

Studies on Highly Regio- and Stereoselective Hydration of 1,2-Allenyllic Sulfoxides

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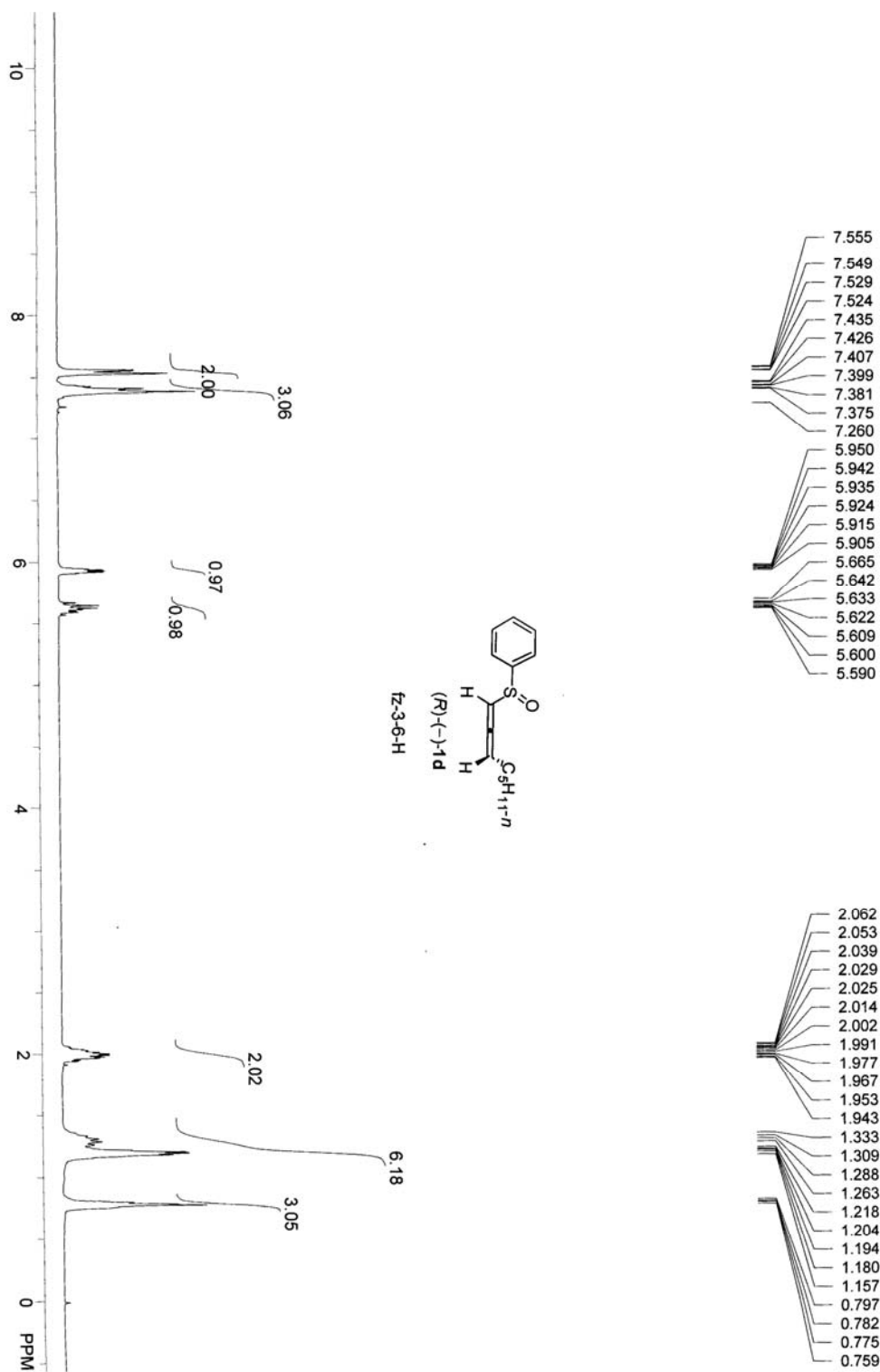
masm@sioc.ac.cn

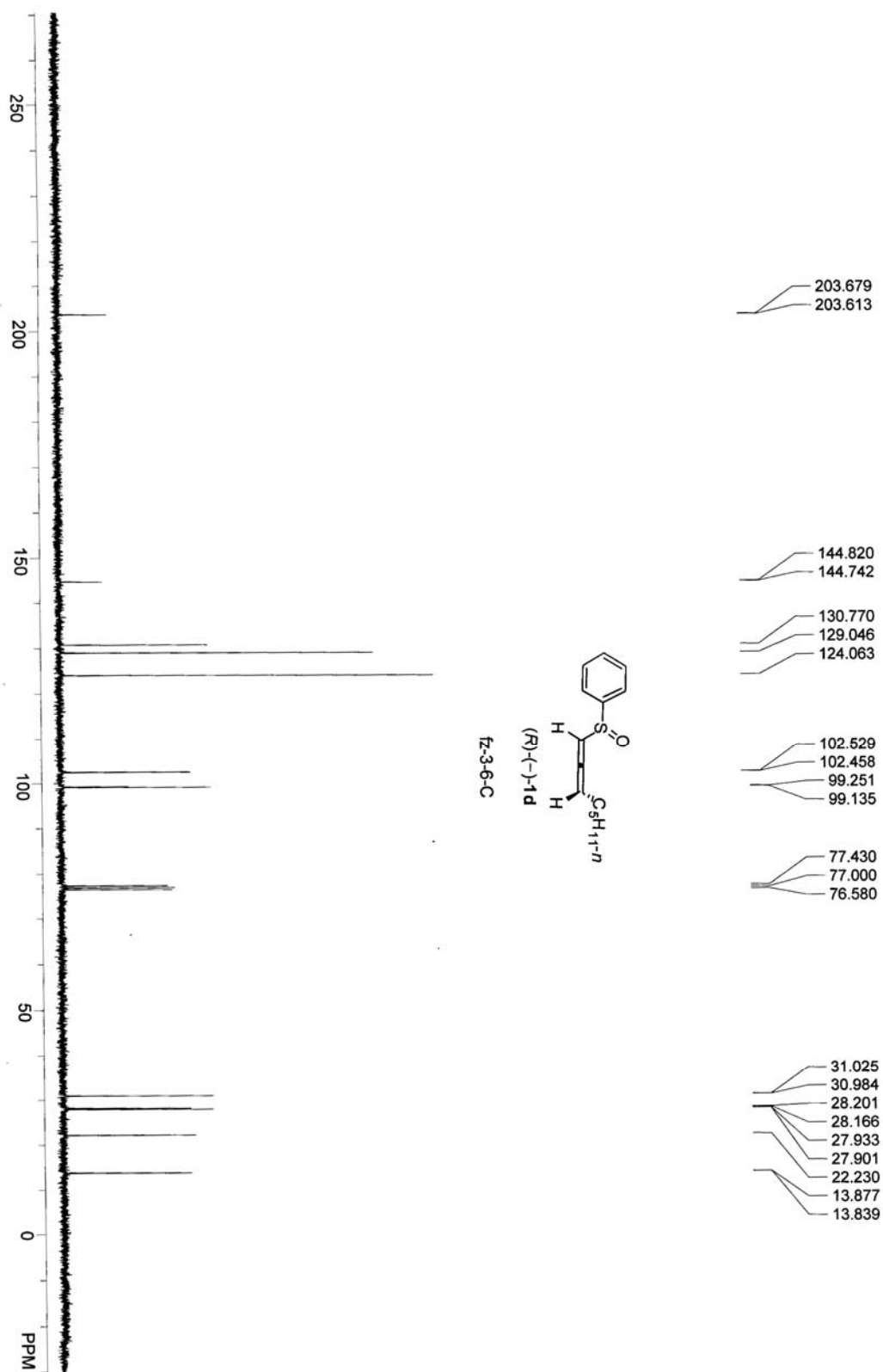
General experimental methods	S2
¹ H NMR, ¹³ C NMR, and HPLC spectra of the products	S2-S85

General experimental methods:

^1H and ^{13}C nuclear magnetic resonance spectra were recorded on an instrument operated at 300 MHz for ^1H NMR and 75 MHz for ^{13}C NMR. Deuteriochloroform (CDCl_3) was used as solvent in all NMR experiments. Chemical shifts (δ) are given in parts per million (ppm). Infrared spectra were recorded on a FT-IR spectrometer. Mass spectra were carried out in EI mode. HRMS spectra were carried out in EI mode. Thin layer chromatography was performed on pre-coated glassback plates and visualized with UV light at 254 nm. Flash column chromatography was performed on silica gel.

^1H NMR, ^{13}C NMR, and HPLC Spectra of the Products



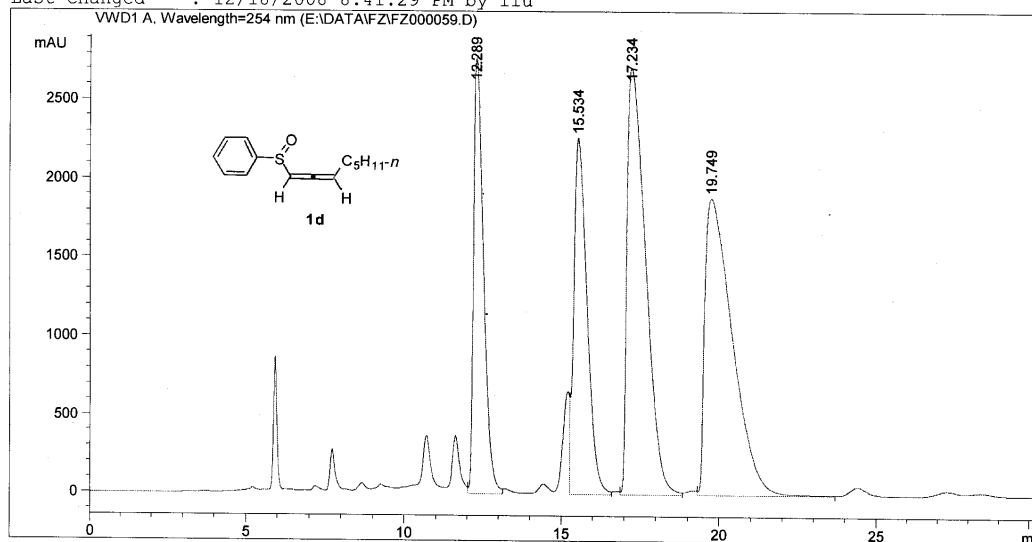


Data File E:\DATA\FZ\FZ000059.D

Sample Name: fz-4-2

chiral OD-H; n-Hexane:i-PrOH=95/5; 254 nm; 0.7 ml/min

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(modified after loading)
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Last changed : 12/18/2008 8:41:29 PM by liu



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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Sample Amount : 1.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	12.289	VV	0.3407	6.12913e4	2774.19287	17.4190
2	15.534	VV	0.4429	6.59609e4	2266.53833	18.7461
3	17.234	VV	0.6518	1.10733e5	2708.01636	31.4702
4	19.749	VV	0.9458	1.13880e5	1887.07410	32.3648

Totals : 3.51865e5 9635.82166

Results obtained with enhanced integrator!

*** End of Report ***

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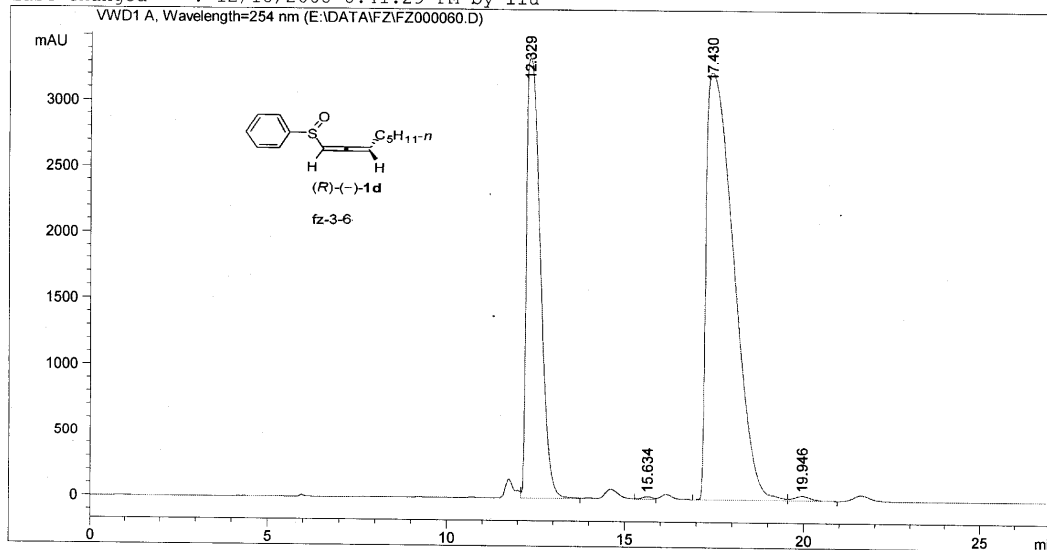
Page 1 of 1

Data File E:\DATA\FZ\FZ000060.D

Sample Name: fz-3-

chiral OD-H; n-Hexane:i-PrOH=95/5; 254 nm; 0.7 ml/min

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(modified after loading)
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Last changed : 12/18/2008 8:41:29 PM by liu
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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Sample Amount : 1.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	12.329	VV	0.4244	9.00749e4	3349.48584	34.1788
2	15.634	VV	0.3485	547.90356	23.68358	0.2079
3	17.430	VV	0.8330	1.71521e5	3240.49878	65.0836
4	19.946	VV	0.5656	1395.75476	36.97234	0.5296

Totals : 2.63540e5 6650.64054

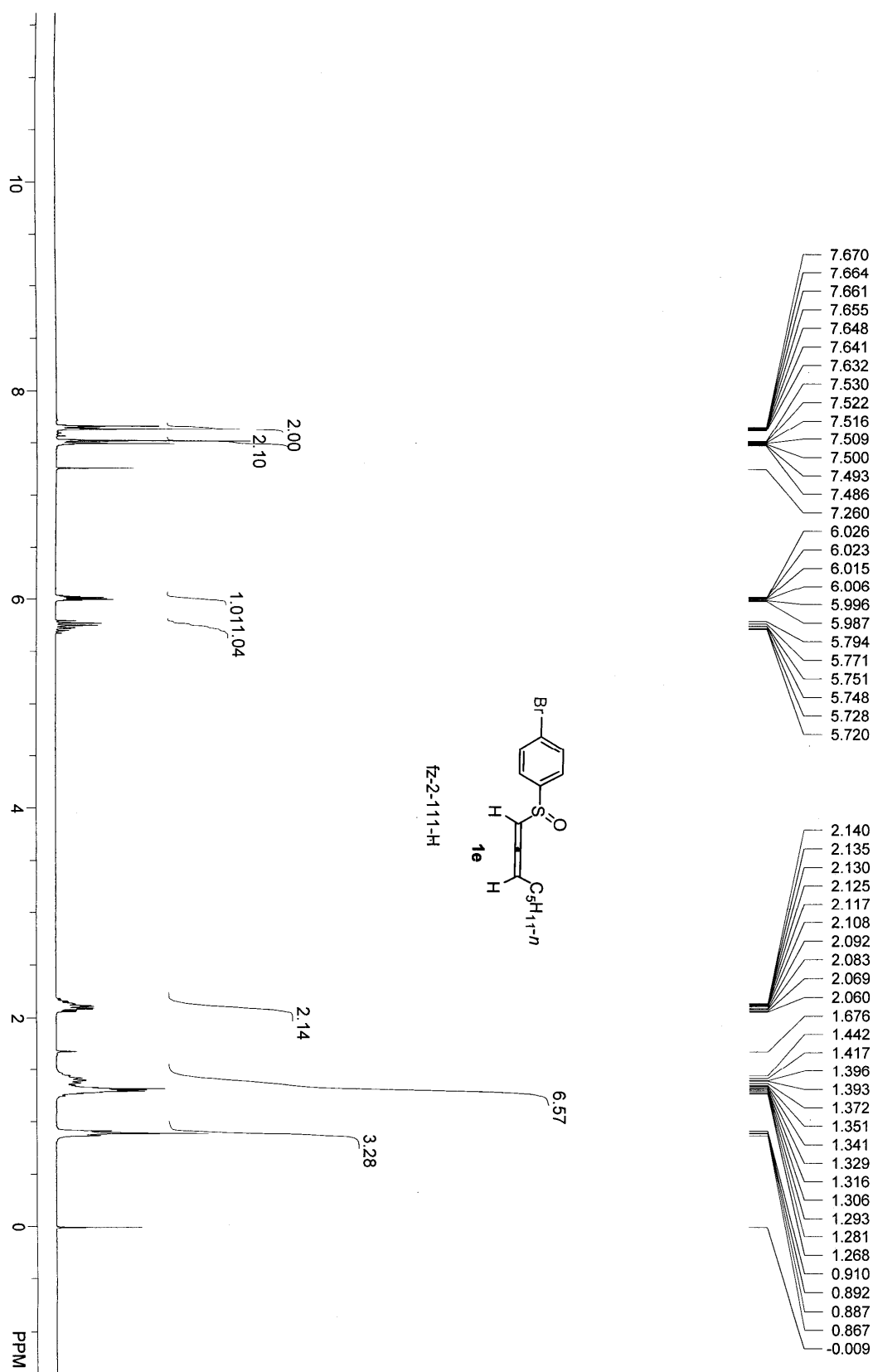
Results obtained with enhanced integrator!

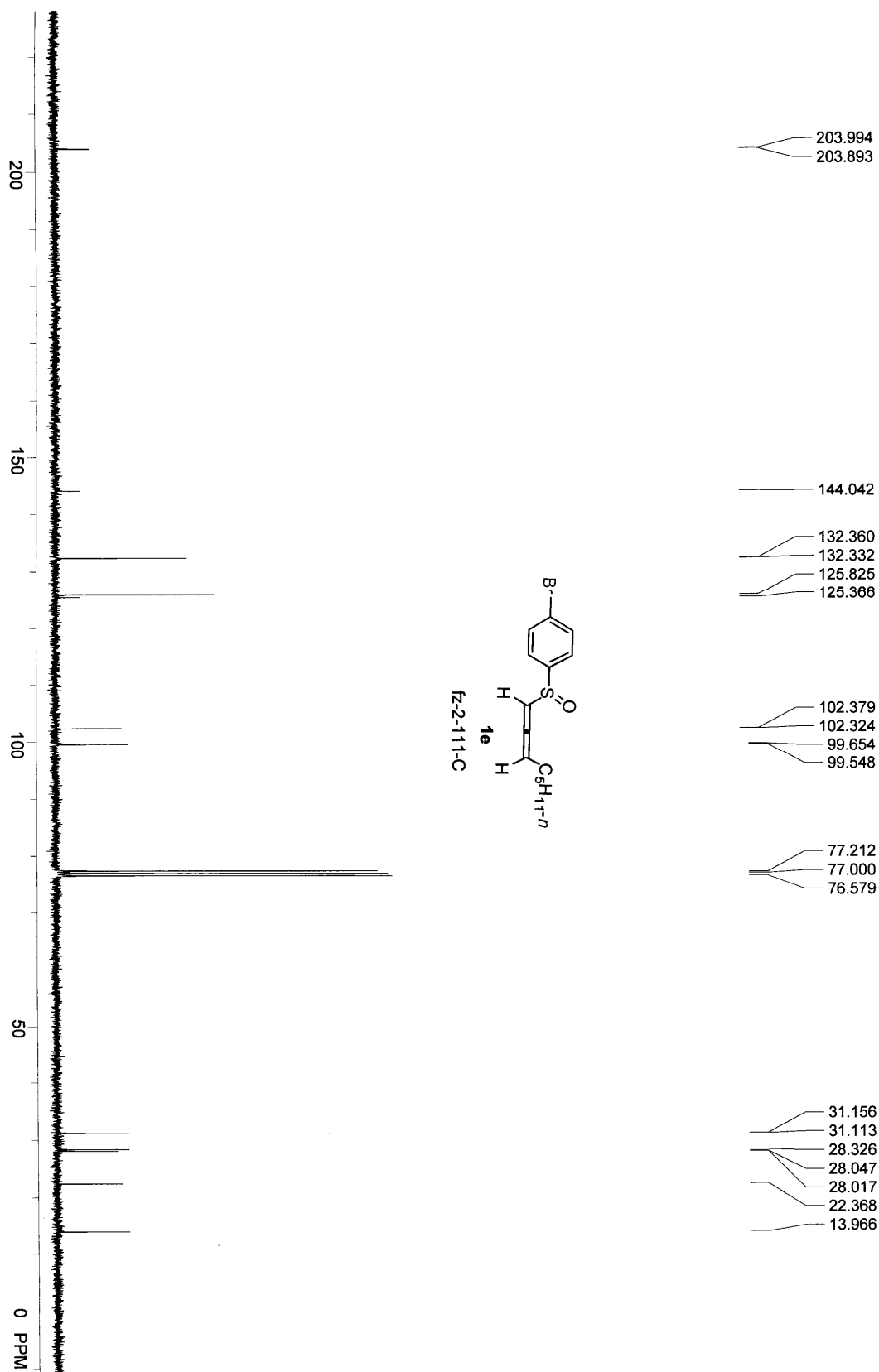
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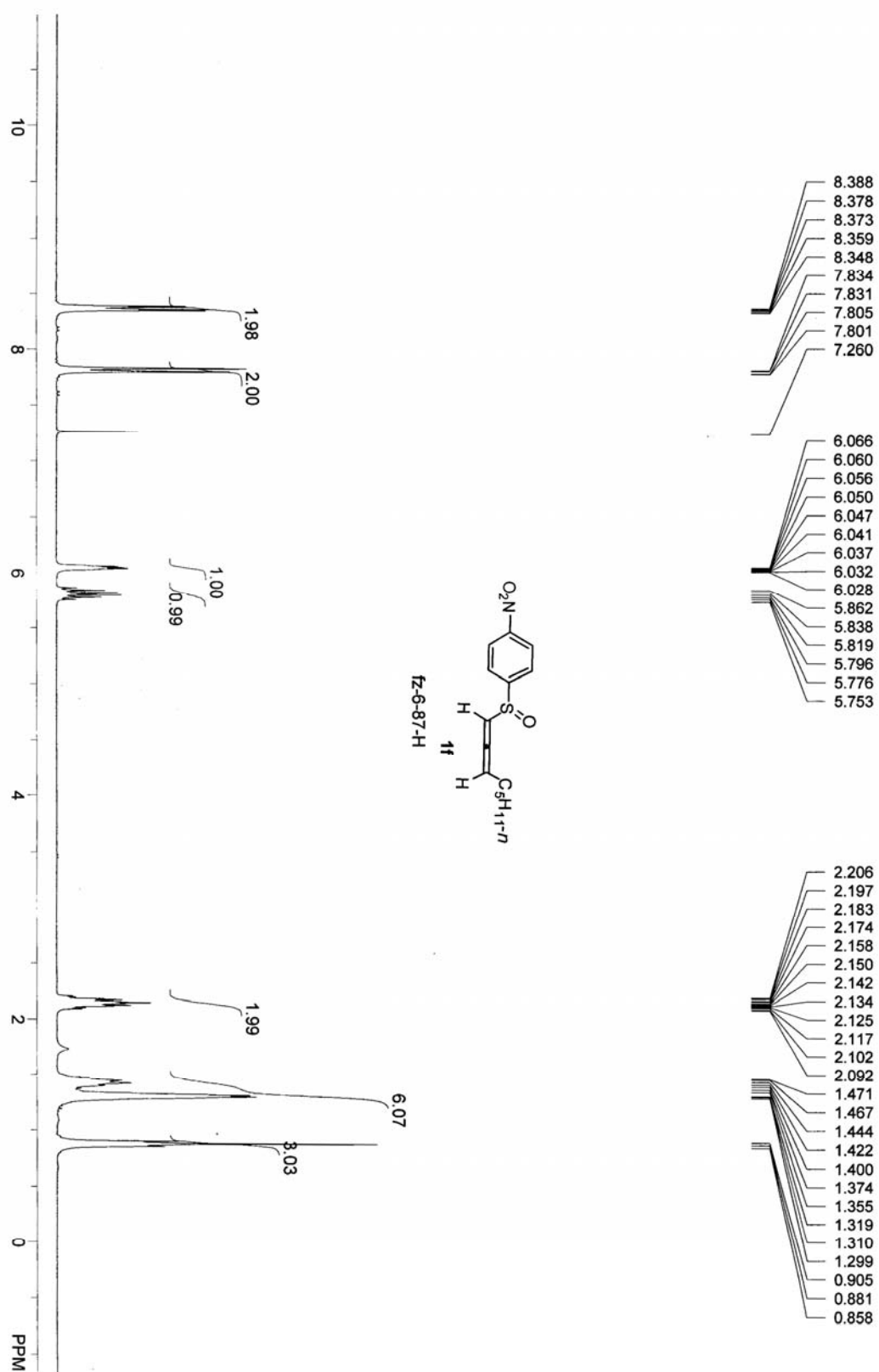
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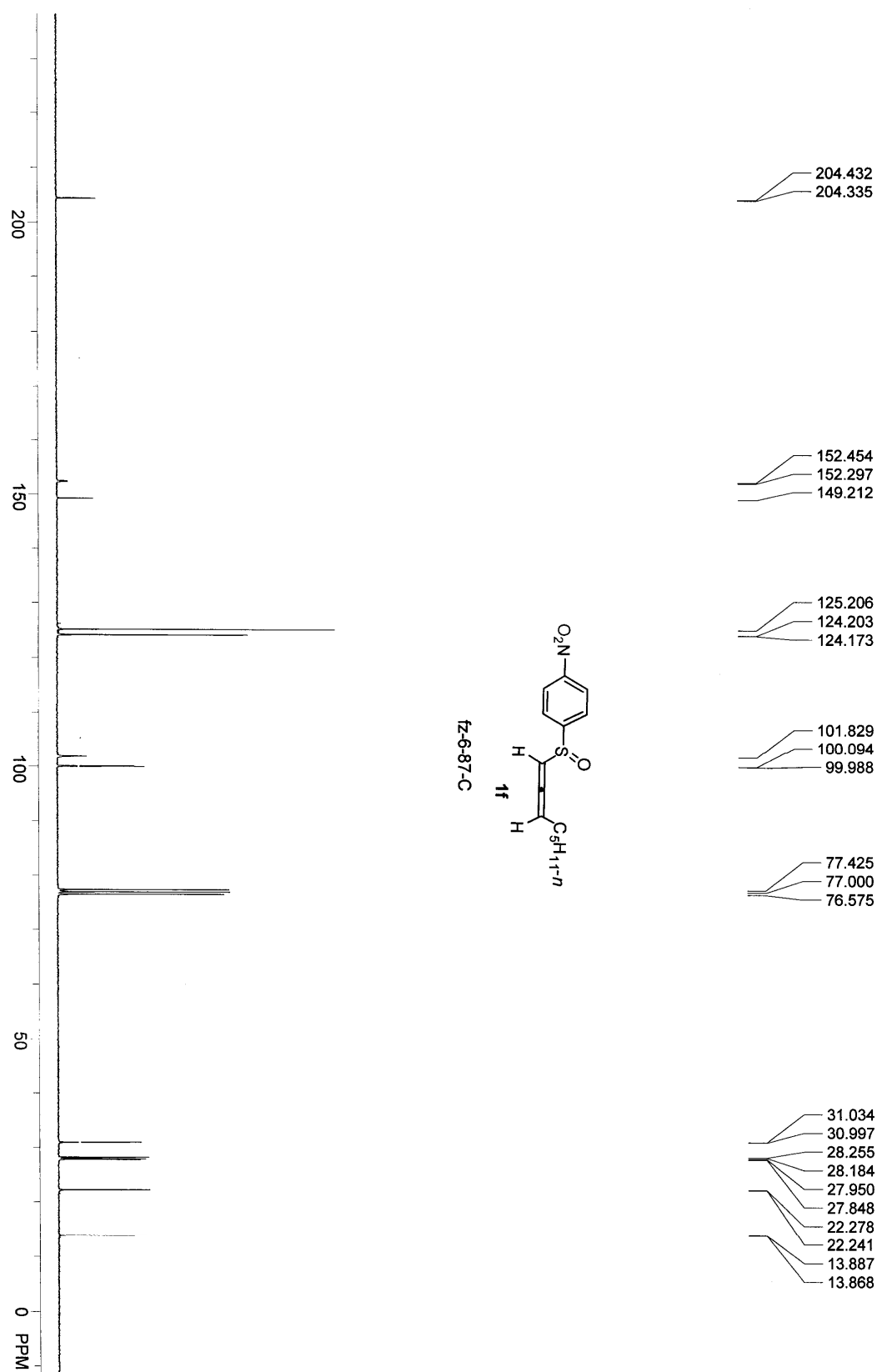
$$dr = \frac{(65.0836 + 0.5296)}{(34.1788 + 0.2079)} = \frac{65.6132}{34.3867} = 1.91$$

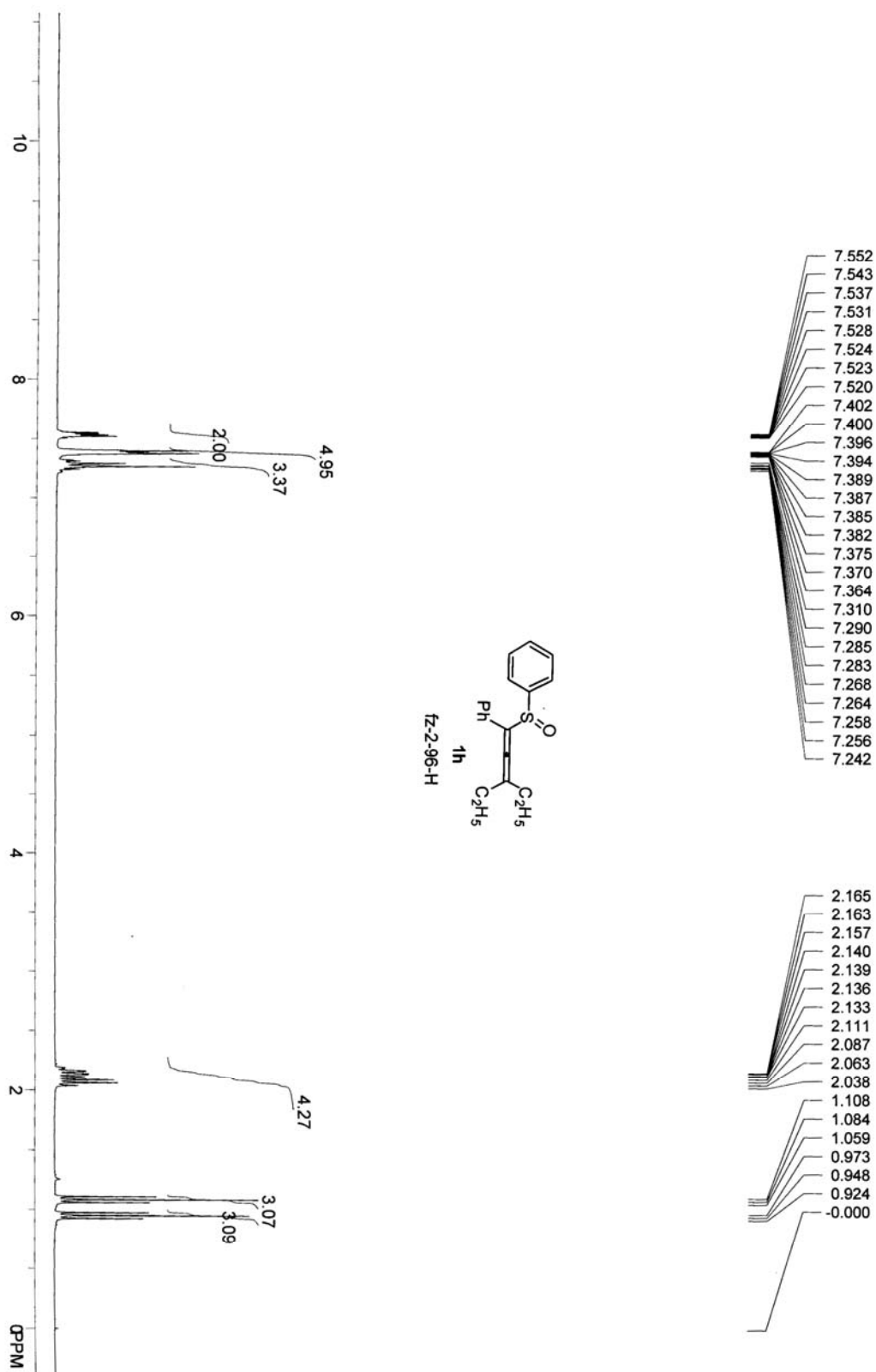
$$ee\% = \frac{34.1788 + 65.0836}{-0.5296 - 0.2079} = 98.59\%$$

