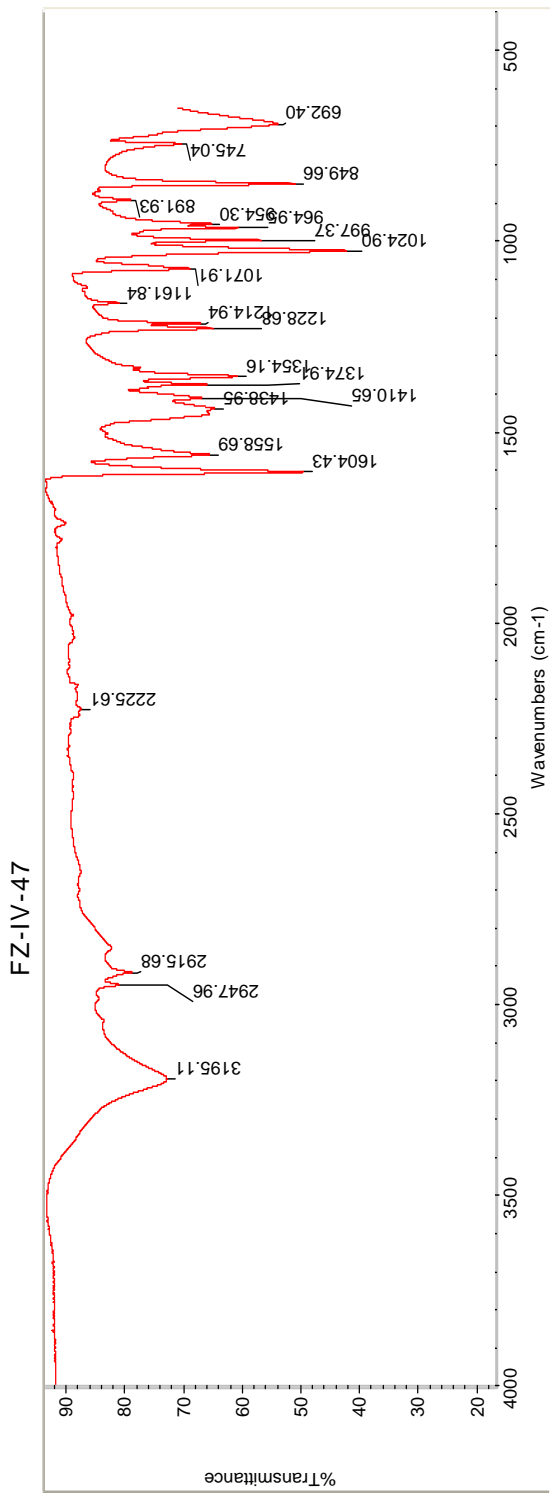
Region	Position	Intensity
FZ-I-26	717.25	Intensiv
4000.00	824.69	Intensiv
400.00	841.37	Intensiv
96.857	933.93	Intensiv
50	989.55	Intensiv
50	1031.24	Intensiv
50	1127.41	Intensiv







Thu Apr 14 17:55:04 2011 (G)

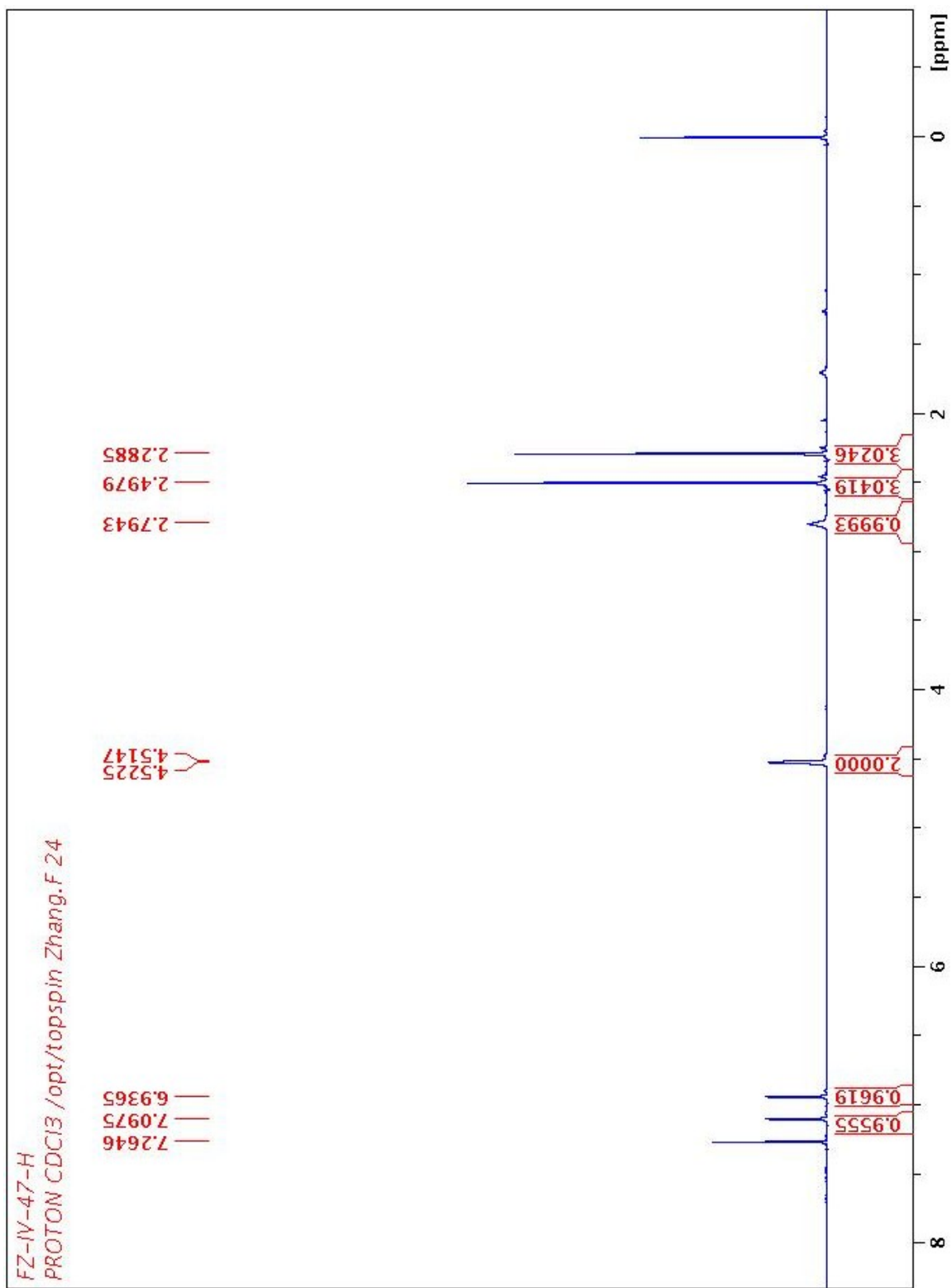


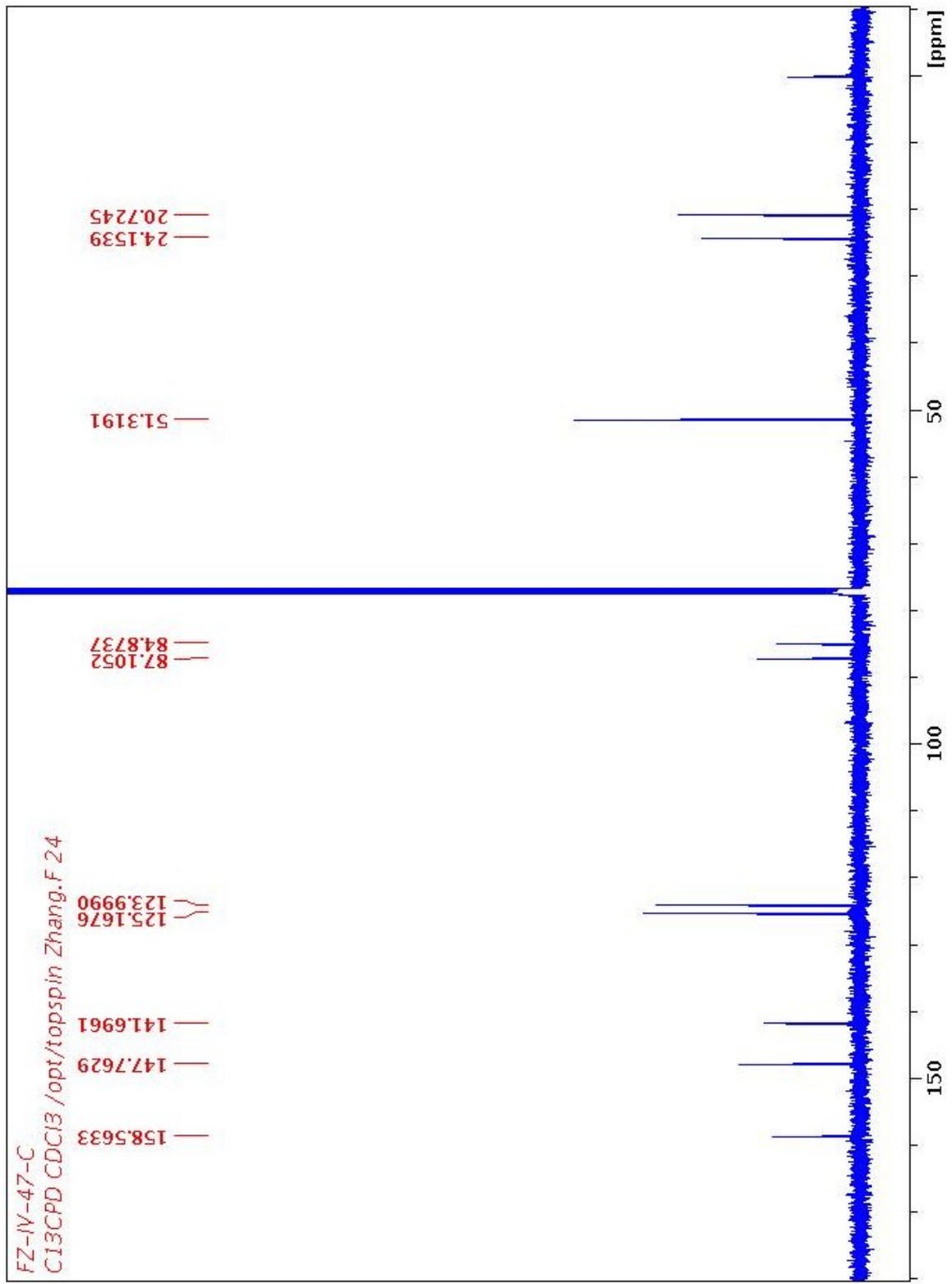
Thu Apr 14 17:55:03 2011 (GMT-04:00)

FIND PEAKS:

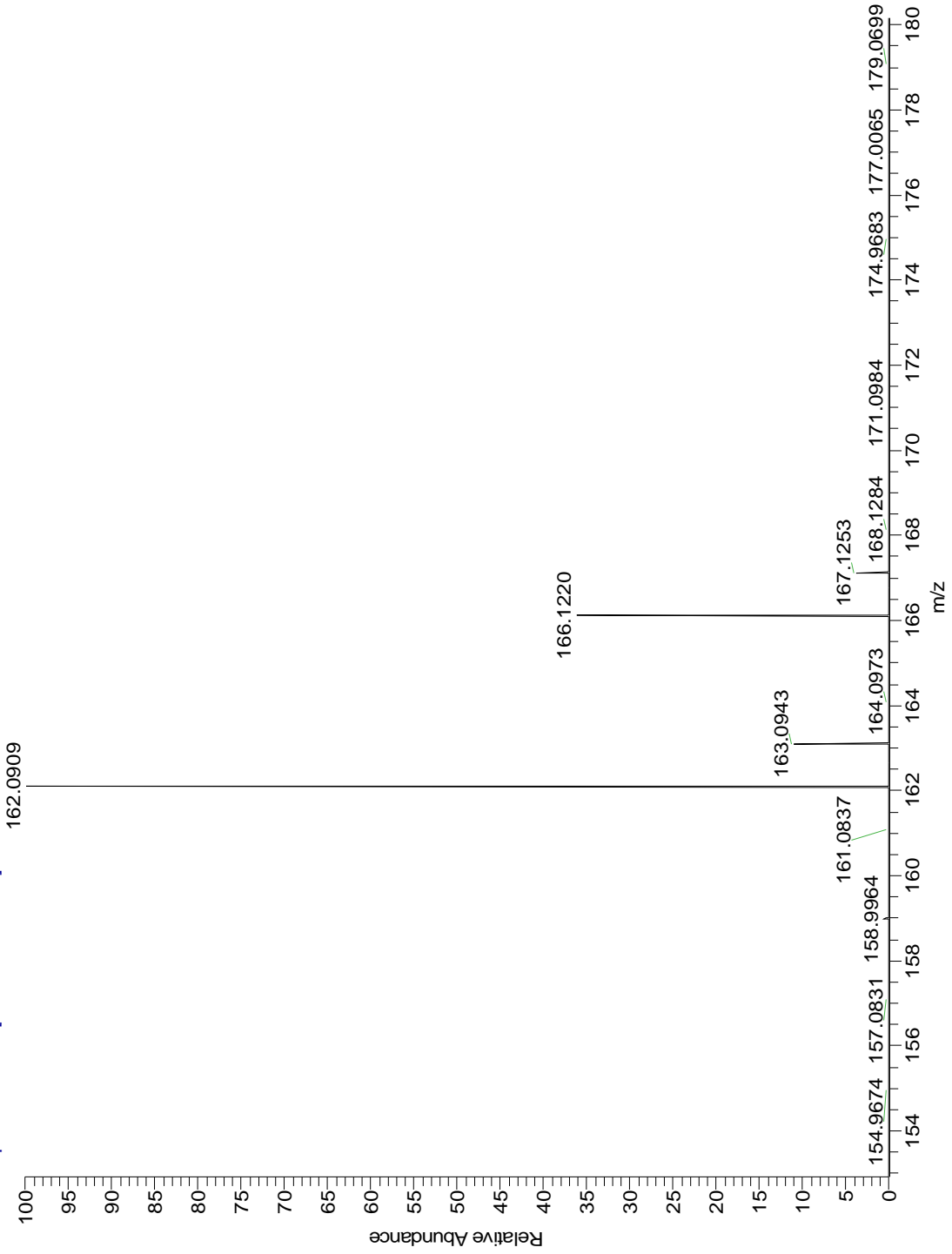
Spectrum:	FZ-IV-47	
Region:	4000.00	400.00
Absolute threshold:	89.638	
Sensitivity:	50	
Peak list:		
Position:	692.40	Intensity:
Position:	745.04	Intensity:
Position:	849.66	Intensity:
Position:	891.93	Intensity:
Position:	954.30	Intensity:
Position:	964.95	Intensity:
Position:	997.37	Intensity:

Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 2.0  
Optical velocity: 0.4747  
Aperture: 80.00





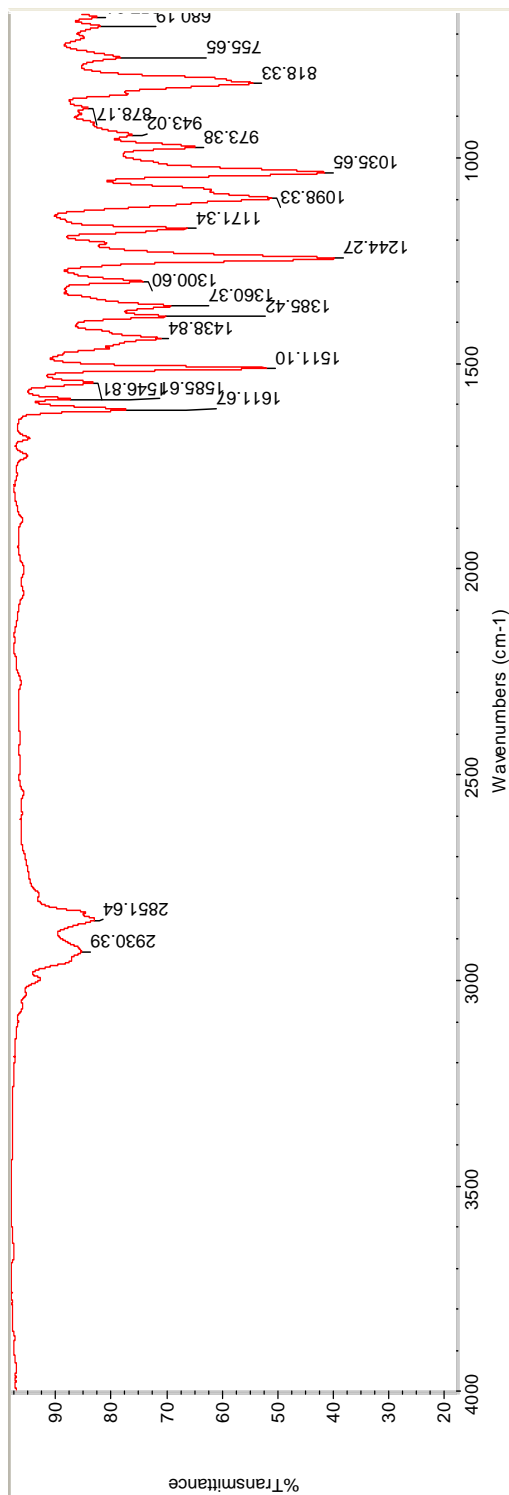
r110809r04 #1-50 RT: 0.00-0.68 AV: 50 NL: 1.87E8  
T: FTMS + p NSIFull.ms [100.00-1500.00]





Thu Apr 14 17:58:29 2011 (G

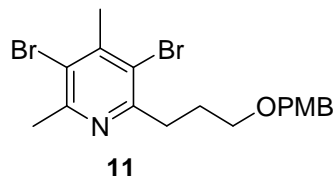
FZ-II-33



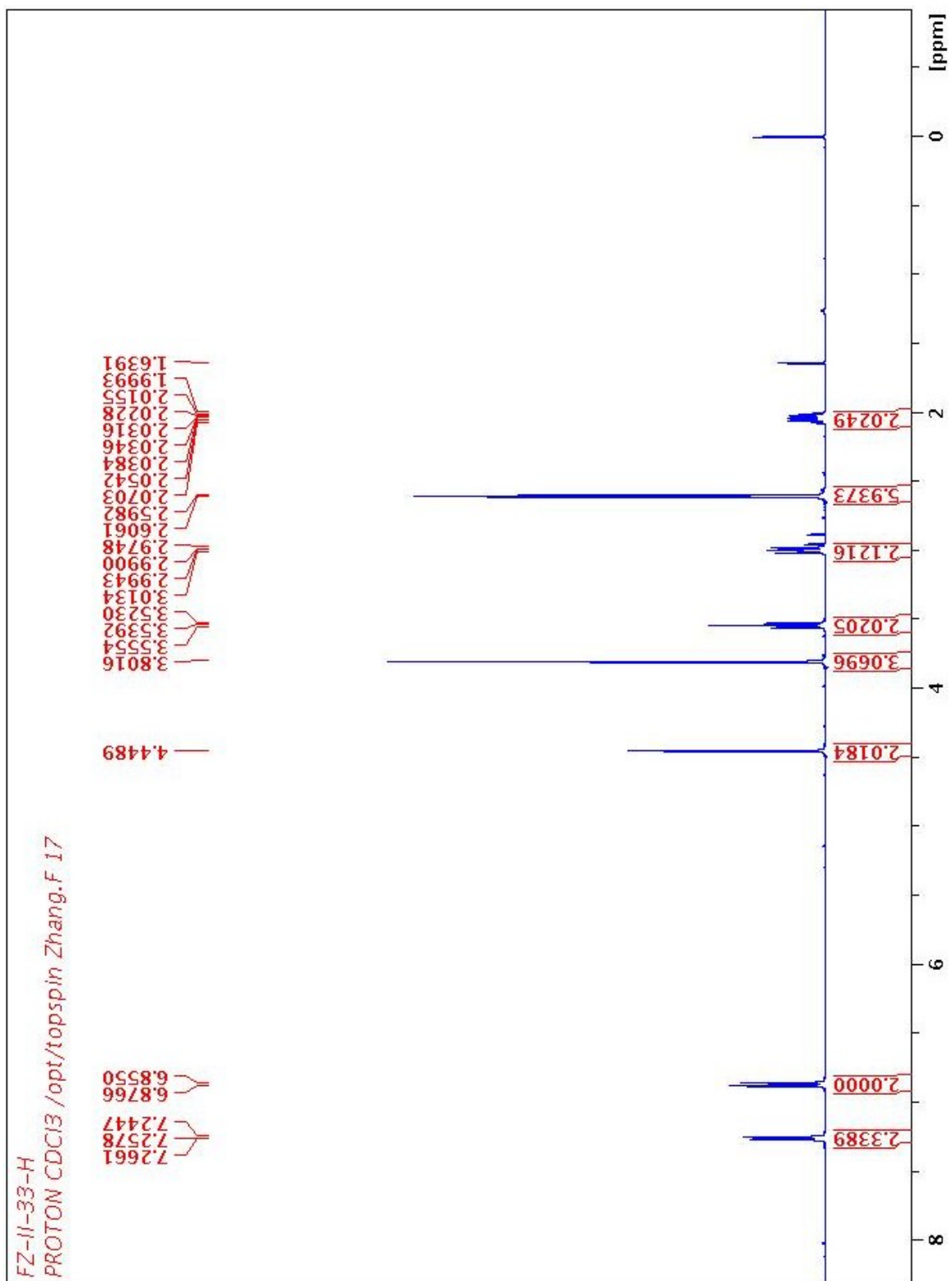
Thu Apr 14 17:58:23 2011 (GMT-04:00)

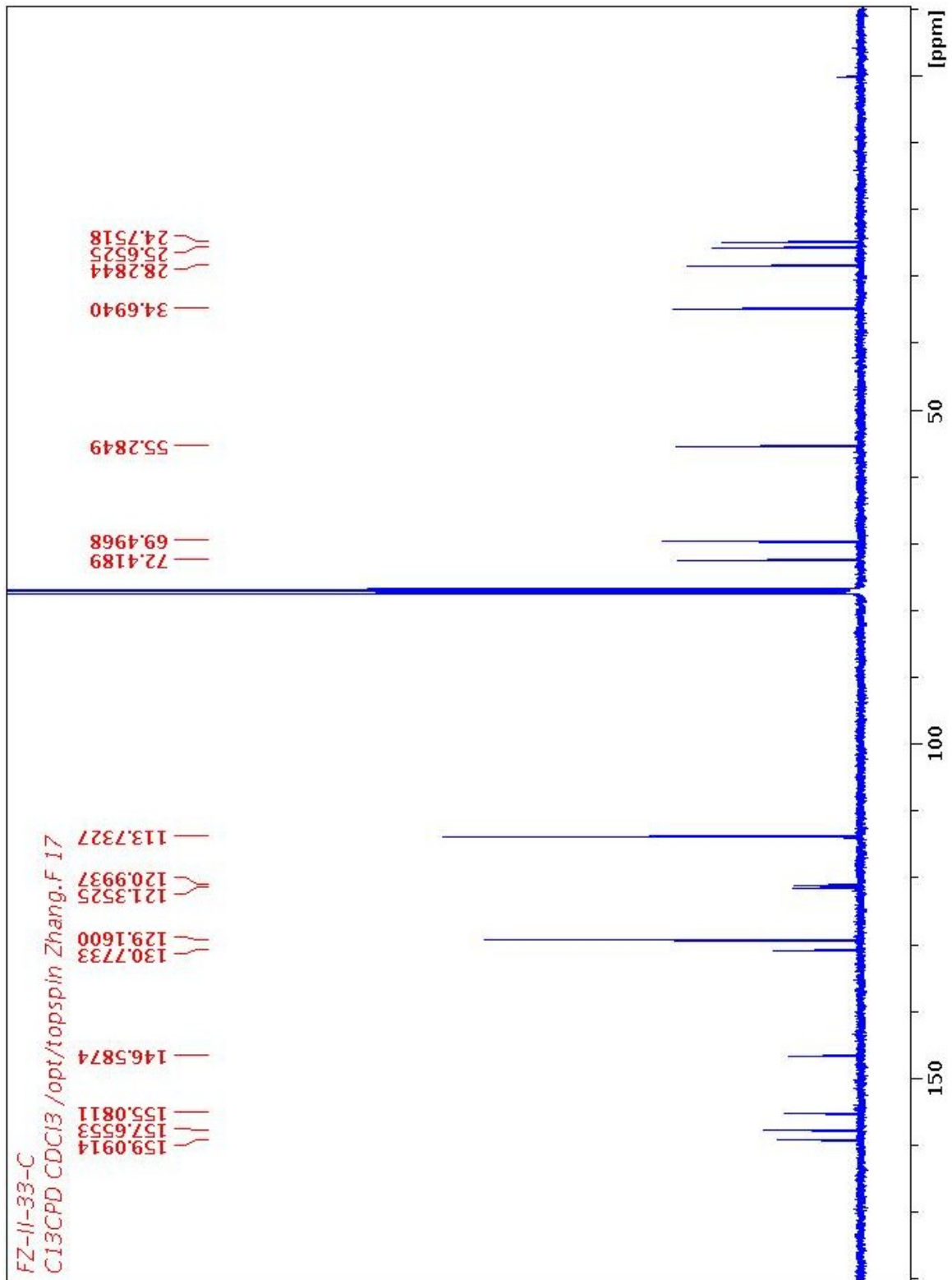
FIND PEAKS:

Spectrum: FZ-II-33  
Region: 4000.12 649.89  
Absolute threshold: 92.730  
Sensitivity: 50  
Peak list:  
Position: 657.91 Intensity:  
Position: 680.19 Intensity:  
Position: 755.65 Intensity:  
Position: 818.33 Intensity:  
Position: 878.17 Intensity:  
Position: 943.02 Intensity:  
Position: 973.38 Intensity:

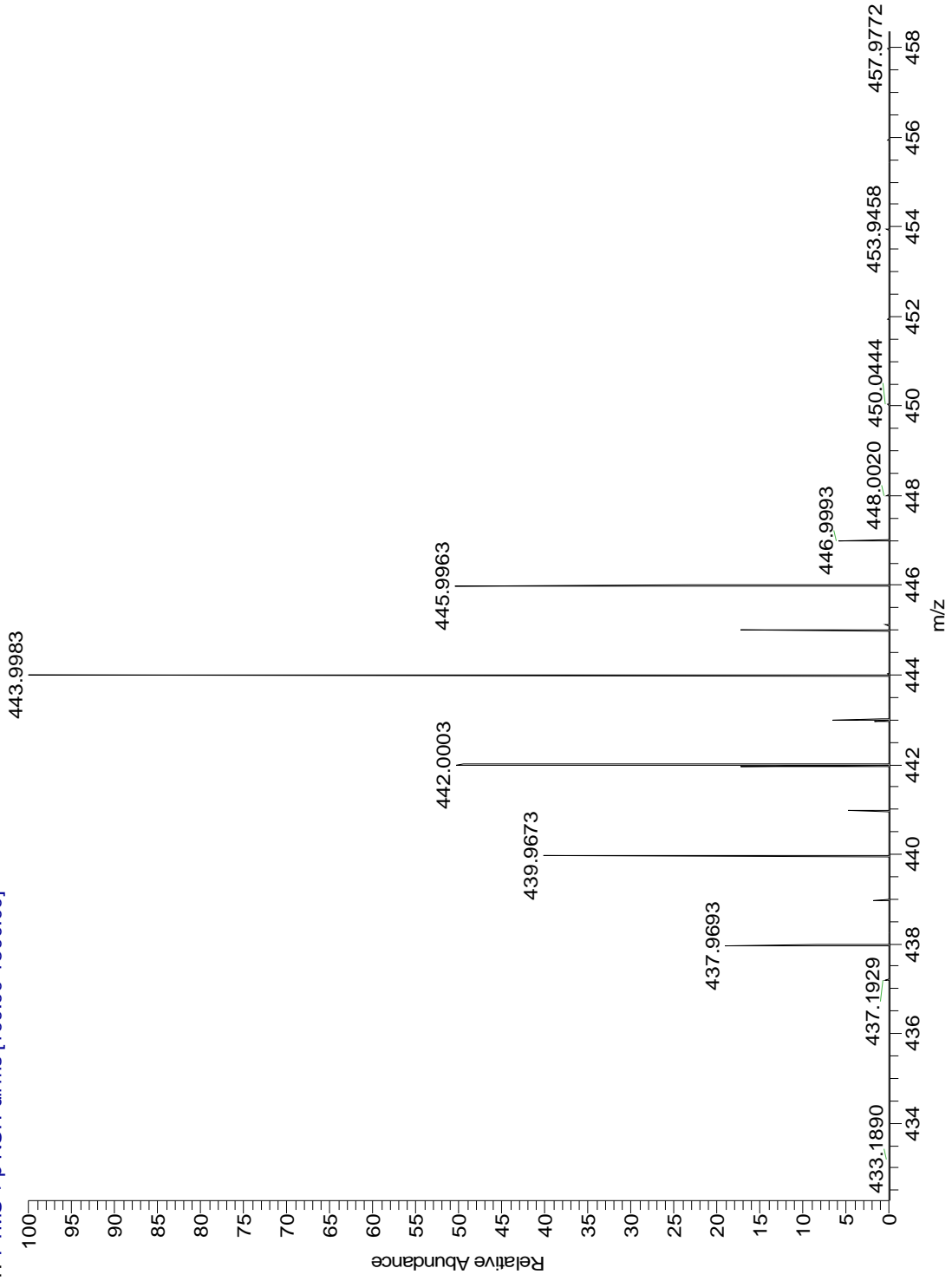


Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00

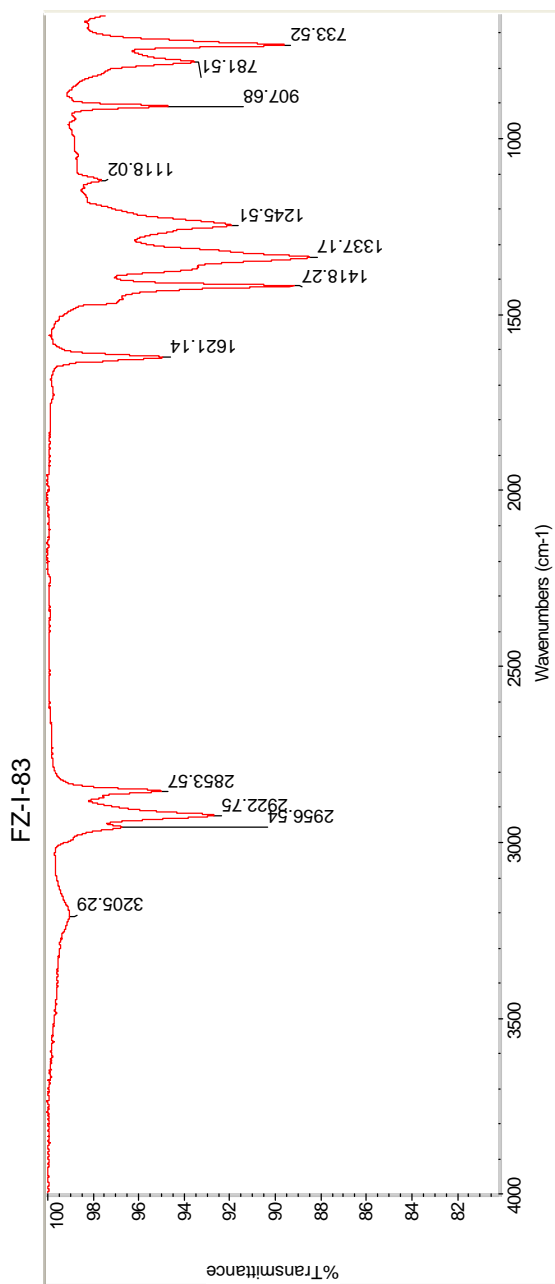




r110809r03 #2-50 RT: 0.02-0.69 AV: 49 NL: 1.91E7  
T: FTMS + p NSI Full ms [100.00-1500.00]



