

## Electronic Supplementary Information

### “Organocatalytic Enantioselective Synthesis of Acyclic Pyrimidine Nucleosides by Aza-Michael Reaction”

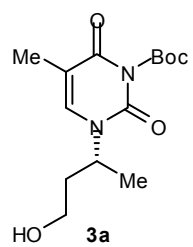
Su-Jeong Lee, Jun-Gi Ahn, Jihwan Seo, Heun-Jong Ha and Chang-Woo Cho\*

*Department of Chemistry and Green-Nano Materials Research Center,  
Kyungpook National University, Daegu 41566, Republic of Korea*

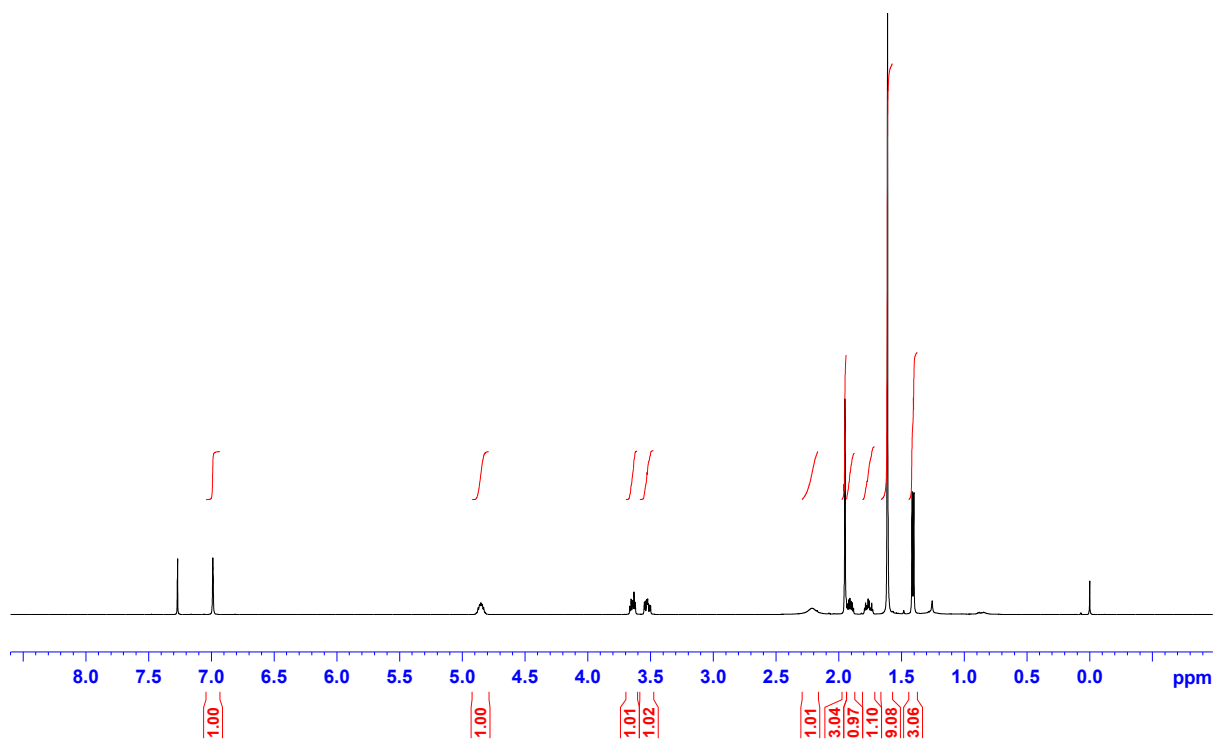
*\*E-mail: cwcho@knu.ac.kr*

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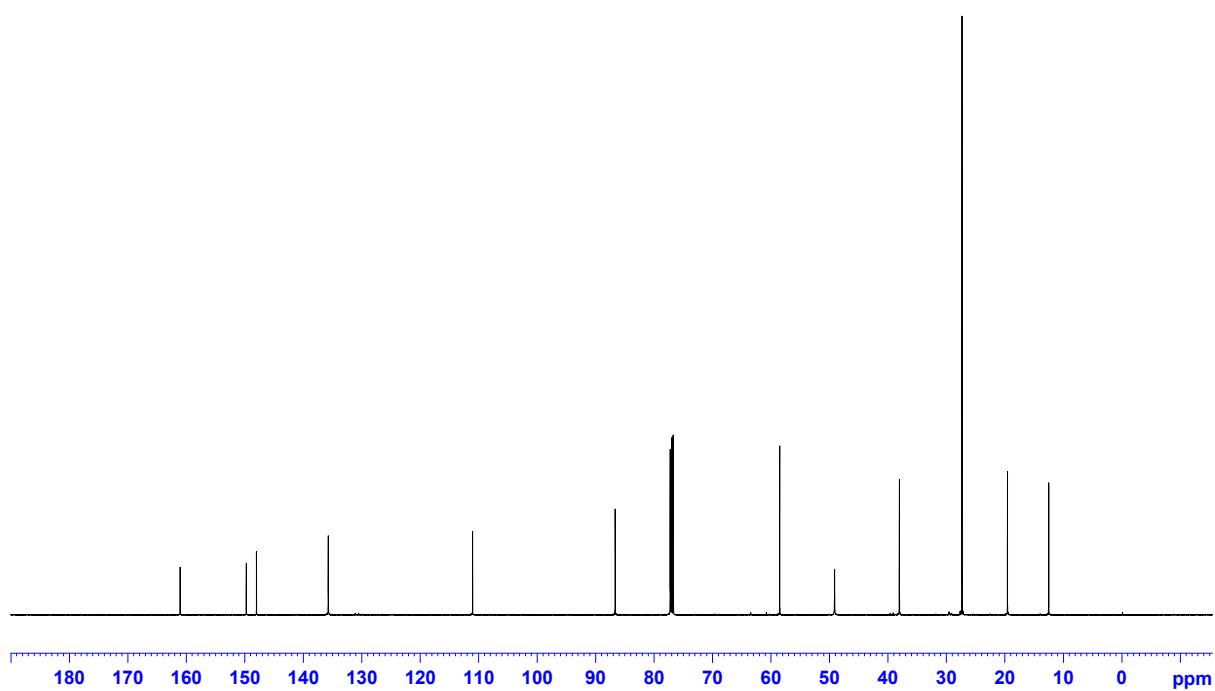
<b>Spectral data and HPLC traces of new compounds</b>	S2–S53
<b>X-Ray crystal structure of 8</b>	S54



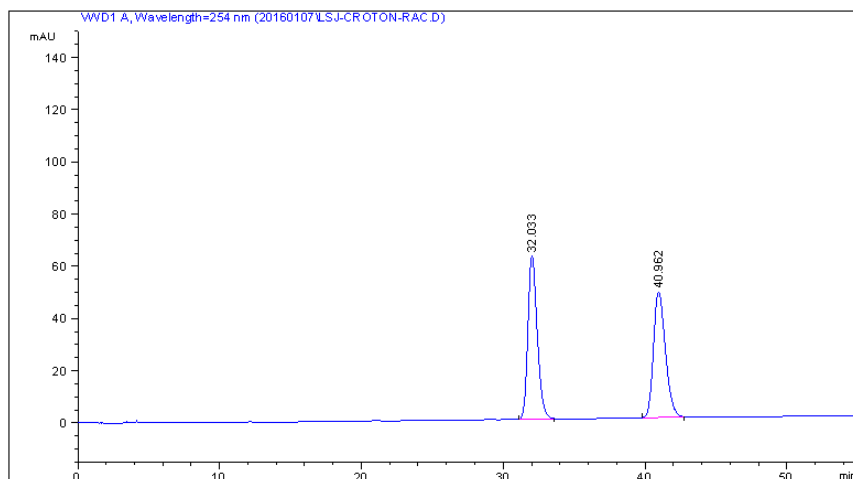
$^1\text{H NMR}$  of **3a**



$^{13}\text{C NMR}$  of **3a**



### Racemate of 3a



#### Area Percent Report

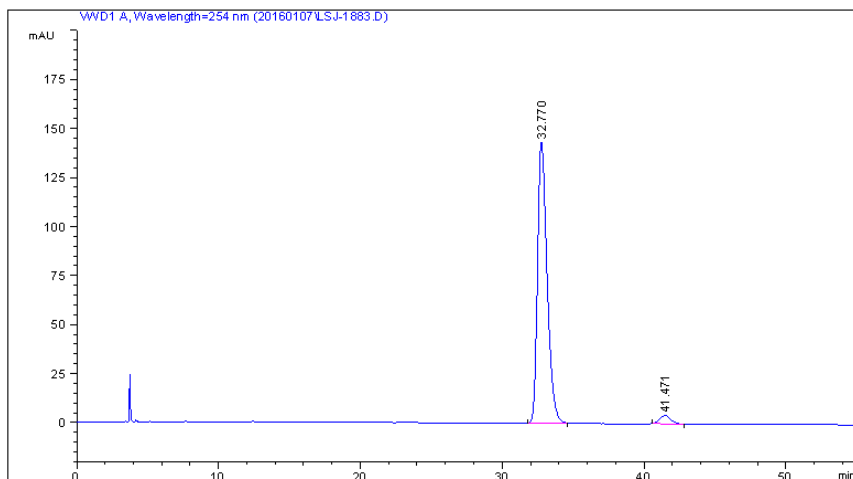
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Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	32.033	BB	0.7020	2864.84839	62.52020	50.4033
2	40.962	BB	0.9074	2818.99805	48.14020	49.5967

Totals : 5683.84644 110.66040

### Enantiomeric excess of 3a: 93%



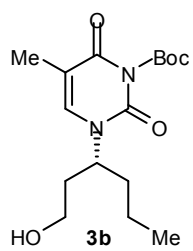
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Use Multiplier & Dilution Factor with ISTDs

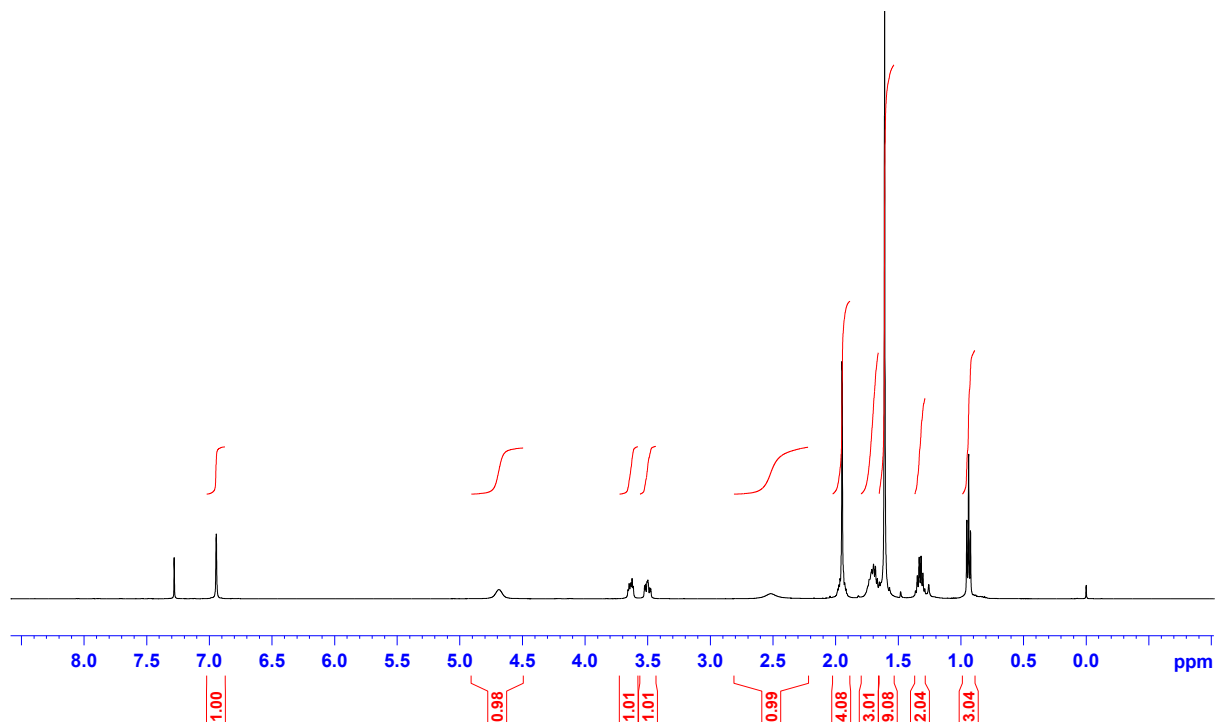
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	32.770	BB	0.7161	6717.59814	143.21561	96.7397
2	41.471	BB	0.8155	226.39282	4.21806	3.2603

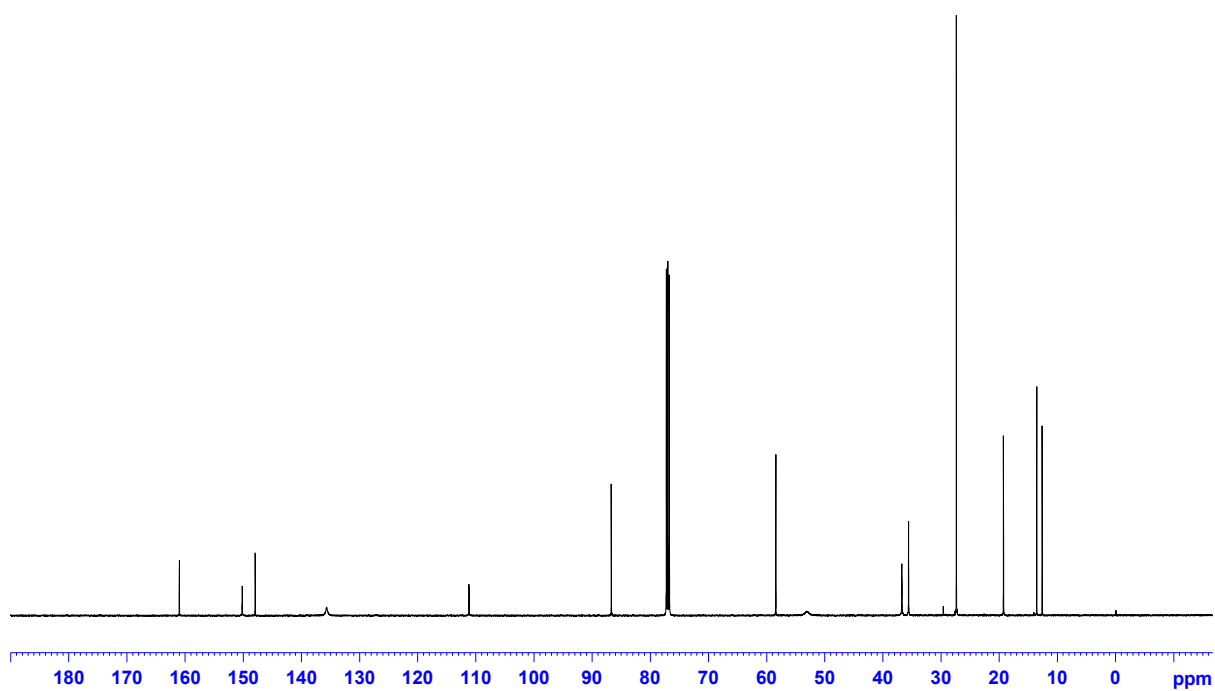
Totals : 6943.99097 147.43366



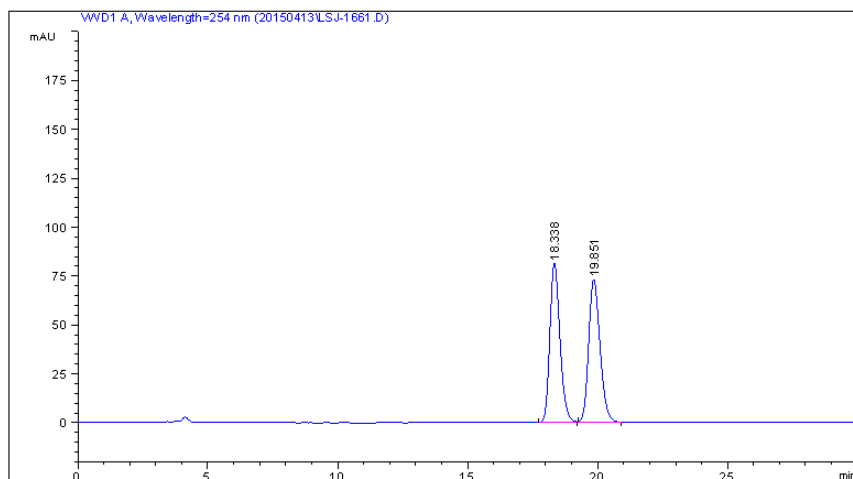
<sup>1</sup>H NMR of **3b**



<sup>13</sup>C NMR of **3b**



*Racemate of 3b*



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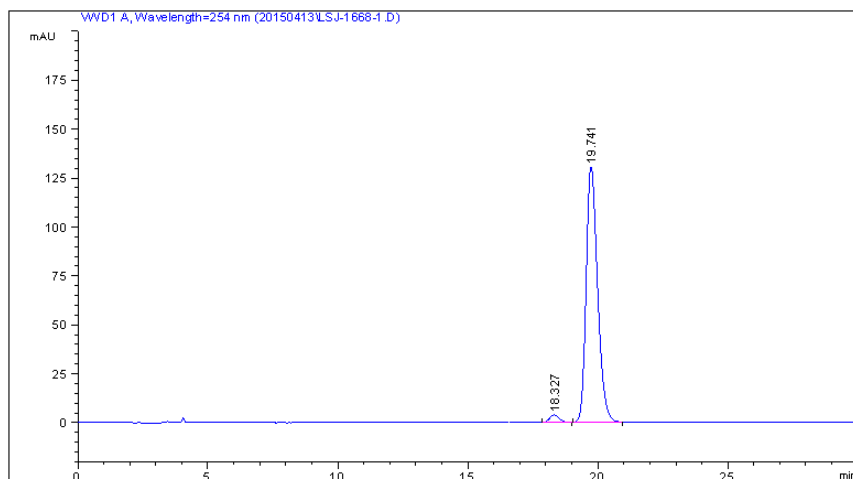
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Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: WWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	18.338	BB	0.4181	2217.85718	81.46687	49.7978
2	19.851	BB	0.4733	2235.87061	73.10355	50.2022

Totals : 4453.72778 154.57041

*Enantiomeric excess of 3b: 95%*



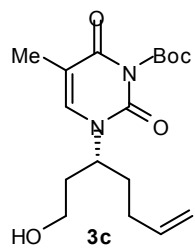
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Use Multiplier & Dilution Factor with ISTDs

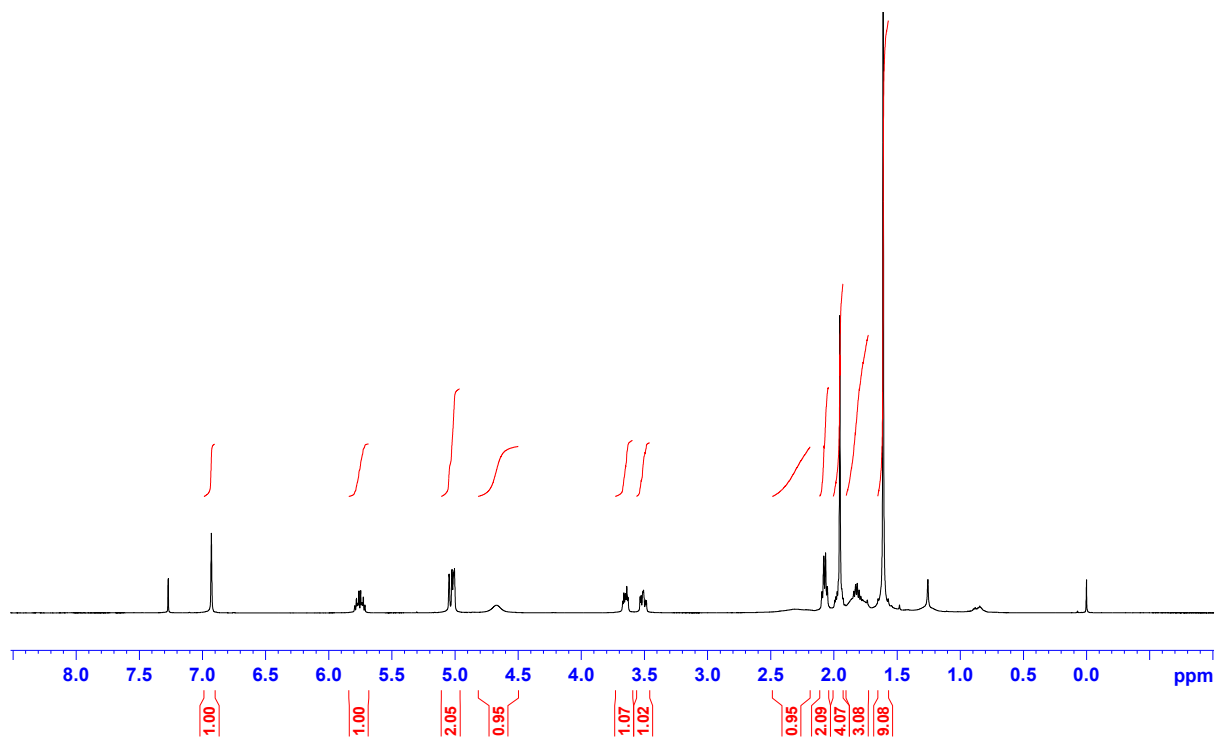
Signal 1: WWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	18.327	BB	0.4070	101.83482	3.87557	2.4909
2	19.741	BB	0.4696	3986.42578	130.61250	97.5091

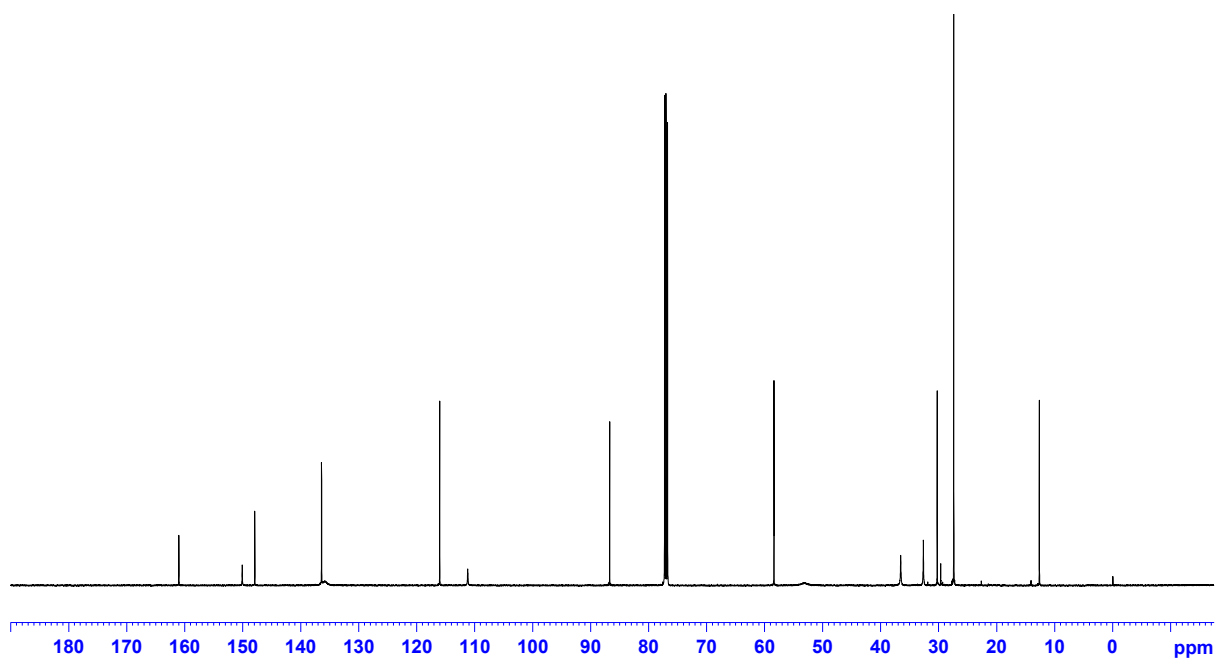
Totals : 4088.26060 134.48807



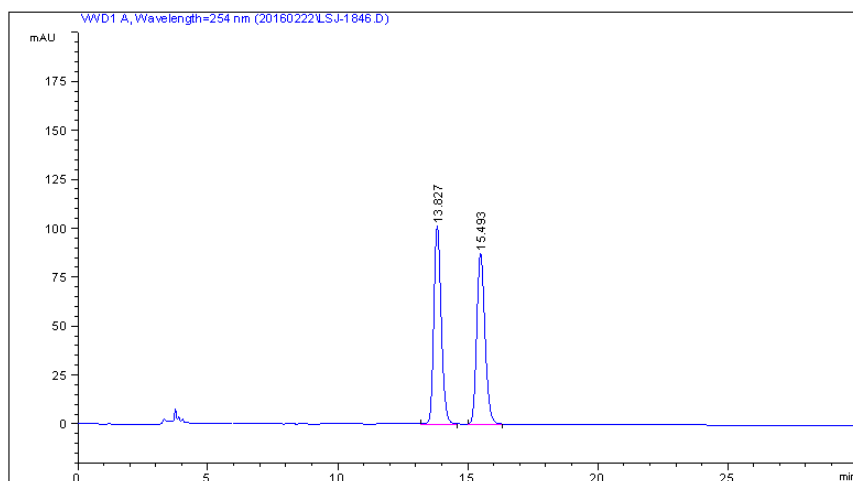
$^1\text{H NMR}$  of **3c**



$^{13}\text{C NMR}$  of **3c**



*Racemate of 3c*



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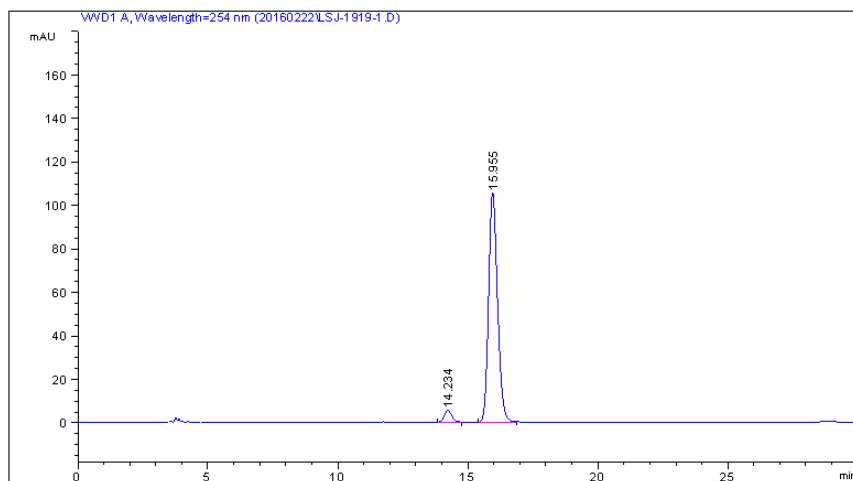
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 Dilution: : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	13.827	BB	0.3042	1993.06494	101.14150	50.8941
2	15.493	BB	0.3384	1923.03735	87.33253	49.1059

Totals : 3916.10229 188.47404

*Enantiomeric excess of 3c: 92%*



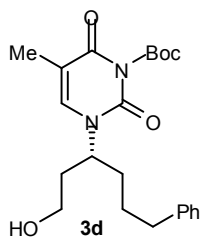
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 Use Multiplier & Dilution Factor with ISTDs

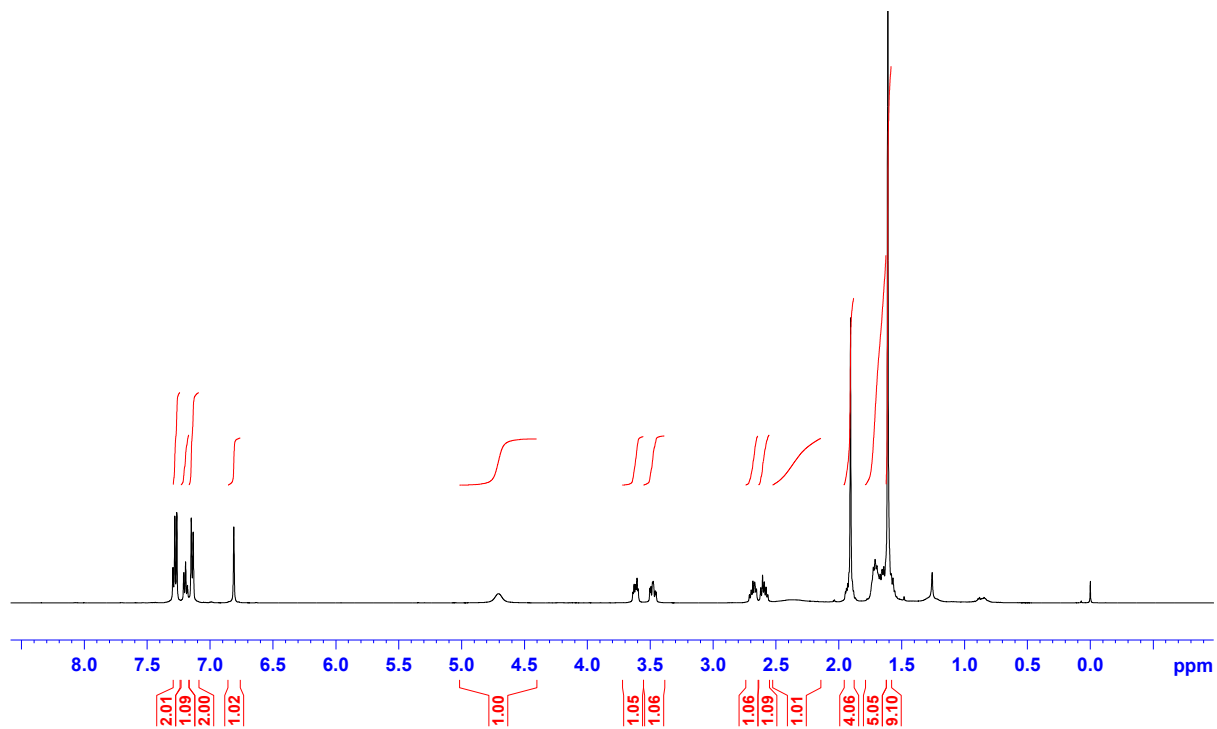
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.234	BB	0.3116	110.34633	5.45808	4.2001
2	15.955	BB	0.3672	2516.90430	105.47299	95.7999