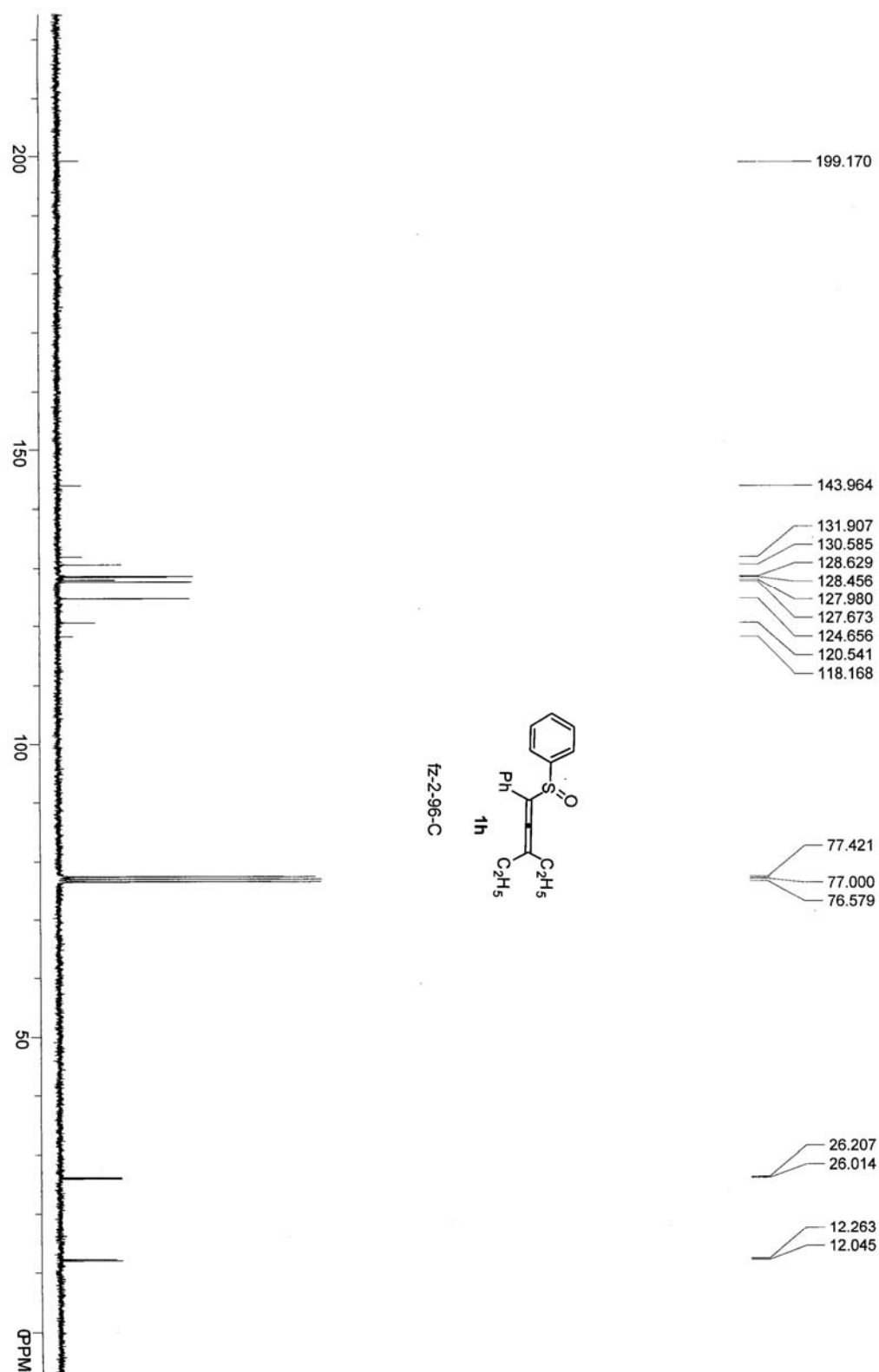


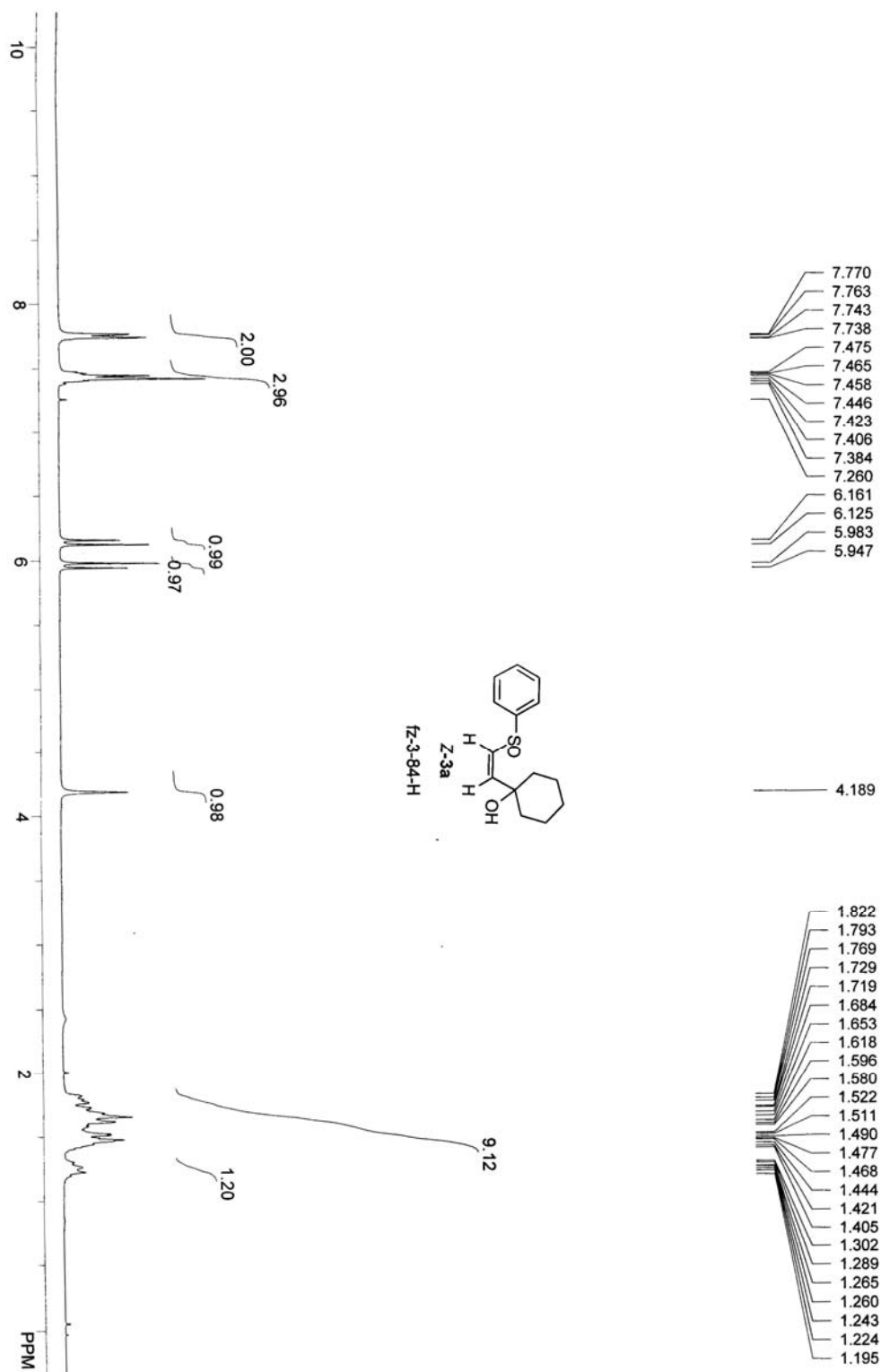


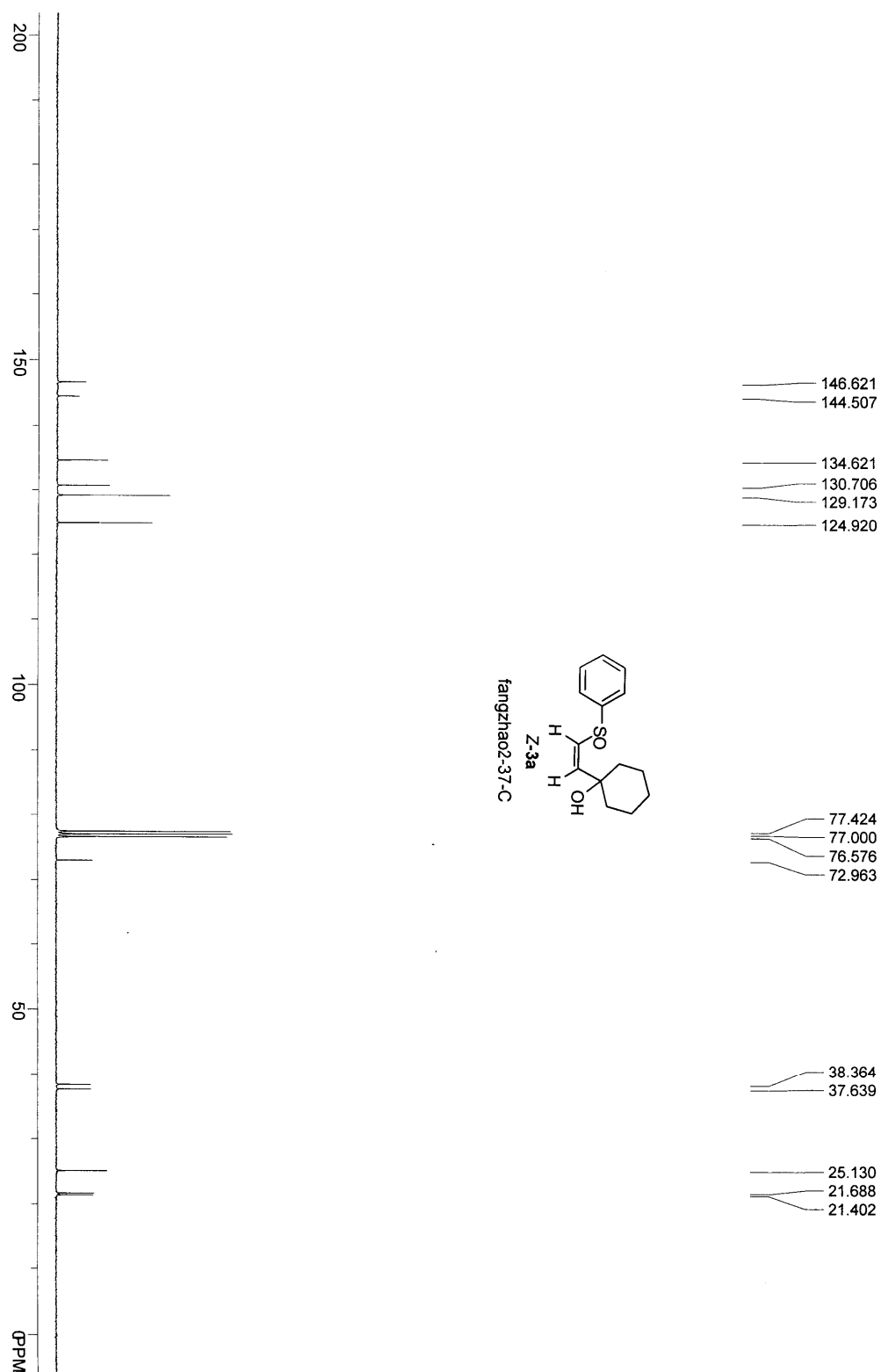


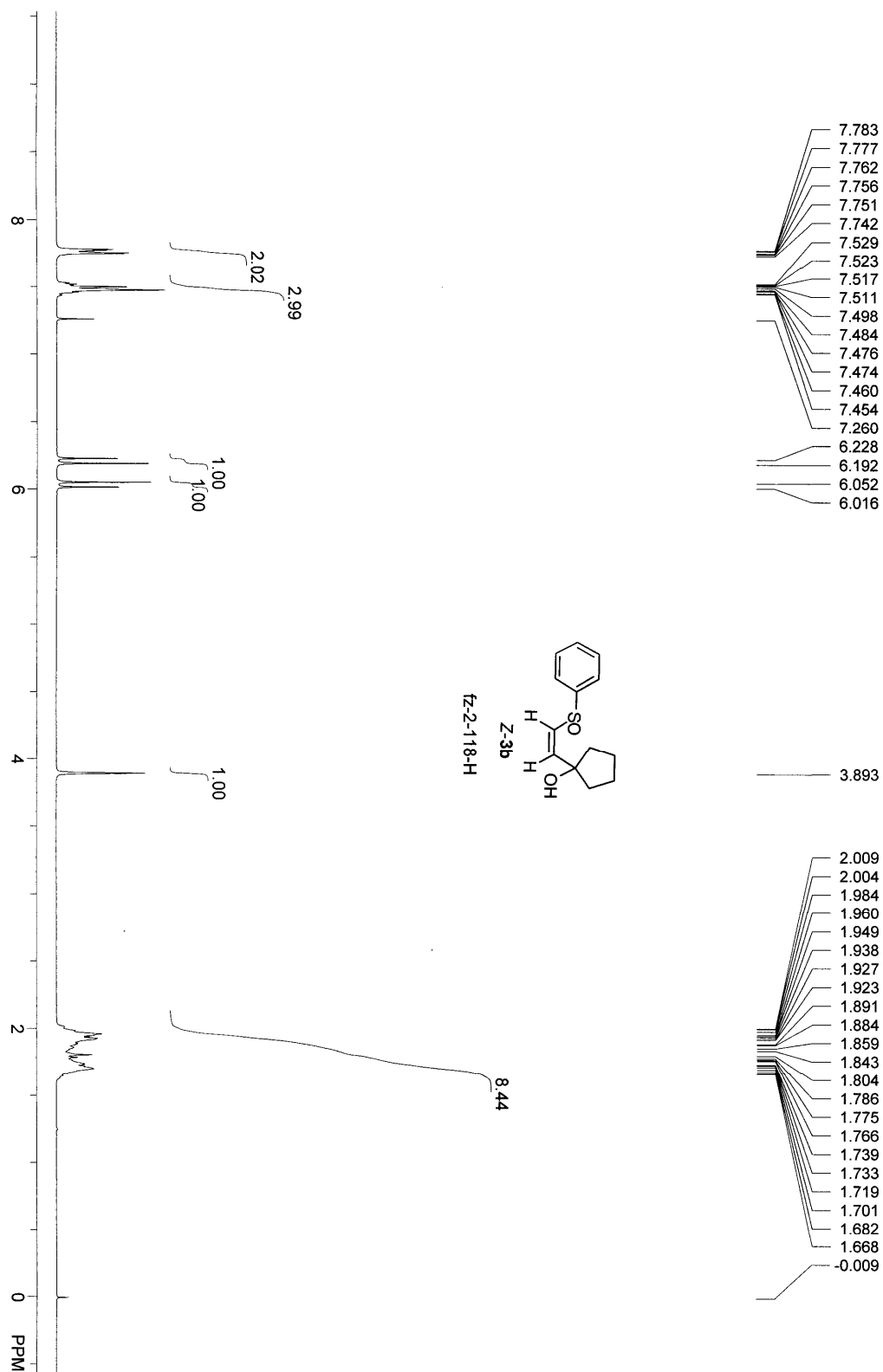


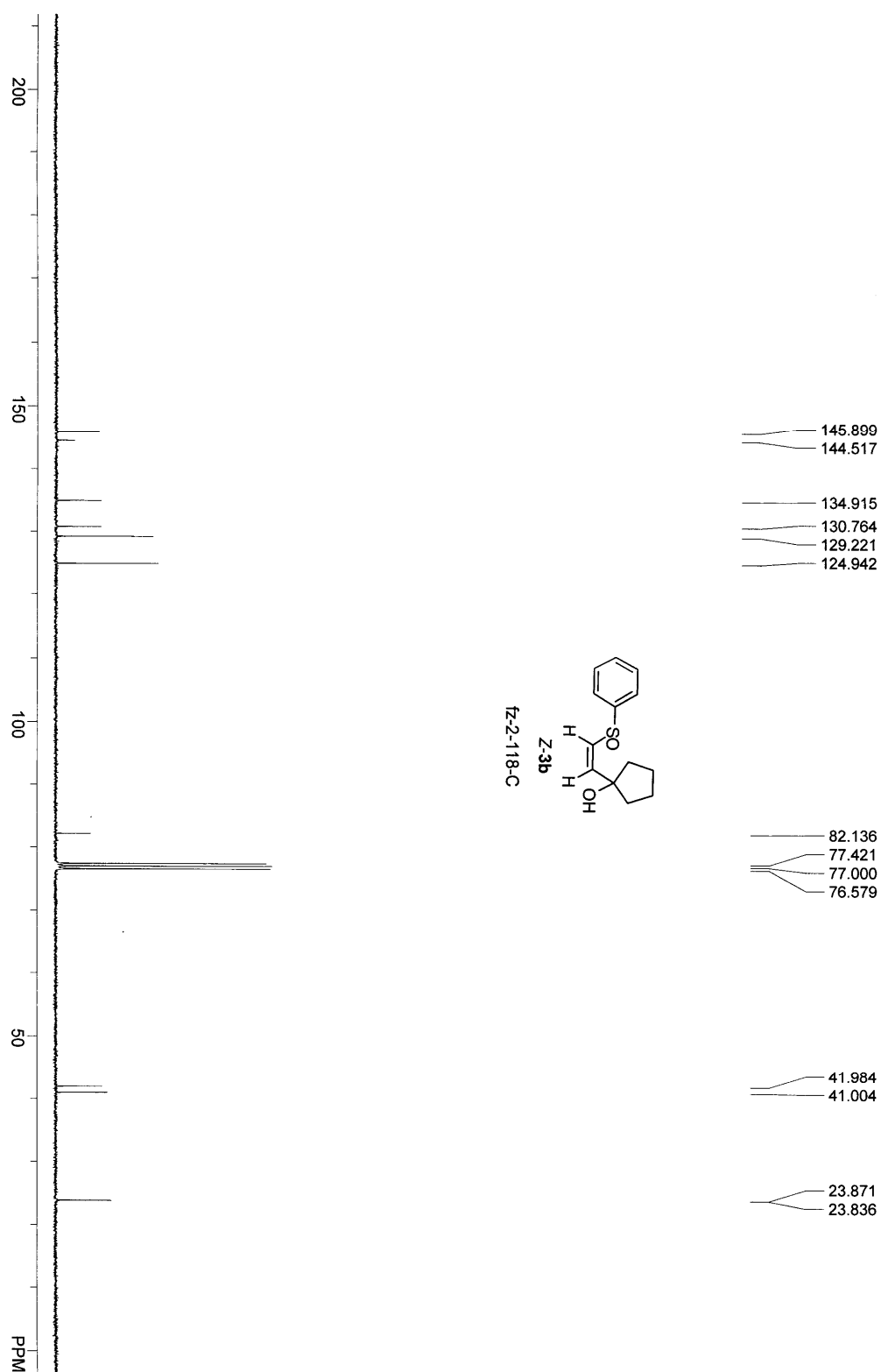


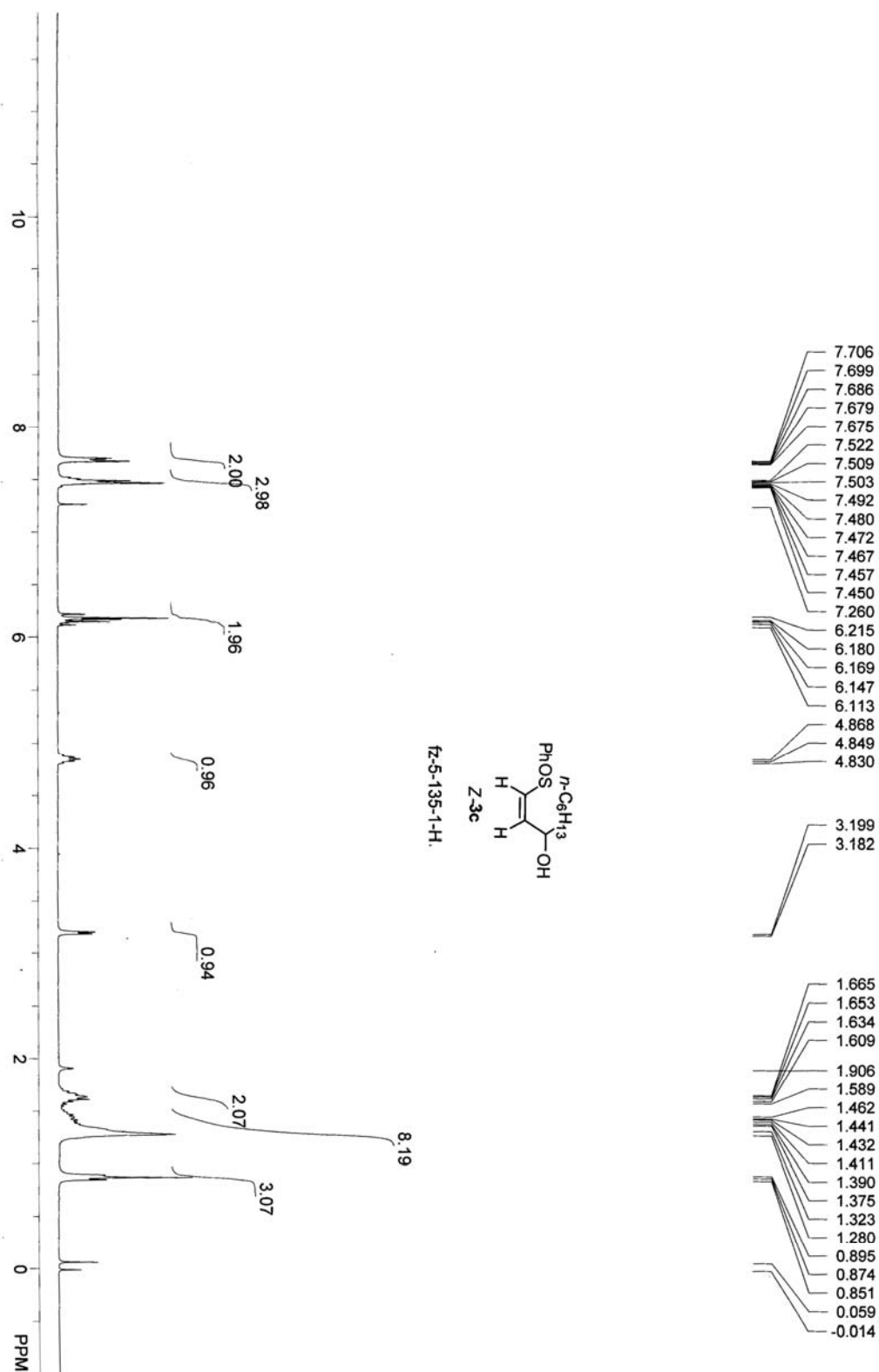


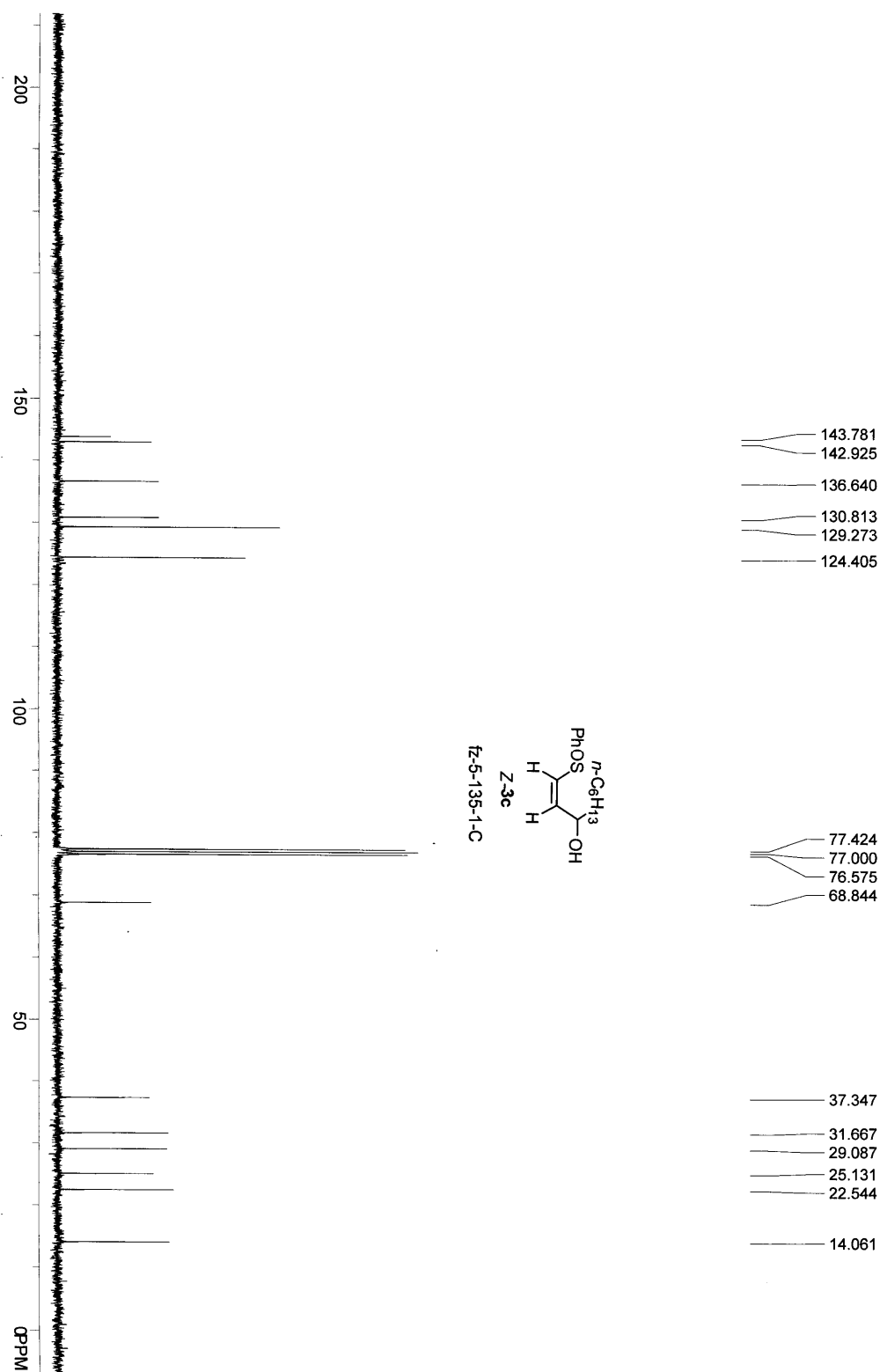


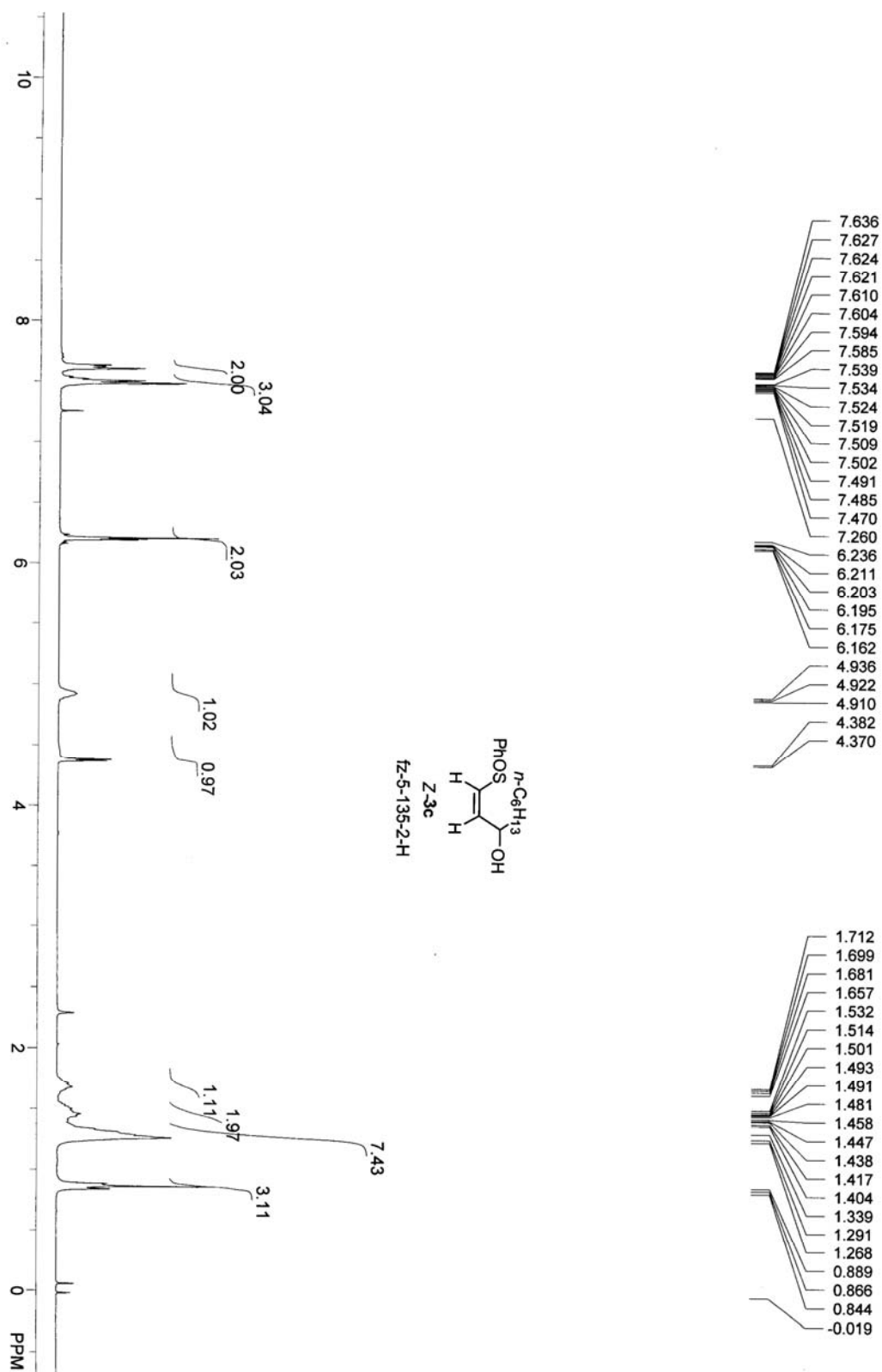


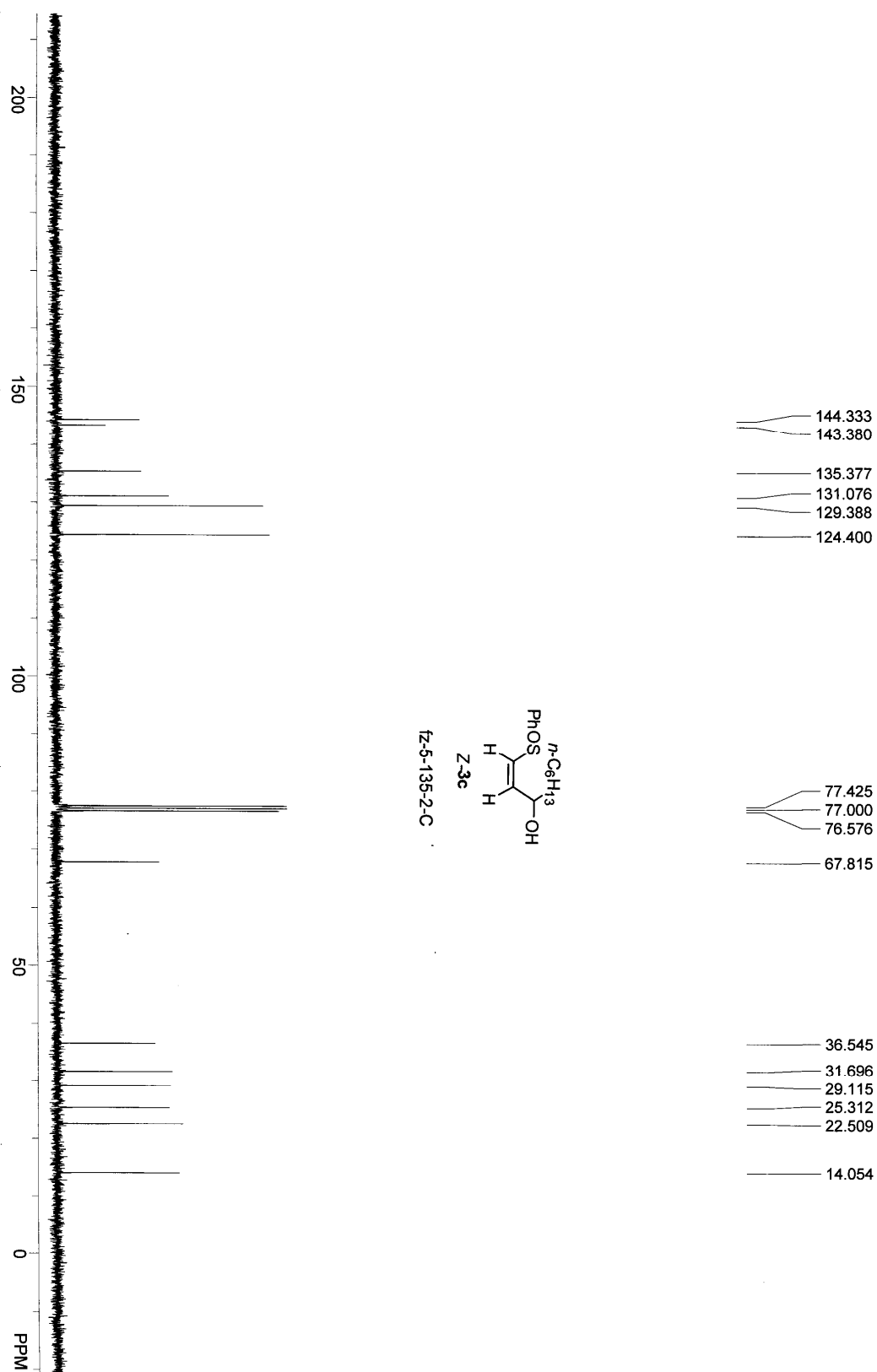


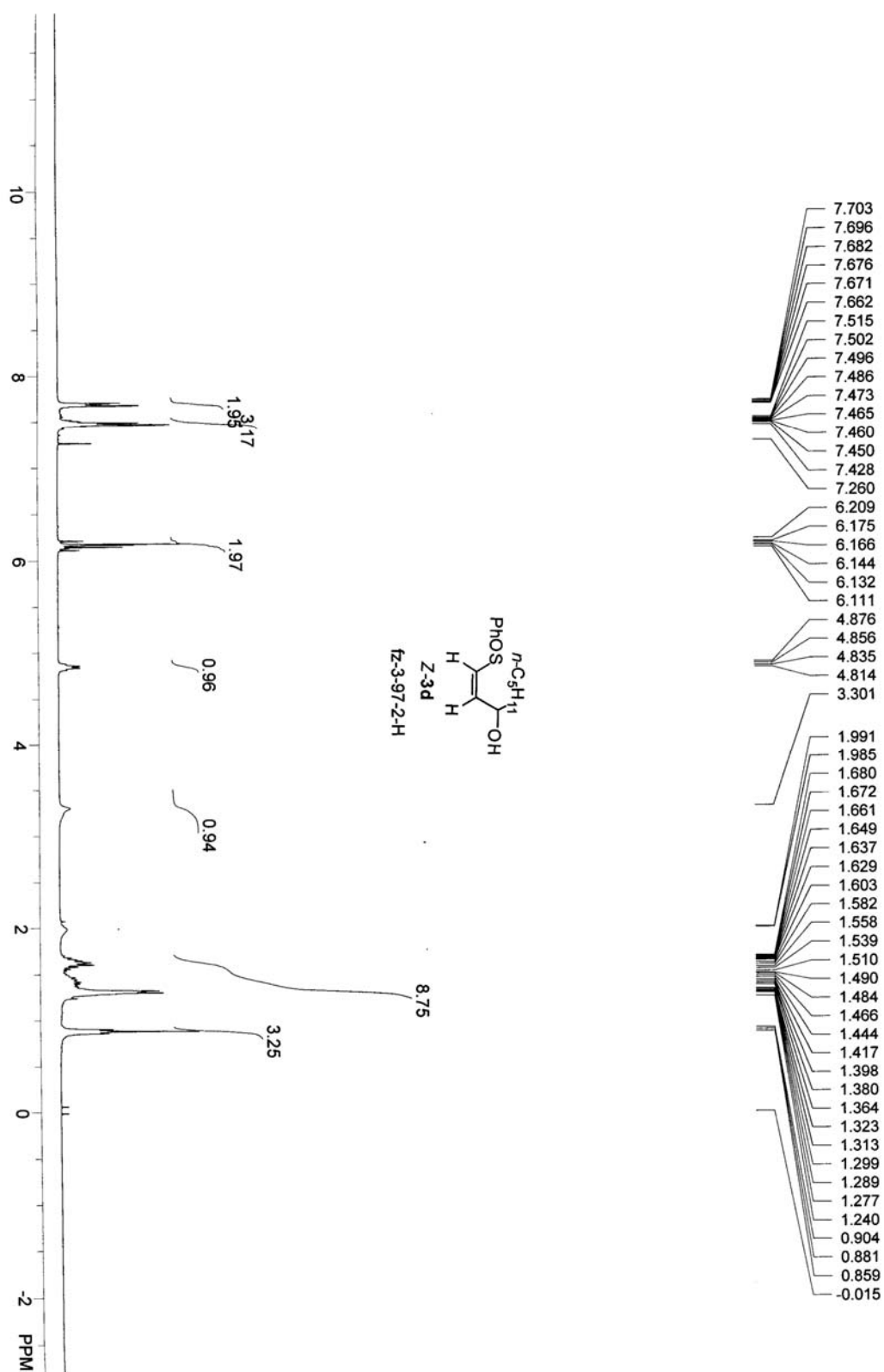


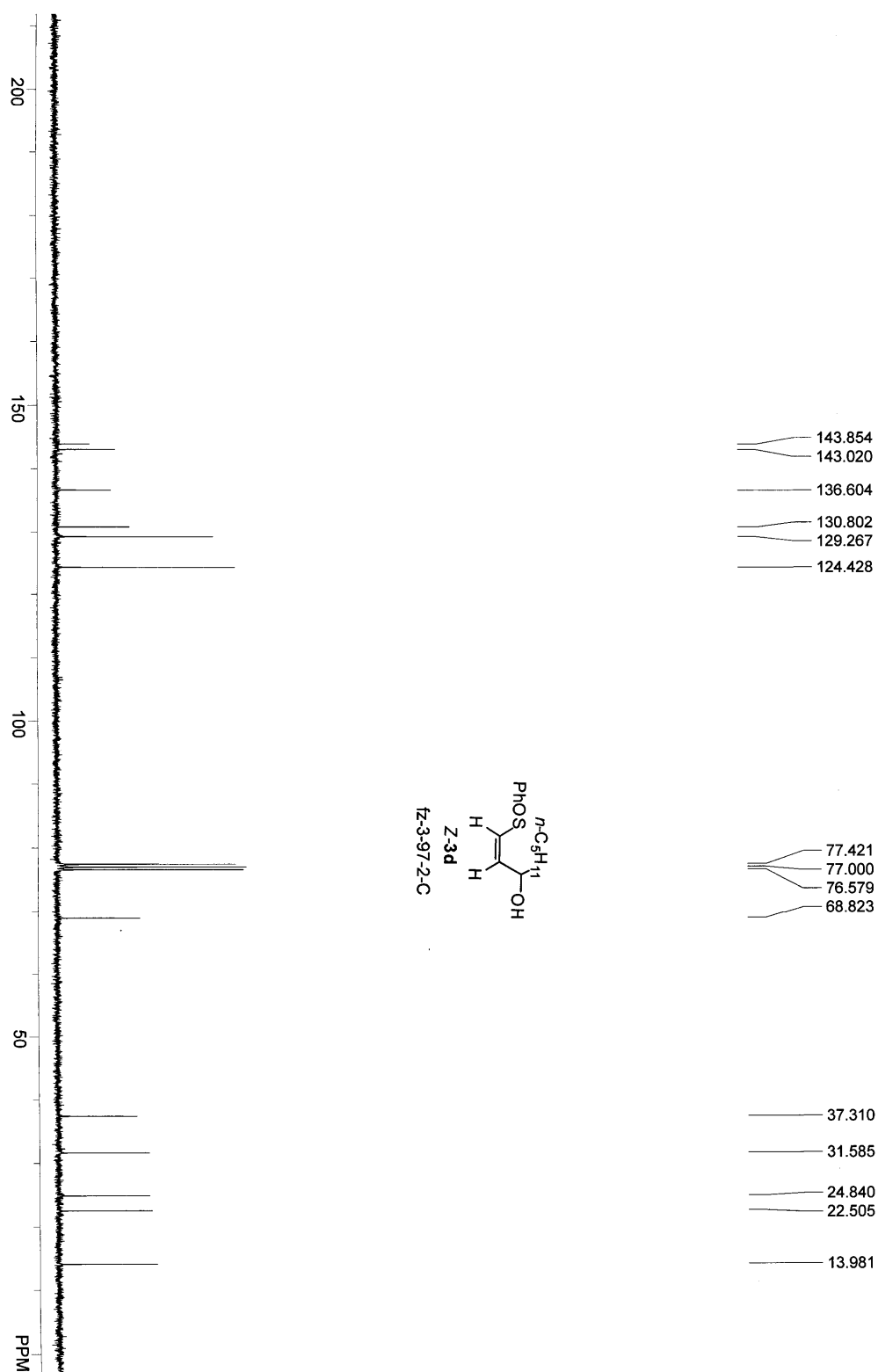


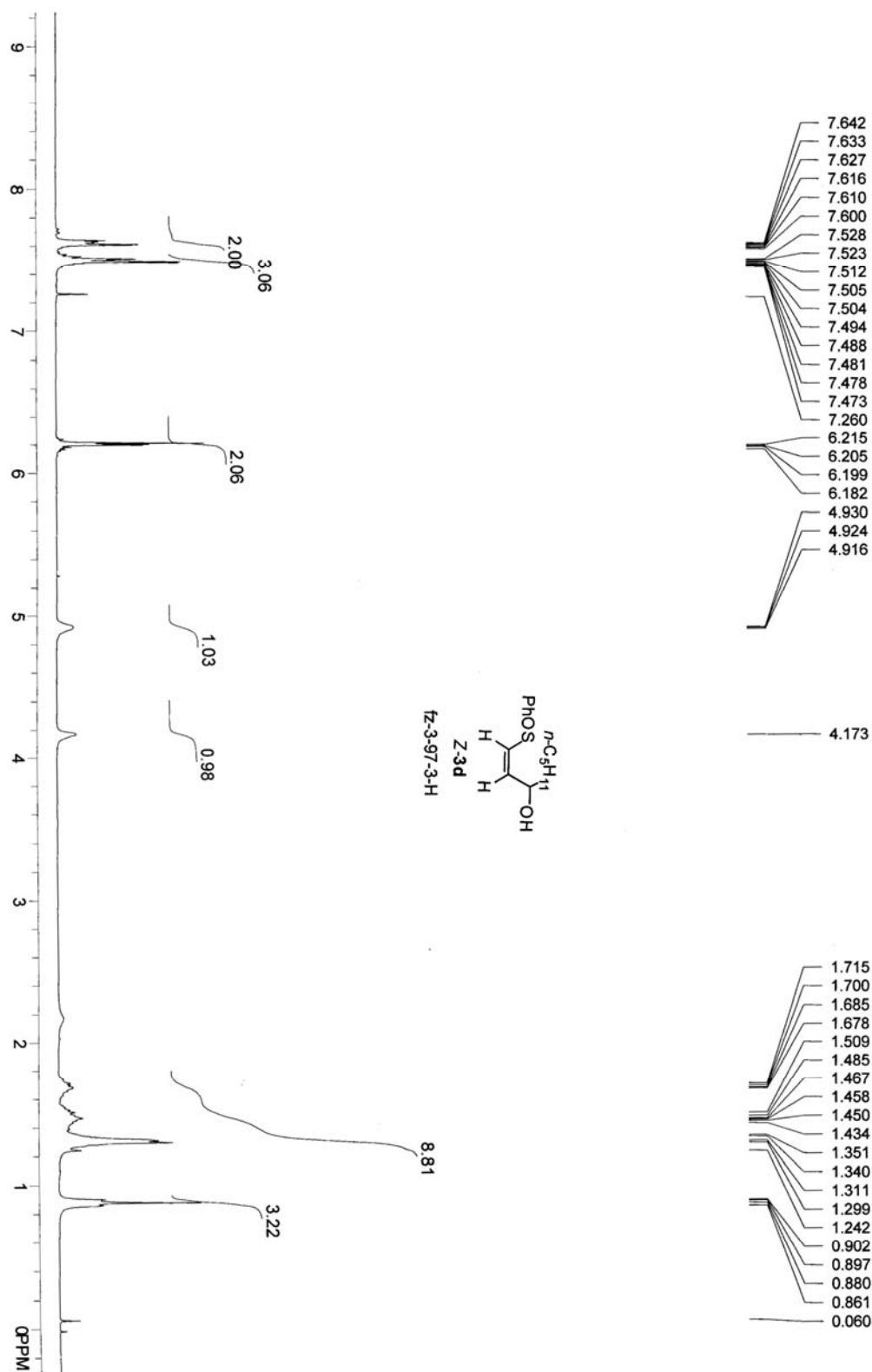


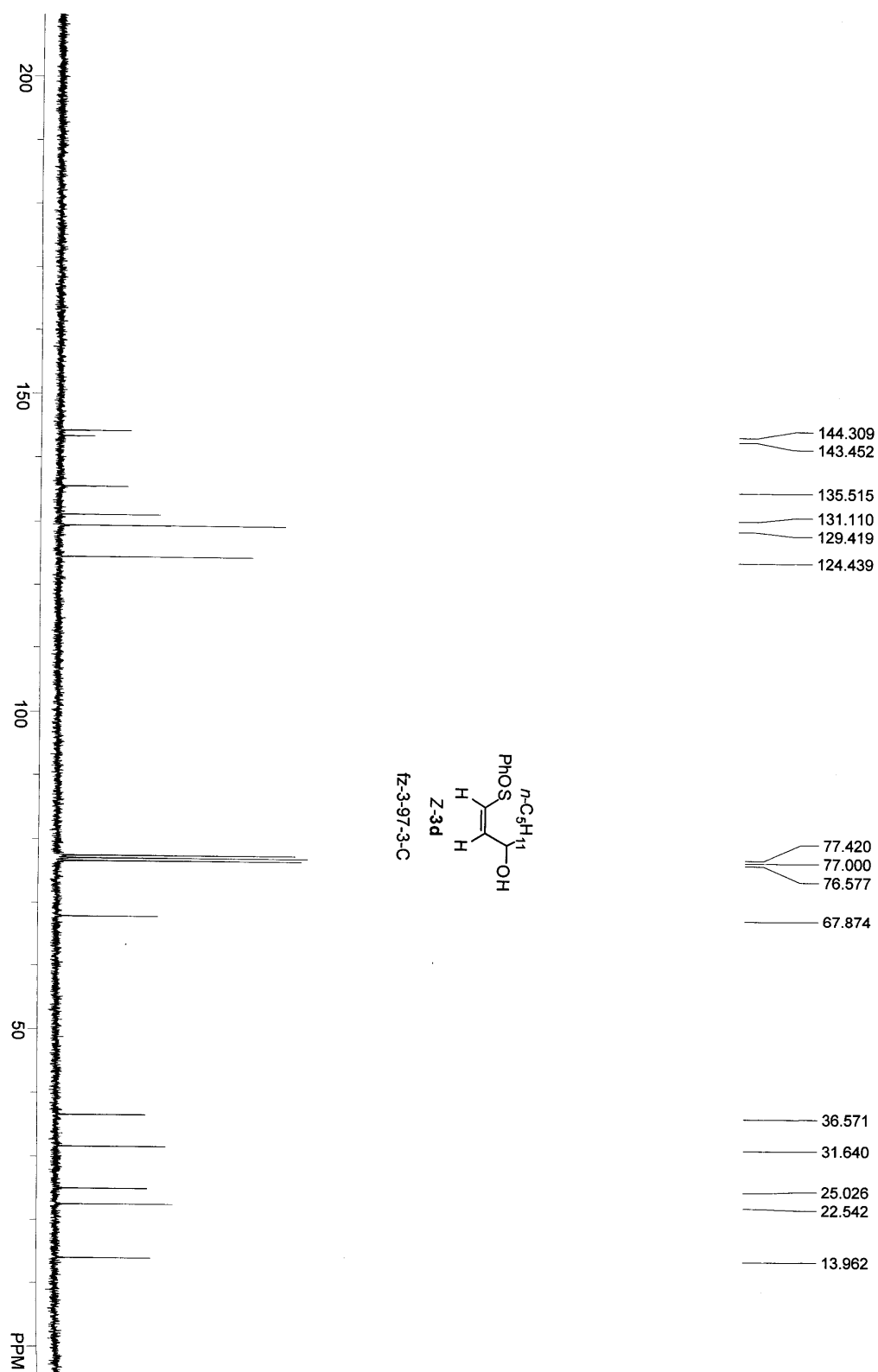


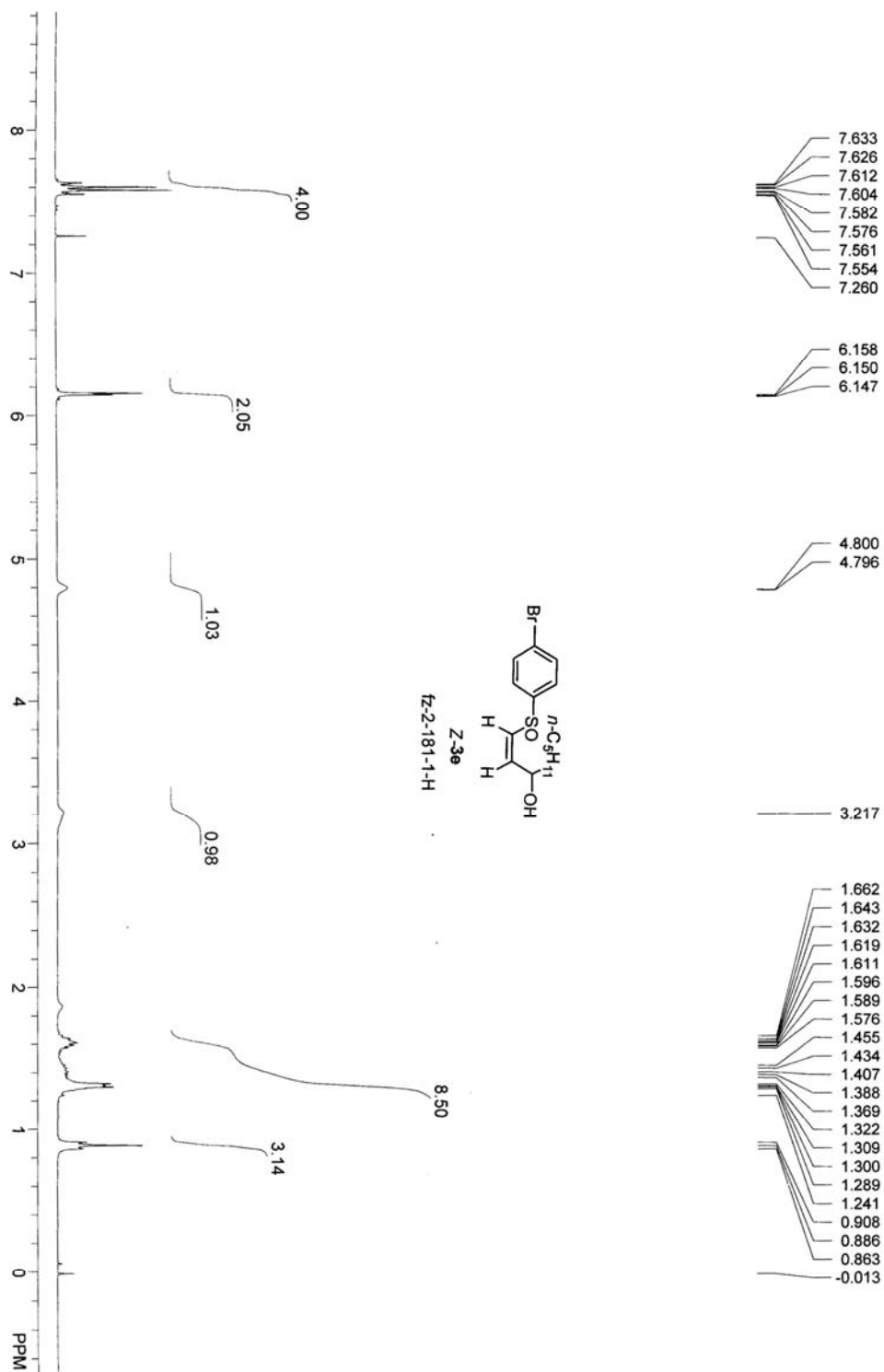


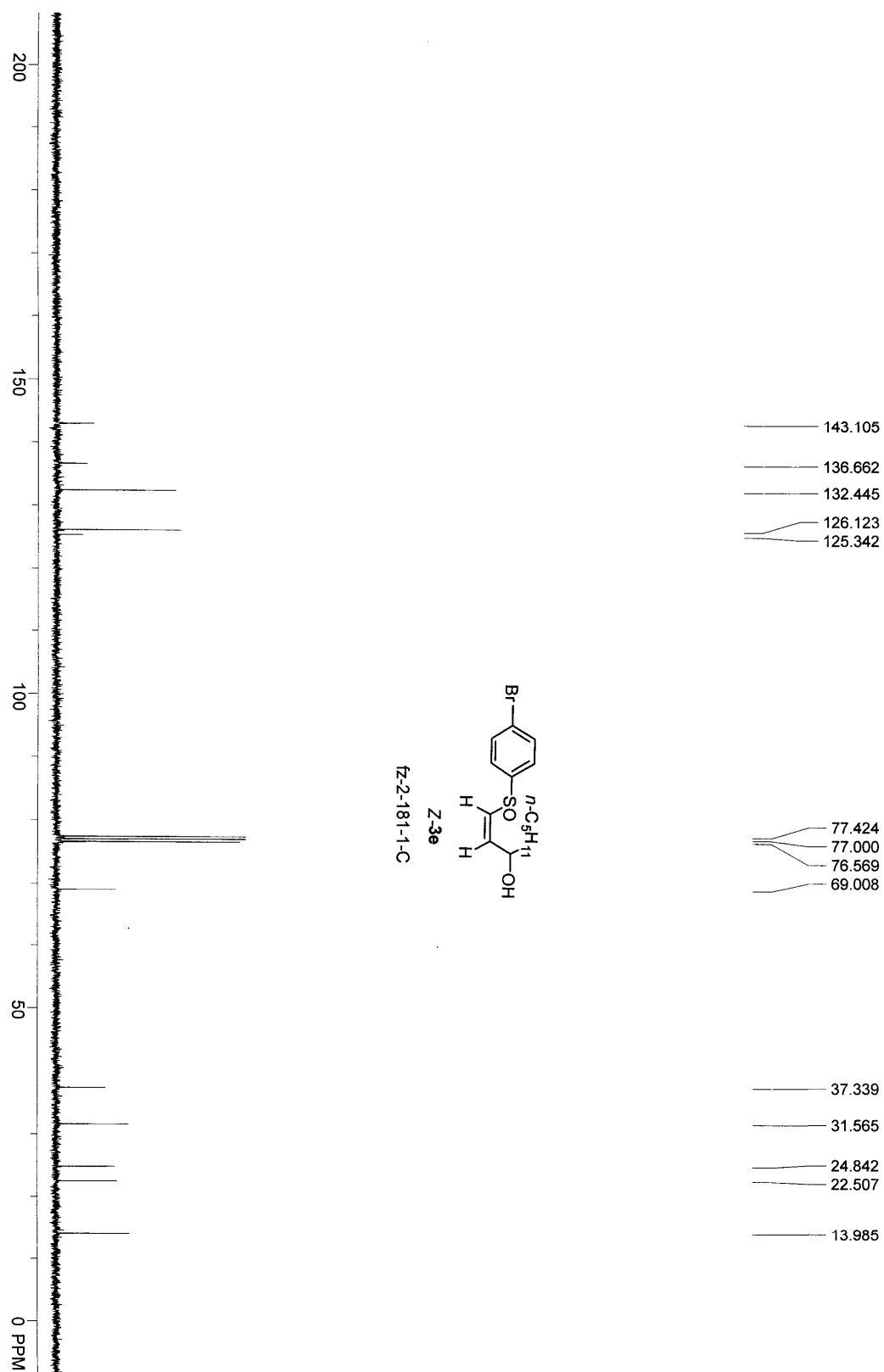


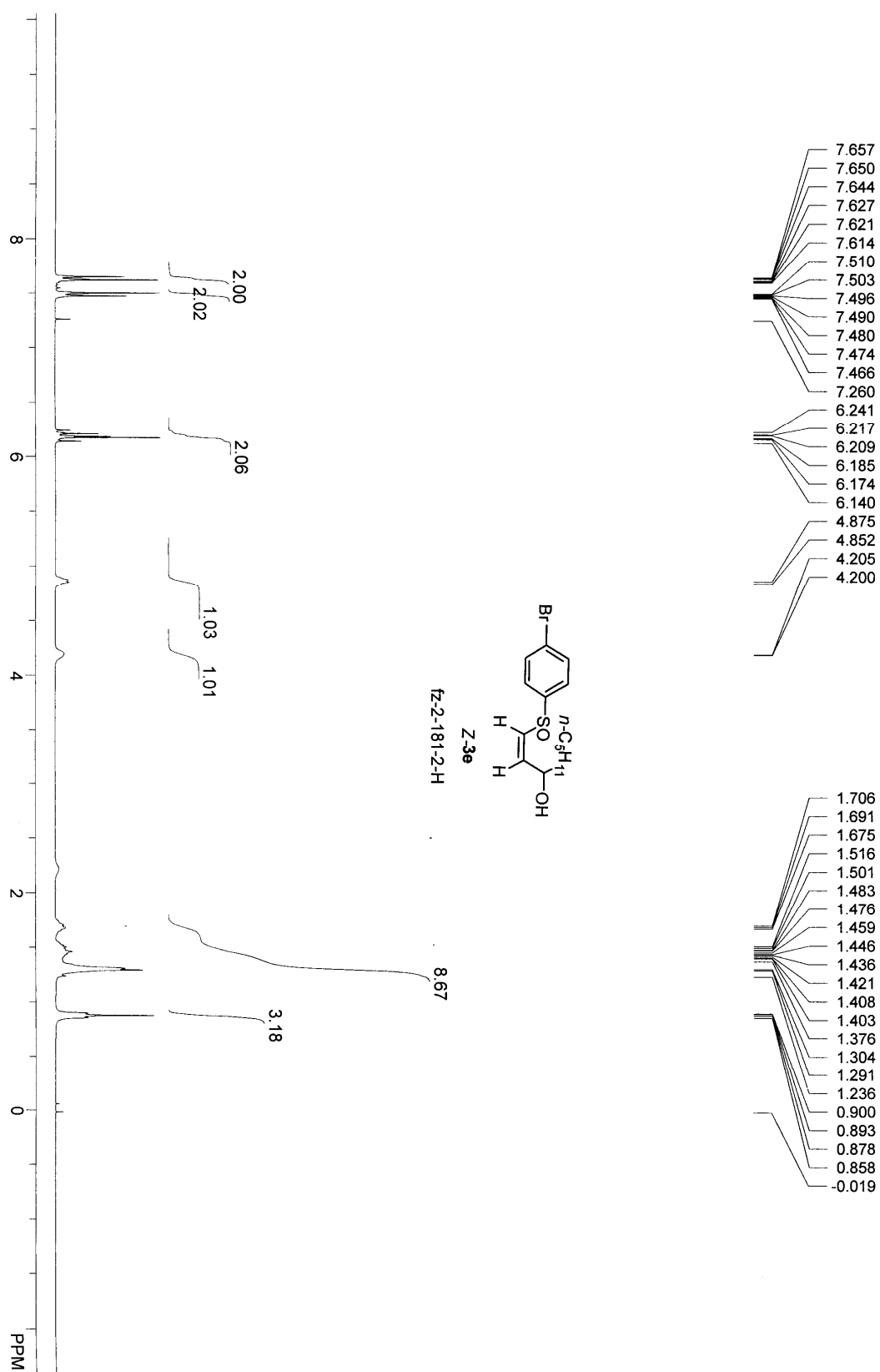


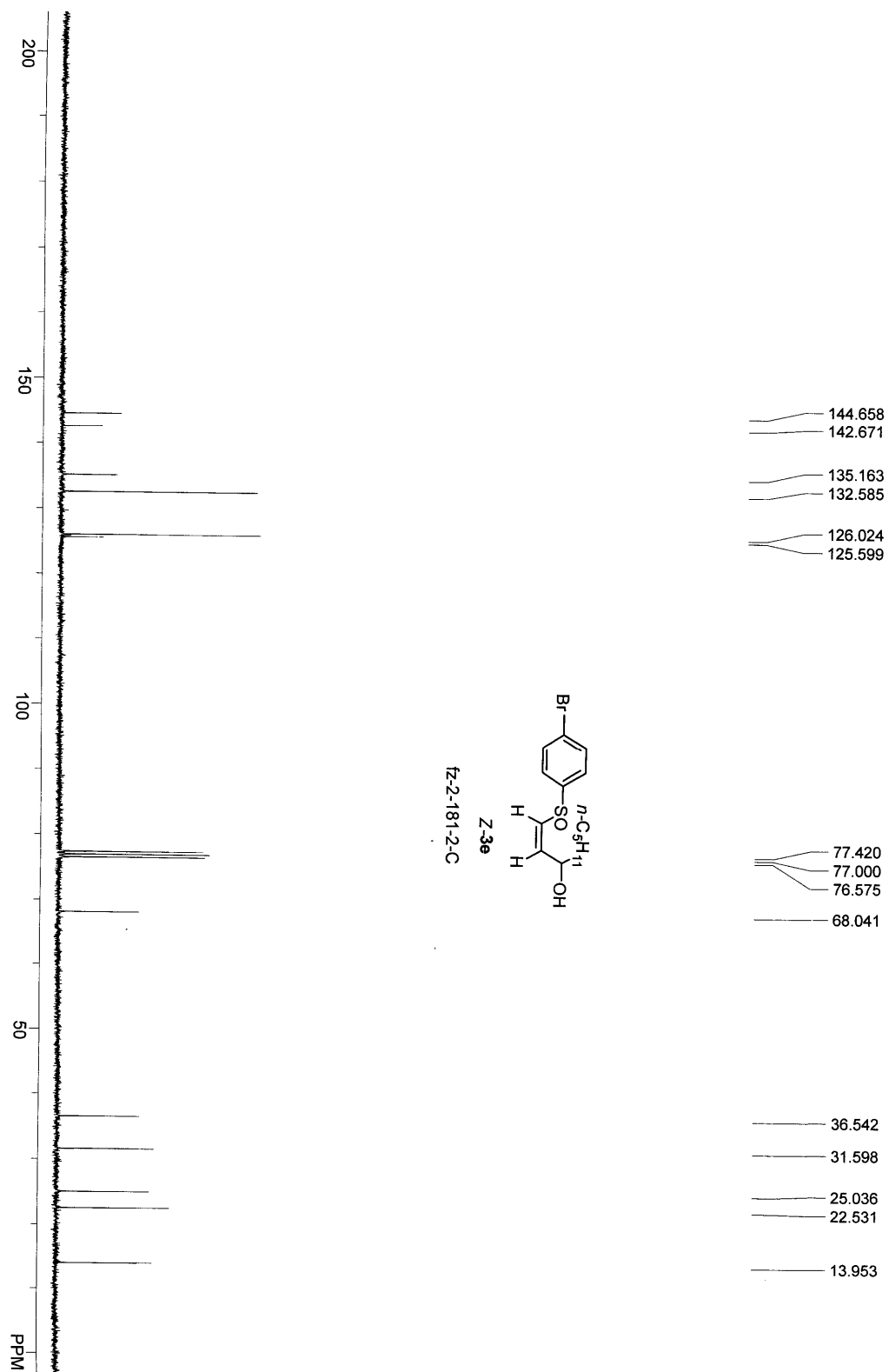


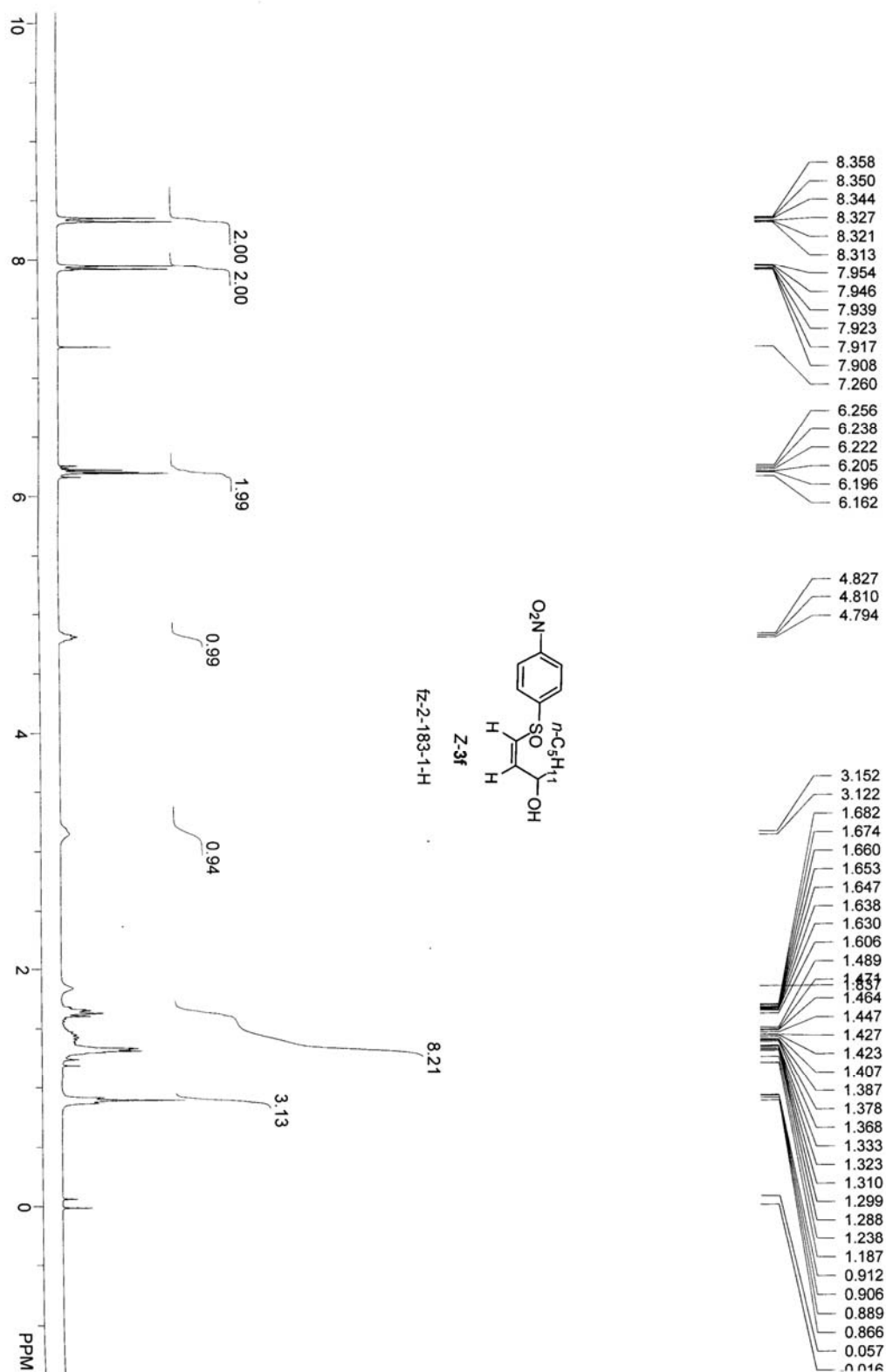


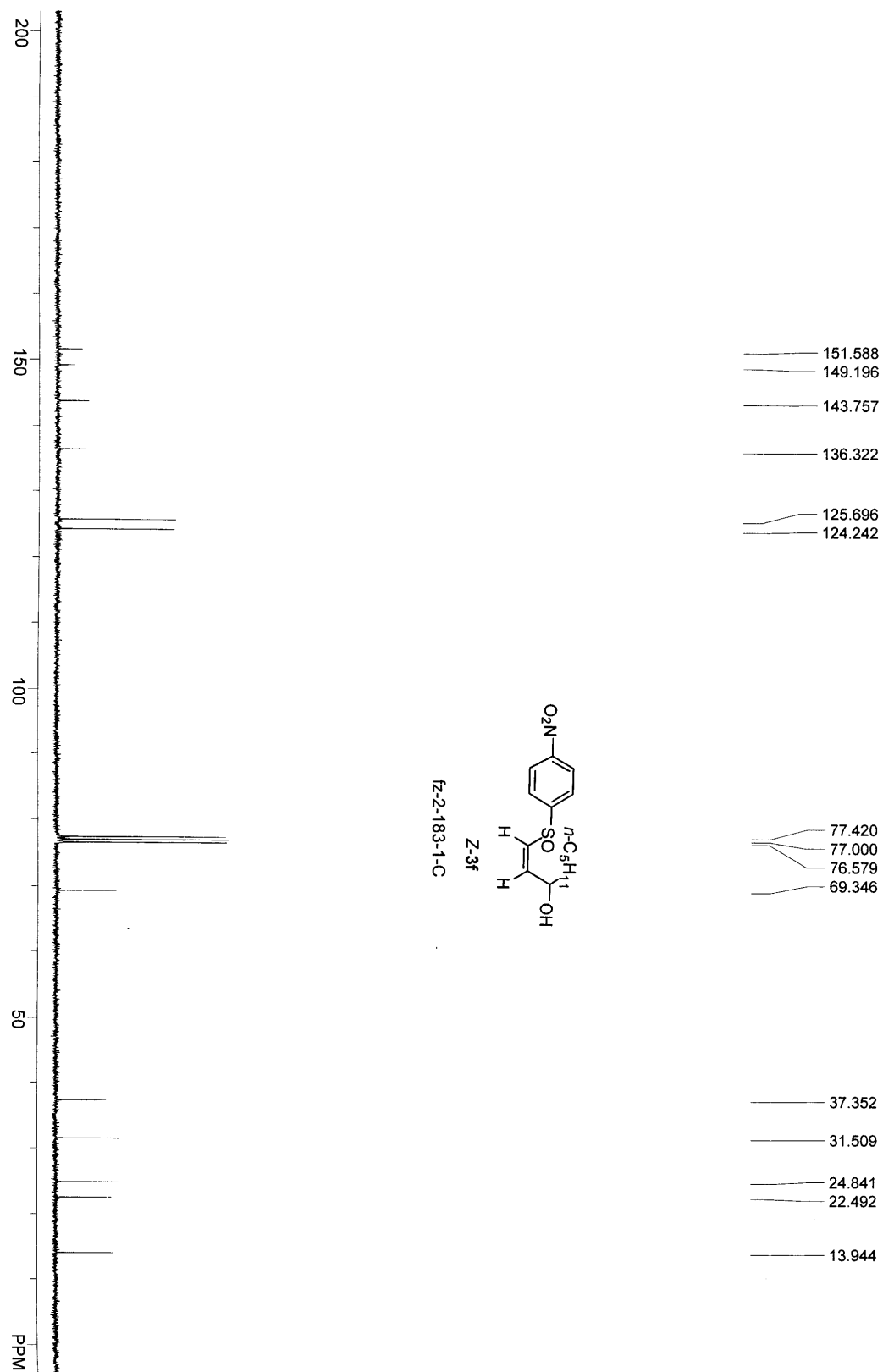


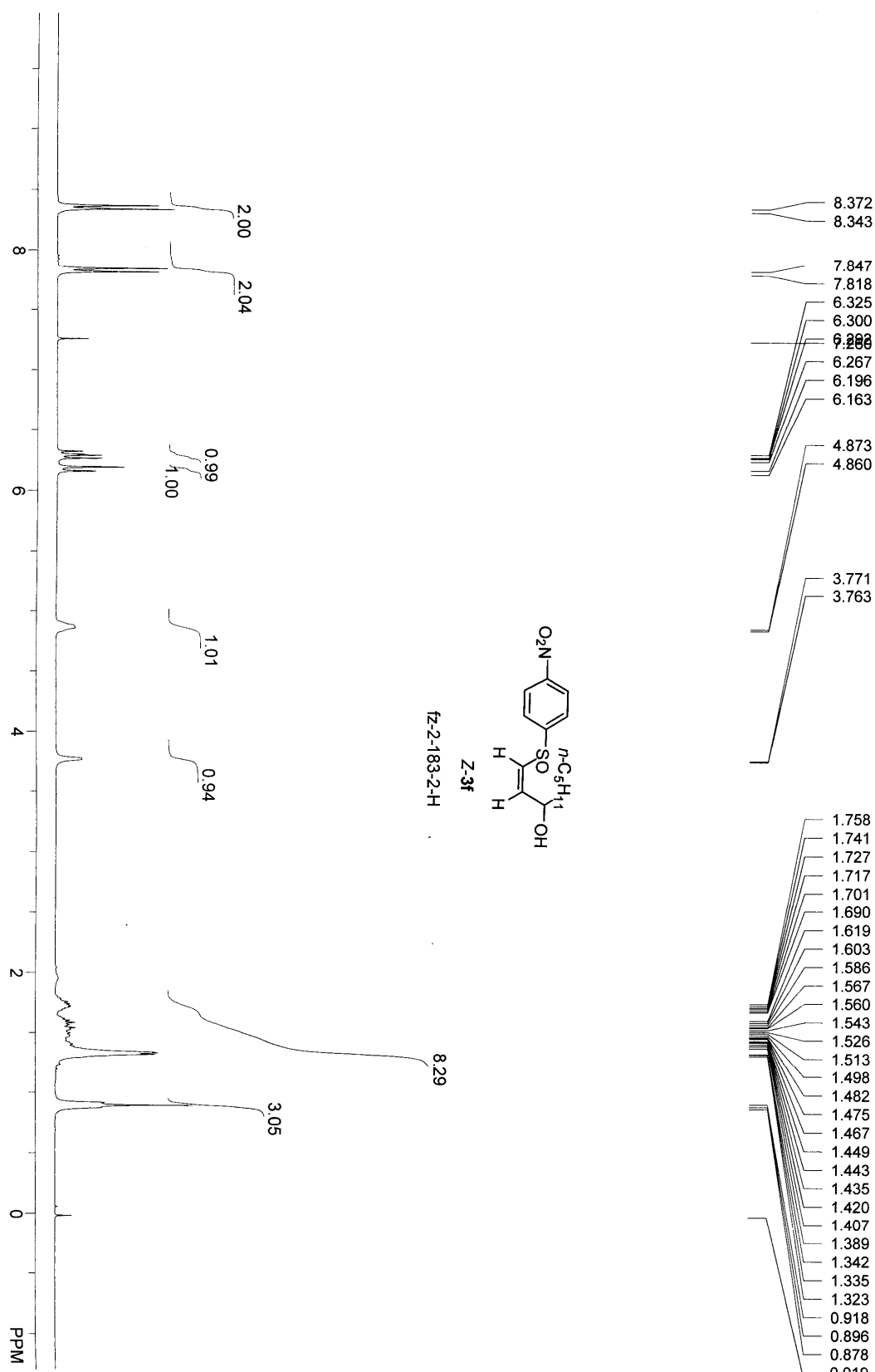


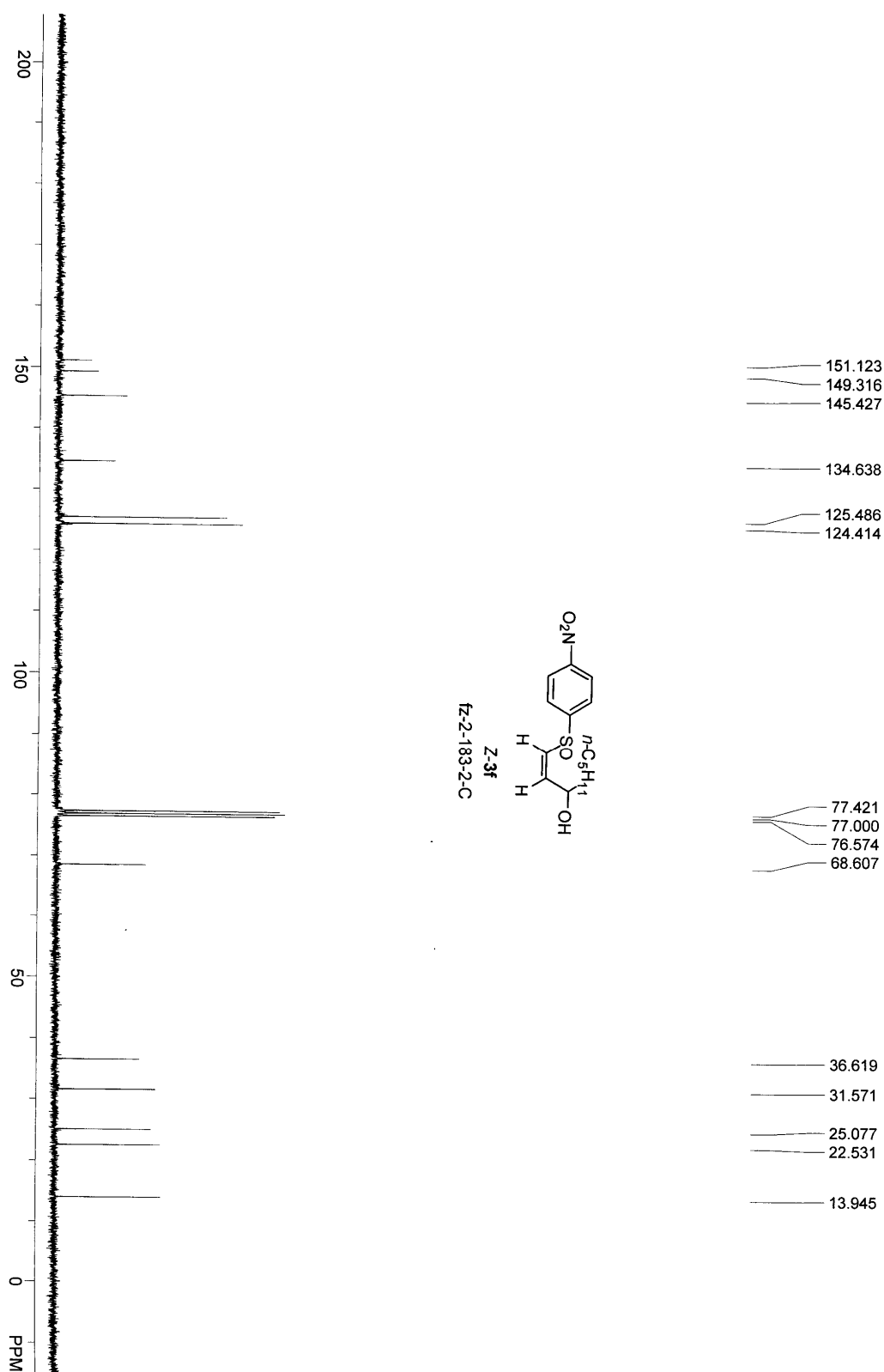


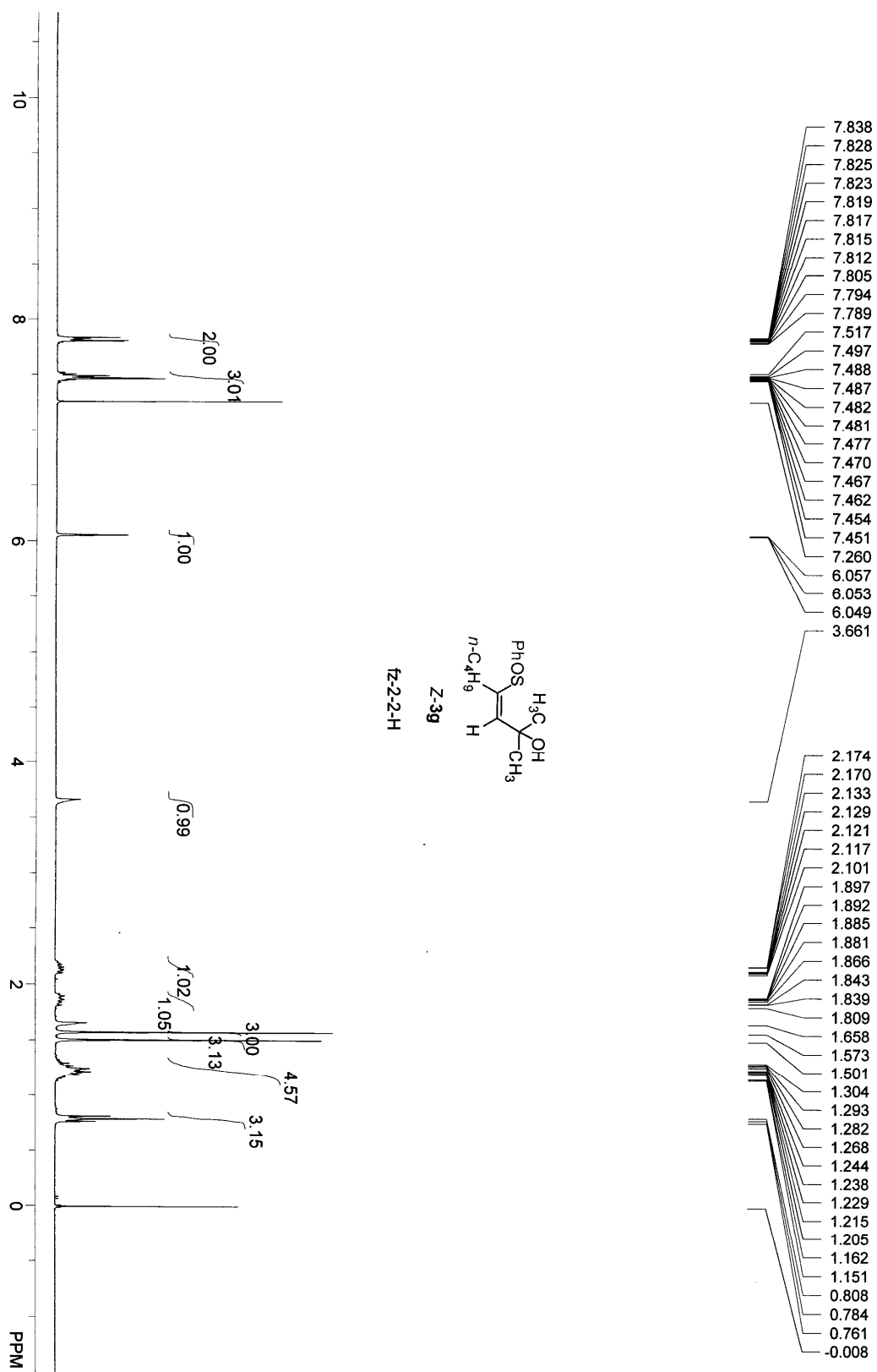


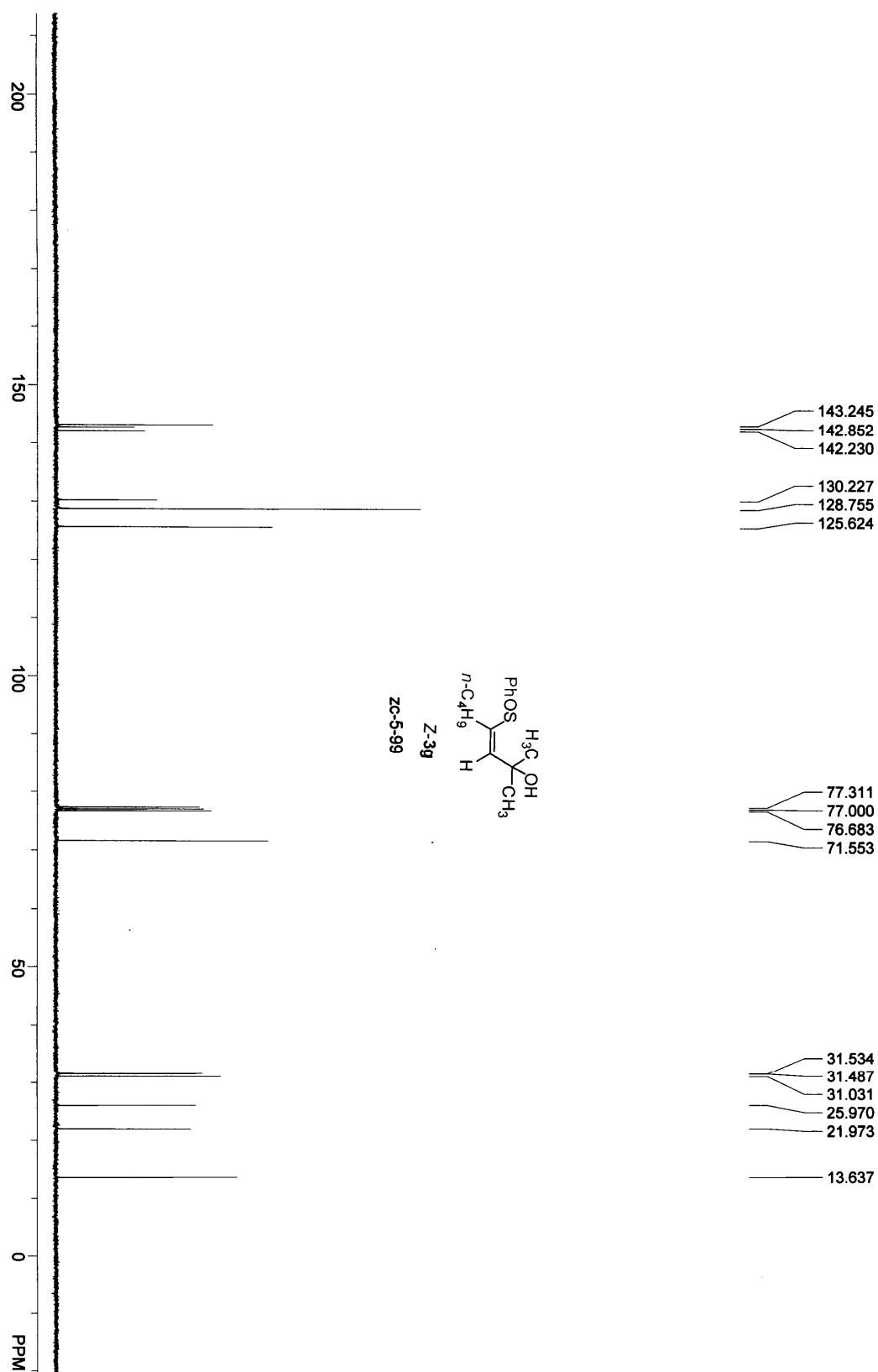


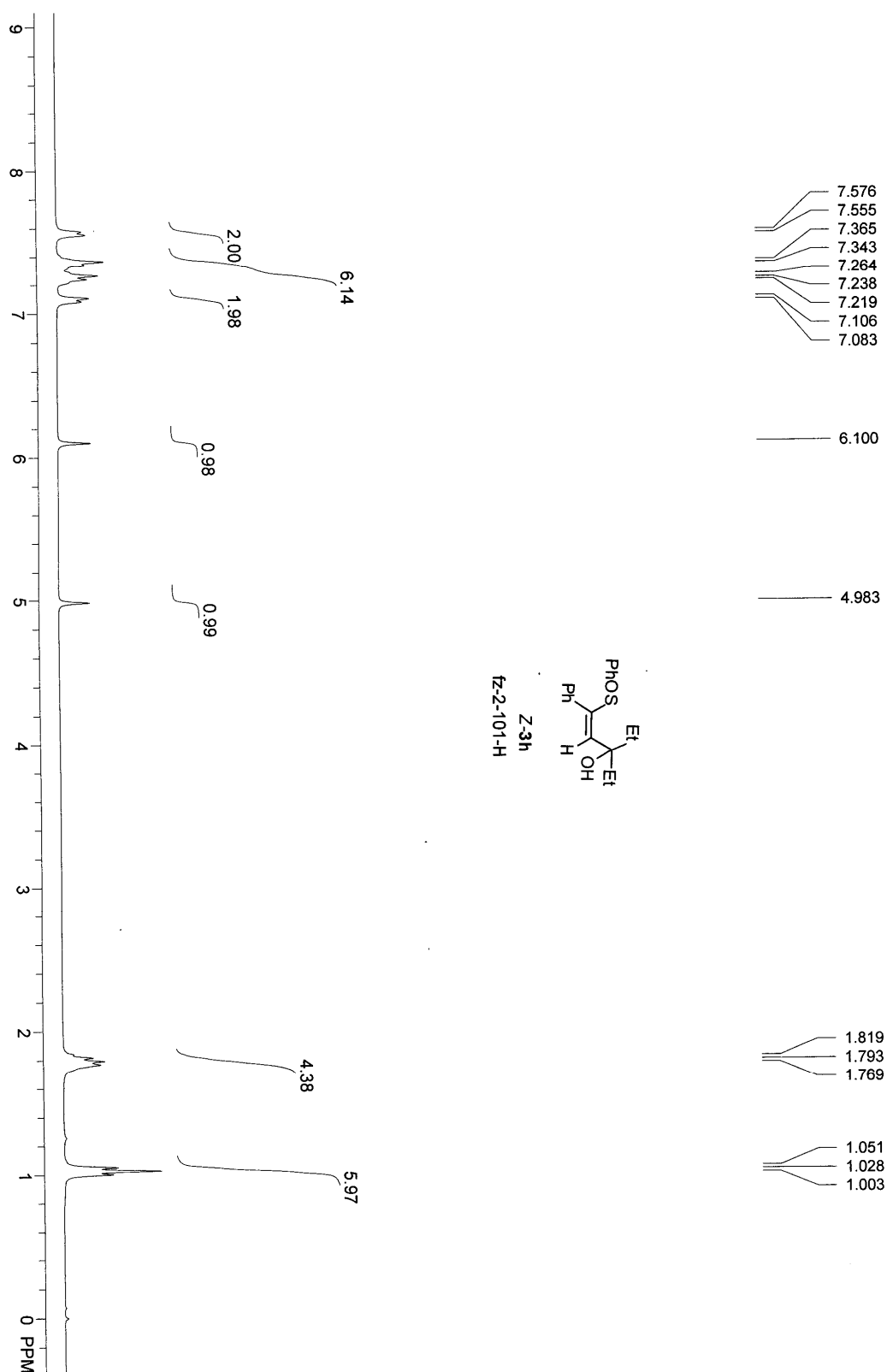


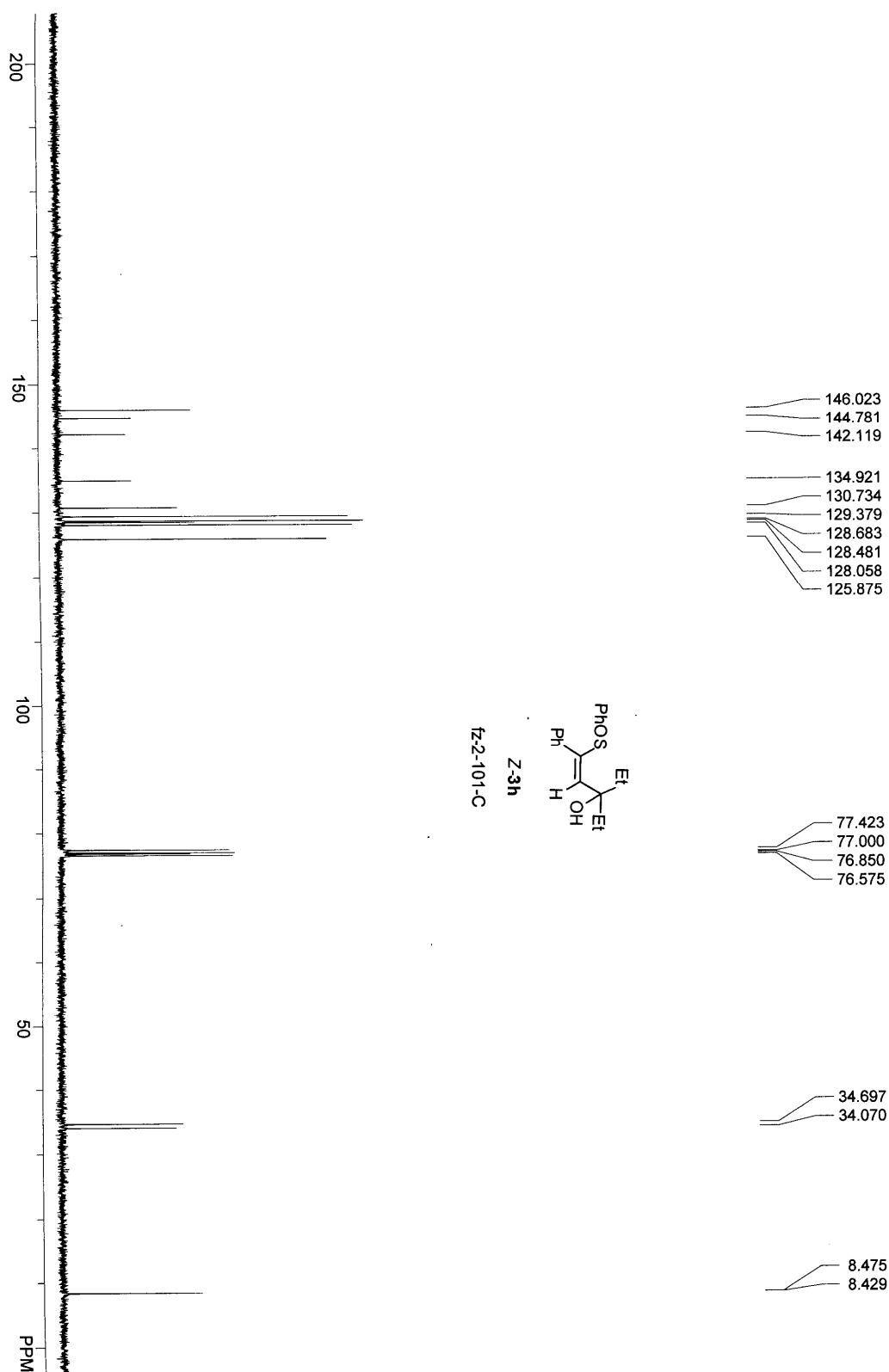


