Supporting Information

Enantioselective Synthesis of α-Methyl Carboxylic Acids from Readily Available Starting Materials via Chemoenzymatic Dynamic Kinetic Resolution

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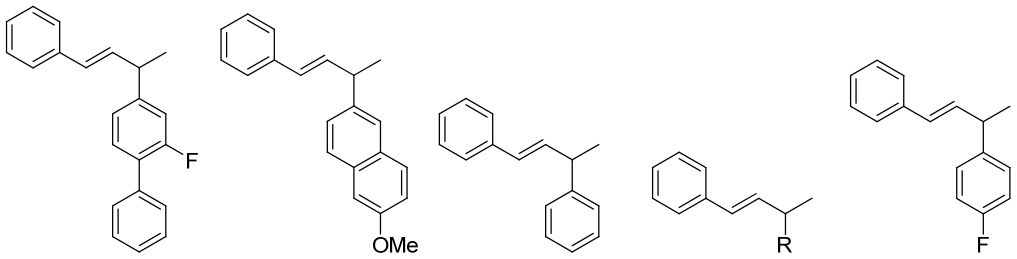
Experimental Section

General: Chemical shifts (δ) for ^{1}H (400 or 300 MHz) and ^{13}C (100 or 75 MHz) NMR spectra are reported in ppm, using residual $CHCl_3$ (7.26 ppm and 77.16 ppm, respectively) or tetramethylsilane as internal standards. Chiral chromatography analyses were performed by HPLC or GC. For HPLC, Chiralcel OD-H and Chiralcel AD columns (0.46 cm Ø * 25 cm) were used, flowrate 0.5 mL/min, unless stated in the text. For GC a CP-Chirasil-Dex CB column (25 m Ø * 0.32 mm) was used, carrier gas: H_2, flowrate: 1.8 mL/min. GC program: isothermal at 100 °C for 5 min, then 4 °C/min until 200° C and thereafter isothermal at 200 °C for 5 min. Silica gel 60 (240-400 mesh) was used for flash chromatography and analytical thin-layer chromatography was performed on precoated silica gel 60-F_{254} plates. All experiments were performed by standard Schlenk techniques under an argon atmosphere. Unless otherwise noted, all materials were obtained from commercial suppliers and used without further purification. Diethyl ether and THF were dried with a solvent purifier.

Characterization of cross-coupling products 5a-5f obtained in the copper-catalyzed allylic substitution reactions.



(*S*)-**5a** (*S*)-**5b** (*S*)-**5c** (*R*)-**5d** R = Bu
(*R*)-**5e** R = Hept (*S*)-**5f**

Supporting information for olefins (*S*)-**5c**, (*R*)-**5d**, and (*R*)-**5d** was previously reported.[1]

(*rac*)-1-phenyl-3-(3-fluoro-4-phenyl)phenyl-1-butene ((rac)-5a). (*rac*)-**5a** was obtained in 97% yield. HPLC analysis (OJ column, *i*-hexane:*i*-PrOH, 85:15; flow 1.0, $t_r(S)$ = 13.6 min, $t_r(R)$ = 18.6 min). ^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.67-7.61 (m, 2H), 7.56-7.36 (m, 8H), 7.34-7.27 (m, 1H), 7.24-7.13 (m, 2H), 6.56 (d, J = 16.0 Hz, 1H), 6.46 (dd, J = 16.0, 6.6 Hz, 1H), 3.76 (dq, J = 7.3, 6.6 Hz, 1H), 1.58 (d, J = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.9 (d, $J_{C\text{-}F}$ = 247.9 Hz), 147.4 (d, $J_{C\text{-}F}$ = 7.3 Hz), 137.4, 135.9, 134.3, 130.7 (d, $J_{C\text{-}F}$ = 4.0 Hz), 129.2, 129.0 (d, $J_{C\text{-}F}$ = 3.1Hz), 128.6 (d, $J_{C\text{-}F}$ = 12.9 Hz), 127.5 (d, $J_{C\text{-}F}$ = 22.9 Hz), 126.9 (d, $J_{C\text{-}F}$ = 13.5 Hz), 126.3, 123.4(d, $J_{C\text{-}F}$ = 3.3 Hz), 114.93 (d, $J_{C\text{-}F}$ = 23.1 Hz), 42.2, 21.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -118.11. HRMS (*m/z*) calculated for $C_{22}H_{19}FNa^+$ $(M+Na)^+$, 325.1363; found 325.1373.

(*R*)-(+)-1-phenyl-3-(3-fluoro-4-phenyl)phenyl-1-butene ((*R*)-5a). (*R*)-**5a** was obtained in 97% yield and >99% ee. $[\alpha]^{27}_D$ = +38.6 (*c* = 1.00, $(CH_3)_2CO$). The optical purity was

determined by HPLC analysis (OJ column, *i*-hexane:*i*-PrOH, 85:15; flow 1.0, $t_r(S)$ = 13.6 min, $t_r(R)$ = 18.6 min).

(*S*)-(–)-1-phenyl-3-(3-fluoro-4-phenyl)phenyl-1-butene ((*S*)-5a). (*S*)-**5a** was obtained in 92% yield and >99% ee. The optical purity was determined by HPLC analysis (OJ column, *i*-hexane:*i*-PrOH, 85:15; flow 1.0, $t_r(S)$ = 13.6 min, $t_r(R)$ = 18.6 min). NMR spectral data were in accordance with published data.[2] $[\alpha]^{27}_D$ = -39.2 (*c* = 1.00, $(CH_3)_2CO$).

(*rac*)-1-phenyl-3-(6-methoxy-2-naphtyl)-1-butene ((*rac*)-5b). (*rac*)-**5b** was obtained in 98% yield. HPLC analysis (OJ column, *i*-hexane:*i*-PrOH, 85:15; flow 1.0, $t_r(R)$ = 25.35, $t_r(S)$ = 29.71 min). ^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.75-7.69 (m, 2H), 7.67-7.63 (m, 1H), 7.43-7.37 (m, 3H), 7.34-7.27 (m, 2H), 7.25-7.19 (m, 1H), 7.18-7.13 (m, 2H), 6.49-6.46 (m, 2H), 3.94 (s, 3H), 3.84-3.76 (m, 1H), 1.57 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.4, 140.8, 137.6, 135.4, 133.3, 129.2, 129.1, 128.7, 128.5, 127.1, 127.0, 126.8, 126.2, 125.1, 118.7, 105.7, 55.3, 42.5, 21.2. $C_{21}H_{20}ONa^+$ (M+Na),$^+$ 311.1406; found 311.1411.

(*R*)-(+)-1-phenyl-3-(6-methoxy-2-naphtyl)-1-butene((*R*)-5b). (*R*)-**5b** was obtained in 99% ee and > 99% ee. The optical purity was determined by HPLC analysis (OJ column, *i*-hexane:*i*-PrOH, 85:15; flow 1.0, $t_r(R)$ = 25.35, $t_r(S)$ = 29.71 min). $[\alpha]^{27}_D$ = +38 (*c* = 1.00, $(CH_3)_2CO$)

(*S*)-(–)-1-phenyl-3-(6-methoxy-2-naphtyl)-1-butene ((*S*)-5b). (*S*)-**5b** was obtained in 98% yield and > 99% ee. The optical purity was determined by HPLC analysis (OJ column, *i*-hexane:*i*-PrOH, 85:15; flow 1.0, $t_r(R)$ = 24.67, $t_r(S)$ = 28.62 min). $[\alpha]^{27}_D$ = -37 (*c* = 1.00, $(CH_3)_2CO$)

(*rac*)-1,3-diphenyl-1-butene ((*rac*)-5c). (*rac*)-**5c** was obtained in 78% yield. NMR spectral data were in accordance with published data.[3] HPLC analysis (OJ column, *i*-hexane:*i*-PrOH, 99:1, $t_r(R)$ = 95.54, $t_r(S)$ = 105.44 min). ^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.41-7.20 (m, 10 H), 6.48-6.38 (m, 2H), 3.68 (dq, J = 7.4, 7.0 Hz, 1 H), 1.50 (d, J = 7.0 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.7, 137.7, 135.4, 128.7, 128.6, 127.5, 127.2, 126.4, 126.3, 42.7, 21.4.

(*R*)-(+)-1,3-diphenyl-1-butene ((*R*)-5c). (*R*)-**5c** was obtained in 78% yield and >99% ee. The optical purity was determined by HPLC analysis (OJ column, *i*-hexane:*i*-PrOH, 99:1, $t_r(R)$ = 95.54, $t_r(S)$ = 105.44 min). $[\alpha]^{27}_D$ = +37 (c = 1.00, $CHCl_3$)

(*S*)-(-)-1,3-diphenyl-1-butene ((*S*)-5c). (*S*)-**5c** was obtained in 79% yield and >99% ee. The optical purity was determined by HPLC analysis (OJ column, *i*-hexane:*i*-PrOH, 99:1, $t_r(R)$ = 95.54, $t_r(S)$ = 105.44 min).

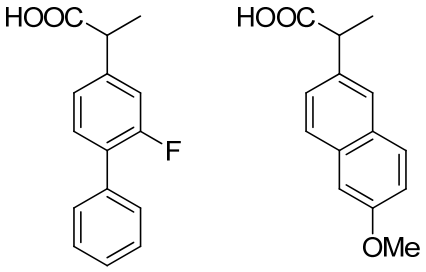
(*rac*)-1-phenyl-3-(4-fluorophenyl)-1-butene ((*rac*)-5f). (*rac*)-**5f** was obtained in 95% yield. NMR spectral data were in accordance with published data.[3] ^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.42-7.21 (m, 7H), 7.07-6.99 (m, 2H), 6.46-6.33 (m, 2H), 3.66 (dq, J = 7.31, 6.92 Hz, 1 H), 1.48 (d, J = 6.92 Hz, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.4 (d, $J_{C\text{-}F}$ = 245 Hz), 141.2 (d, $J_{C\text{-}F}$ = 3.0 Hz), 137.4, 135.0, 128.7 (d, $J_{C\text{-}F}$ = 7.7 Hz), 128.7, 128.6, 127.2, 126.2, 115.2 (d, $J_{C\text{-}F}$ = 21.0 Hz), 41.8, 21.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -117.2. HPLC analysis (OJ column, *i*-hexane:*i*-PrOH, 99:1, $t_r(R)$ = 92.40, $t_r(S)$ = 81.59 min).

(*R*)-(+)-1-phenyl-3-(4-fluorophenyl)-1-butene ((*R*)-5f). (*R*)-**5f** was obtained in 94% yield and >99% ee. NMR spectral data were in accordance with published data.[3] The optical purity

was determined by HPLC analysis (OJ column, *i*-hexane:*i*-PrOH, 99:1, $t_r(R)$ = 92.40, $t_r(S)$ = 81.59 min). $[\alpha]^{27}_D$ = +33 (*c* = 1.00, $CHCl_3$).