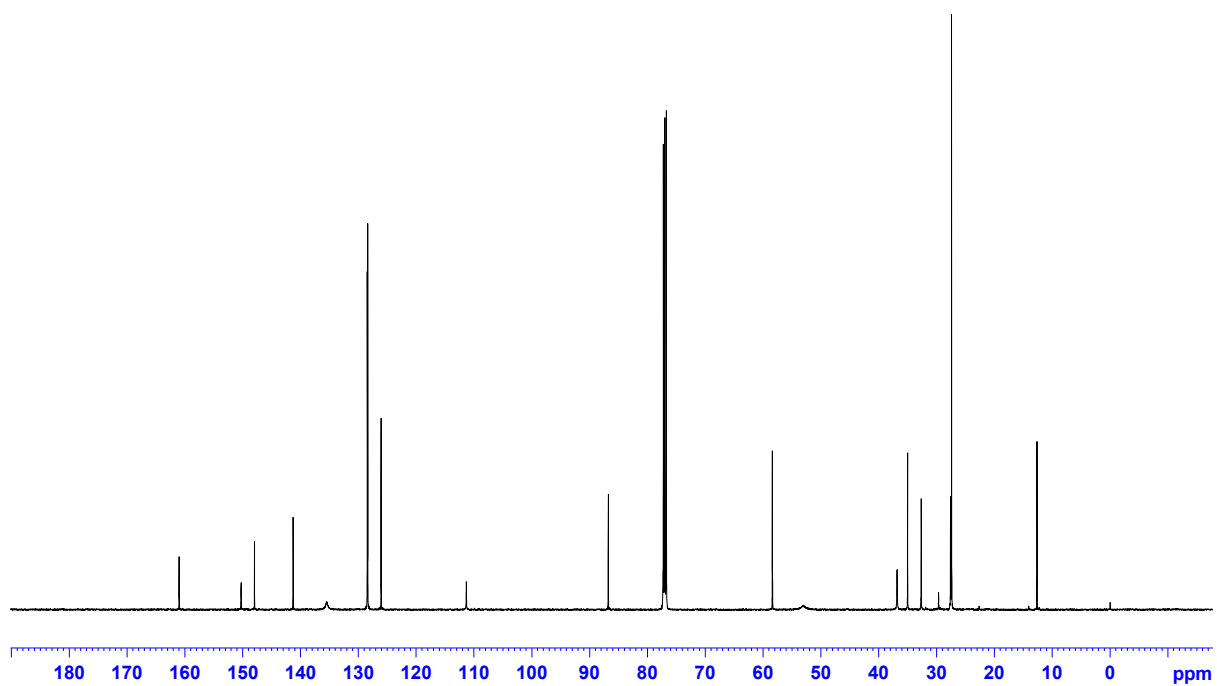
Totals : 2627.25063 110.93108



$^1\text{H NMR}$  of **3d**

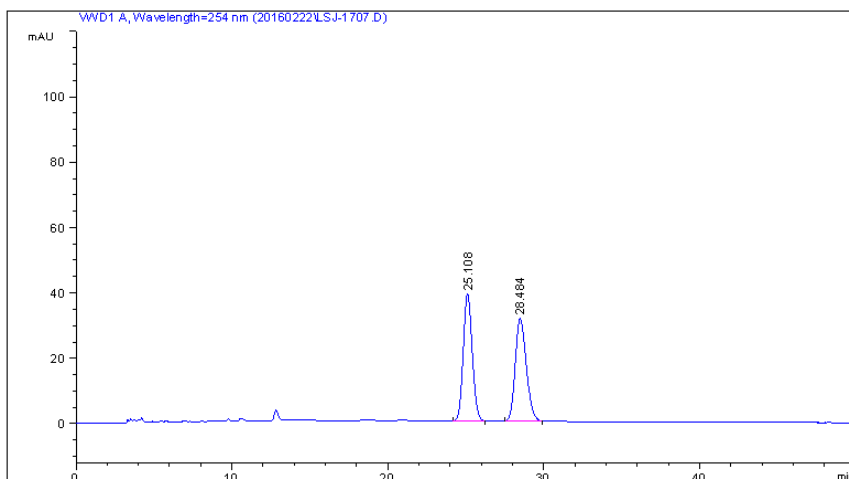


$^{13}\text{C NMR}$  of **3d**





*Racemate of 3d*



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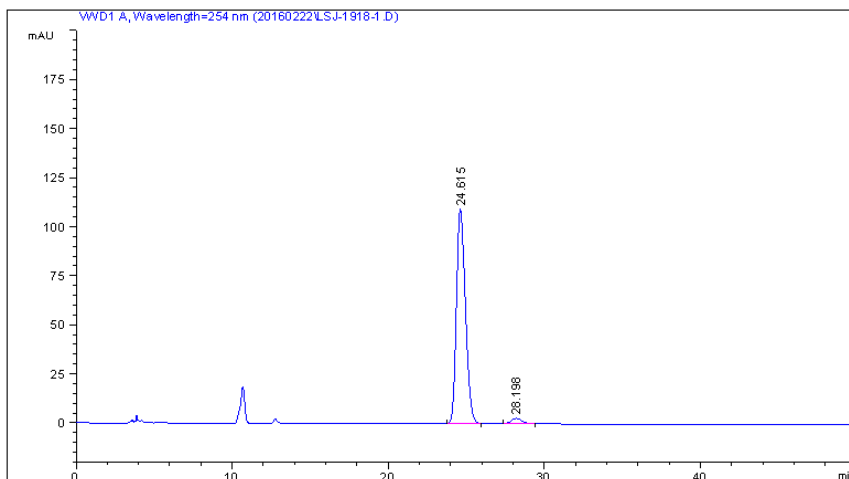
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	25.108	BB	0.6269	1563.03955	38.83009	50.1532
2	28.484	BB	0.7628	1553.48755	31.36421	49.8468

Totals : 3116.52710 70.19430

*Enantiomeric excess of 3d: 94%*



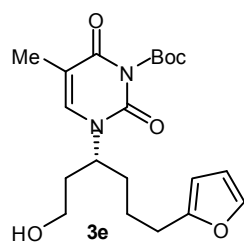
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Use Multiplier & Dilution Factor with ISTDs

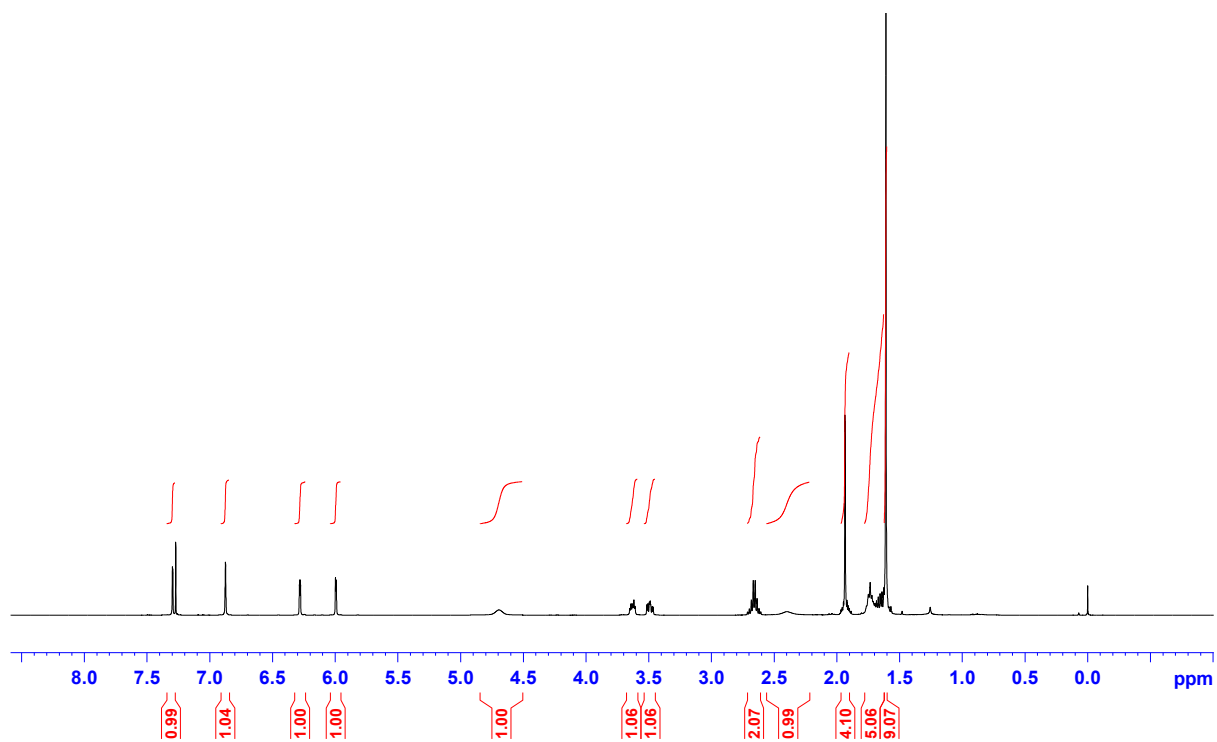
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	24.615	BB	0.6213	4377.87549	109.36605	97.0448
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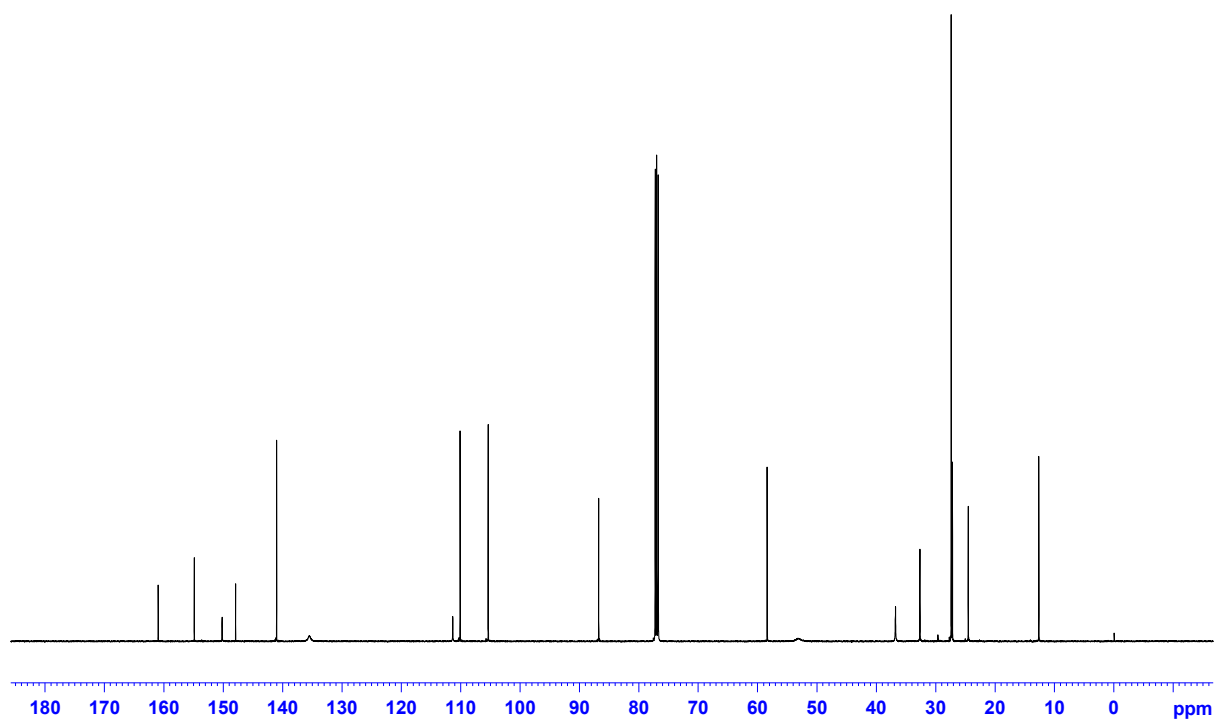
Totals : 4511.18829 112.17606



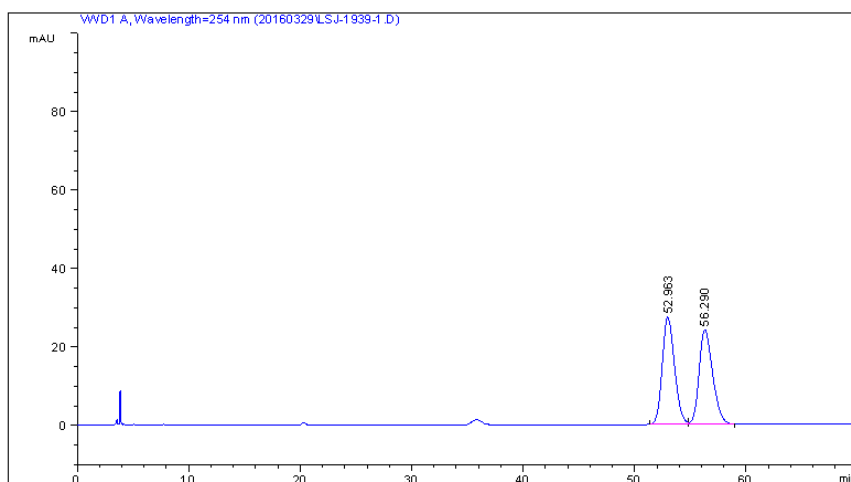
$^1\text{H NMR}$  of **3e**



$^{13}\text{C NMR}$  of **3e**



## Racemate of **3e**



### Area Percent Report

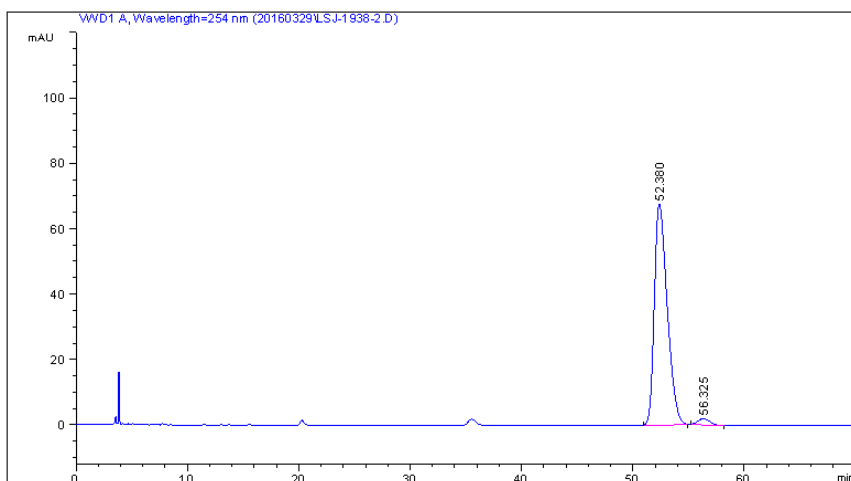
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: WVD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	52.963	BV	1.1945	2103.75146	27.34833	50.5511	
2	56.290	VB	1.2766	2057.88574	24.15050	49.4489	

Totals : 4161.63721 51.49883

## Enantiomeric excess of **3e**: 95%



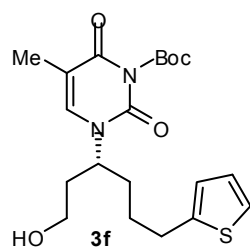
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Use Multiplier & Dilution Factor with ISTDs

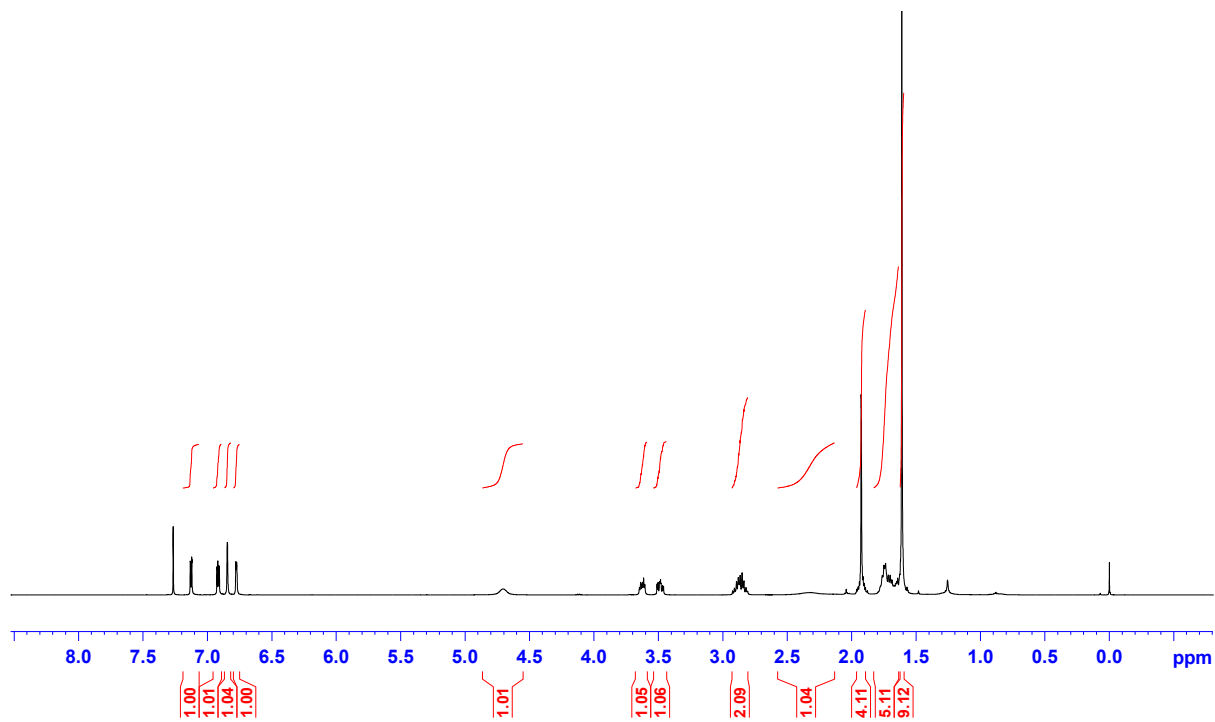
Signal 1: WVD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	52.380	BB	1.2345	5434.72949	67.52699	97.4186	
2	56.325	BB	0.9357	144.00957	1.91465	2.5814	

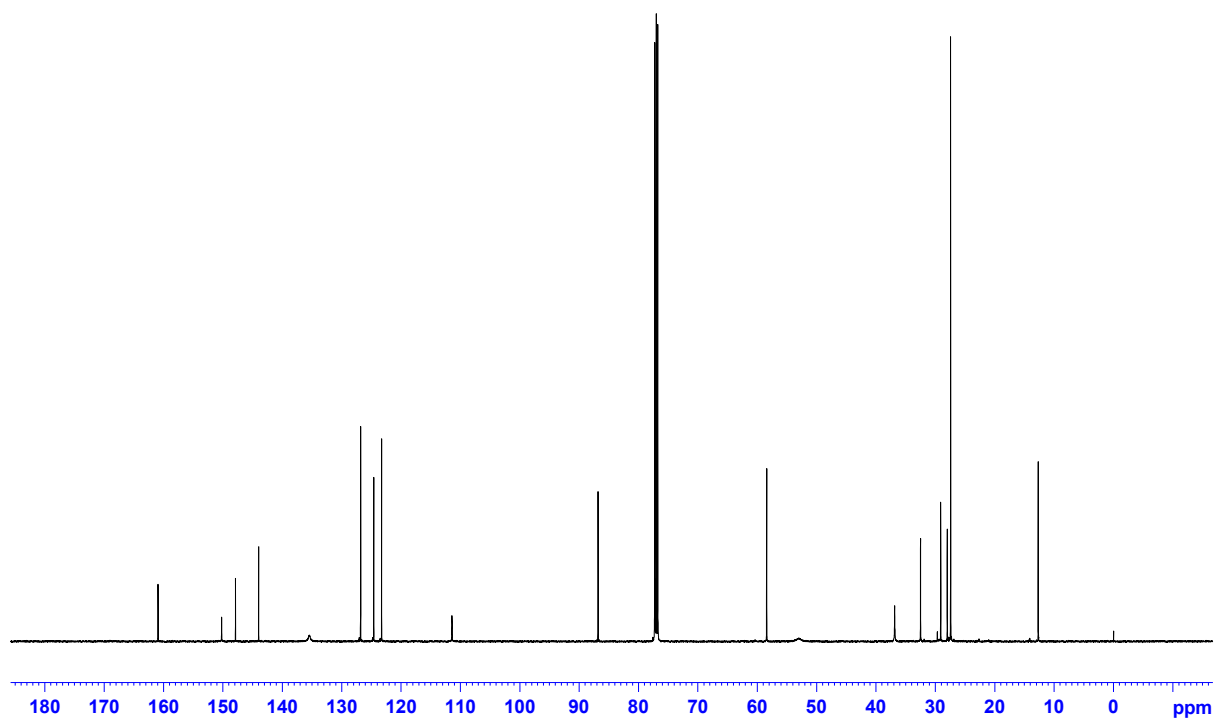
Totals : 5578.73906 69.44164



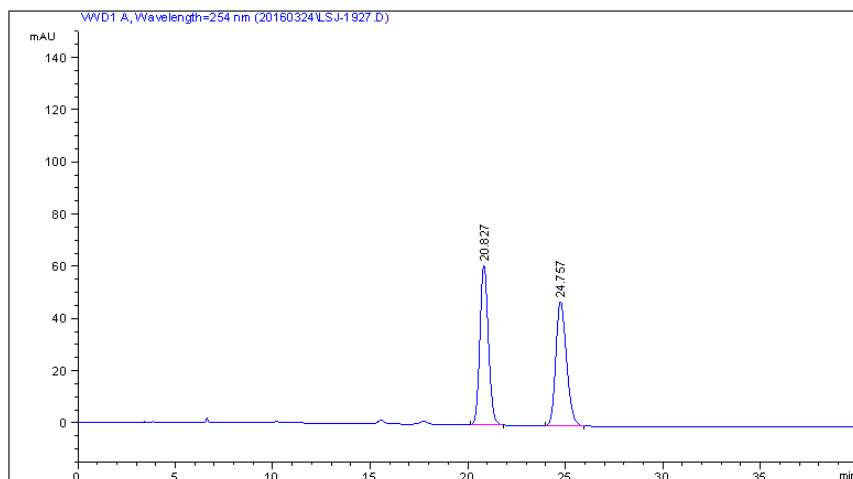
$^1\text{H NMR}$  of **3f**



$^{13}\text{C NMR}$  of **3f**



*Racemate of 3f*



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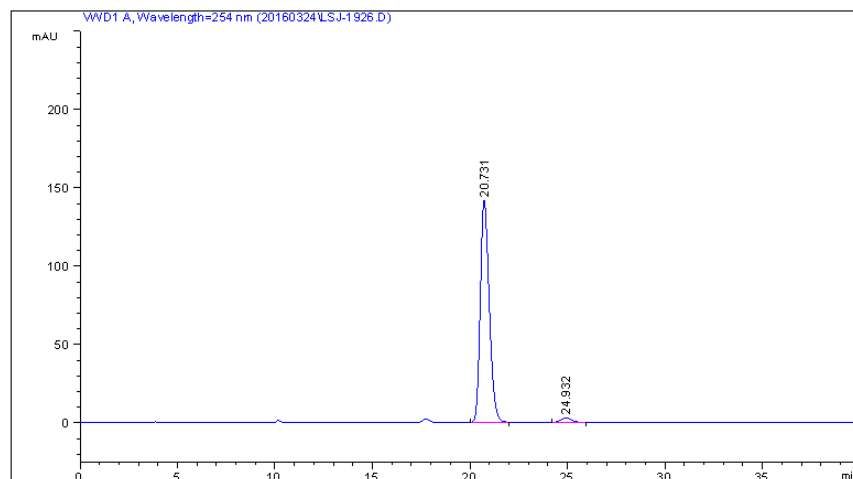
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Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	20.827	BB	0.4709	1858.70581	61.17733	50.4993
2	24.757	BB	0.5933	1821.95032	47.63438	49.5007

Totals : 3680.65613 108.81172

*Enantiomeric excess of 3f: 95%*



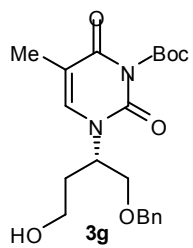
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Area Percent Report  
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Use Multiplier & Dilution Factor with ISTDs

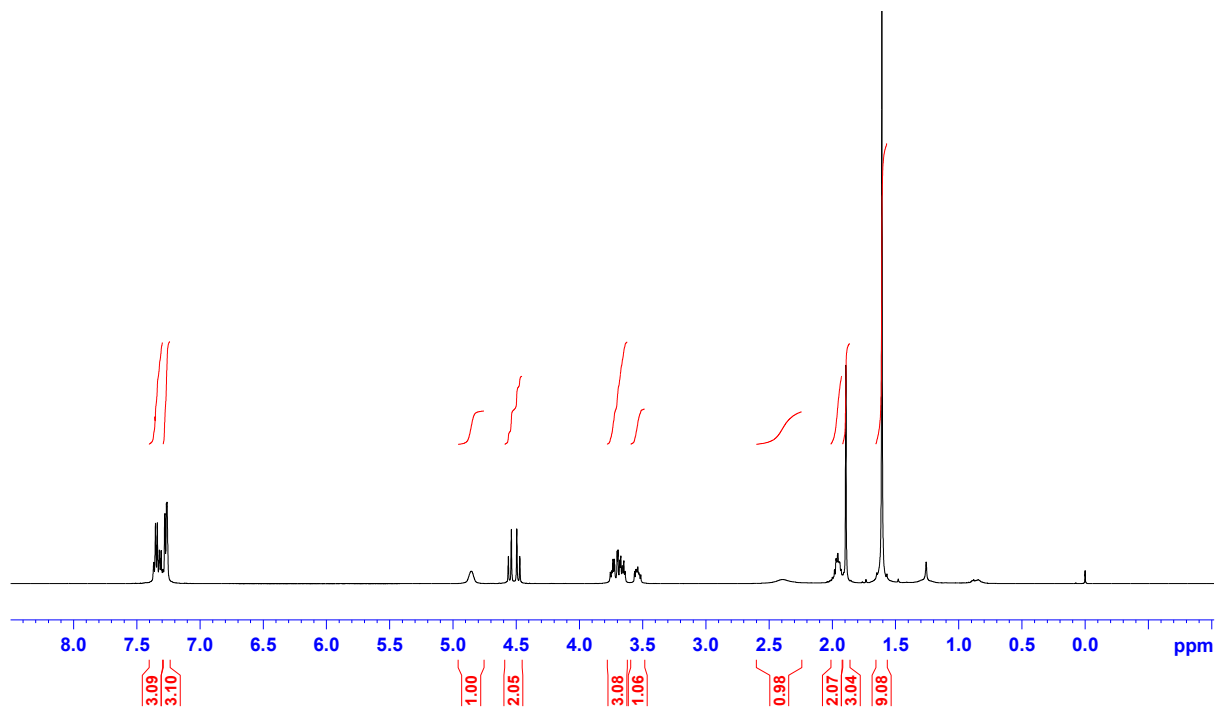
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	20.731	BB	0.4949	4540.33008	141.61728	97.4861
2	24.932	BB	0.5768	117.08242	3.01498	2.5139

