

Electronic Supplementary Information

Catalytic enantioselective synthesis of carboxy-substituted 2-isoxazolines by cascade oxa-Michael-cyclization

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Chang-Woo Cho^{*a}

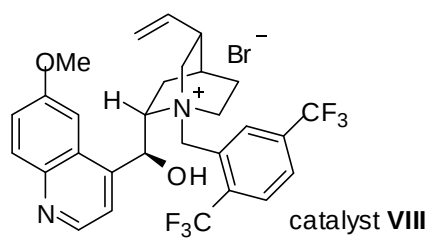
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Kyungpook National University, Daegu 41566, Republic of Korea*

^b*Center for Eco-Friendly New Materials, Korea Research Institute of Chemical
Technology, Daejeon 34114, Republic of Korea*

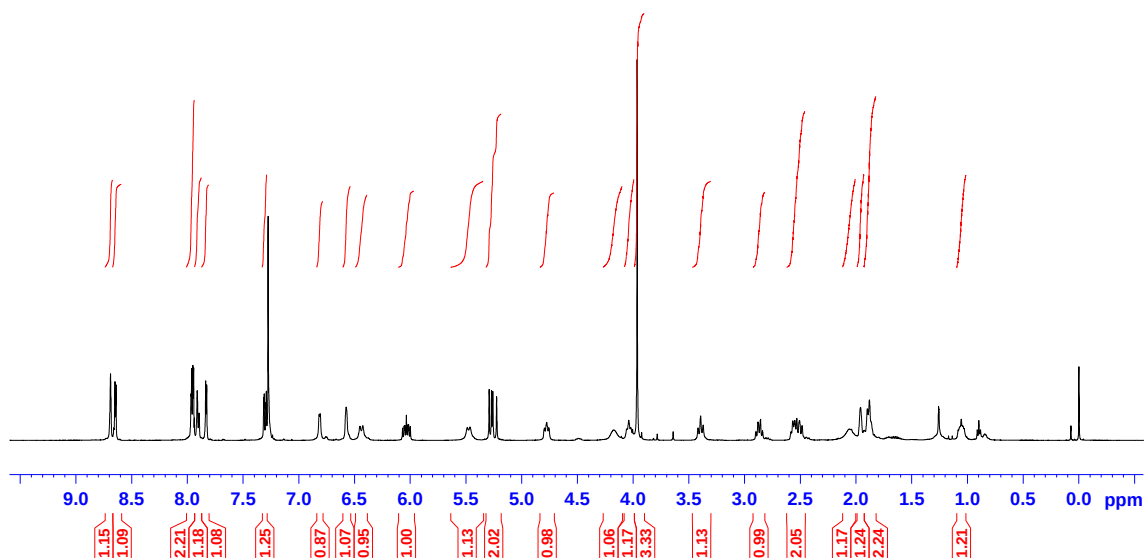
**E-mail: cwcho@knu.ac.kr*

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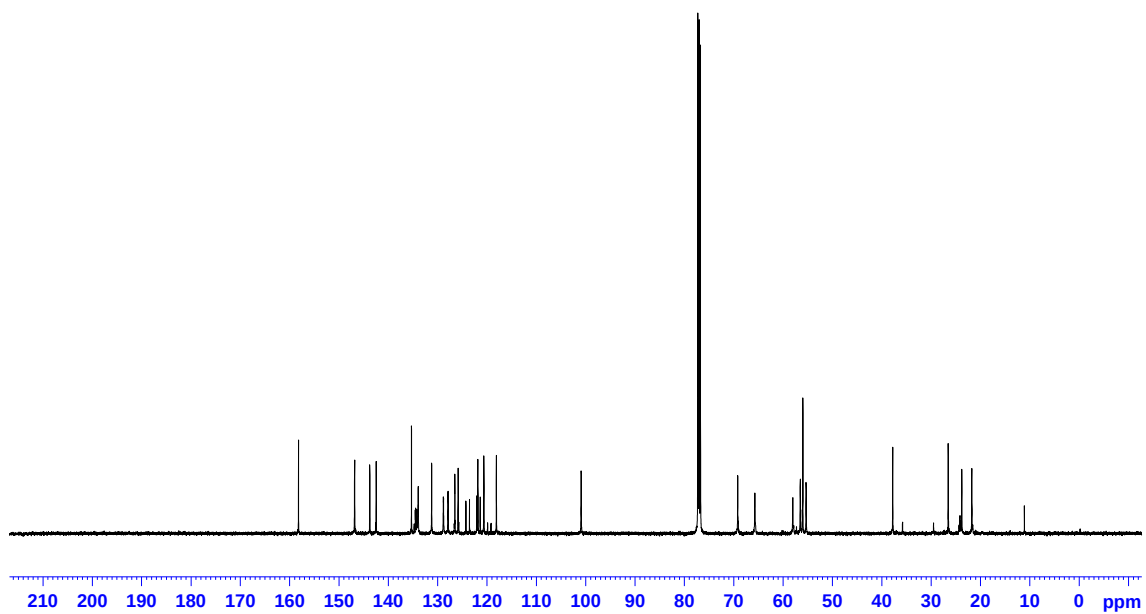
NMR spectra and chiral HPLC traces of new compounds	S2-S41
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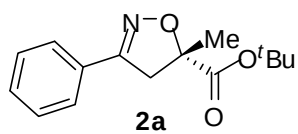