(*S*)-(–)-1-phenyl-3-(4-fluorophenyl)-1-butene ((*S*)-5f). (*S*)-**5f** was obtained in 97% yield and >99% ee. The optical purity was determined by HPLC analysis (OJ column, *i*-hexane:*i*-PrOH, 99:1, $t_r(R)$ = 92.40, $t_r(S)$ = 81.59 min). $[\alpha]^{27}_D$ = -32 (*c* = 1.00, $CHCl_3$).

Characterization of oxidation products 7a-7b.



7a **7b**

(*rac*)-Flurbiprofen. (*rac*)-**7a**. GC analysis (flow rate; 1.5 mL/min. GC program: From 100 °C to 200 °C at a rate of 10 °C/min, isothermal at 200 °C for 40 min; $t_r(S)$ = 25.6, $t_r(R)$ = 26.3 min). Spectroscopic data were in agreement with the literature data.[4]

(*R*)-2-((3-fluoro-4-phenyl)phenyl)propionic acid ((*R*)-Flurbiprofen (*R*)-**7a**).

Method [A] (*R*)-**7a** was obtained in 93% yield and >99% ee. The optical purity was determined by GC analysis (flow rate; 1.5 mL/min. GC program: From 100 °C to 200 °C at a rate of 10 °C/min, isothermal at 200 °C for 40 min; $t_r(S)$ = 25.6, $t_r(R)$ = 26.3 min). $[\alpha]^{27}_D$ = -42.7 (*c* = 0.8, $CDCl_3$). Spectroscopic data were in agreement with the literature data.[4]

Method [B] (*R*)-**7a** was obtained in 44% yield and >99% ee. The optical purity was determined by GC analysis (flow rate; 1.5 mL/min. GC program: From 100 °C to 200 °C at a rate of 10 °C/min, isothermal at 200 °C for 40 min; t_r(*S*) = 25.6, t_r(*R*) = 26.3 min). $[\alpha]^{27}_D$ = -40.6 (*c* = 0.5, $CDCl_3$). Spectroscopic data were in agreement with the literature data.[4]

(*S*)-2-((3-fluoro-4-phenyl)phenyl)propionic acid ((*S*)-Flurbiprofen (*S*)-**7a**).

Method [A] (*S*)-**7a** was obtained in 76% yield and >99% ee. The optical purity was determined by GC analysis (flow rate; 1.5 mL/min. GC program: From 100 °C to 200 °C at a rate of 10 °C/min, isothermal at 200 °C for 40 min; t_r(*S*) = 25.6, t_r(*R*) = 26.3 min). $[\alpha]^{27}_D$ = +42.2 (*c* = 1.0, $CDCl_3$). Spectroscopic data were in agreement with the literature data.[4]

(*S*)-2-(6-methoxy-2-naphtyl)propionic acid ((*S*)-Naproxen, (*S*)-**7b**).

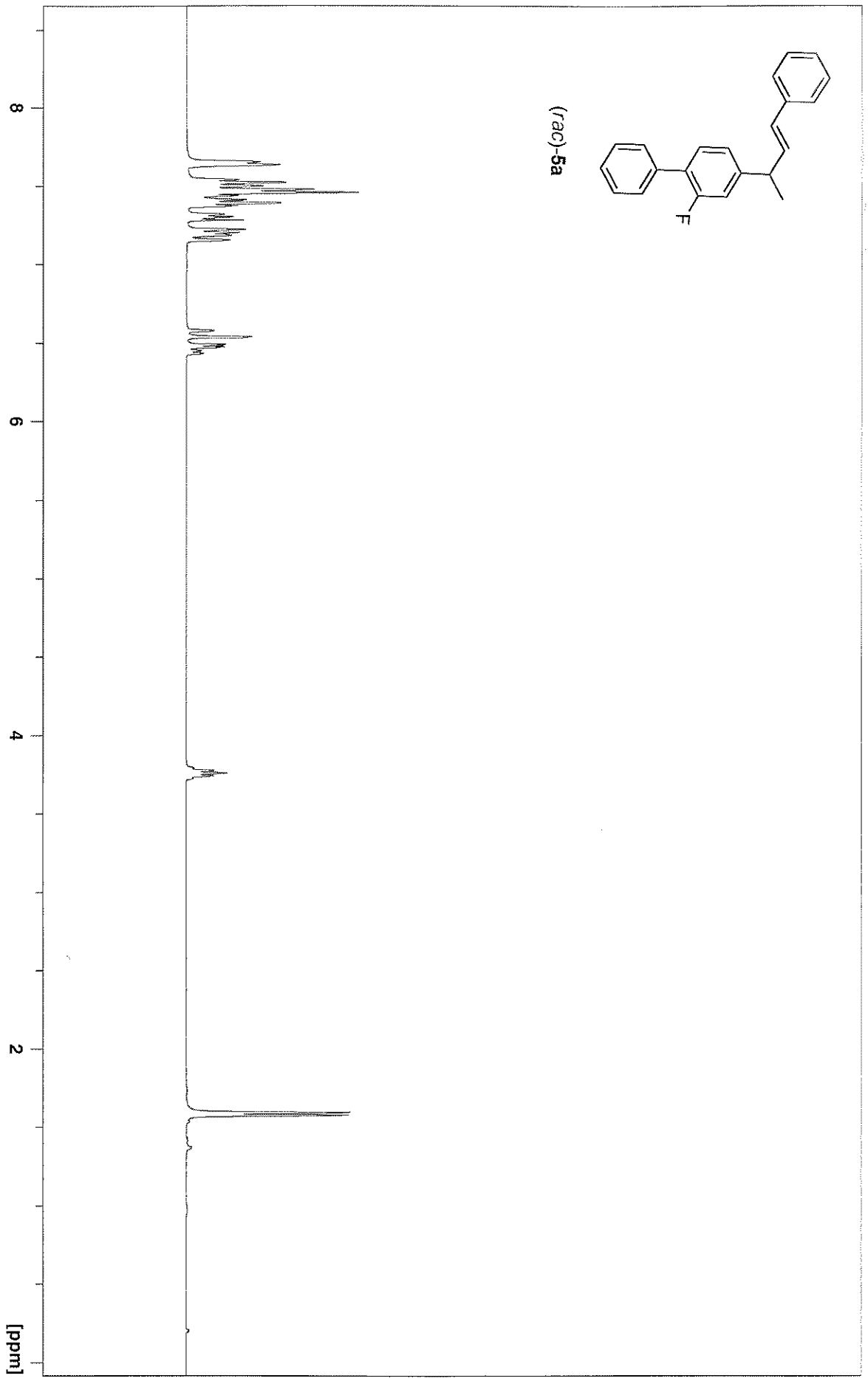
Method [B] (*S*)-**7b** was obtained in 42% yield and >99% ee. The optical purity (>99% ee) was determined by GC analysis (flow rate; 1.5 mL/min. GC program: From 100 °C to 200 °C at a rate of 10 °C/min, isothermal at 200 °C for 40 min; t_r(*S*) = 28.5, t_r(*R*) = 29.2 min). $[\alpha]^{27}_D$ = +60.8 (*c* = 0.5, $CDCl_3$). Spectroscopic data were in agreement with the literature data.[5]

Method [C] (*S*)-**7b** was obtained in 51% yield and >99% ee. The optical purity (>99% ee) was determined by GC analysis (flow rate; 1.5 mL/min. GC program: From 100 °C to 200 °C at a rate of 10 °C/min, isothermal at 200 °C for 40 min; t_r(*S*) = 28.5, t_r(*R*) = 29.2 min). Spectroscopic data were in agreement with the literature data.[5]

References

1. Norinder, J.; Bogar, K.; Kanupp, L.; Bäckvall, J.-E. *Org. Lett.* **2007**, *9*, 5095–5098.
2. Rodriguez, D.; Perez Sestelo, J.; Sarandeses, L. A. *J. Org. Chem.* **2004**, *69*, 8136–8139.
3. Mauleón, P.; Alonso, I.; Rivero, M. R.; Carretero, J. C. *J. Org. Chem.* **2007**, *72*, 9924–9935.