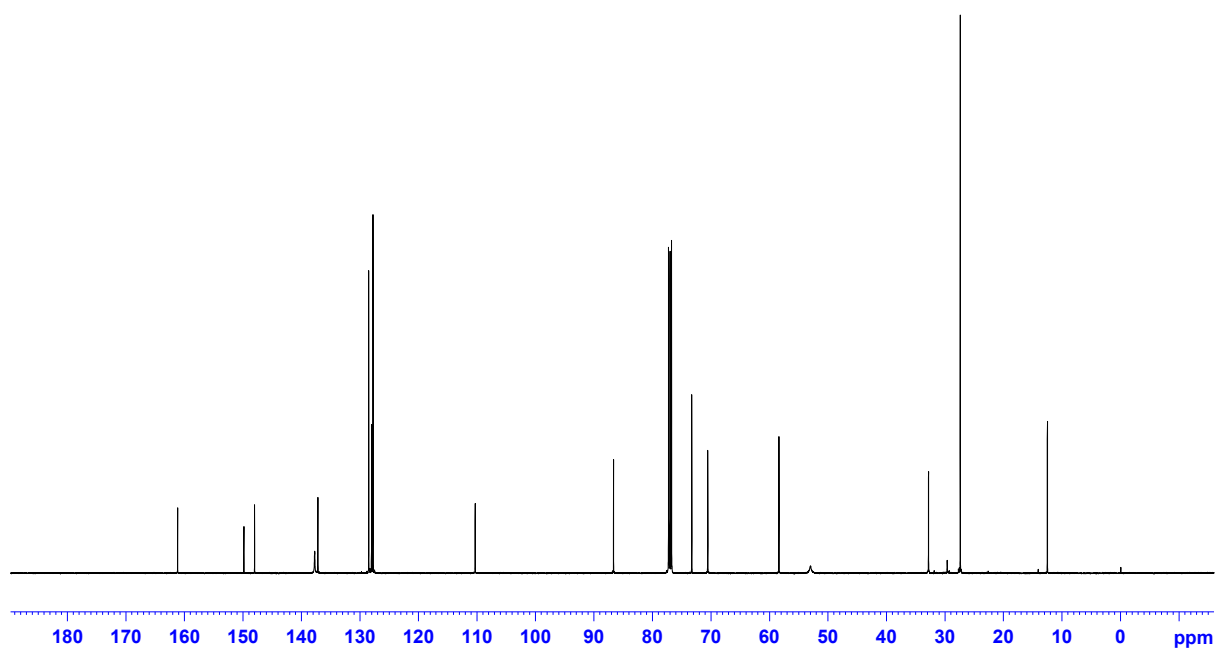
Totals : 4657.41250 144.63226



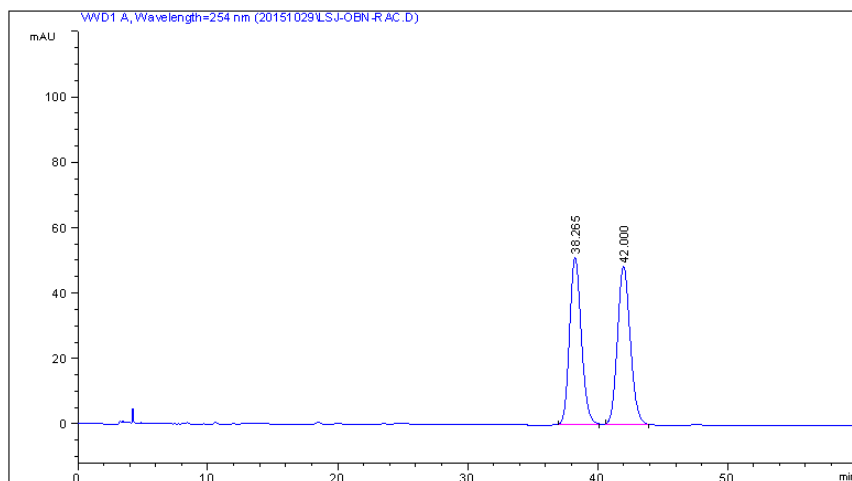
$^1\text{H NMR}$  of **3g**



$^{13}\text{C NMR}$  of **3g**



### Racemate of 3g



#### Area Percent Report

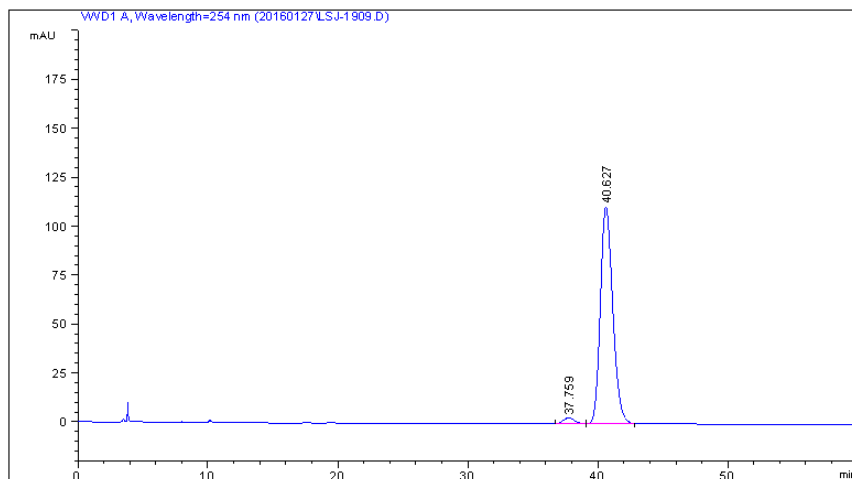
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Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	38.265	BB	0.9726	3209.04614	51.12160	49.2230
2	42.000	BB	1.0779	3310.35229	48.28510	50.7770

Totals : 6519.39844 99.40670

### Enantiomeric excess of 3g: 95%



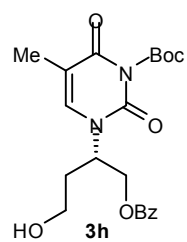
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Use Multiplier & Dilution Factor with ISTDs

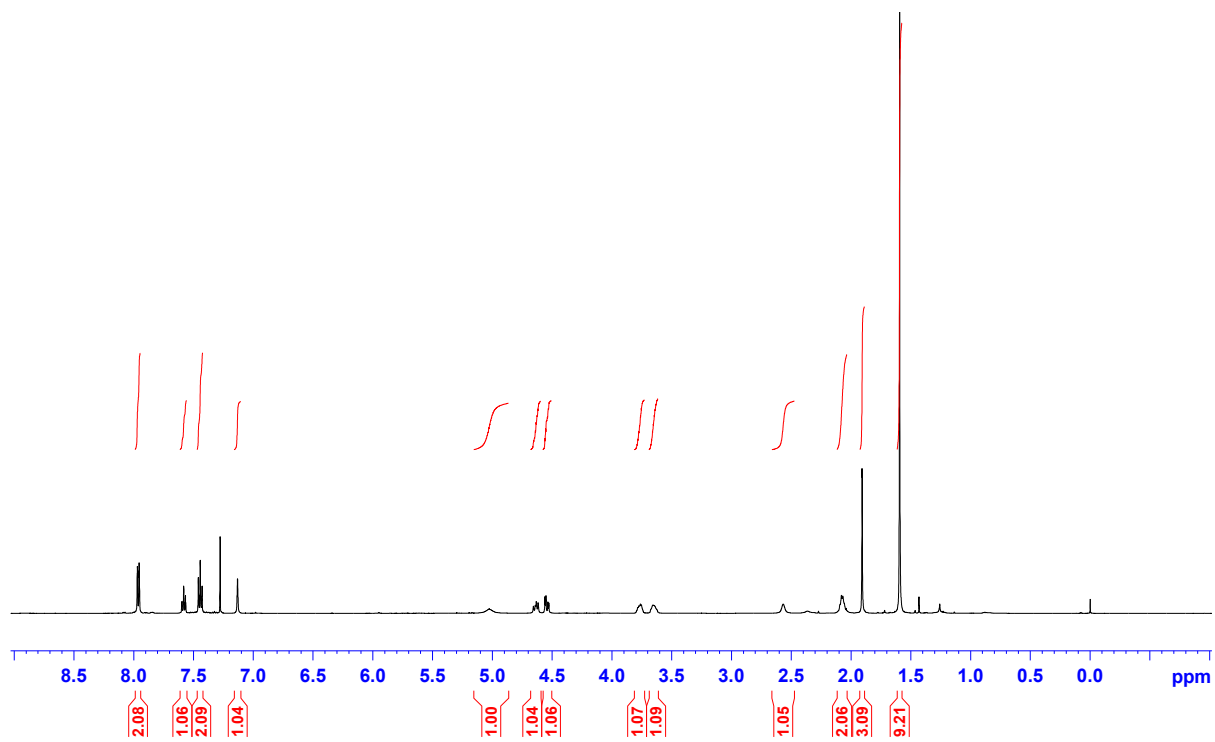
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	37.759	BV	0.8729	179.89629	3.01230	2.3900
2	40.627	VB	1.0202	7347.04102	110.72124	97.6100

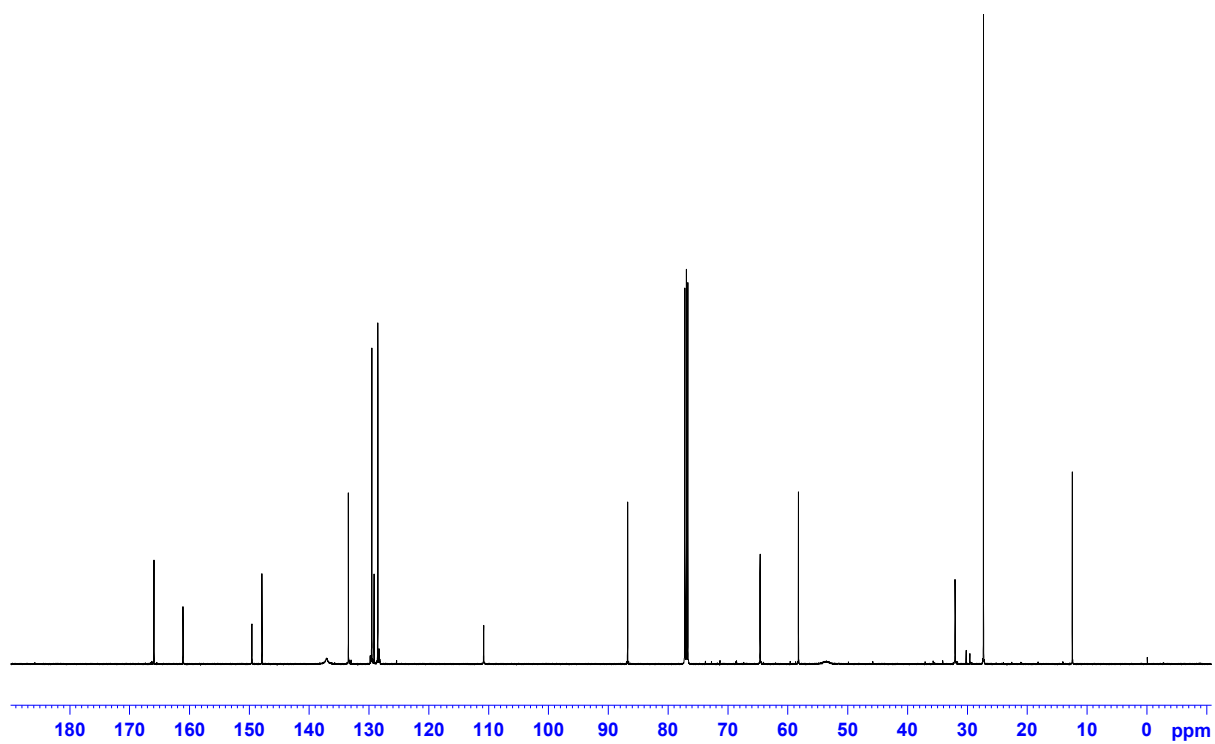
Totals : 7526.93730 113.73354



$^1\text{H NMR}$  of **3h**

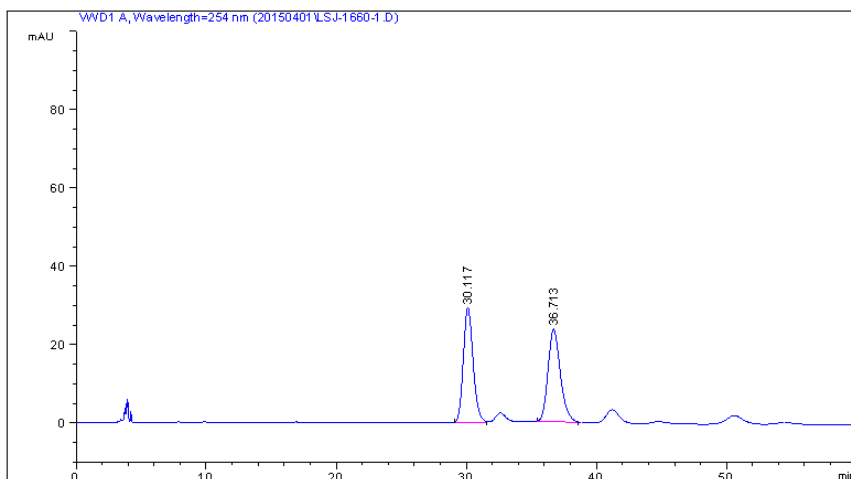


$^{13}\text{C NMR}$  of **3h**





### Racemate of **3h**



#### Area Percent Report

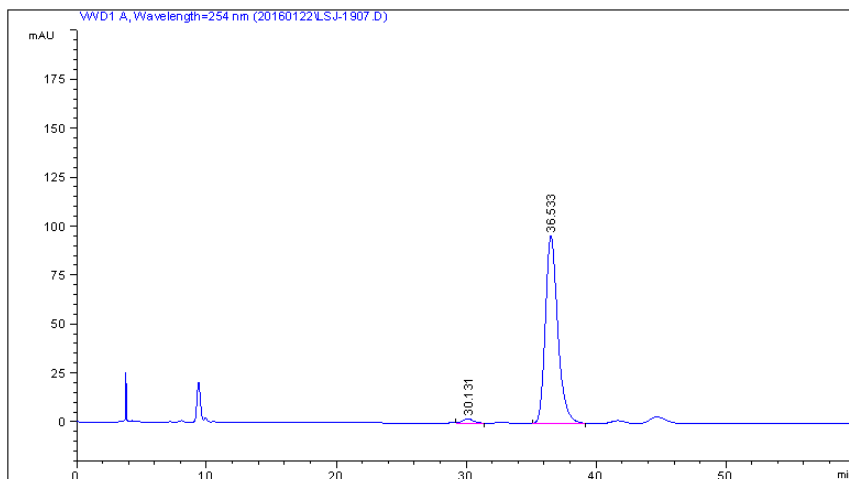
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Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	30.117	BB	0.8160	1531.80530	29.26505	49.4721
2	36.713	BB	1.0155	1564.49695	23.63260	50.5279

Totals : 3096.30225 52.89765

### Enantiomeric excess of **3h**: 96%



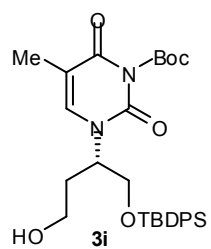
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Use Multiplier & Dilution Factor with ISTDs

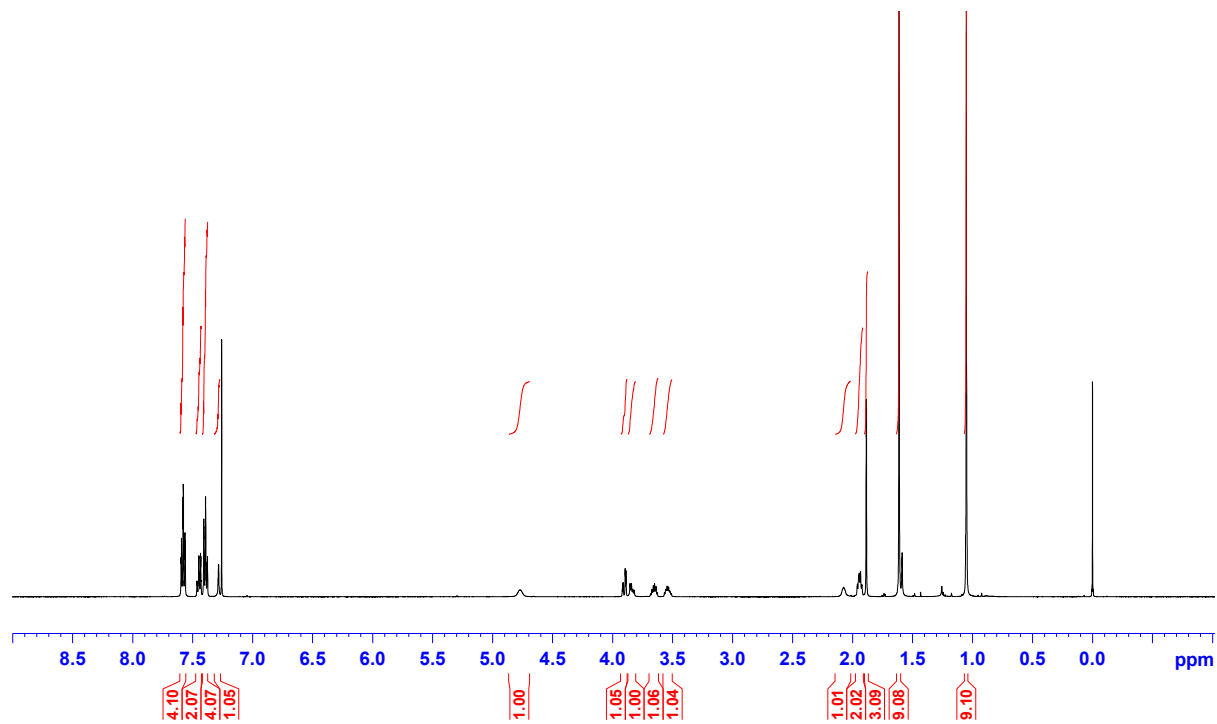
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	30.131	BB	0.7769	121.88227	2.32742	1.8843
2	36.533	BB	1.0292	6346.55811	95.79405	98.1157

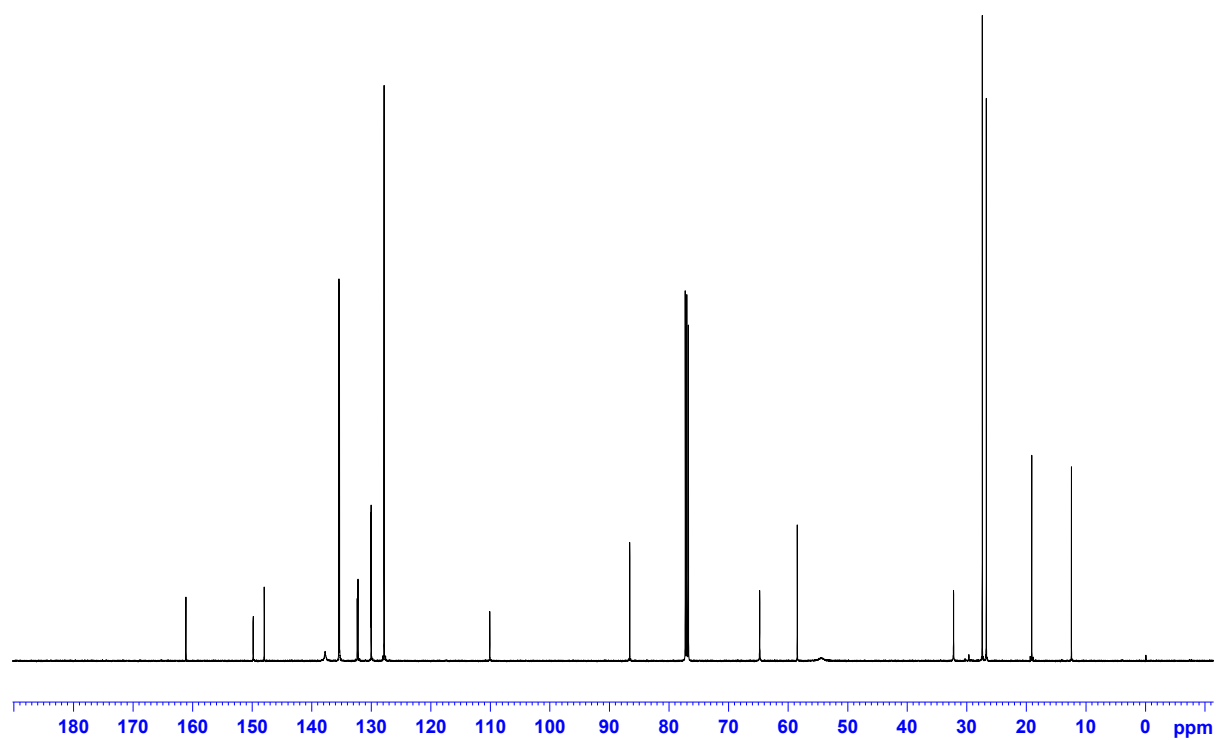
Totals : 6468.44038 98.12148



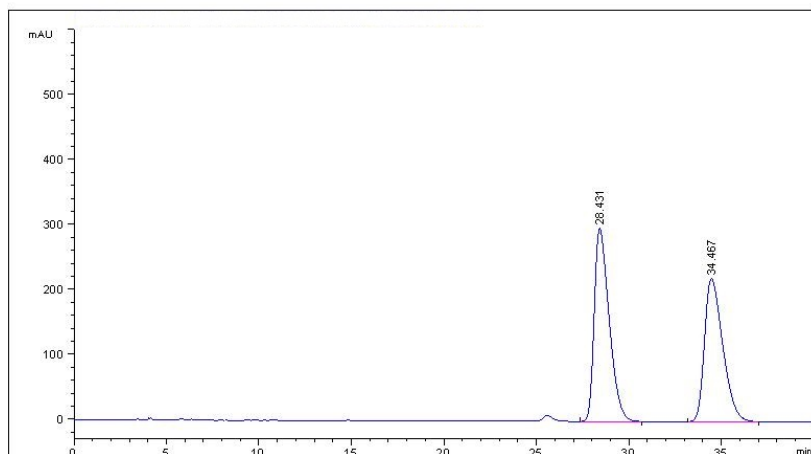
$^1\text{H NMR}$  of **3i**



$^{13}\text{C NMR}$  of **3i**



### Racemate of **3i**



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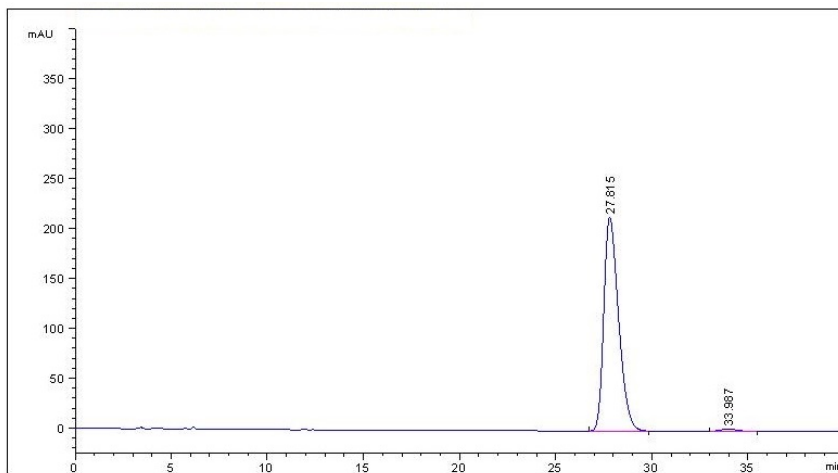
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	28.431	BB	0.8536	1.66290e4	297.25372	52.3704
2	34.467	BB	1.0535	1.51237e4	220.11441	47.6296

Totals : 3.17527e4 517.36813

### Enantiomeric excess of **3i**: 98%



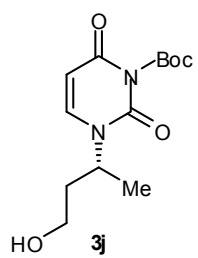
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Multiplier: : 1.0000  
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Use Multiplier & Dilution Factor with ISTDs

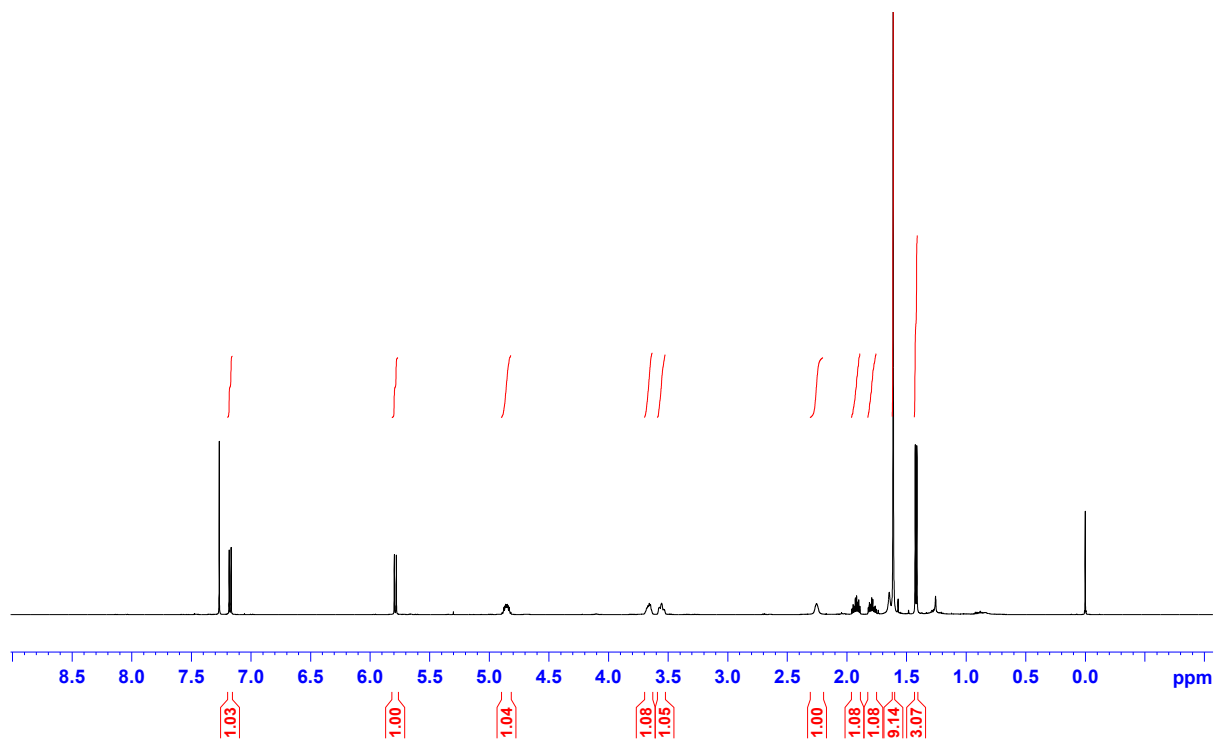
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	27.815	BB	0.8256	1.14519e4	214.36505	98.7520
2	33.987	BB	0.7988	144.73178	2.36371	1.2480