^1H NMR of catalyst **VIII**

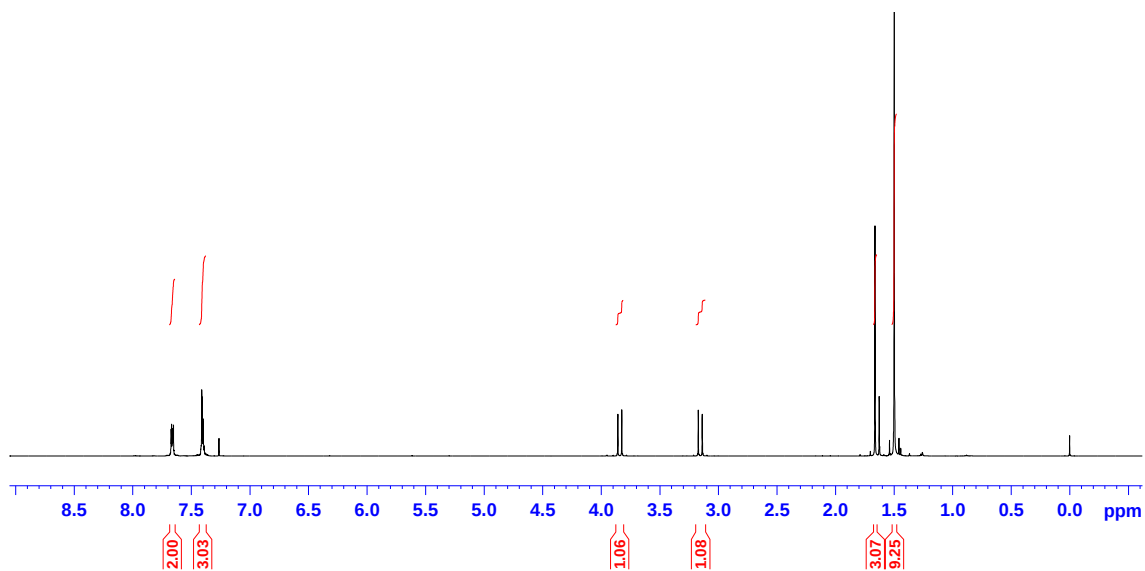


^{13}C NMR of catalyst **VIII**

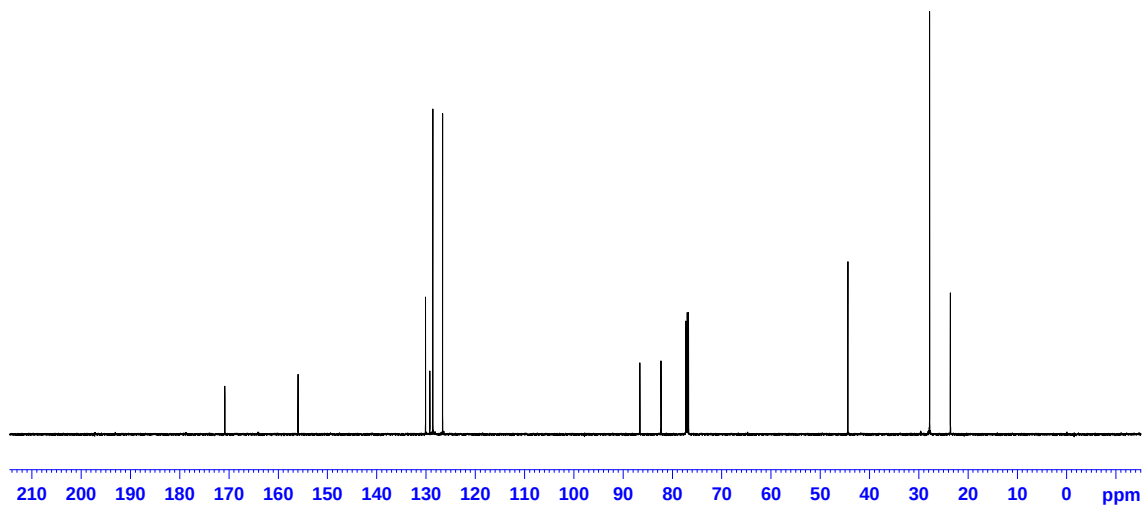




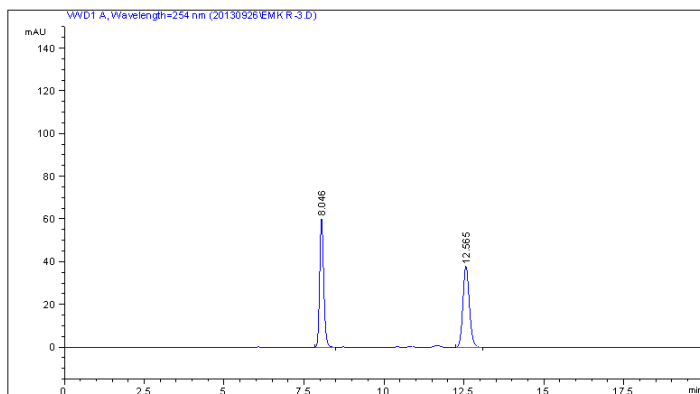
^1H NMR of **2a**



^{13}C NMR of **2a**



Racemate of **2a**



Area Percent Report

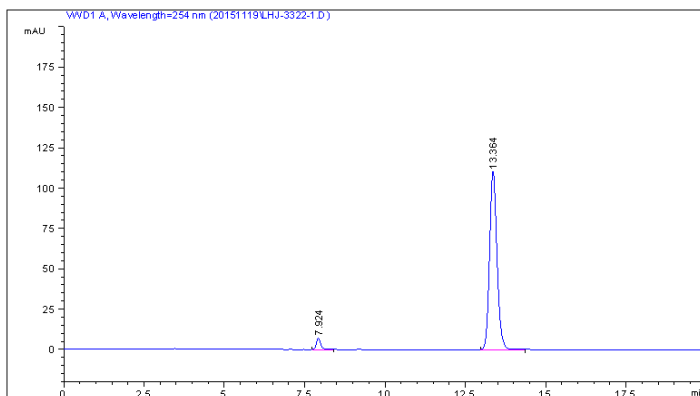
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Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	8.046	BB	0.1356	535.34106		60.29088	49.9913
2	12.565	BB	0.2168	535.52808		38.01197	50.0087

Totals : 1070.86914 98.30285

Enantiomeric excess of **2a**: 93%



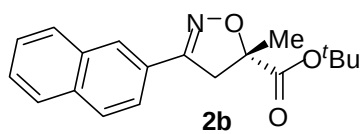
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Use Multiplier & Dilution Factor with ISTDs