4. Schlosser, M.; Geneste, H. *Chem. Eur. J.* **1998**, *4*, 1969–1973.
5. Boyd, E.; Coulbeck, E.; Coumbarides, G. S.; Chavda, S.; Dingjan, M.; Eames, J.; Flinn, A.; Motevalli, M.; Northen, J.; Yohannes, Y. *Tetrahedron: Asymmetry* **2007**, *18*, 2515–2530.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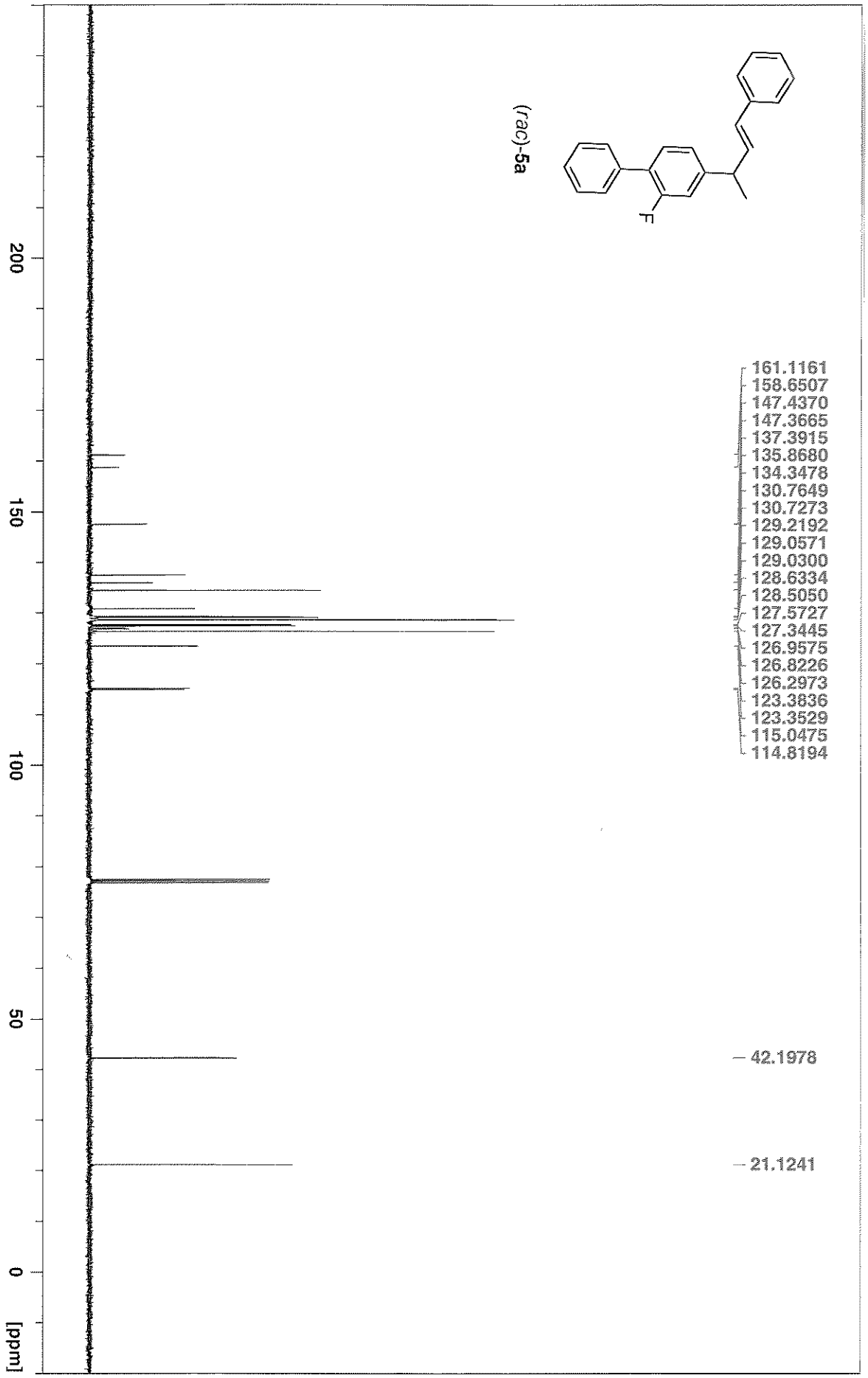
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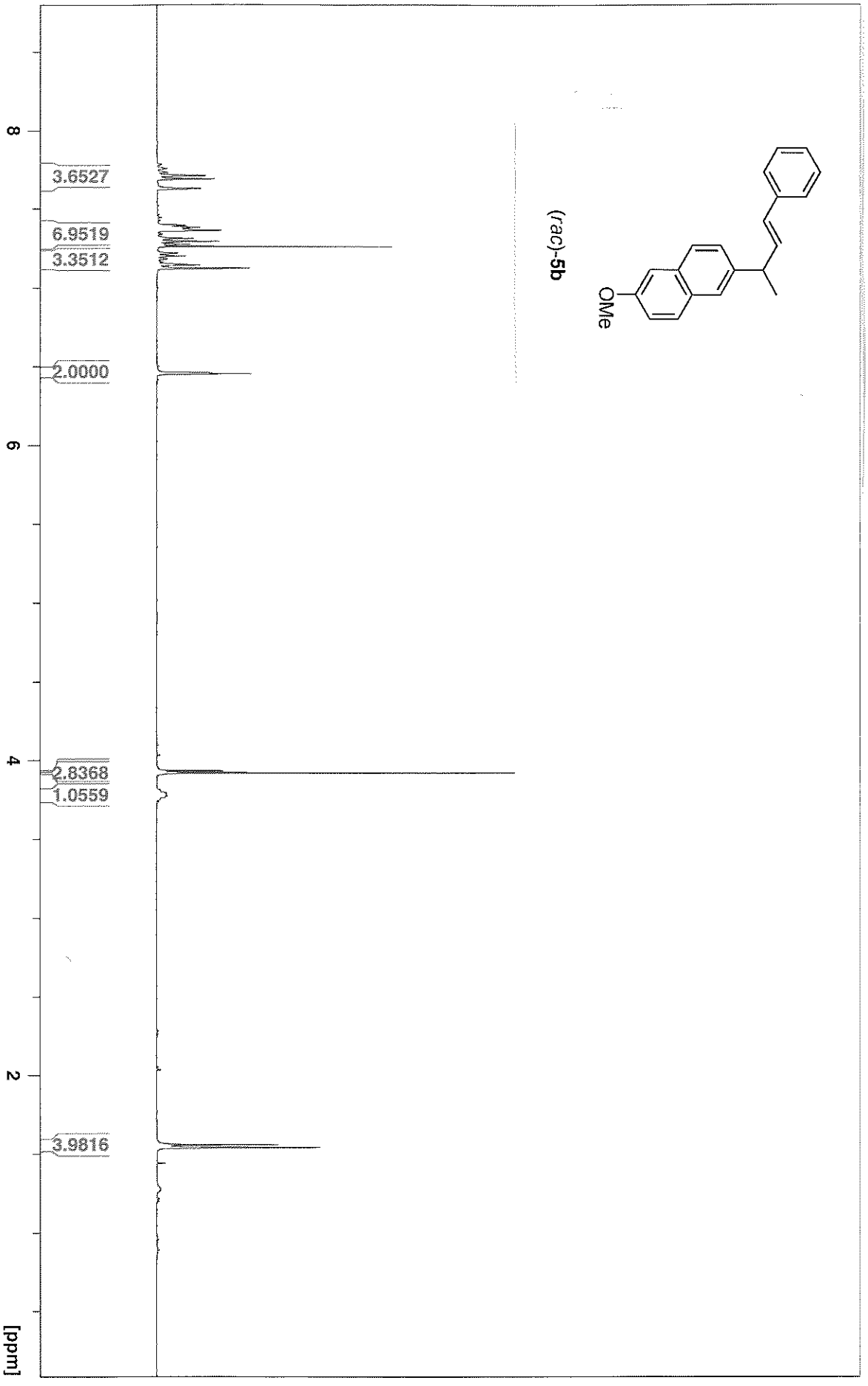
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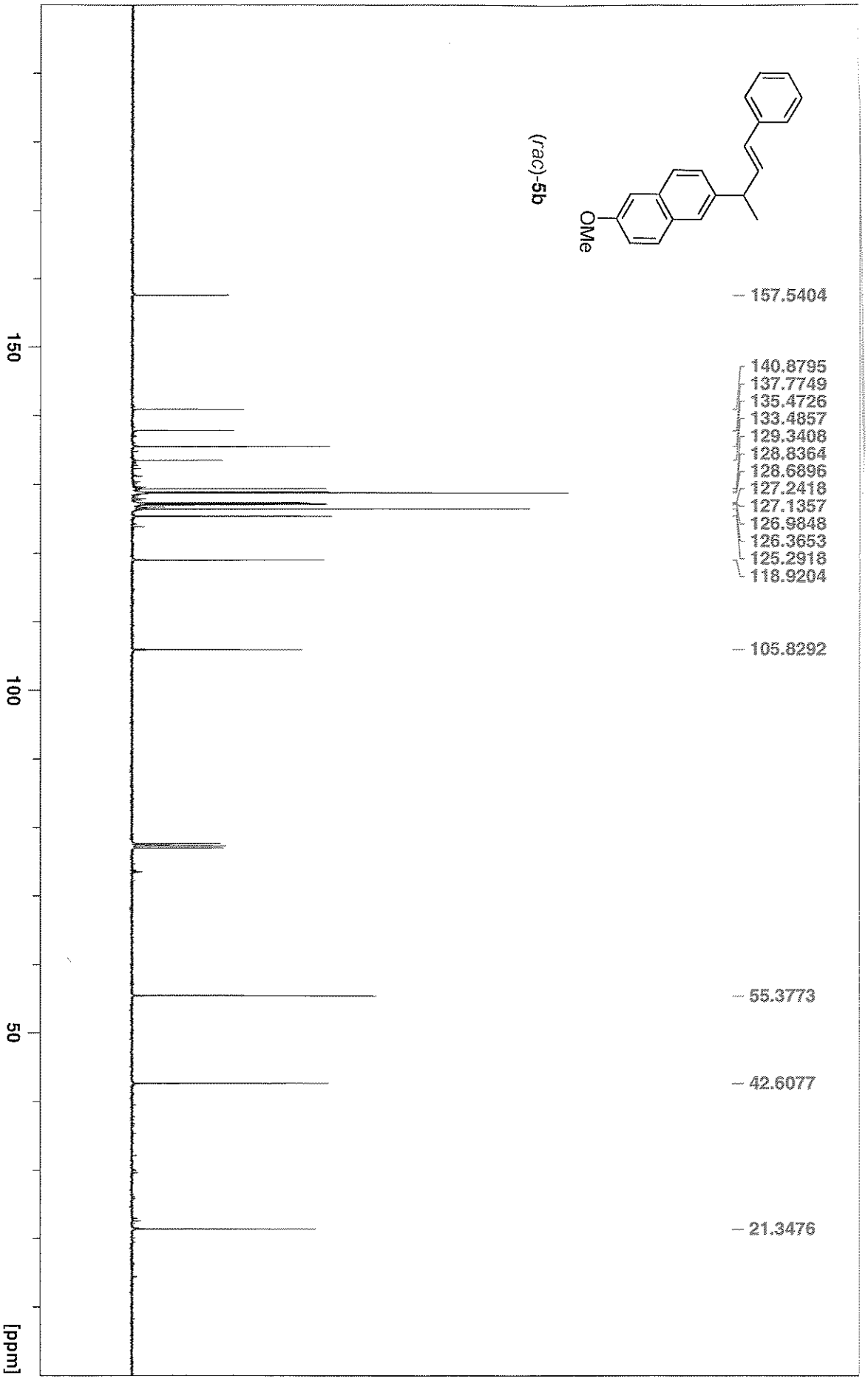
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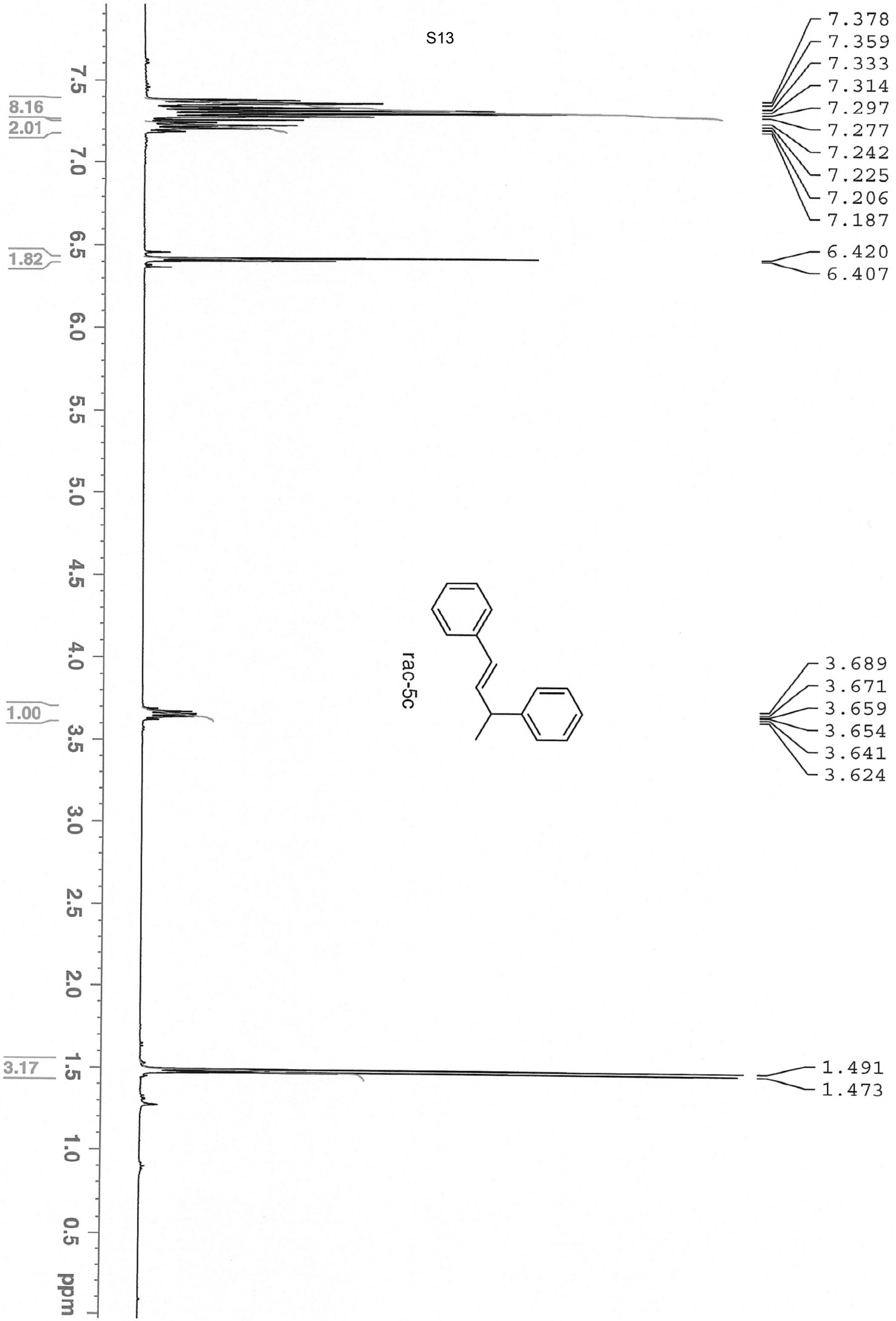
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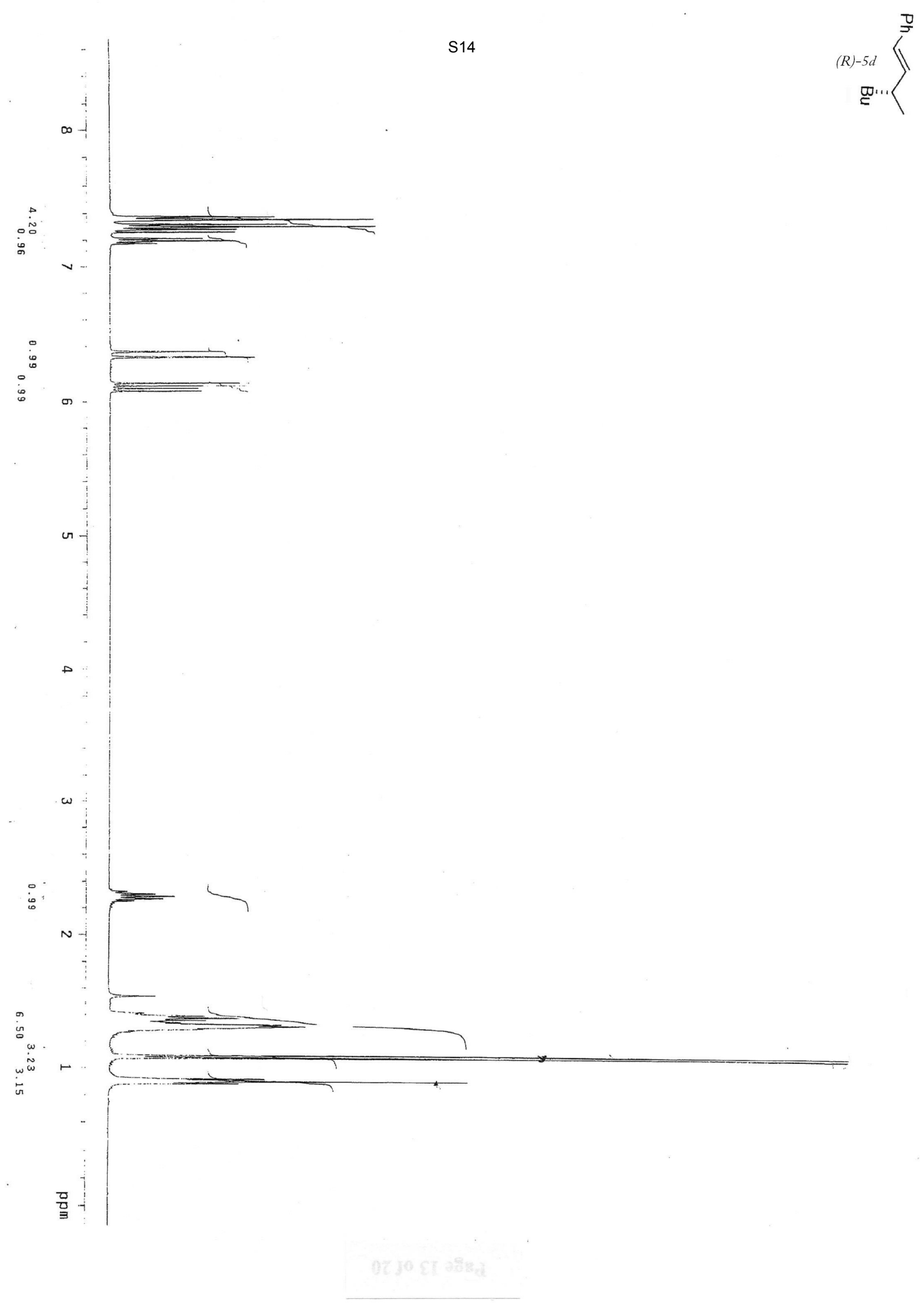