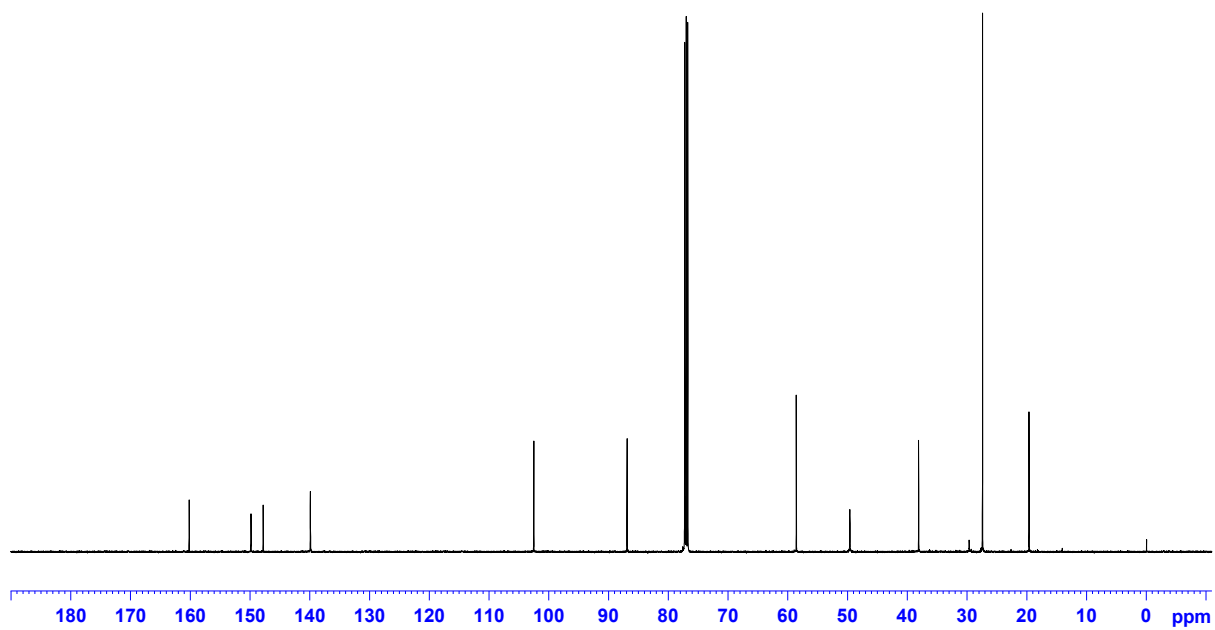
Totals : 1.15967e4 216.72876



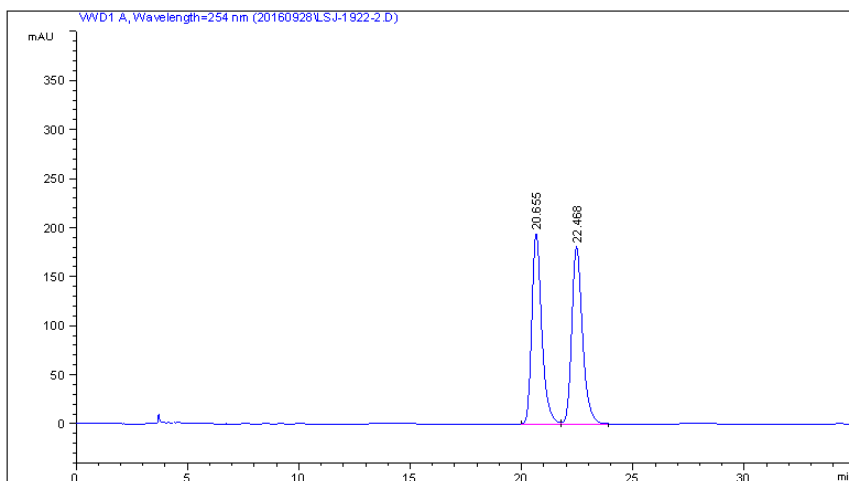
$^1\text{H NMR}$  of **3j**



$^{13}\text{C NMR}$  of **3j**



### Racemate of 3j



#### Area Percent Report

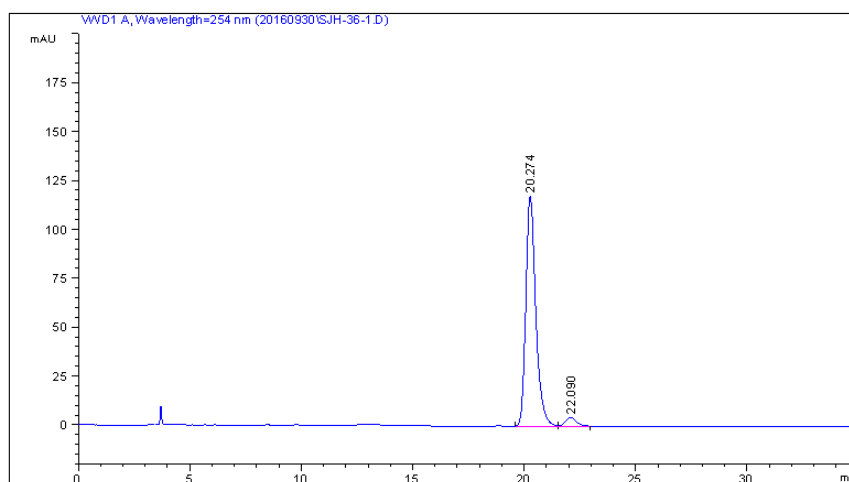
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	20.655	BV	0.4738	6038.74316	193.98862	49.8696
2	22.468	VB	0.5114	6070.31250	180.65408	50.1304

Totals : 1.21091e4 374.64270

### Enantiomeric excess of 3j: 92%



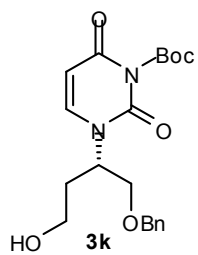
#### Area Percent Report

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

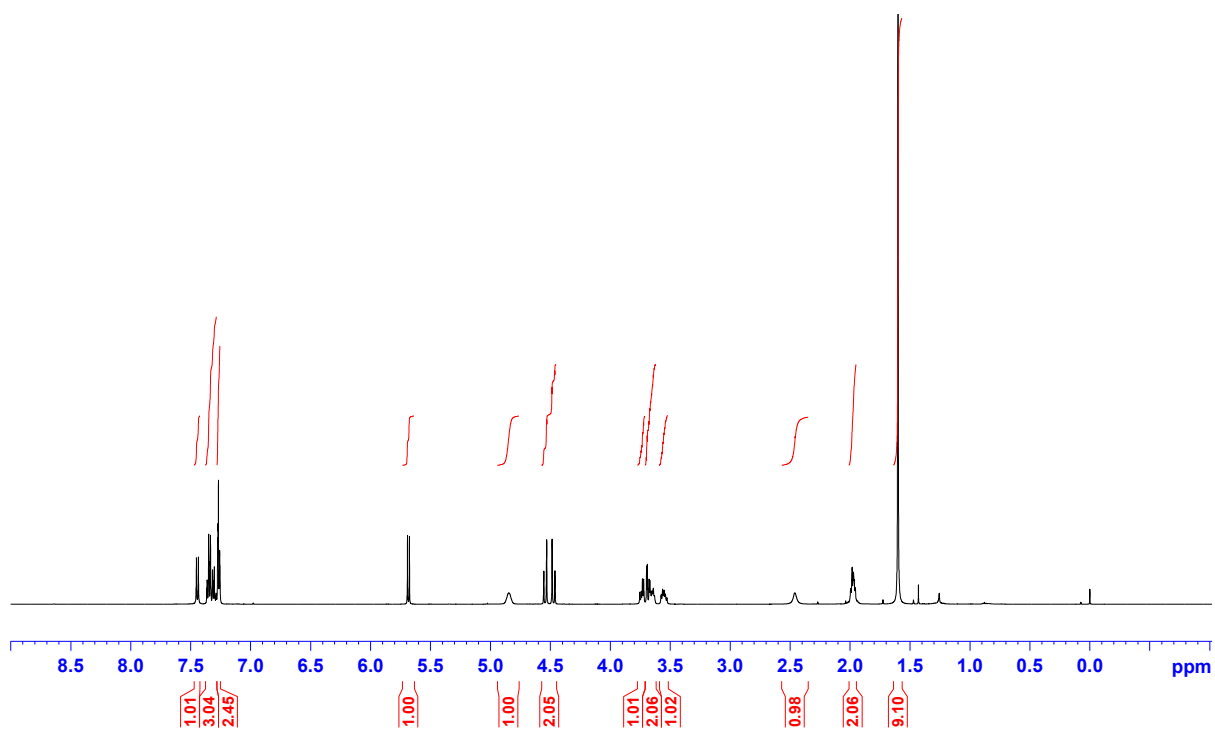
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	20.274	BB	0.4690	3641.14160	117.60153	95.9639
2	22.090	BB	0.5103	153.14223	4.55391	4.0361

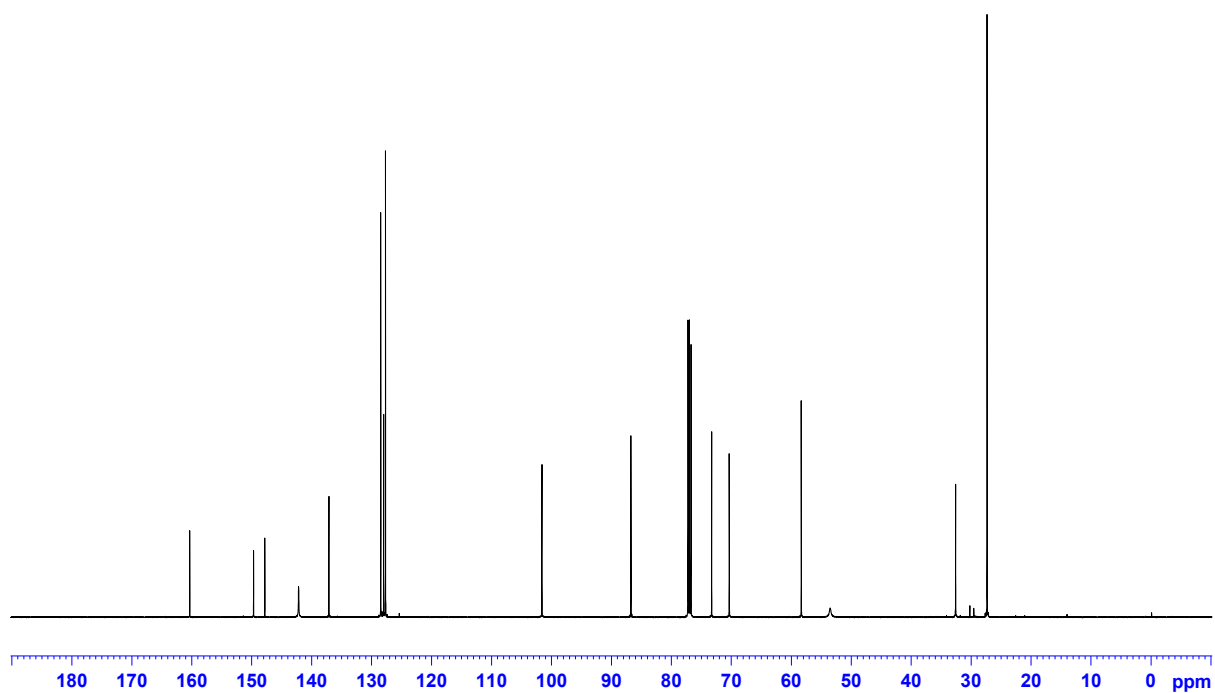
Totals : 3794.28383 122.15544



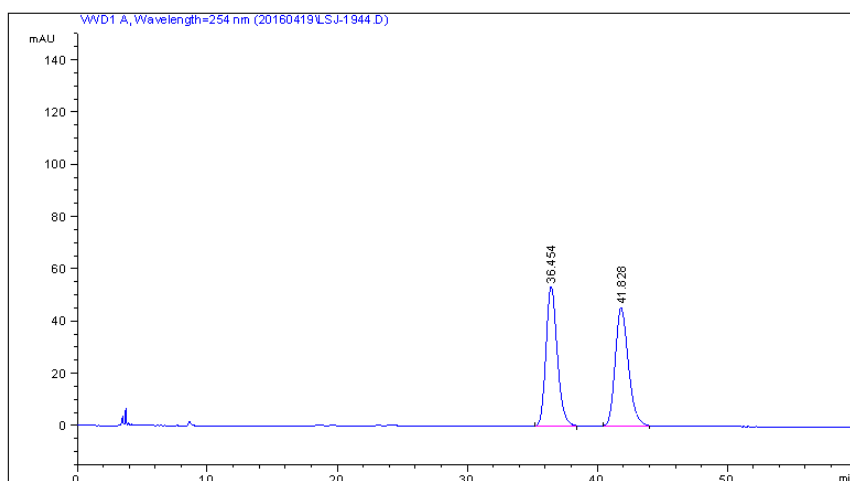
$^1\text{H NMR}$  of **3k**



$^{13}\text{C NMR}$  of **3k**



## Racemate of **3k**



### Area Percent Report

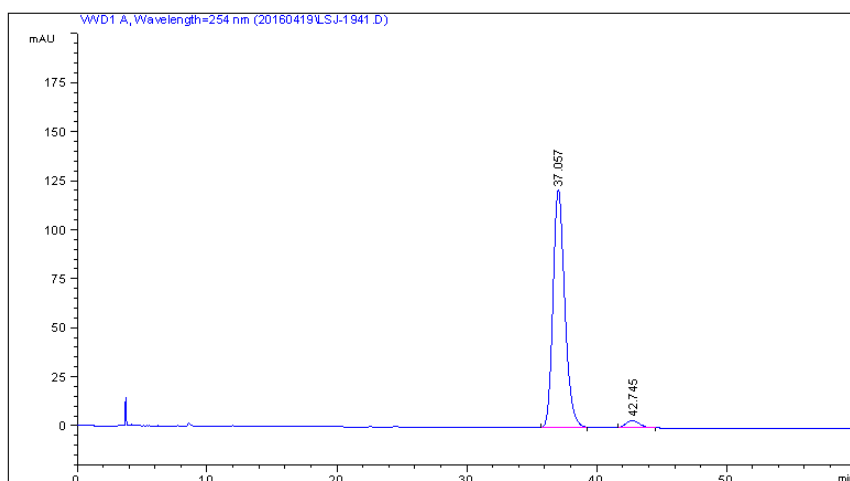
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	36.454	BB	0.9250	3226.00366	53.37684	50.2897
2	41.828	BB	1.0705	3188.83032	45.36346	49.7103

Totals : 6414.83398 98.74031

## Enantiomeric excess of **3k**: 93%



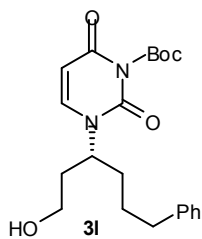
### Area Percent Report

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

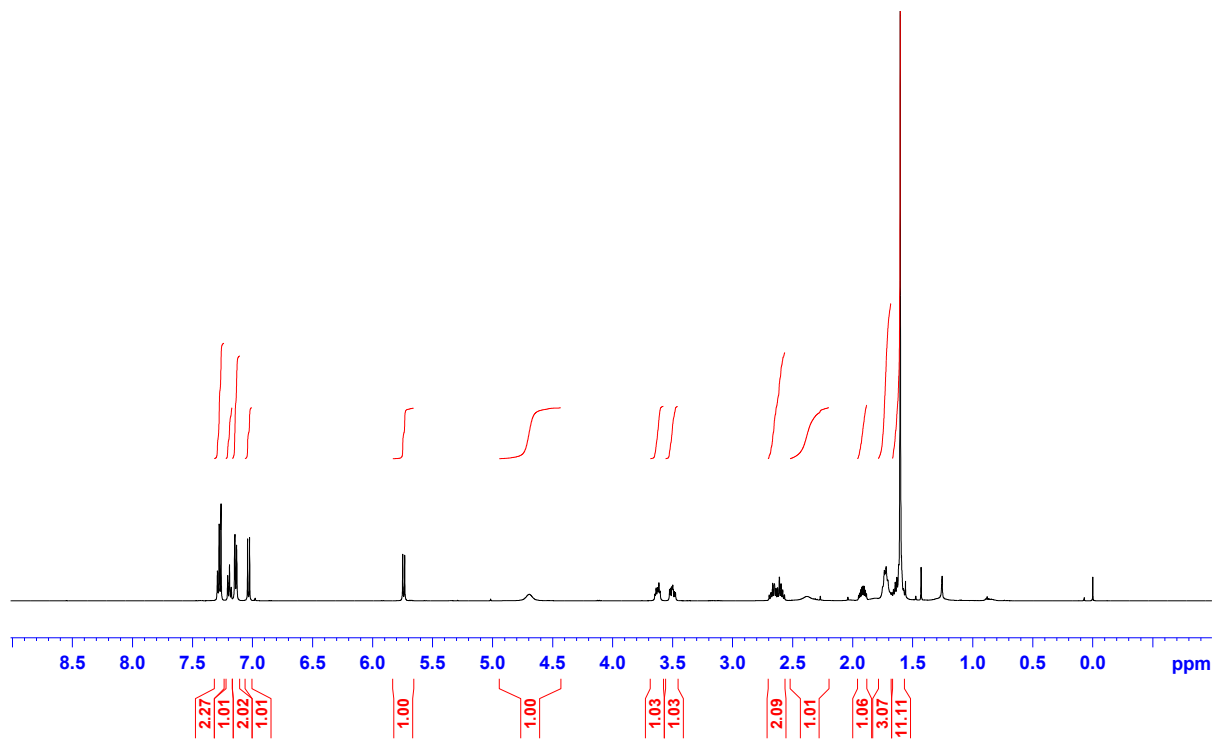
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	37.057	BB	0.9589	7620.50635	121.01651	96.6602
2	42.745	BB	1.0108	263.30606	3.71275	3.3398

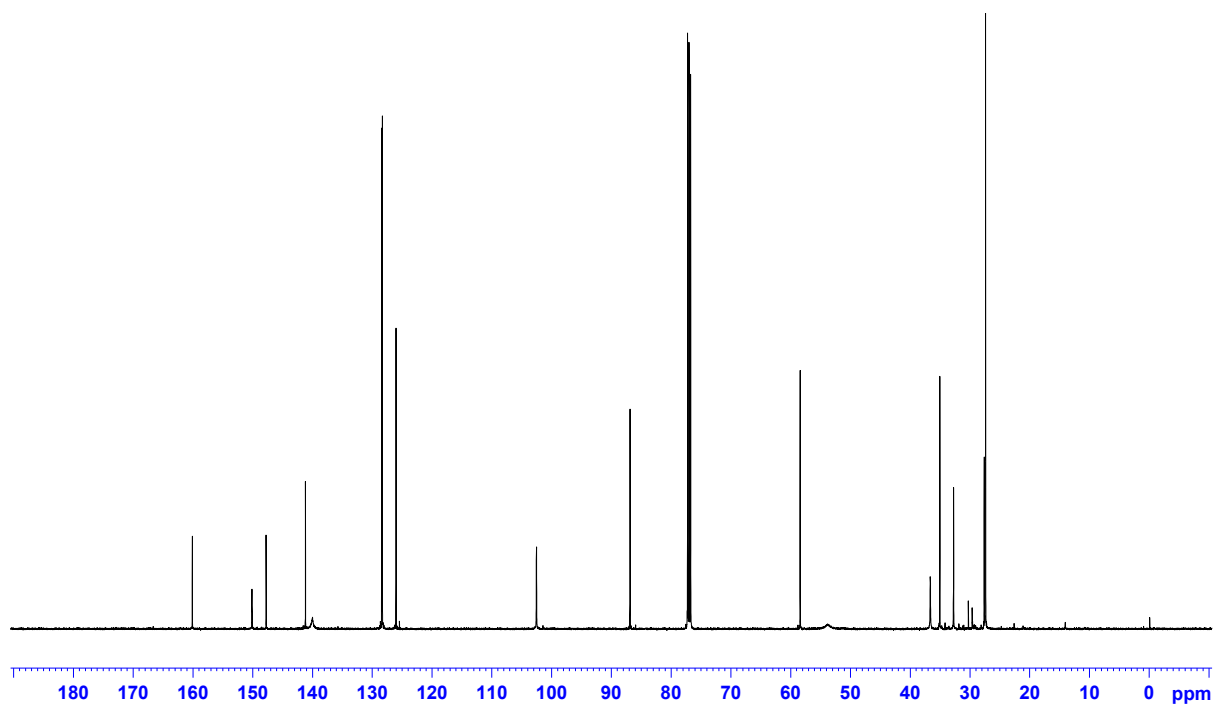
Totals : 7883.81241 124.72926



$^1\text{H NMR}$  of **3I**

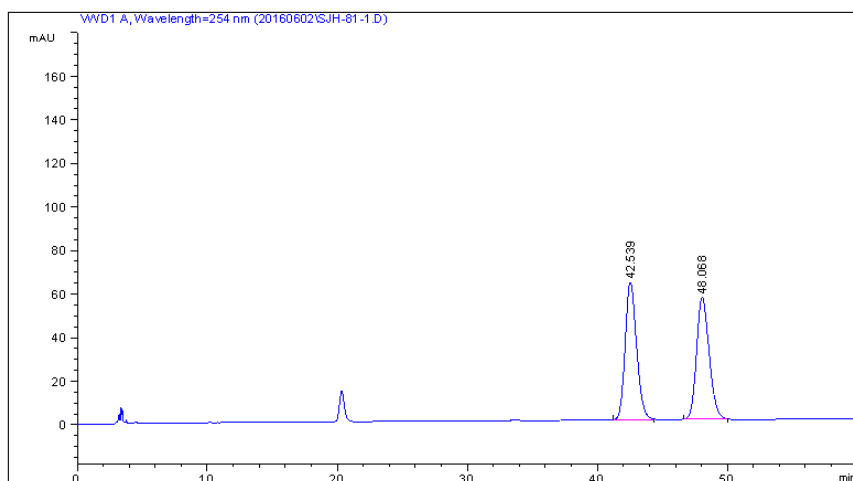


$^{13}\text{C NMR}$  of **3I**





### Racemate of **3l**



#### Area Percent Report

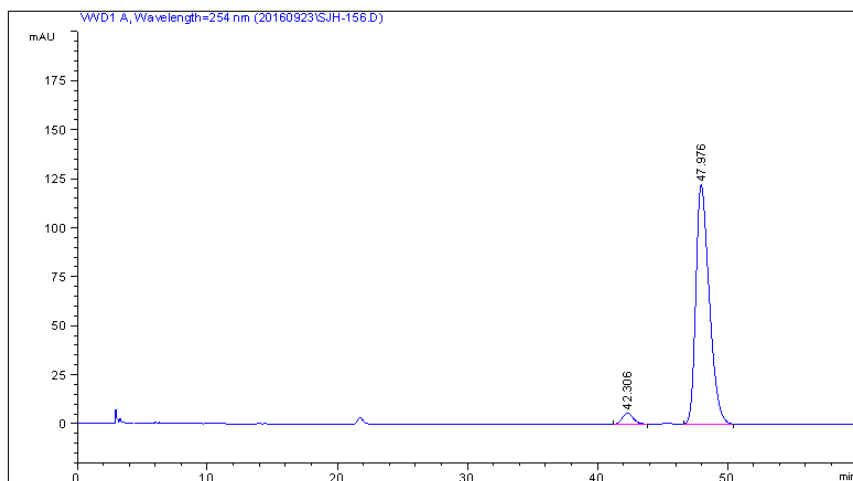
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	42.539	BB	0.9368	3843.25317	62.92355	50.4316
2	48.068	BB	1.0381	3777.46362	55.95325	49.5684

Totals : 7620.71680 118.87681

### Enantiomeric excess of **3l**: 92%



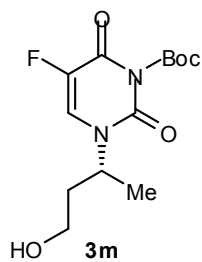
#### Area Percent Report

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

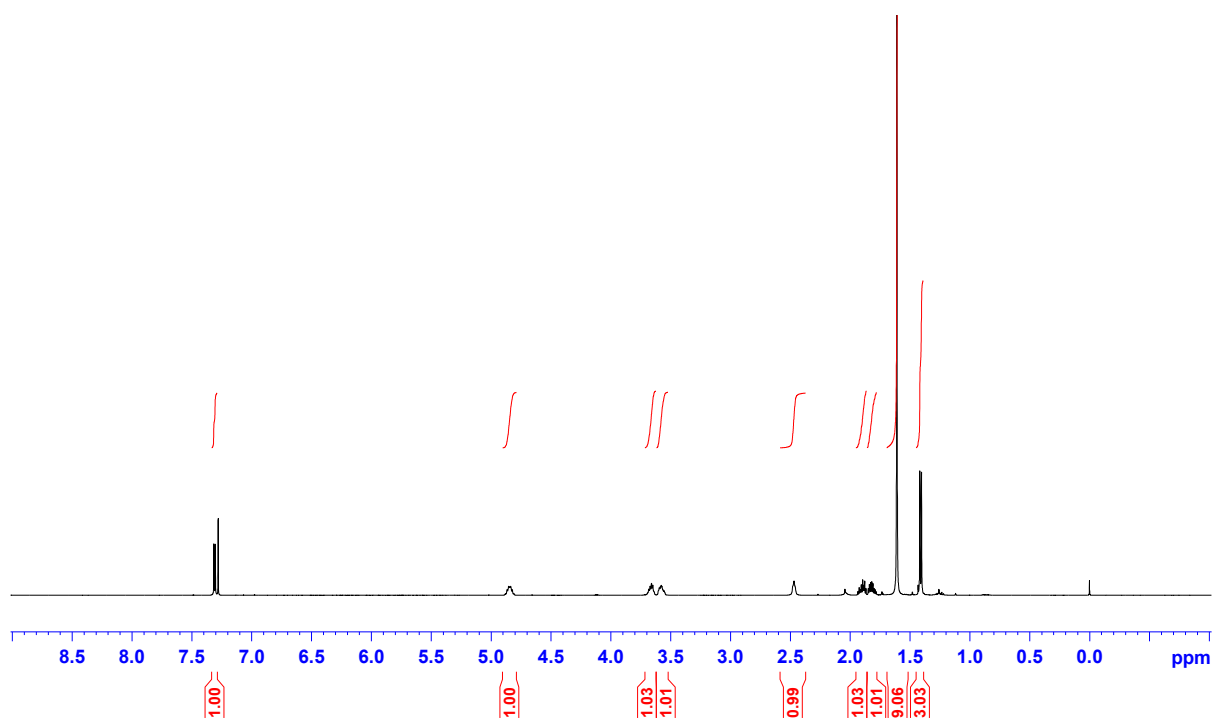
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	42.306	BB	0.8992	342.76016	5.70325	3.7675
2	47.976	BB	1.0974	8754.96582	122.06538	96.2325

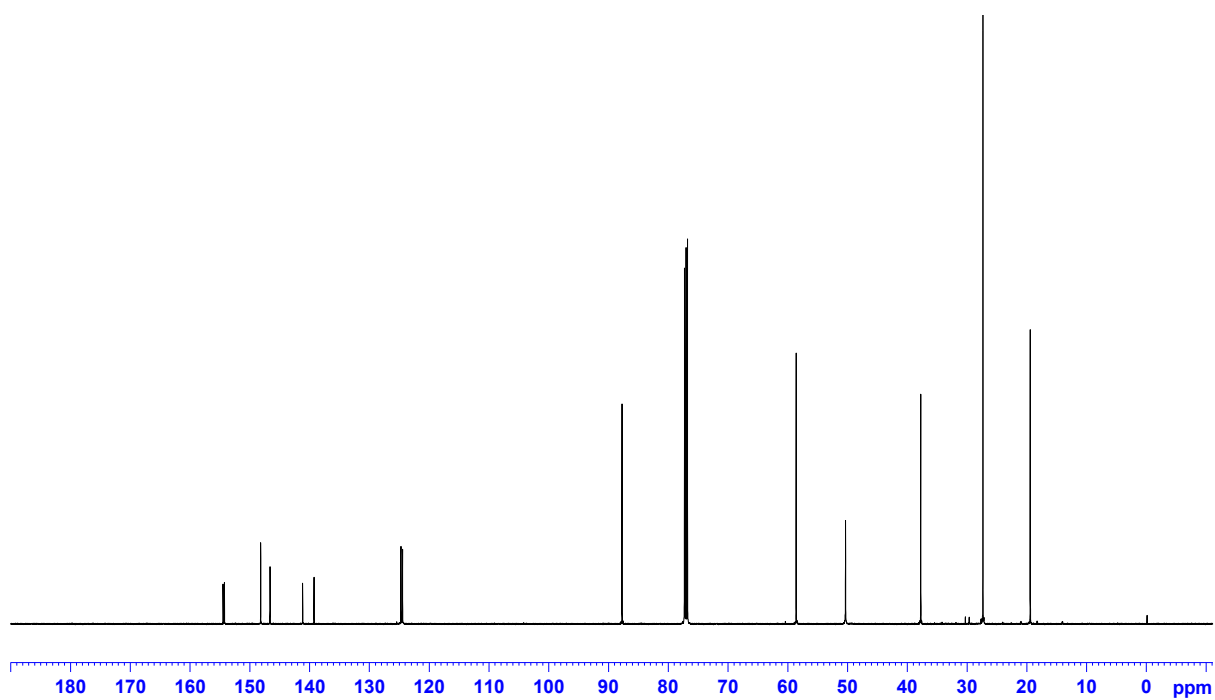
Totals : 9097.72598 127.76863



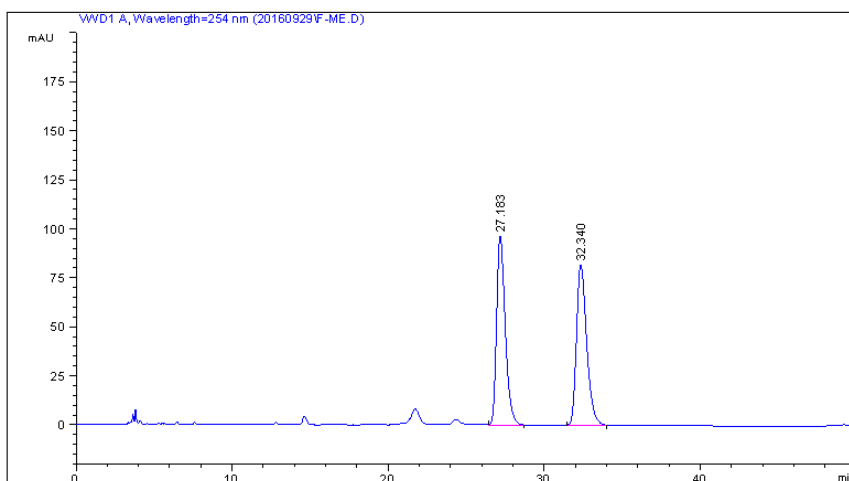
$^1\text{H}$  NMR of **3m**



$^{13}\text{C}$  NMR of **3m**



## Racemate of 3m



### Area Percent Report

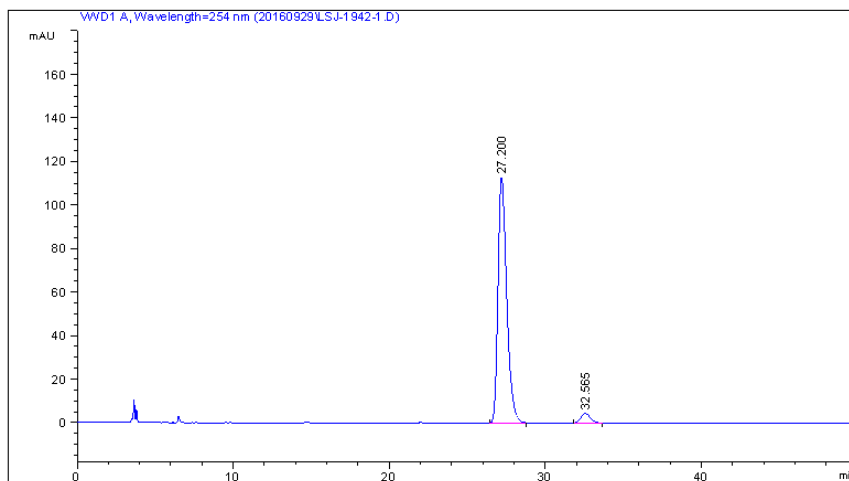
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	27.183	BB	0.5906	3729.53564		96.50521	50.1009
2	32.340	BB	0.6892	3714.51953		81.91311	49.8991