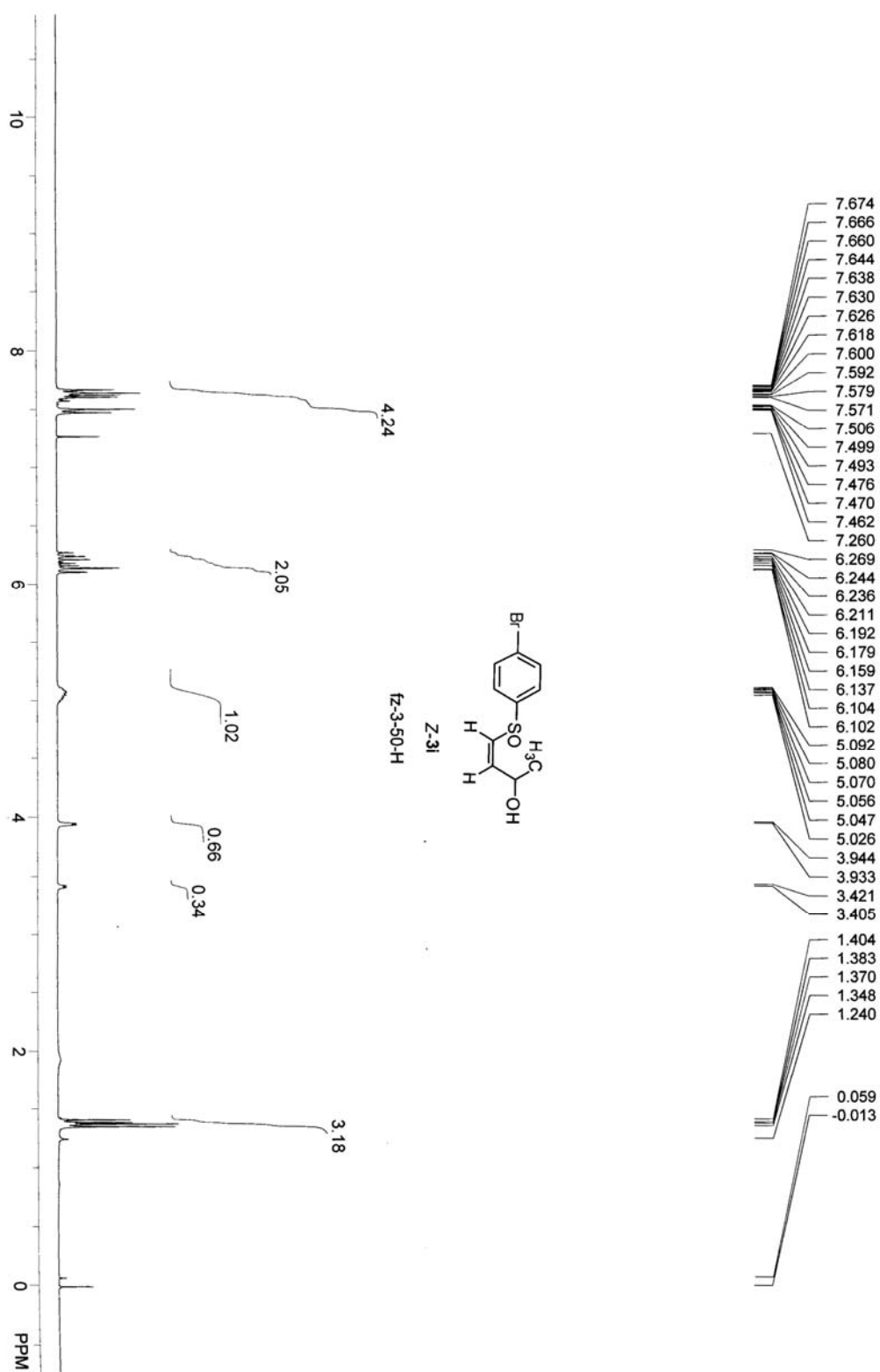


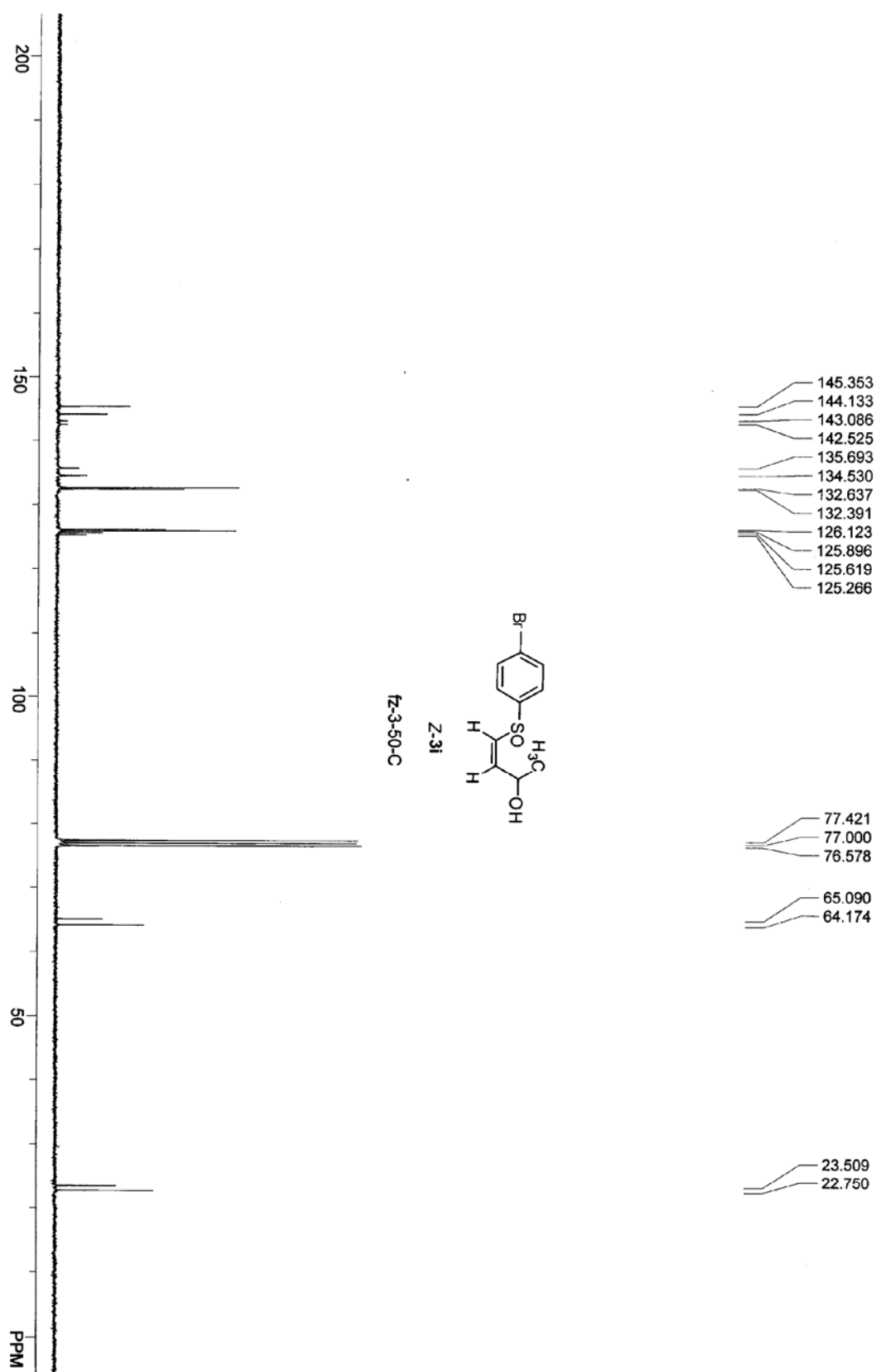


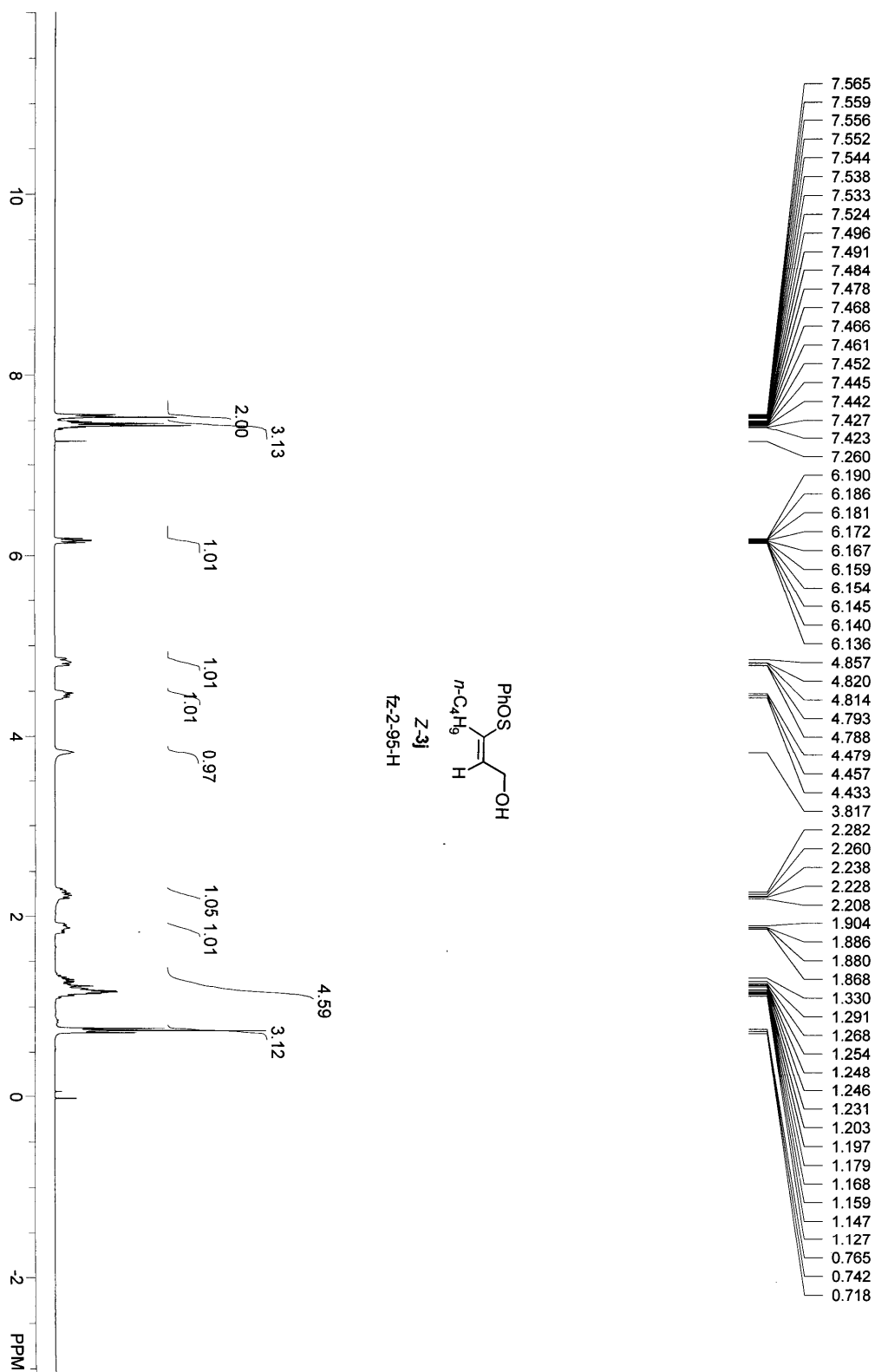


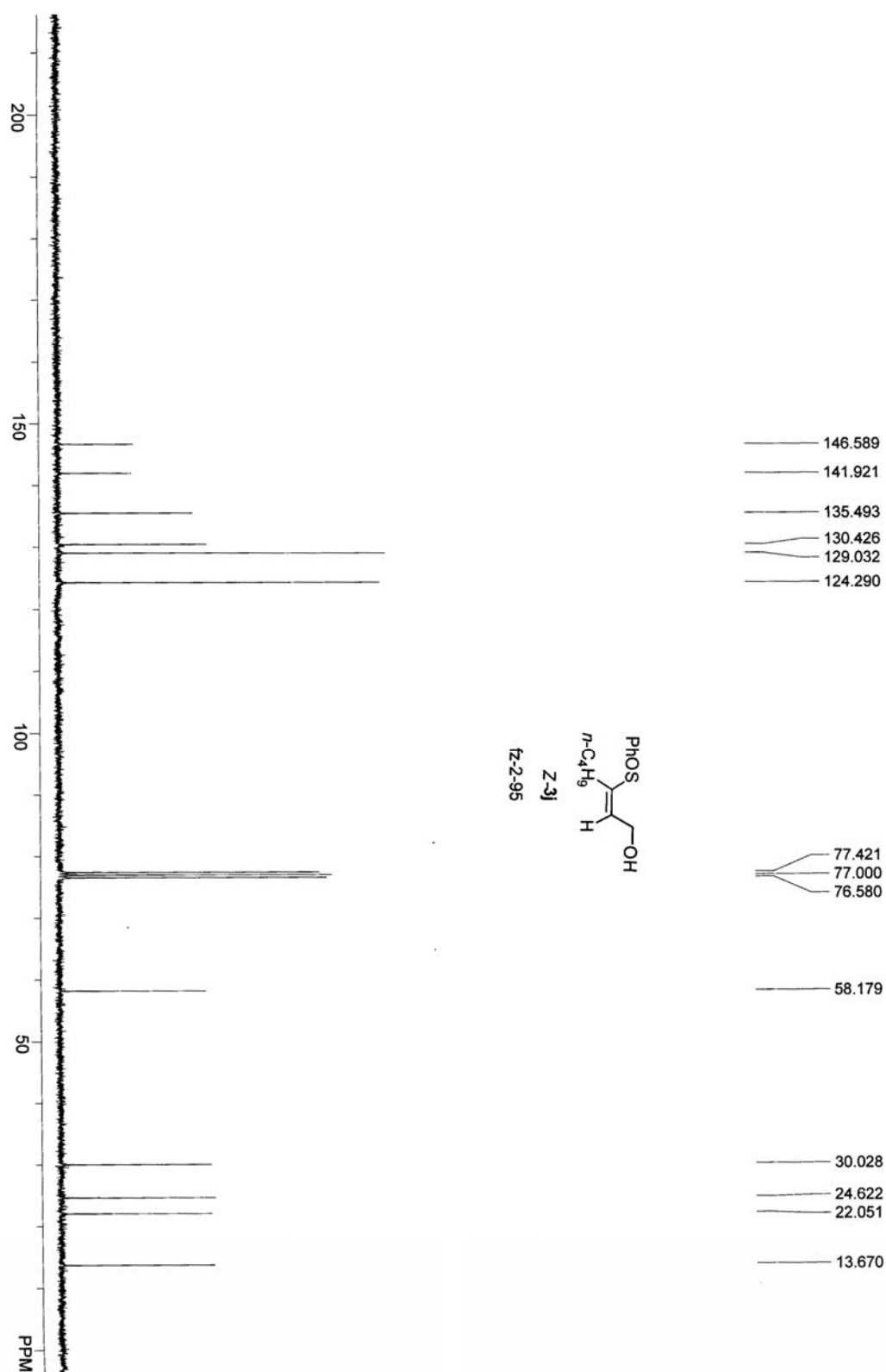


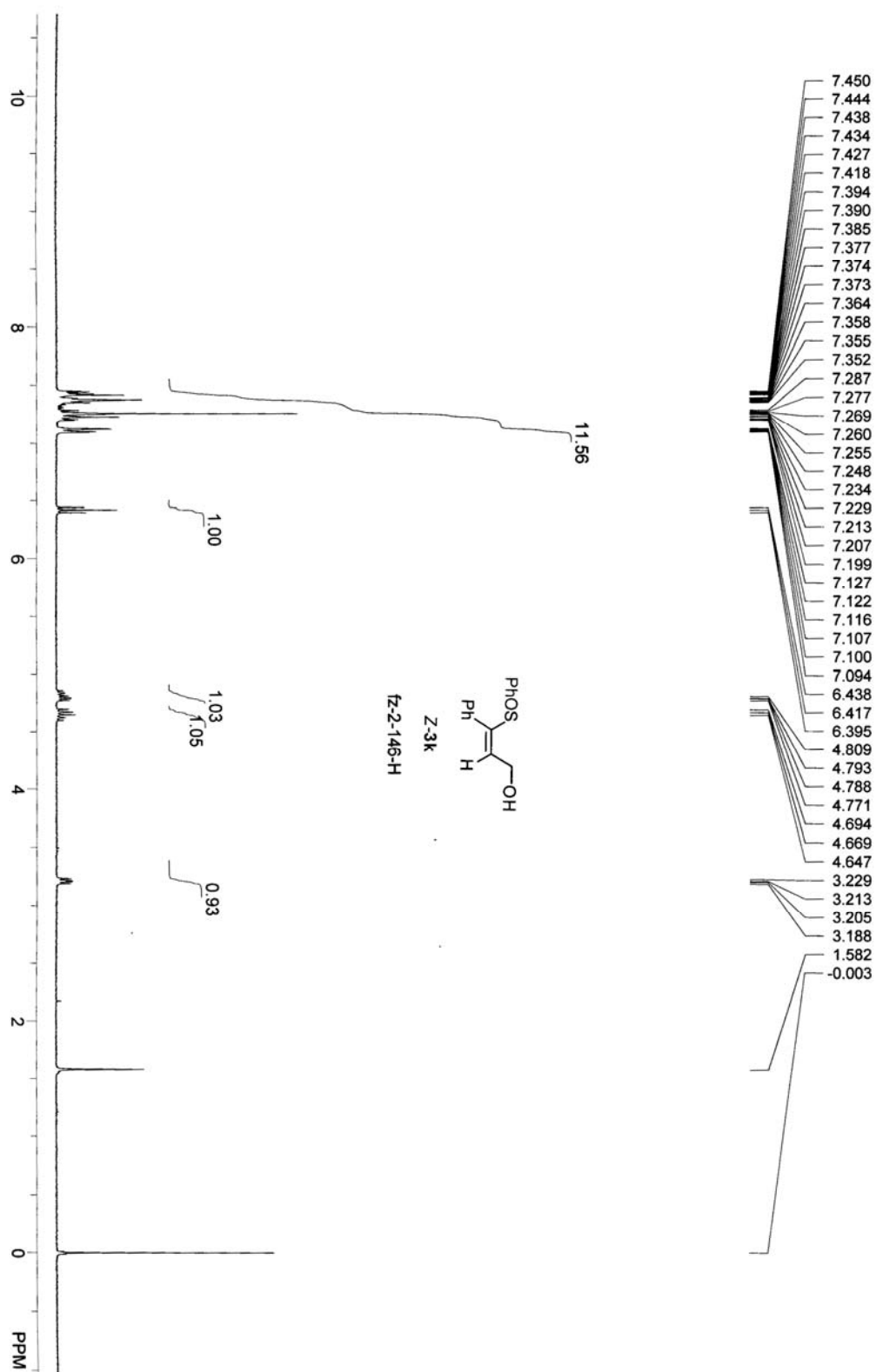


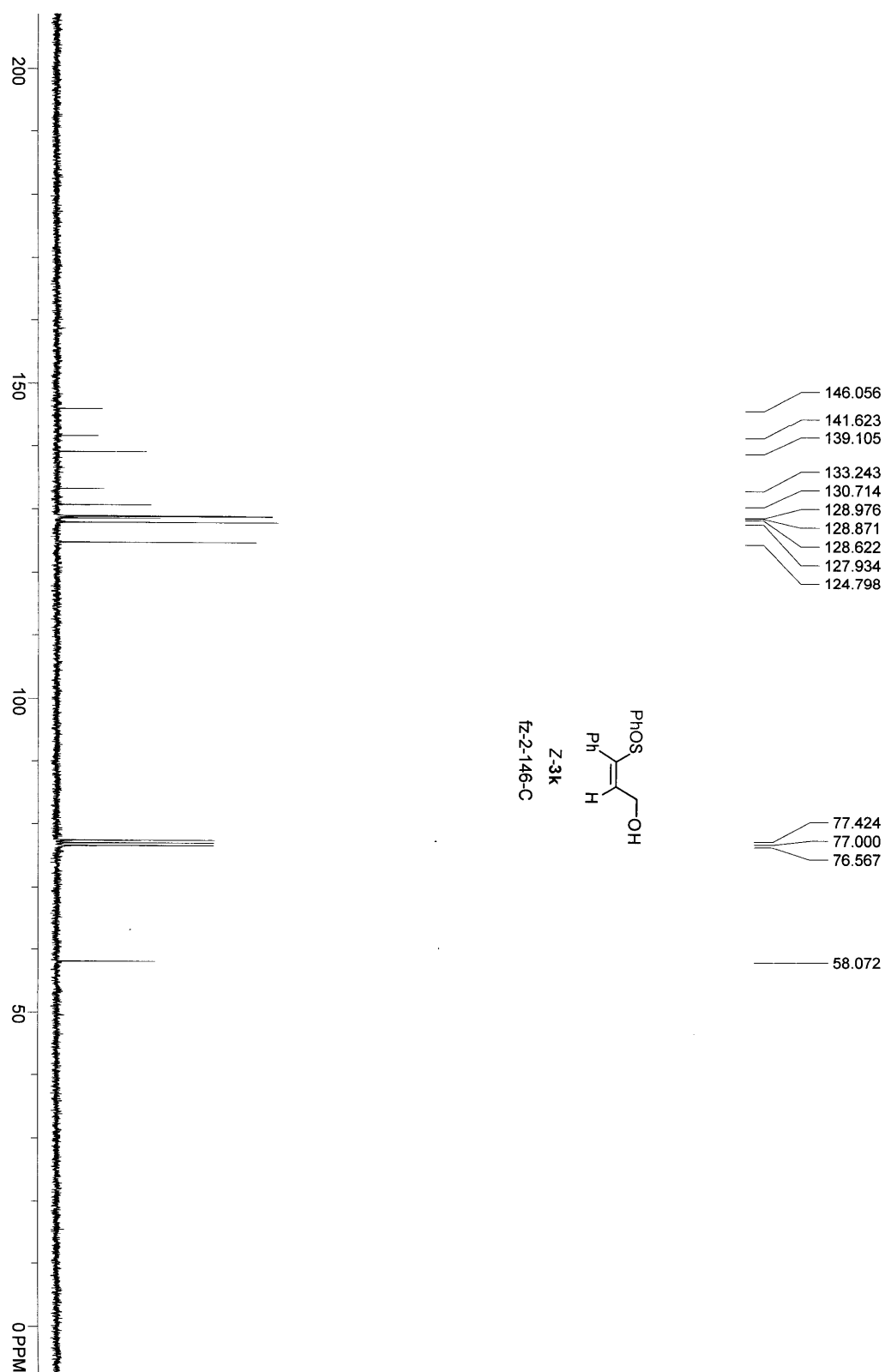


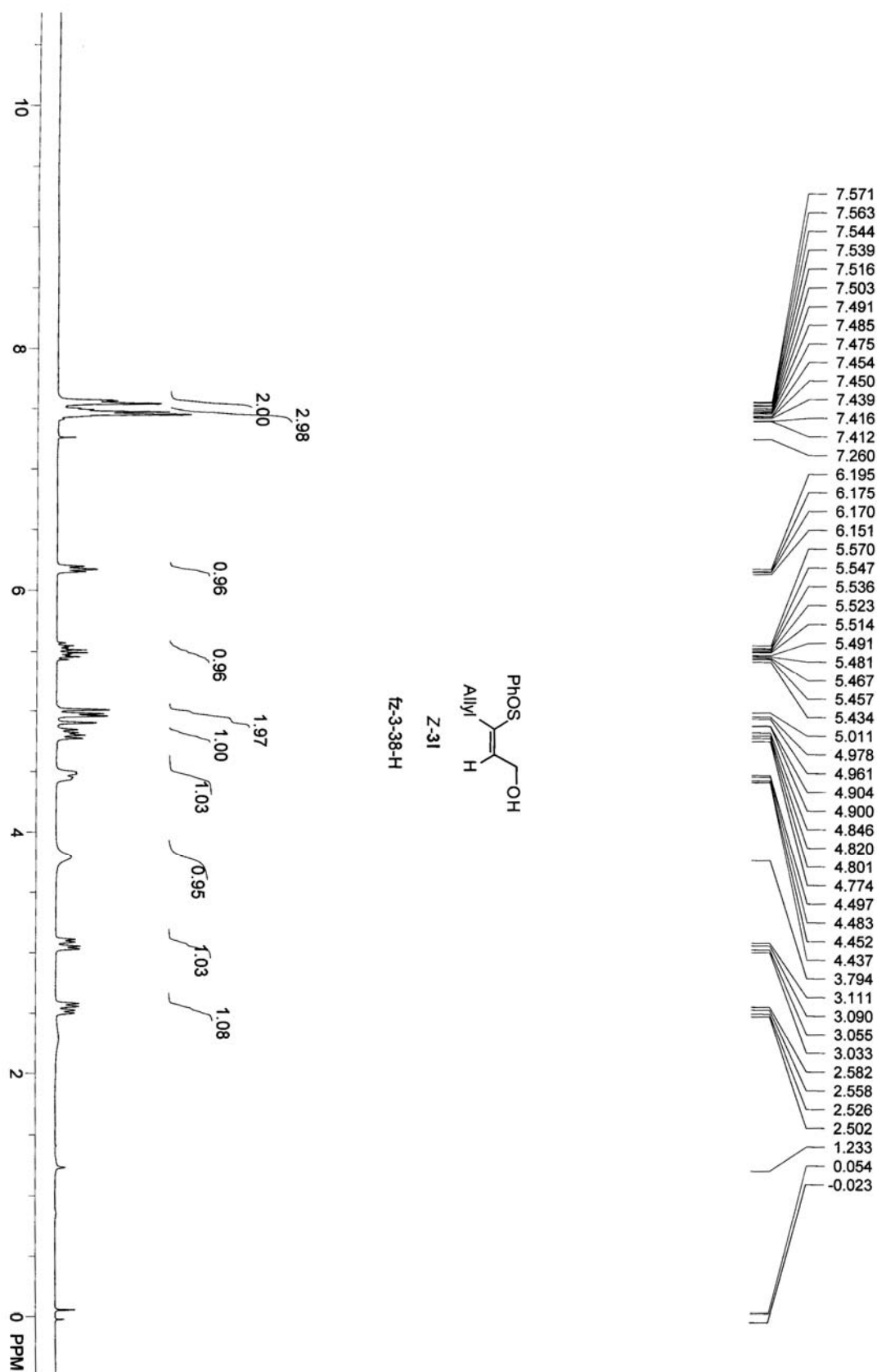


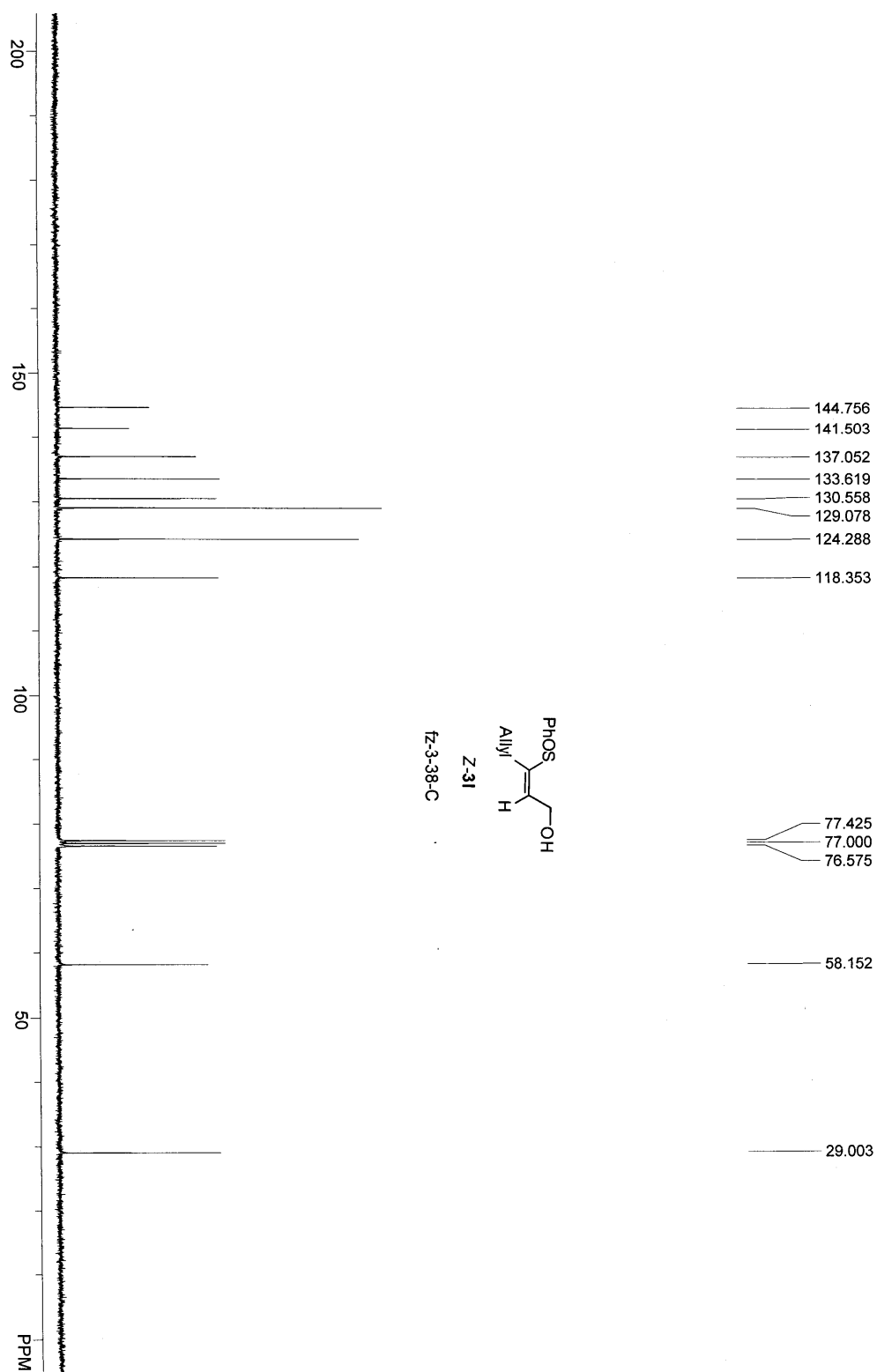


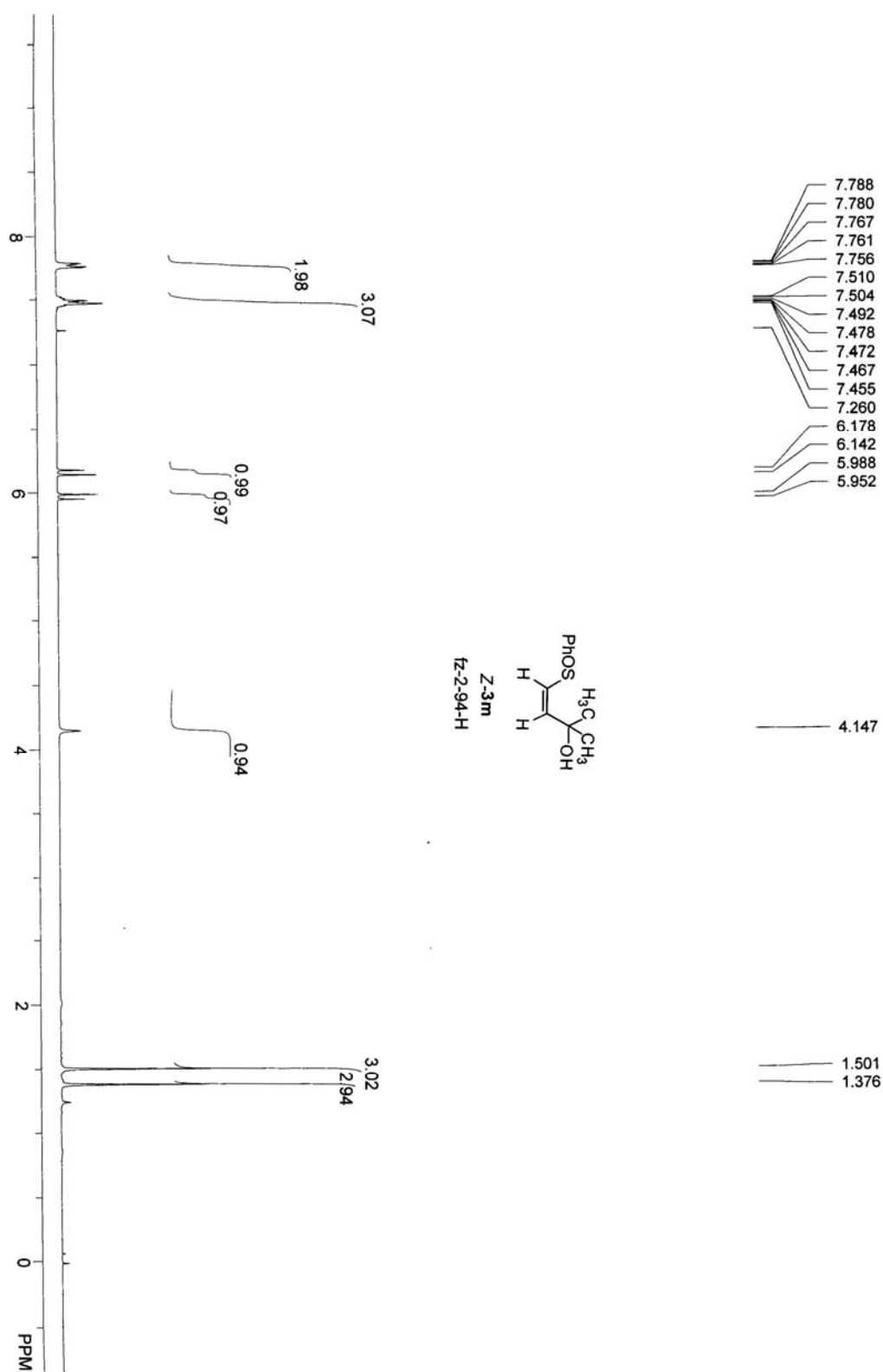


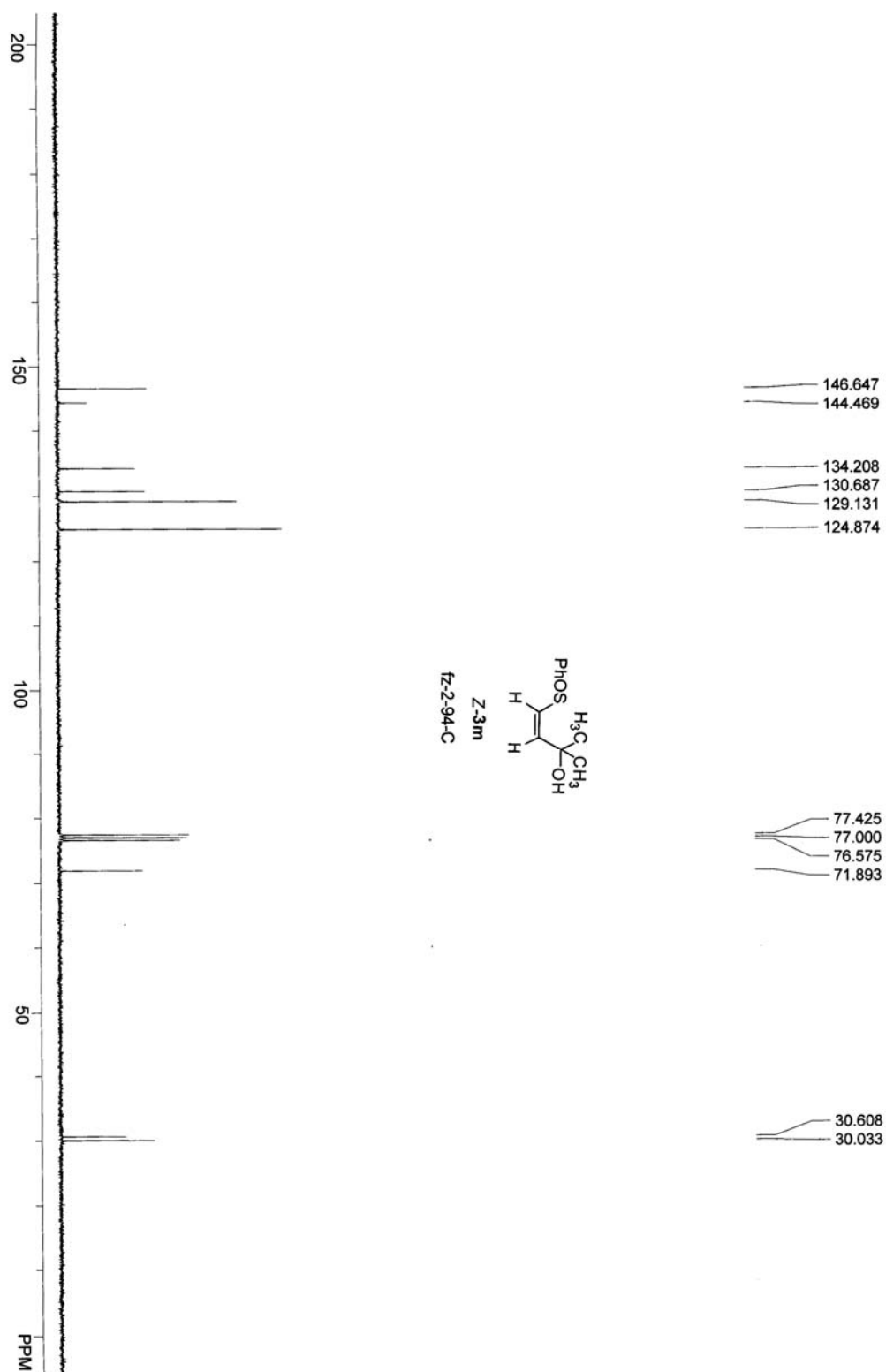


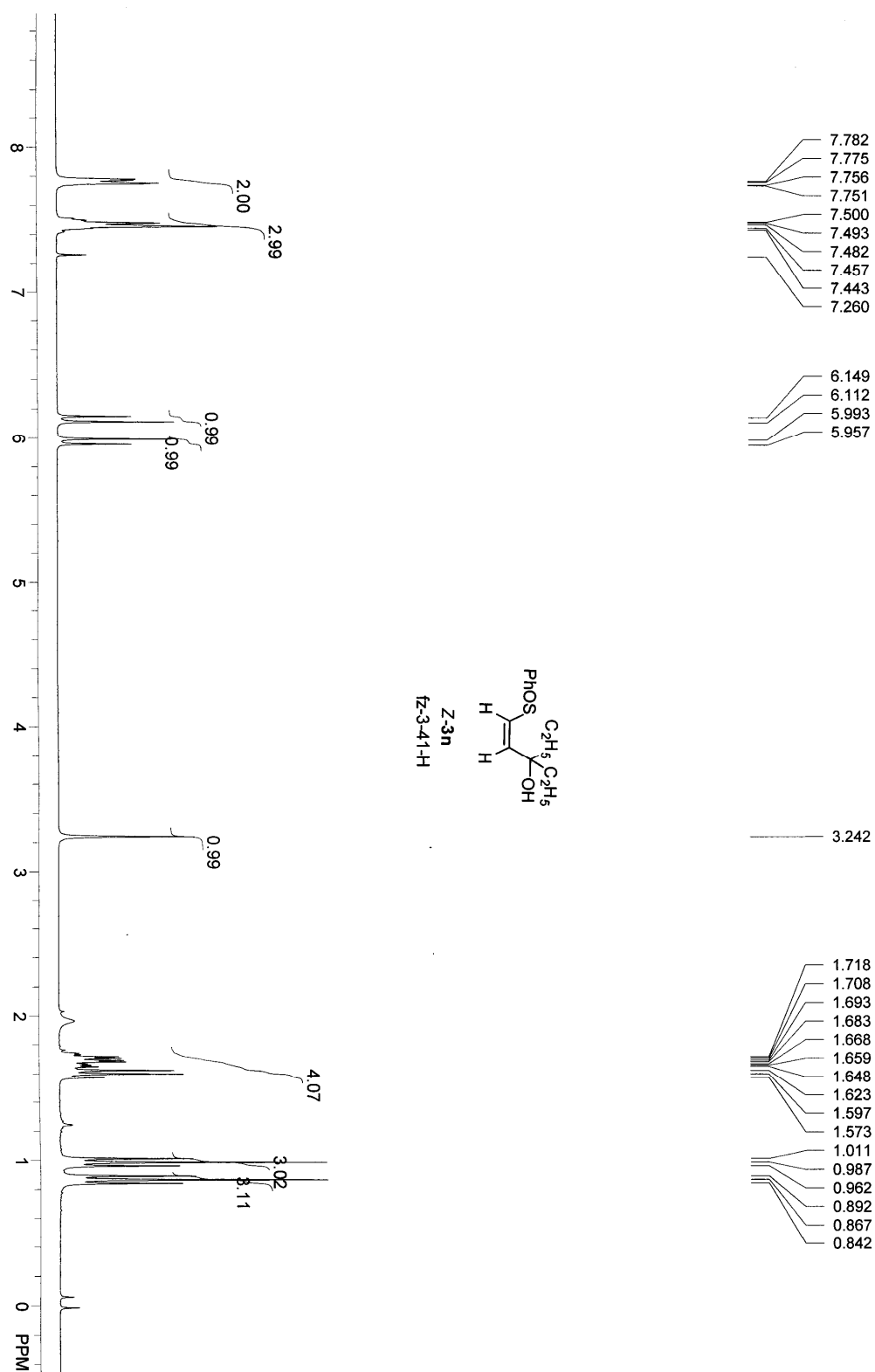


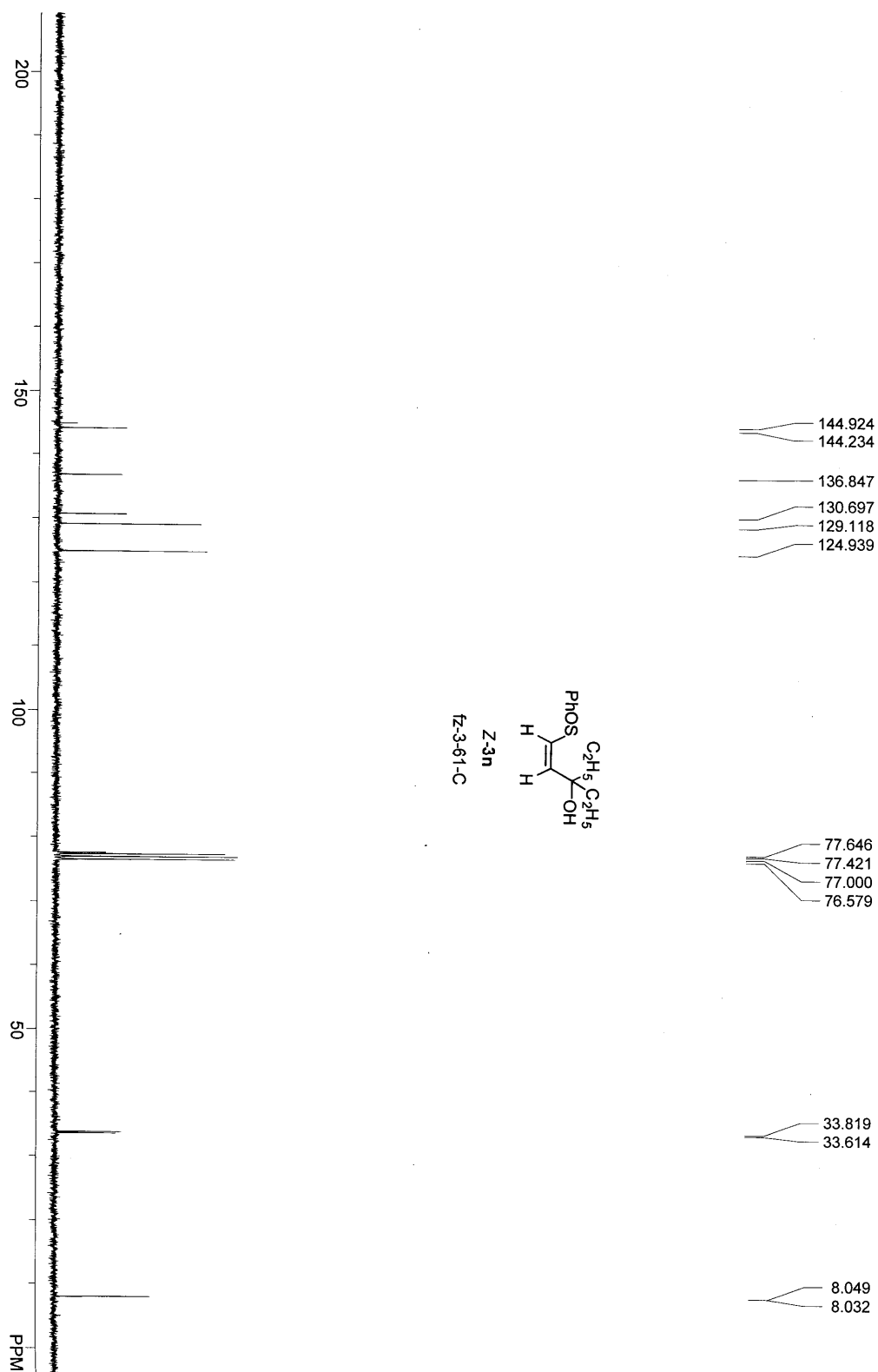


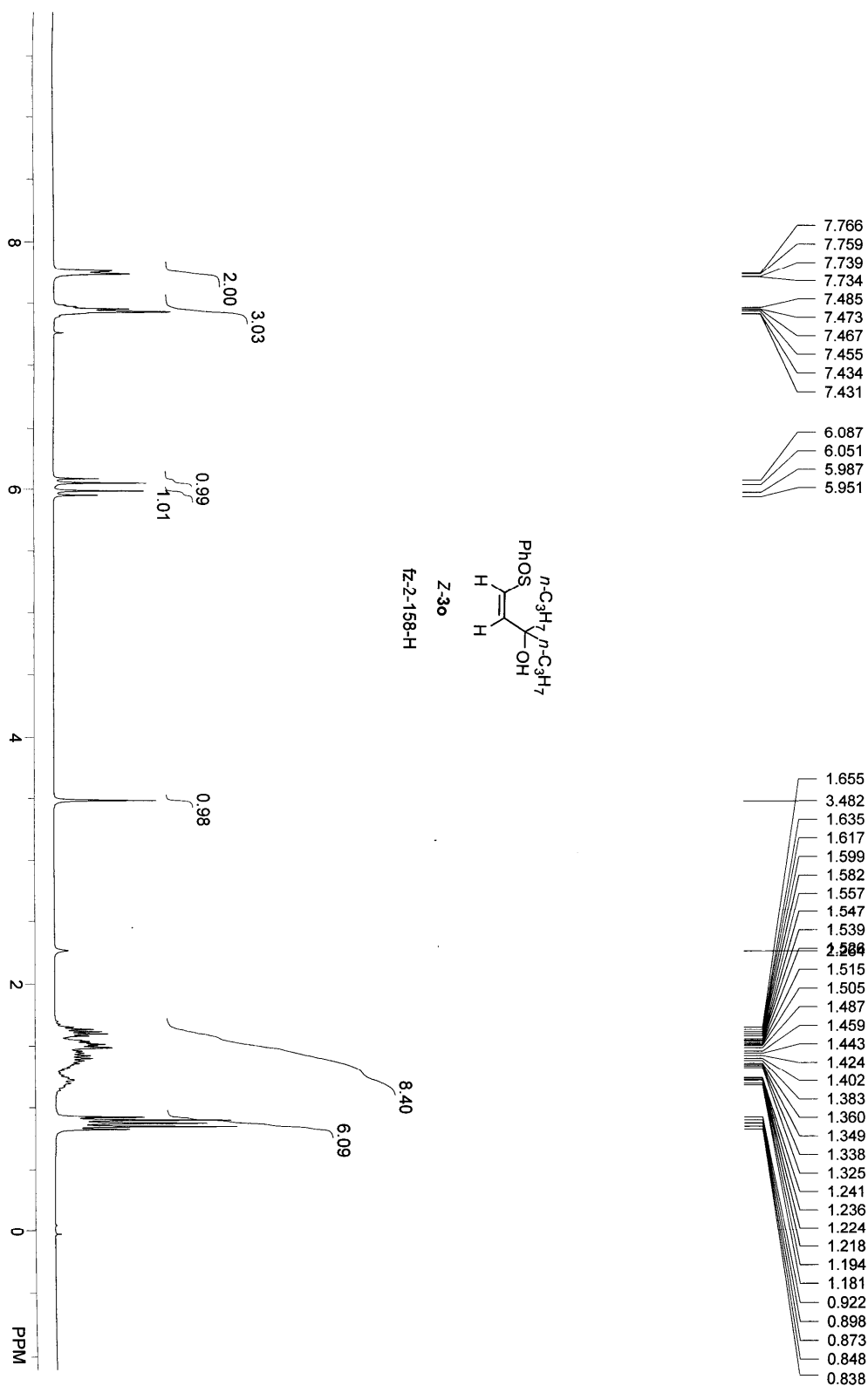


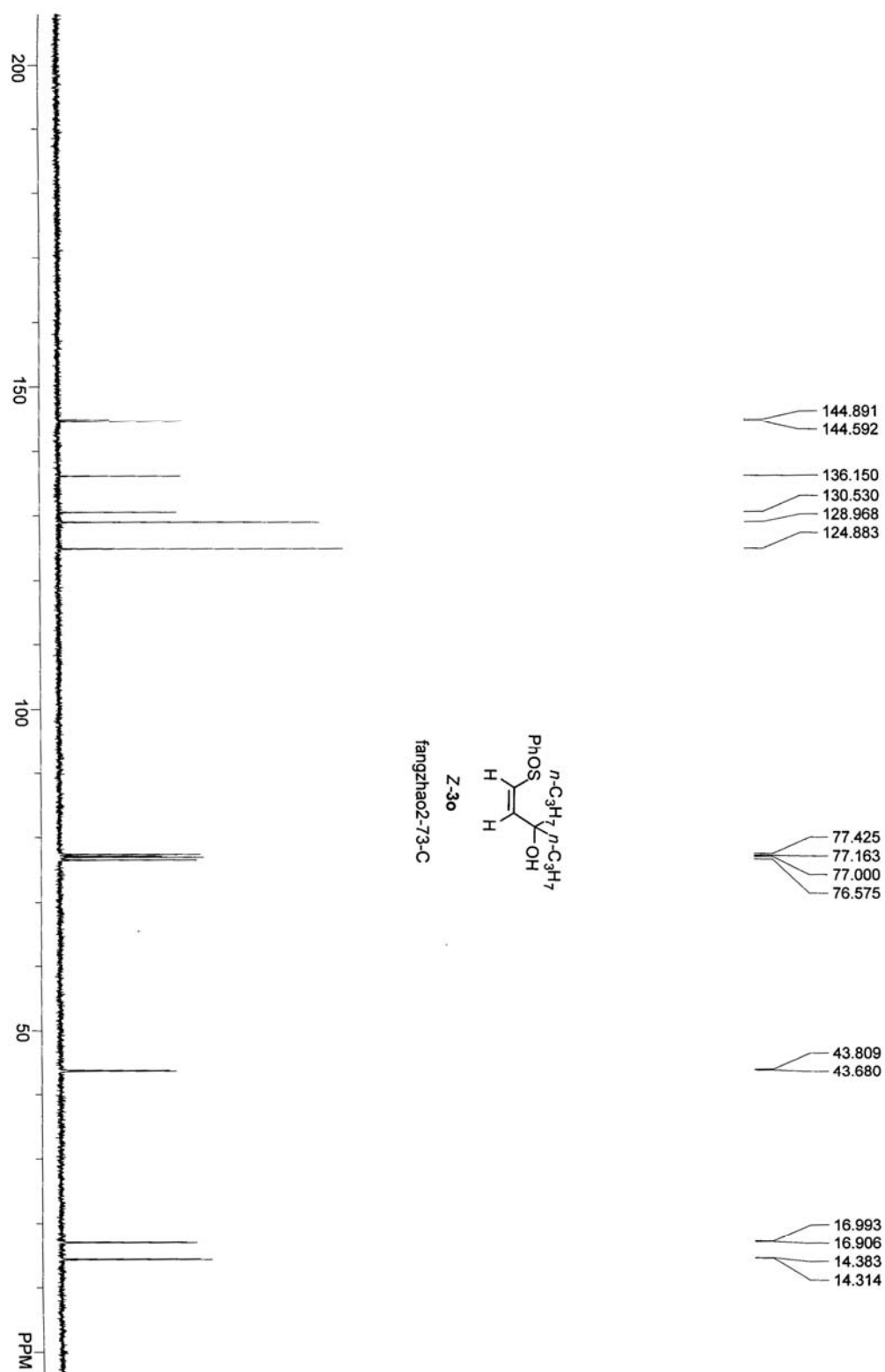


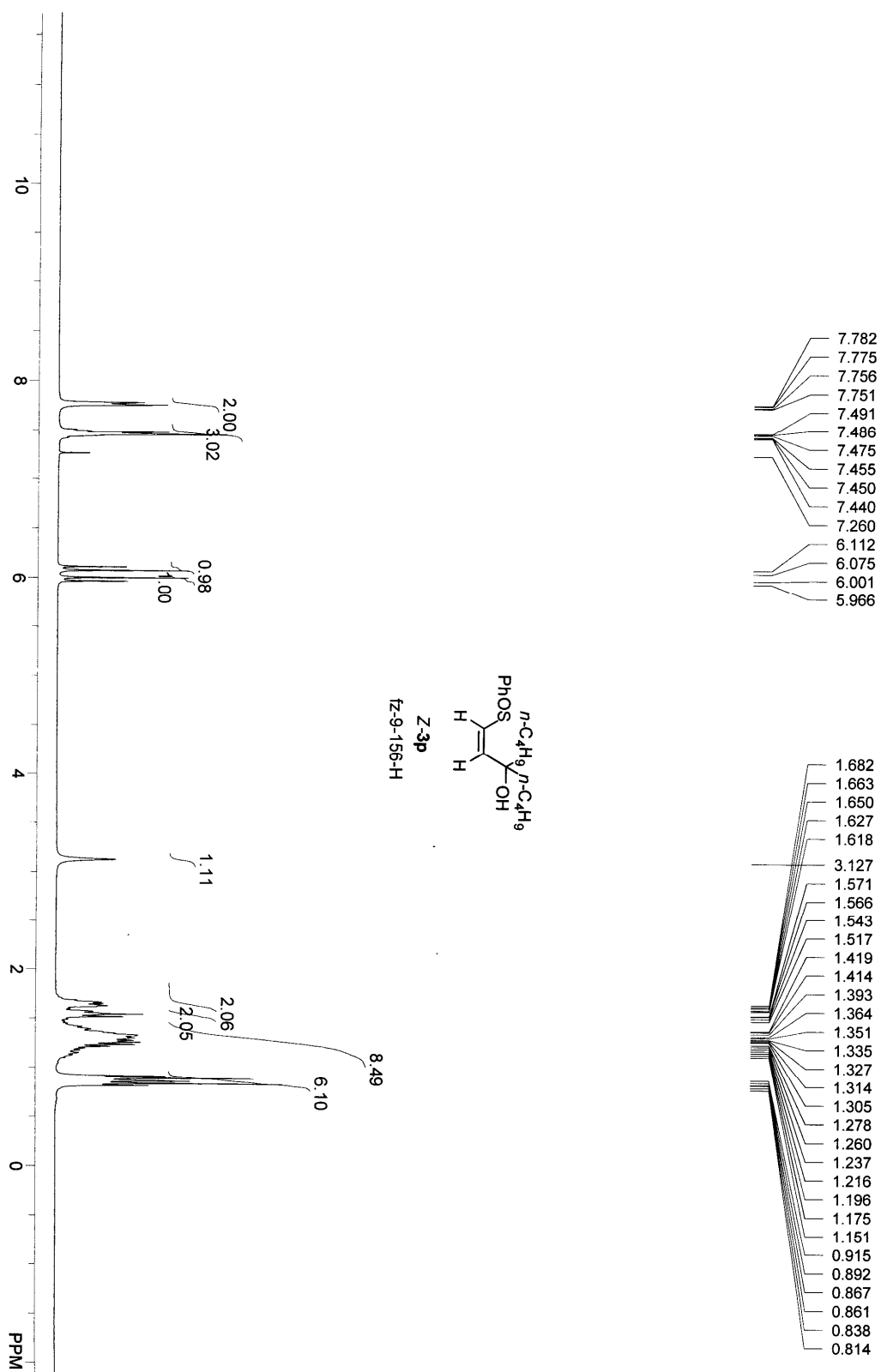


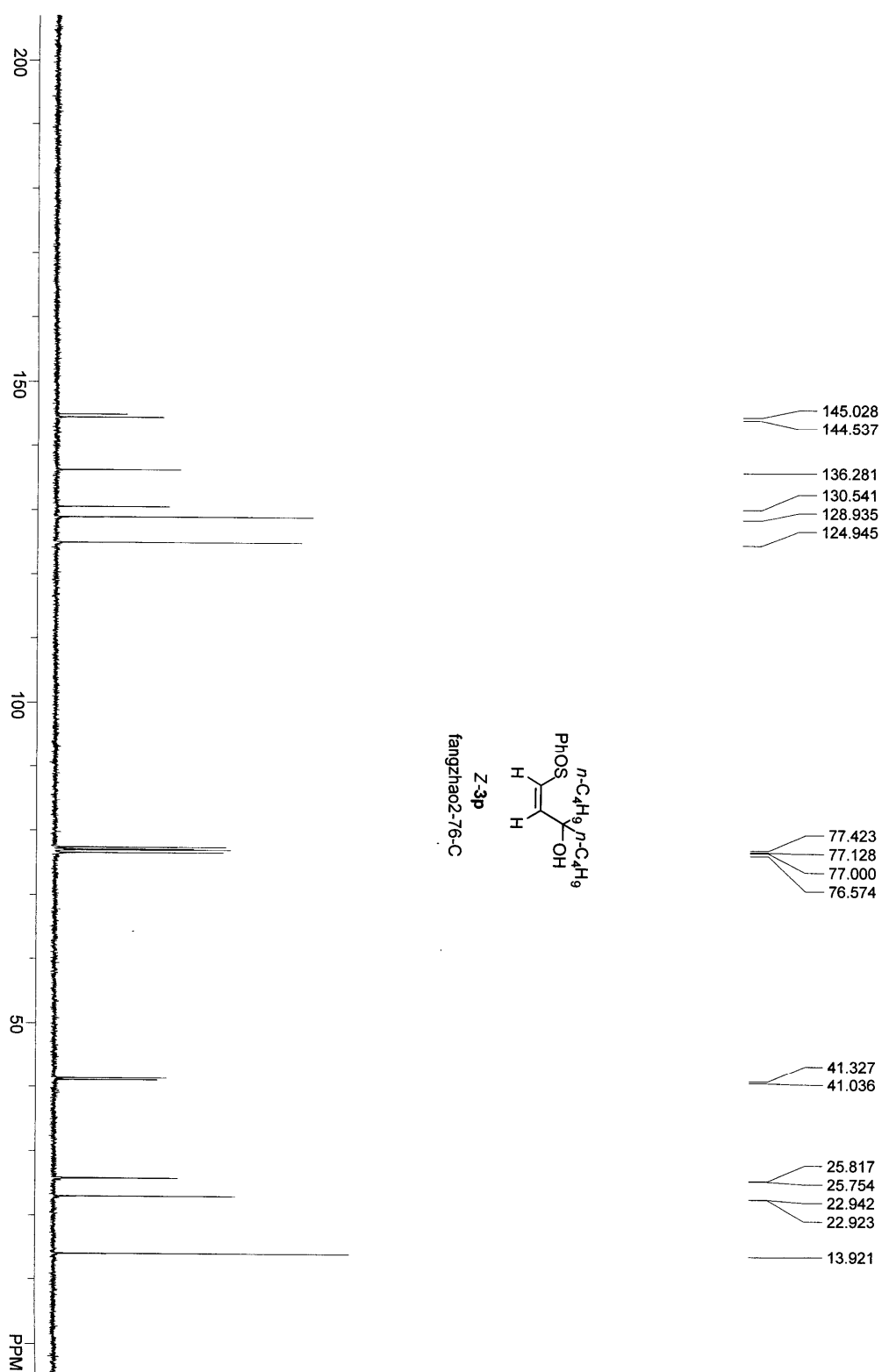


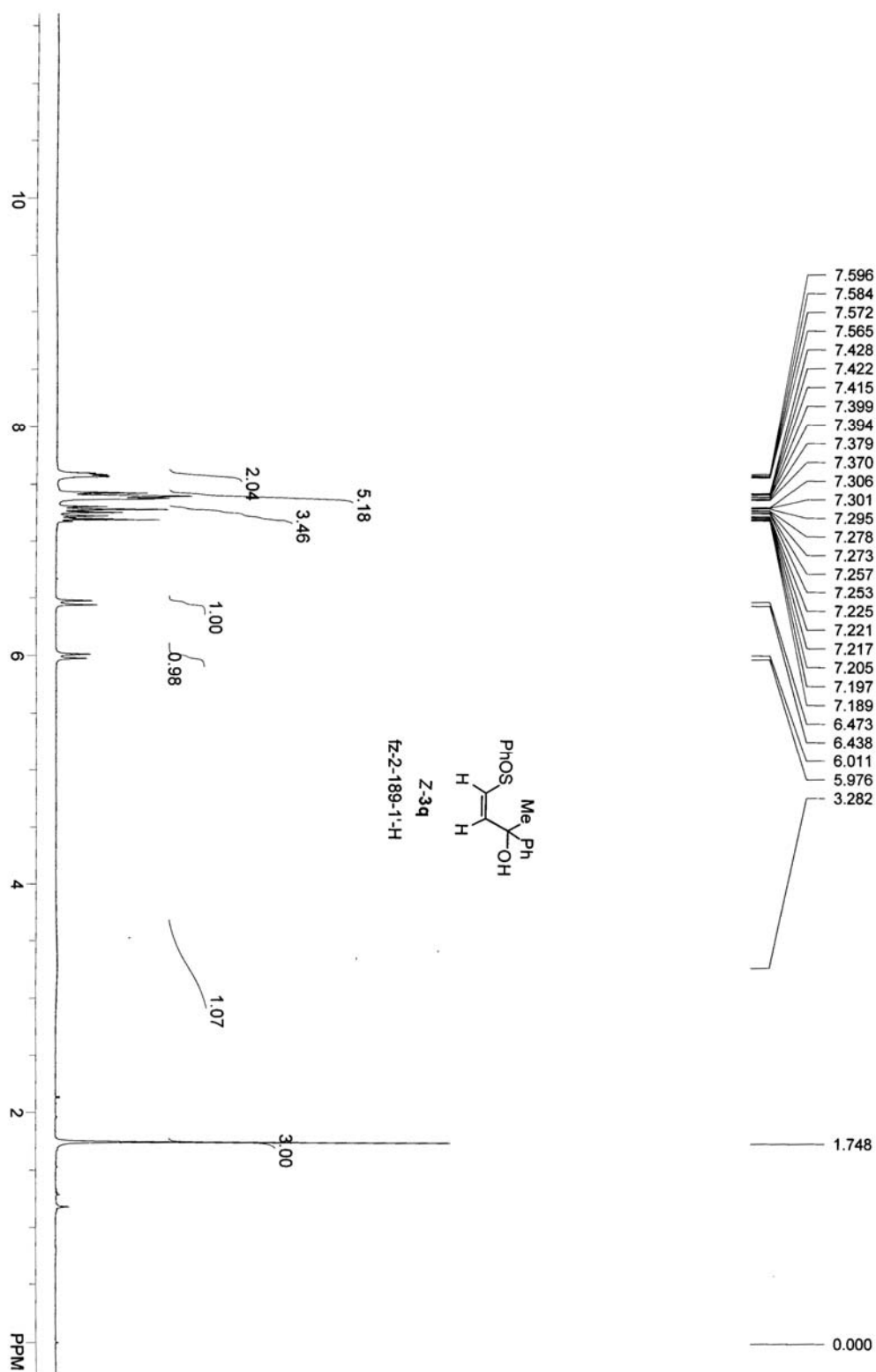


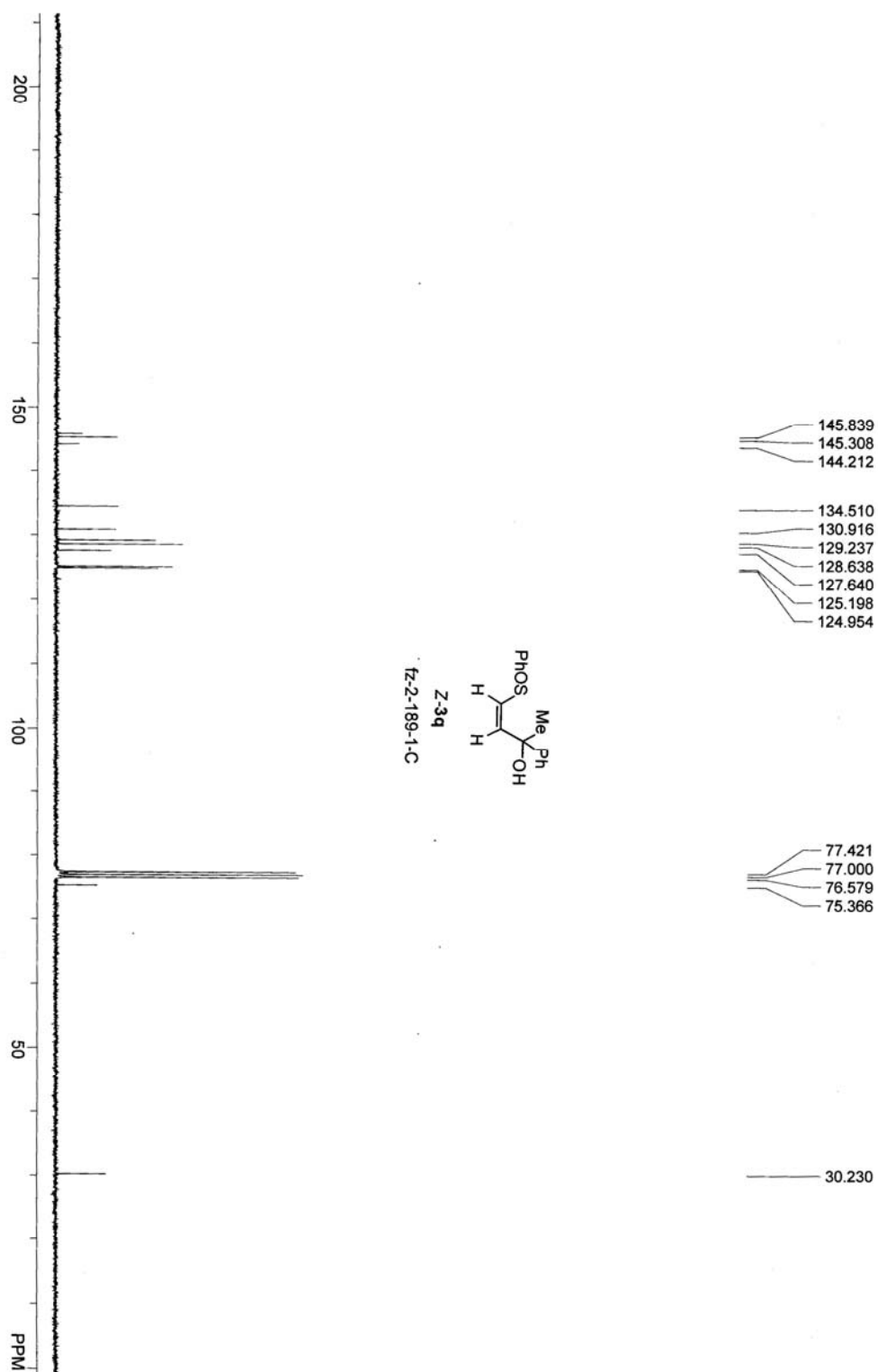


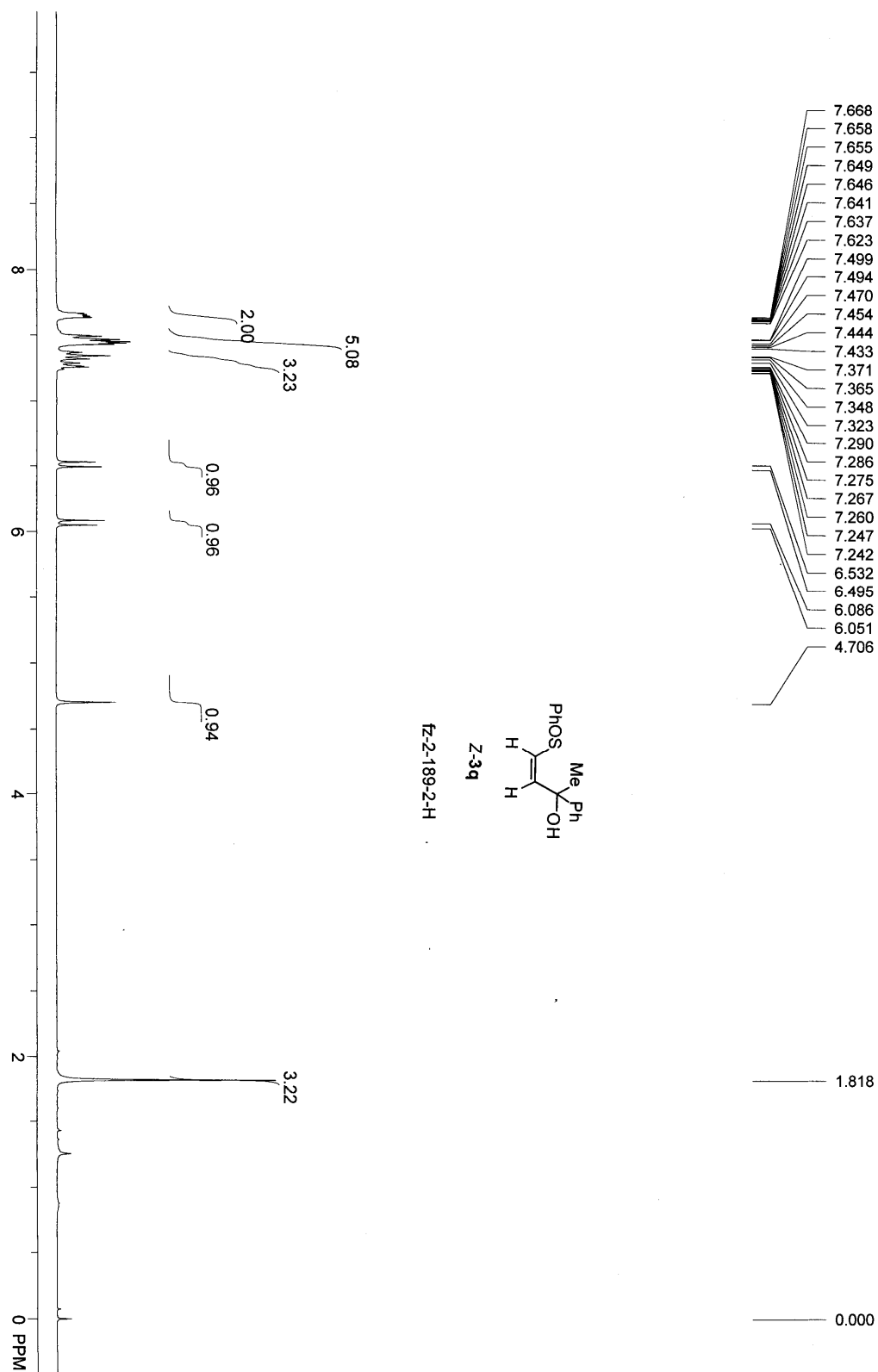


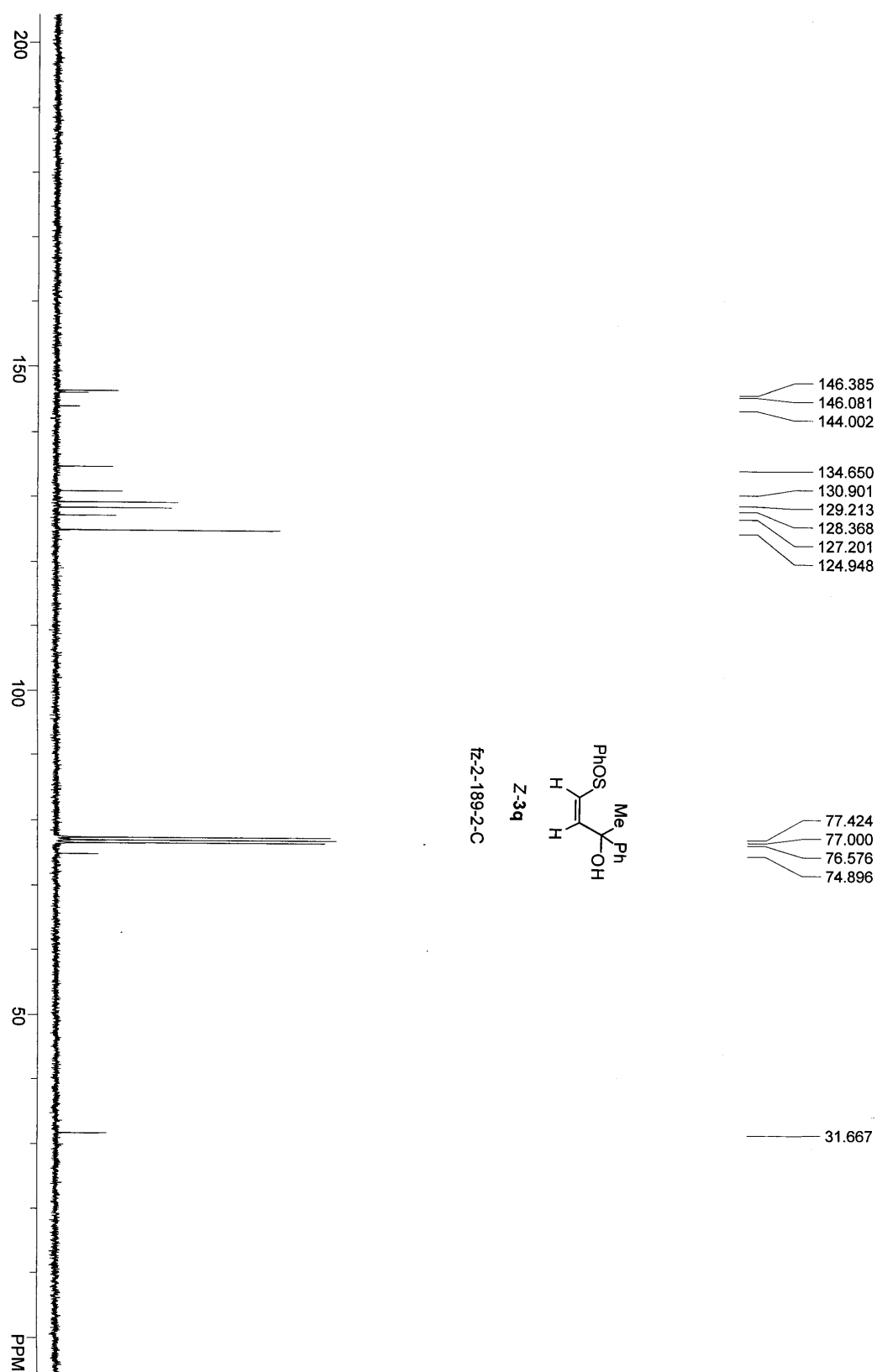


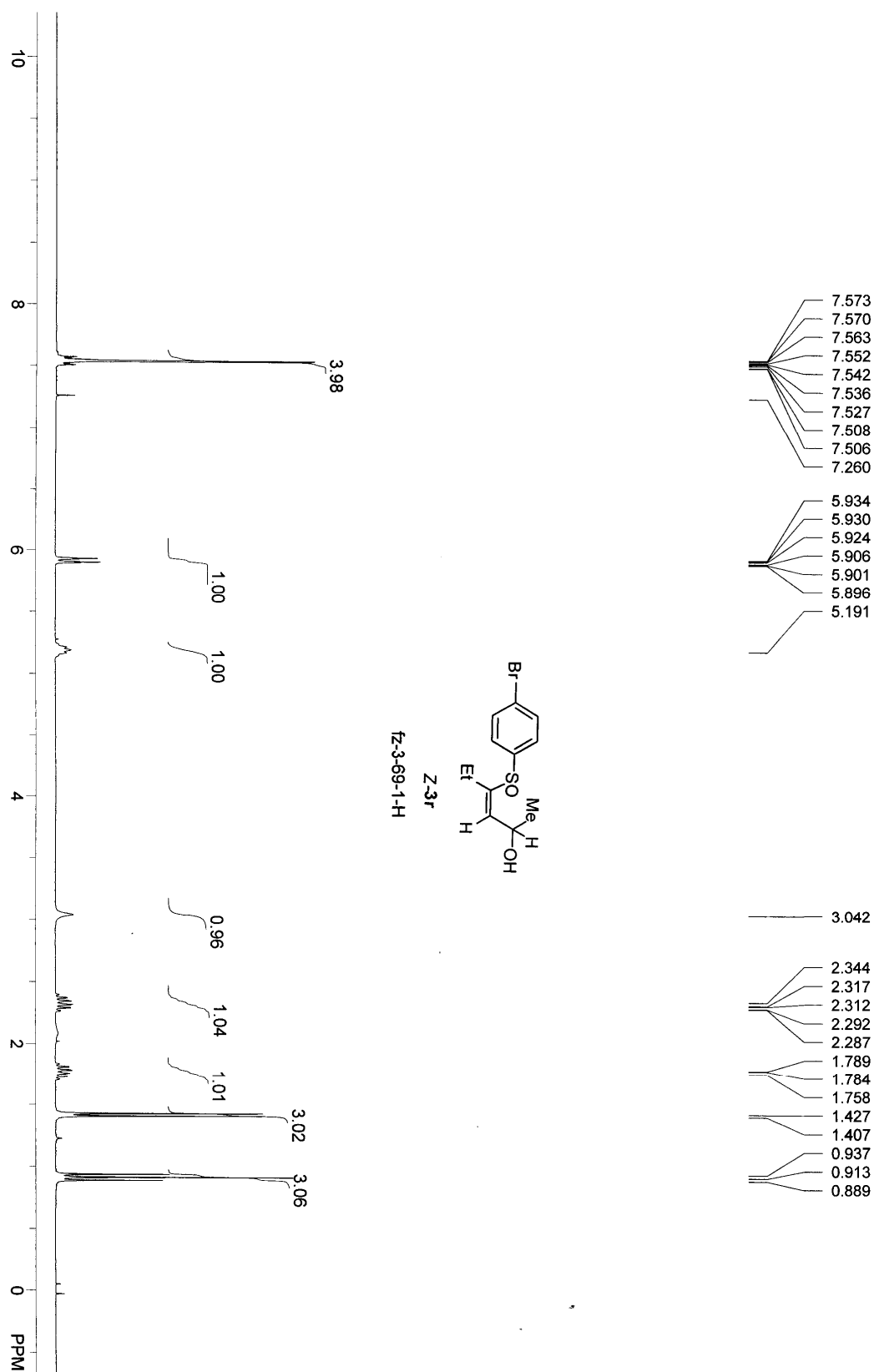


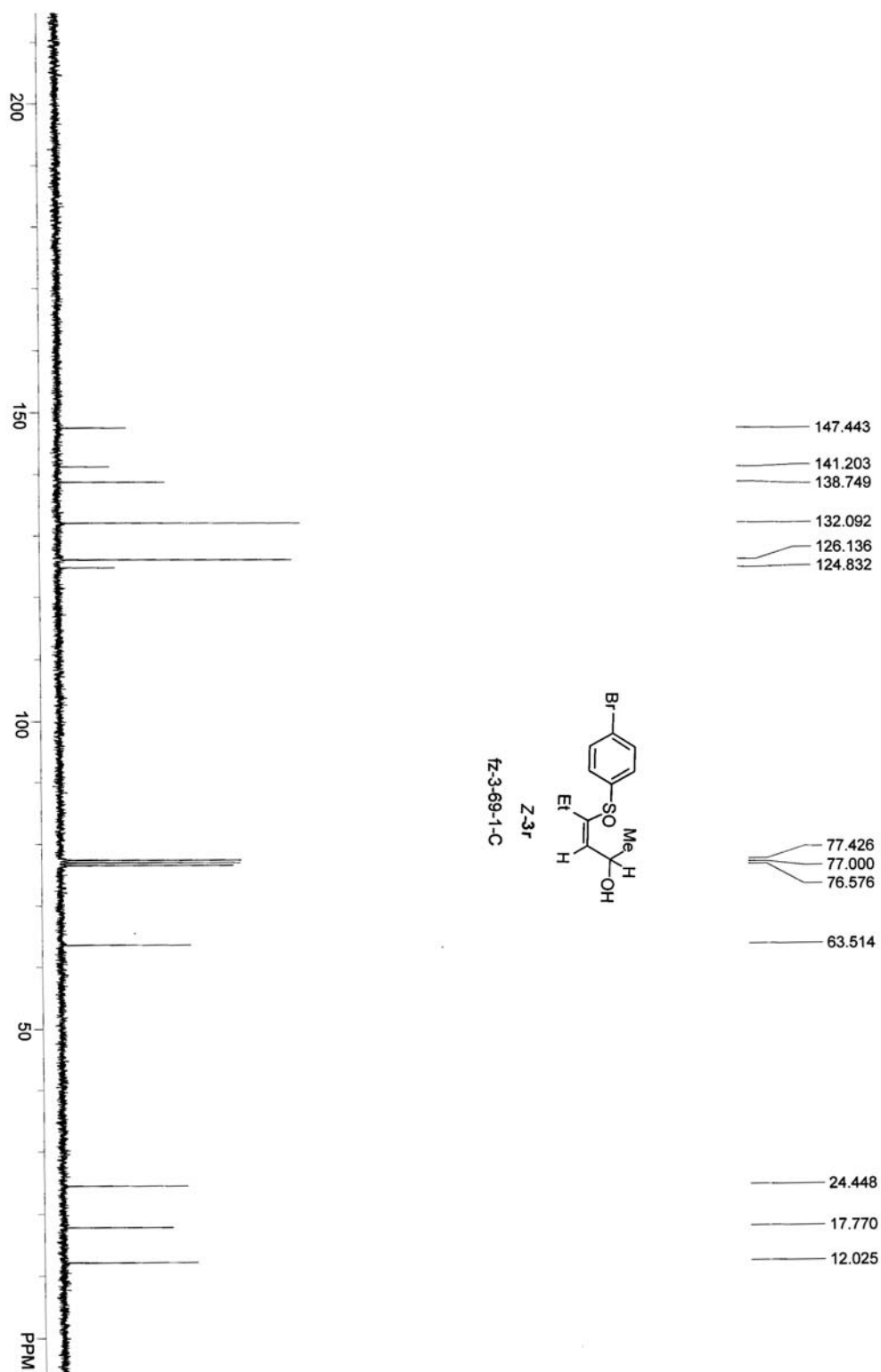


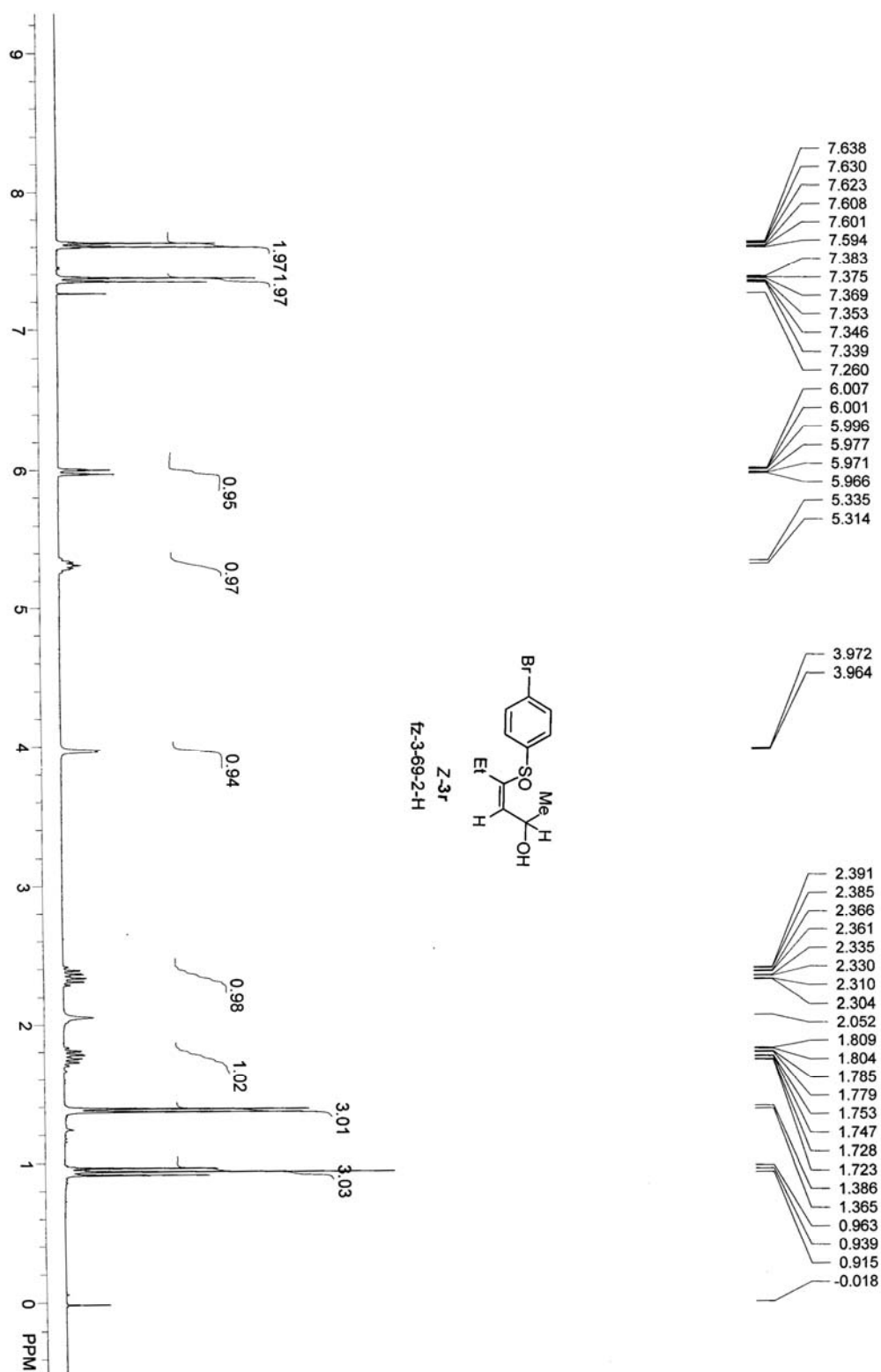


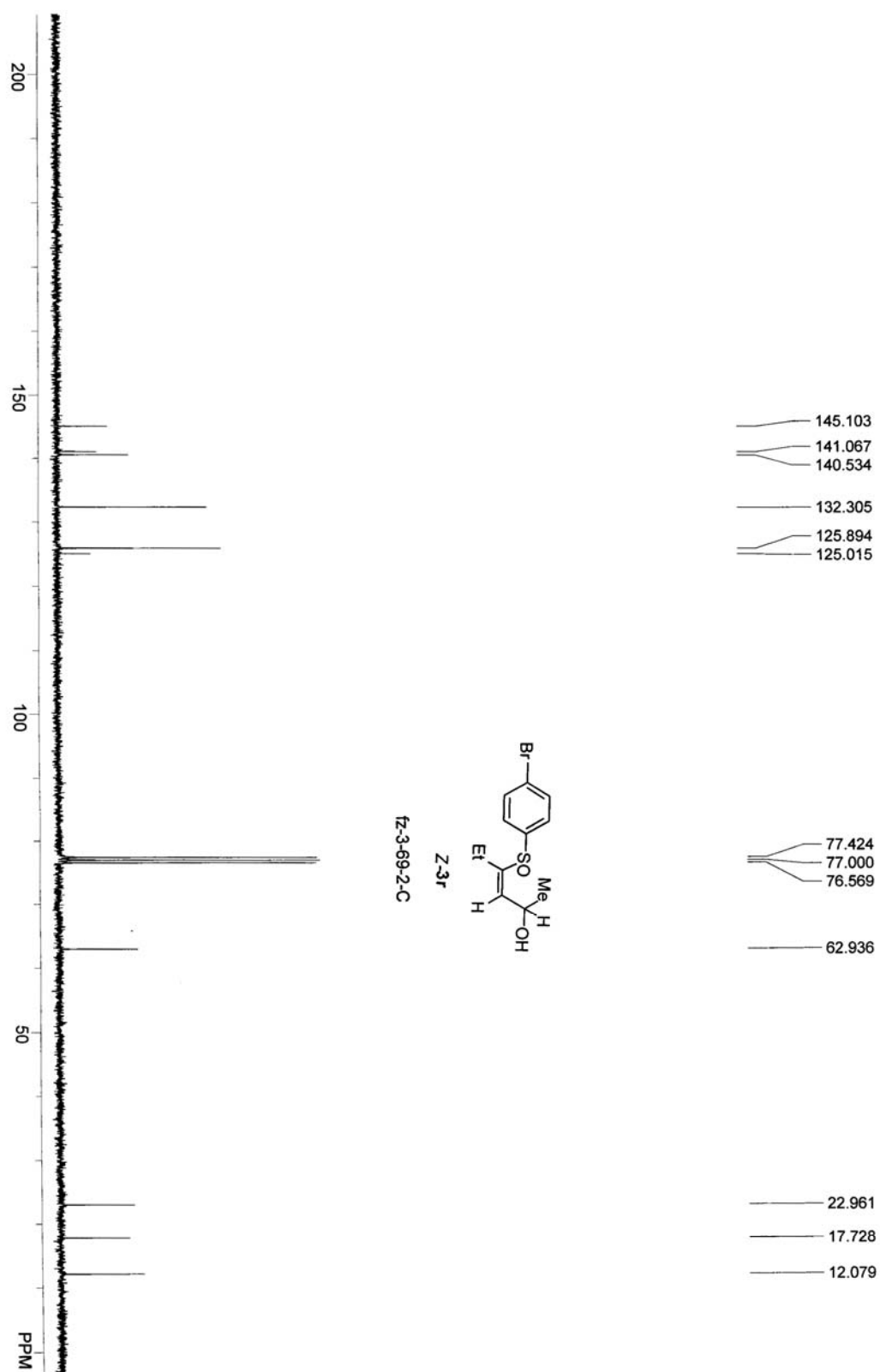


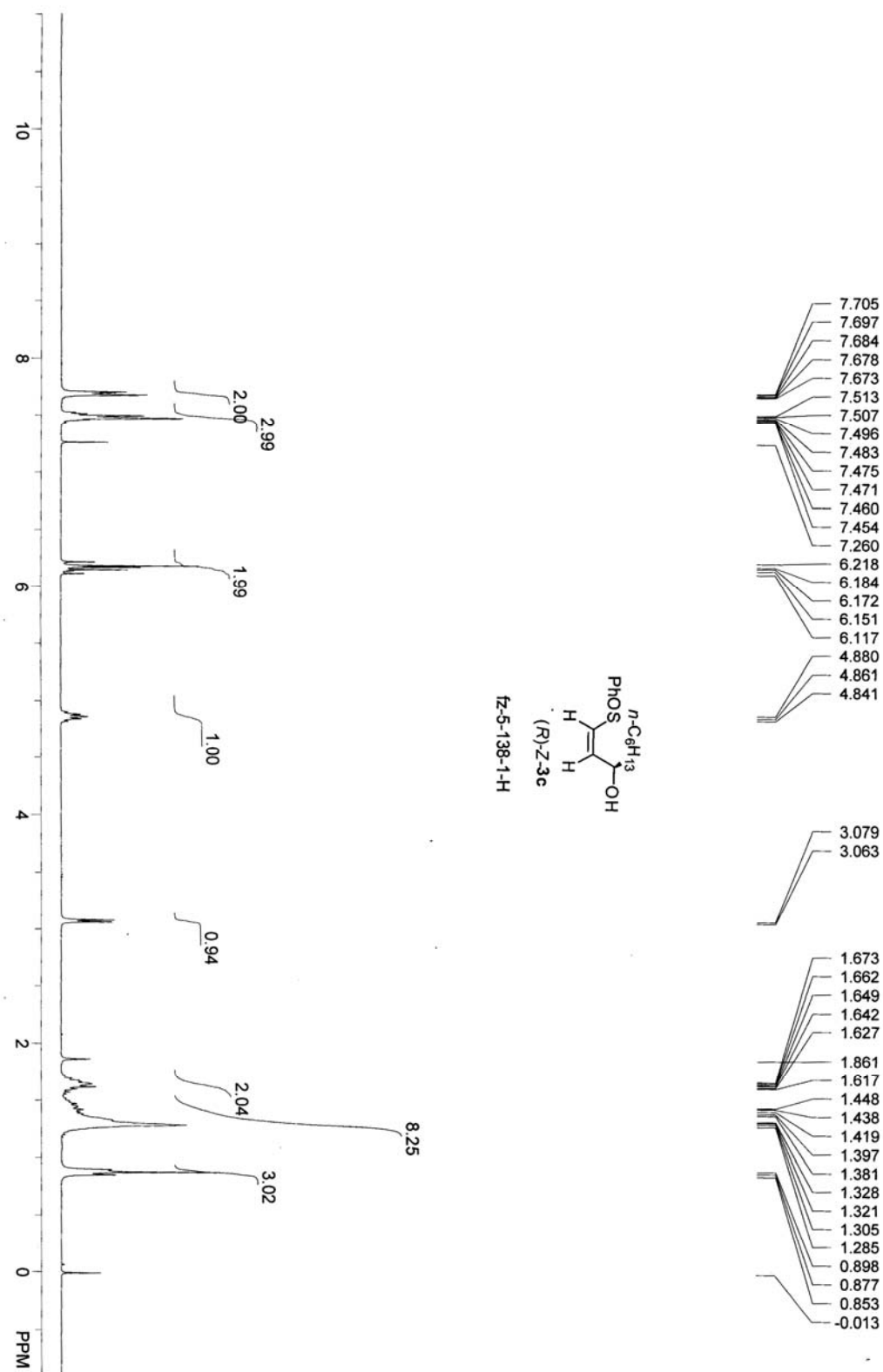