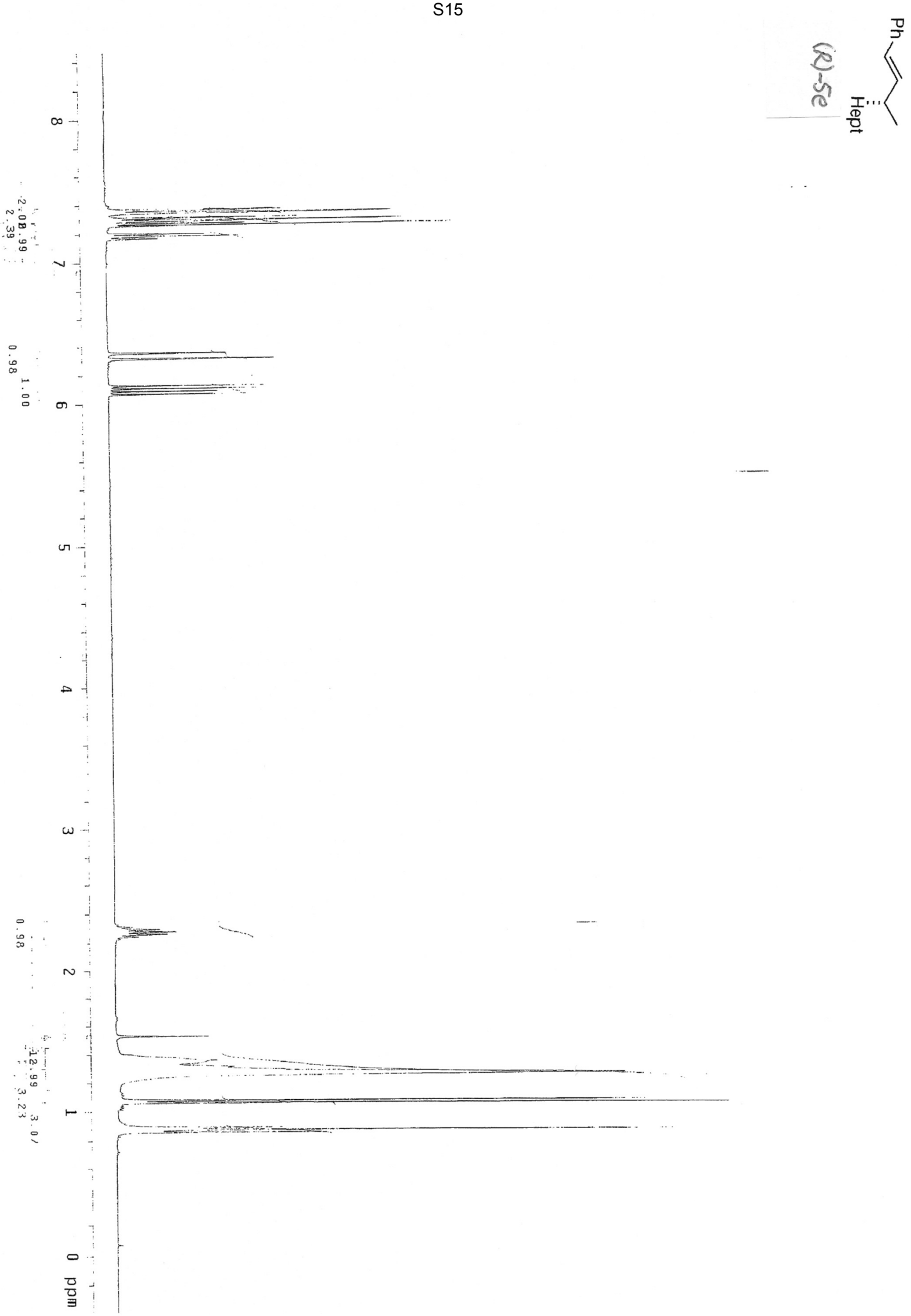
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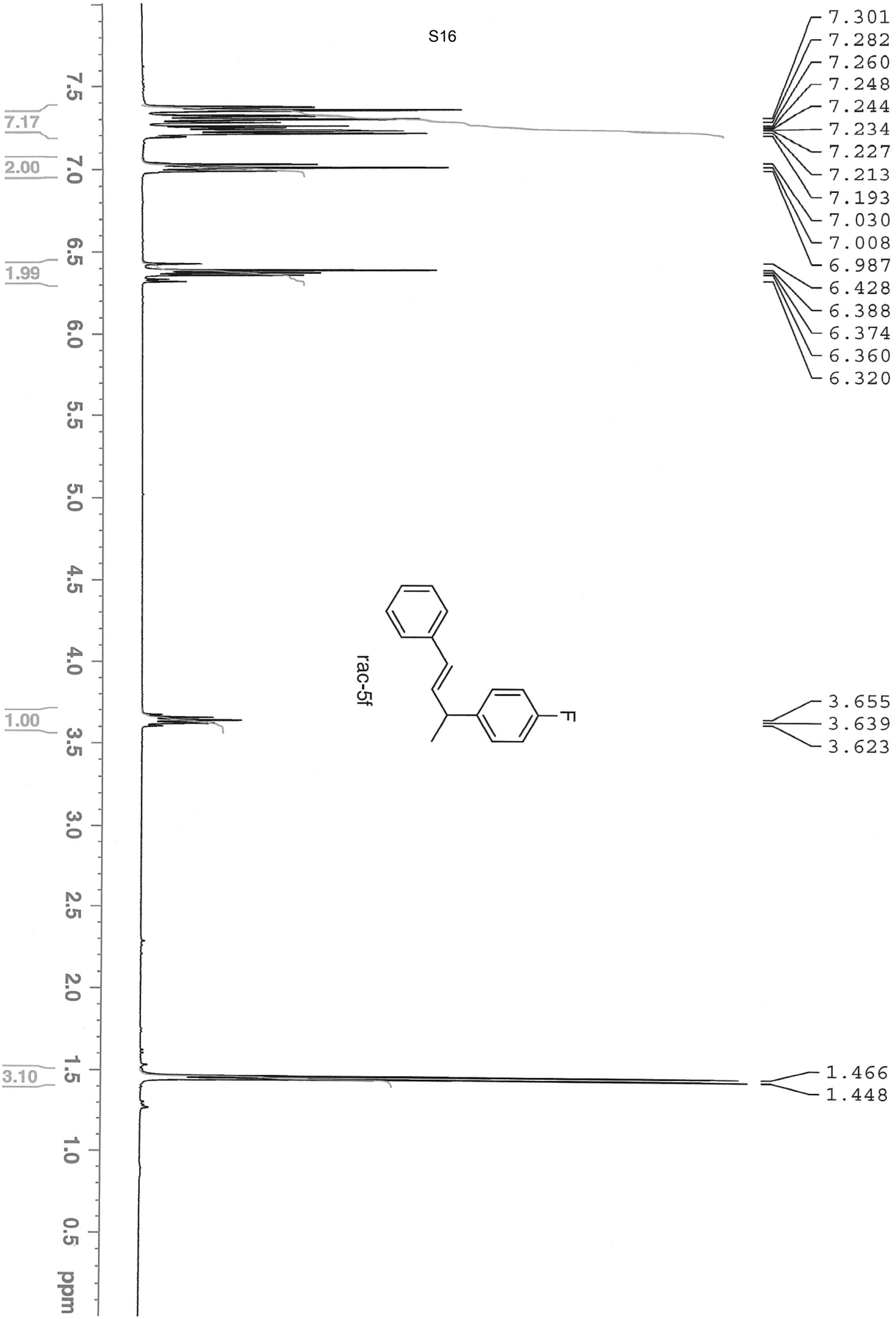
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KB-360