Totals : 7444.05518 178.41832

## Enantiomeric excess of 3m: 92%



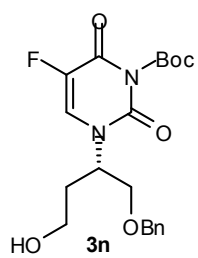
### Area Percent Report

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

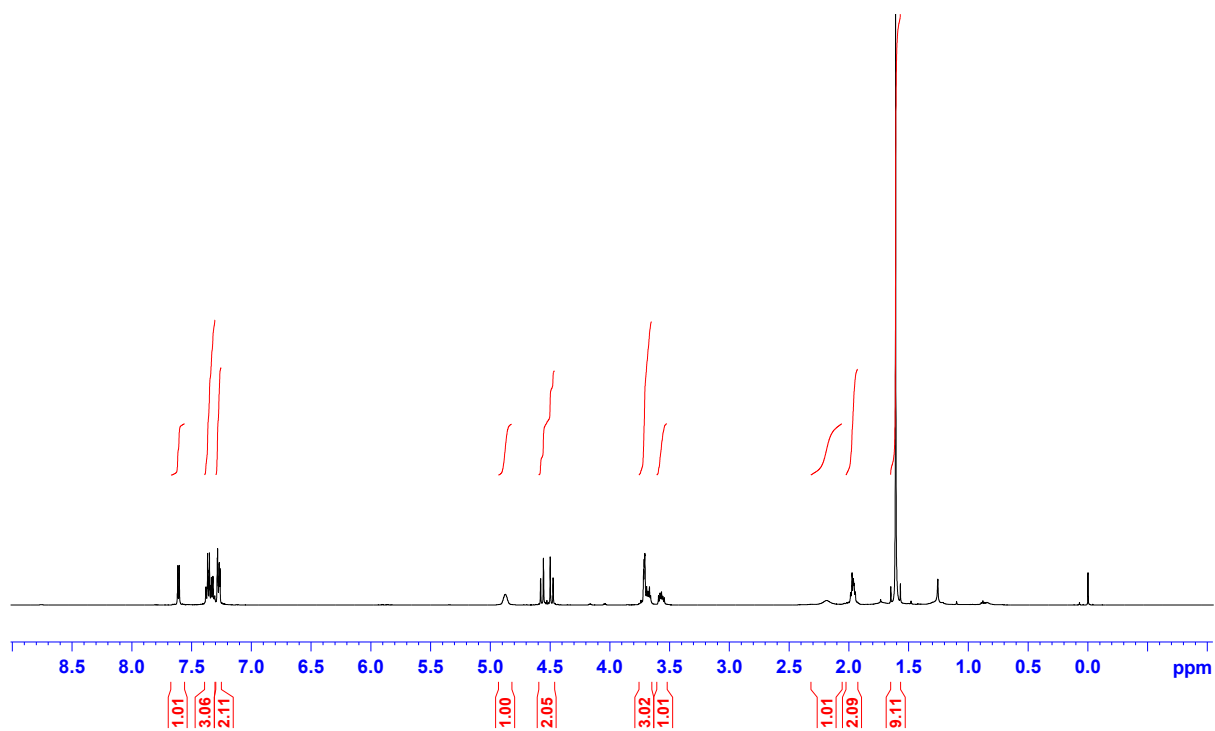
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	27.200	BB	0.5951	4403.79395		112.84711	95.7544
2	32.565	BB	0.6559	195.25688		4.48963	4.2456

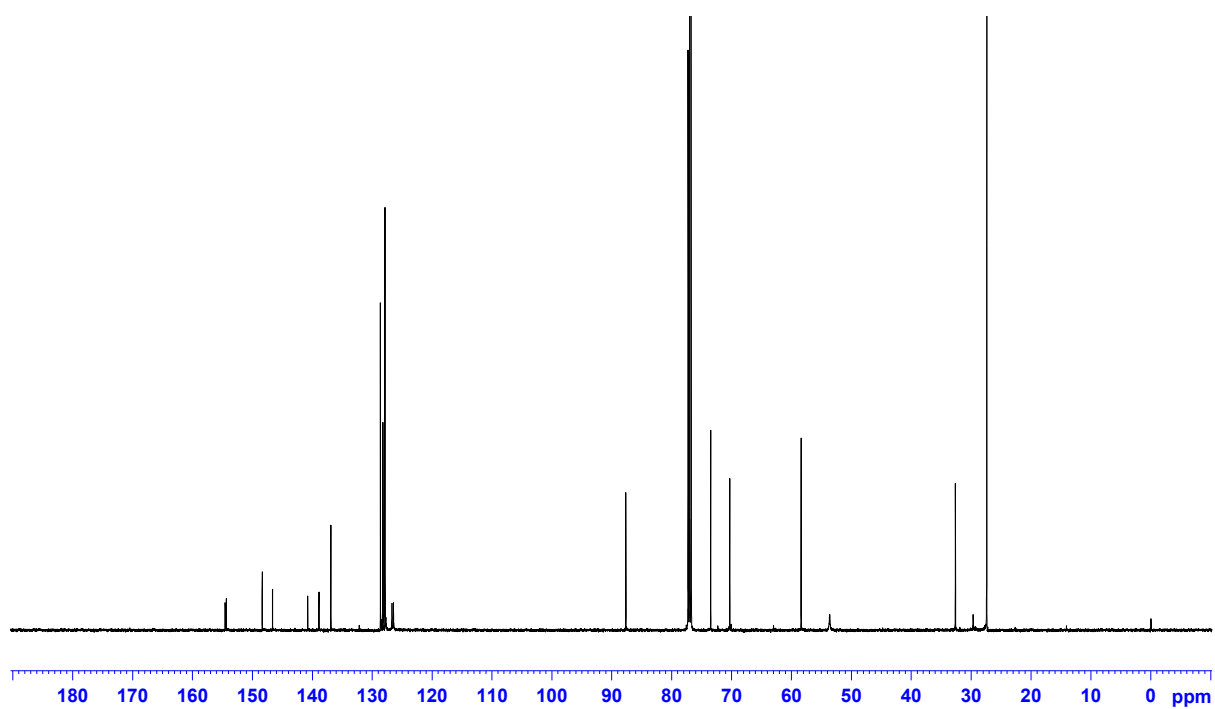
Totals : 4599.05083 117.33675



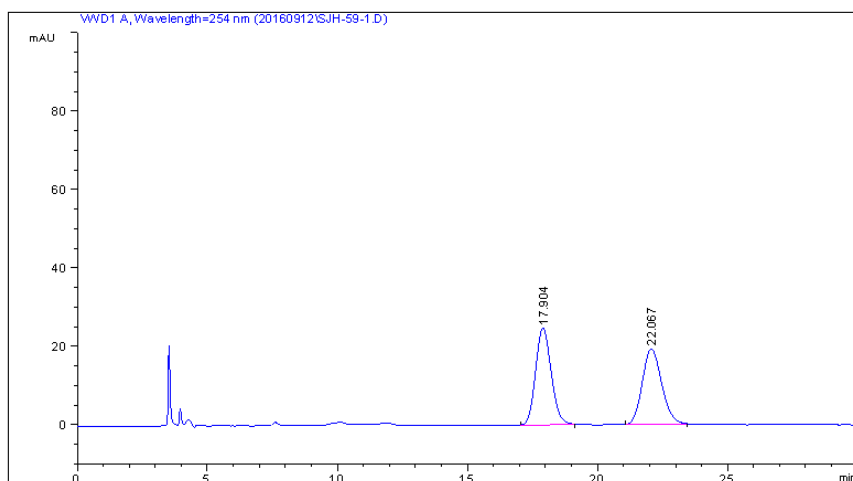
<sup>1</sup>H NMR of **3n**



<sup>13</sup>C NMR of **3n**



Racemate of **3n**



Area Percent Report

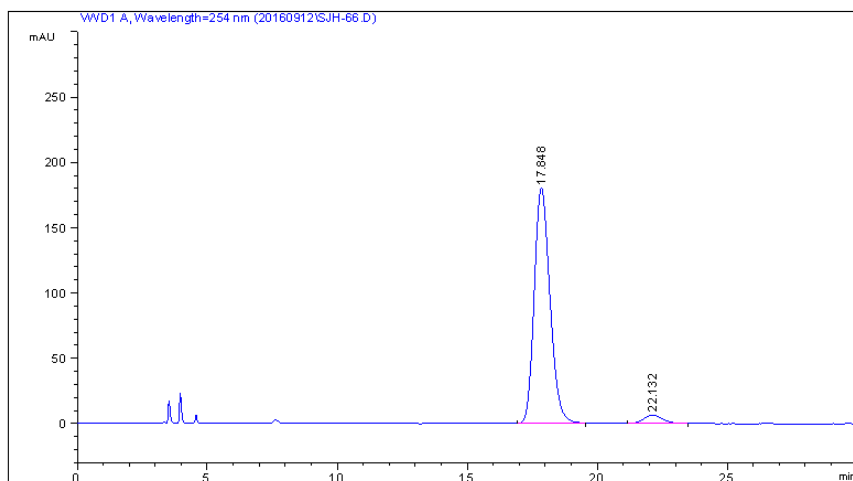
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	17.904	BB	0.6467	1031.70447	24.73944	50.7486
2	22.067	BB	0.7890	1001.26855	19.24340	49.2514

Totals : 2032.97302 43.98284

Enantiomeric excess of **3n**: 91%



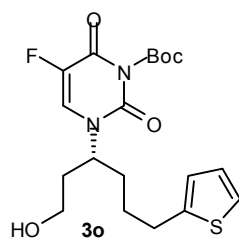
Area Percent Report

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

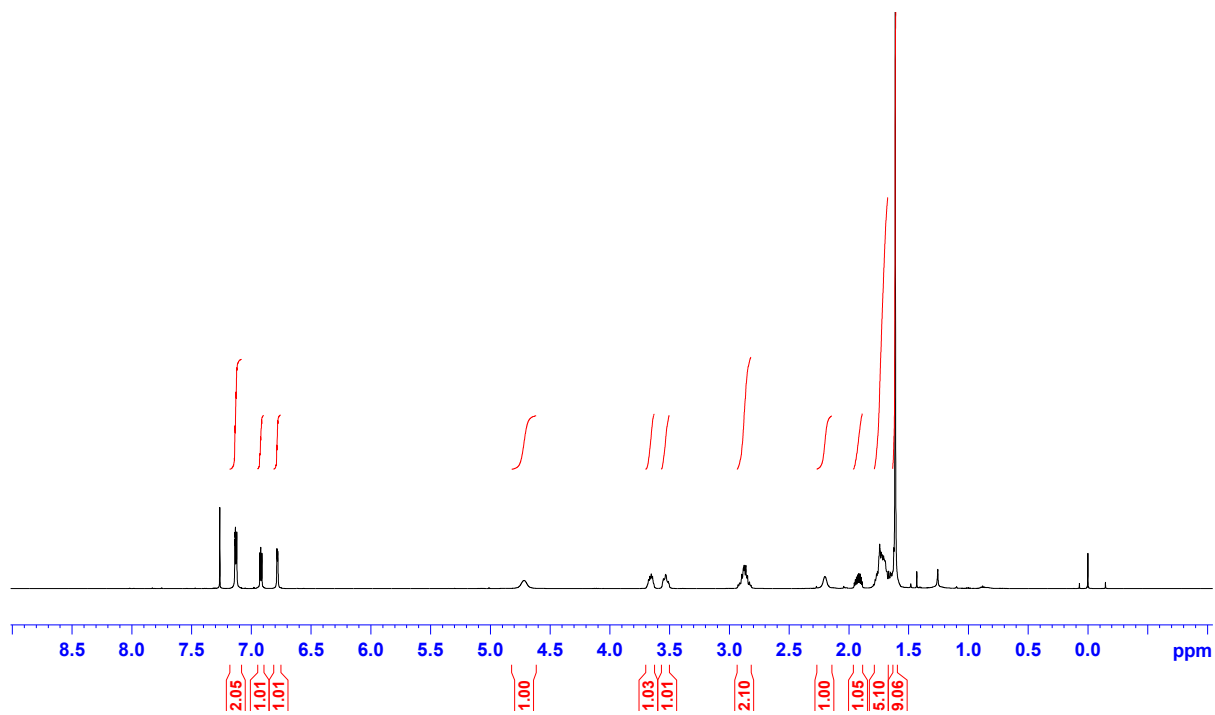
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	17.848	BB	0.6513	7595.12012	180.41788	95.7060
2	22.132	BB	0.7982	340.77109	6.54431	4.2940

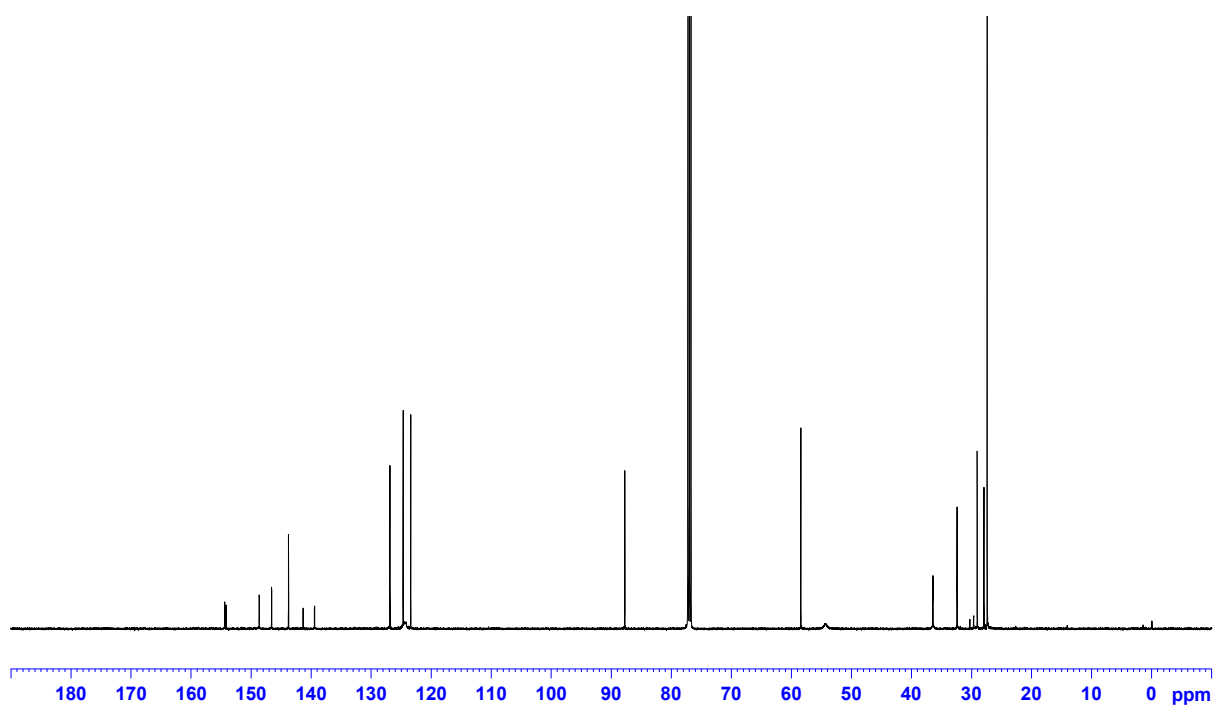
Totals : 7935.89120 186.96219



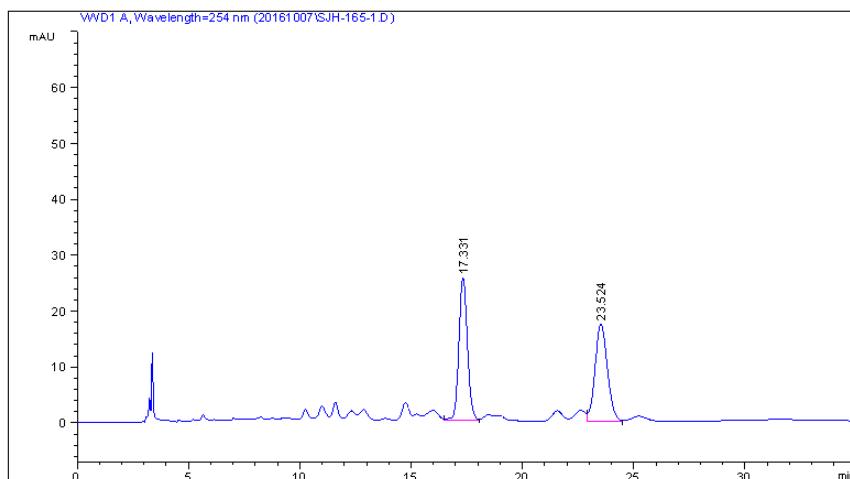
$^1\text{H NMR}$  of **3o**



$^{13}\text{C NMR}$  of **3o**



*Racemate of 3o*



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

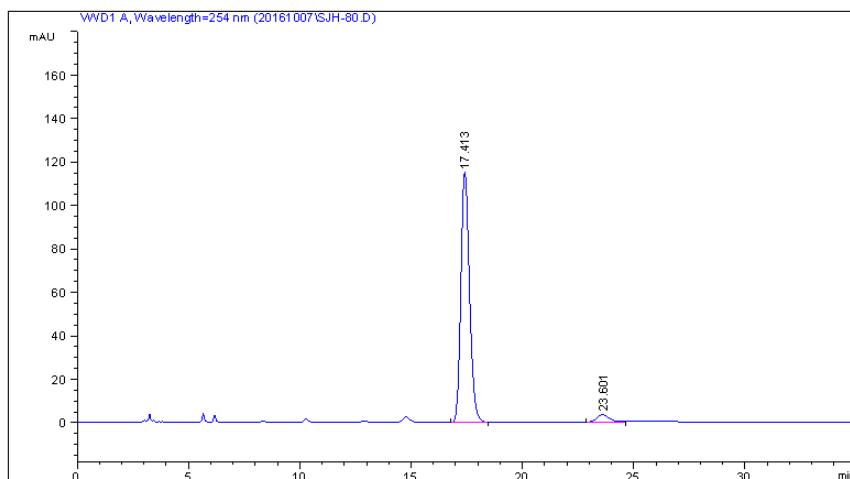
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	17.331	VB	0.4127	684.63605	25.58125	50.1531
2	23.524	VB	0.6013	680.45526	17.47751	49.8469

Totals : 1365.09131 43.05875

*Enantiomeric excess of 3o: 92%*



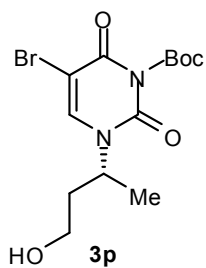
=====  
Area Percent Report  
=====

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

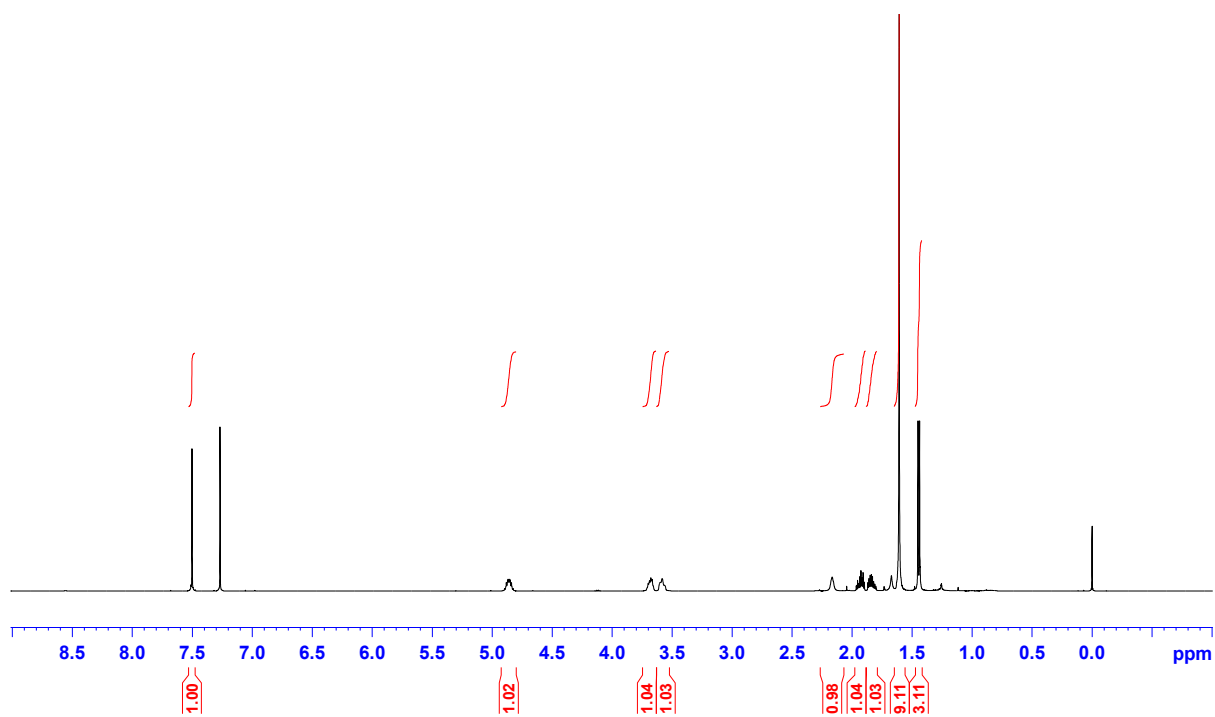
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	17.413	BB	0.4167	3104.36353	115.05789	96.0038
2	23.601	BB	0.5968	129.22102	3.39629	3.9962

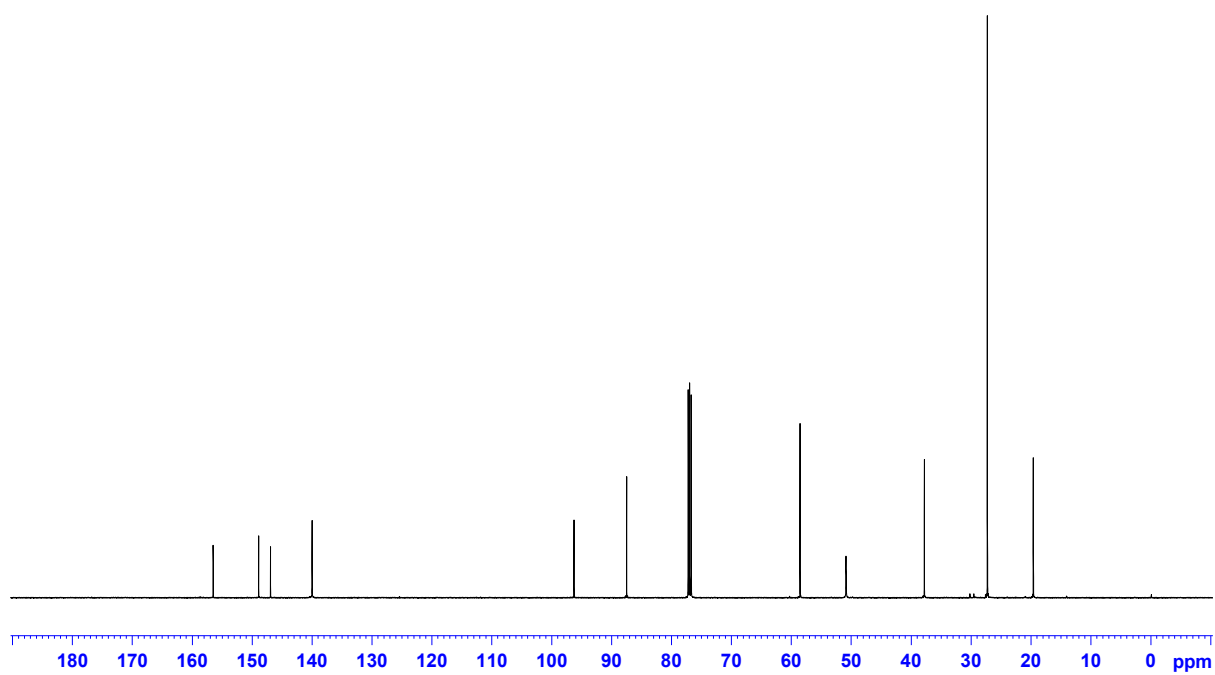
Totals : 3233.58455 118.45418



$^1\text{H NMR}$  of **3p**

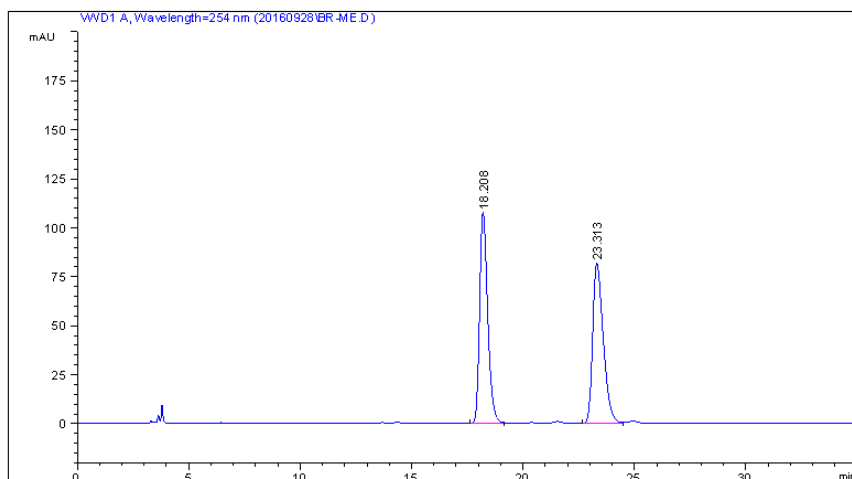


$^{13}\text{C NMR}$  of **3p**





*Racemate of 3p*



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

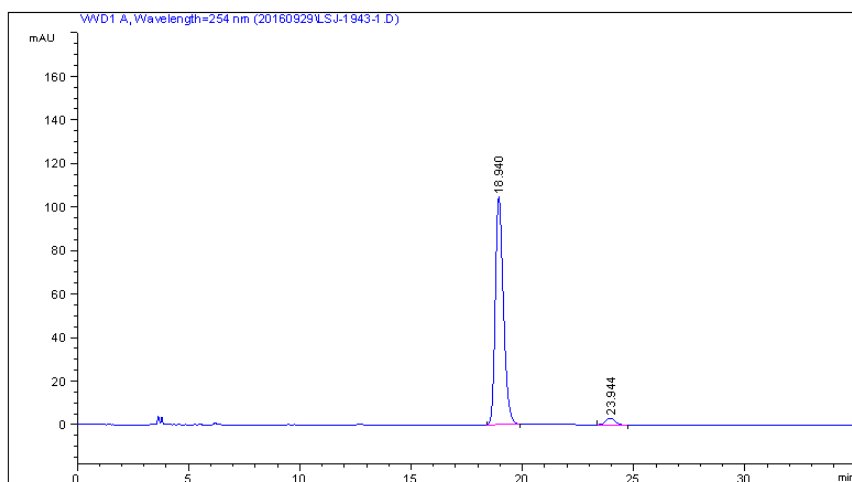
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	18.208	BB	0.3836	2706.42383	107.65462	49.9521
2	23.313	BB	0.5068	2711.61304	81.65504	50.0479