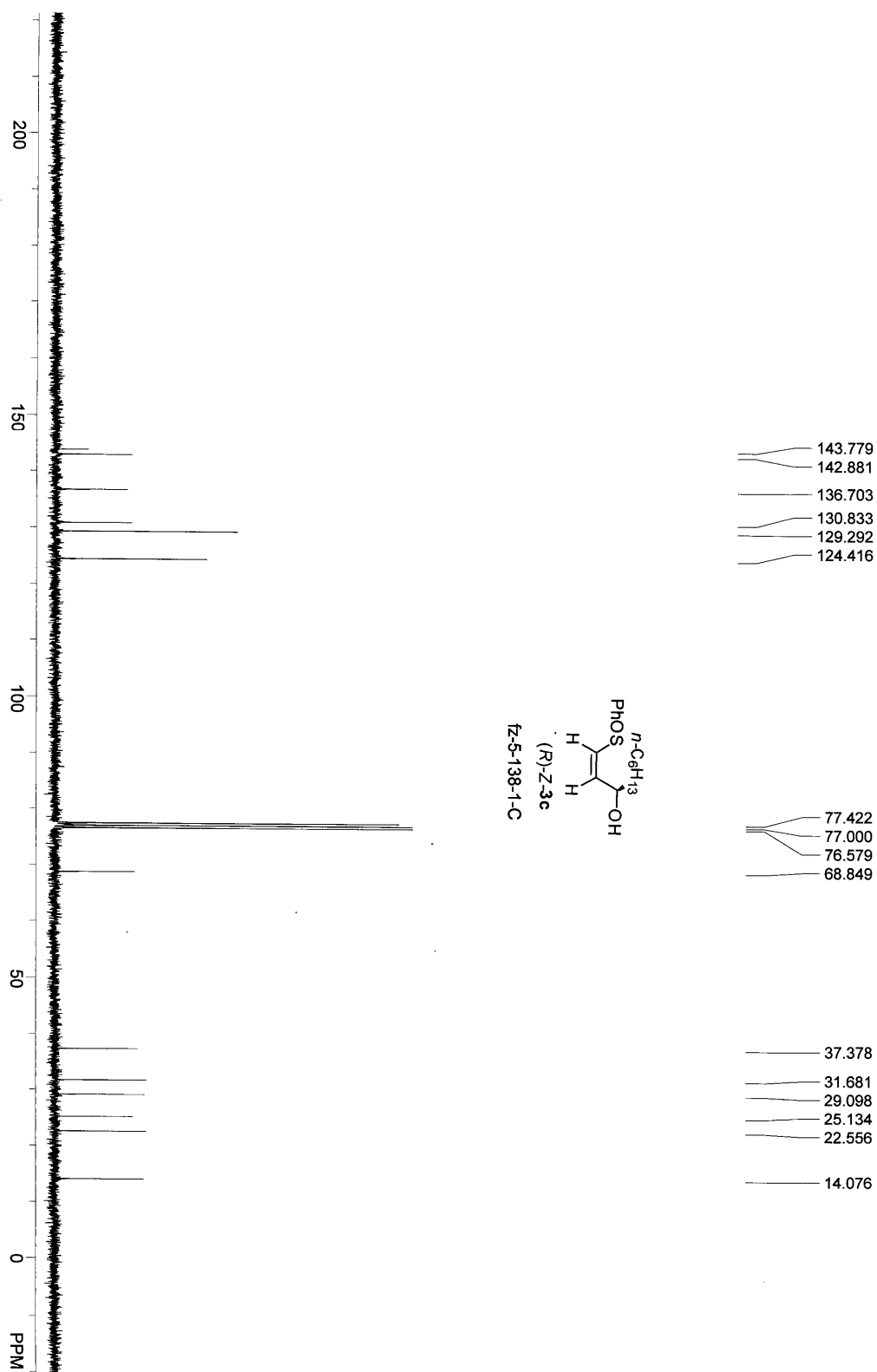










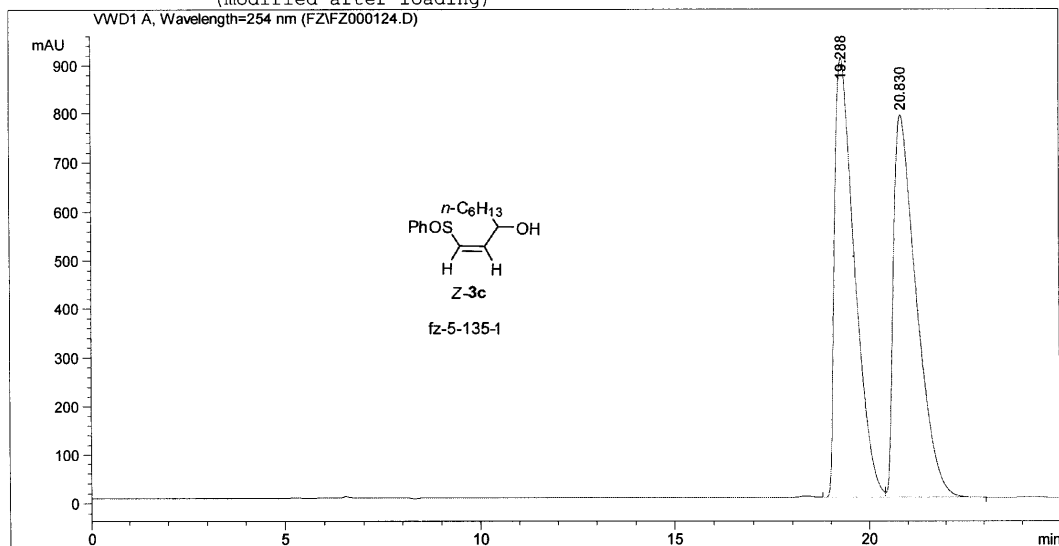


Data File D:\HPCHEM\1\DATA\FZ\FZ000124.D

Sample Name: fz-5-135-1

OJ-H; hexane/i-PrOH=95:5; 0.5 mL/min; 254nm

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Acq. Operator : fz
Method : D:\HPCHEM\1\DATA\LJ\LJ000012.D\DEF_XFX.M
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(modified after loading)



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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	19.288	VV	0.5474	3.24940e4	904.28009	49.7787
2	20.830	VB	0.6274	3.27829e4	784.40448	50.2213

Totals : 6.52770e4 1688.68457

Results obtained with enhanced integrator!

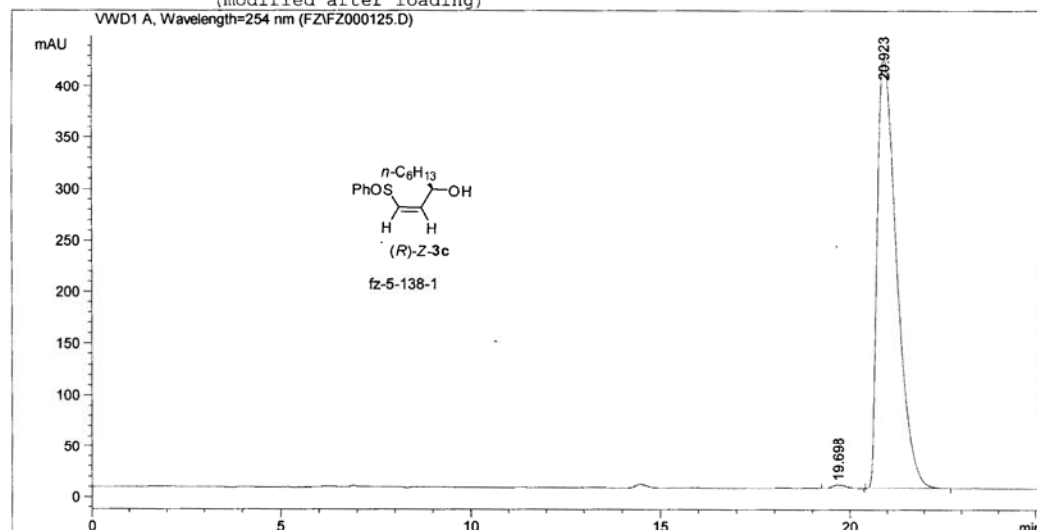
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Data File D:\HPCHEM\1\DATA\FZ\FZ000125.D

Sample Name: fz-5-138-1

OJ-H; hexane/i-PrOH=95:5; 0.5 mL/min; 254nm

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Injection Date   : 3/1/2009 12:18:20 PM
Sample Name      : fz-5-138-1                Location :   -
Acq. Operator    : fz