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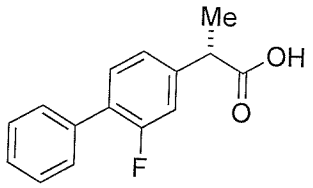
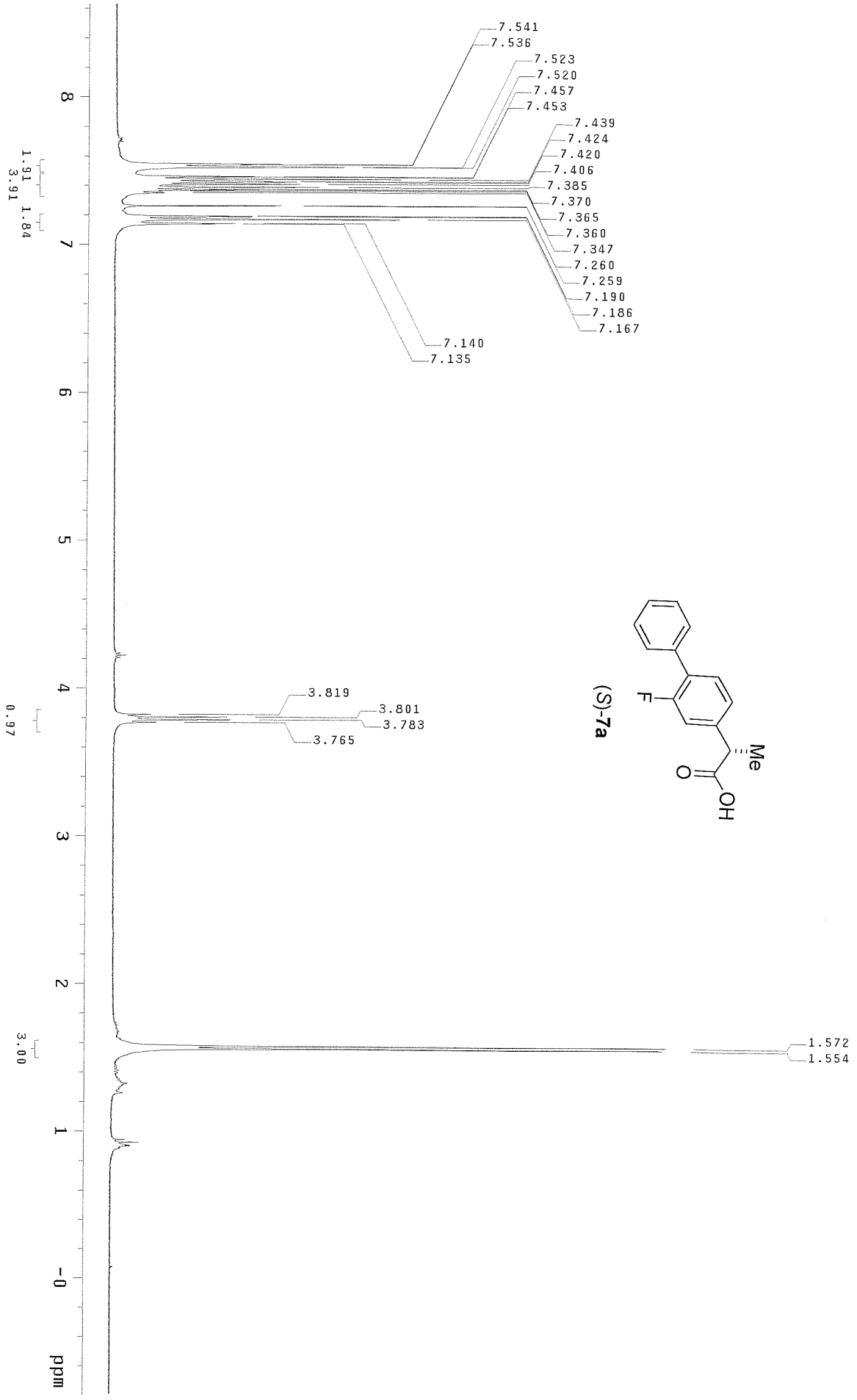


(*S*)-**7a**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(S)-7a
ppm

Empower software

lisa

Reported by User: HPLC User (User)

Project Name: Lisa

SAMPLE INFORMATION

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Injection Volume:	10,00 ul	Processing Method:	Default
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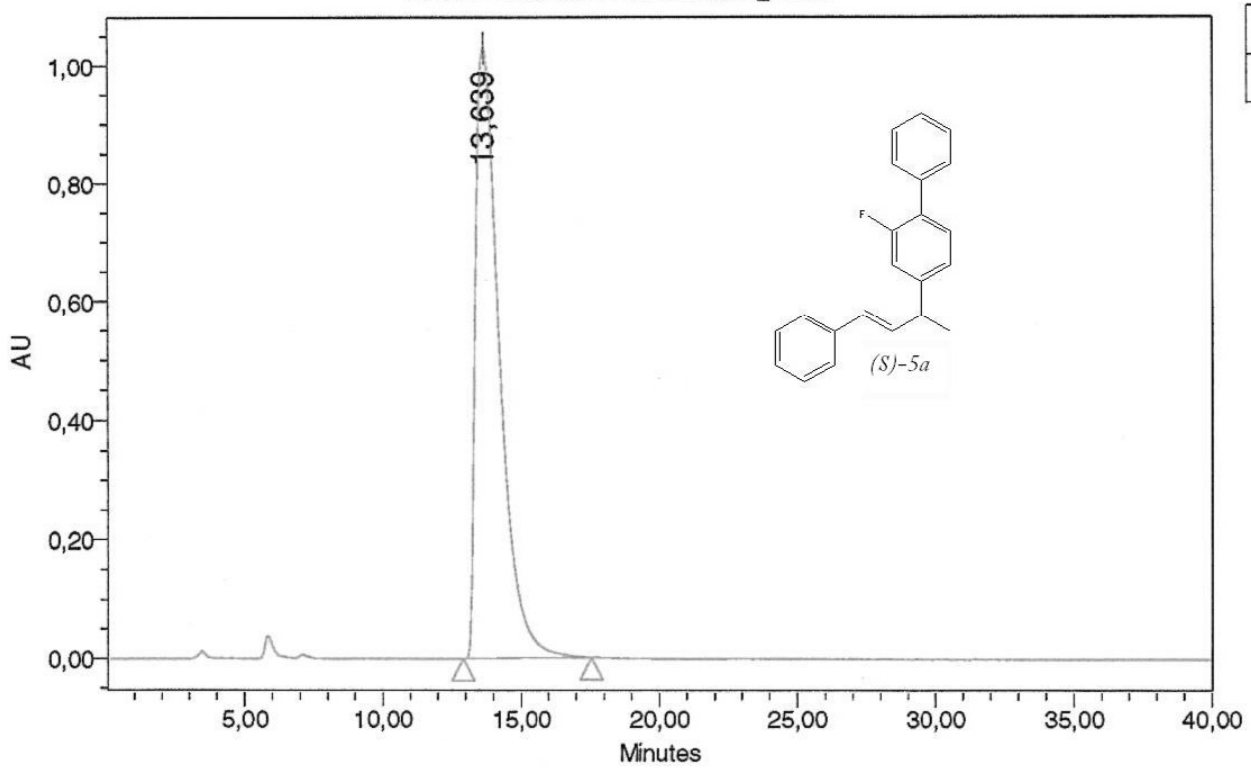
Auto-Scaled Chromatogram



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Empower software

lisa

Reported by User: HPLC User (User)

Project Name: Lisa

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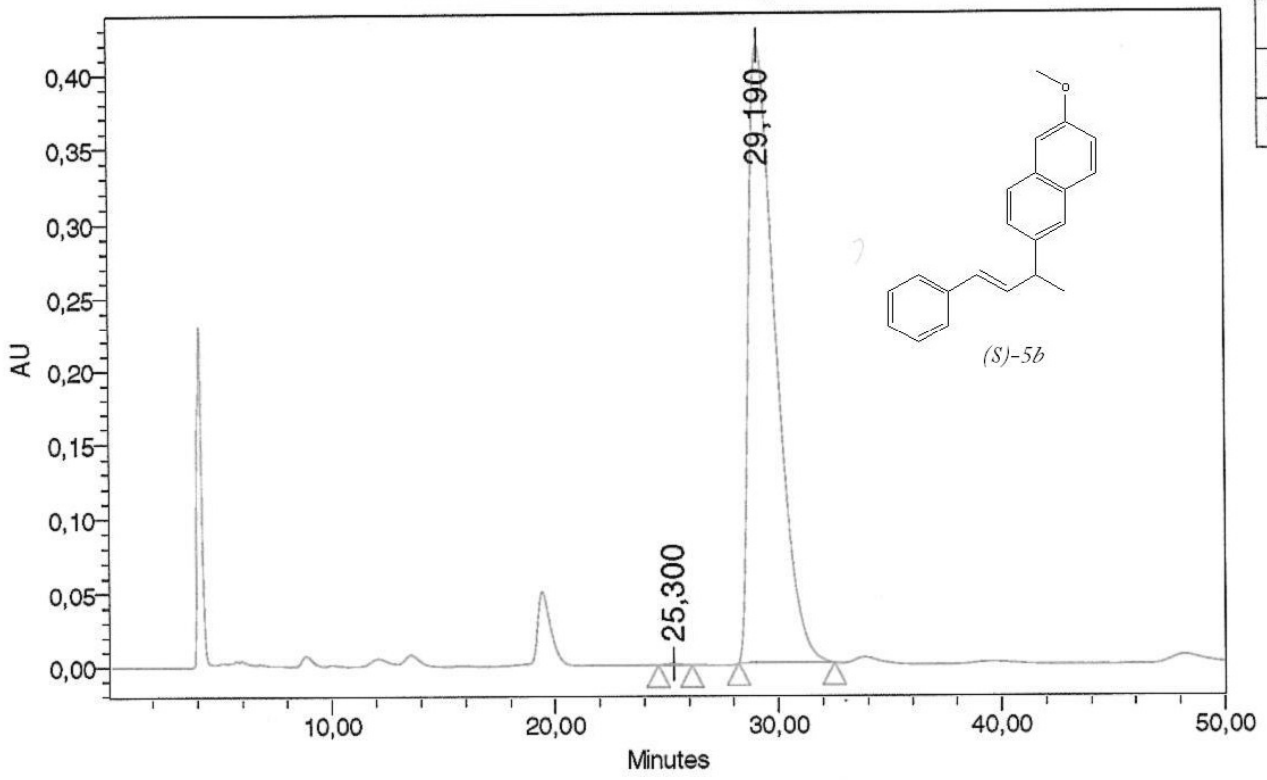
Auto-Scaled Chromatogram