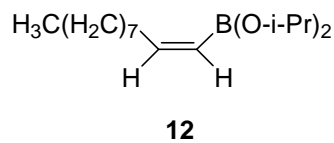
Fri Jun 10 12:17:32 2011 (GI)

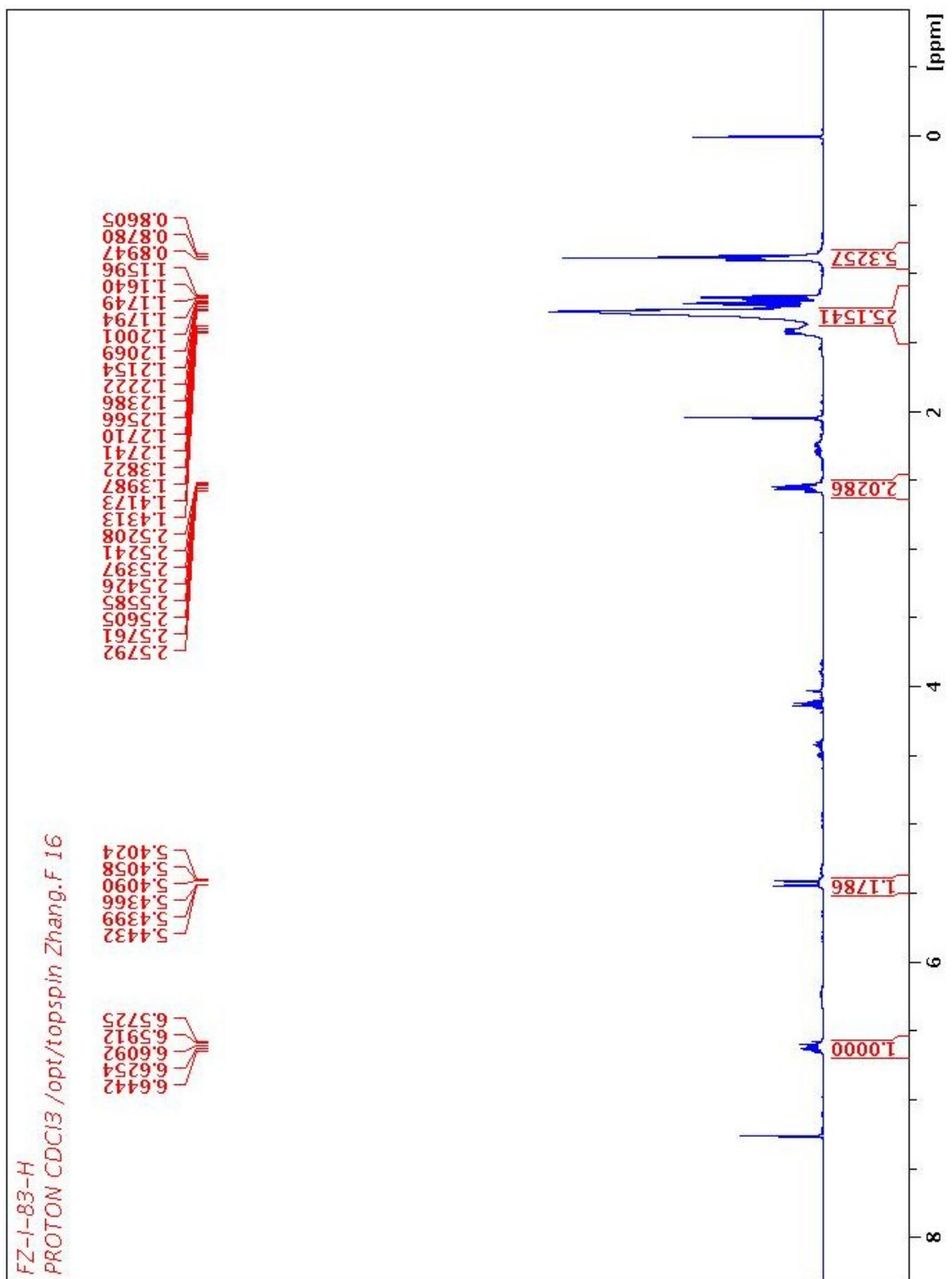


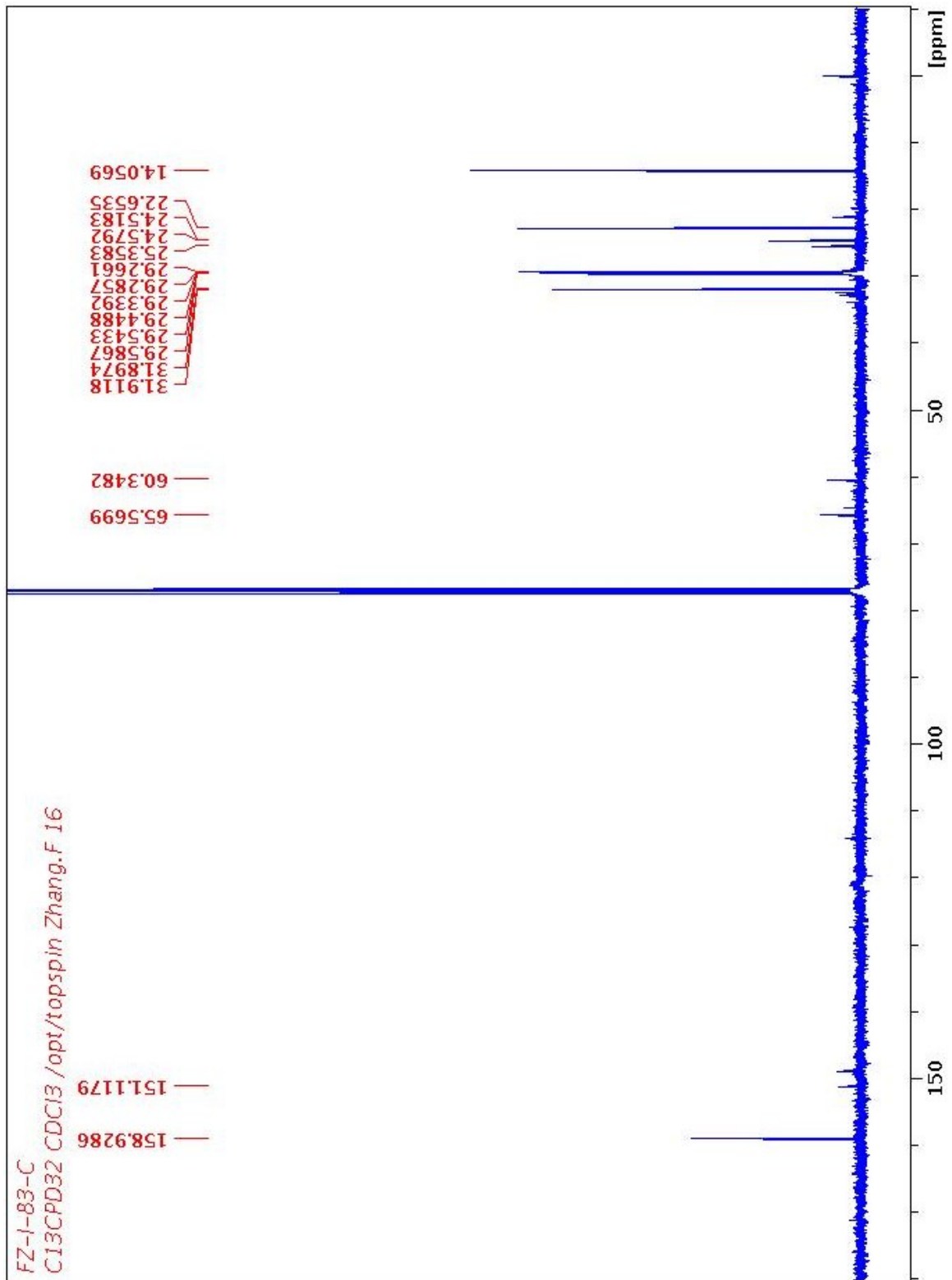
Fri Jun 10 12:17:26 2011 (GMT-04:00)

Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00

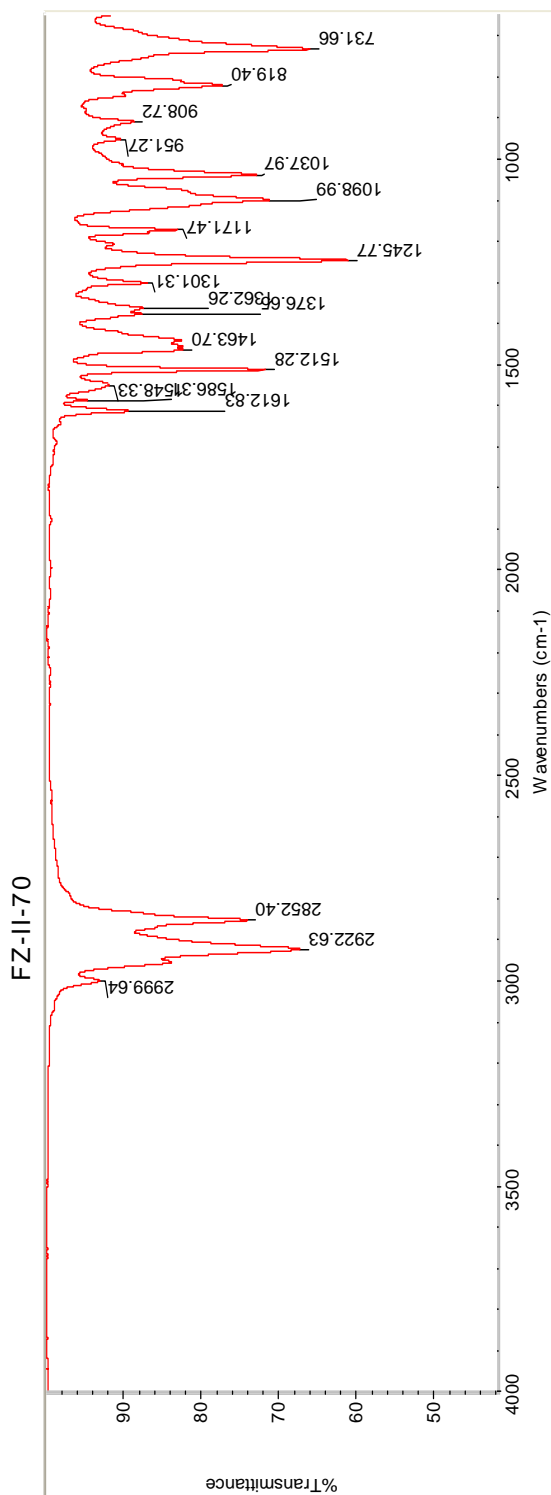
FIND PEAKS: FZ-I-83  
Region: 4000.00 400.00  
Absolute threshold: 99.112  
Sensitivity: 50  
Peak list:  
Position: 733.52 Intensity:  
Position: 781.51 Intensity:  
Position: 907.68 Intensity:  
Position: 1118.02 Intensity:  
Position: 1245.51 Intensity:  
Position: 1337.17 Intensity:  
Position: 1418.27 Intensity:







Thu Apr 14 18:00:52 2011 (G

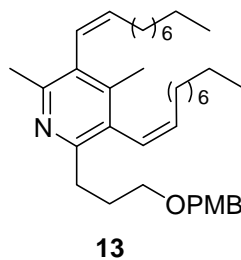


Thu Apr 14 18:00:47 2011 (GMT-04:00)

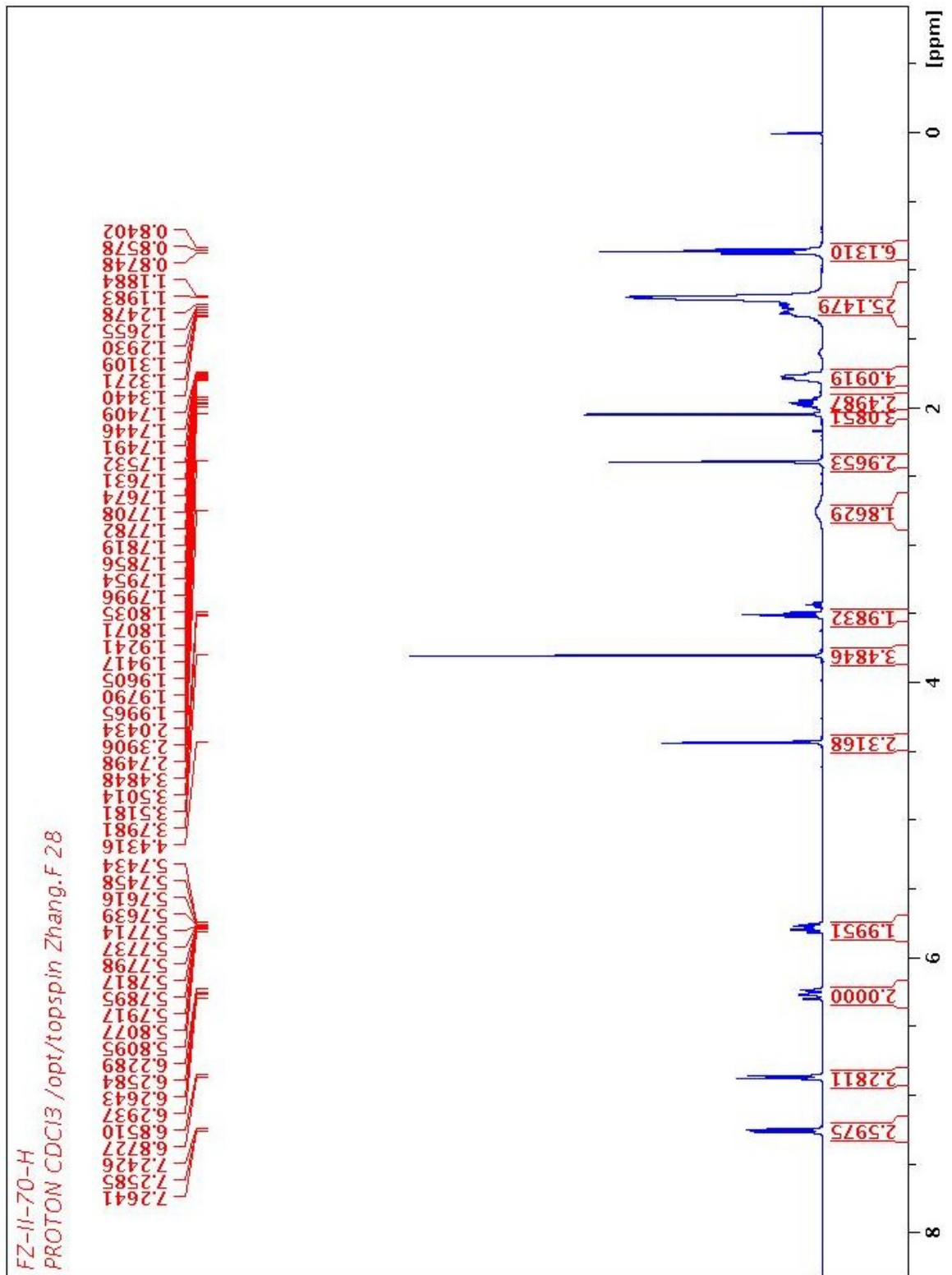
FIND PEAKS:

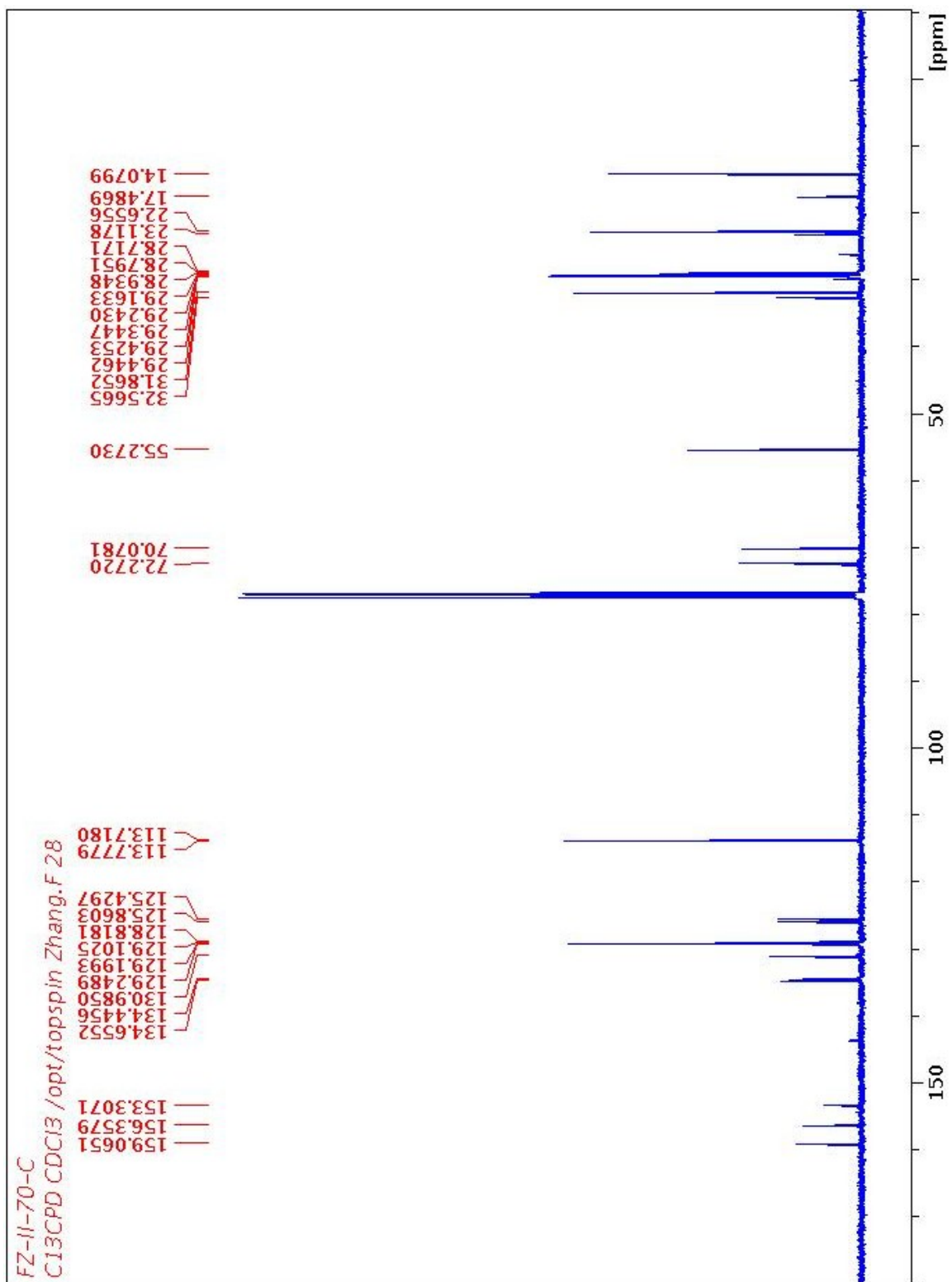
Position	Intensity
731.66	Intensiv
819.40	Intensiv
908.72	Intensiv
951.27	Intensiv
1037.97	Intensiv
1098.99	Intensiv
1171.47	Intensiv

Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00

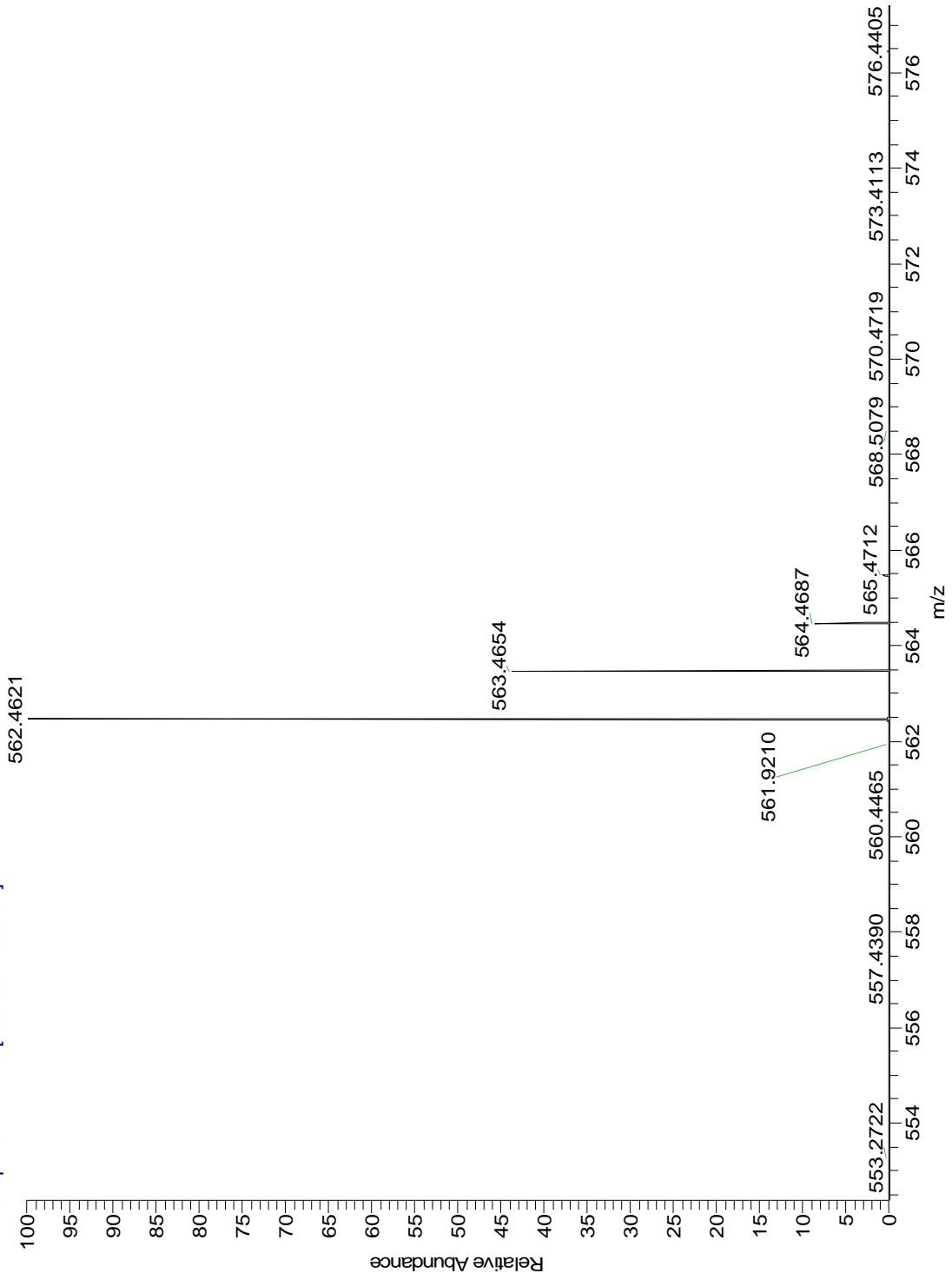




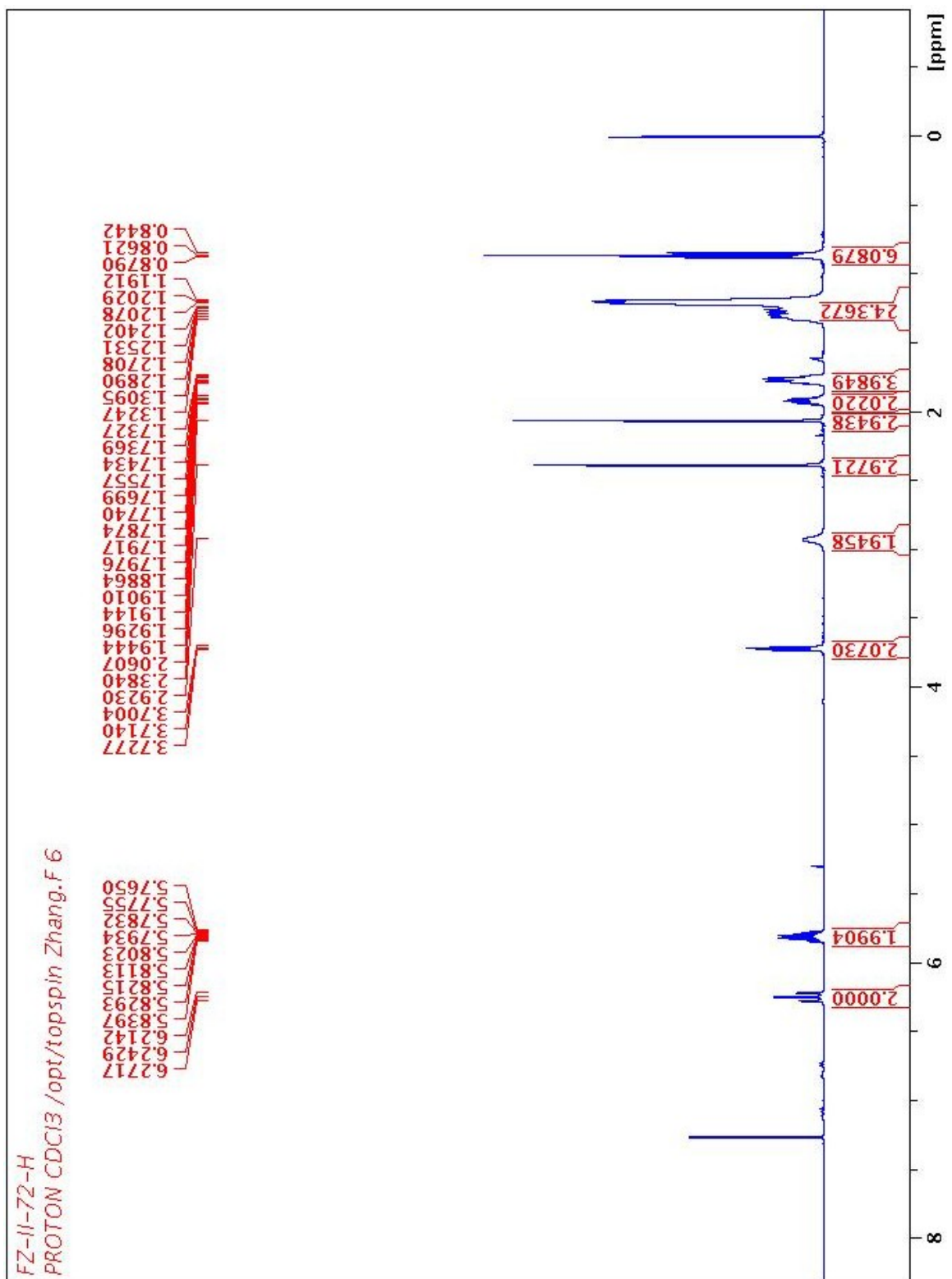


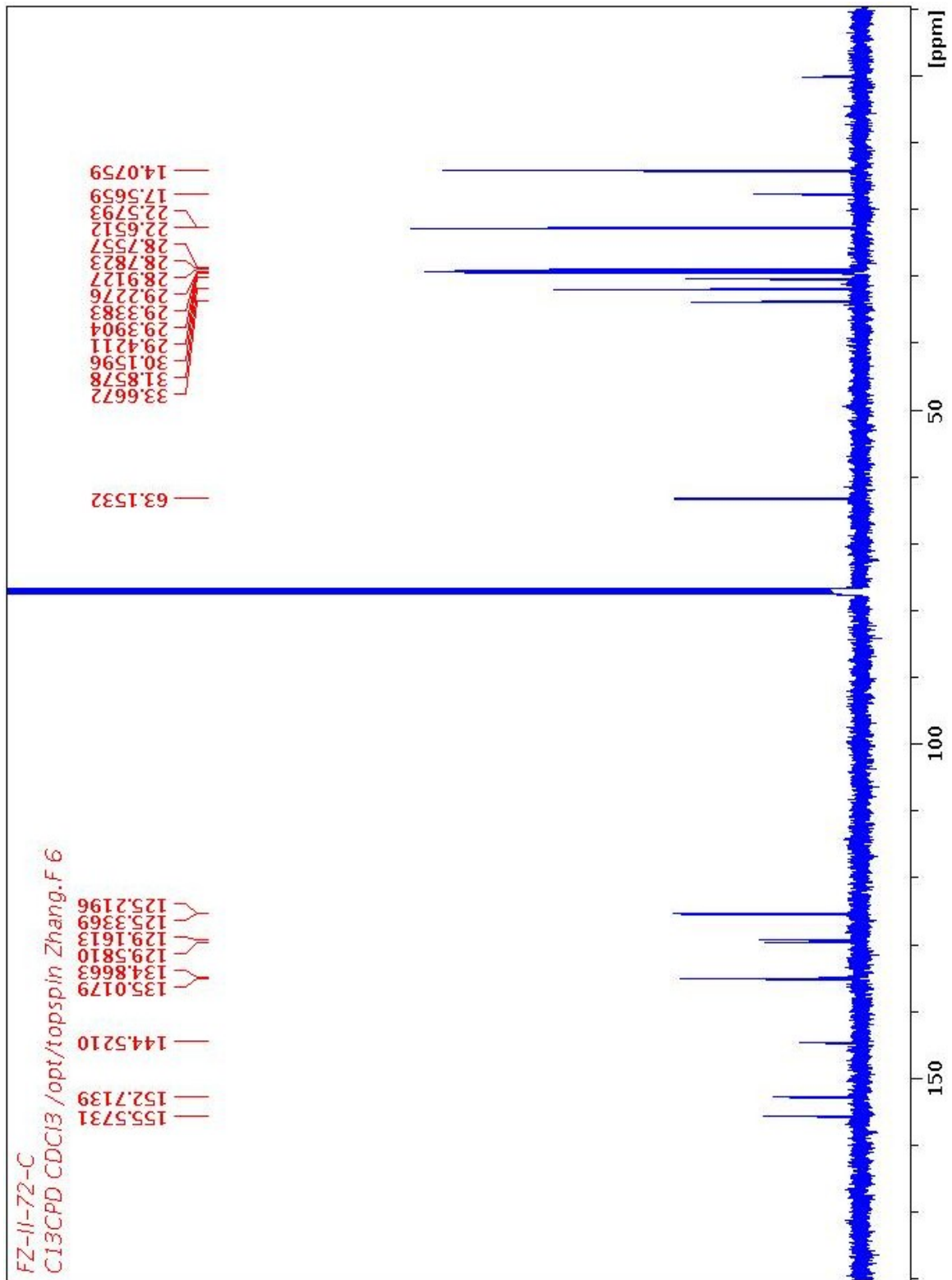


r110809r05 #1-49 RT: 0.01-0.68 AV: 49 NL: 1.51E7  
T: FTMS + p NSIFull.ms [300.00-1500.00]