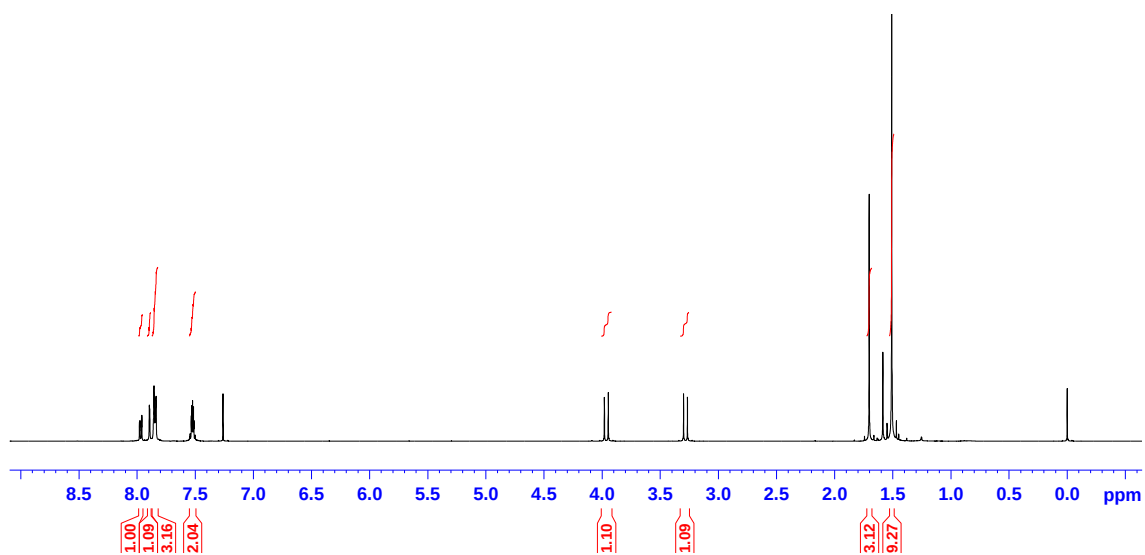
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	7.924	BB	0.1464	68.57644		7.17755	3.7083
2	13.364	BB	0.2494	1780.69409		110.34338	96.2917

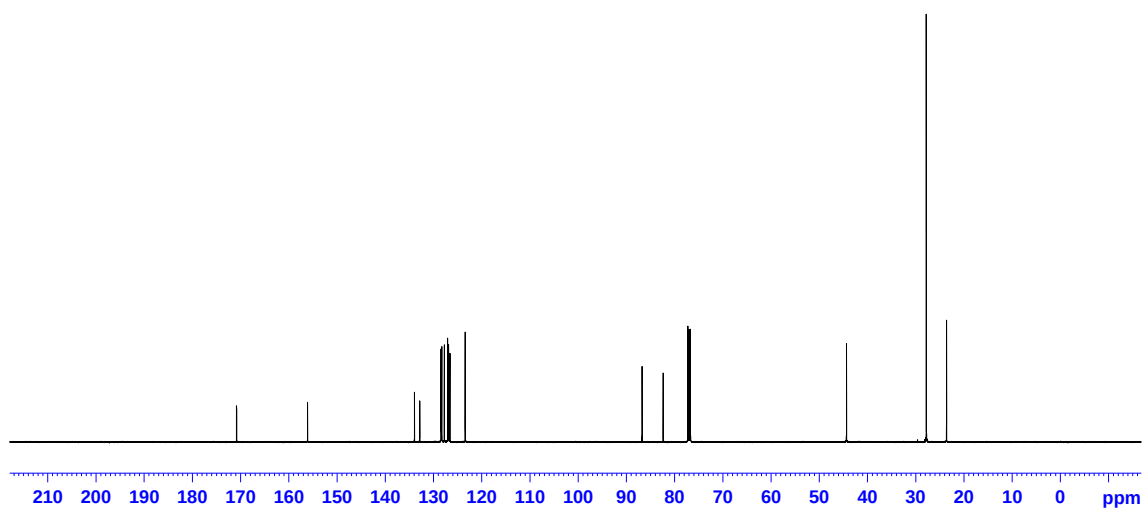
Totals : 1849.27053 117.52094



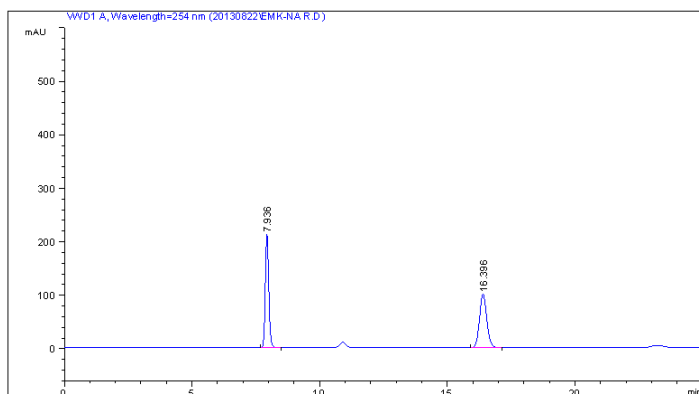
^1H NMR of **2b**



^{13}C NMR of **2b**



Racemate of **2b**



Area Percent Report

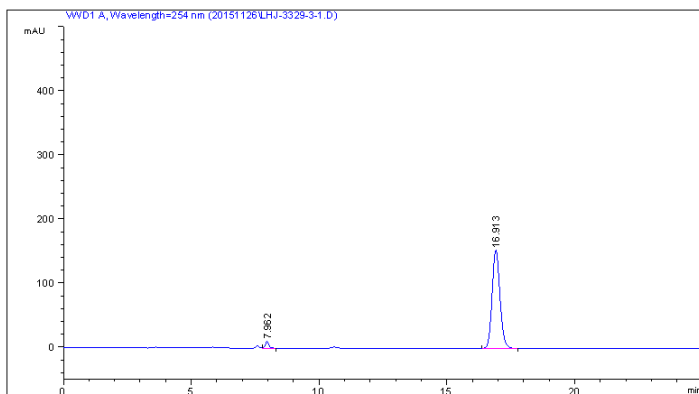
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Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	7.936	VB	0.1463	1989.25146		211.25790	50.0375
2	16.396	BB	0.3092	1986.27051		99.86577	49.9625

Totals : 3975.52197 311.12367

Enantiomeric excess of **2b**: 94%



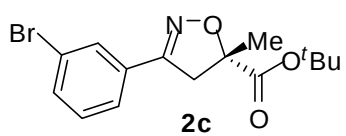
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Use Multiplier & Dilution Factor with ISTDs