(S)-5b

Peak Results

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Empower software

lisa

Reported by User: HPLC User (User)

Project Name: Lisa

SAMPLE INFORMATION

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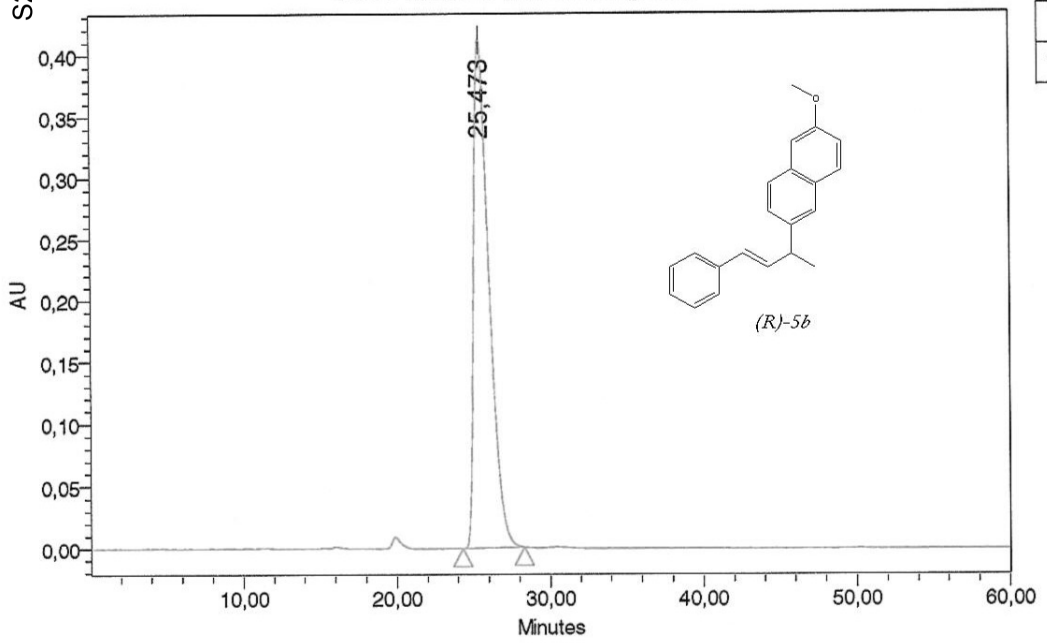
S21

Auto-Scaled Chromatogram



(R)-5b

Peak Results

	Name	RT	Area	Height	Amount	Units
1		25,473	28275219	411698		

Empower software

lisa

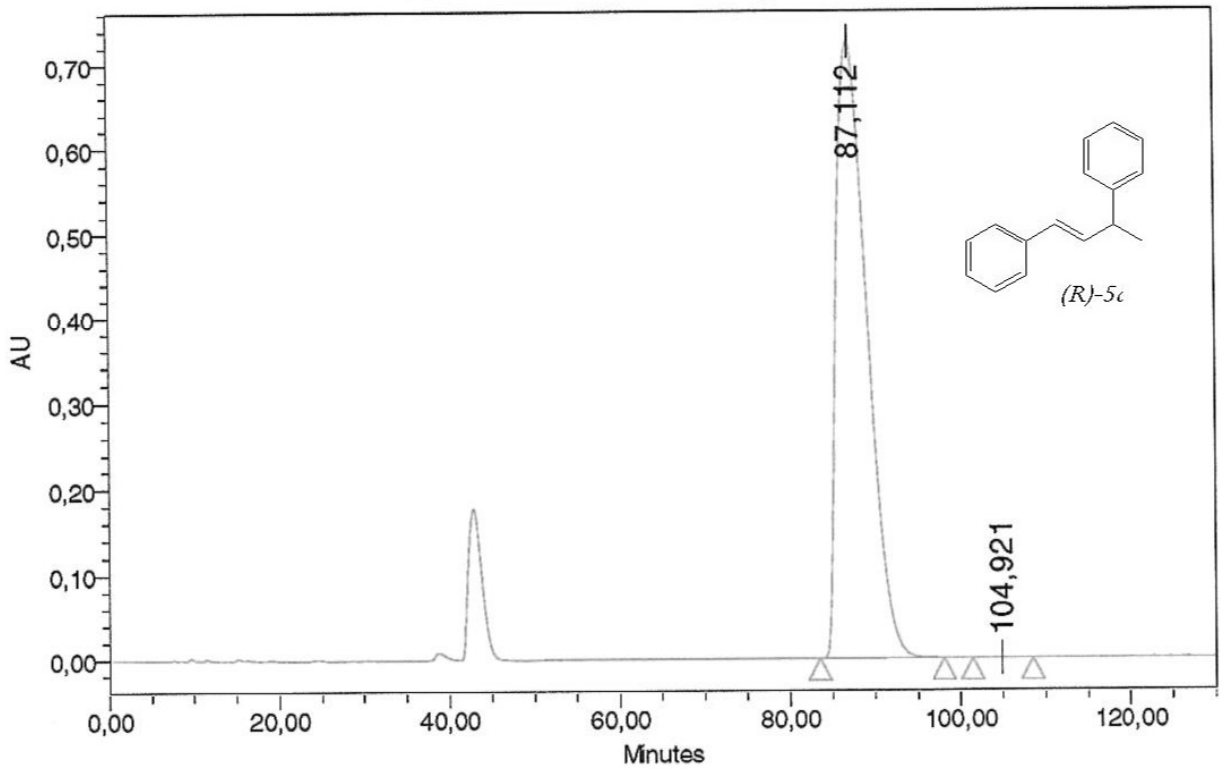
Reported by User: HPLC User (User)

Project Name: Lisa

SAMPLE INFORMATION

Sample Name:	LMK-E-154-crude	Acquired By:	User
Sample Type:	Unknown	Date Acquired:	2010-02-24 14:48:07
Vial:	84	Acq. Method Set:	0_01_0_999
Injection #:	1	Date Processed:	2010-07-02 16:27:30
Injection Volume:	10,00 ul	Processing Method:	Default
Run Time:	130,0 Minutes	Channel Name:	254 nm
Sample Set Name:	20100224_LMK_E_154_155_OJ	Proc. Chnl. Descr.:	PDA 254,0 nm

Auto-Scaled Chromatogram



(R)-5c

Peak Results

	Name	RT	Area	Height	Amount	Units
1		87,112	181068387	725736		
2		104,921	16403	147		

Empower software

lisa

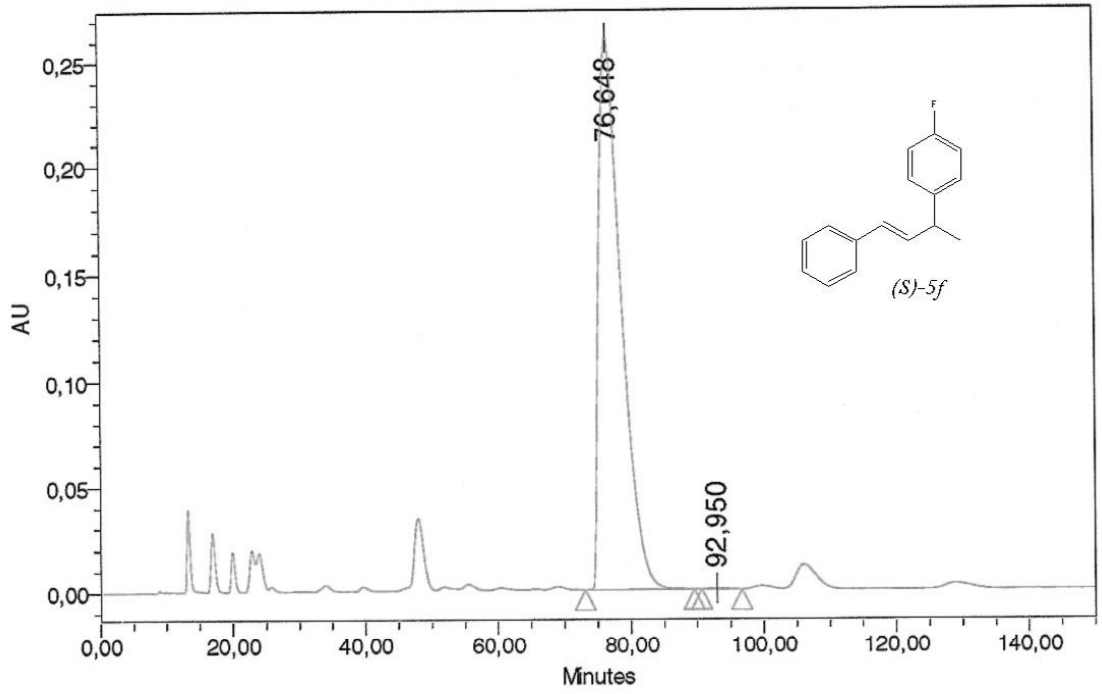
Reported by User: HPLC User (User)

Project Name: Lisa

SAMPLE INFORMATION

Sample Name:	LMK-D-101-S-PHF_OJ_01-999	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	2009-03-26 04:29:46
Vial:	9	Acq. Method Set:	0_01_0_999
Injection #:	1	Date Processed:	2010-07-02 16:20:42
Injection Volume:	10,00 ul	Processing Method:	Default
Run Time:	150,0 Minutes	Channel Name:	254 nm
Sample Set Name:		Proc. Chnl. Descr.:	PDA 254,0 nm

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	Height	Amount	Units
1		76,648	61169669	260482		
2		92,950	106959	650		