Method           : D:\HPCHEM\1\DATA\LJ\LJ000012.D\DEF_XFX.M
Last changed     : 3/1/2009 10:34:17 AM by fz
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Area Percent Report

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Sorted By       :      Signal
Multiplier      :      1.0000
Dilution        :      1.0000
Use Multiplier & Dilution Factor with ISTDs
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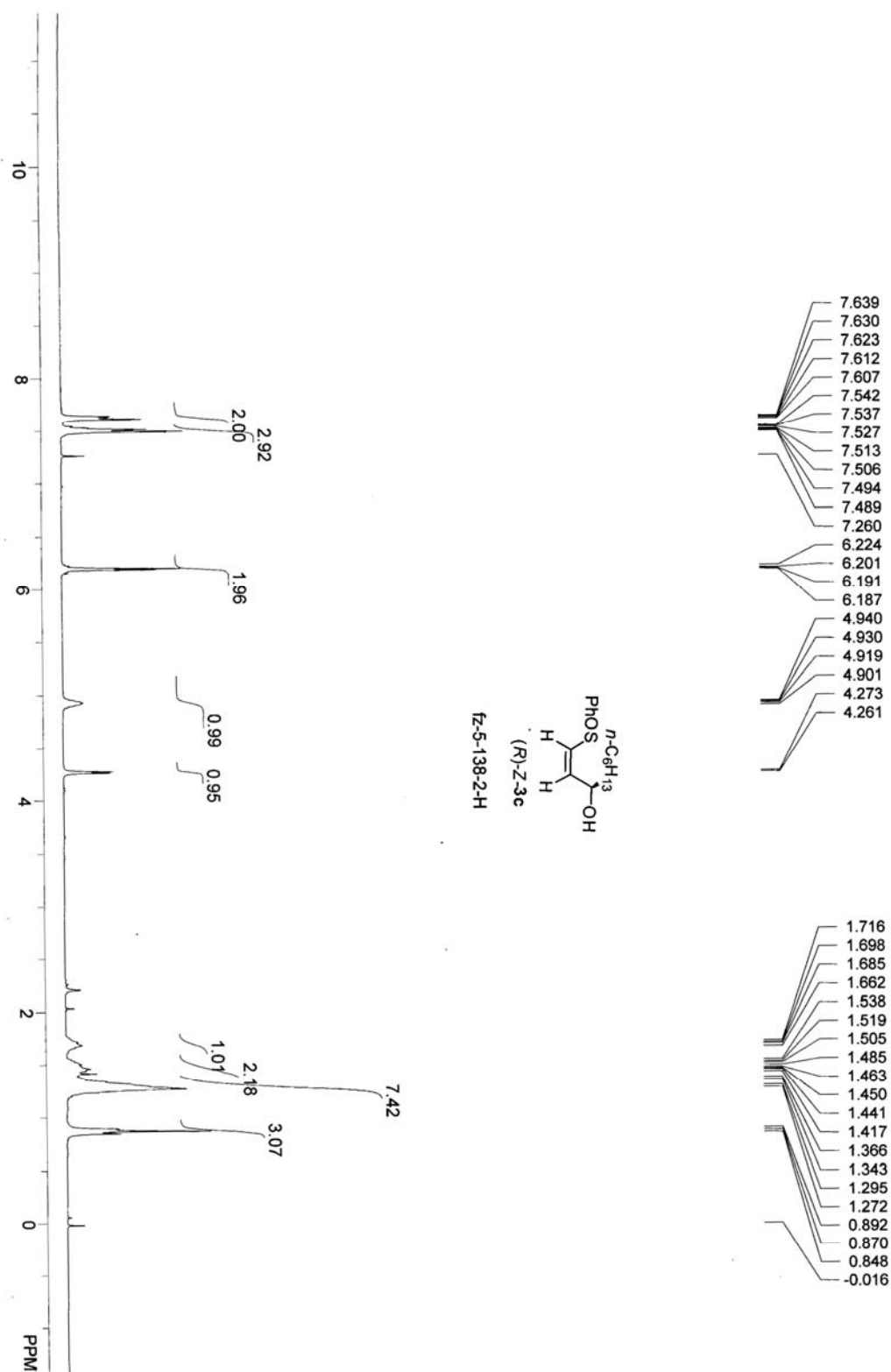
Signal 1: VWD1 A, Wavelength=254 nm

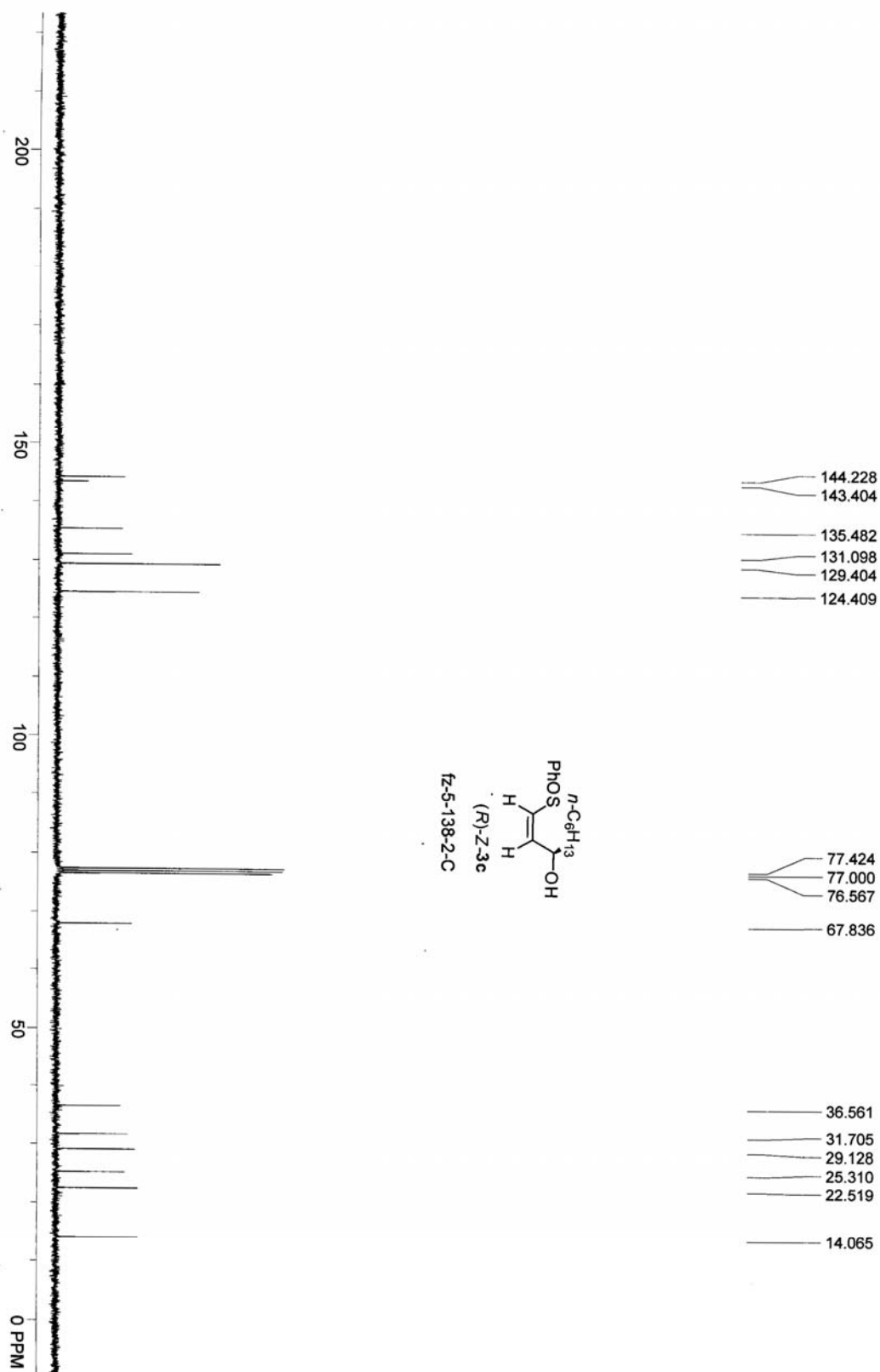
Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	19.698	BP	0.3847	86.11472	3.34642	0.5620
2	20.923	BB	0.5565	1.52356e4	419.24820	99.4380

Totals : 1.53217e4 422.59462

Results obtained with enhanced integrator!

*** End of Report ***



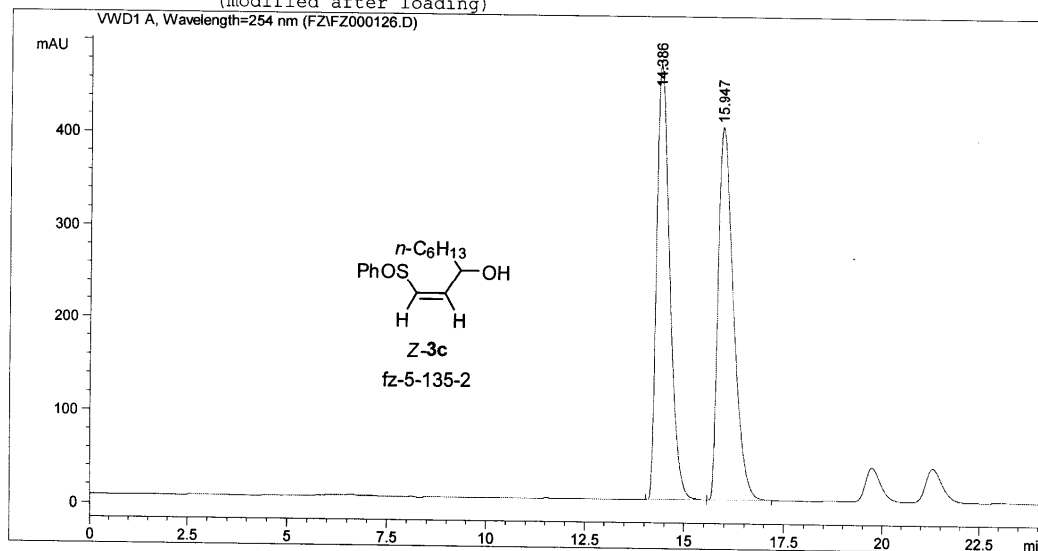


Data File D:\HPCHEM\1\DATA\FZ\FZ000126.D

Sample Name: fz-5-135-2

OJ-H; hexane/i-PrOH=95:5; 0.5 mL/min; 254nm

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Acq. Operator : fz
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(modified after loading)