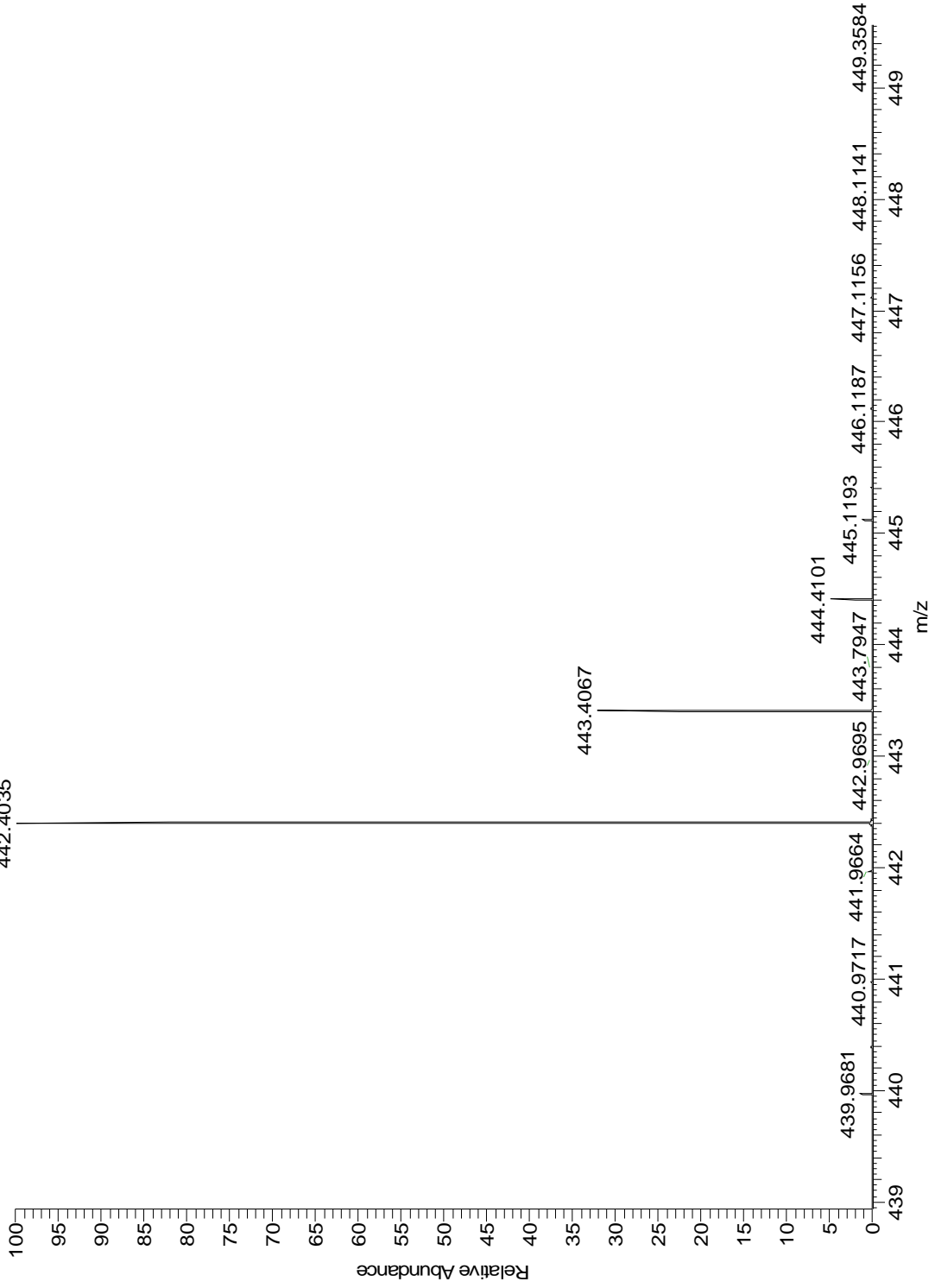






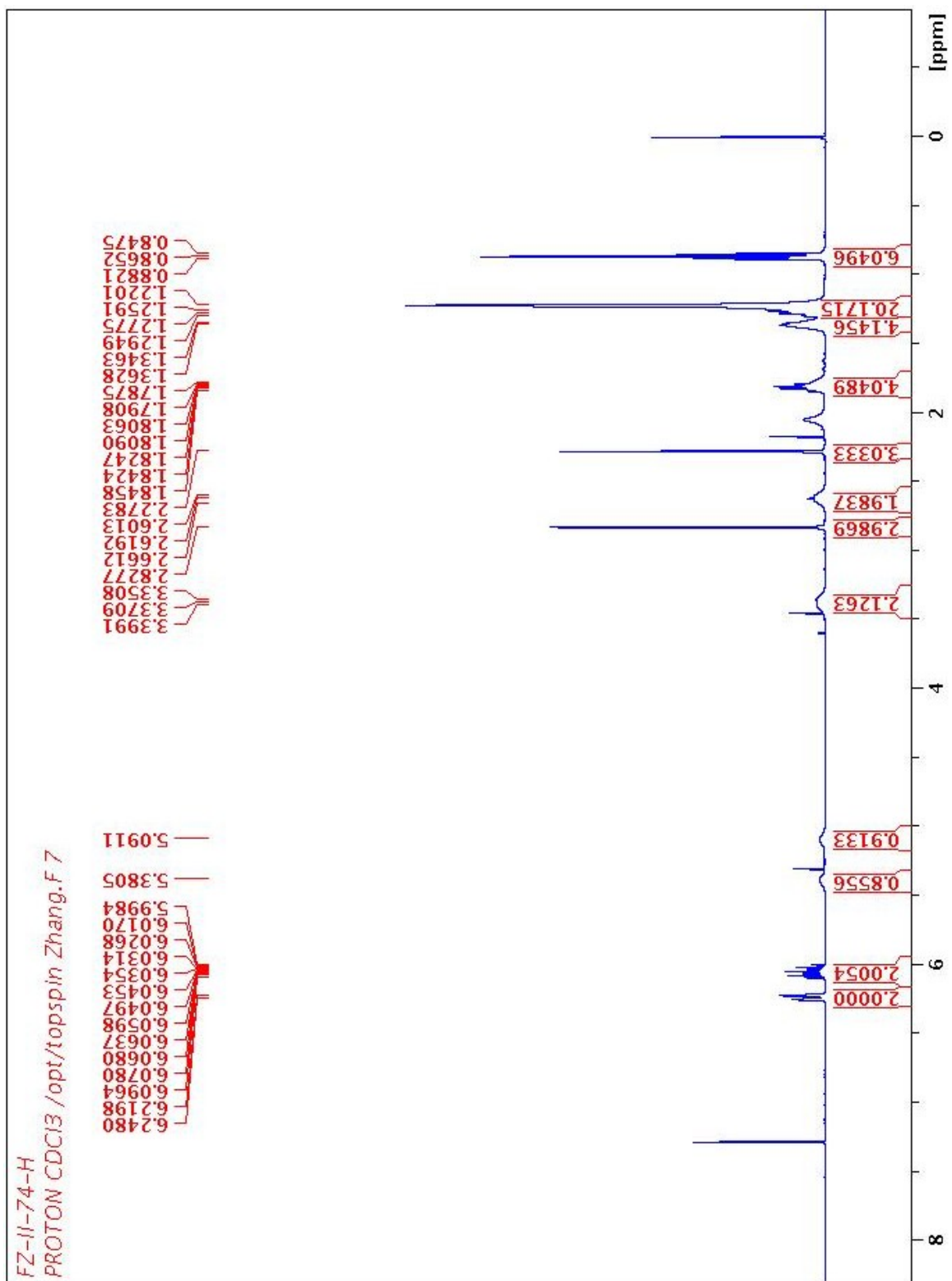


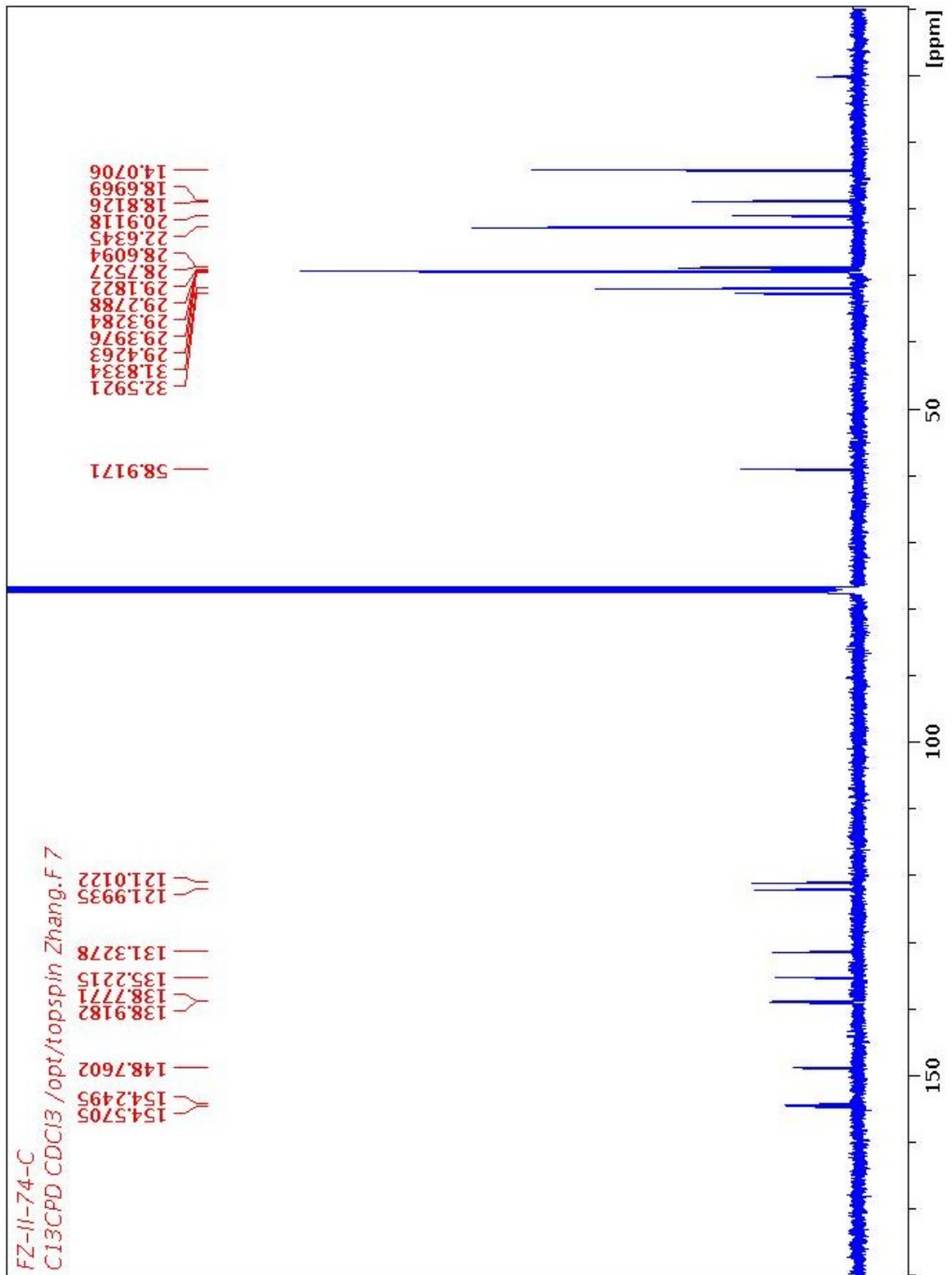
r110809r06 #31-50 RT: 0.43-0.70 AV: 20 NL: 2.28E7  
T: FTMS + p NSI Full ms [300.00-1500.00]



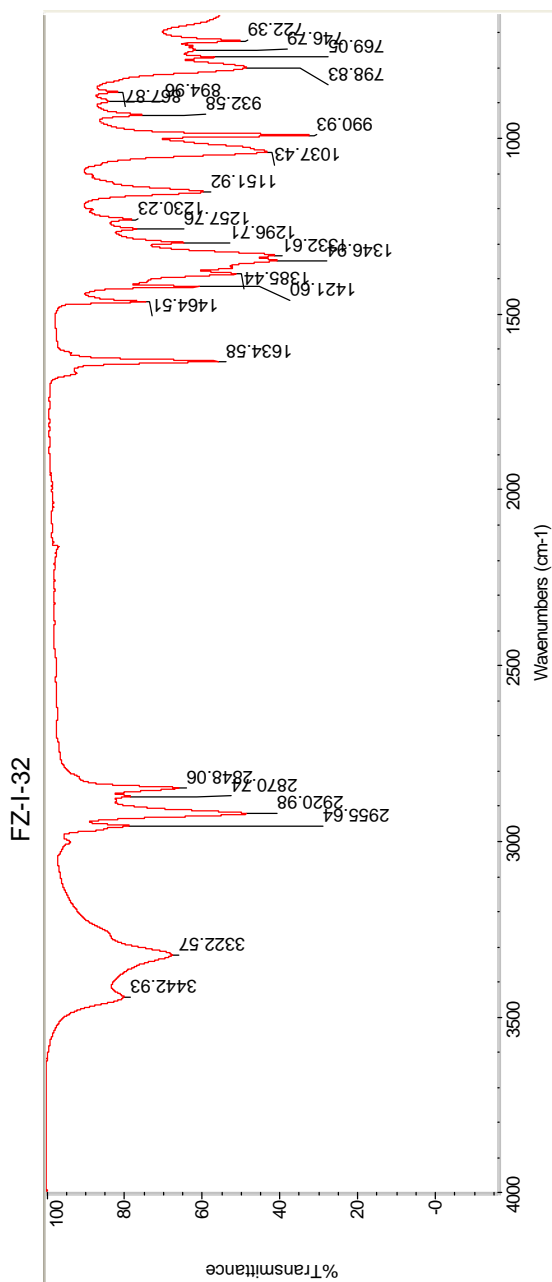








Fri Jun 10 12:14:37 2011 (GI)

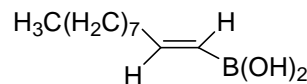


Fri Jun 10 12:14:27 2011 (GMT-04:00)

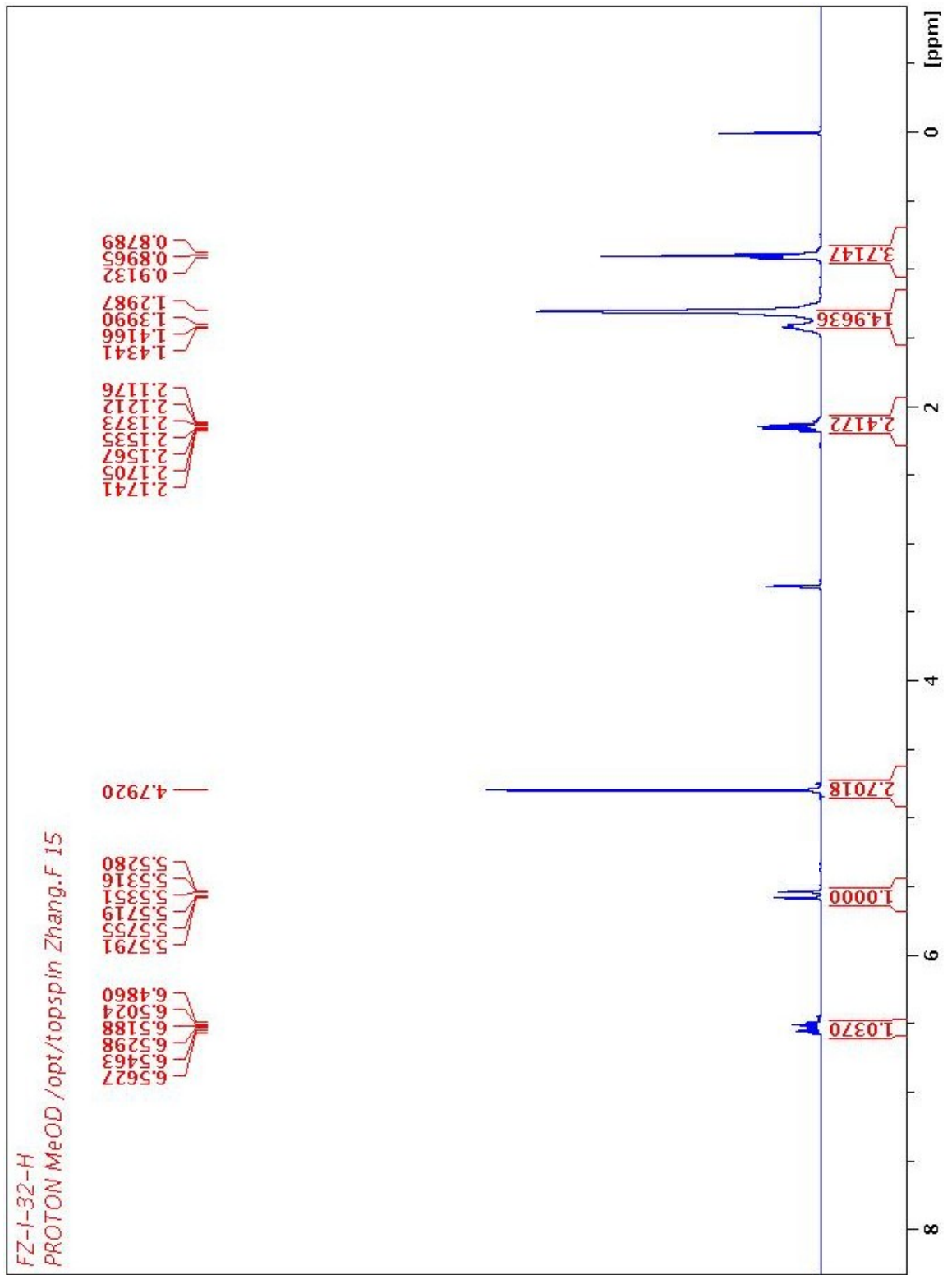
FIND PEAKS:

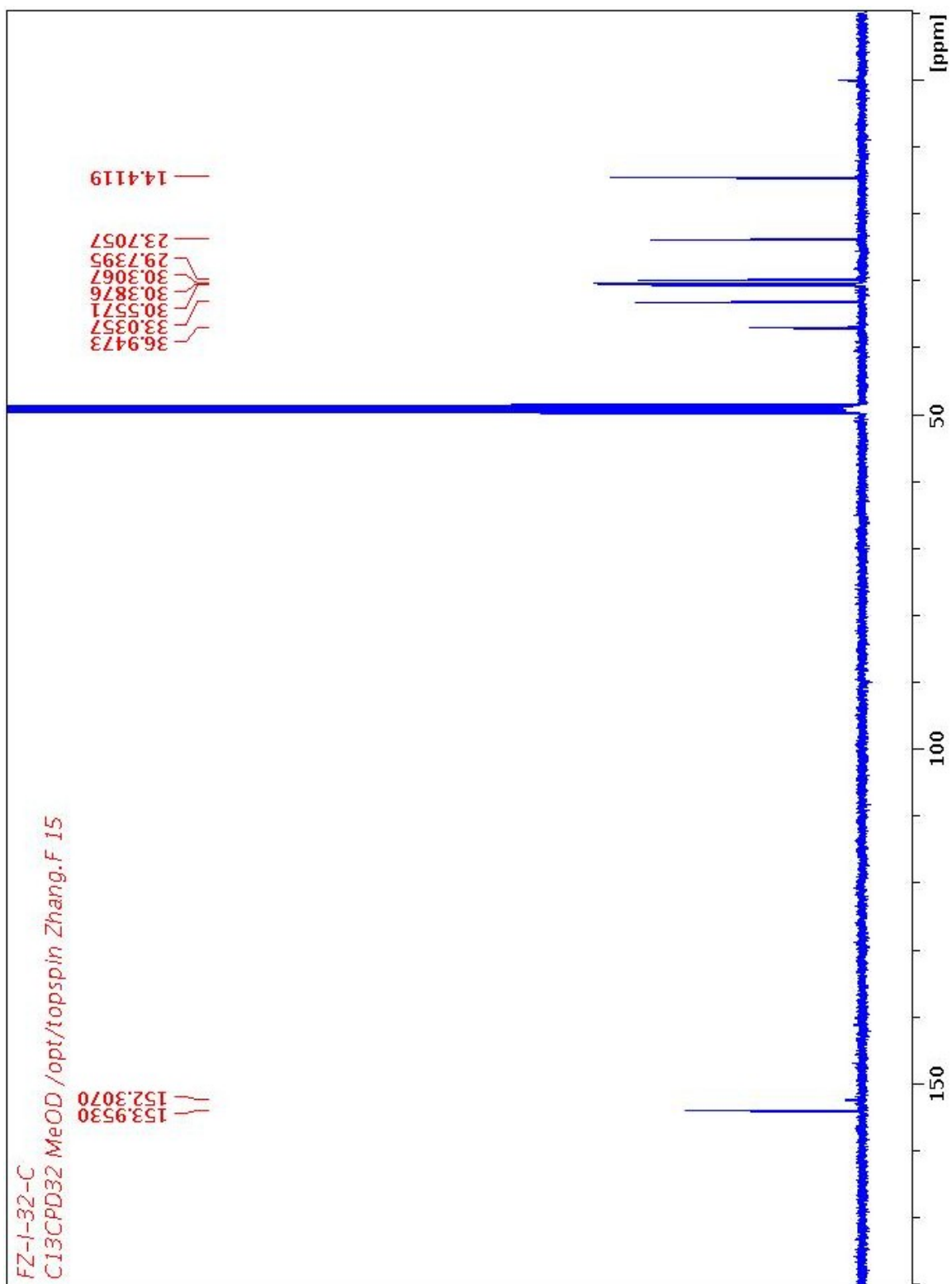
Spectrum:	FZ-I-32
Region:	4000.12
Absolute threshold:	649.89
Sensitivity:	90.470
Peak list:	
Position:	722.39
Intensity:	Intensiv:
Position:	746.79
Intensity:	Intensiv:
Position:	769.05
Intensity:	Intensiv:
Position:	798.83
Intensity:	Intensiv:
Position:	867.87
Intensity:	Intensiv:
Position:	894.96
Intensity:	Intensiv:
Position:	932.58
Intensity:	Intensiv:

Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00

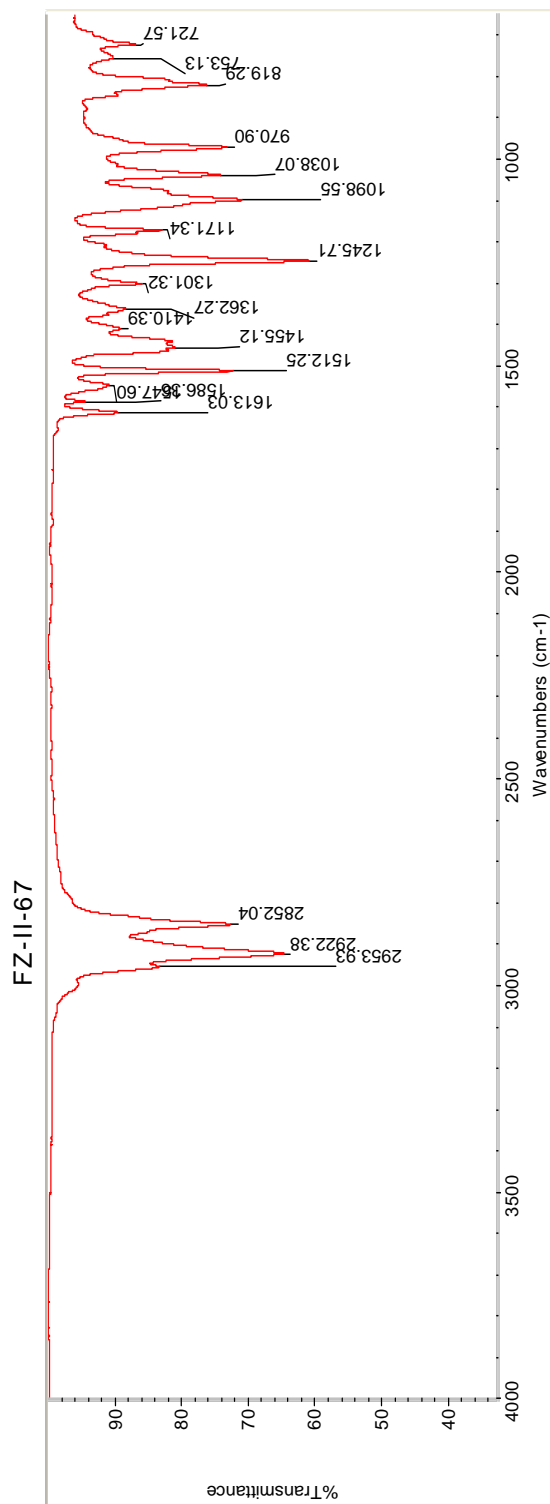


15





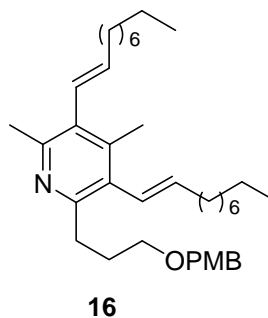
Thu Apr 14 17:59:10 2011 (G

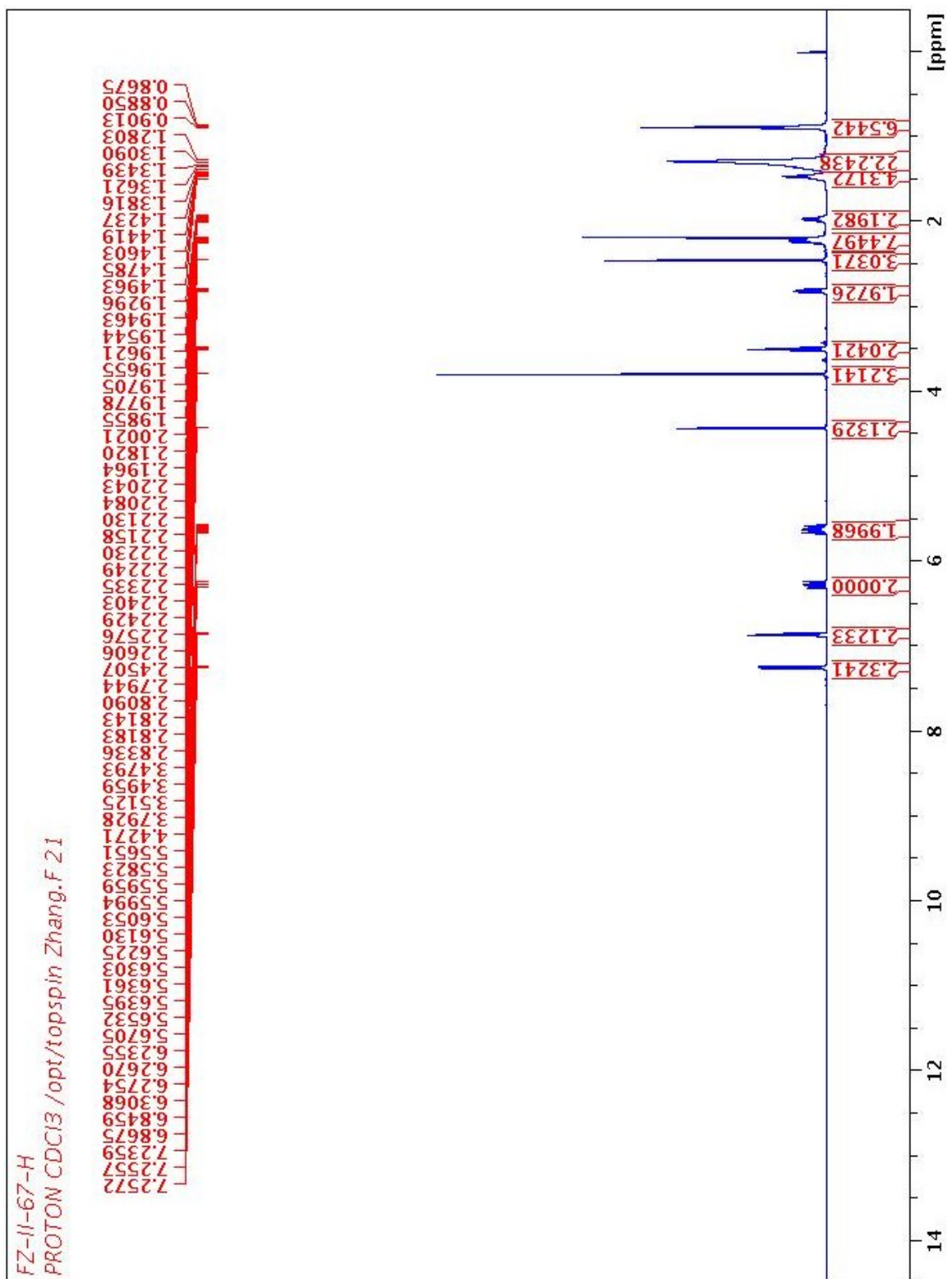


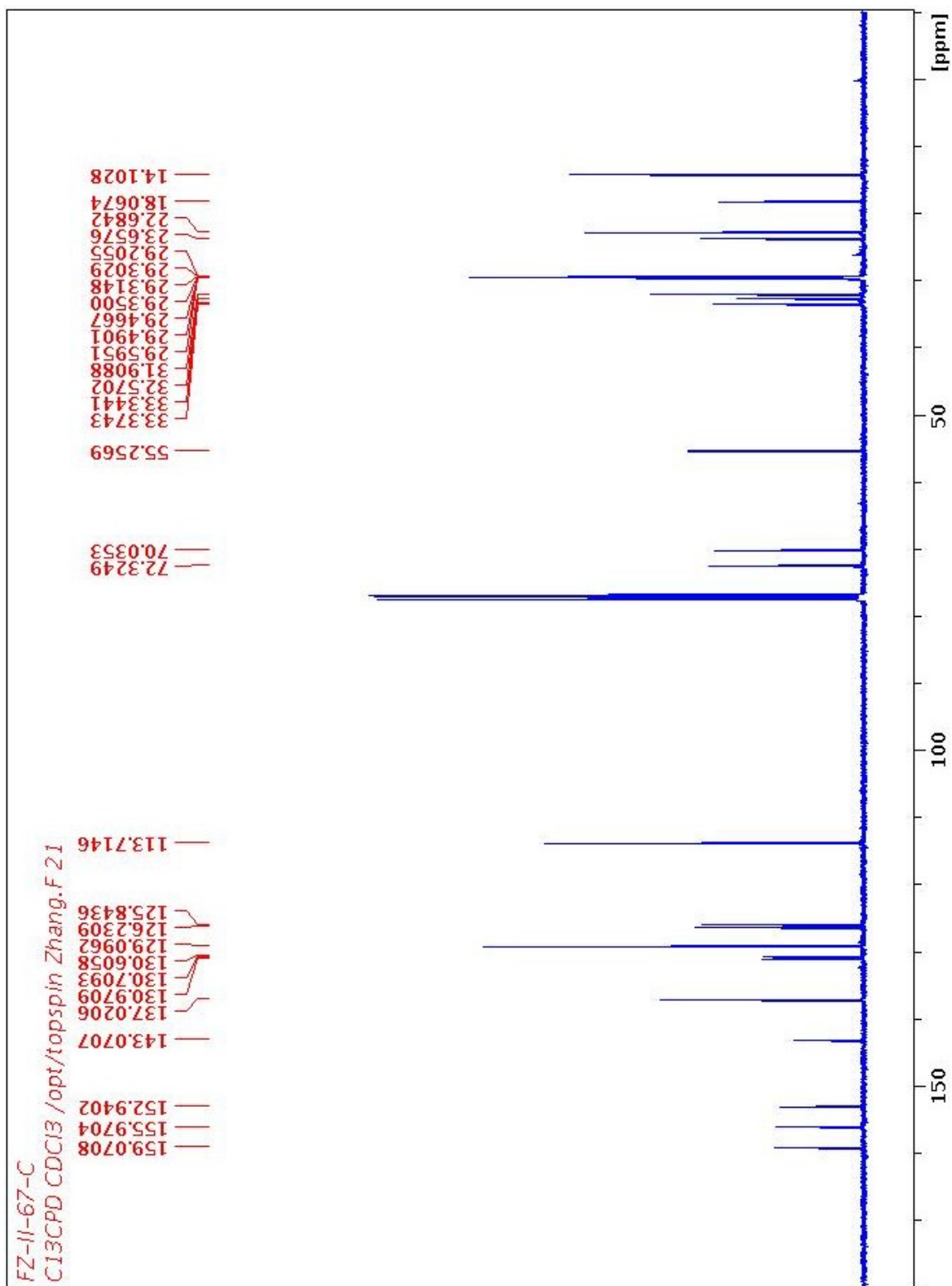
Thu Apr 14 17:59:05 2011 (GMT-04:00)

Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00

FIND PEAKS:  
Spectrum: FZ-II-67  
Region: 4000.12 649.89  
Absolute threshold: 97.735  
Sensitivity: 50  
Peak list:  
Position: 721.57 Intensity:  
Position: 753.13 Intensity:  
Position: 819.29 Intensity:  
Position: 970.90 Intensity:  
Position: 1038.07 Intensity:  
Position: 1098.55 Intensity:  
Position: 1171.34 Intensity:

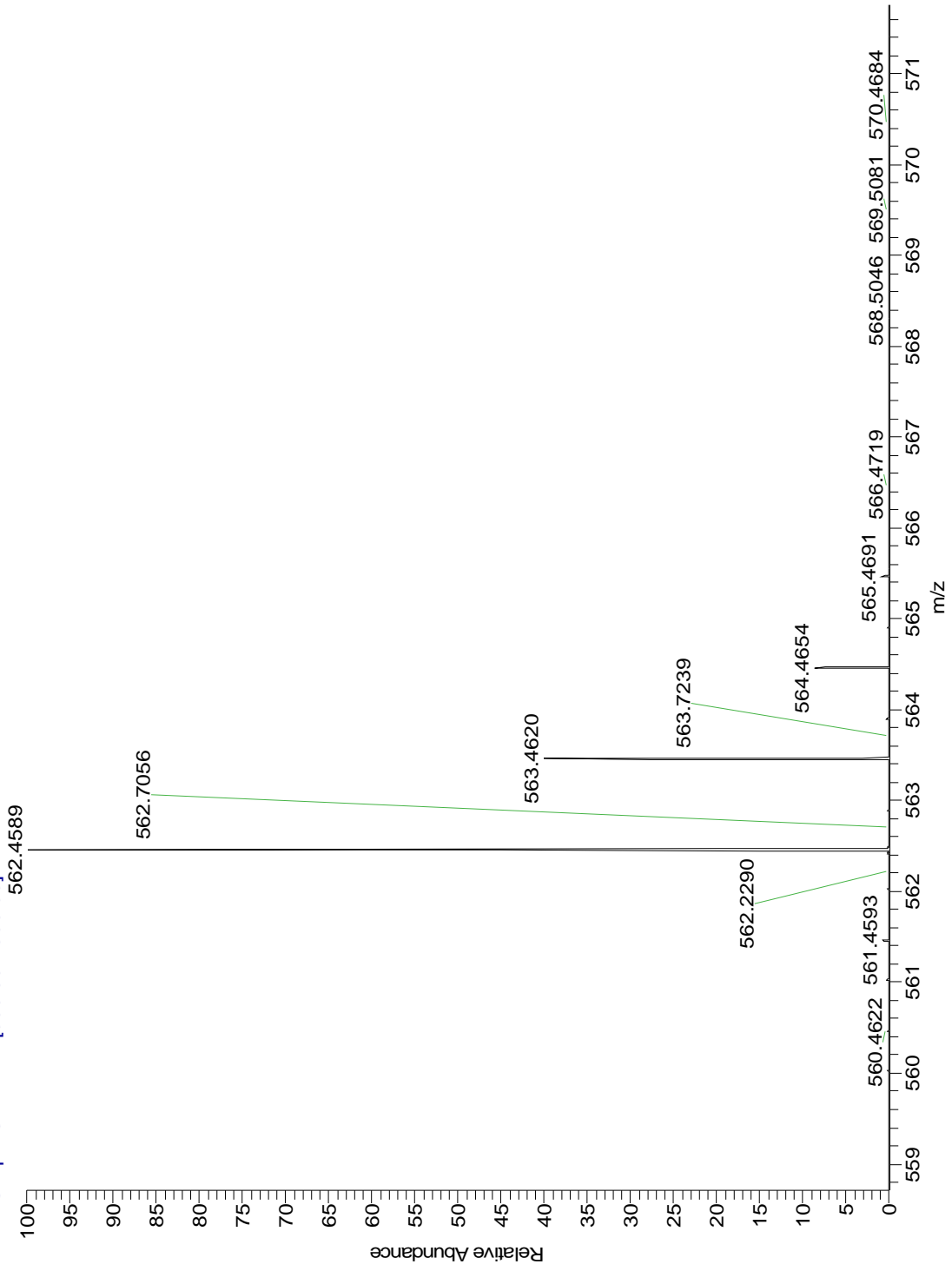




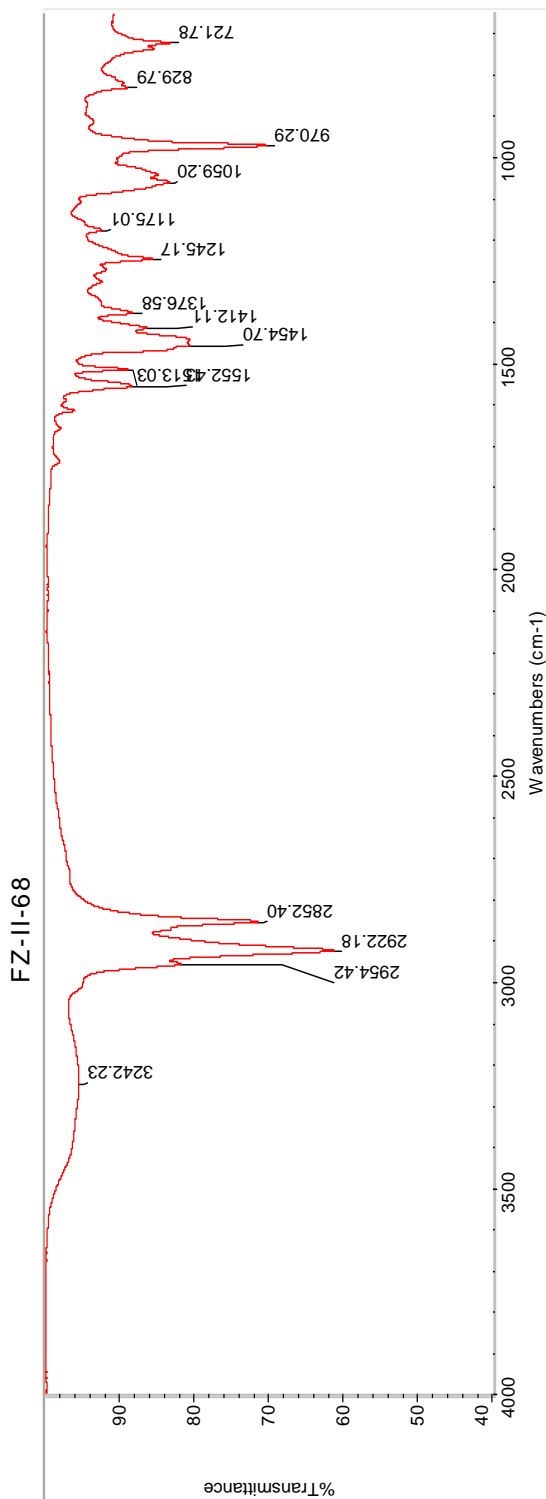




r110809r07 #1-49 RT: 0.01-0.68 AV: 49 NL: 4.47E8  
T: FTMS + p NSI Full ms [300.00-1500.00]



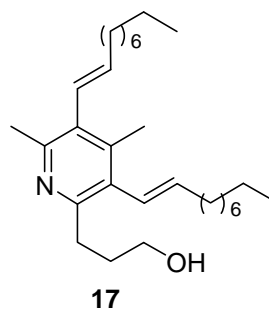
Thu Apr 14 17:59:41 2011 (G

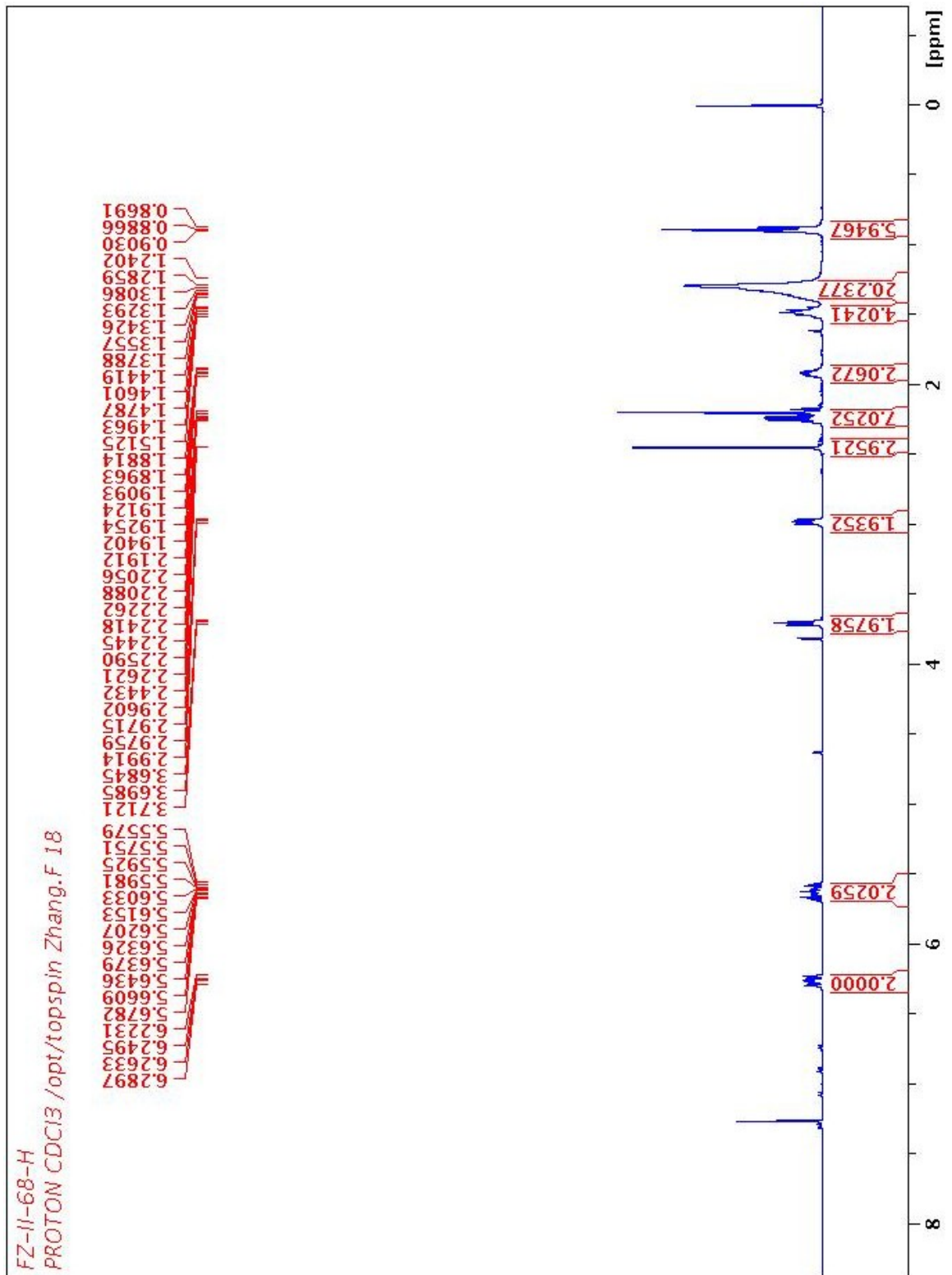


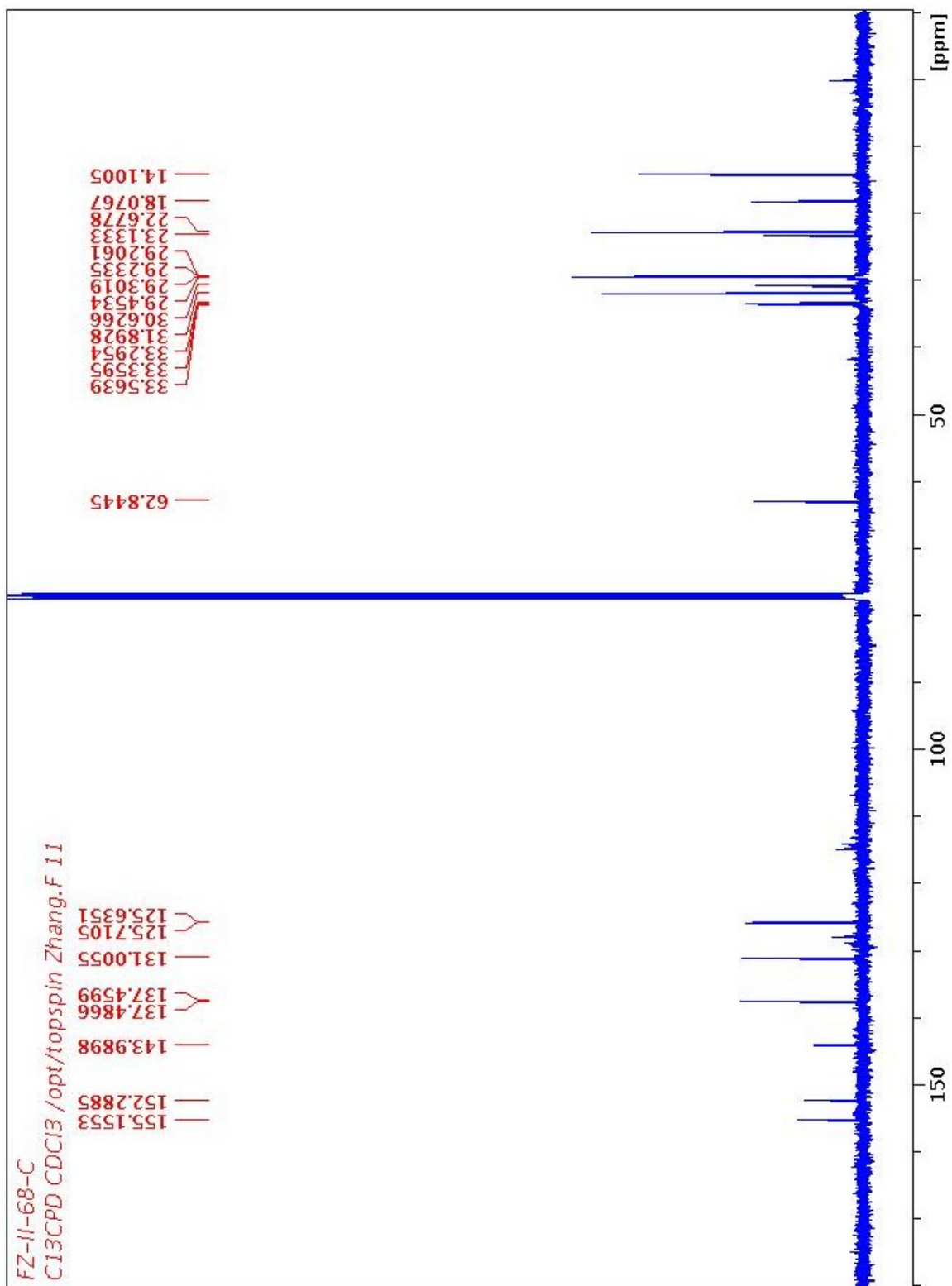
Thu Apr 14 17:59:37 2011 (GMT-04:00)

Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00

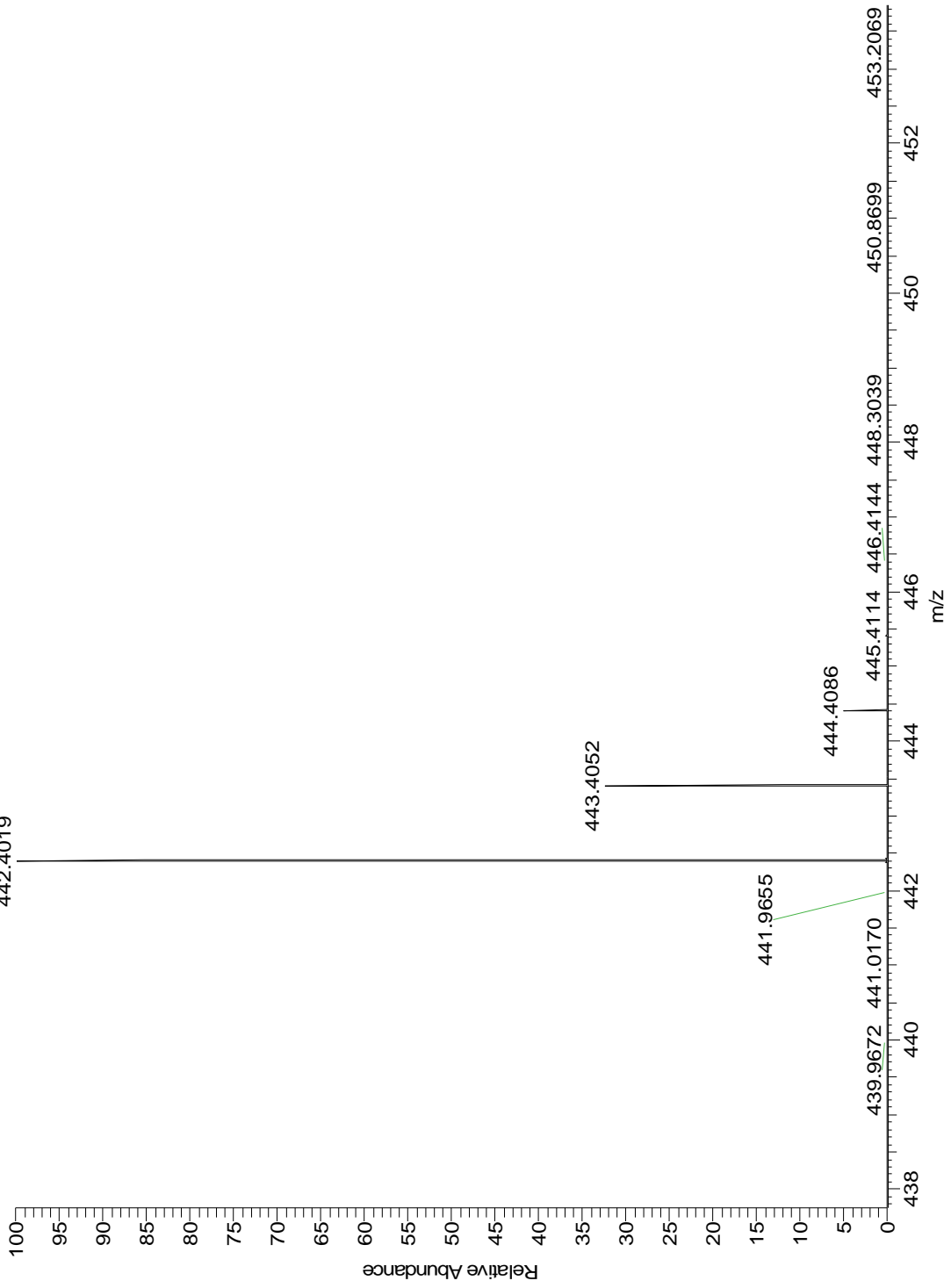
FIND PEAKS:  
Spectrum: FZ-II-68  
Region: 4000.12 649.89  
Absolute threshold: 95.383  
Sensitivity: 50  
Peak list:  
Position: 721.78 Intensity:  
Position: 829.79 Intensity:  
Position: 970.29 Intensity:  
Position: 1059.20 Intensity:  
Position: 1175.01 Intensity:  
Position: 1245.17 Intensity:  
Position: 1376.58 Intensity:



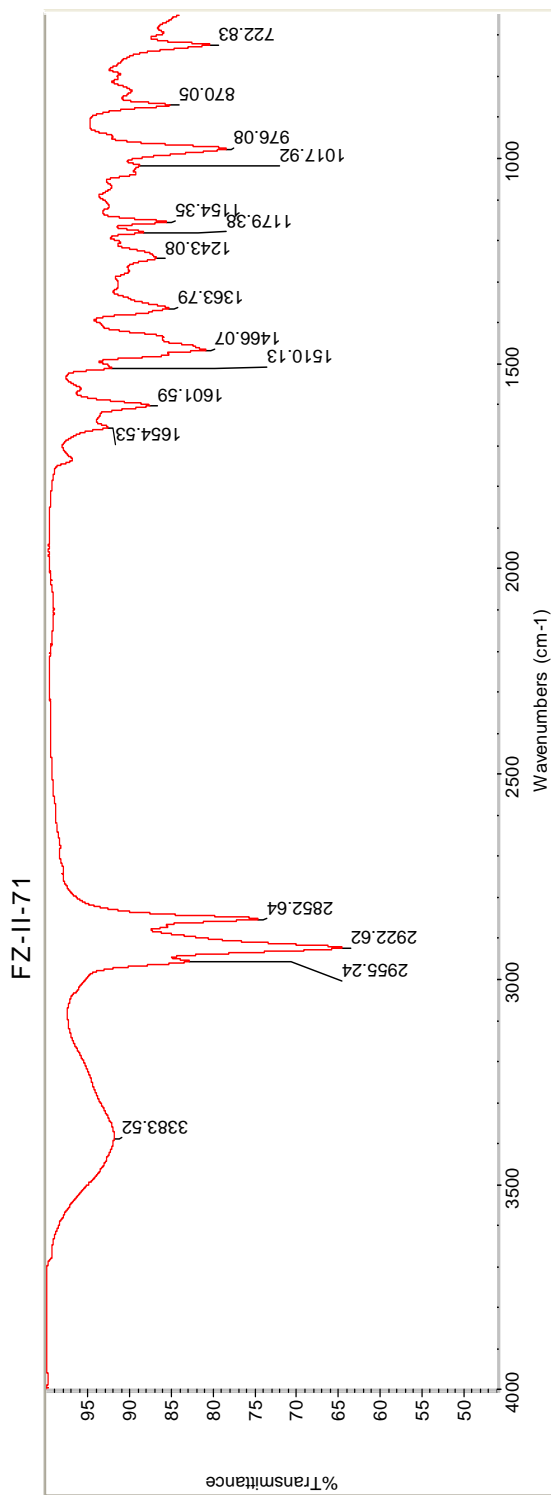




r110809r08 #22-50 RT: 0.29-0.68 AV: 29 NL: 6.59E8  
T: FTMS + p NSIFull ms [300.00-1500.00]



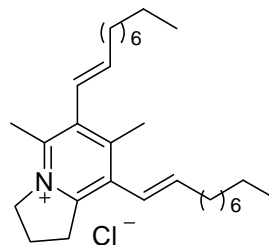
Thu Apr 14 18:00:17 2011 (G



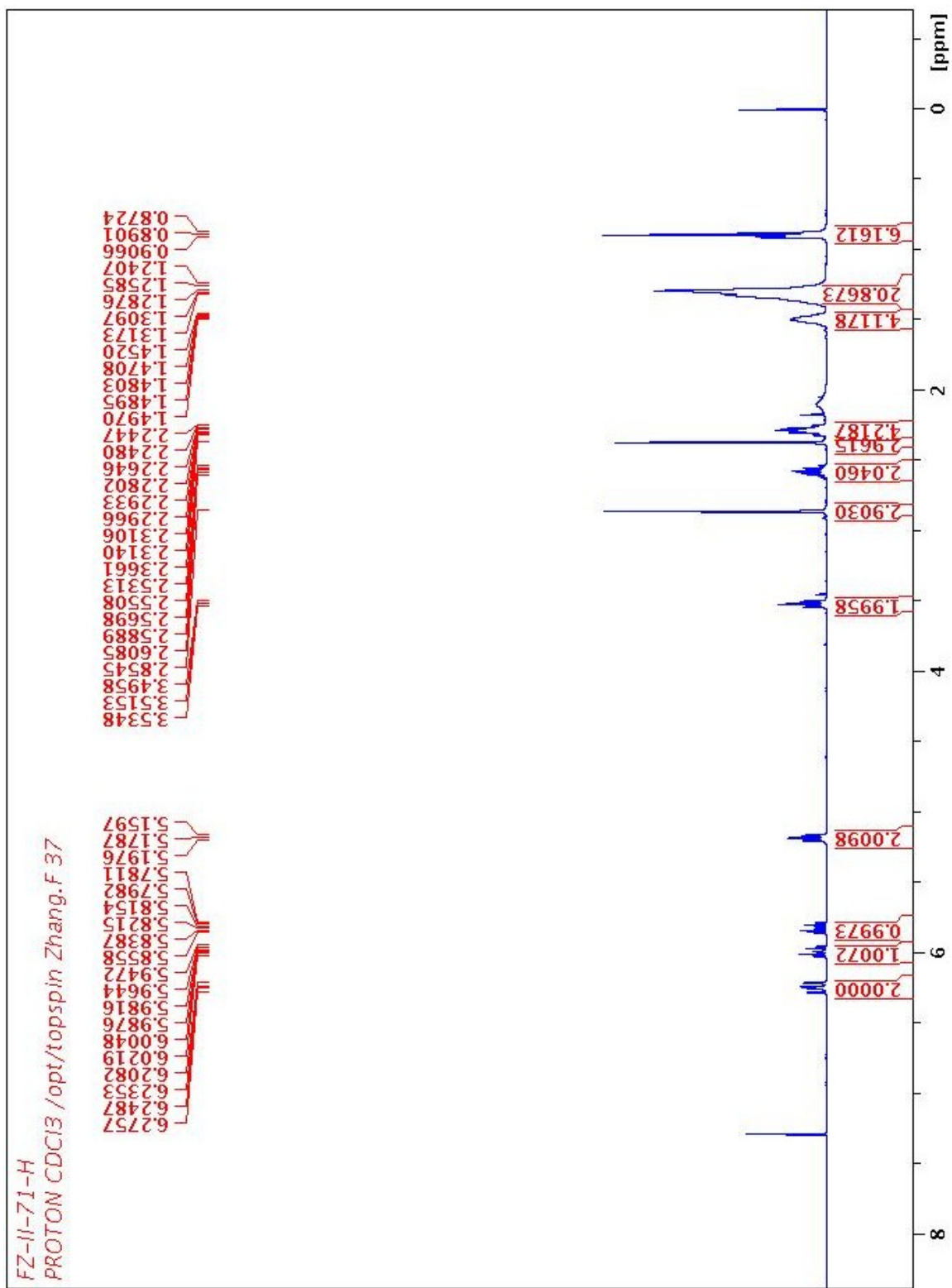
Thu Apr 14 18:00:11 2011 (GMT-04:00)