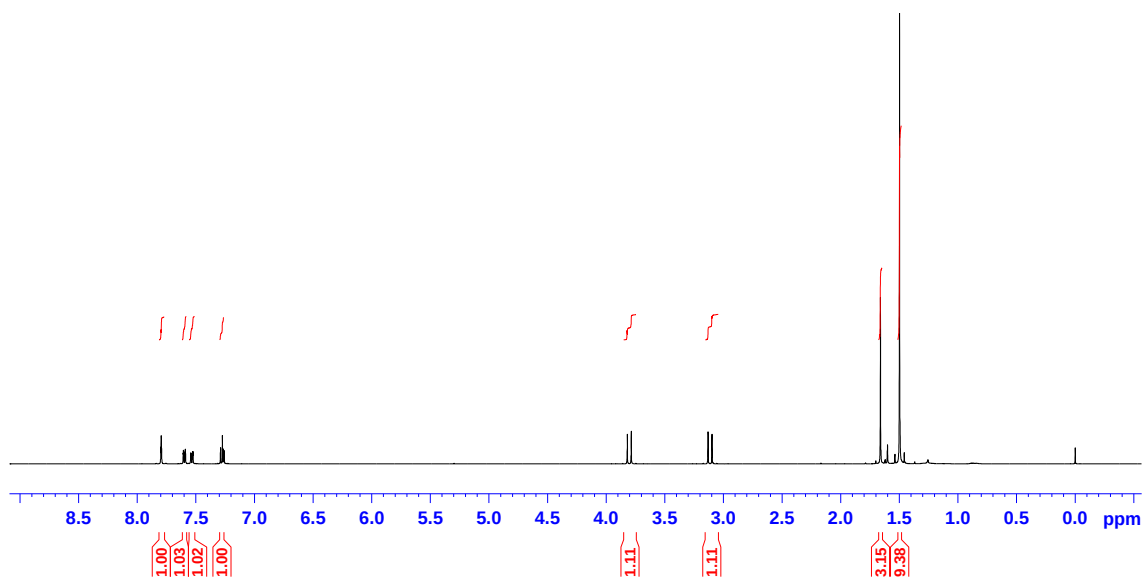
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	7.962	VB	0.1408	92.29984		9.90441	2.7513
2	16.913	BB	0.3289	3262.49805		152.98415	97.2487

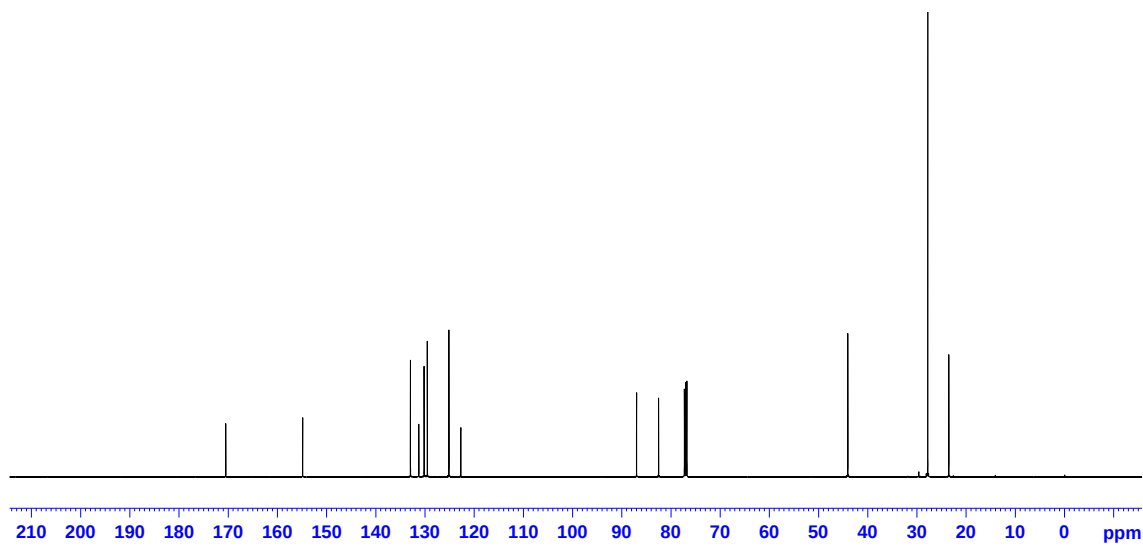
Totals : 3354.79789 162.88856



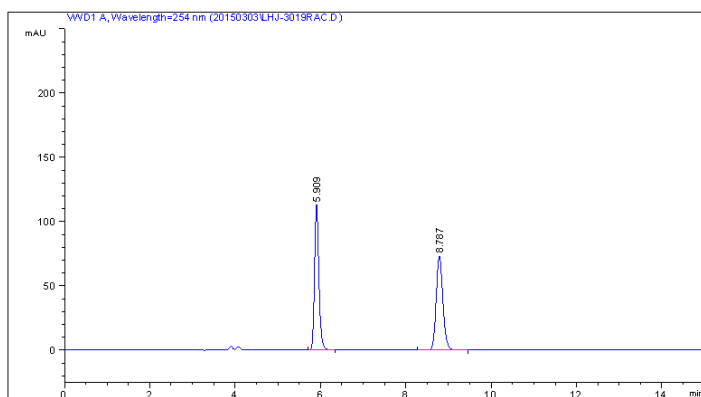
^1H NMR of **2c**



^{13}C NMR of **2c**



Racemate of 2c



Area Percent Report

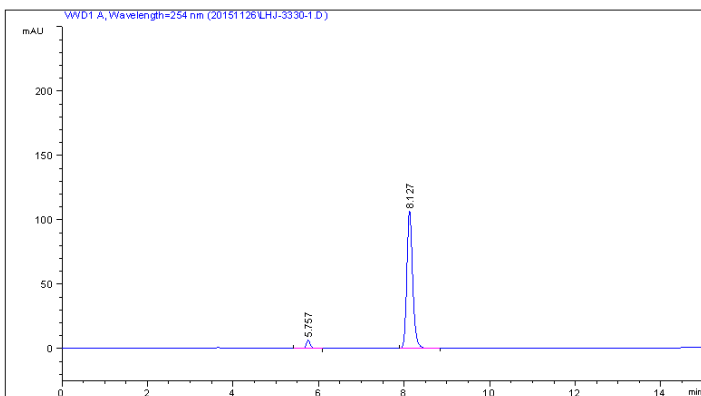
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	5.909	BV	0.1091	804.65979		113.24727	49.9423
2	8.787	VB	0.1692	806.52002		73.27828	50.0577

Totals : 1611.17981 186.52555

Enantiomeric excess of 2c: 92%



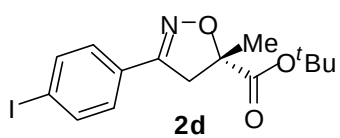
Area Percent Report

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Use Multiplier & Dilution Factor with ISTDs