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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.386	PB	0.3508	1.07082e4	469.04782	50.0115
2	15.947	BB	0.4077	1.07032e4	400.78946	49.9885

Totals : 2.14114e4 869.83728

Results obtained with enhanced integrator!

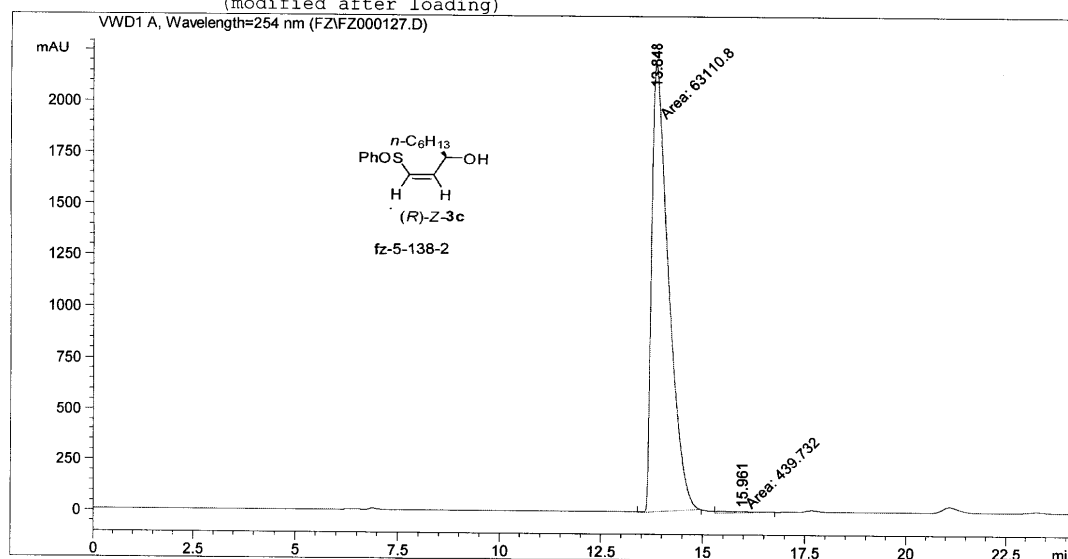
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Data File D:\HPCHEM\1\DATA\FZ\FZ000127.D

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OJ-H; hexane/i-PrOH=95:5; 0.5 mL/min; 254nm

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Area Percent Report

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Multiplier      : 1.0000
Dilution        : 1.0000
Use Multiplier & Dilution Factor with ISTDs
=====
```

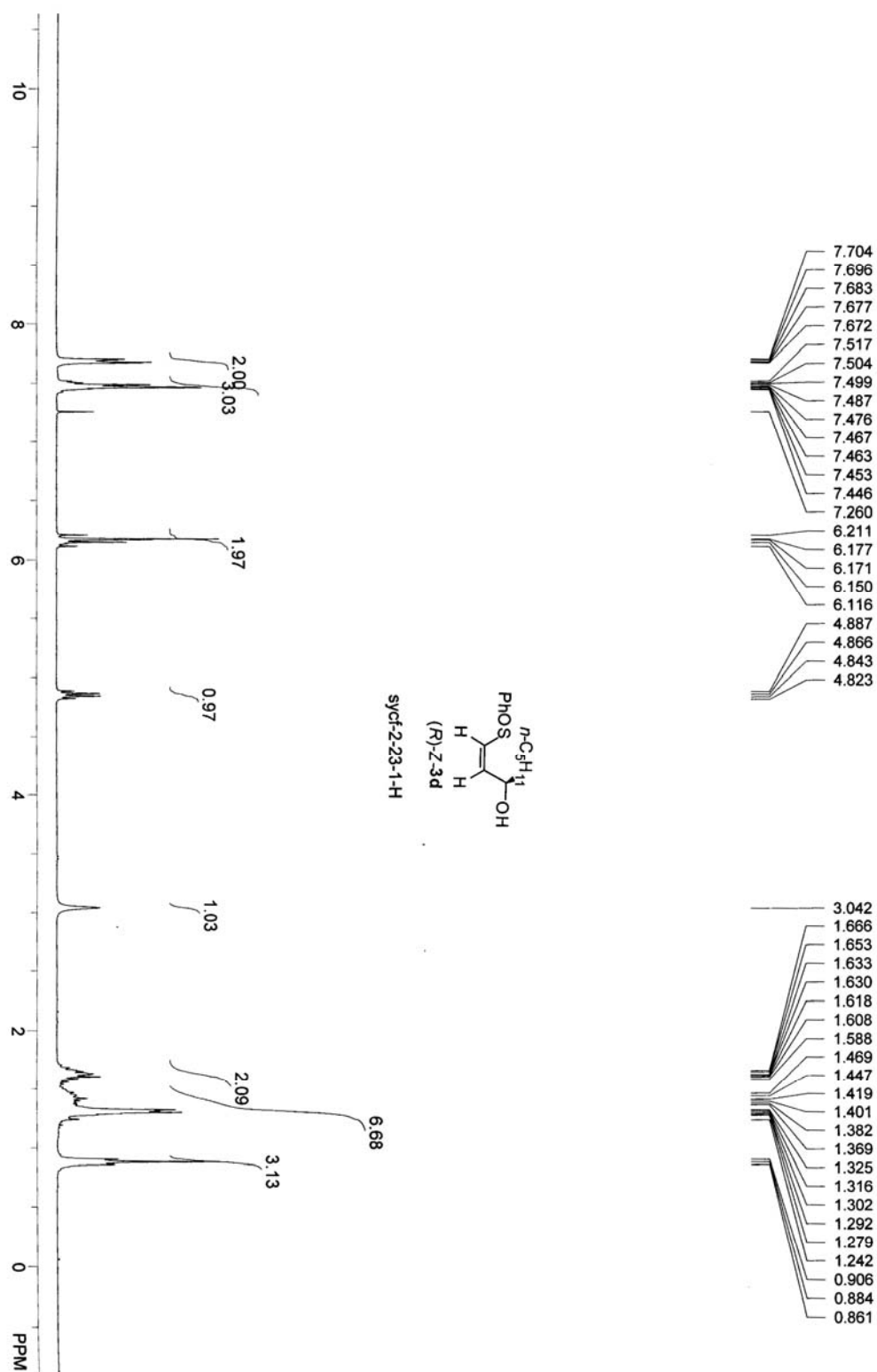
Signal 1: VWD1 A, Wavelength=254 nm

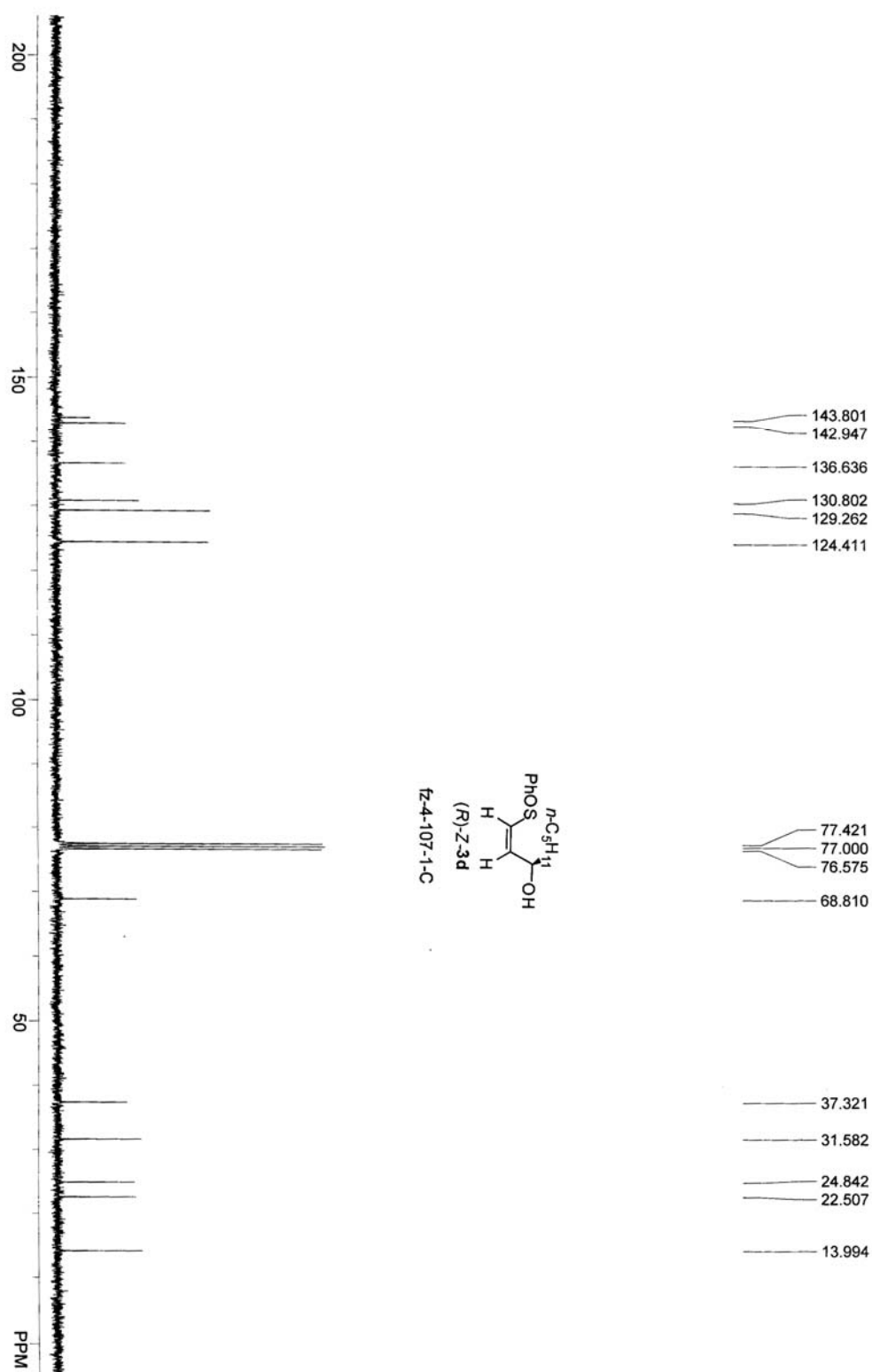
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	13.848	MM	0.4815	6.31108e4	2184.57861	99.3081	
2	15.961	MM	0.7864	439.73233	7.10781	0.6919	

Totals : 6.35505e4 2191.68643

Results obtained with enhanced integrator!