Totals : 5418.03687 189.30965

*Enantiomeric excess of 3p: 93%*



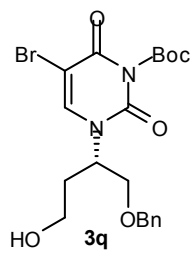
=====  
Area Percent Report  
=====

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

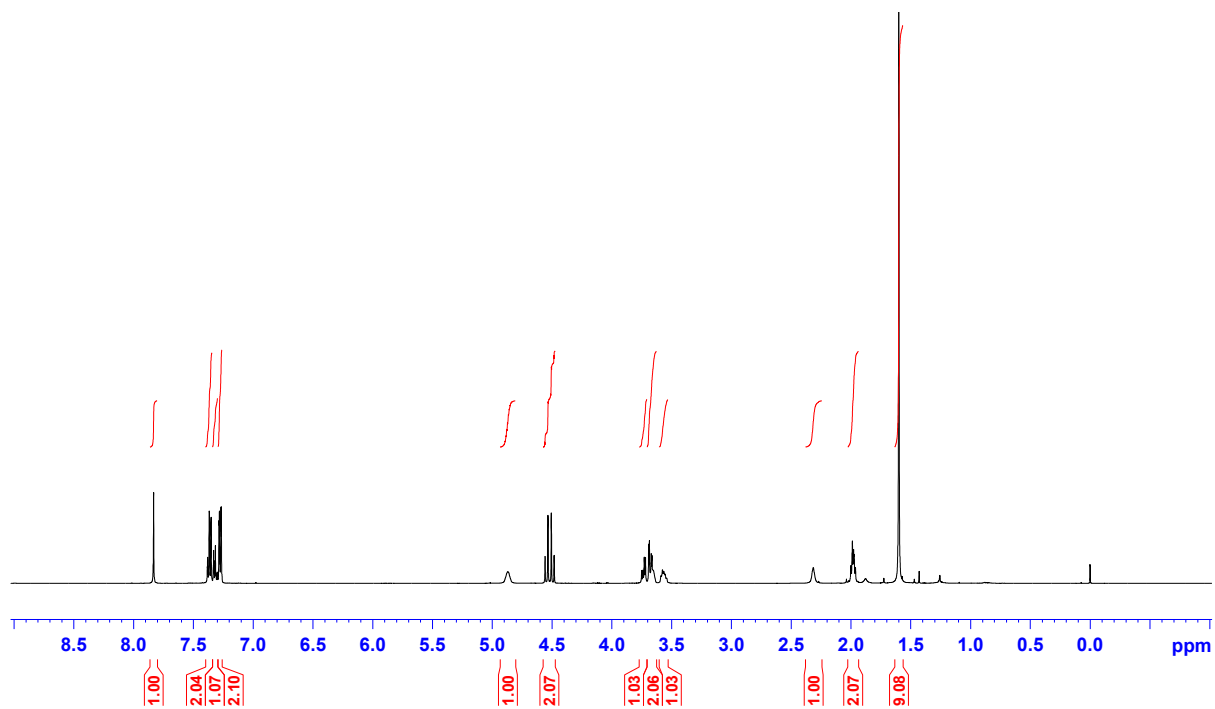
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	18.940	BB	0.3892	2652.86646	104.55978	96.4599
2	23.944	BB	0.4743	97.36208	3.17473	3.5401

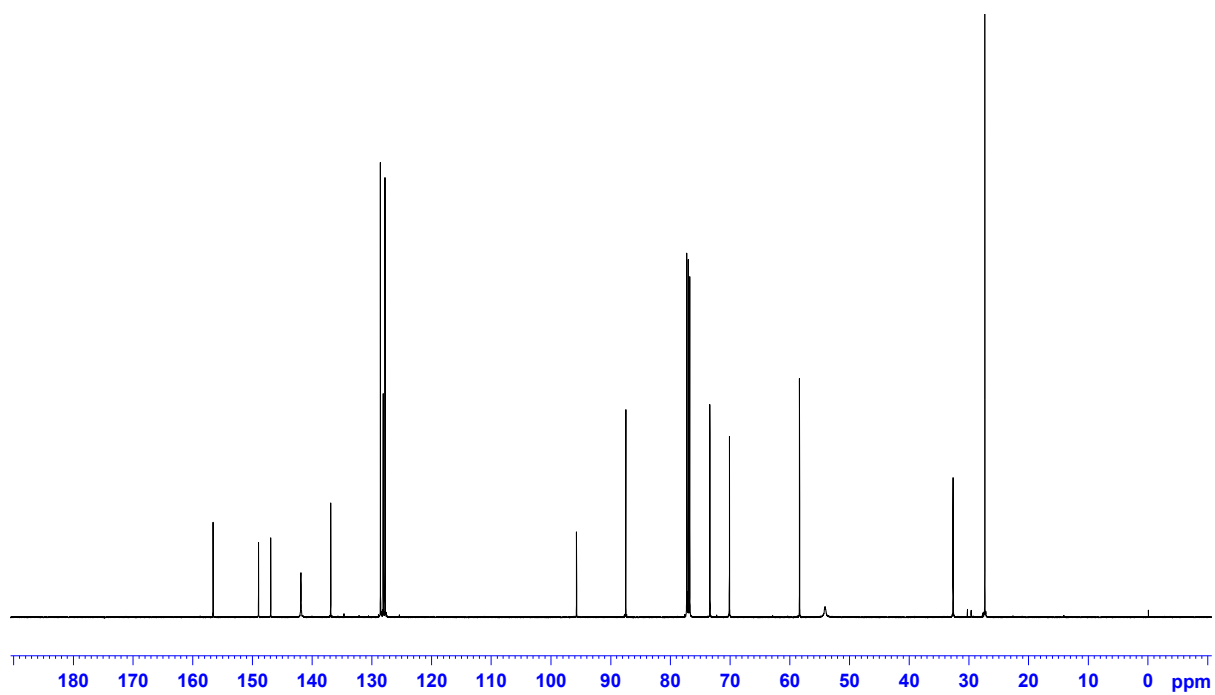
Totals : 2750.22853 107.73450



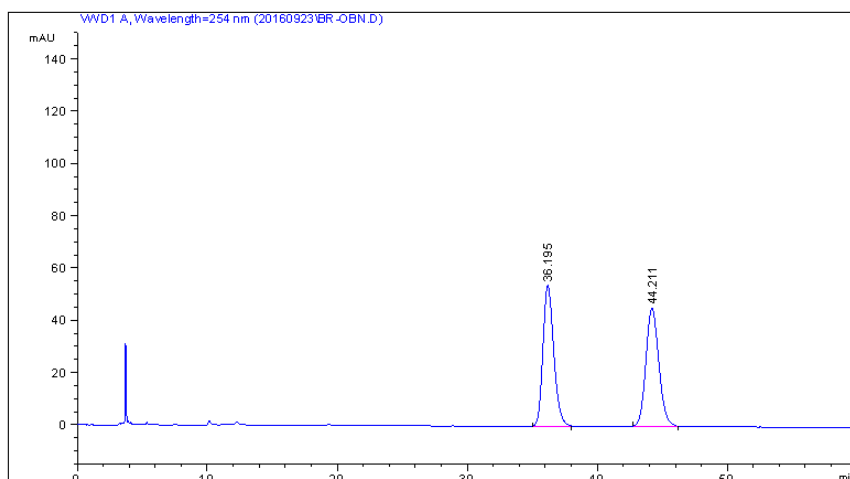
$^1\text{H NMR}$  of **3q**



$^{13}\text{C NMR}$  of **3q**



### Racemate of 3q



#### Area Percent Report

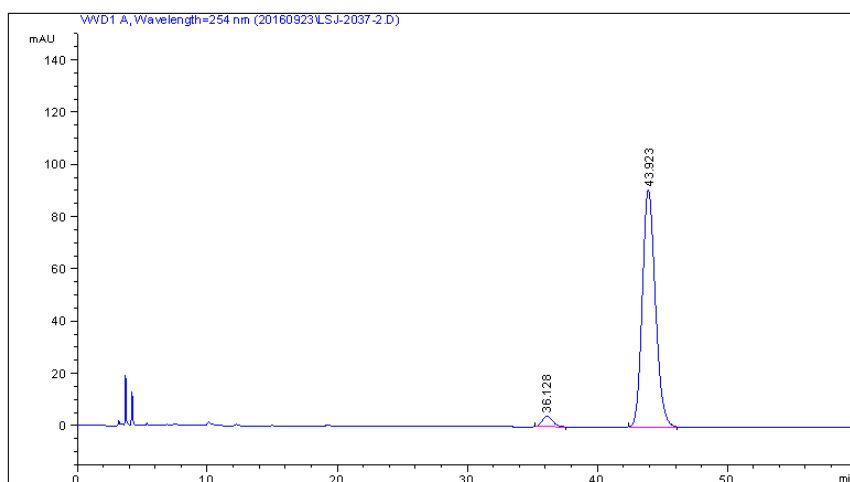
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	36.195	BB	0.8966	3123.47827	53.96434	49.8296
2	44.211	BB	1.0755	3144.83667	45.34634	50.1704

Totals : 6268.31494 99.31068

### Enantiomeric excess of 3q: 93%



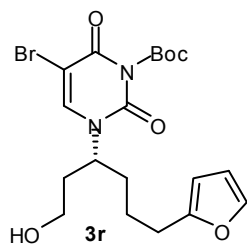
#### Area Percent Report

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

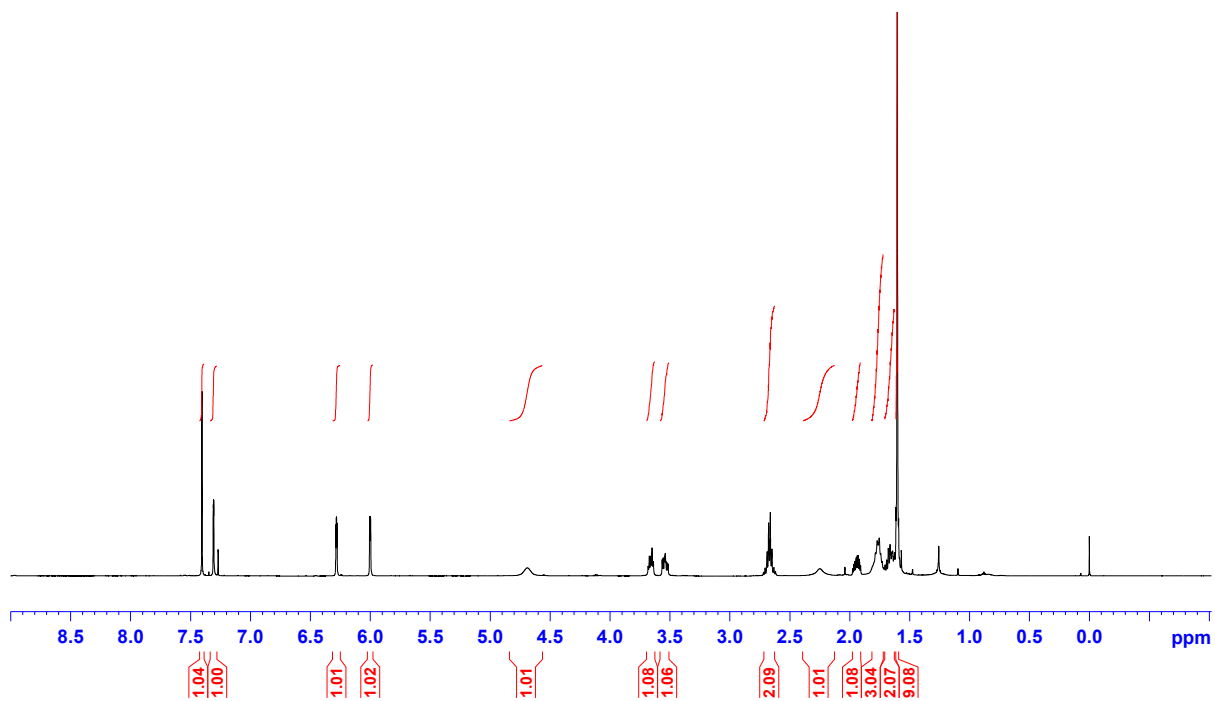
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	36.128	BB	0.8237	229.51941	4.09840	3.5121
2	43.923	BB	1.0730	6305.51514	90.72053	96.4879

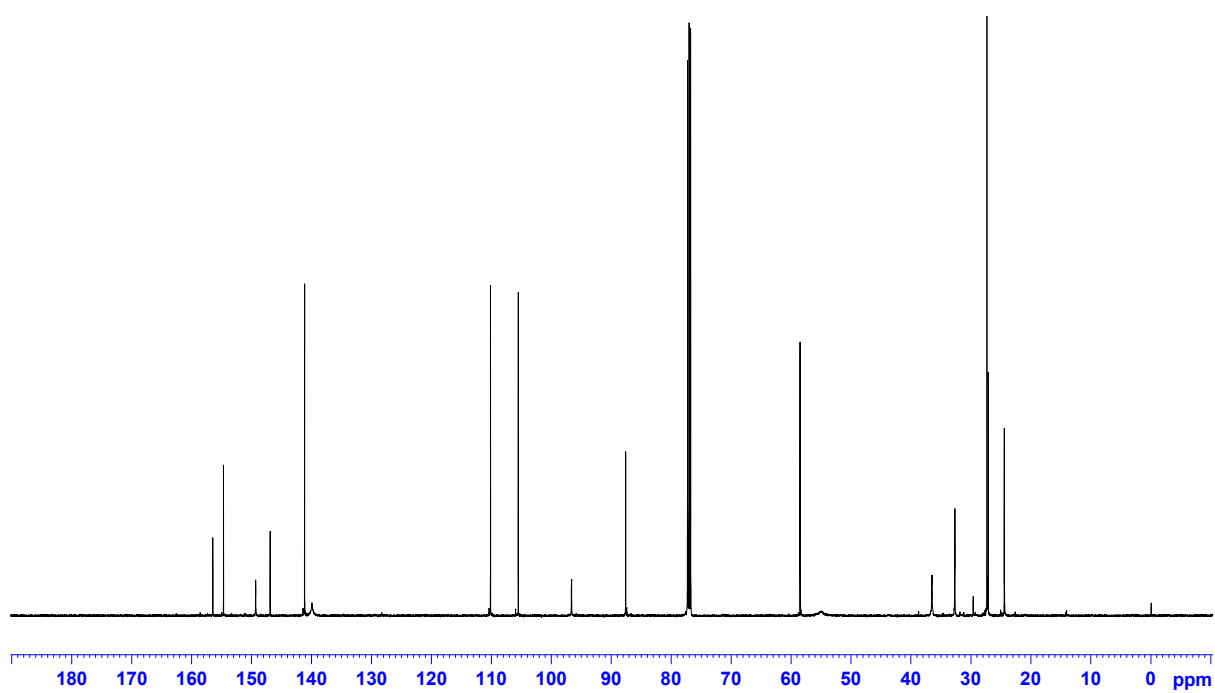
Totals : 6535.03455 94.81892



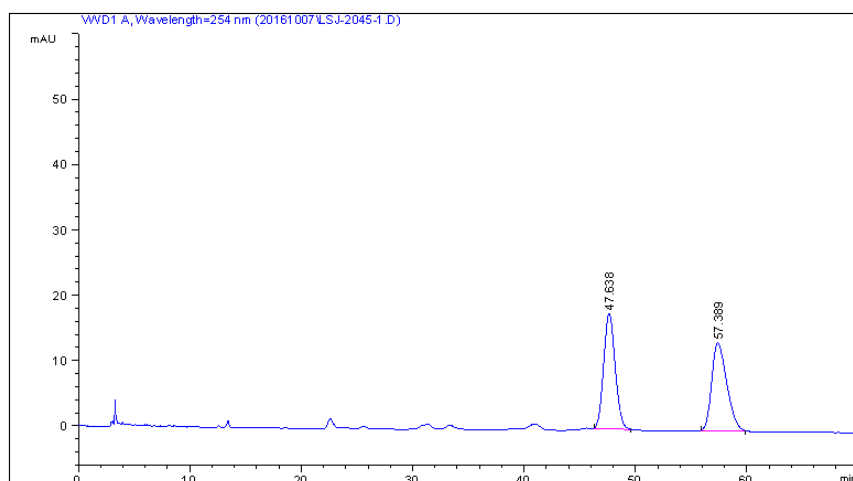
$^1\text{H NMR}$  of **3r**



$^{13}\text{C NMR}$  of **3r**



## Racemate of 3r



### Area Percent Report

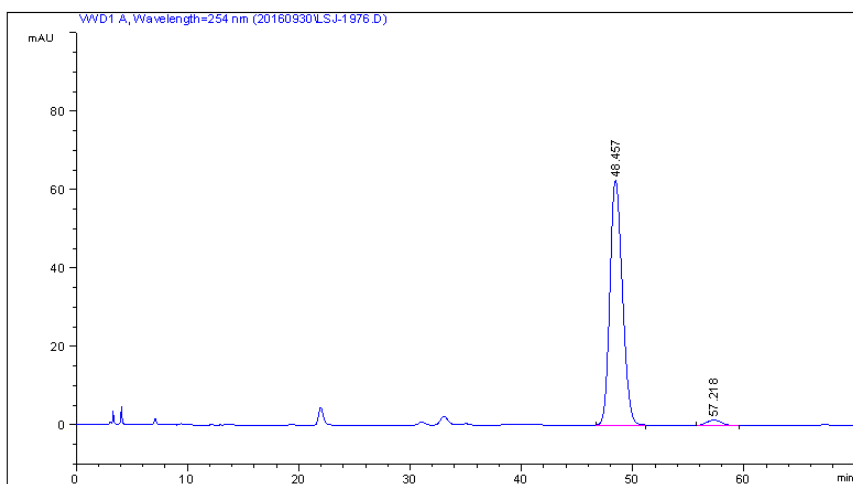
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	47.638	BB	1.0987	1271.05676	17.66425	50.1179
2	57.389	BB	1.3574	1265.07654	13.43938	49.8821

Totals : 2536.13330 31.10363

## Enantiomeric excess of 3r: 95%



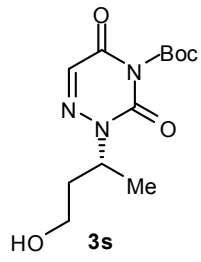
### Area Percent Report

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

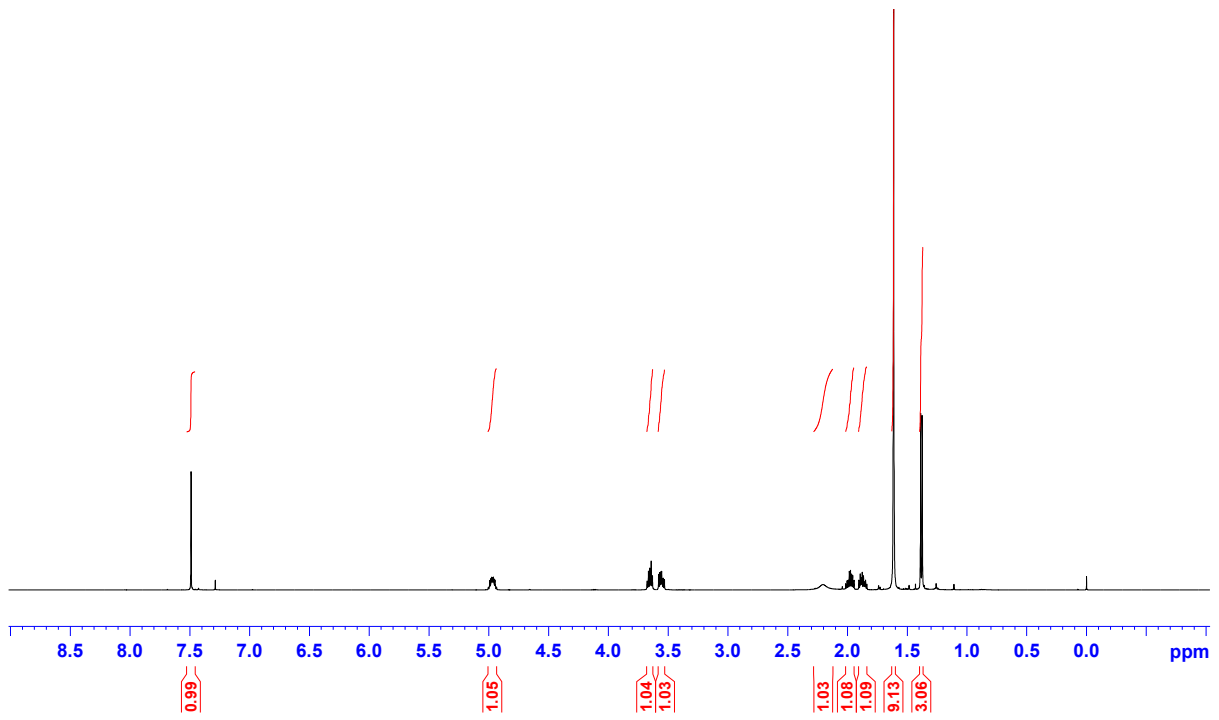
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	48.457	BB	1.2019	4872.06982	62.41705	97.3623
2	57.218	BB	1.0746	131.99260	1.44471	2.6377

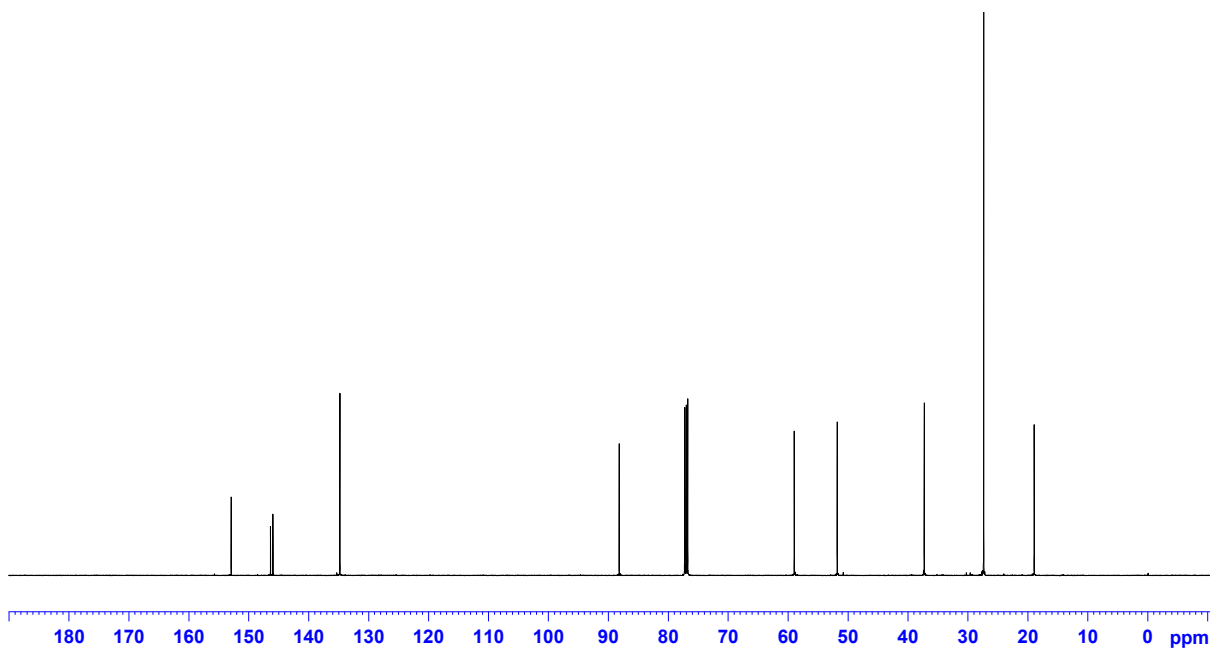
Totals : 5004.06242 63.86176



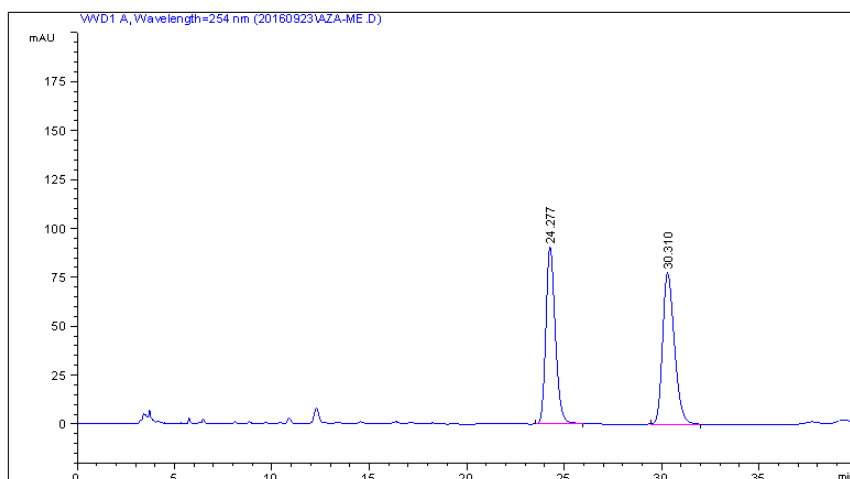
$^1\text{H NMR}$  of **3s**



$^{13}\text{C NMR}$  of **3s**



### Racemate of 3s



#### Area Percent Report

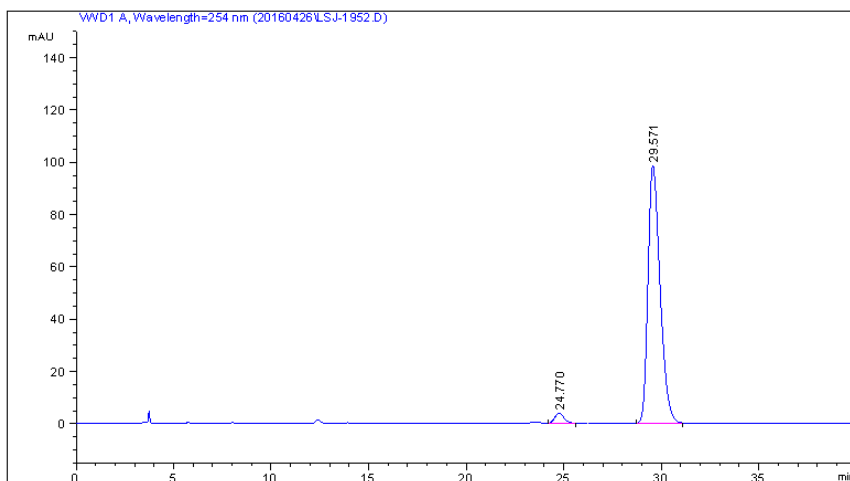
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: WVD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	24.277	BB	0.5199	3054.30322	90.28773	48.1861
2	30.310	BB	0.6528	3284.25391	77.31559	51.8139

Totals : 6338.55713 167.60332

### Enantiomeric excess of 3s: 94%



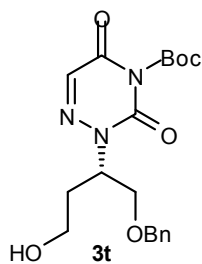
#### Area Percent Report

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

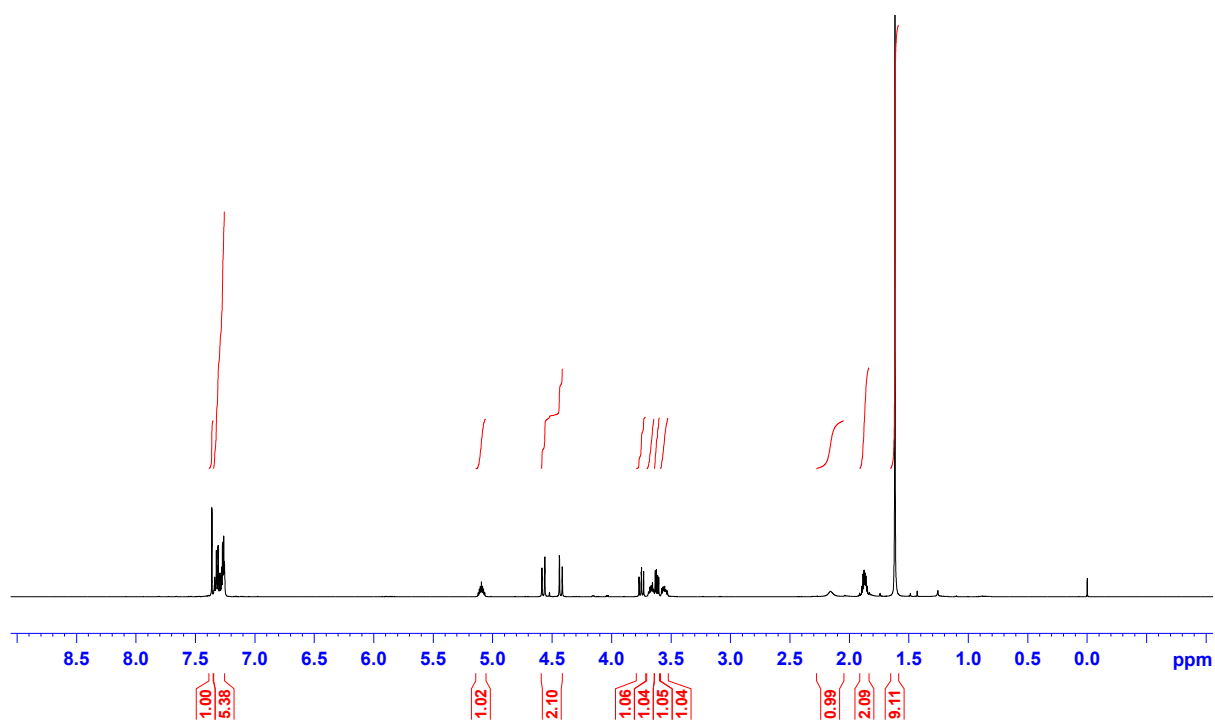
Signal 1: WVD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	24.770	BB	0.5152	127.77089	3.83642	2.9311
2	29.571	BB	0.6613	4231.37207	98.51534	97.0689