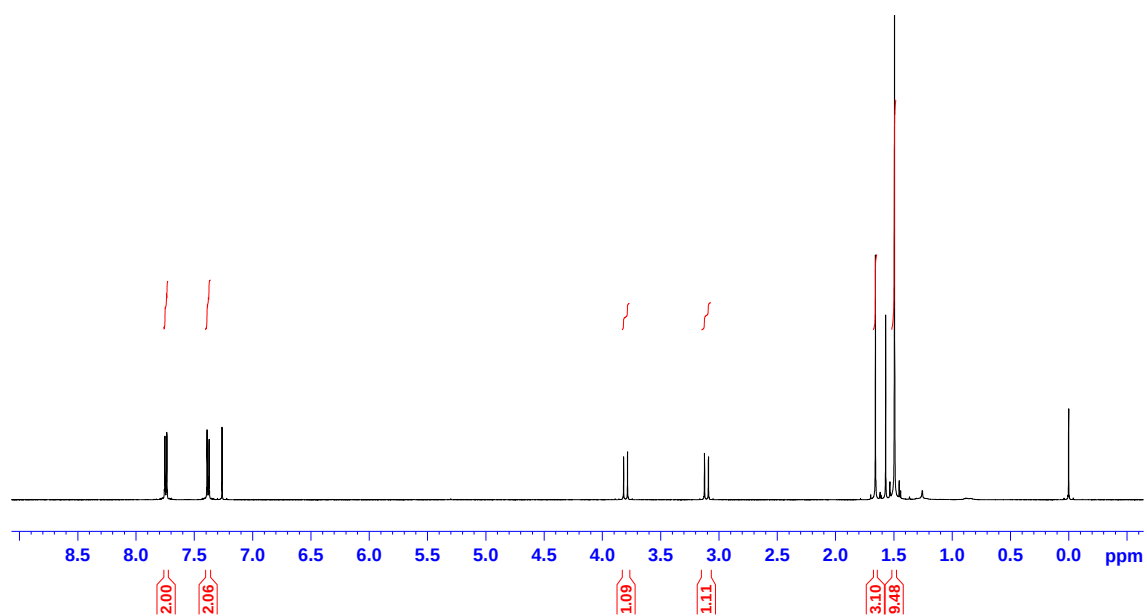
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	5.757	BB	0.1025	43.07316		6.34771	4.0713
2	8.127	BB	0.1464	1014.88800		106.23417	95.9287

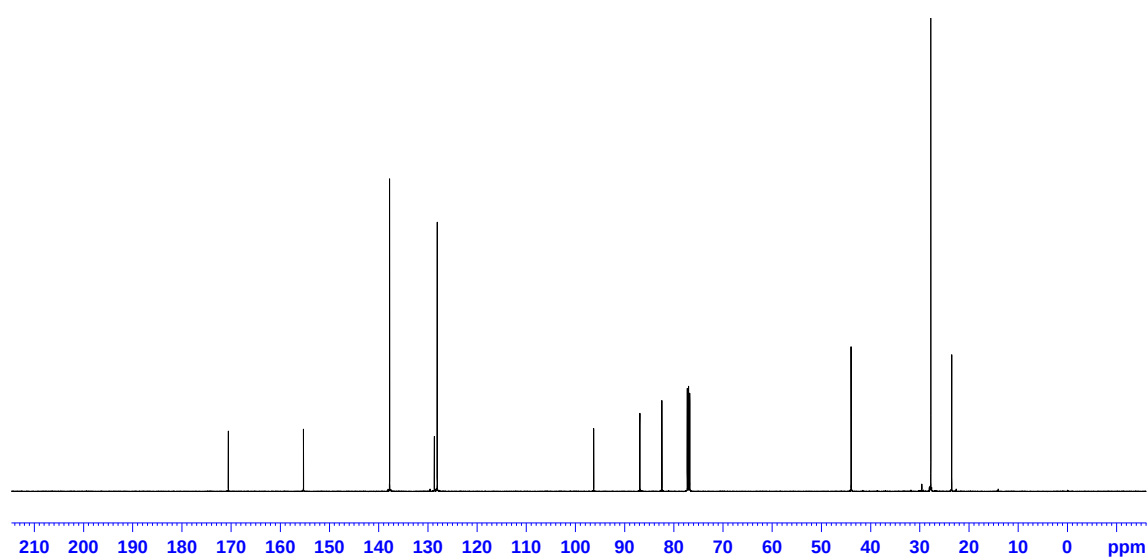
Totals : 1057.96116 112.58188



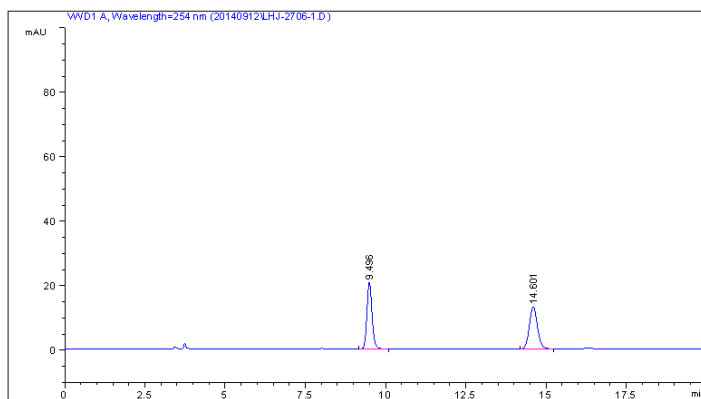
^1H NMR of **2d**



^{13}C NMR of **2d**



Racemate of **2d**



Area Percent Report

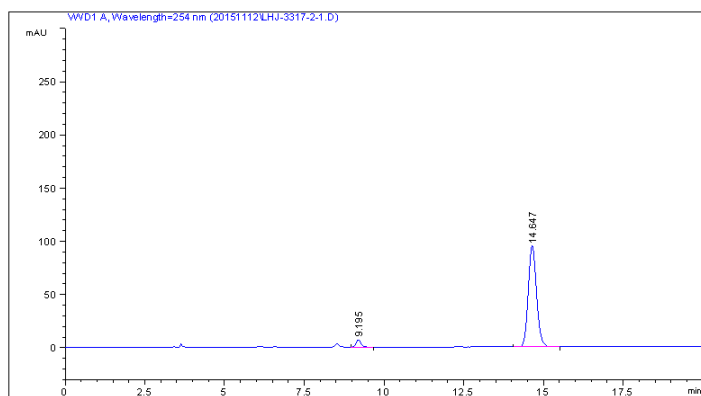
Sorted By : Signal
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Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VMD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	9.496	BB	0.1699	228.09161		20.61439	49.9988
2	14.601	BB	0.2693	228.10240		13.05830	50.0012