*** End of Report ***



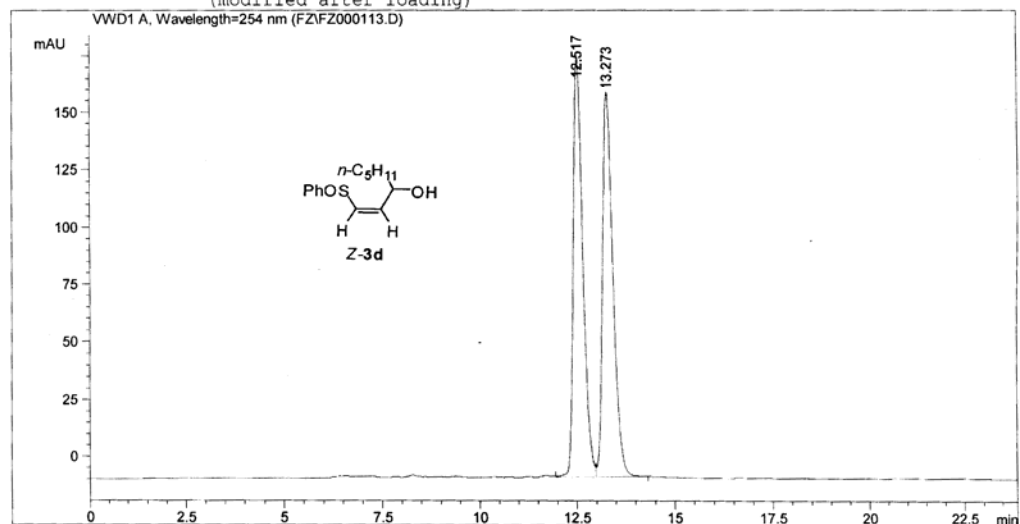


Data File D:\HPCHEM\1\DATA\FZ\FZ000113.D

Sample Name: fz-4-106-1

OJ-H column; Hexane:iPrOH = 90:10; 0.5ml/min; 254nm

=====
Injection Date : 12/20/2008 12:43:46 PM
Sample Name : fz-4-106-1 Location : -
Acq. Operator : fz
Method : D:\HPCHEM\1\METHODS\XFX_LC.M
Last changed : 12/20/2008 11:42:12 AM By fz
(modified after loading)



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	12.517	VV	0.2600	3133.24756	183.82214	50.1613
2	13.273	VB	0.2838	3113.10132	167.52574	49.8387

Totals : 6246.34888 351.34789

Results obtained with enhanced integrator!

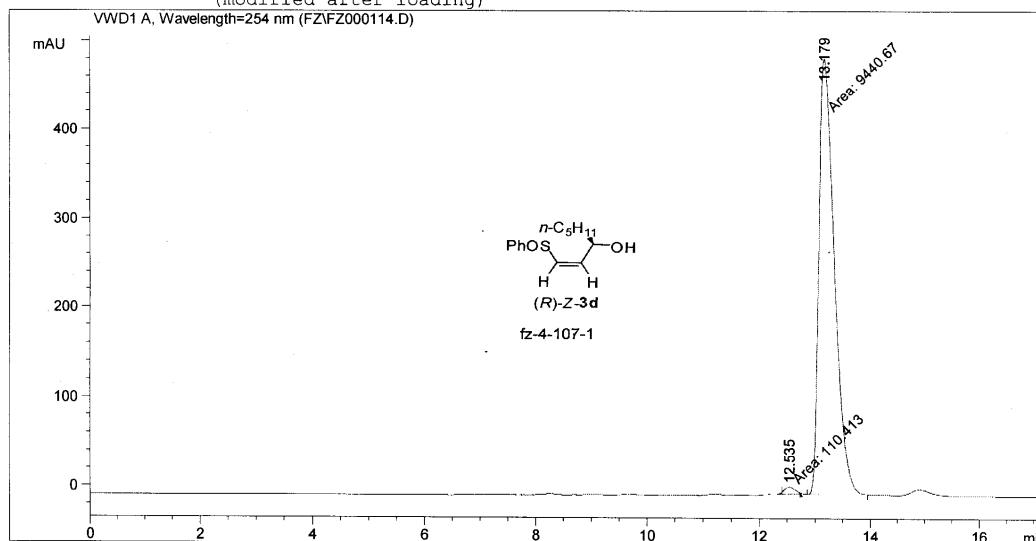
=====
*** End of Report ***

Data File D:\HPCHEM\1\DATA\FZ\FZ000114.D

Sample Name: fz-4-107-1

OJ-H column; Hexane:iPrOH = 90:10; 0.5ml/min; 254nm

```
=====
Injection Date   : 12/20/2008 1:10:06 PM
Sample Name     : fz-4-107-1
Acq. Operator   : fz
Method          : D:\HPCHEM\1\METHODS\XFX_LC.M
Last changed    : 12/20/2008 11:42:12 AM by fz
                  (modified after loading)
Location        : -
=====
```



Area Percent Report