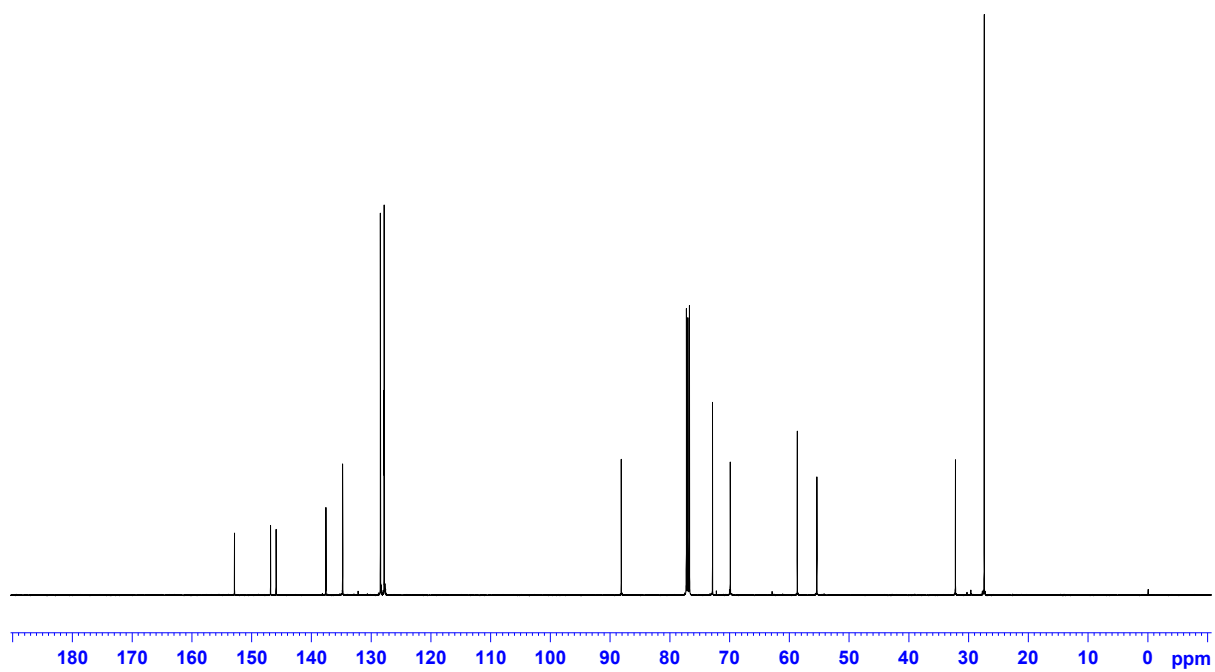
Totals : 4359.14296 102.35176



$^1\text{H NMR}$  of **3t**

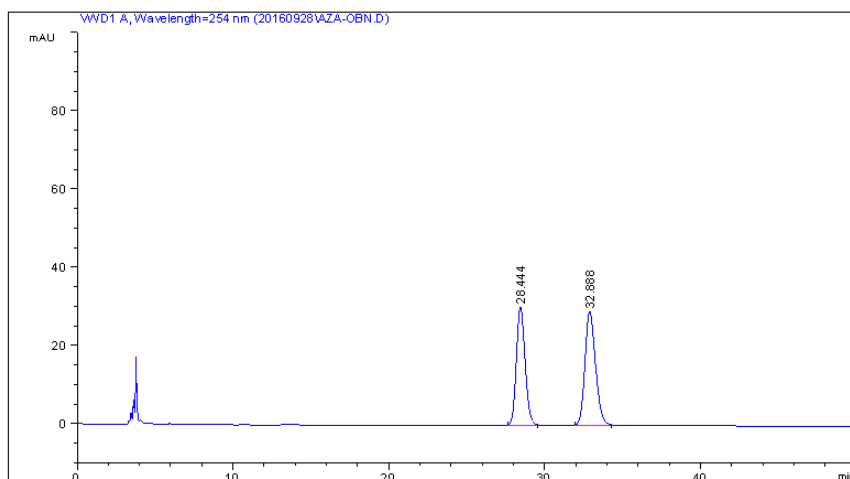


$^{13}\text{C NMR}$  of **3t**





### Racemate of **3t**



#### Area Percent Report

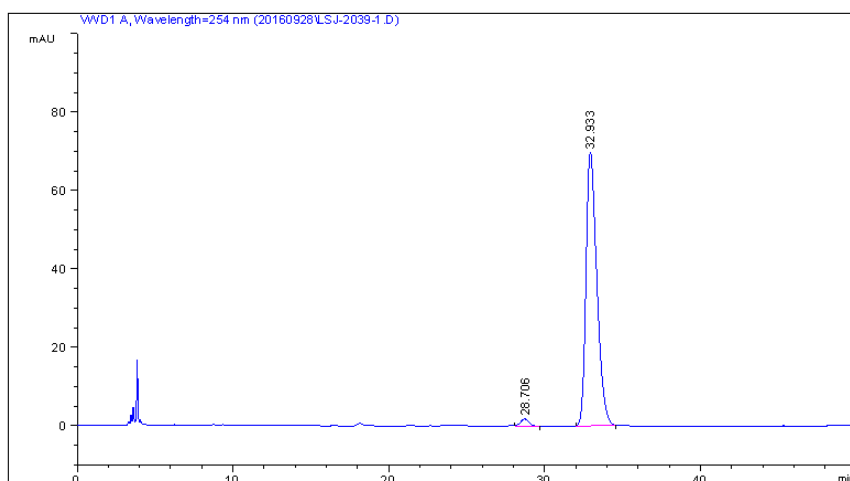
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	28.444	BB	0.6036	1179.41089	30.13647	46.2898	
2	32.888	BB	0.7257	1368.47253	28.97477	53.7102	

Totals : 2547.88342 59.11124

### Enantiomeric excess of **3t**: 96%



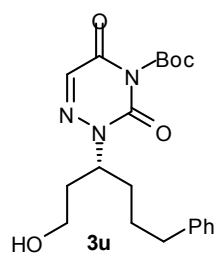
#### Area Percent Report

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

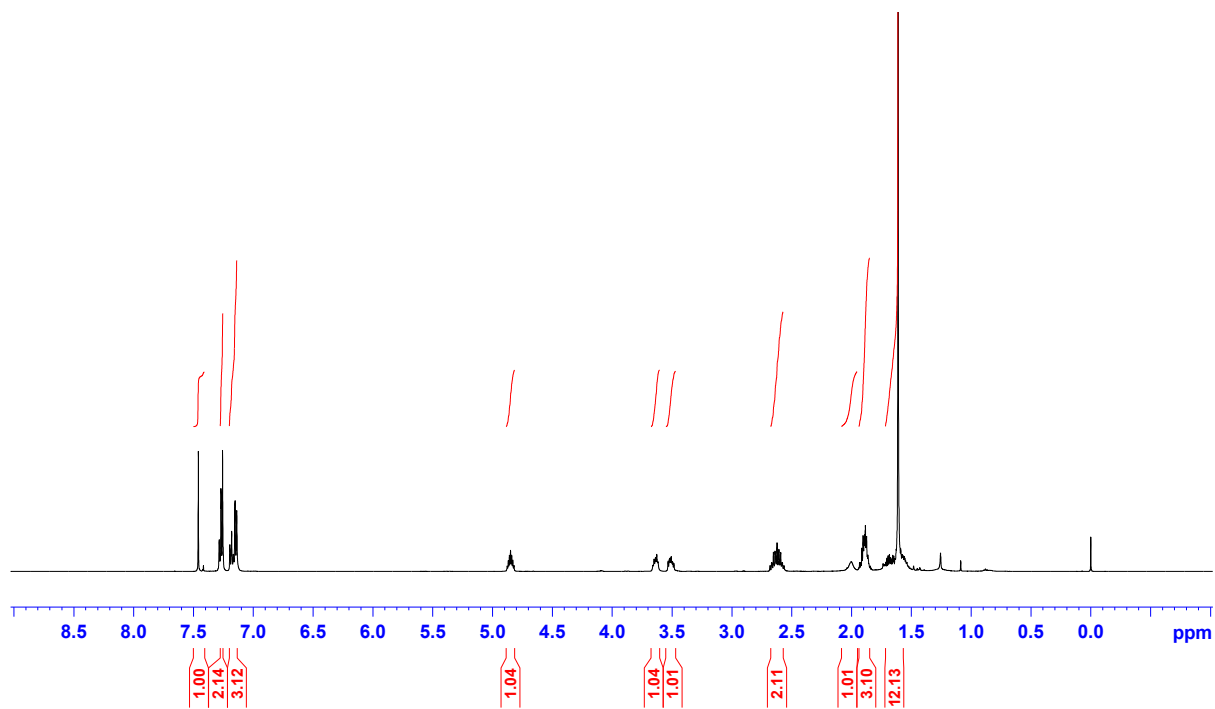
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	28.706	BB	0.5685	66.64995	1.80129	1.9338	
2	32.933	BB	0.7419	3379.89307	69.69822	98.0662	

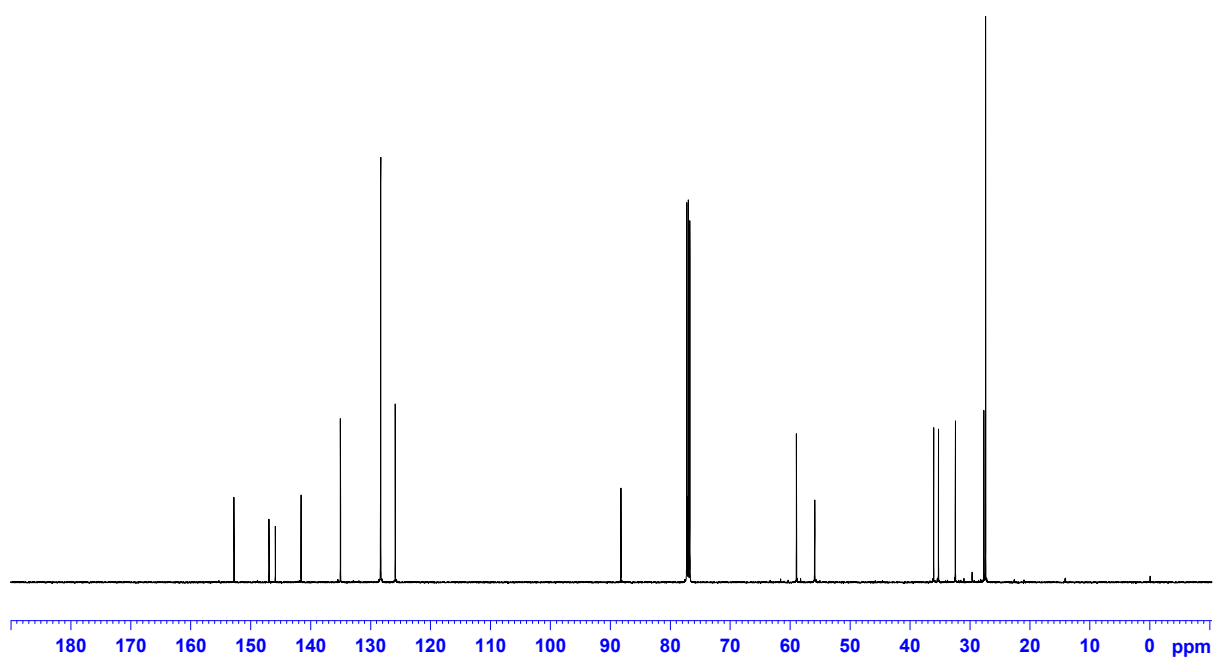
Totals : 3446.54301 71.49951



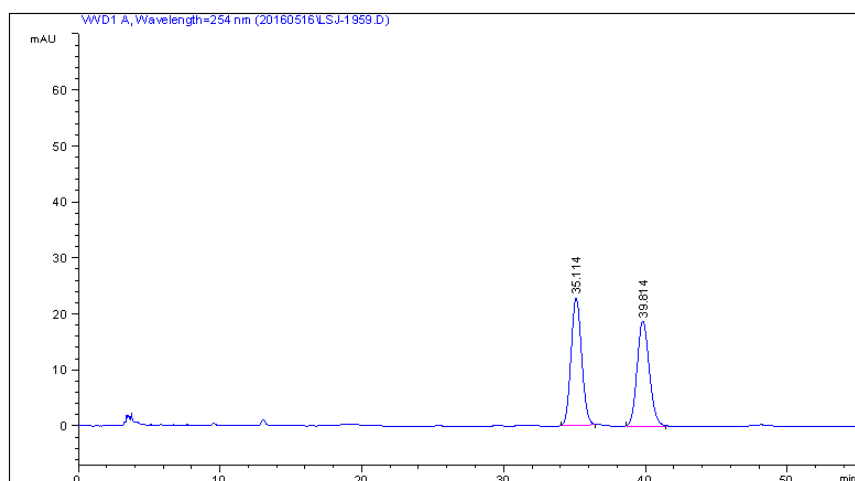
$^1\text{H NMR}$  of **3u**



$^{13}\text{C NMR}$  of **3u**



### Racemate of **3u**



#### Area Percent Report

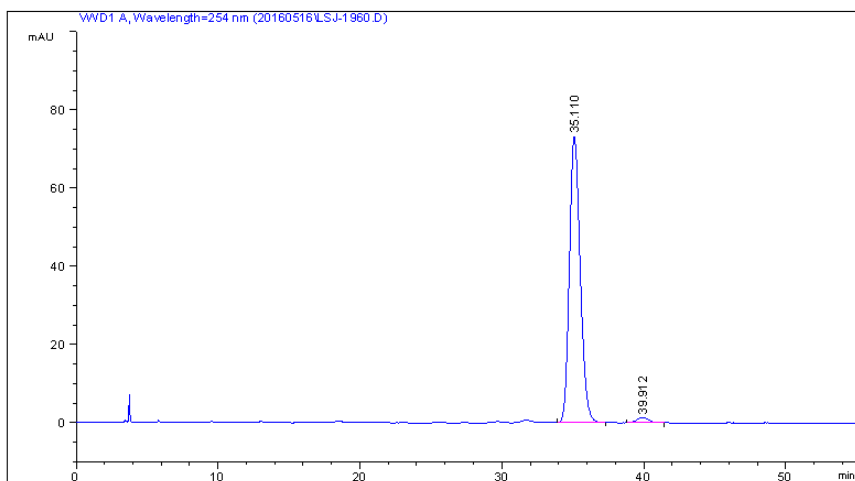
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	35.114	BB	0.8122	1184.84485	22.77767	51.3760
2	39.814	BB	0.9322	1121.37610	18.70915	48.6240

Totals : 2306.22095 41.48682

### Enantiomeric excess of **3u**: 96%



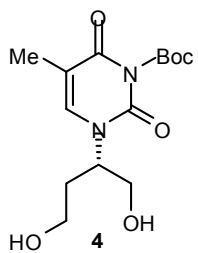
#### Area Percent Report

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

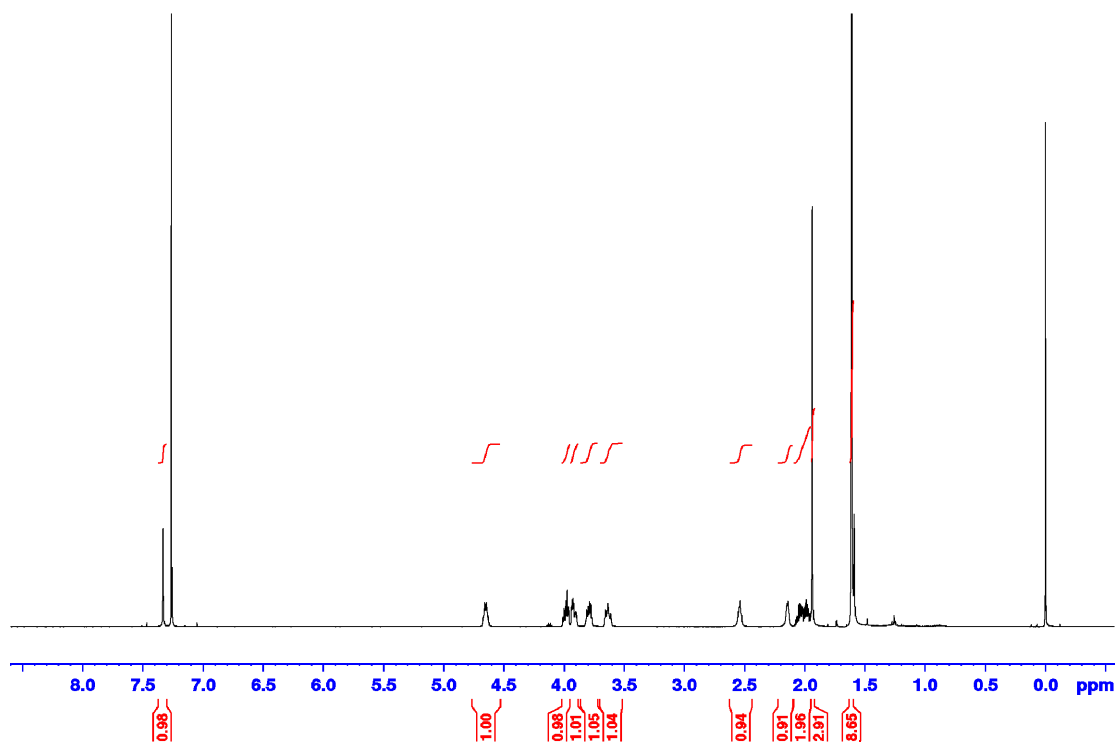
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	35.110	BB	0.8204	3885.35596	73.17531	97.9742
2	39.912	BB	0.8161	80.33545	1.33408	2.0258

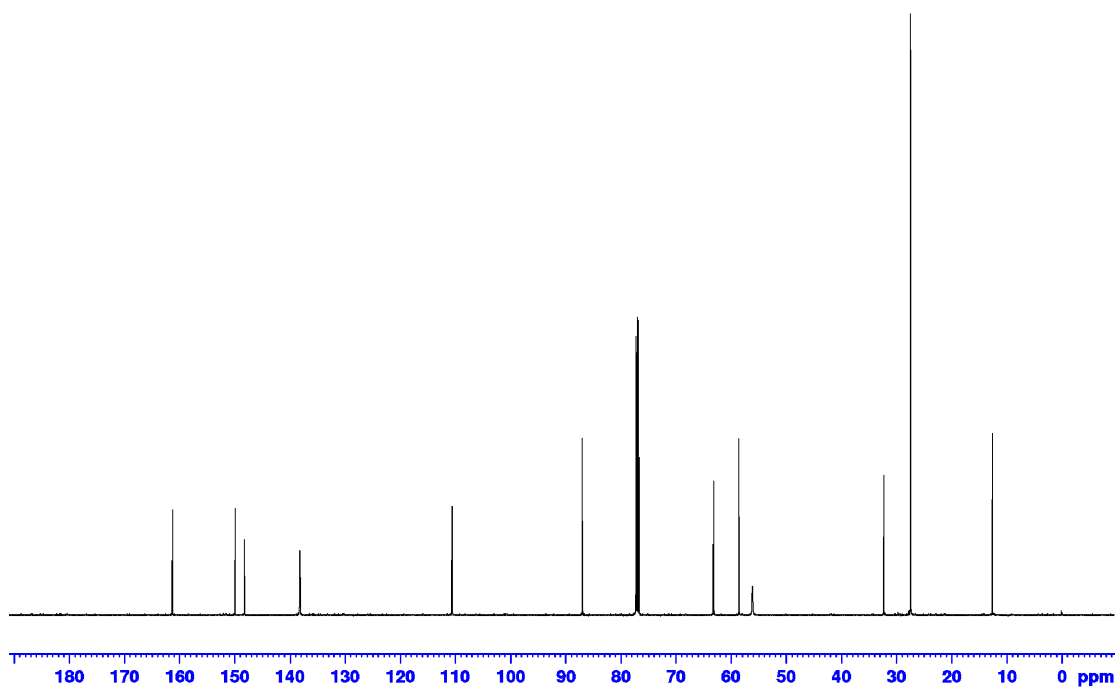
Totals : 3965.69141 74.50939



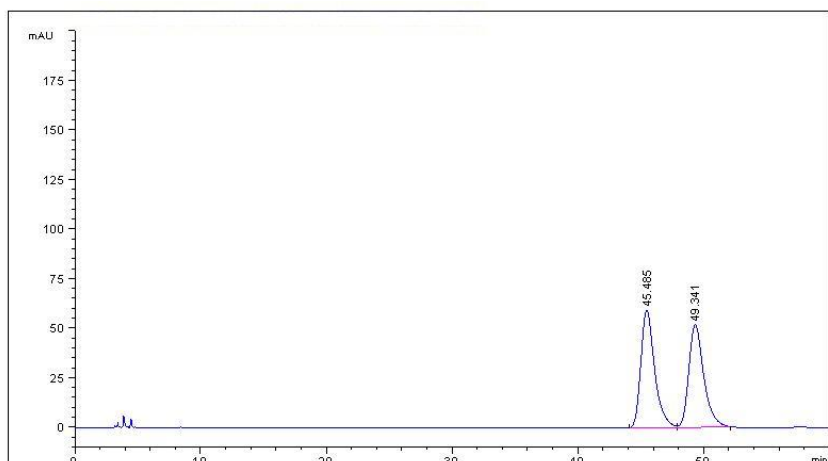
$^1\text{H NMR}$  of **4**



$^{13}\text{C NMR}$  of **4**



### Racemate of 4



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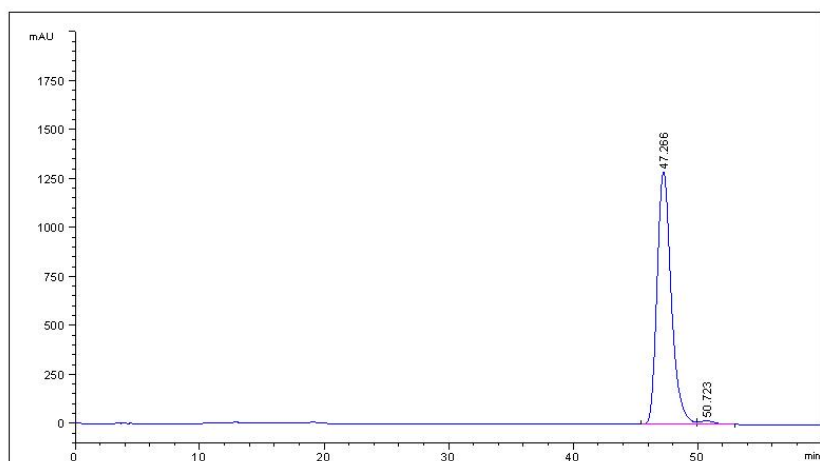
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	45.485	BB	1.1550	4534.15771	59.53031	51.3761	
2	49.341	BB	1.2338	4291.27148	51.90907	48.6239	

Totals : 8825.42920 111.43937

### Enantiomeric excess of 4: 97%



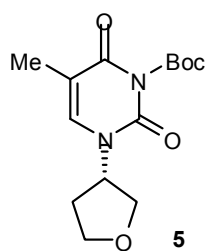
=====  
Area Percent Report  
=====

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

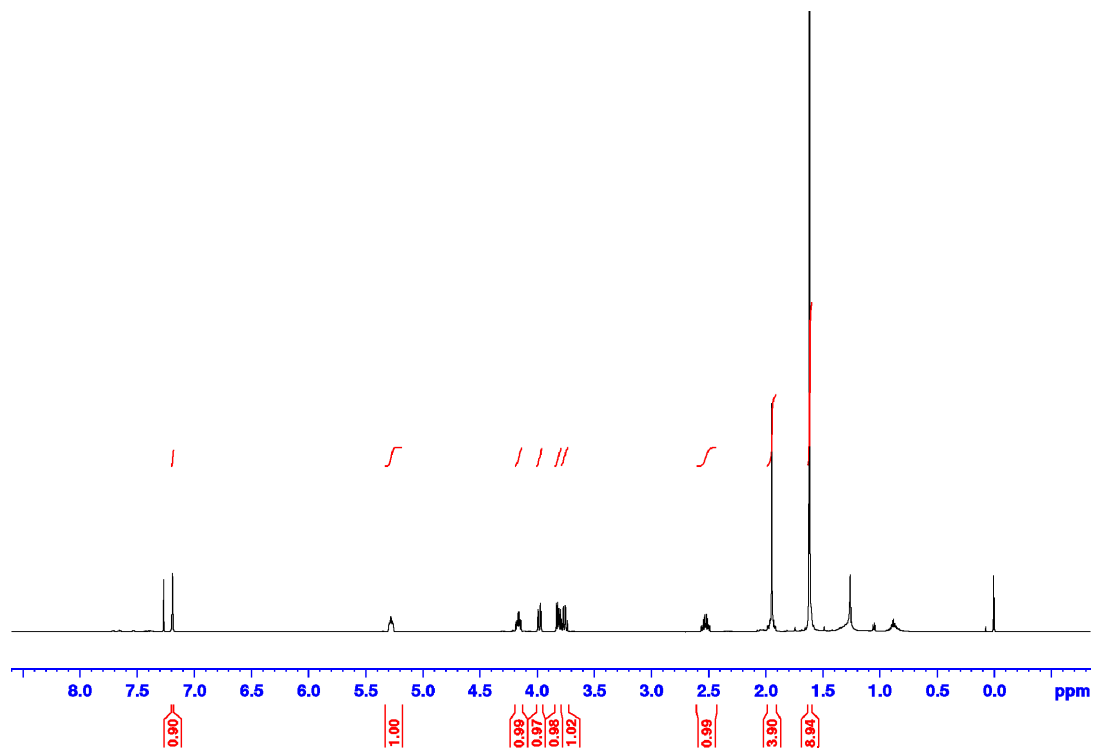
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	47.266	BV	1.2089	1.01933e5	1287.74377	98.5795	
2	50.723	VB	1.2013	1468.87231	17.72451	1.4205	

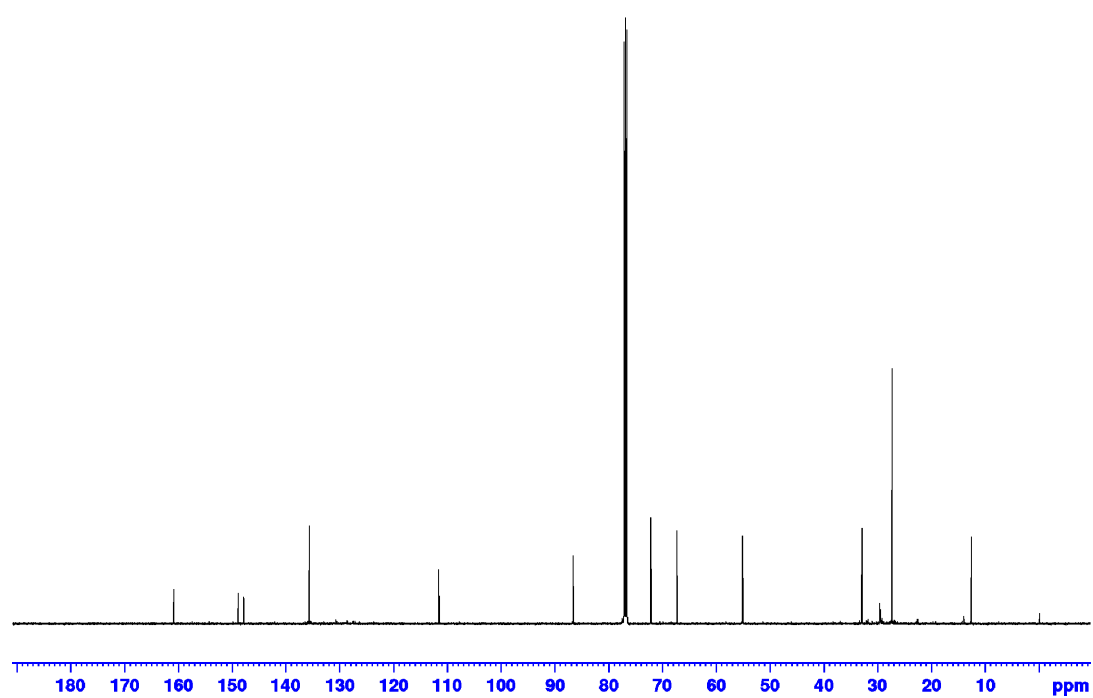
Totals : 1.03402e5 1305.46828



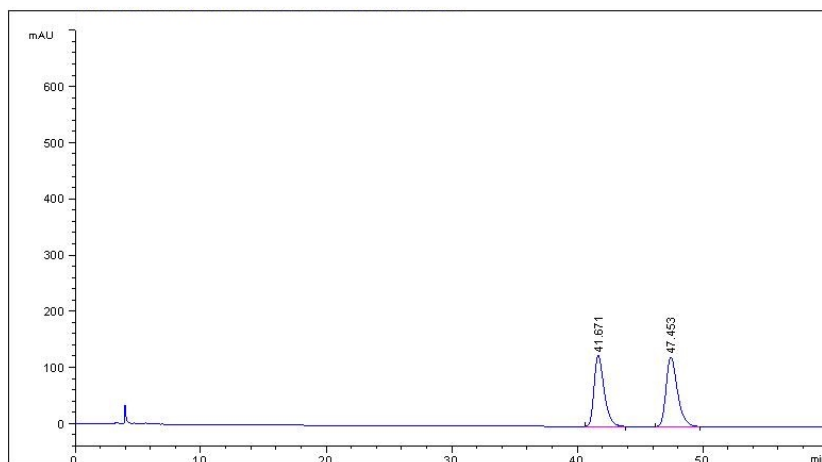
$^1\text{H NMR}$  of **5**



$^{13}\text{C NMR}$  of **5**



Racemate of 5



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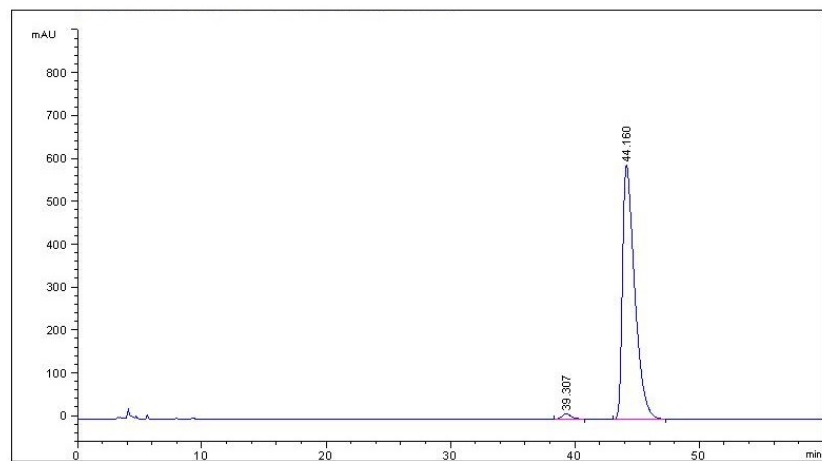
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	41.671	BB	0.8479	7035.47314	126.29169	47.4499
2	47.453	BB	0.9591	7791.70215	123.69643	52.5501