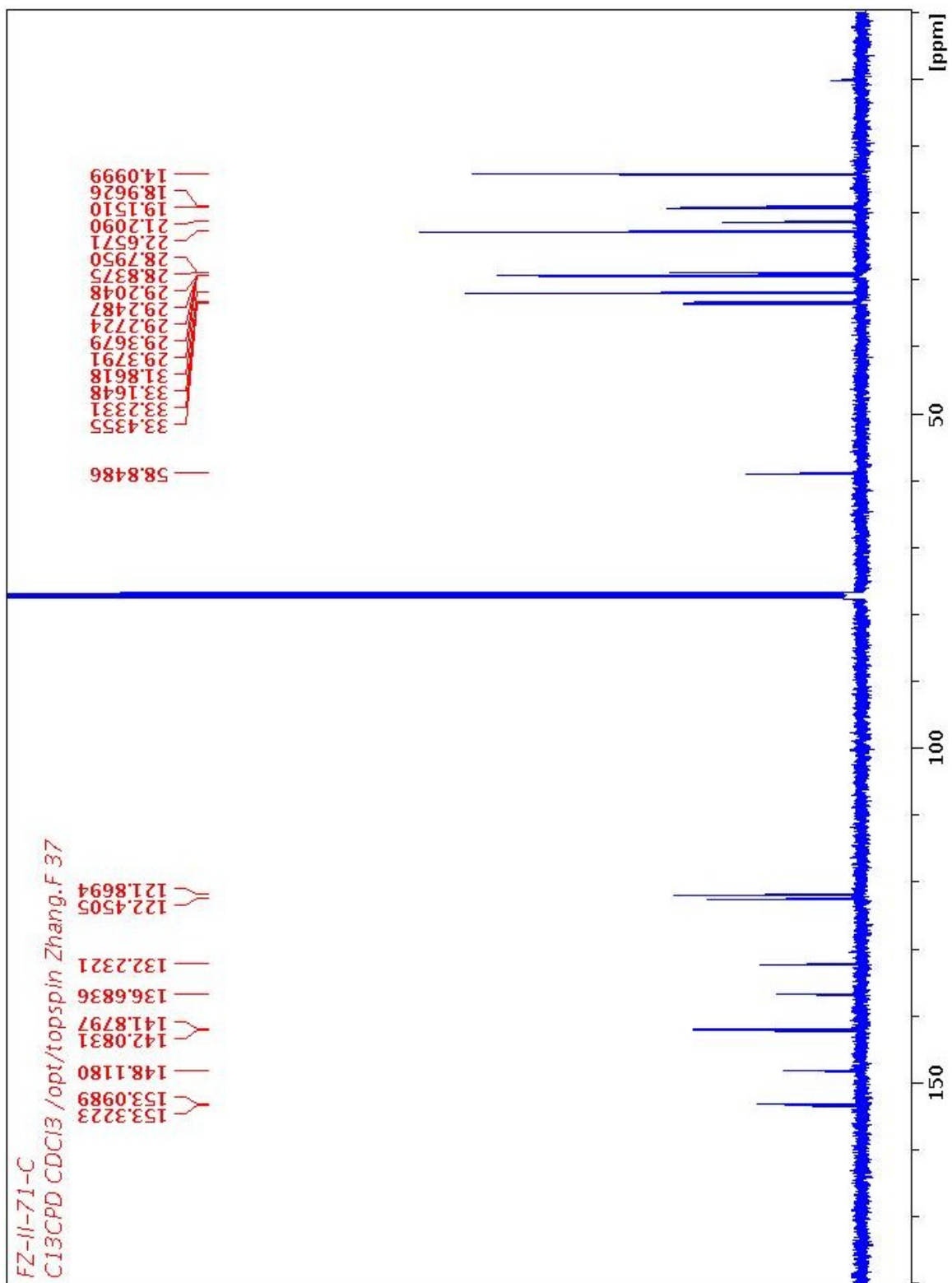
Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00

FIND PEAKS:  
Spectrum: FZ-II-71  
Region: 4000.12 649.89  
Absolute threshold: 98.696  
Sensitivity: 50  
Peak list:  
Position: 722.83 Intensity:  
Position: 870.05 Intensity:  
Position: 976.08 Intensity:  
Position: 1017.92 Intensity:  
Position: 1154.35 Intensity:  
Position: 1179.38 Intensity:  
Position: 1243.08 Intensity:



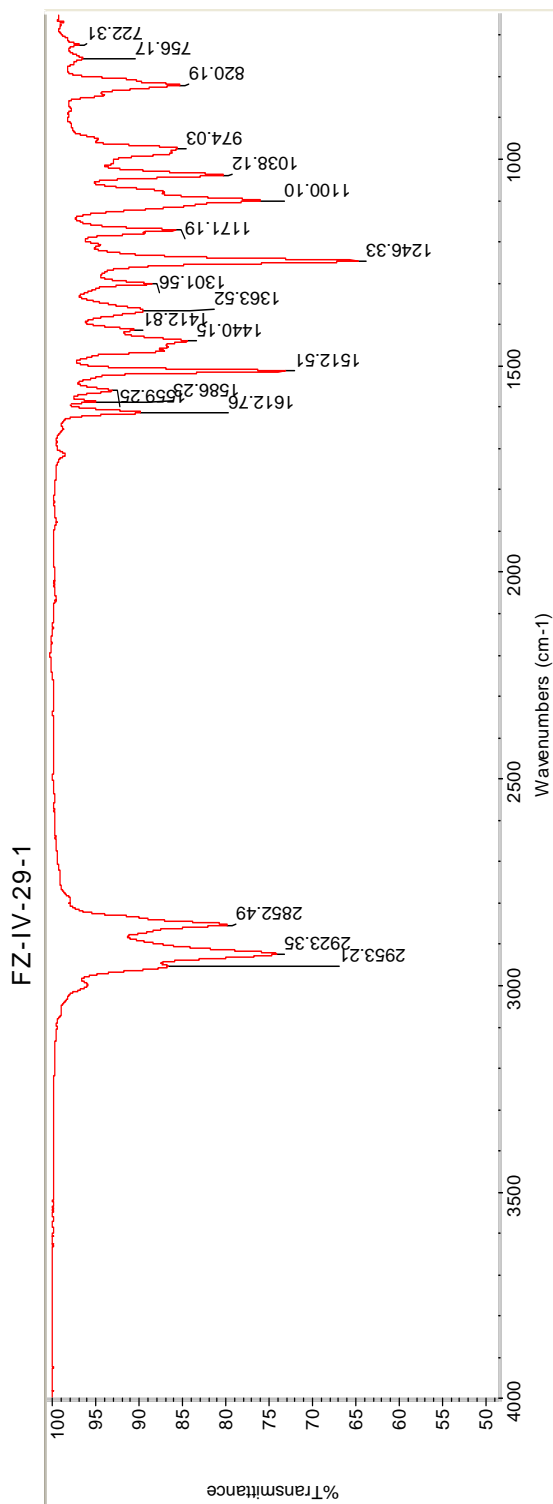
2 (11E,22E)







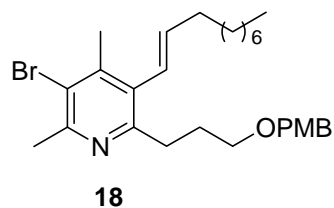
Thu Apr 14 18:05:29 2011 (G

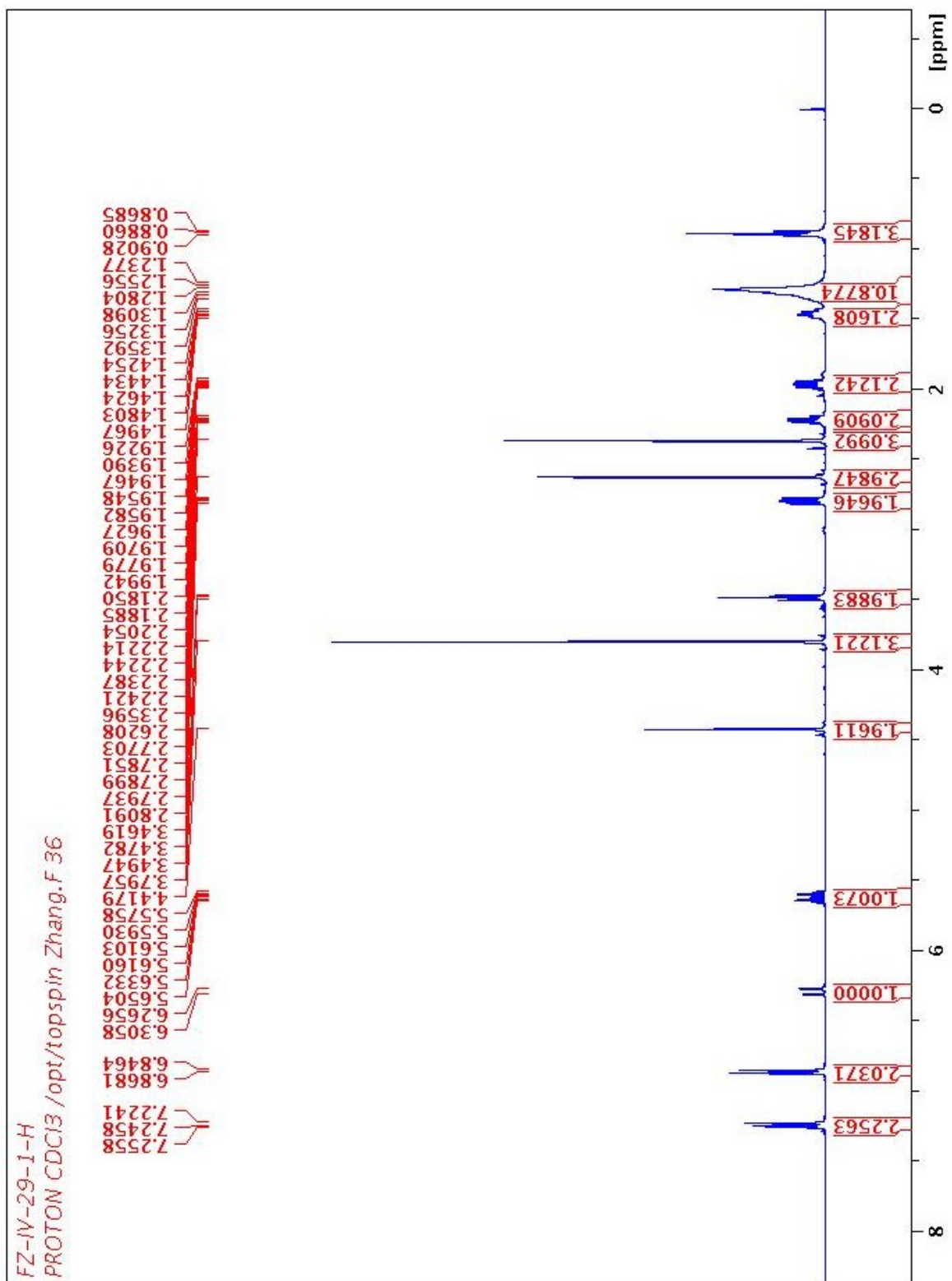


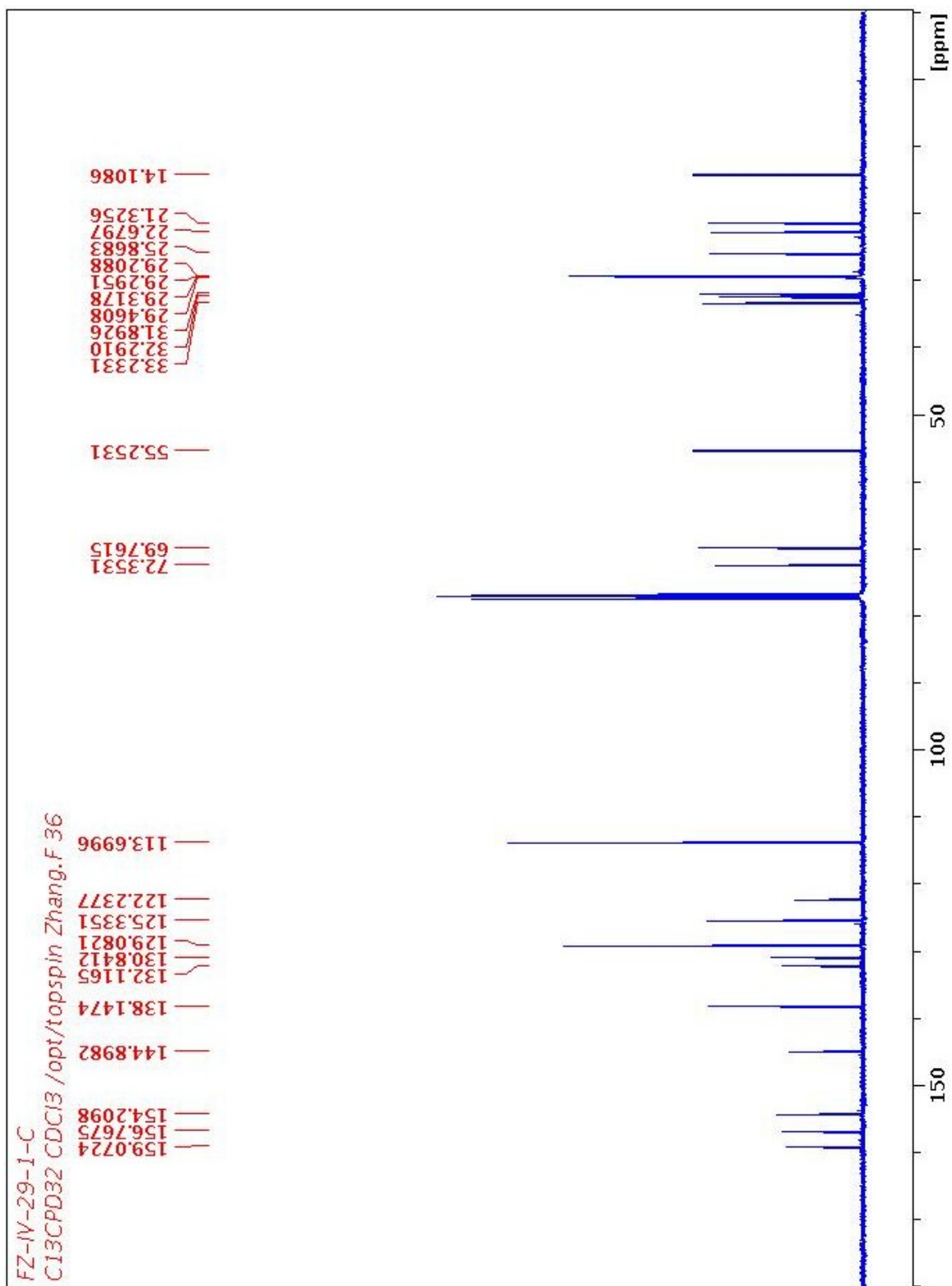
Thu Apr 14 18:05:20 2011 (GMT-04:00)

Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00

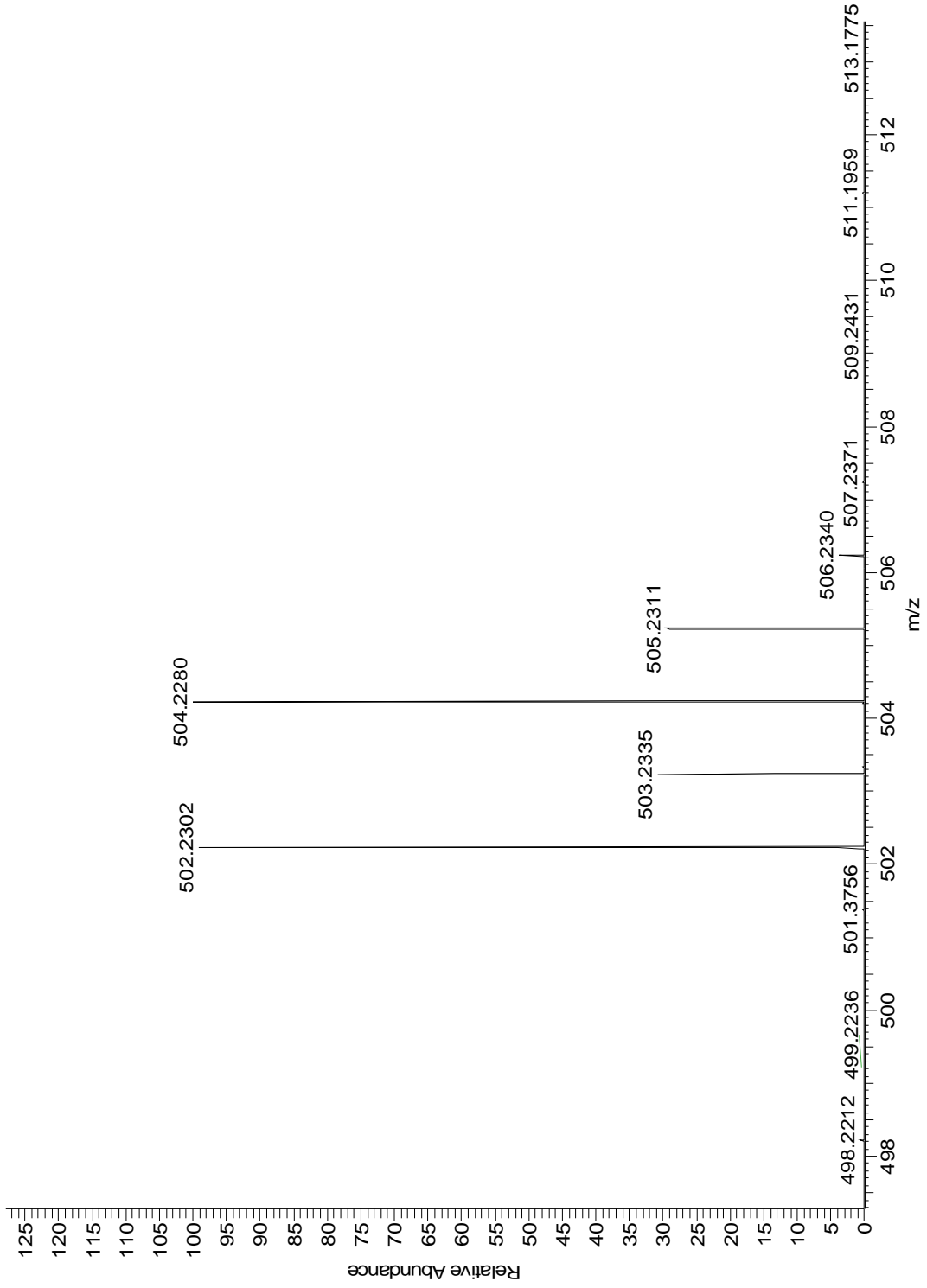
Find Peaks:  
Spectrum: FZ-IV-29-1  
Region: 4000.12 649.89  
Absolute threshold: 97.767  
Sensitivity: 59  
Peak list:  
Position: 722.31 Intensity: Intensive  
Position: 756.17 Intensity: Intensive  
Position: 820.19 Intensity: Intensive  
Position: 974.03 Intensity: Intensive  
Position: 1038.12 Intensity: Intensive  
Position: 1100.10 Intensity: Intensive  
Position: 1171.19 Intensity: Intensive



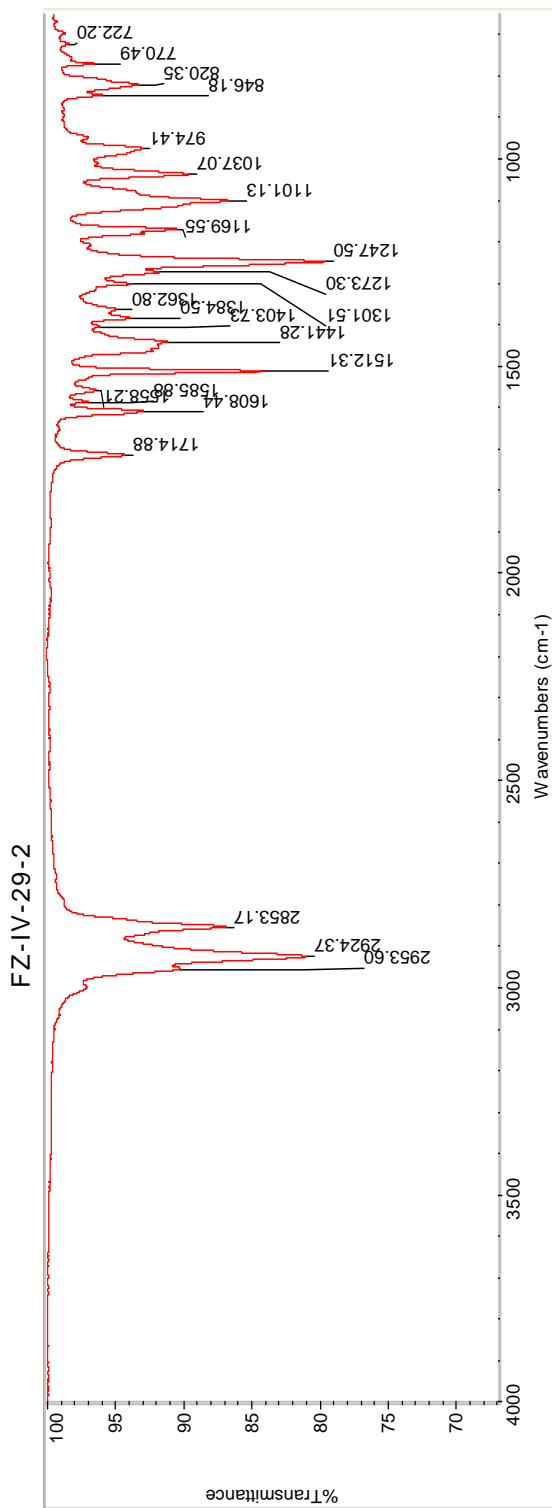




r11080909 #4-49 RT: 0.04-0.67 AV: 46 NL: 2.18E8  
T: FTMS + p NSI Full ms [300.00-1500.00]



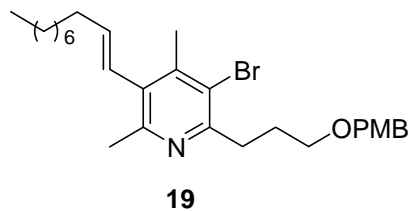
Thu Apr 14 18:02:39 2011 (G

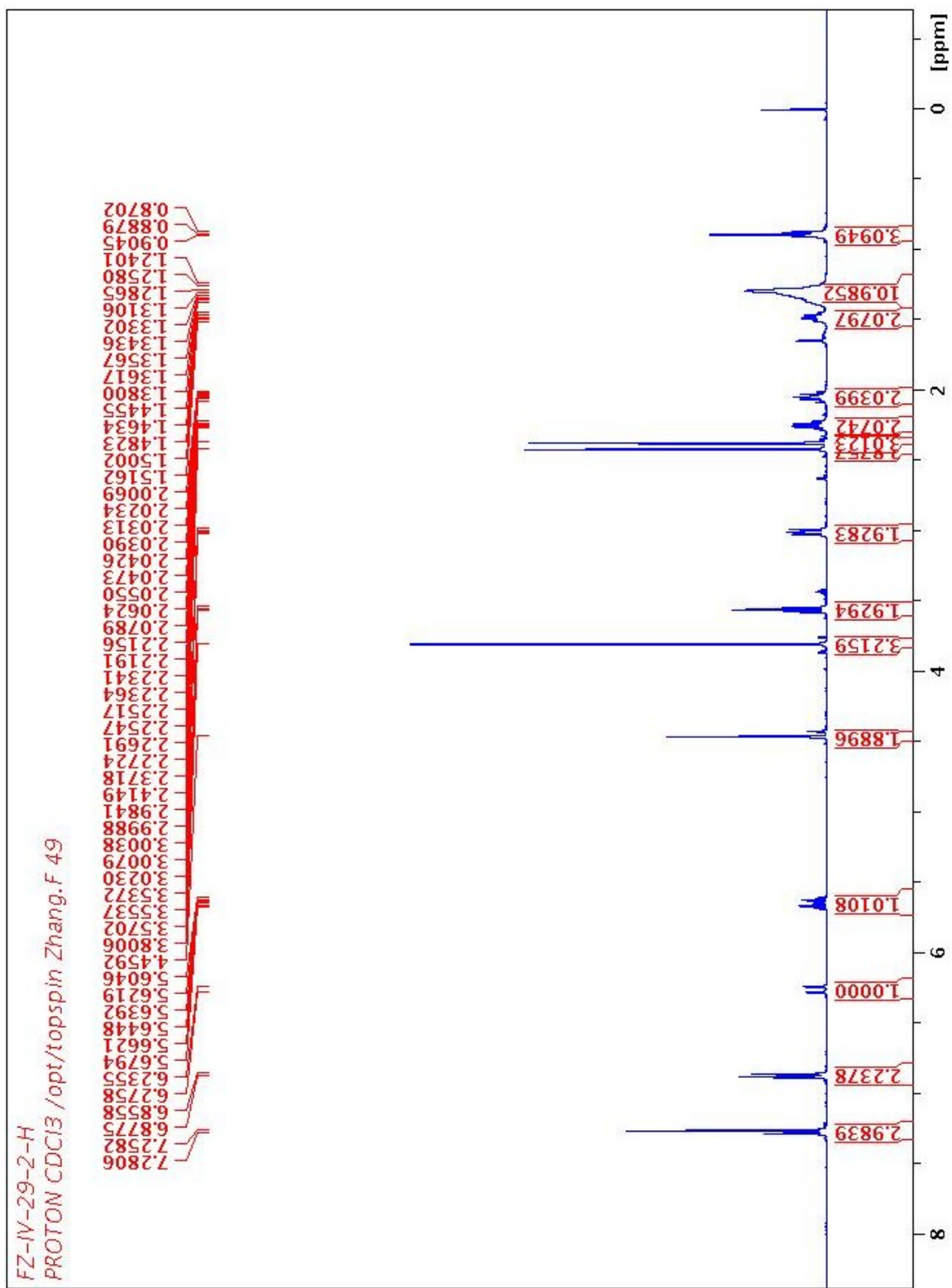


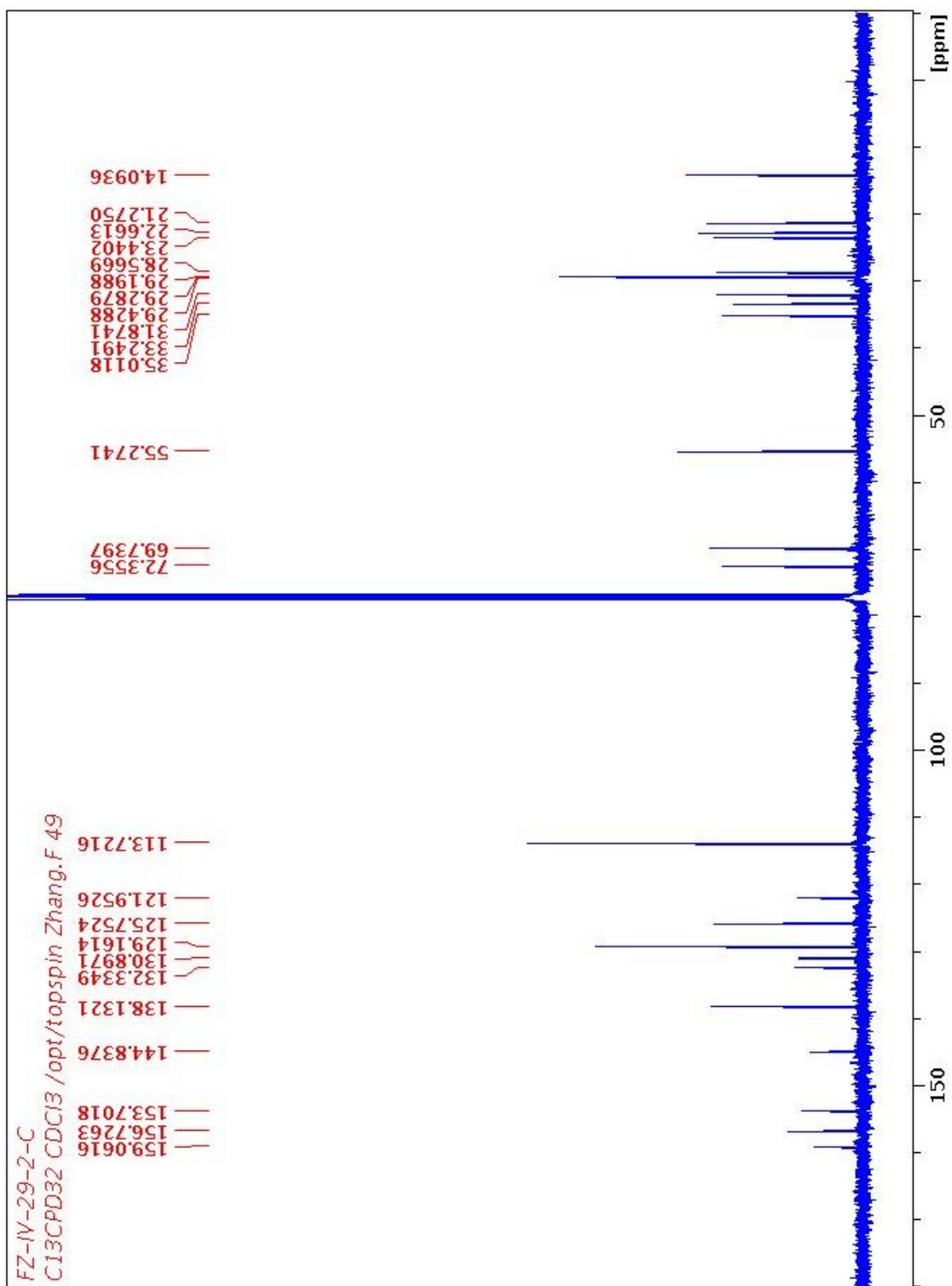
Thu Apr 14 18:02:35 2011 (GMT-04:00)

Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00

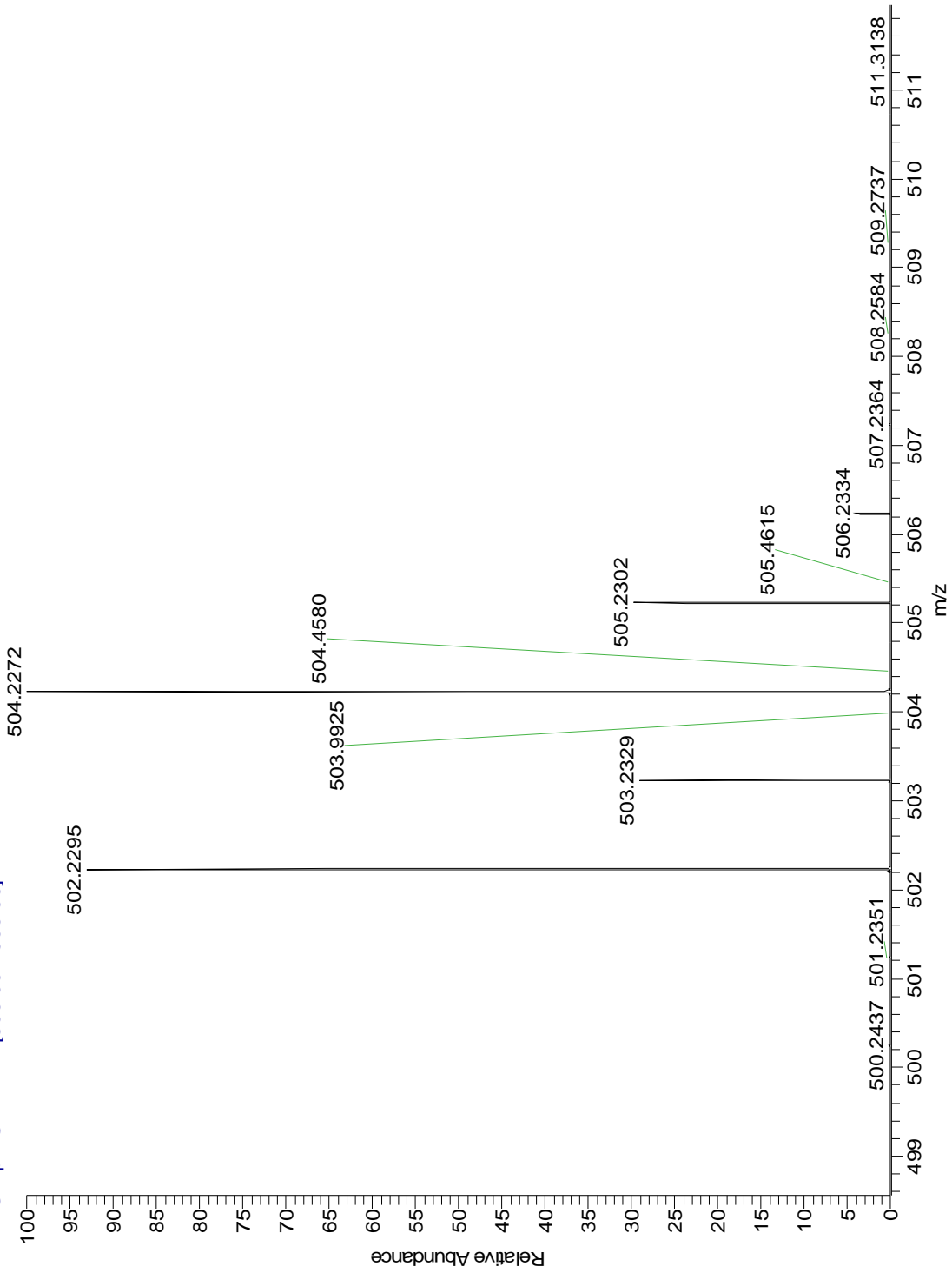
FIND PEAKS:  
Spectrum: FZ-IV-29-2  
Region: 4000.12 649.89  
Absolute threshold: 98.848  
Sensitivity: 55  
Peak list:  
Position: 722.20 Intensity: Intensive  
Position: 770.49 Intensity: Intensive  
Position: 820.35 Intensity: Intensive  
Position: 846.18 Intensity: Intensive  
Position: 974.41 Intensity: Intensive  
Position: 1037.07 Intensity: Intensive  
Position: 1101.13 Intensity: Intensive





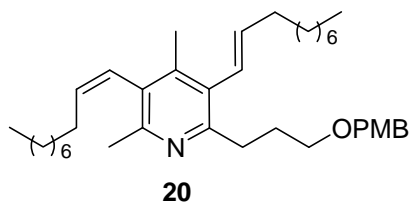
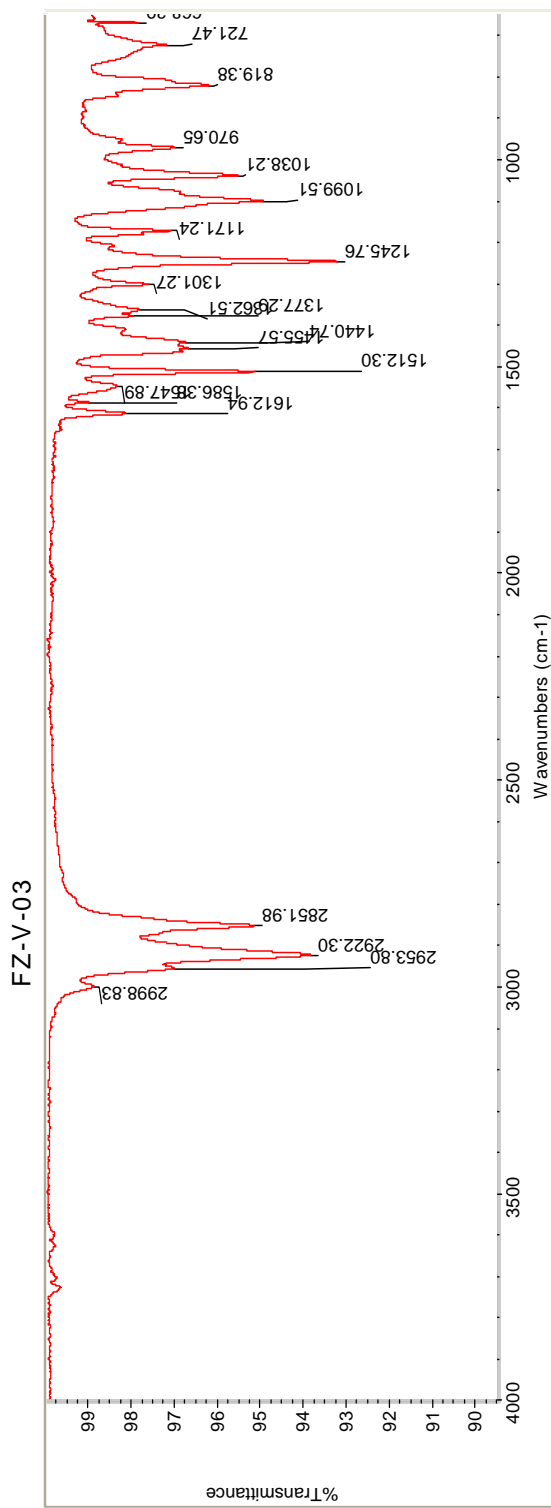


r110809r11 #5-50 RT: 0.07-0.69 AV: 46 NL: 2.14E8  
T: FTMS + p NSIFull ms [300.00-1500.00]





Thu Apr 14 18:06:13 2011 (G



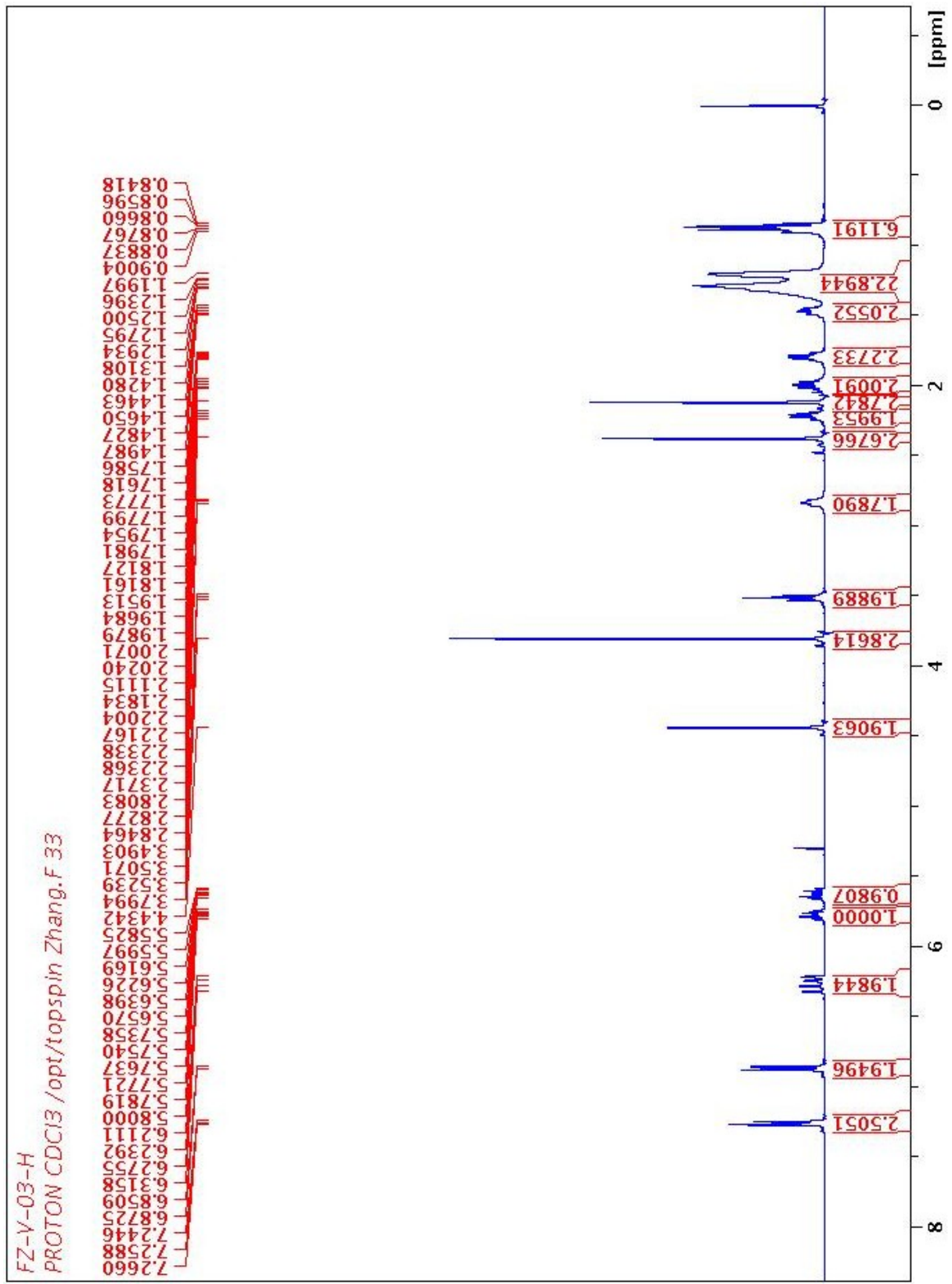
Thu Apr 14 18:06:08 2011 (GMT-04:00)

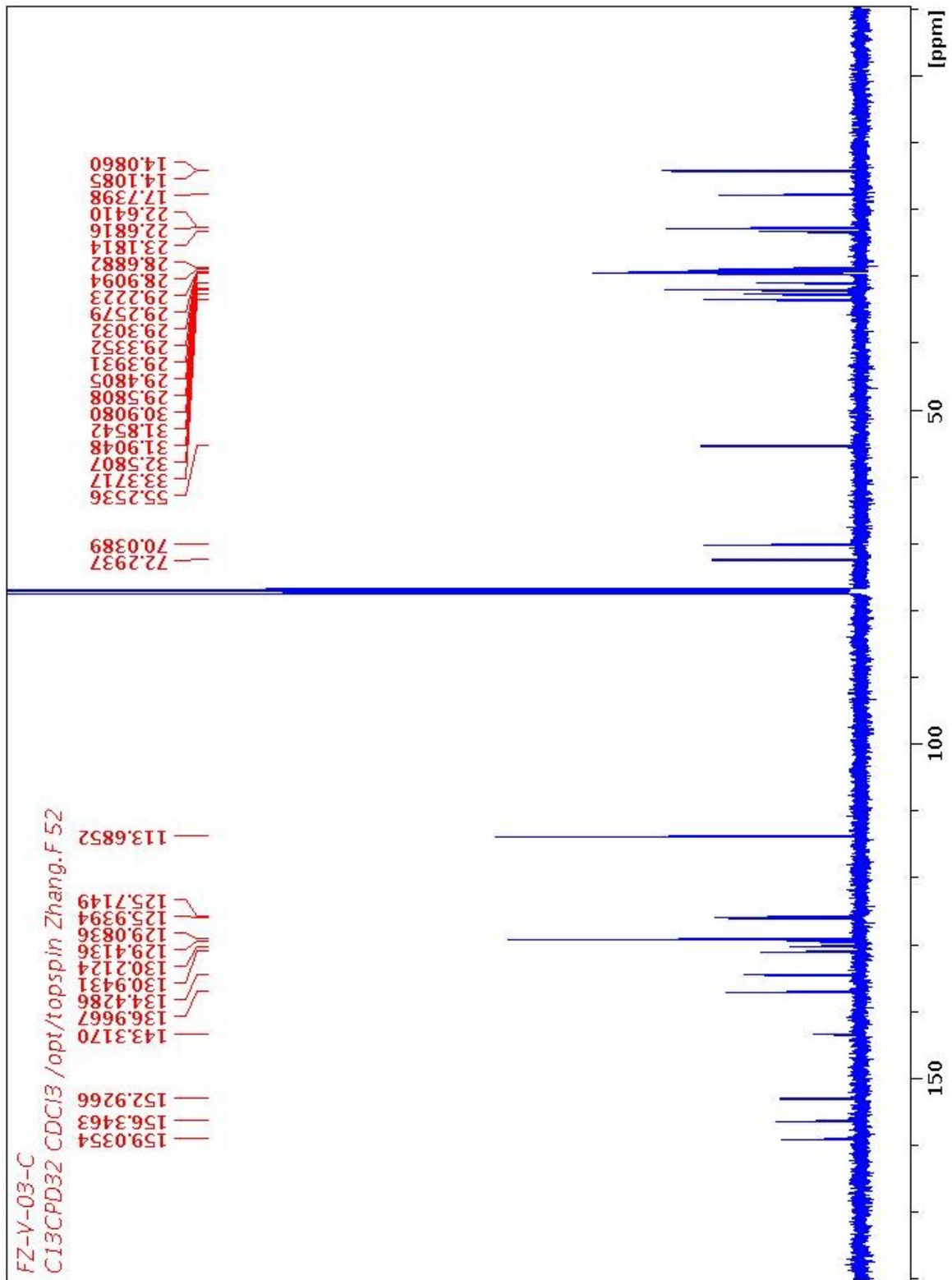
FIND PEAKS:

Position	Intensity
668.39	Intensiv
721.47	Intensiv
819.38	Intensiv
970.65	Intensiv
1038.21	Intensiv
1099.51	Intensiv
1171.24	Intensiv

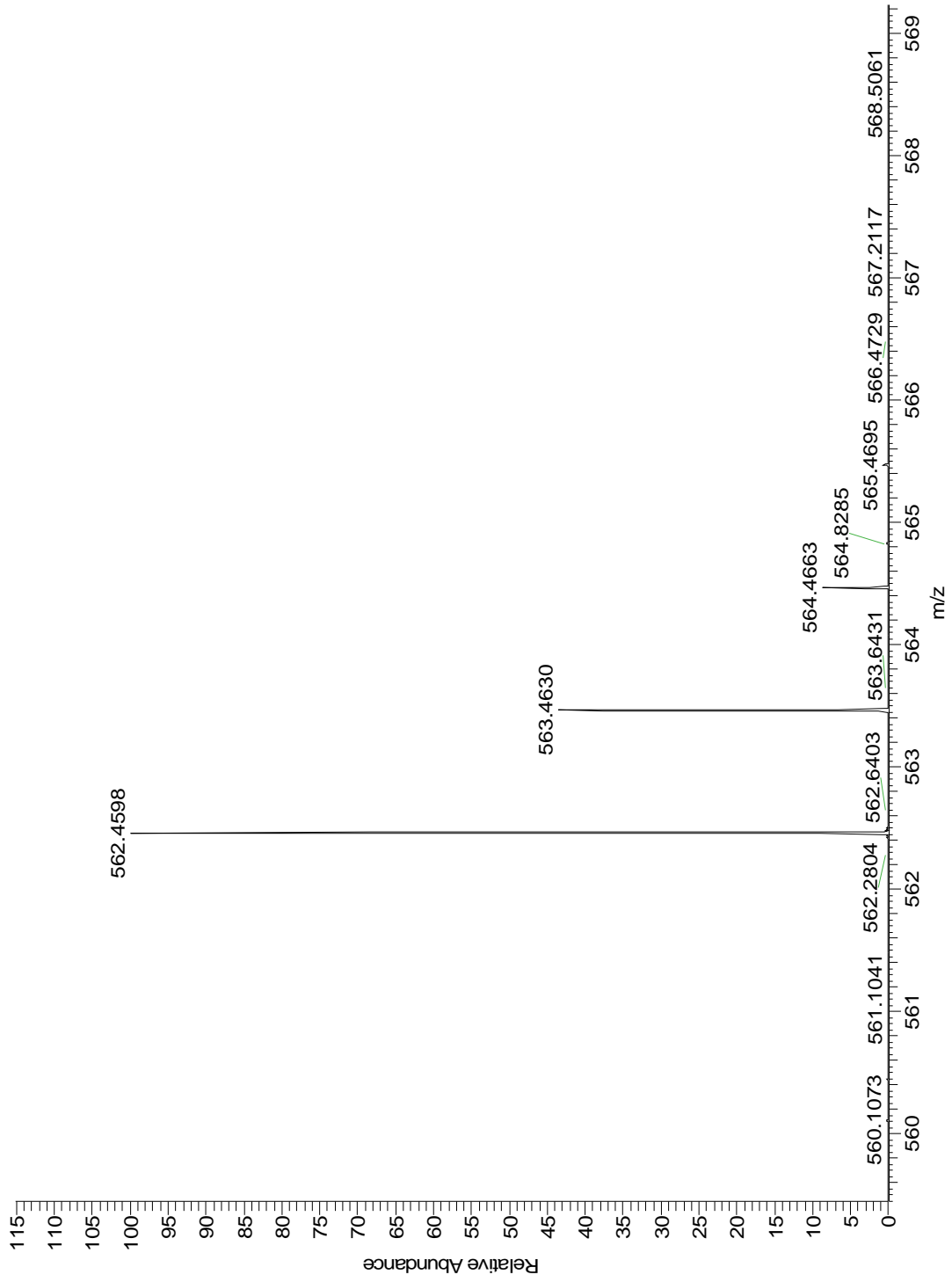
Position	Intensity
2998.83	Intensiv
2953.80	Intensiv
2922.30	Intensiv
2851.98	Intensiv

Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00

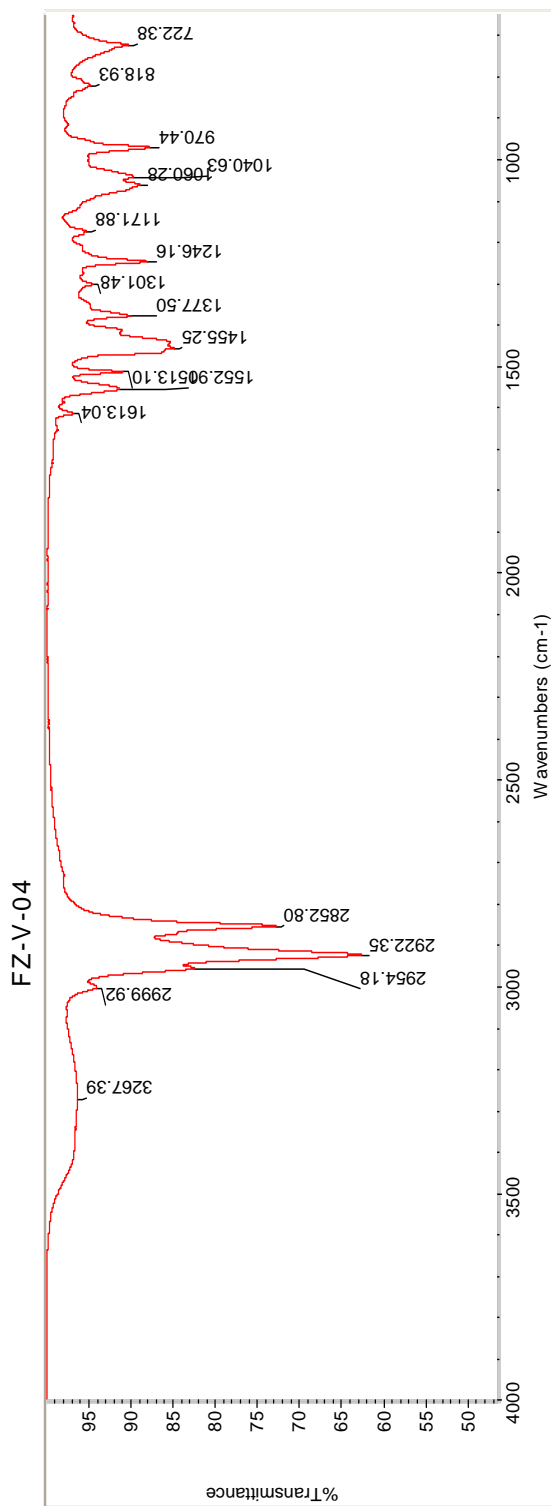




r110809r10 #7-49 RT: 0.09-0.68 AV: 43 NL: 1.09E8  
T: FTMS + p NSIFull.ms [300.00-1500.00]



Thu Apr 14 18:06:46 2011 (G

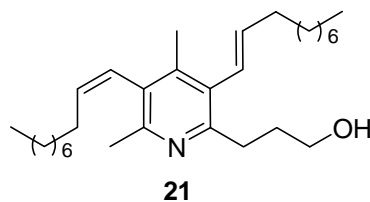


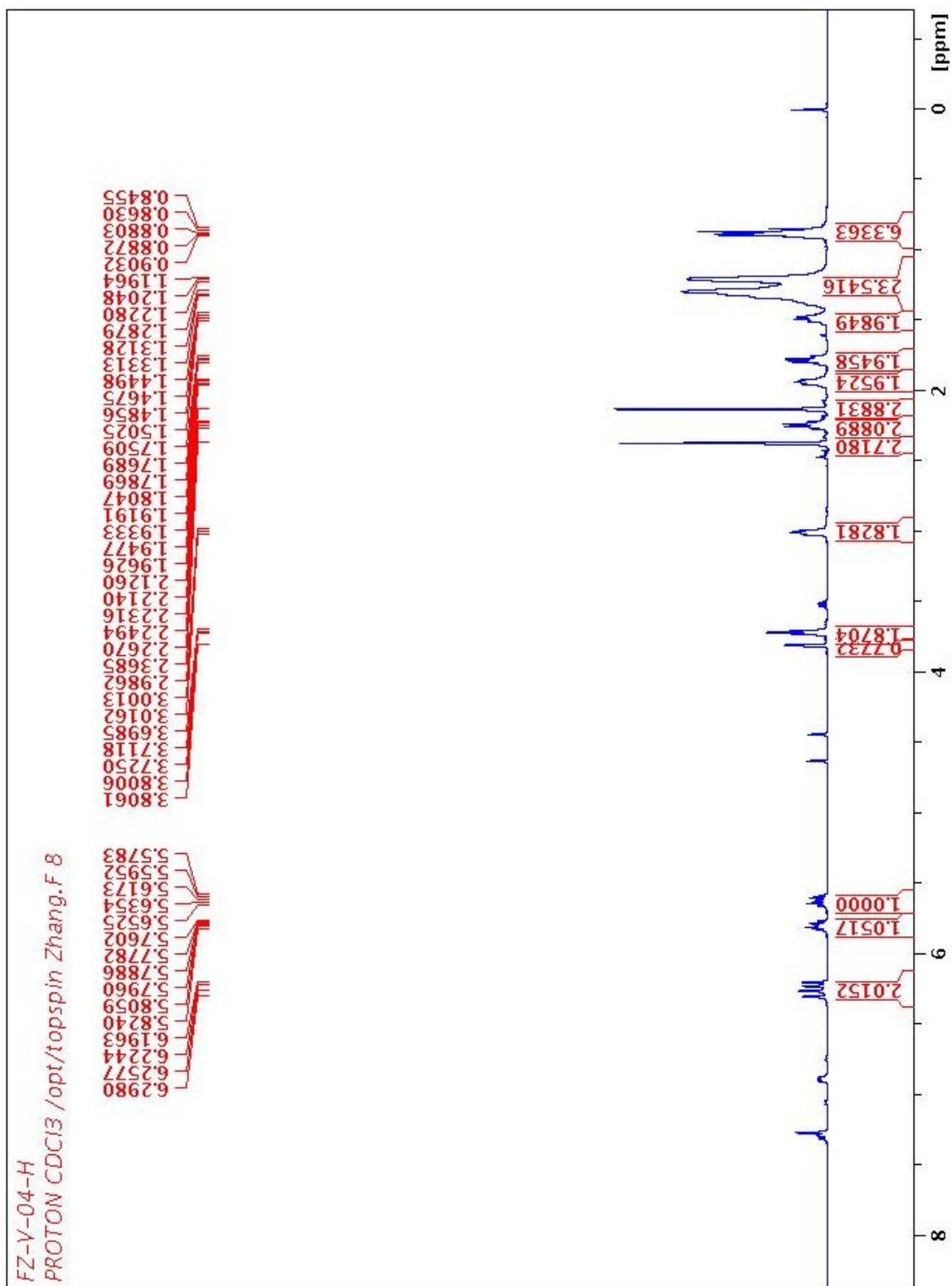
Thu Apr 14 18:06:41 2011 (GMT-04:00)

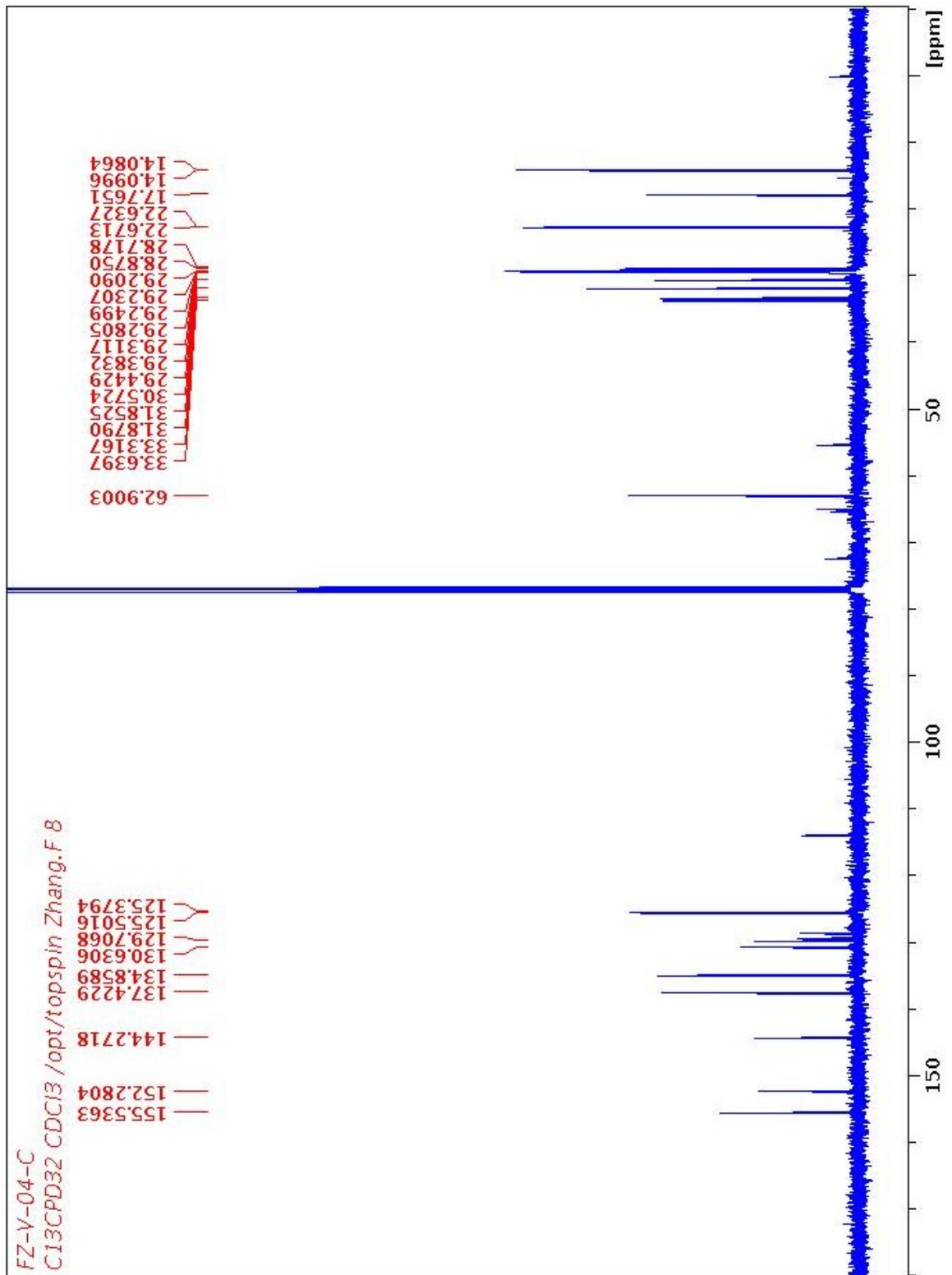
Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00