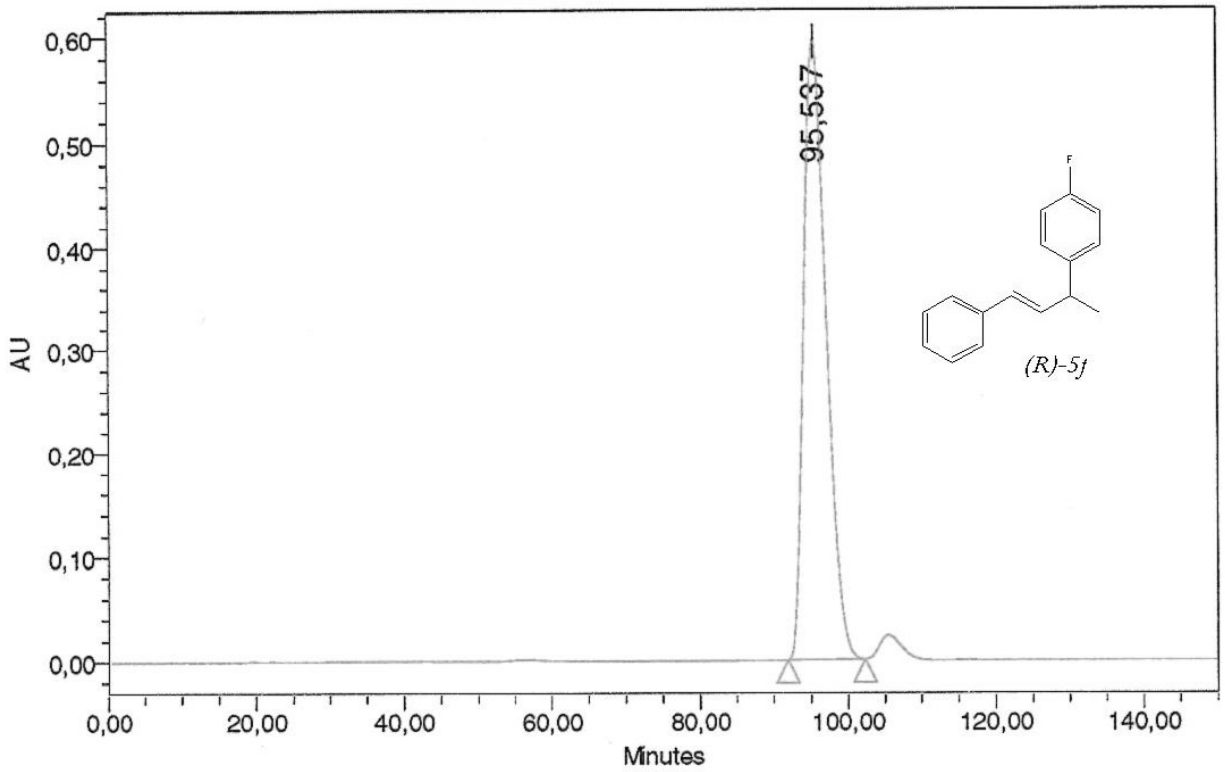
Reported by User: HPLC User (User)

Project Name: Lisa

SAMPLE INFORMATION

Sample Name:	LMK-D-96-R-Ph_OJ_01-999	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	2009-03-25 21:57:22
Vial:	6	Acq. Method Set:	0_01_0_999
Injection #:	1	Date Processed:	2010-07-05 15:25:58
Injection Volume:	10,00 ul	Processing Method:	Default
Run Time:	150,0 Minutes	Channel Name:	254 nm
Sample Set Name:		Proc. Chnl. Descr.:	PDA 254,0 nm

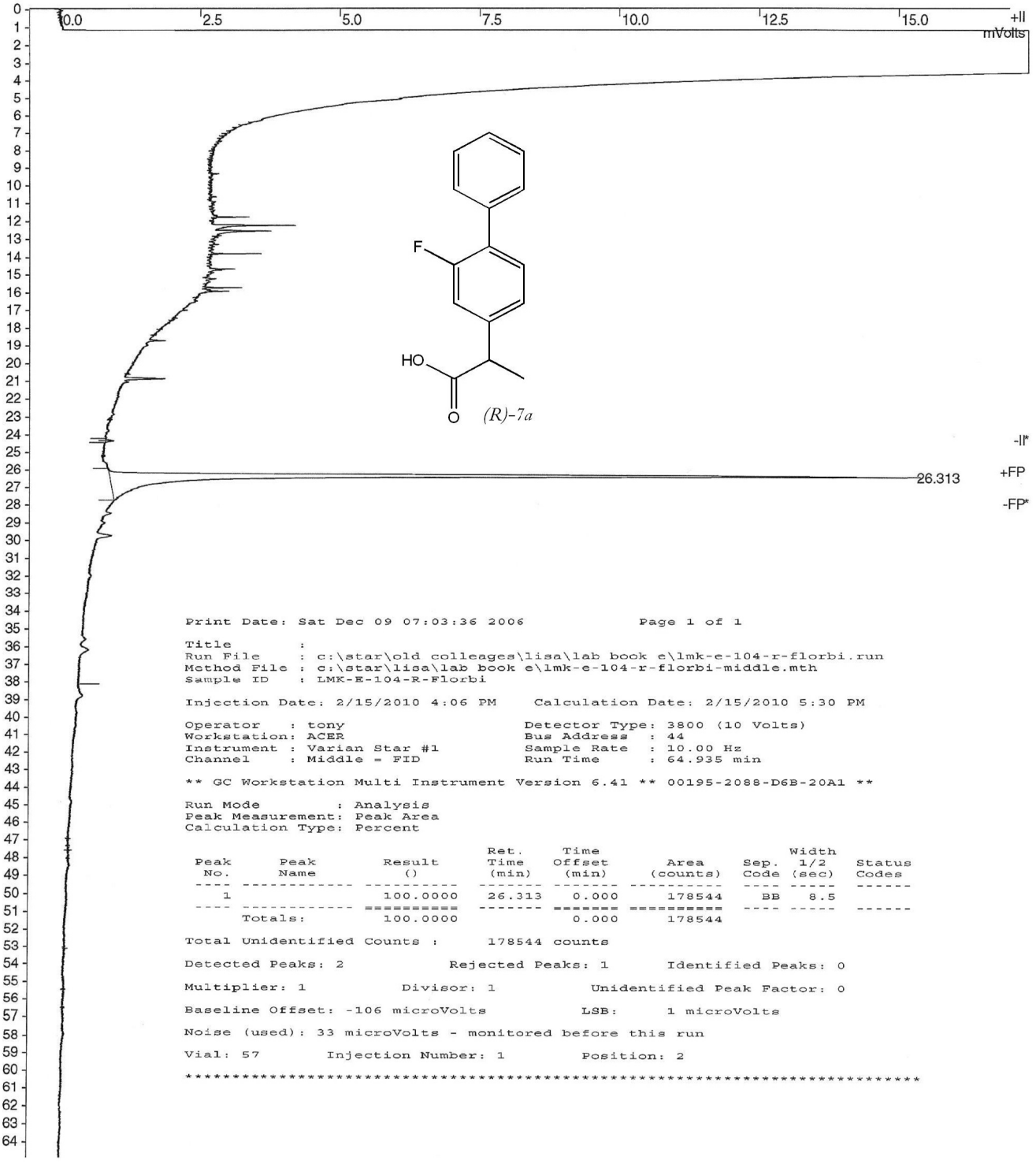
Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	Height	Amount	Units
1		95,537	125718292	593596		

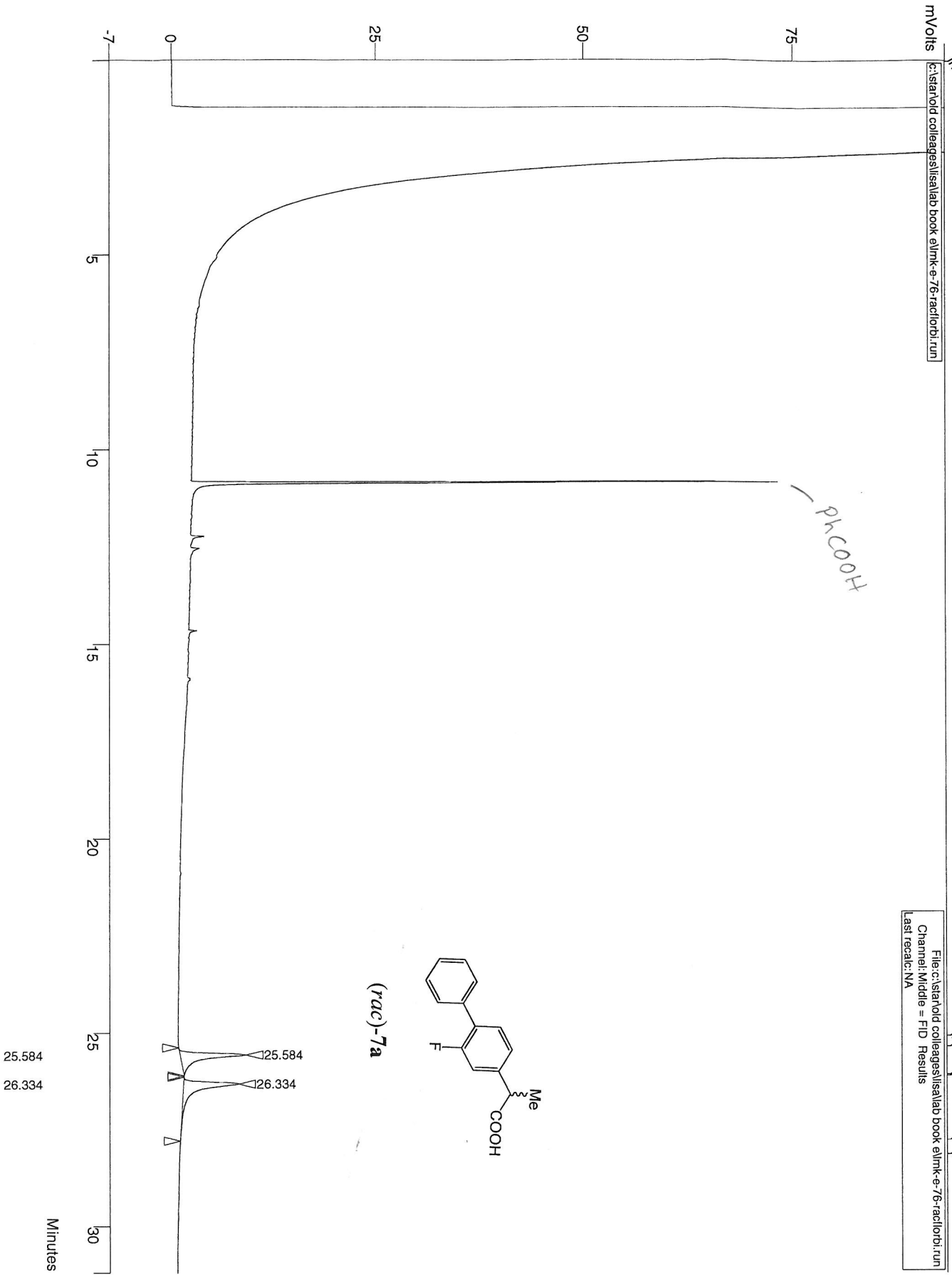
```
Title       :
Run File    : c:\star\old colleages\lisa\lab book e\lmk-e-104-r-florbi.run
Method File : c:\star\lisa\lab book e\lmk-e-104-r-florbi-middle.mth
Sample ID   : LMK-E-104-R-Florbi

Injection Date: 2/15/2010 4:06 PM    Calculation Date: 2/15/2010 5:30 PM

Operator    : tony                   Detector Type: 3800 (10 Volts)
Workstation: ACER                    Bus Address  : 44
Instrument : Varian Star #1          Sample Rate  : 10.00 Hz
Channel    : Middle = FID            Run Time     : 64.935 min

** GC Workstation Multi Instrument Version 6.41 ** 00195-2088-D6B-20A1 **

Chart Speed =    0.30 cm/min   Attenuation = 7              Zero Offset = 3%
Start Time  =    0.000   min    End Time    = 64.935  min   Min / Tick  = 1.00
```