Totals : 1.48272e4 249.98812

Enantiomeric excess of 5: 97%



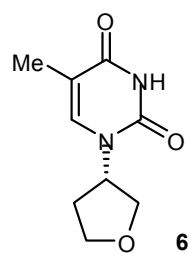
=====  
Area Percent Report  
=====

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

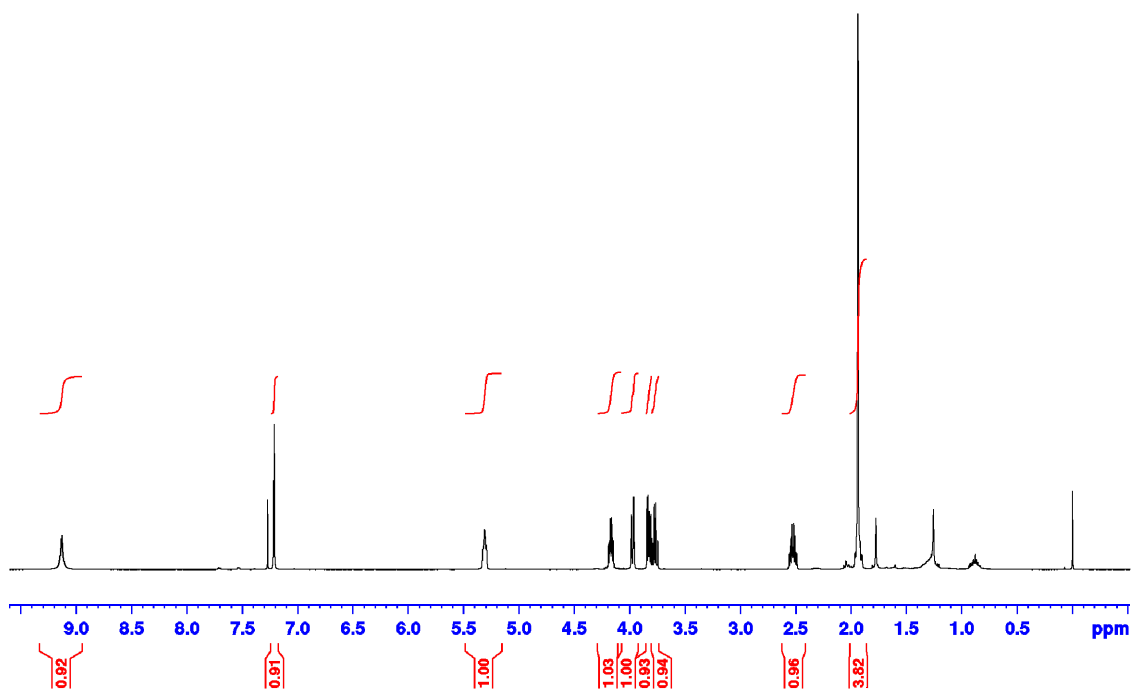
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	39.307	BB	0.7990	607.58551	11.59889	1.4870
2	44.160	BB	1.0269	4.02510e4	591.50342	98.5130

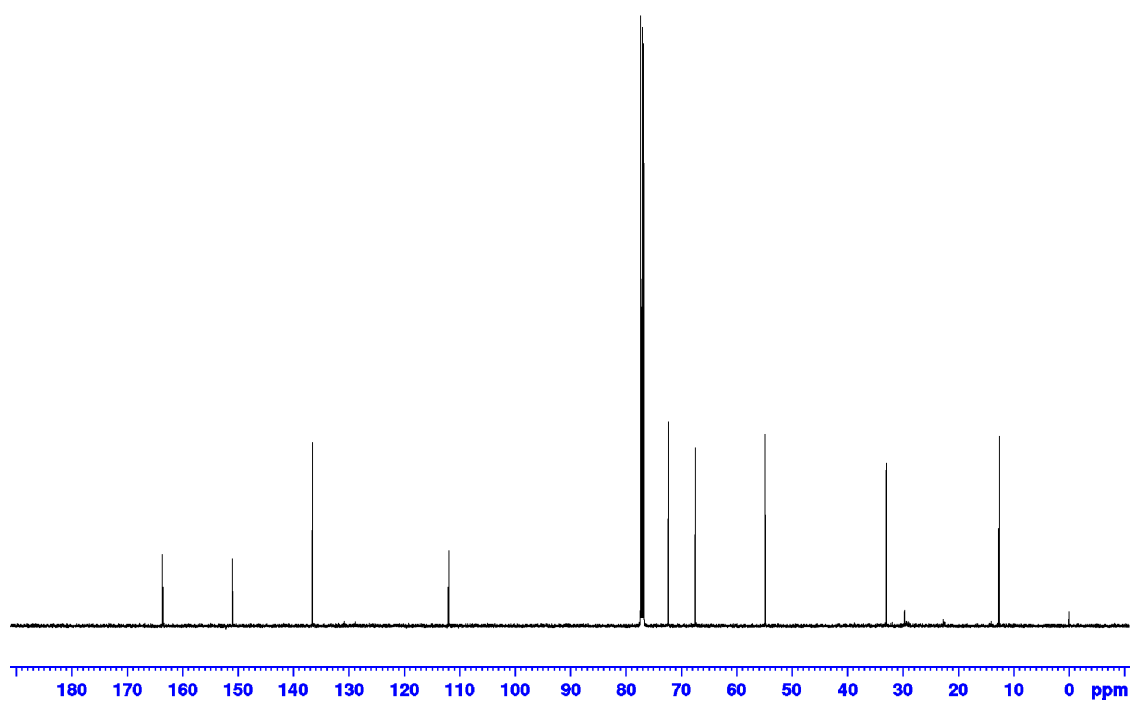
Totals : 4.08586e4 603.10231



$^1\text{H NMR}$  of **6**

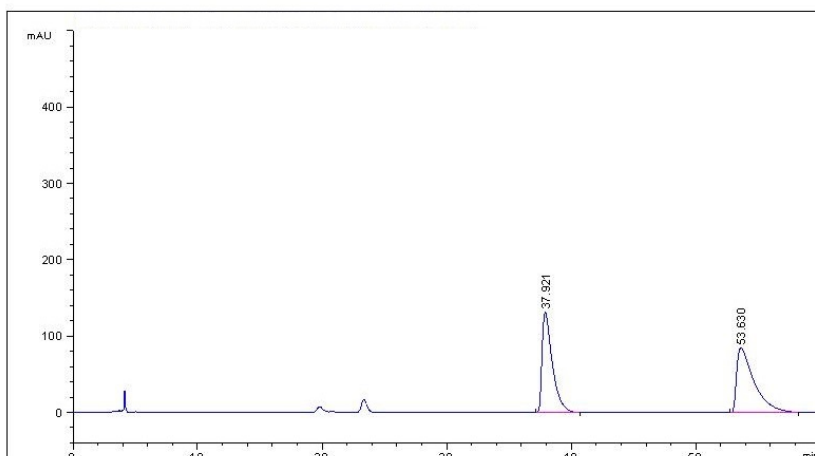


$^{13}\text{C NMR}$  of **6**





## Racemate of 6



### Area Percent Report

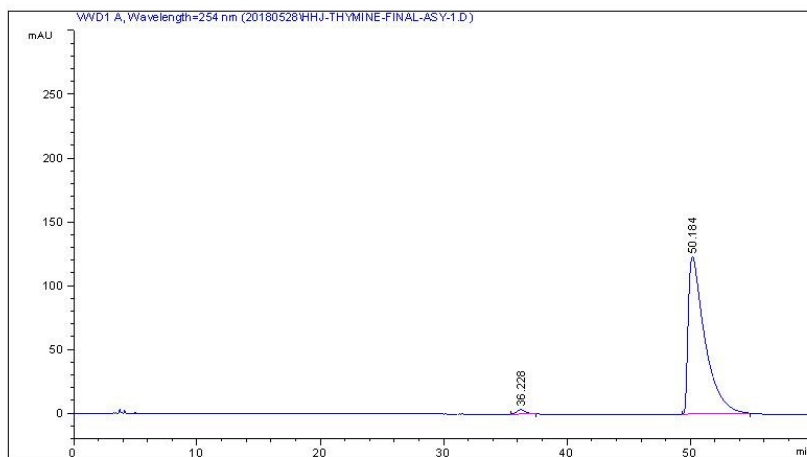
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	37.921	BB	0.8591	7605.03613	131.32484	47.7913
2	53.630	BB	1.4266	8307.98633	84.93492	52.2087

Totals : 1.59130e4 216.25977

## Enantiomeric excess of 6: 97%



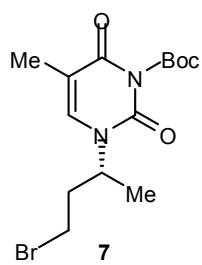
### Area Percent Report

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

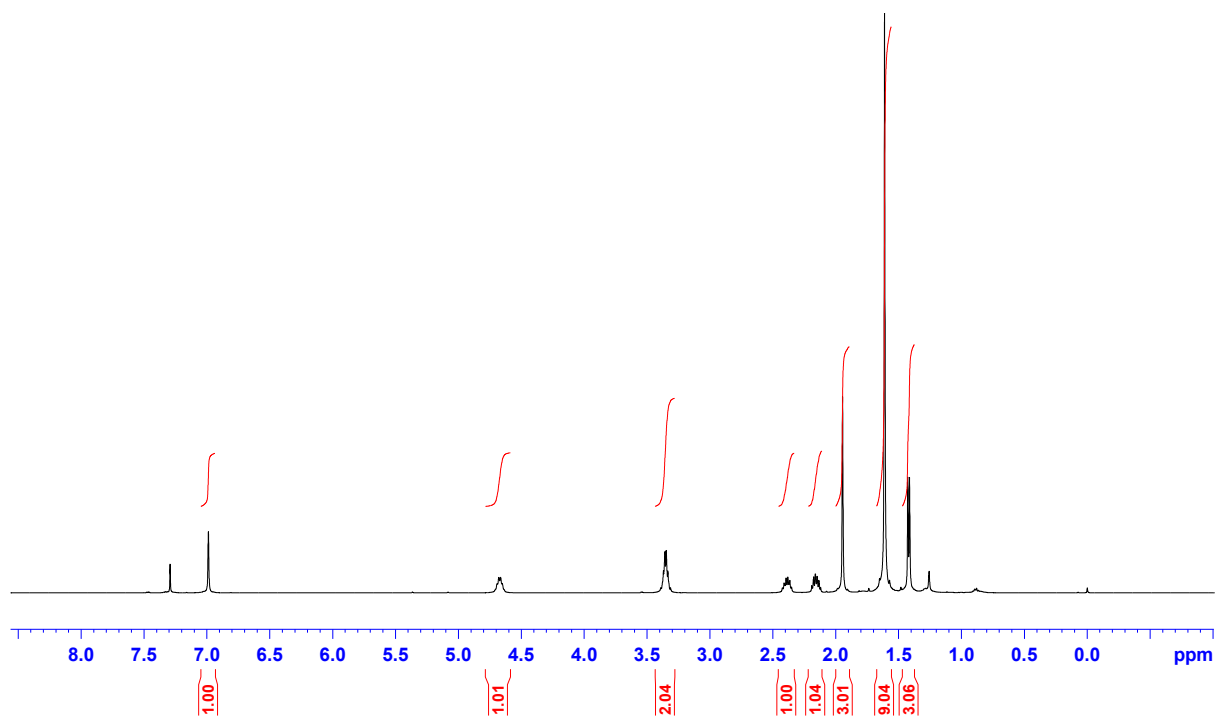
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	36.228	BB	0.7221	170.65524	3.37662	1.4573
2	50.184	BB	1.3369	1.15398e4	123.42179	98.5427

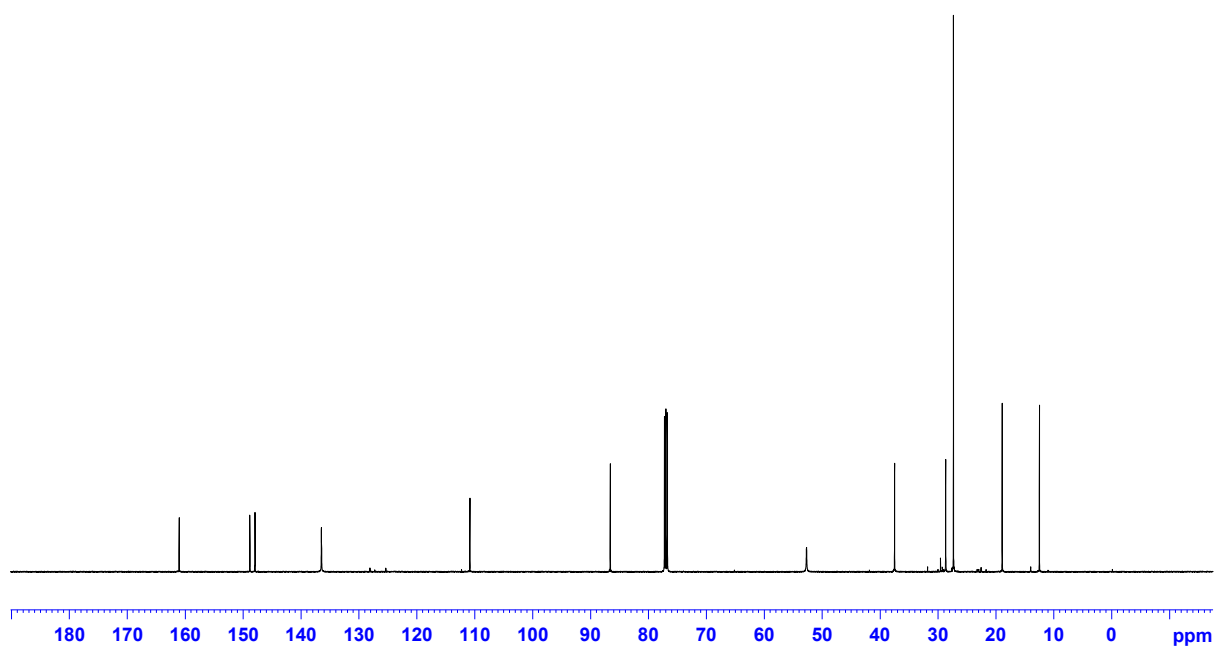
Totals : 1.17104e4 126.79841



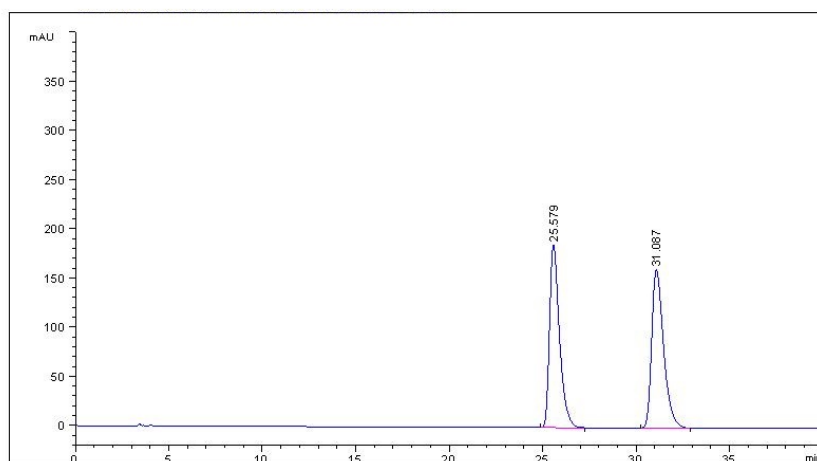
$^1\text{H NMR}$  of 7



$^{13}\text{C NMR}$  of 7



Racemate of 7



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Area Percent Report  
=====

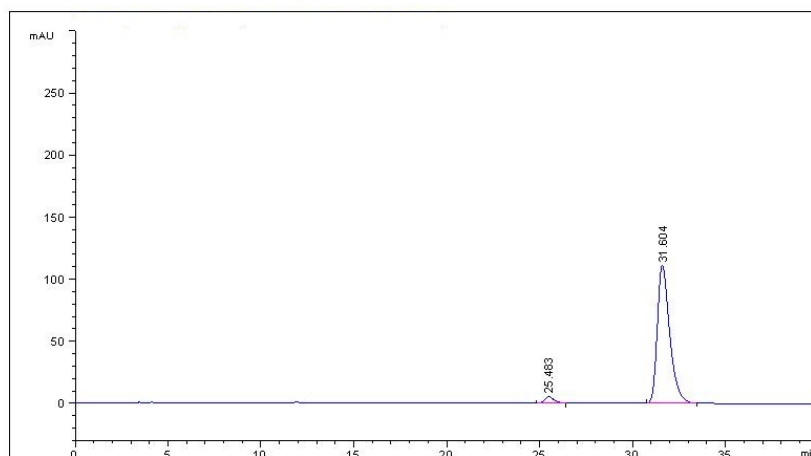
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	25.579	BB	0.5599	6855.47168	185.84795	49.1337
2	31.087	BB	0.6680	7097.22949	161.18871	50.8663

Totals : 1.39527e4 347.03665

Enantiomeric excess of 7: 93%



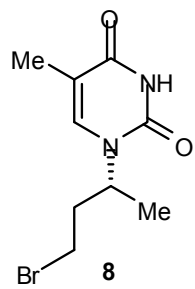
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Area Percent Report  
=====

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

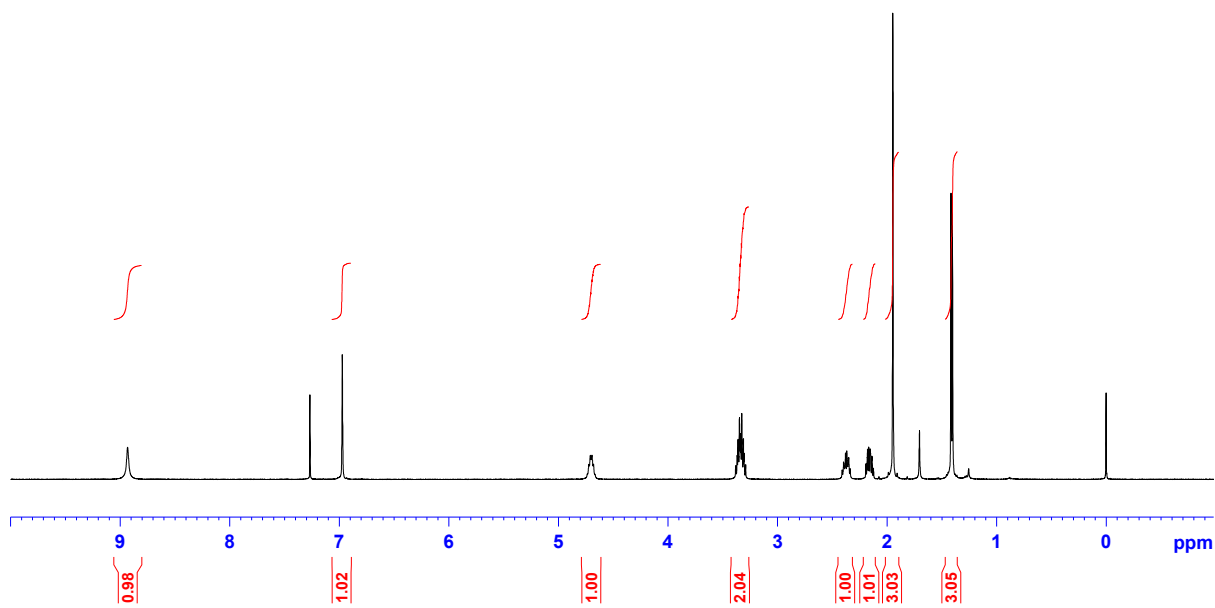
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	25.483	BB	0.5467	191.23438	5.29390	3.5768
2	31.604	BB	0.7077	5155.23535	111.02760	96.4232

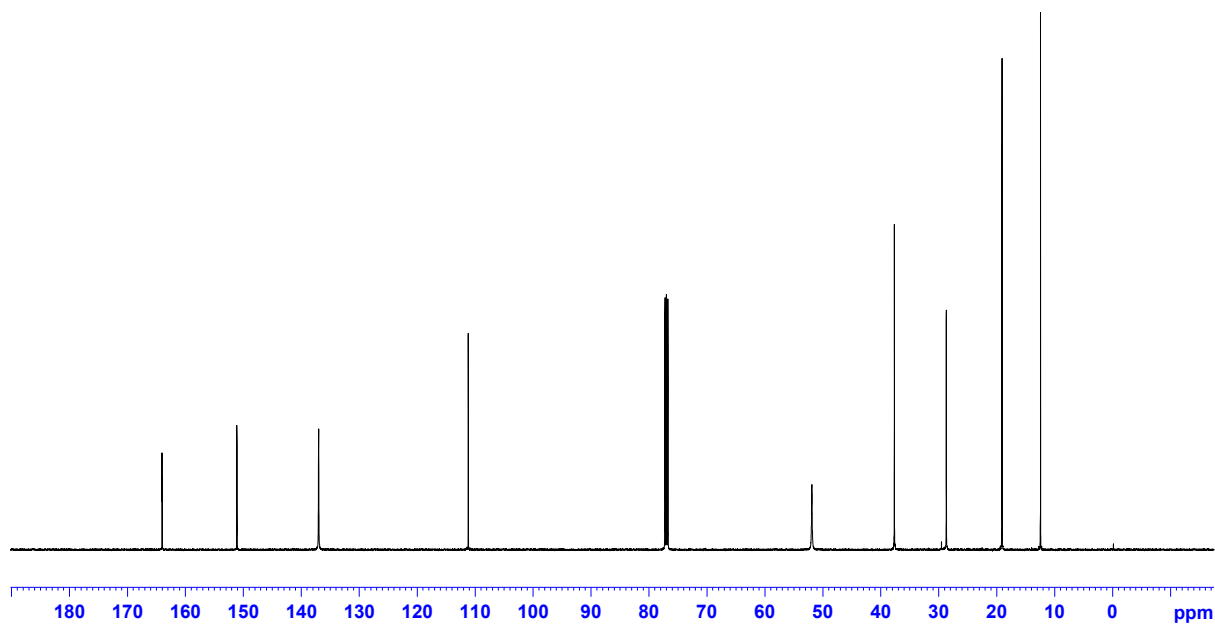
Totals : 5346.46973 116.32150



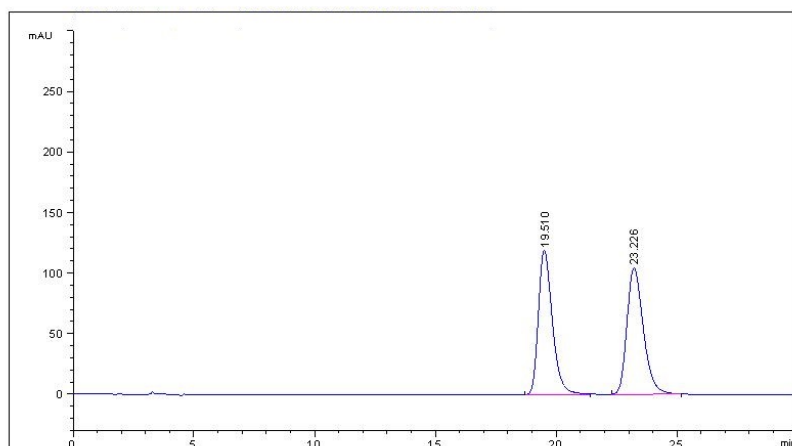
$^1\text{H NMR}$  of **8**



$^{13}\text{C NMR}$  of **8**



Racemate of **8**



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Area Percent Report  
=====

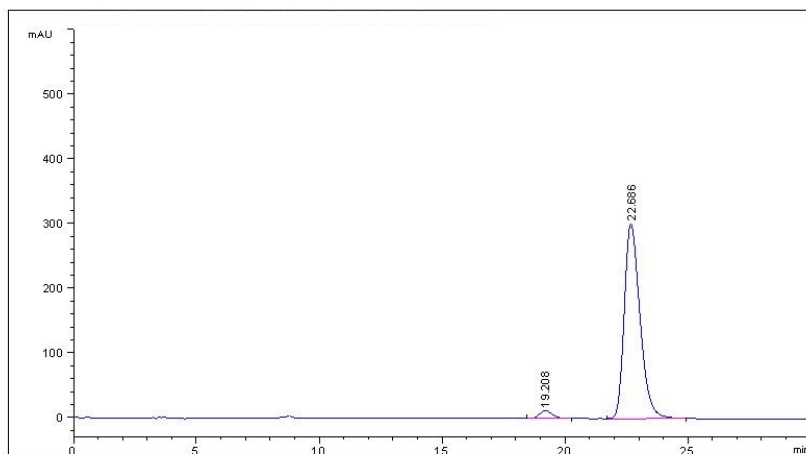
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	19.510	BB	0.6141	4779.98877	119.02715	49.1990
2	23.226	BB	0.7261	4935.63184	104.43660	50.8010

Totals : 9715.62061 223.46375

Enantiomeric excess of **8**: 94%



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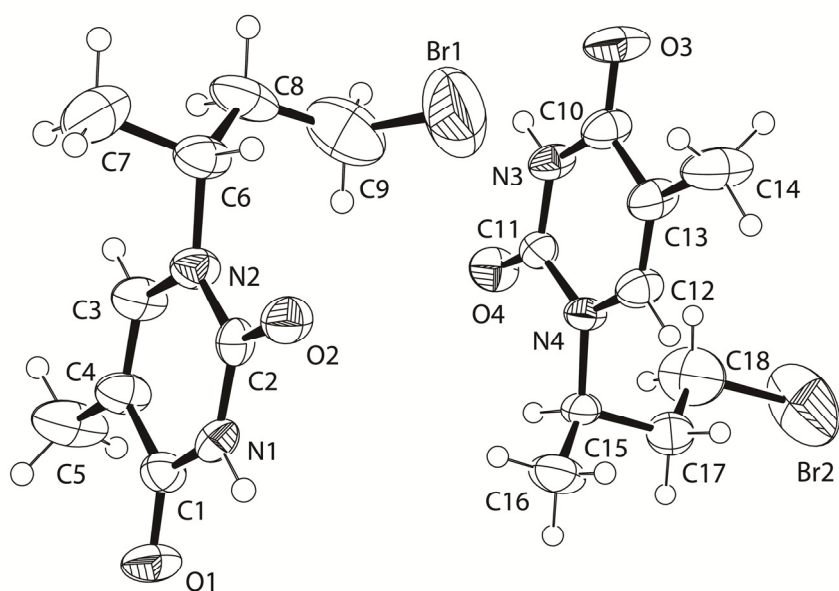
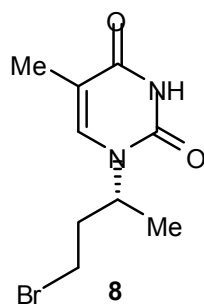
Sorted By : Signal  
Multiplier: : 1.0000  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	19.208	BB	0.5597	448.92688	12.21799	3.2499
2	22.686	BB	0.6813	1.33645e4	300.87344	96.7501

Totals : 1.38135e4 313.09143

**X-Ray crystal structure of 8 (CCDC-1868522)**



*Thermal ellipsoids are drawn at the 50% probability level*