Totals : 456.19402 33.67269

Enantiomeric excess of **2d**: 92%



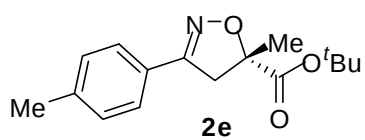
Area Percent Report

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Use Multiplier & Dilution Factor with ISTDs

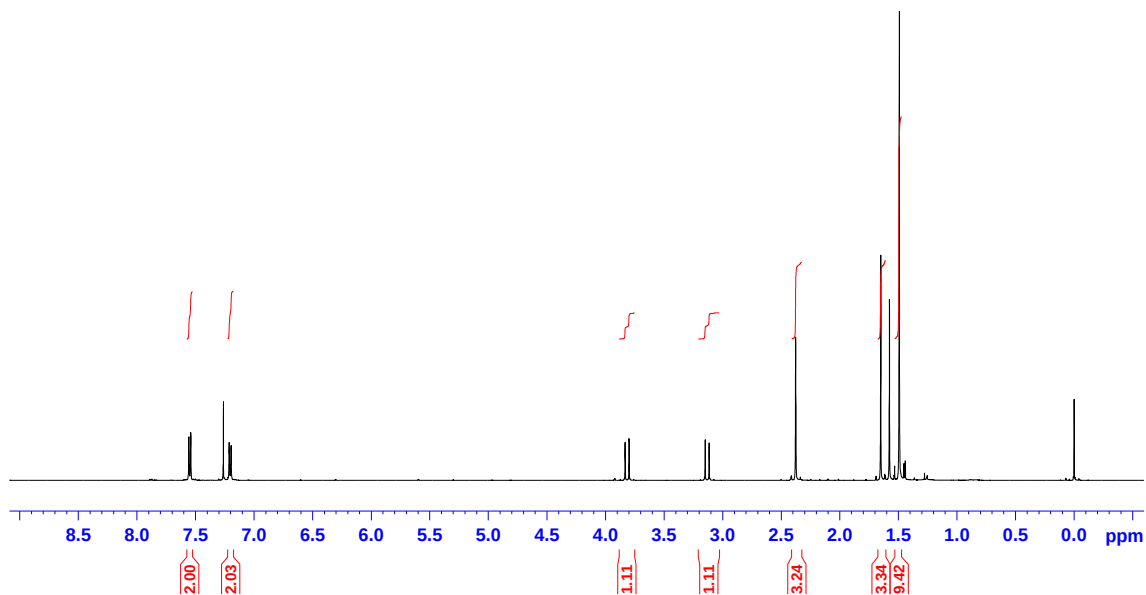
Signal 1: VMD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	9.195	BB	0.1729	75.84350		6.84546	4.2108
2	14.647	VB	0.2819	1725.33948		94.95502	95.7892

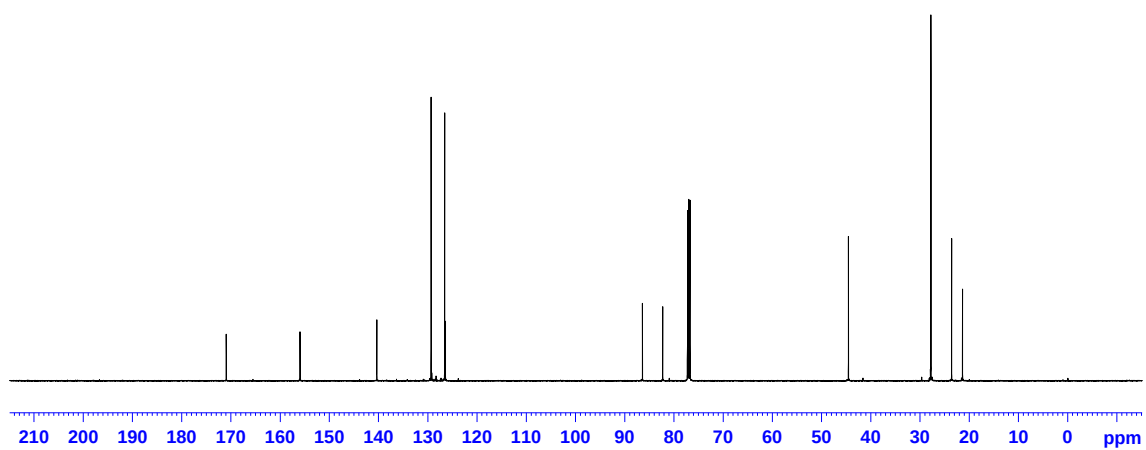
Totals : 1801.18298 101.80048



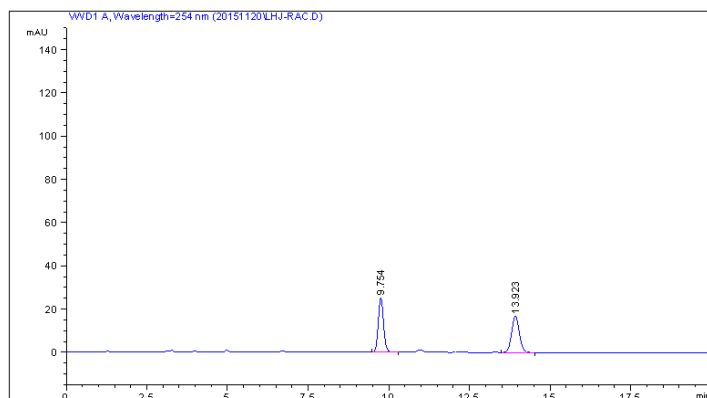
^1H NMR of **2e**



^{13}C NMR of **2e**



Racemate of **2e**



Area Percent Report

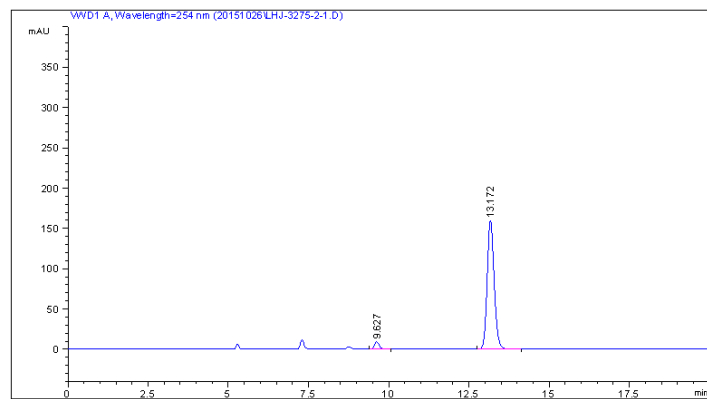
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	9.754	BB	0.1729	281.70807	25.16016	49.9806
2	13.923	VB	0.2585	281.92670	16.92047	50.0194