```
=====
Sorted By       : Signal
Multiplier      : 1.0000
Dilution        : 1.0000
Use Multiplier & Dilution Factor with ISTDs
=====
```

Signal 1: VWD1 A, Wavelength=254 nm

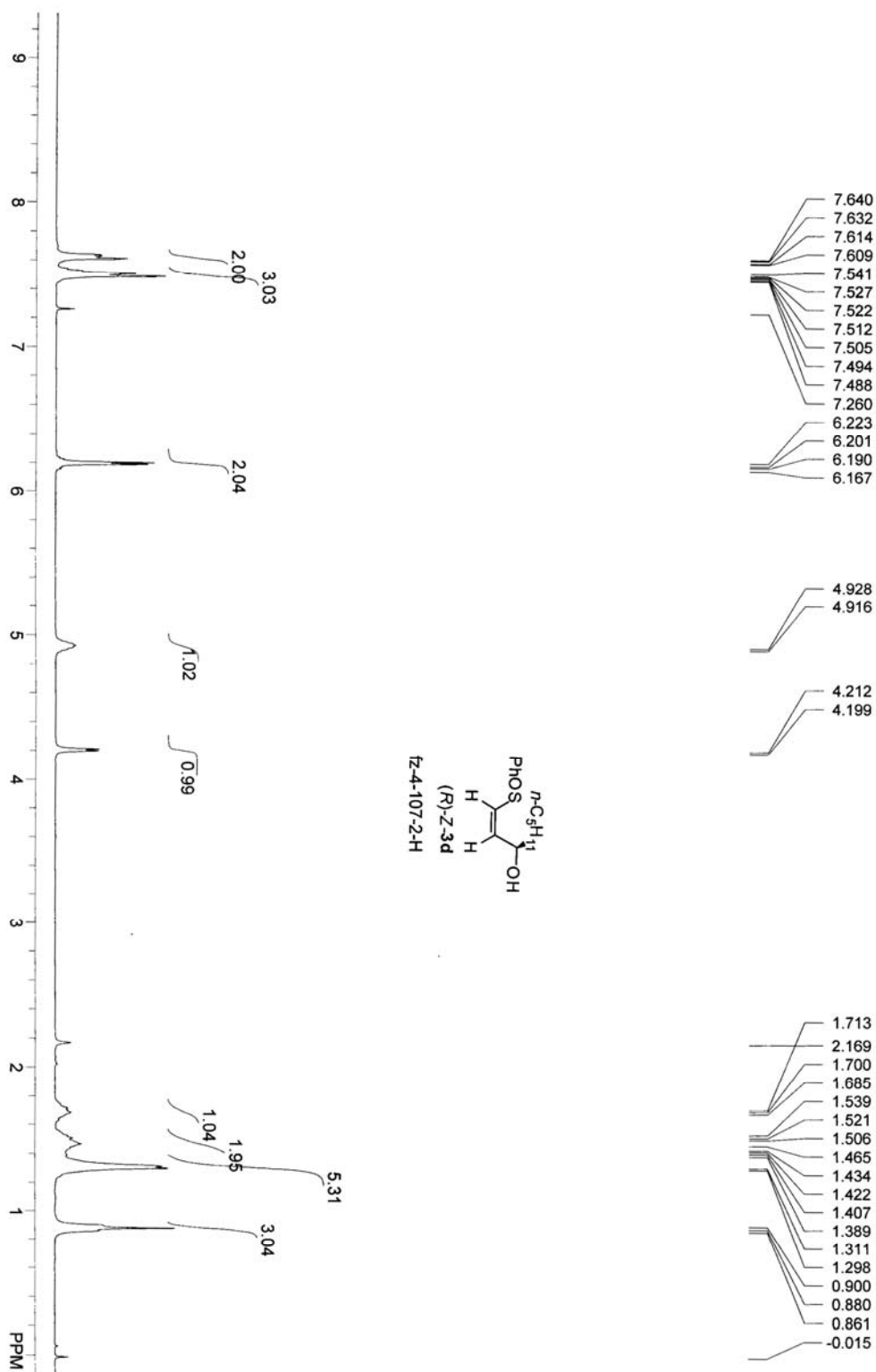
Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	12.535	MM	0.2250	110.41331	8.17980	1.1560
2	13.179	MM	0.3221	9440.66602	488.53577	98.8440

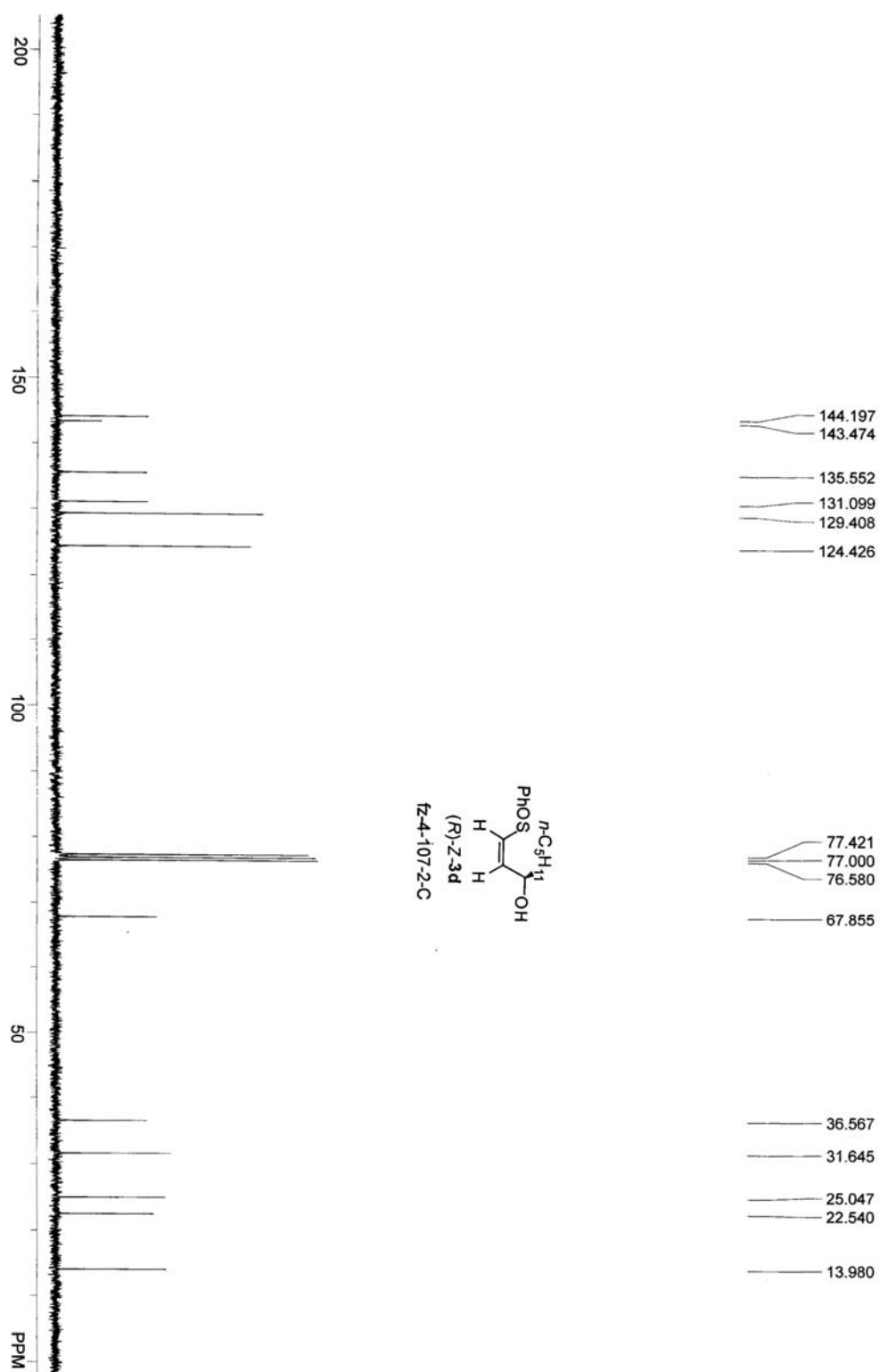
Totals : 9551.07933 496.71556

Results obtained with enhanced integrator!

*** End of Report ***

$$e\% = \frac{988440 - 11560}{988440} = 97.69\%$$



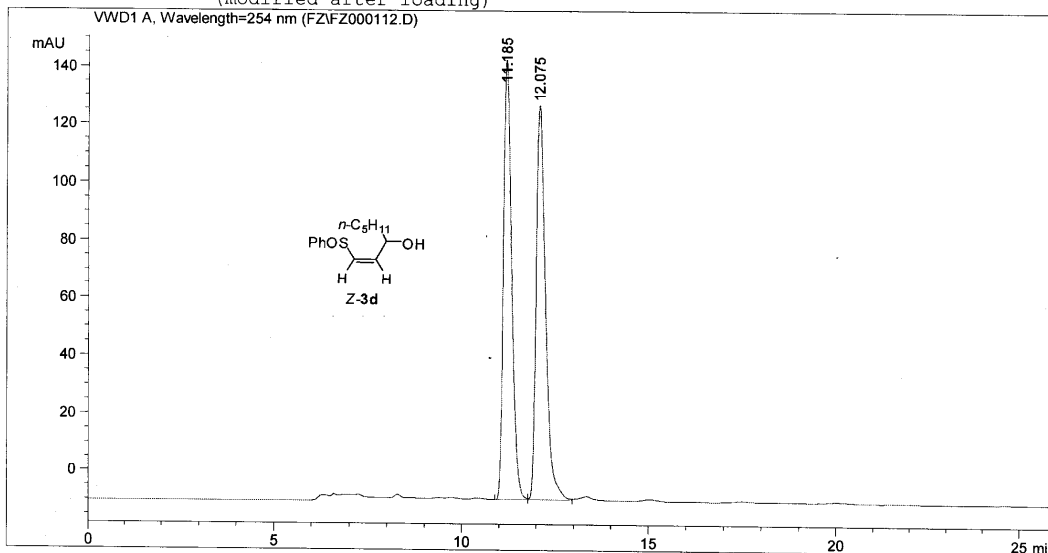


Data File D:\HPCHEM\1\DATA\FZ\FZ000112.D

Sample Name: fz-4-106-2

OJ-H column; Hexane:iPrOH = 90:10; 0.5ml/min; 254nm

=====
Injection Date : 12/20/2008 12:16:01 PM
Sample Name : fz-4-106-2 Location : -
Acq. Operator : fz
Method : D:\HPCHEM\1\METHODS\XFX LC.M
Last changed : 12/20/2008 11:42:12 AM By fz
(modified after loading)
=====



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	11.185	BV	0.2348	2344.03174	152.35619	49.3969
2	12.075	VB	0.2679	2401.27148	136.46500	50.6031

Totals : 4745.30322 288.82118

Results obtained with enhanced integrator!

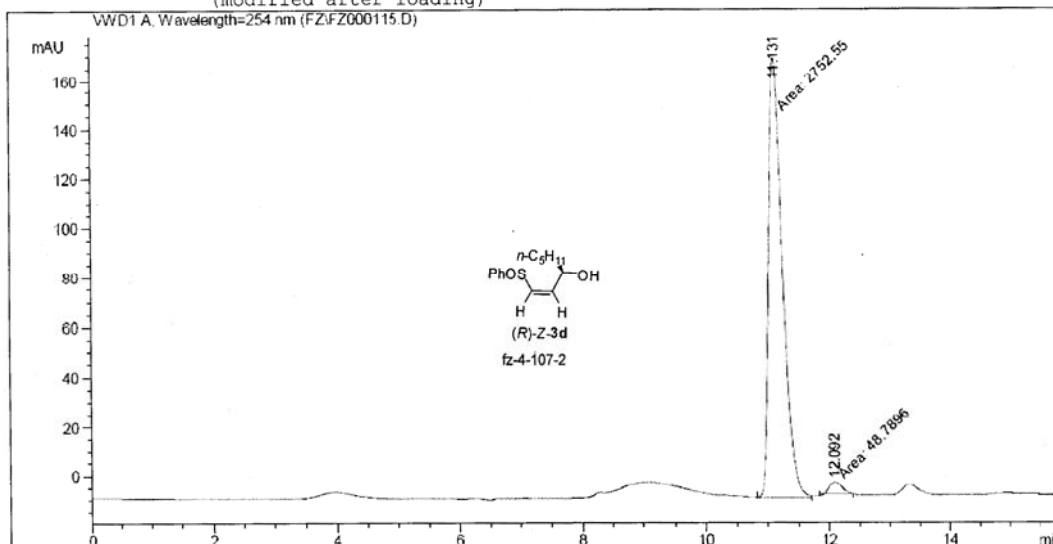
=====
*** End of Report ***
=====

Data File D:\HPCHEM\1\DATA\FZ\FZ000115.D

Sample Name: fz-4-107-2

OJ-H column; Hexane:iPrOH = 90:10; 0.5ml/min; 254nm

=====
Injection Date : 12/20/2008 1:30:29 PM
Sample Name : fz-4-107-2 Location : -
Acq. Operator : fz
Method : D:\HPCHEM\1\METHODS\XFX LC.M
Last changed : 12/20/2008 11:42:12 AM by fz
(modified after loading)



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

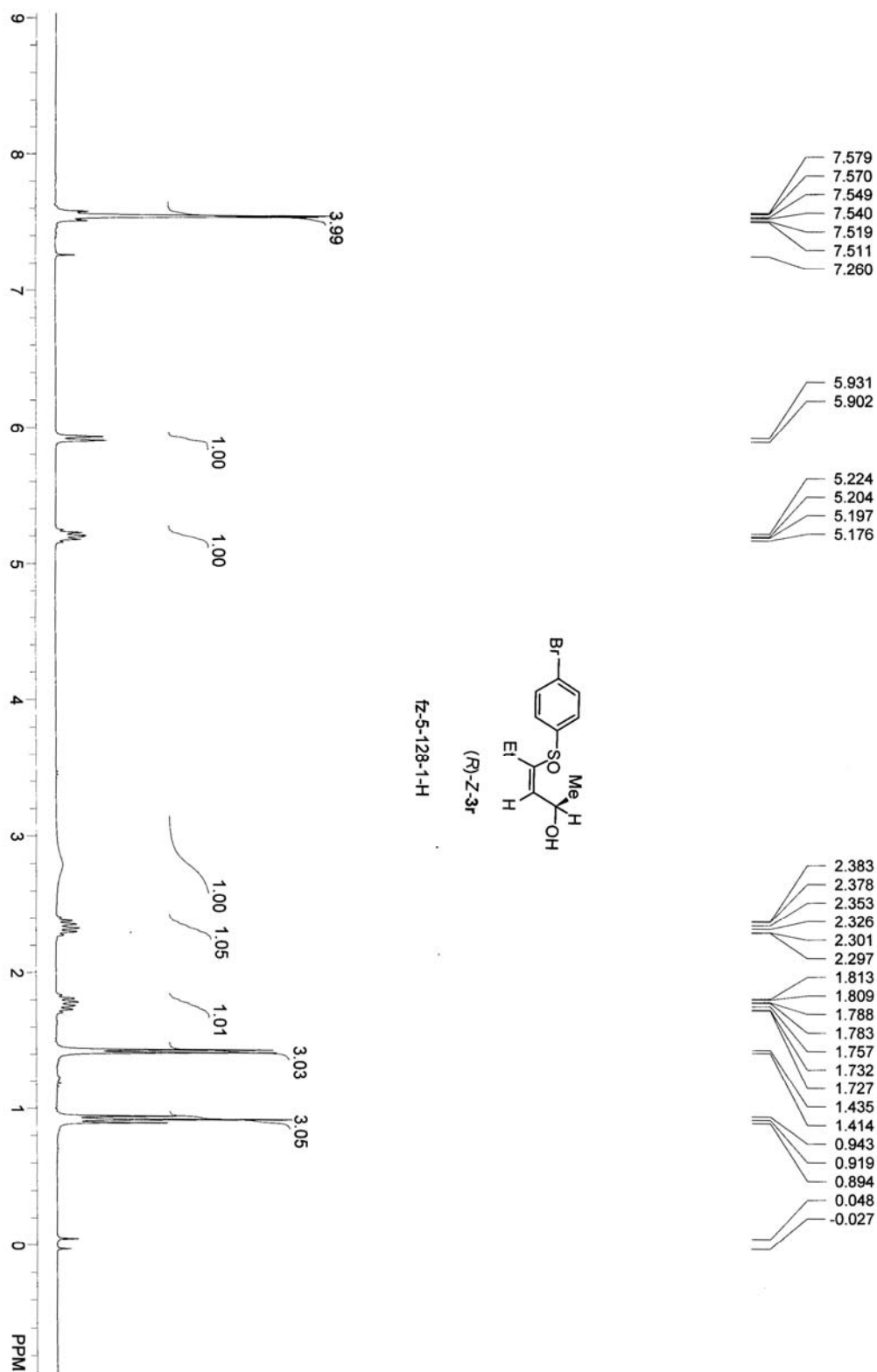
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.131	MM	0.2569	2752.55225	178.55991	98.2583
2	12.092	MM	0.1940	48.78958	4.19074	1.7417

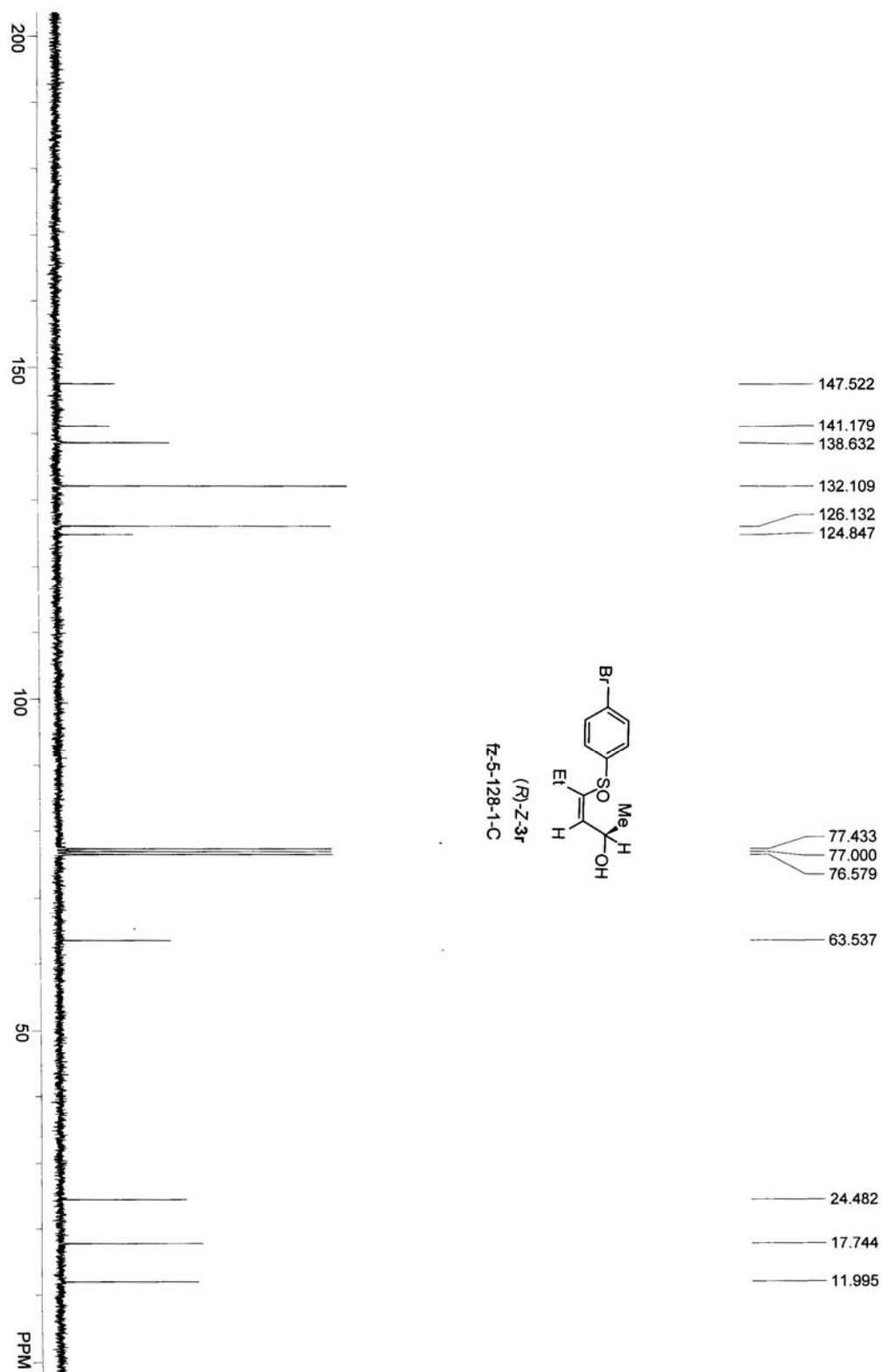
Totals : 2801.34182 182.75065

Results obtained with enhanced integrator!

=====
*** End of Report ***

ee% = 98.2583 - 1.7417
= 96.5%



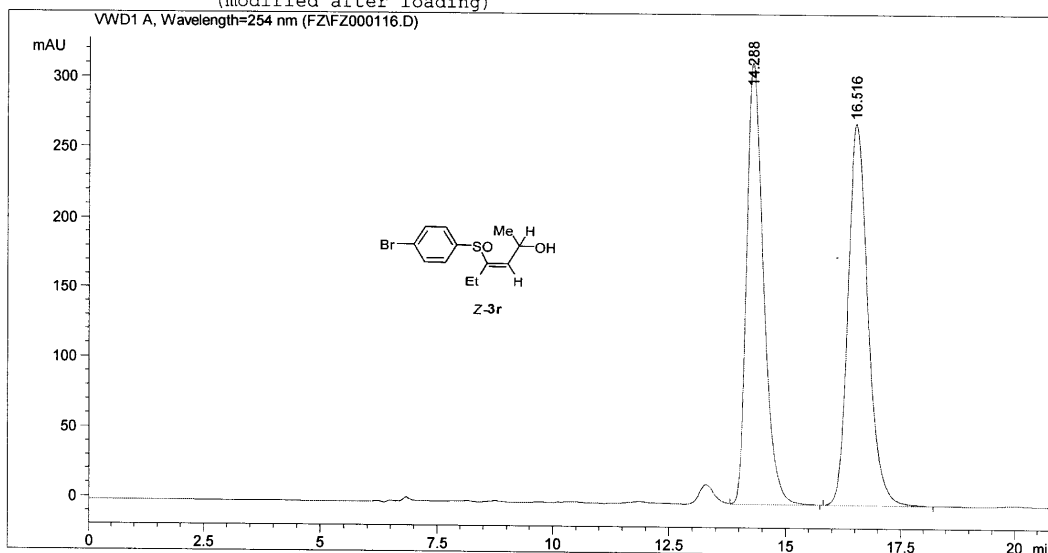


Data File D:\HPCHEM\1\DATA\FZ\FZ000116.D

Sample Name: fz-5-119-1

OJ-H; hexane/i-PrOH=90:10; 0.5 mL/min; 254nm

=====
Injection Date : 2/24/2009 10:15:12 AM
Sample Name : fz-5-119-1 Location : -
Acq. Operator : fz
Method : D:\HPCHEM\1\DATA\LJ\LJ000012.D\DEF_XFX.M
Last changed : 2/24/2009 9:56:29 AM by xfx
(modified after loading)



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	14.288	VB	0.3864	7987.59619	314.68600	49.1776
2	16.516	BB	0.4622	8254.73926	271.70612	50.8224

Totals : 1.62423e4 586.39212

Results obtained with enhanced integrator!

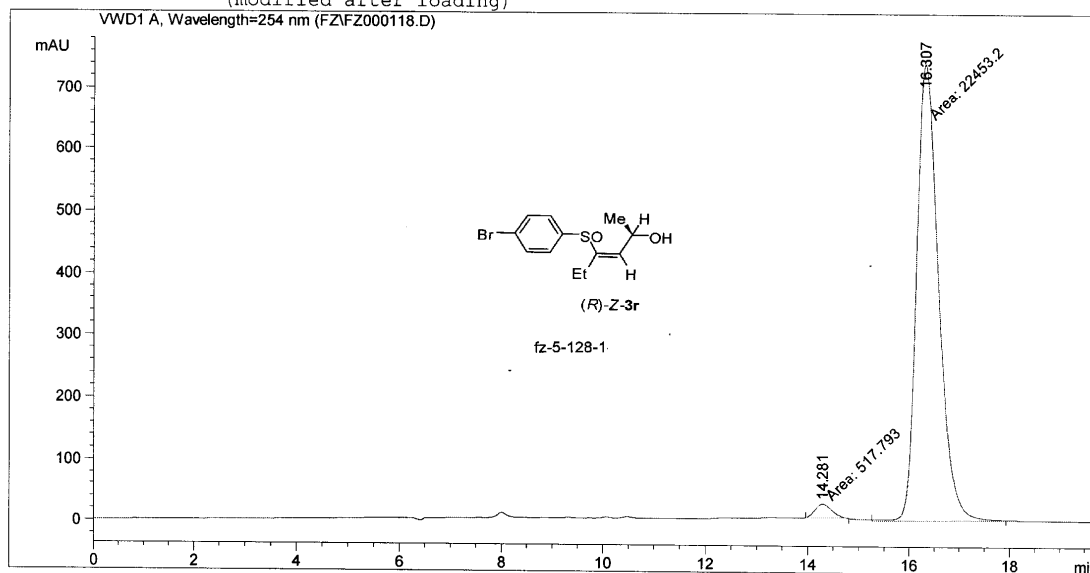
=====
*** End of Report ***

Data File D:\HPCHEM\1\DATA\FZ\FZ000118.D

Sample Name: fz-5-128-1

OJ-H; hexane/i-PrOH=90:10; 0.5 mL/min; 254nm

```
=====
Injection Date   : 2/24/2009 11:02:58 AM
Sample Name      : fz-5-128-1
Acq. Operator    : fz
Method           : D:\HPCHEM\1\DATA\LJ\LJ000012.D\DEF_XFX.M
Last changed     : 2/24/2009 9:56:29 AM by xfx
                  (modified after loading)
=====
```



Area Percent Report

```
=====
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
=====
```

Signal 1: VWD1 A, Wavelength=254 nm

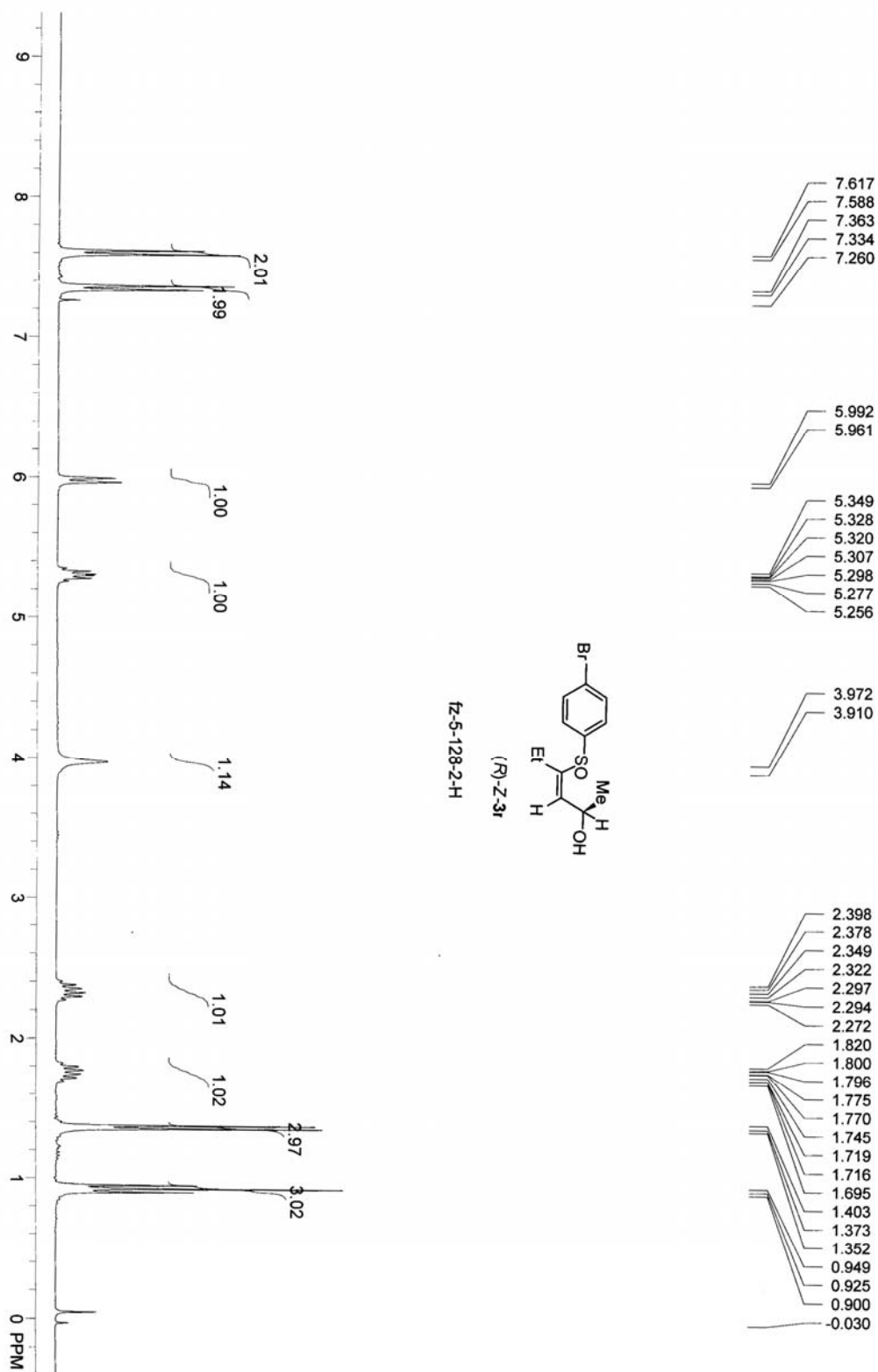
Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	14.281	MM	0.3826	517.79327	22.55390	2.2541
2	16.307	MM	0.5078	2.24532e4	736.90546	97.7459

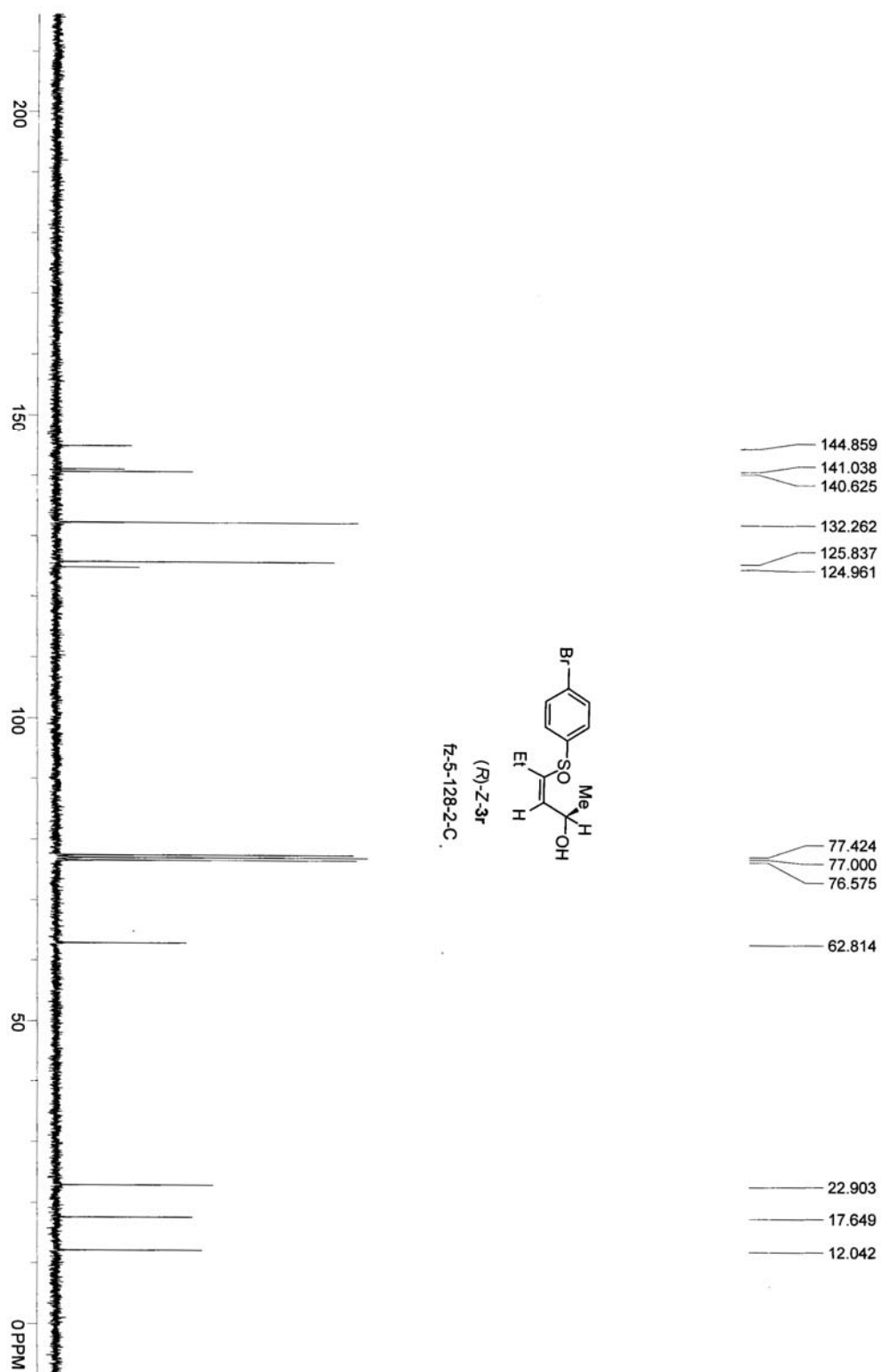
Totals : 2.29709e4 759.45935

Results obtained with enhanced integrator!

*** End of Report ***

ee: $97.7459 - 2.2541 = 95.491$



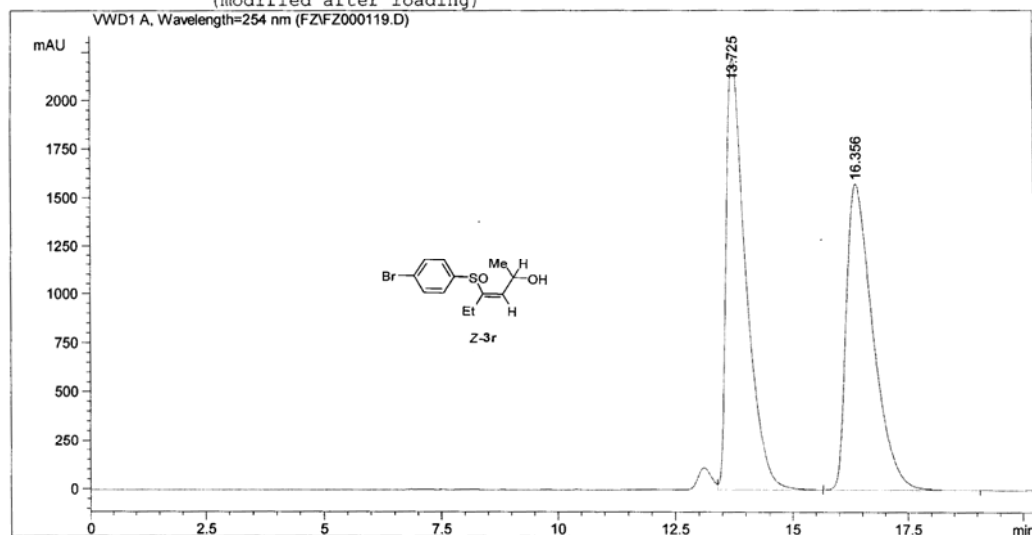


Data File D:\HPCHEM\1\DATA\FZ\FZ000119.D

Sample Name: fz-5-119-2

OJ-H; hexane/i-PrOH=90:10; 0.5 mL/min; 254nm

```
=====
Injection Date   : 2/24/2009 12:13:00 PM
Sample Name      : fz-5-119-2
Acq. Operator    : fz
Method           : D:\HPCHEM\1\DATA\LJ\LJ000012.D\DEF_XFX.M
Last changed     : 2/24/2009 9:56:29 AM by xfx
                  (modified after loading)
=====
```



Area Percent Report

```
=====
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
=====
```

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	13.725	VB	0.4319	6.48742e4	2224.86621	50.6855	
2	16.356	BB	0.6061	6.31193e4	1574.22498	49.3145	

Totals : 1.27994e5 3799.09119

Results obtained with enhanced integrator!

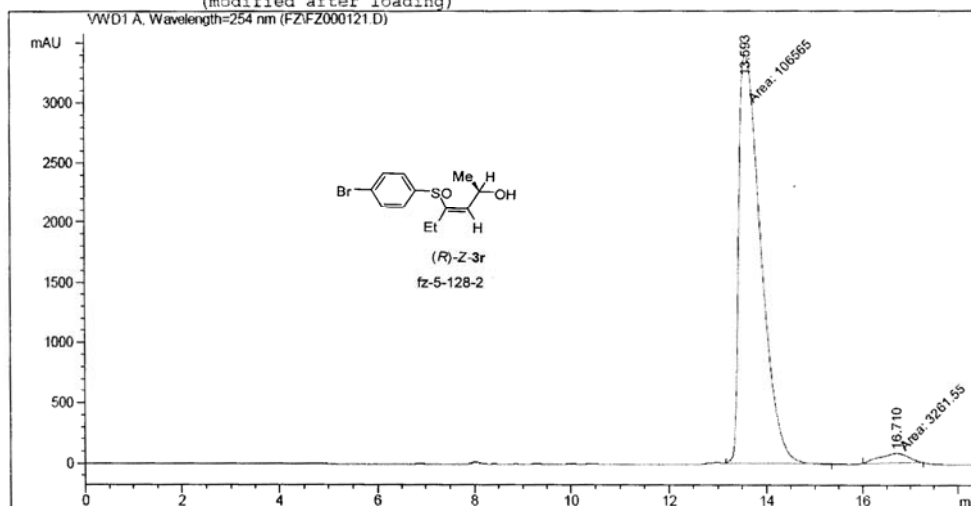
*** End of Report ***

Data File D:\HPCHEM\1\DATA\FZ\FZ000121.D

Sample Name: fz-5-128-2

OJ-H; hexane/i-PrOH=90:10; 0.5 mL/min; 254nm

=====
Injection Date : 2/24/2009 1:00:52 PM
Sample Name : fz-5-128-2 Location : -
Acq. Operator : fz
Method : D:\HPCHEM\1\DATA\LJ\LJ000012.D\DEF_XFX.M
Last changed : 2/24/2009 9:56:29 AM by xfx
(modified after loading)



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	13.593	MM	0.5230	1.06565e5	3396.19458	97.0303
2	16.710	MM	0.6987	3261.54688	77.79647	2.9697

Totals : 1.09826e5 3473.99105

Results obtained with enhanced integrator!

=====
*** End of Report ***

ee: 97.0303 - 2.9697
= 94.1