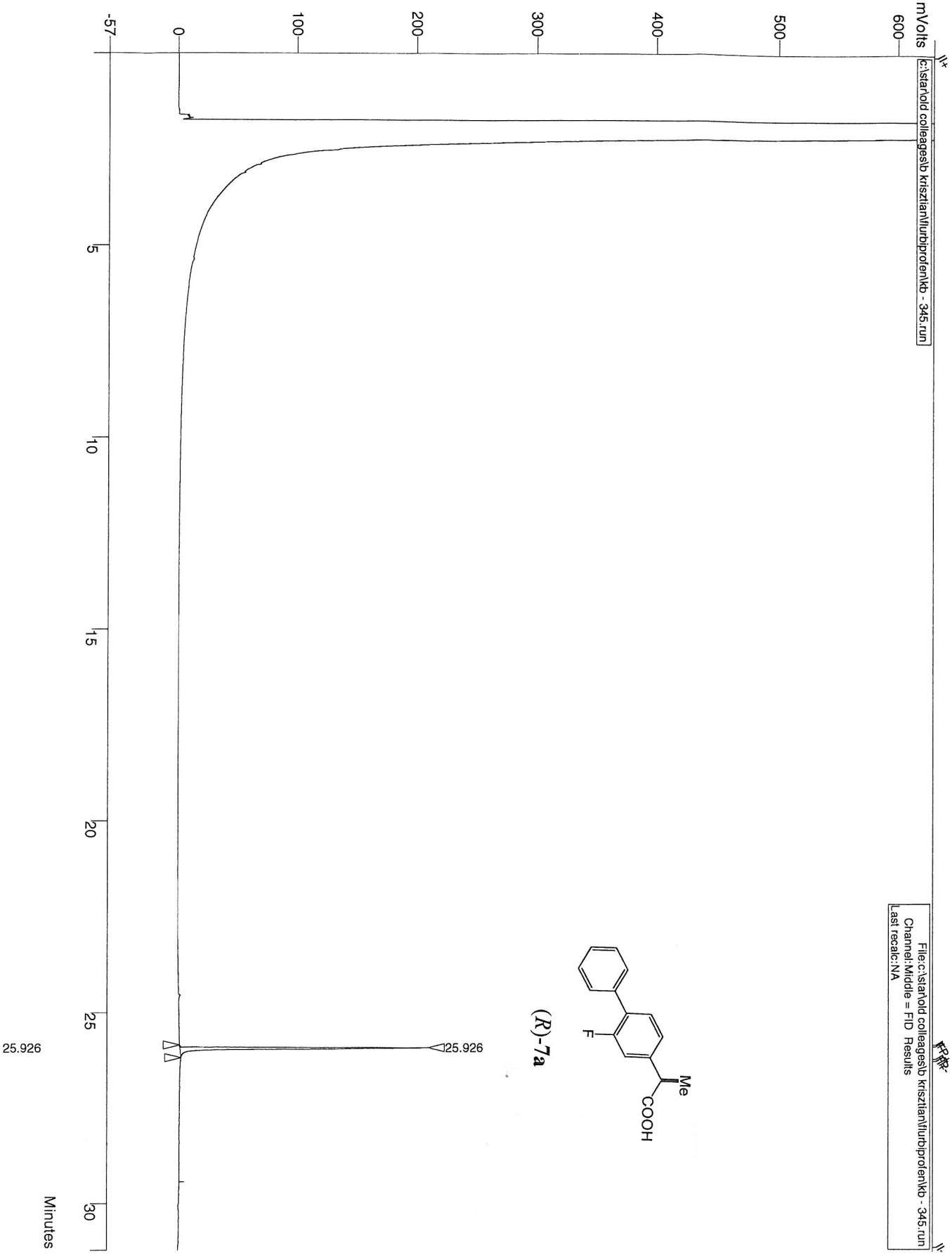

```
Print Date: Sat Dec 09 07:03:36 2006            Page 1 of 1

Title       :
Run File    : c:\star\old colleages\lisa\lab book e\lmk-e-104-r-florbi.run
Method File : c:\star\lisa\lab book e\lmk-e-104-r-florbi-middle.mth
Sample ID   : LMK-E-104-R-Florbi

Injection Date: 2/15/2010 4:06 PM    Calculation Date: 2/15/2010 5:30 PM

Operator    : tony                   Detector Type: 3800 (10 Volts)
Workstation: ACER                    Bus Address  : 44
Instrument : Varian Star #1          Sample Rate  : 10.00 Hz
Channel    : Middle = FID            Run Time     : 64.935 min

** GC Workstation Multi Instrument Version 6.41 ** 00195-2088-D6B-20A1 **

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		100.0000	26.313	0.000	178544	BB	8.5	
Totals:		100.0000		0.000	178544			

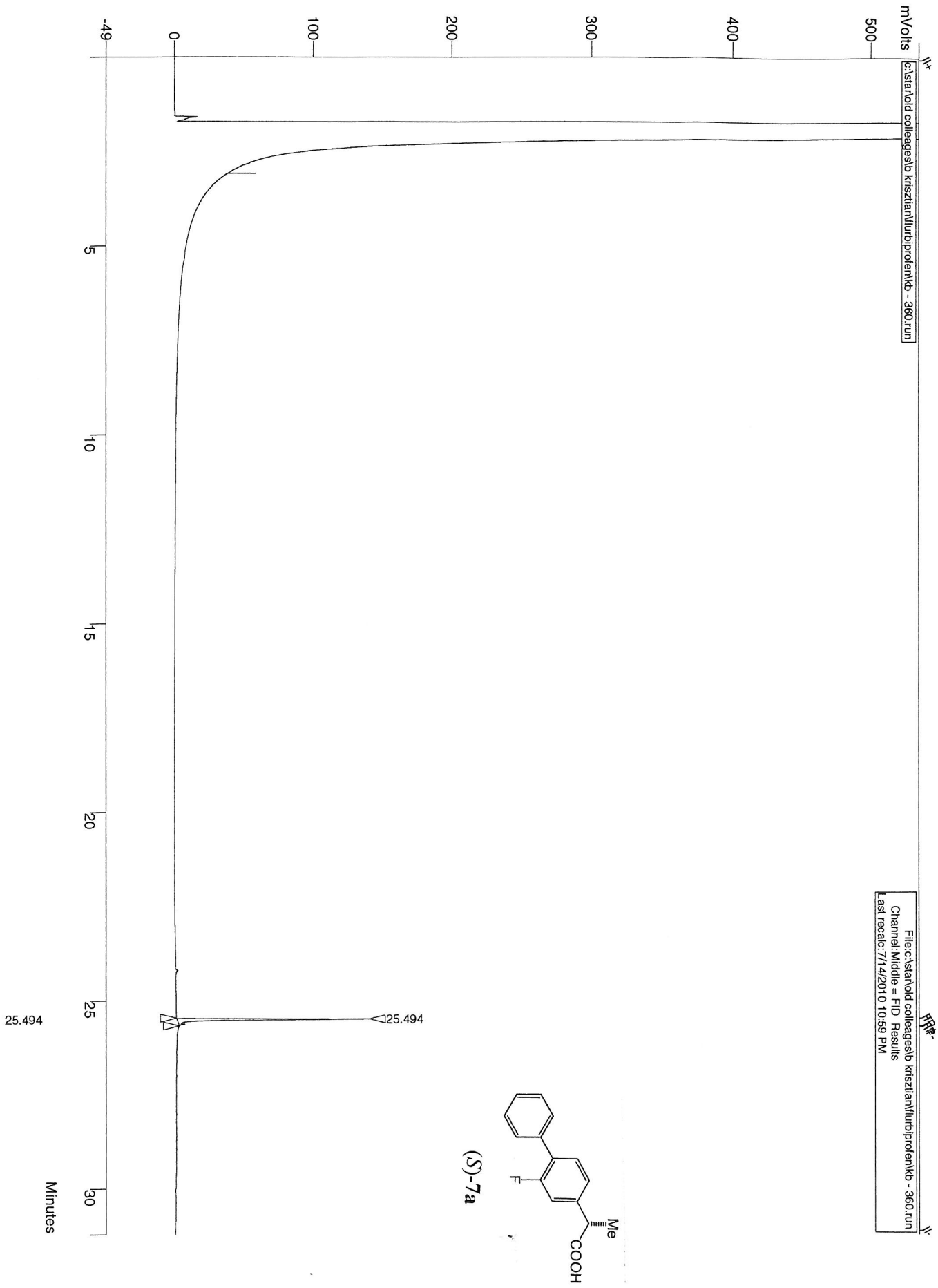
```
Total Unidentified Counts :      178544 counts

Detected Peaks: 2            Rejected Peaks: 1       Identified Peaks: 0

Multiplier: 1           Divisor: 1           Unidentified Peak Factor: 0

Baseline Offset: -106 microVolts          LSB:      1 microVolts

Noise (used): 33 microVolts - monitored before this run

Vial: 57       Injection Number: 1         Position: 2

********************************************************************************
```


mVolts
c:\star\old colleages\lisa\lab book e\lmk-e-76-racflorbi.run
PhCOOH
File:c:\star\old colleages\lisa\lab book e\lmk-e-76-racflorbi.run
Channel:Middle = FID Results
Last recalc:NA
F
Me
COOH
25.584
26.334
Minutes

(*rac*)-**7a**


mVolts
600
500
400
300
200
100
0
-57
c:\star\old colleages\b krisztian\flurbiprofen\kb - 345.run
File:c:\star\old colleages\b krisztian\flurbiprofen\kb - 345.run
Channel:Middle = FID Results
Last recalc:NA
5
10
15
20
25
30
Minutes
25.926
25.926
F
Me
COOH

(*R*)-**7a**


mVolts
500
400
300
200
100
0
-49
c:\star\old colleages\b krisztian\flurbiprofen\kb - 360.run
File:c:\star\old colleages\b krisztian\flurbiprofen\kb - 360.run
Channel:Middle = FID Results
Last recalc:7/14/2010 10:59 PM
5
10
15
20
25
30
Minutes
25.494
25.494
F
Me
COOH

(*S*)-**7a**