**FIND PEAKS:**  
Spectrum: FZ-V-04  
Region: 4000.12 649.89  
Absolute threshold: 98.387  
Sensitivity: 59  
Peak list:

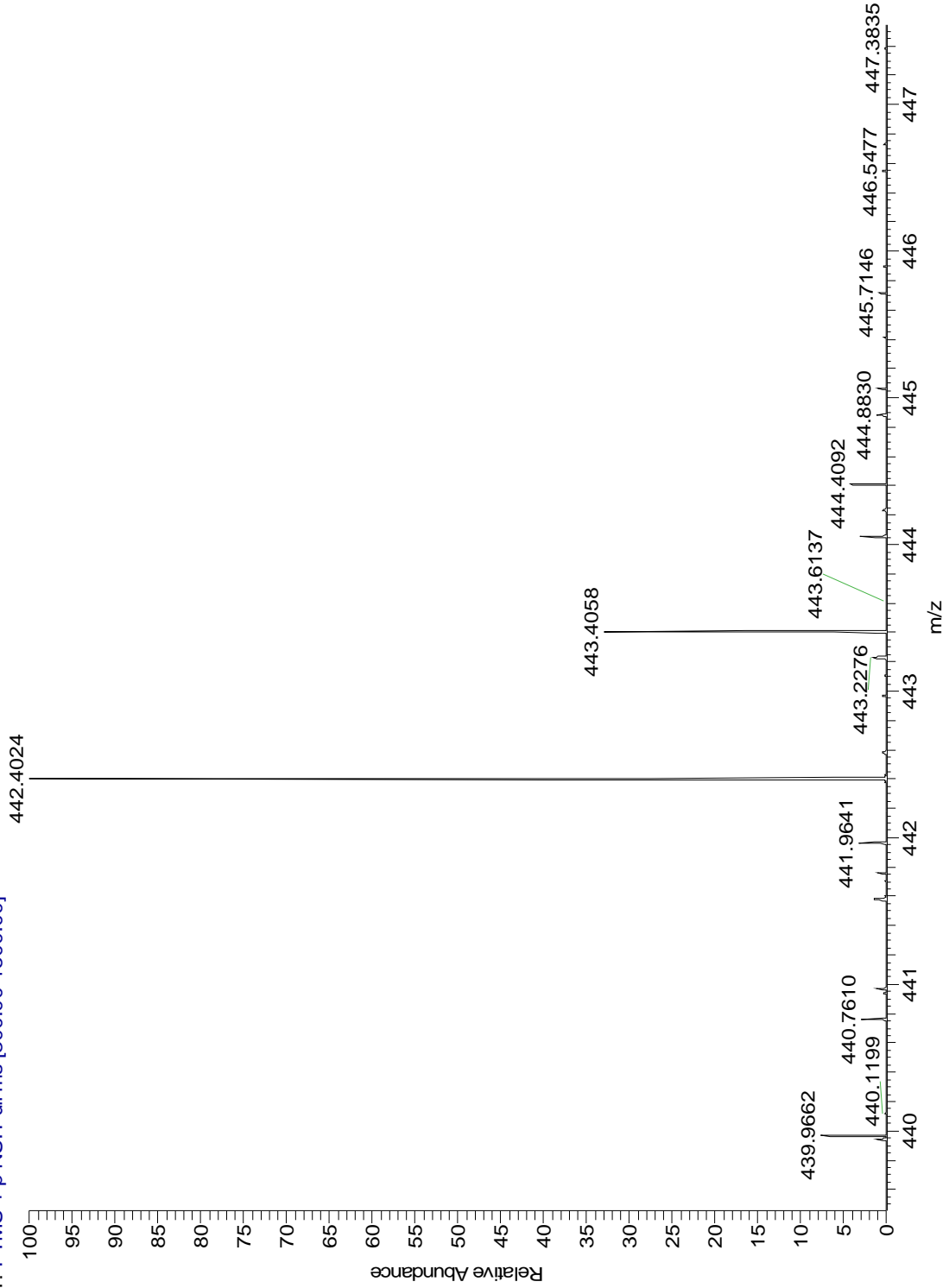
Position	Intensity
722.38	Intensiv
818.93	Intensiv
970.44	Intensiv
1040.63	Intensiv
1060.28	Intensiv
1171.88	Intensiv
1246.16	Intensiv





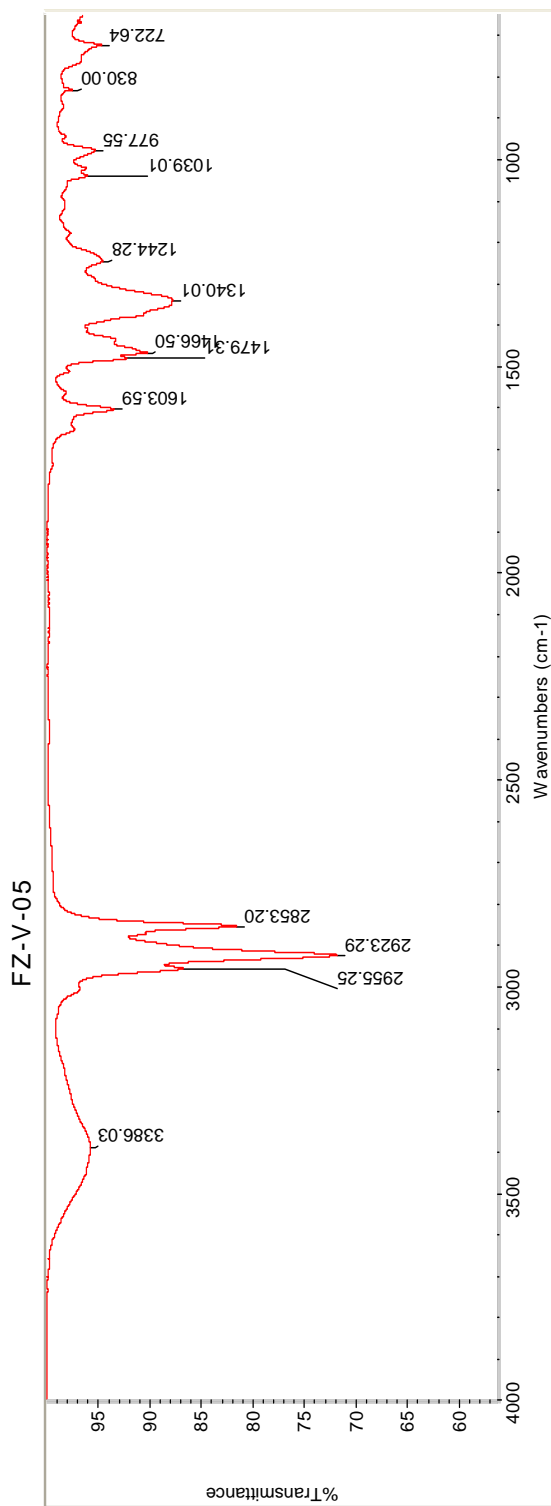


r11080912 #4-48 RT: 0.04-0.65 AV: 45 NL: 2.29E7  
T: FTMS + p NSI Full ms [300.00-1500.00]





Thu Apr 14 18:07:20 2011 (G

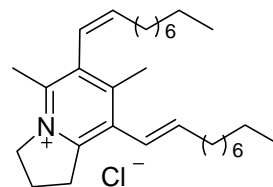


Thu Apr 14 18:07:14 2011 (GMT-04:00)

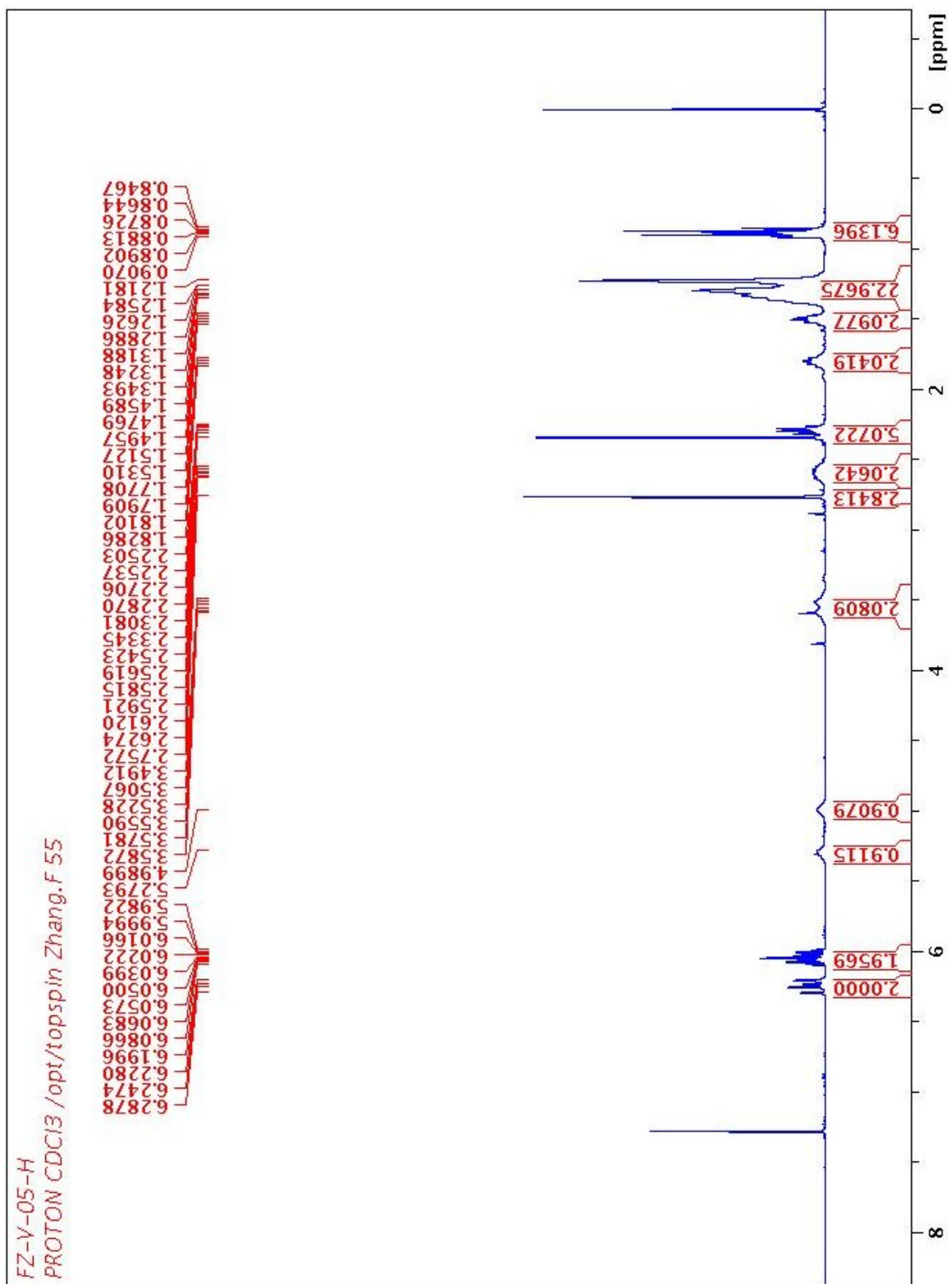
Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00

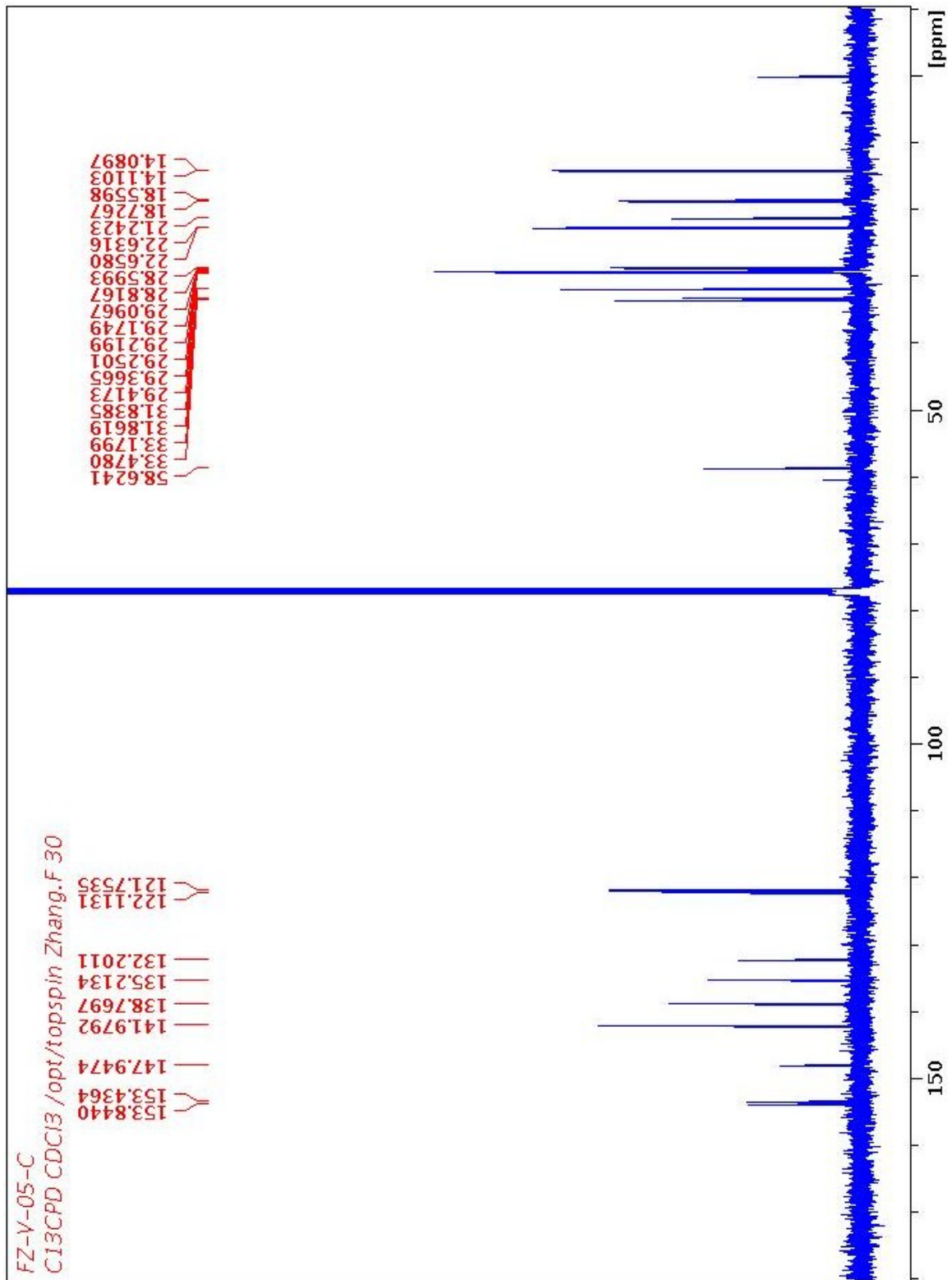
**FIND PEAKS:**

Region	Position	Intensity
FZ-V-05	722.64	Intensiv
	830.00	Intensiv
	977.55	Intensiv
	1039.01	Intensiv
	1244.28	Intensiv
	1340.01	Intensiv
	1466.50	Intensiv
	1603.59	Intensiv
	2853.20	Intensiv
	2923.29	Intensiv
	2955.25	Intensiv
	3386.03	Intensiv
Absolute threshold:	59	
Sensitivity:	59	
Peak list:		

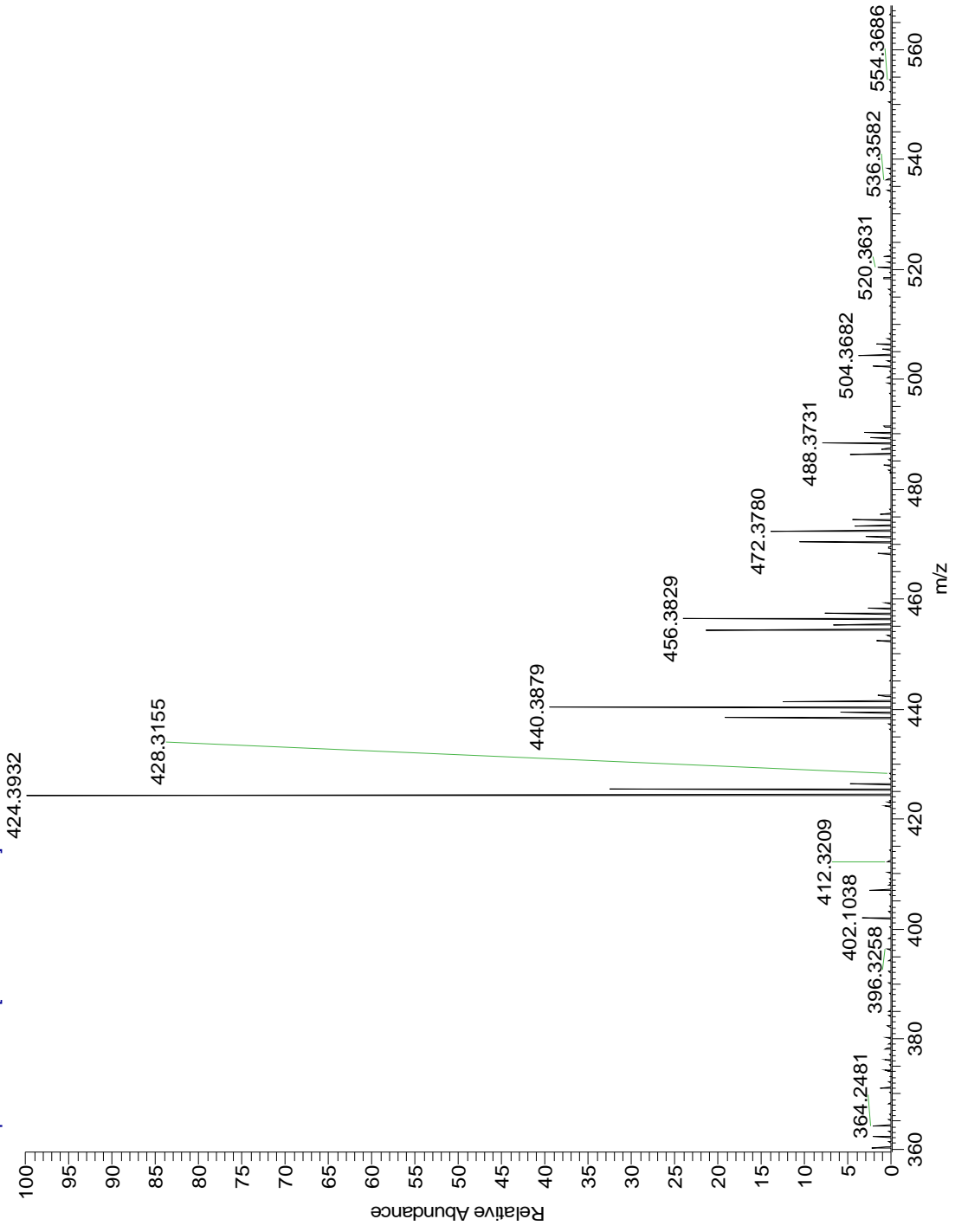


**3 (11Z,22E)**

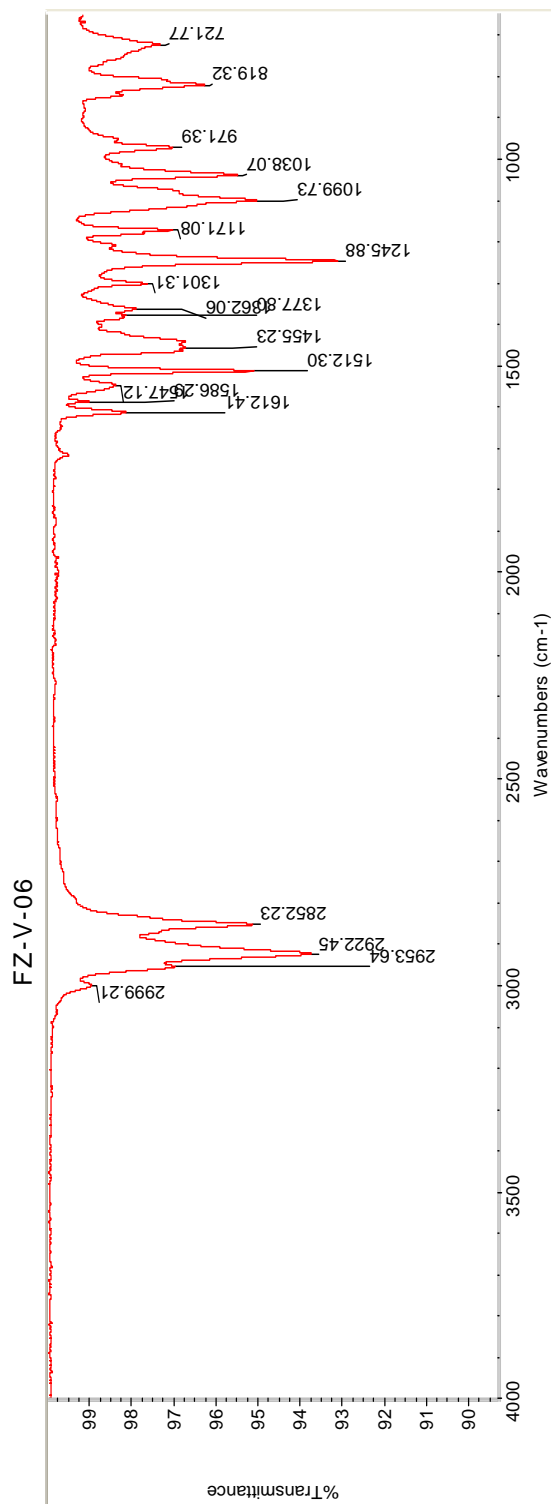




r110622r02 #3-34 RT: 0.03-0.46 AV: 32 NL: 1.03E8  
T: FTMS + p NSI Full ms [300.00-2000.00]



Thu Apr 14 18:03:21 2011 (G

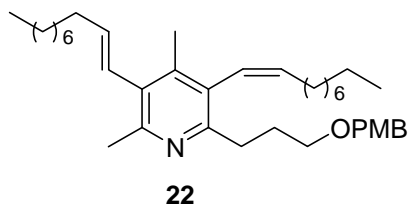


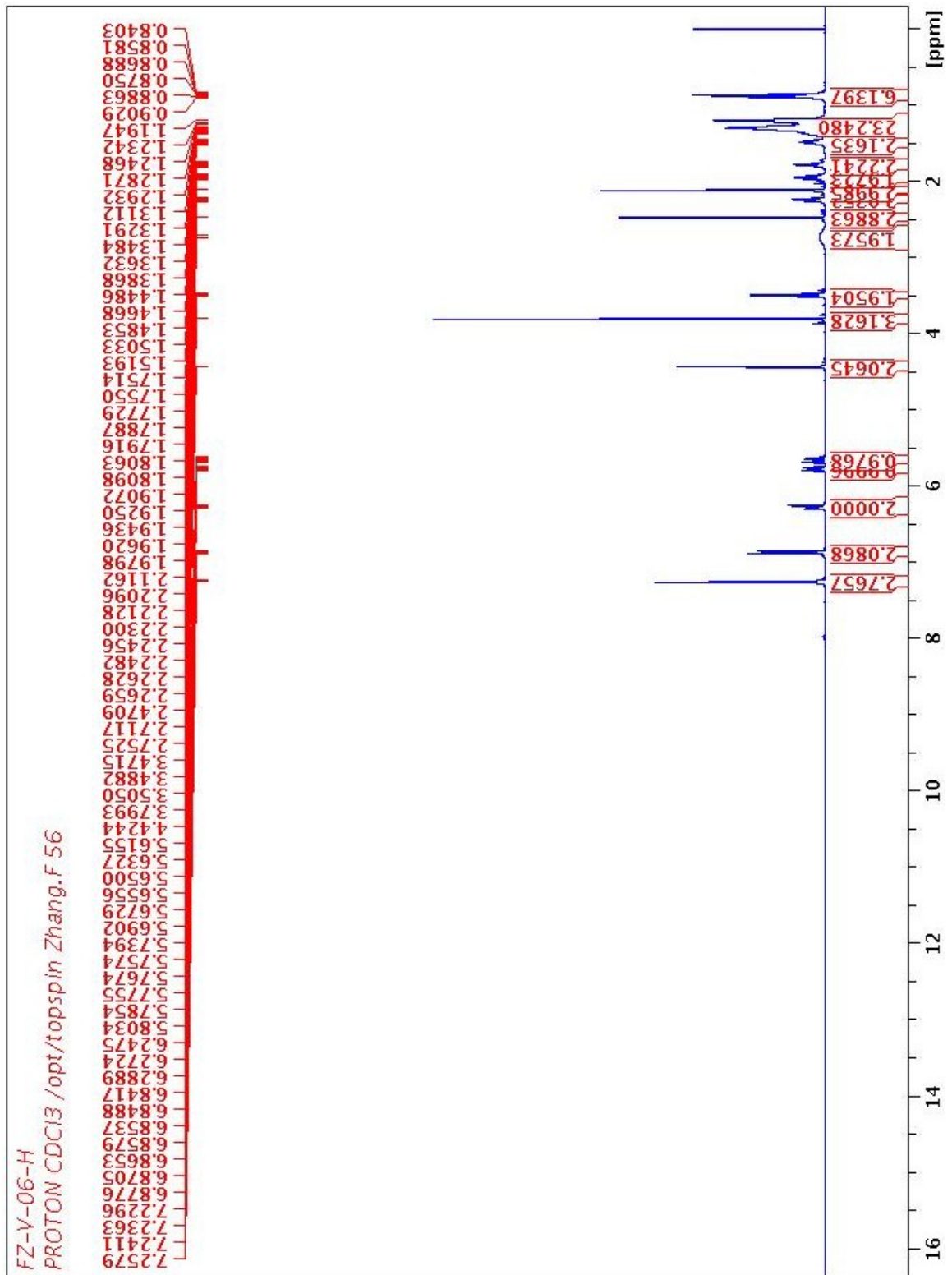
Thu Apr 14 18:03:16 2011 (GMT-04:00)

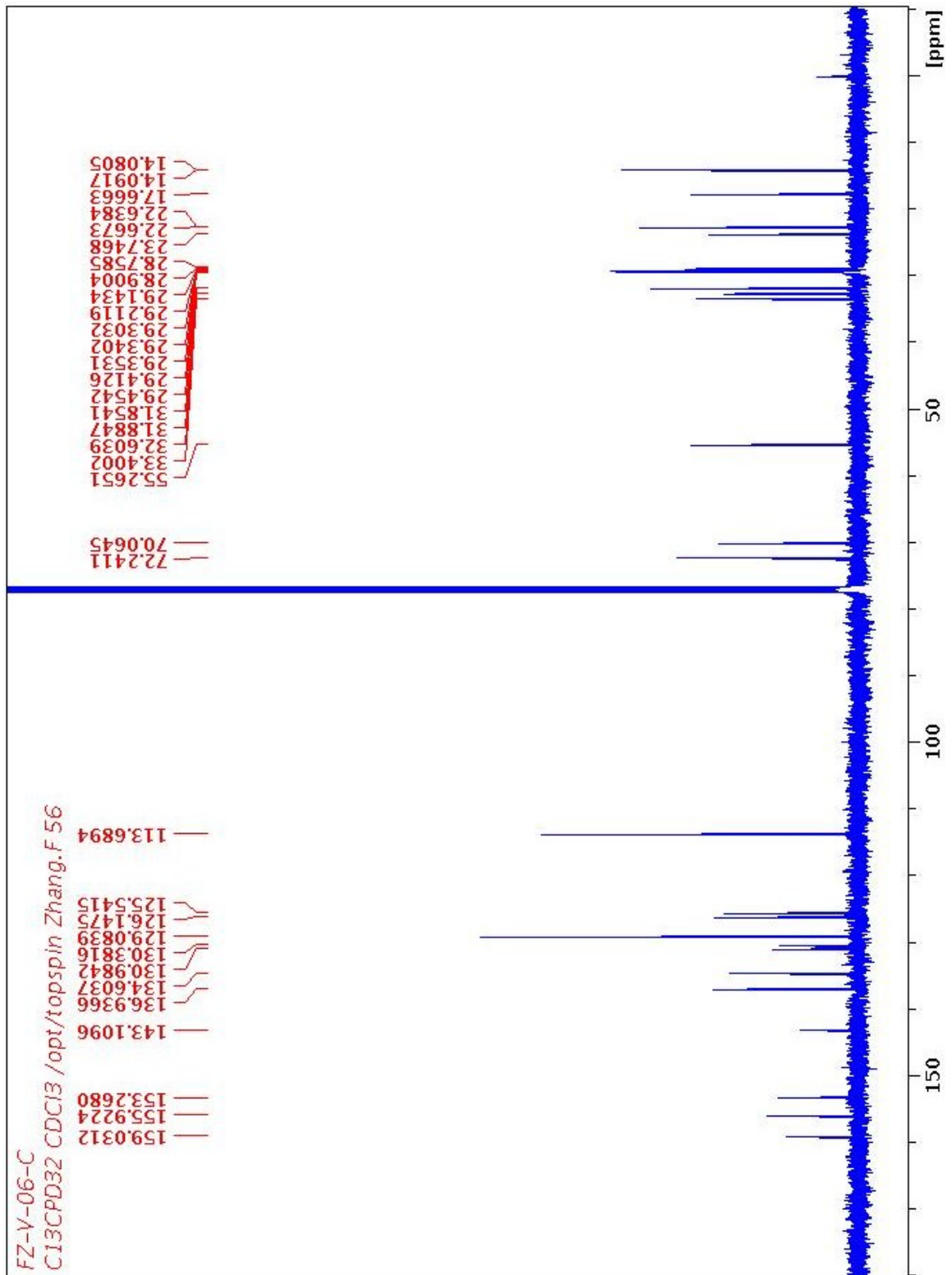
Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00

FIND PEAKS:

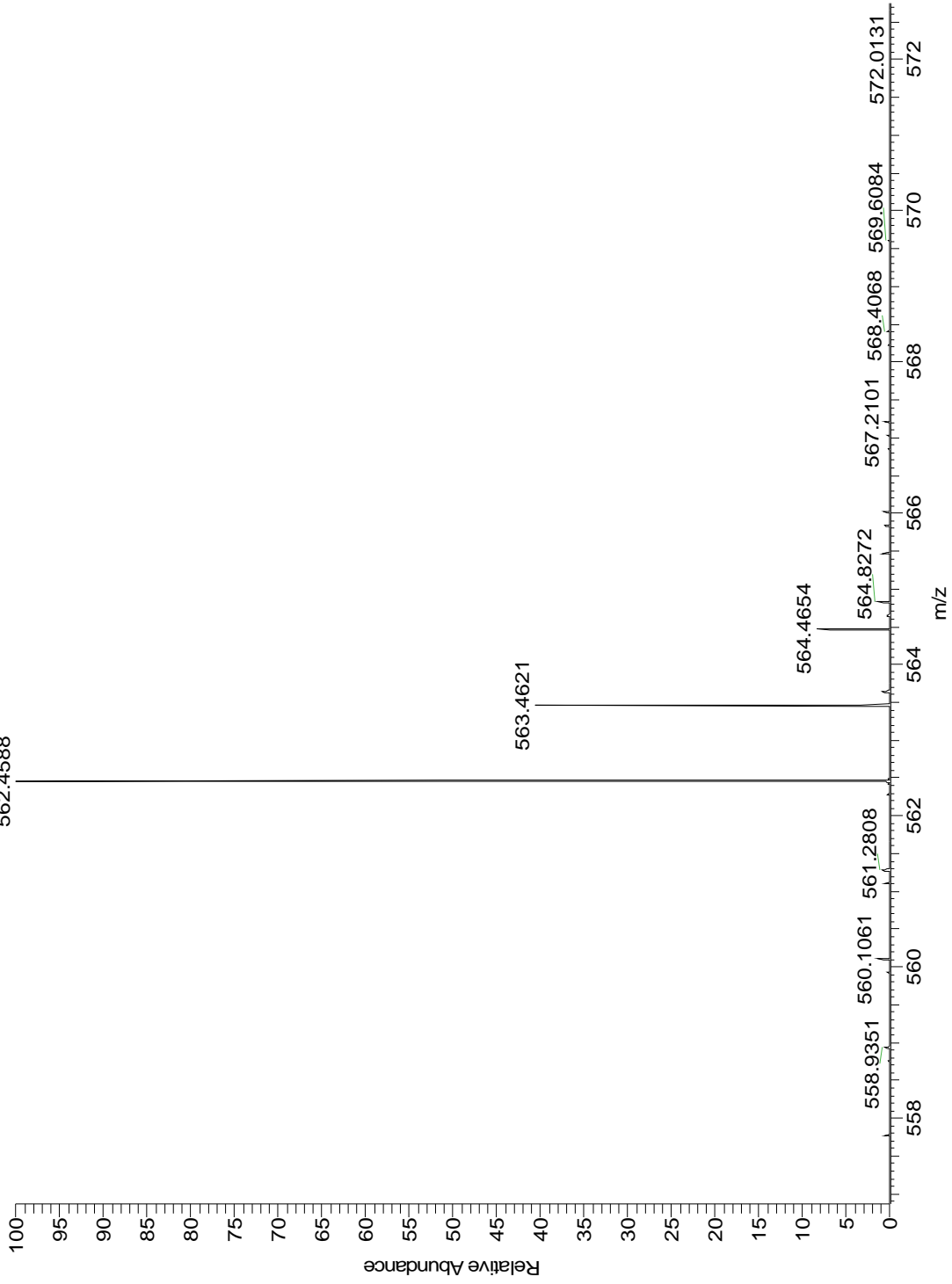
Region	Spectrum	Position	Intensity
4000.12	FZ-V-06	2999.21	99.218
649.89		721.77	Intensiv
99.218		819.32	Intensiv
		971.39	Intensiv
		1038.07	Intensiv
		1099.73	Intensiv
		1171.08	Intensiv
		1245.88	Intensiv







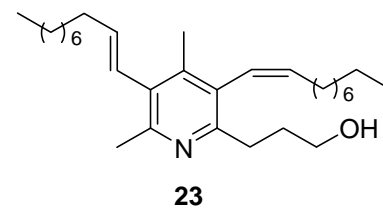
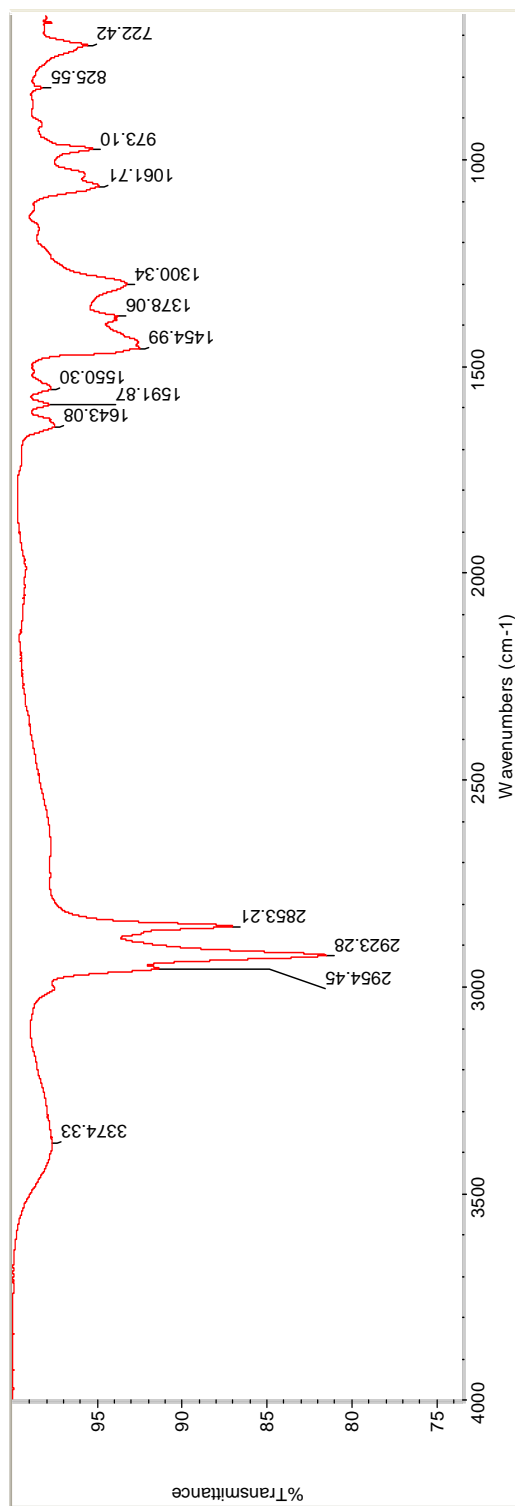
r11080913 #2-49 RT: 0.02-0.67 AV: 48 NL: 5.74E7  
T: FTMS + p NSIFull ms [300.00-1500.00]





Thu Apr 14 18:03:59 2011 (G

FZ-V-07

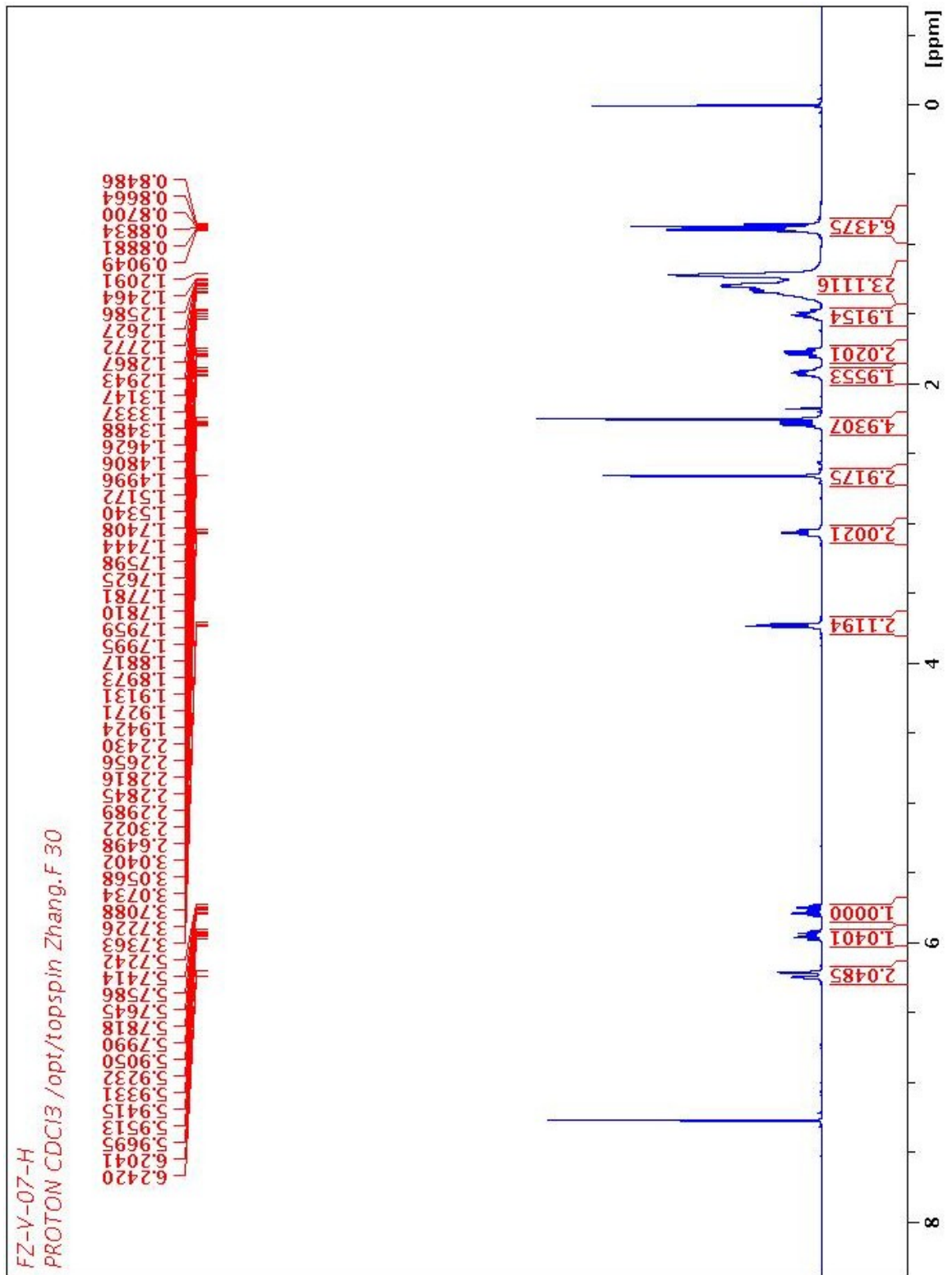


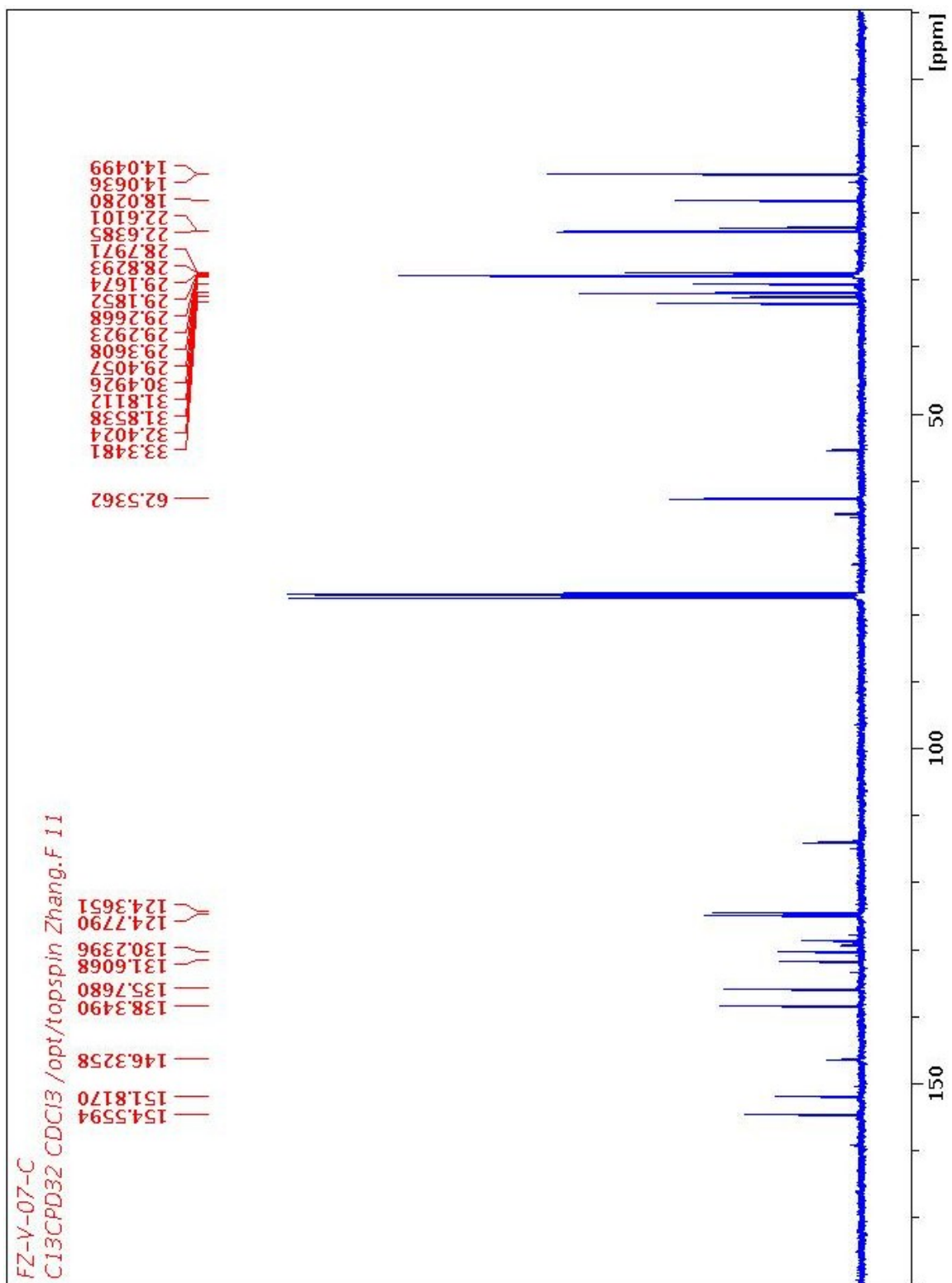
Thu Apr 14 18:03:55 2011 (GMT-04:00)

Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00

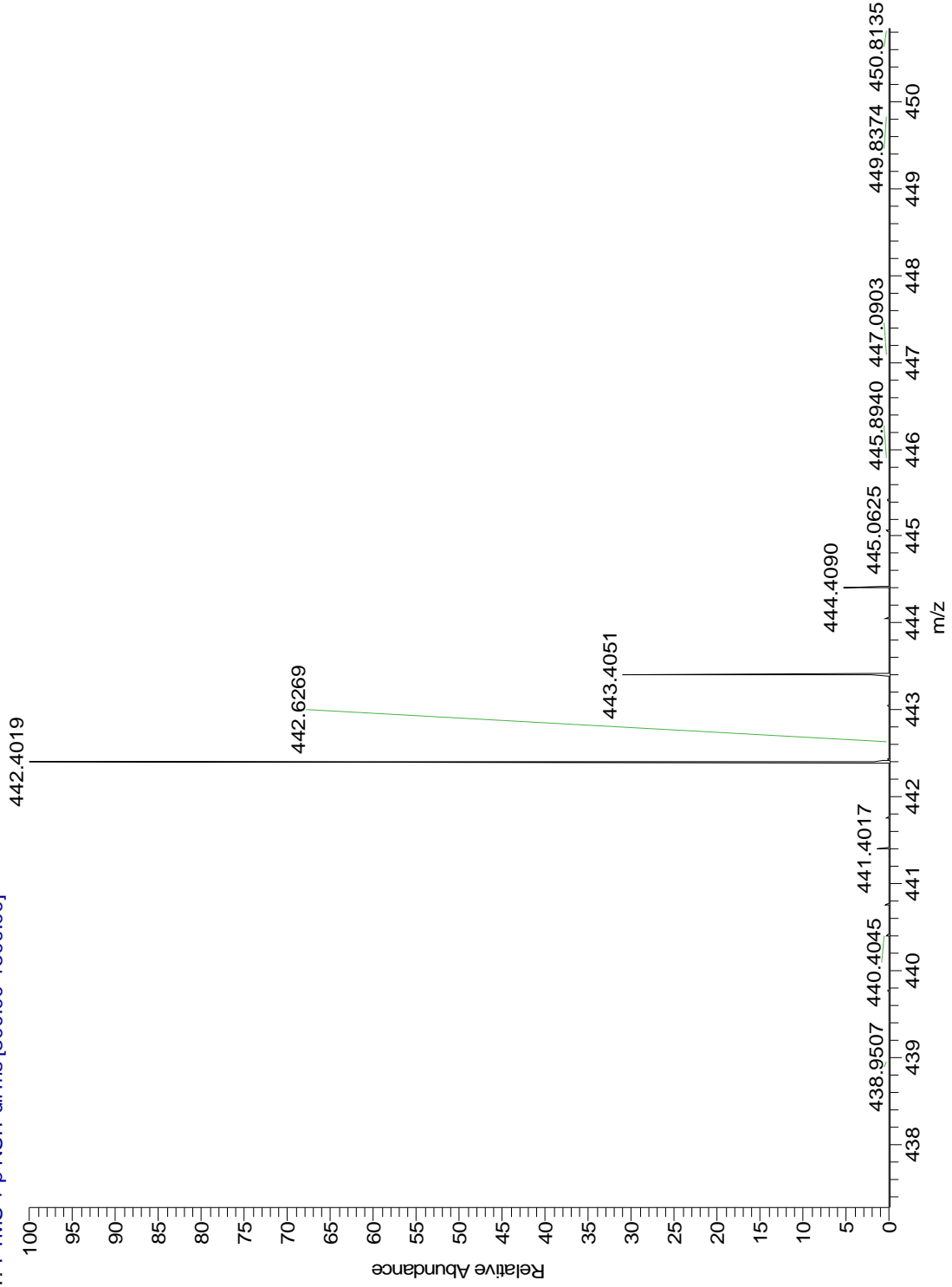
FIND PEAKS:

Spectrum:	FZ-V-07
Region:	4000.12
Absolute threshold:	649.89
Sensitivity:	98.773
Peak list:	55
Position:	722.42
Intensity:	Intensiv
Position:	825.55
Intensity:	Intensiv
Position:	973.10
Intensity:	Intensiv
Position:	1061.71
Intensity:	Intensiv
Position:	1300.34
Intensity:	Intensiv
Position:	1378.06
Intensity:	Intensiv
Position:	1454.99
Intensity:	Intensiv

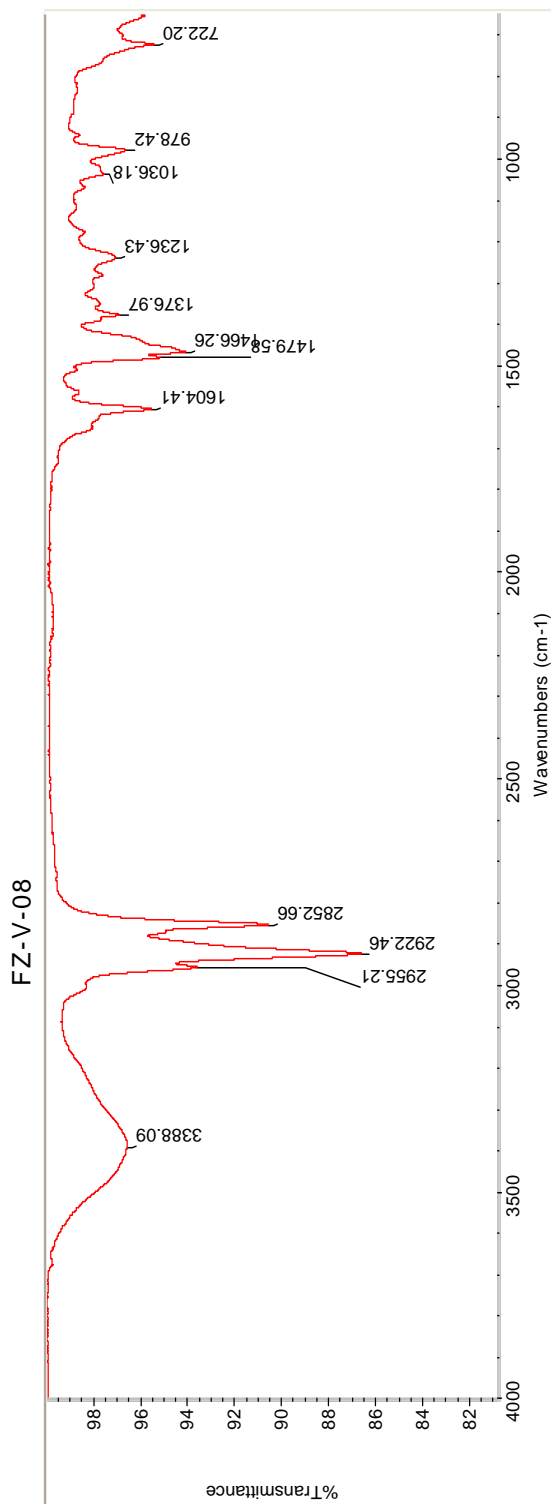




r110809r14 #6-49 RT: 0.07-0.67 AV: 44 NL: 1.22E9  
T: FTMS + p NSIFull ms [300.00-1500.00]



Thu Apr 14 18:04:43 2011 (G



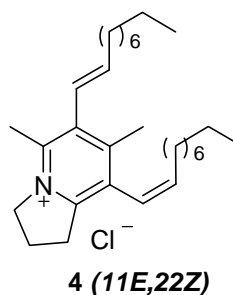
Thu Apr 14 18:04:38 2011 (GMT-04:00)

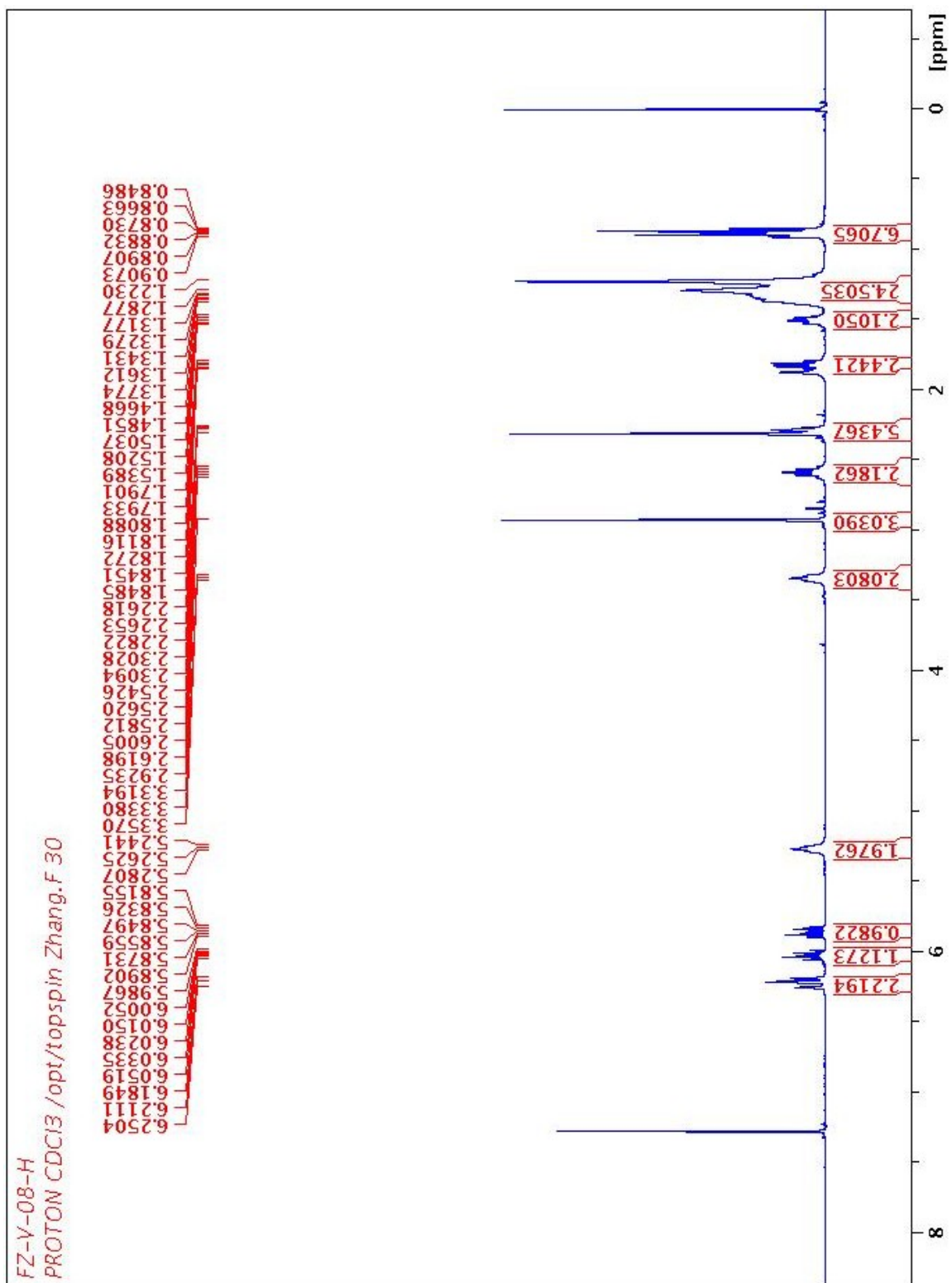
Number of sample scans: 16  
Number of background scans: 16  
Resolution: 4.000  
Sample gain: 1.0  
Optical velocity: 0.4747  
Aperture: 80.00

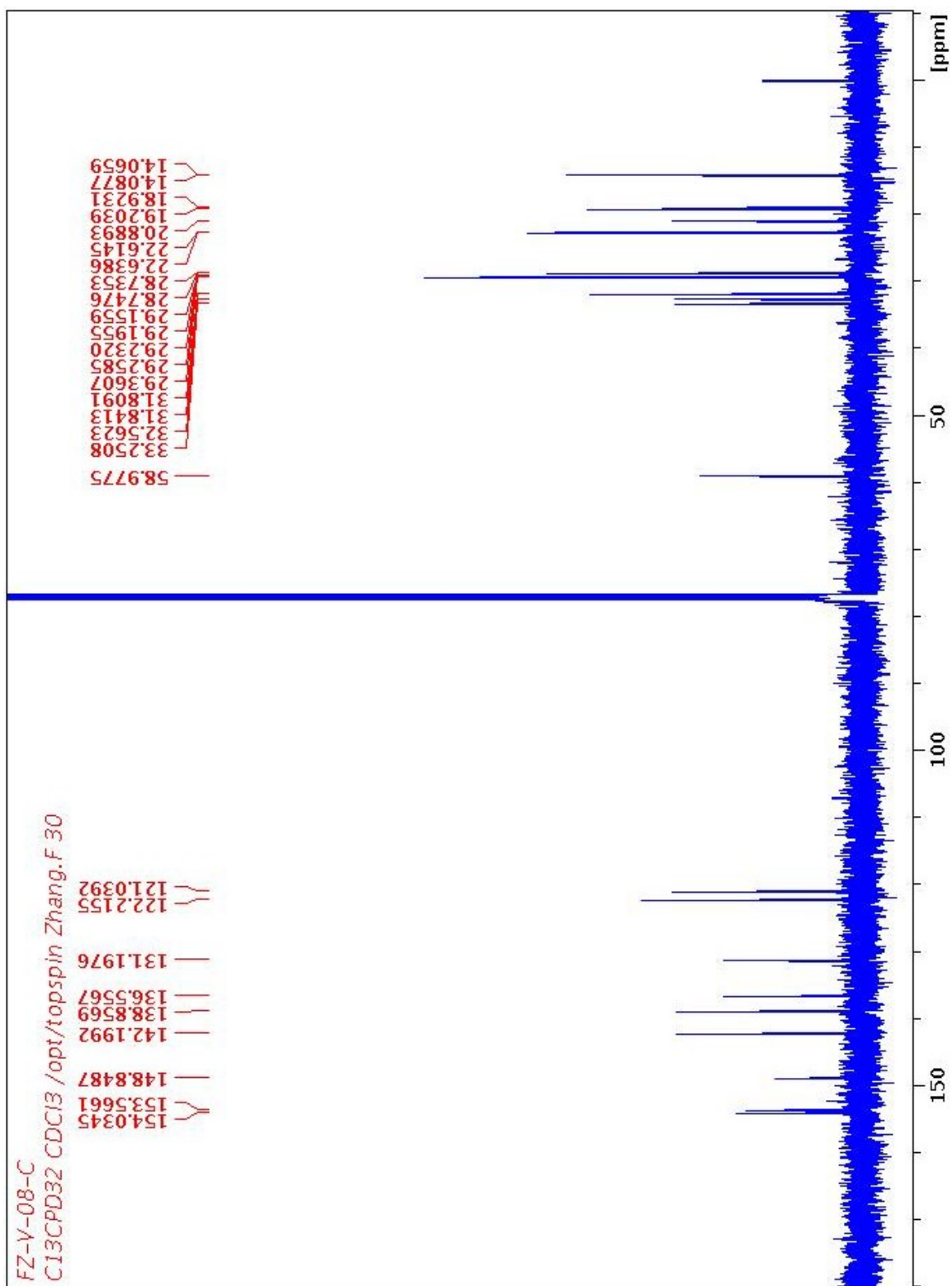
Find Peaks:

Region	Position	Intensity
FZ-V-08	722.20	Intensiv
	978.42	Intensiv
	1036.18	Intensiv
	1236.43	Intensiv
	1376.97	Intensiv
	1466.26	Intensiv
	1479.58	Intensiv
	2922.46	
	2852.66	
	2955.21	

Absolute threshold: 99.012  
Sensitivity: 55  
Peak list:







r110622r03 #2-49 RT: 0.02-0.67 AV: 48 NL: 5.94E8  
T: FTMS + p NSIFull.ms [300.00-2000.00]