Totals : 563.63477 42.08063

Enantiomeric excess of **2e**: 92%



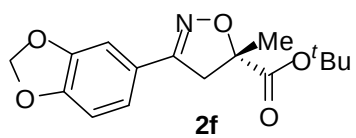
Area Percent Report

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Use Multiplier & Dilution Factor with ISTDs

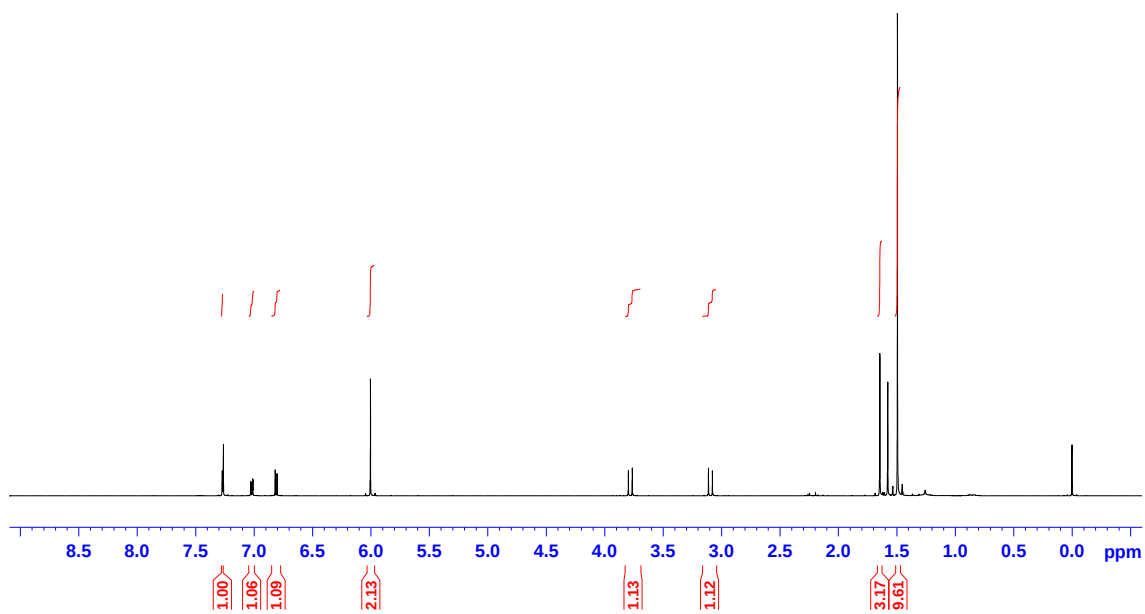
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	9.627	BB	0.1665	96.93569	8.99720	3.8445
2	13.172	BB	0.2353	2424.48901	159.71883	96.1555

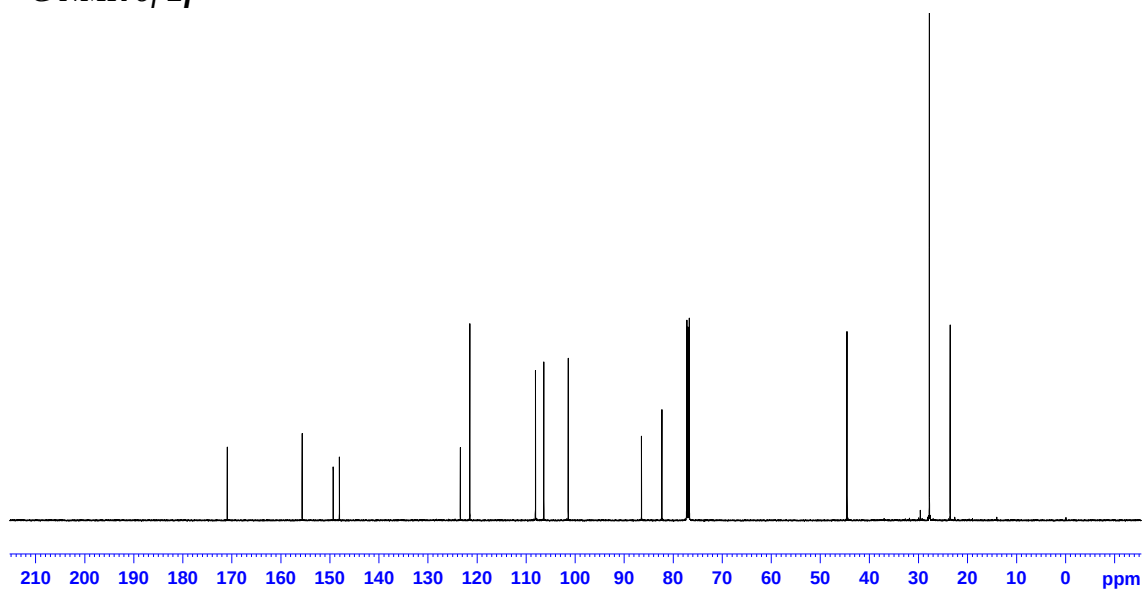
Totals : 2521.42471 168.71603



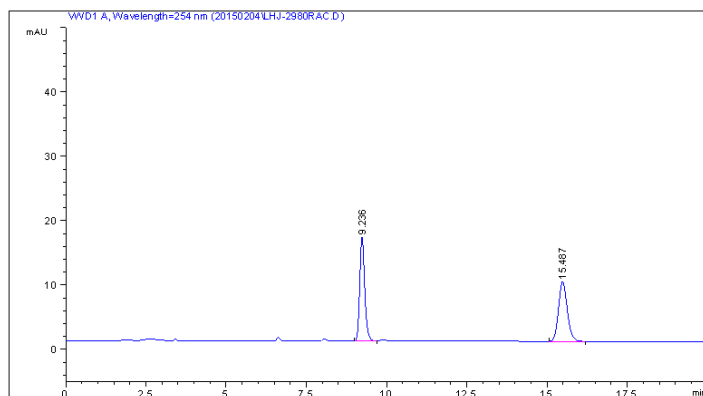
^1H NMR of **2f**



^{13}C NMR of **2f**



Racemate of **2f**



Area Percent Report

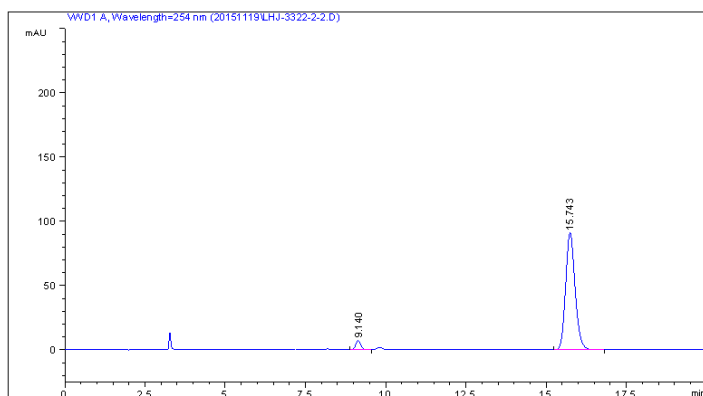
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Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	9.236	BV	0.1663	175.26360	16.10583	50.0860
2	15.487	BB	0.2909	174.66153	9.28113	49.9140

Totals : 349.92513 25.38697

Enantiomeric excess of **2f**: 91%



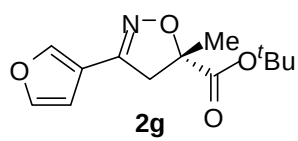
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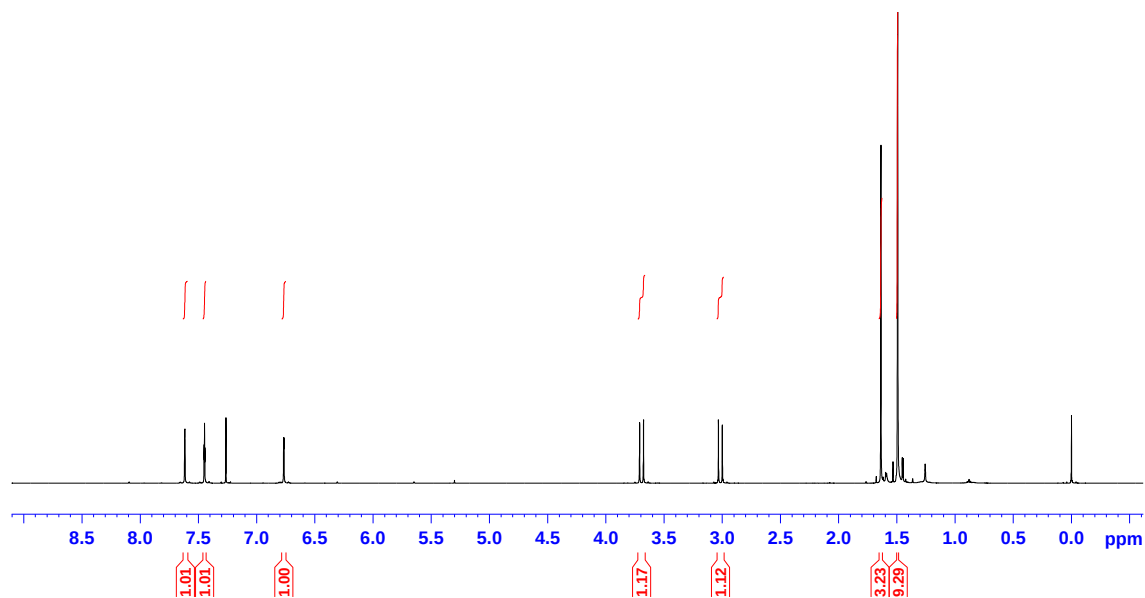
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	9.140	BV	0.1775	83.42481	7.27053	4.2778
2	15.743	BB	0.3148	1866.74634	91.08116	95.7222

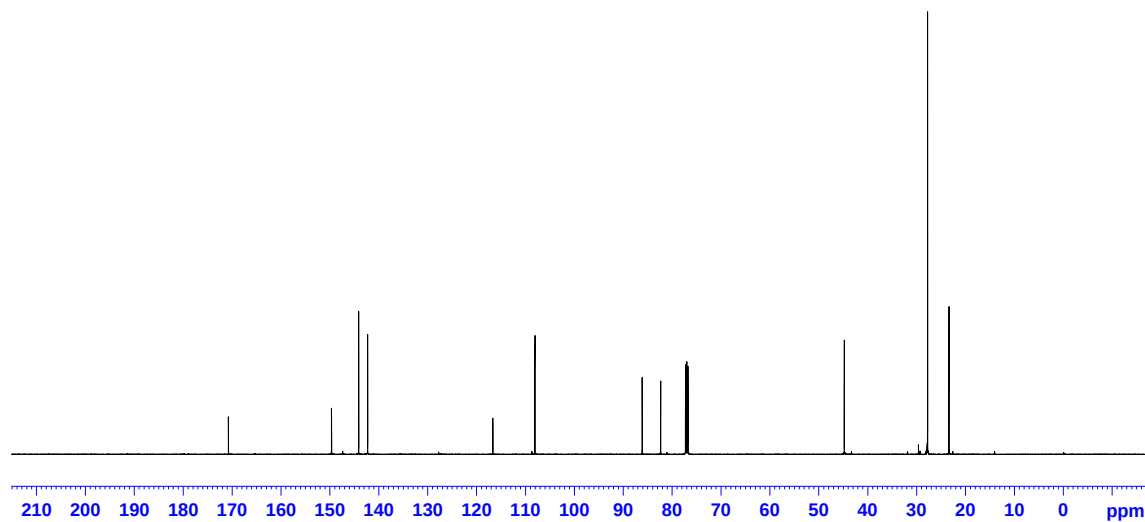
Totals : 1950.17115 98.35169



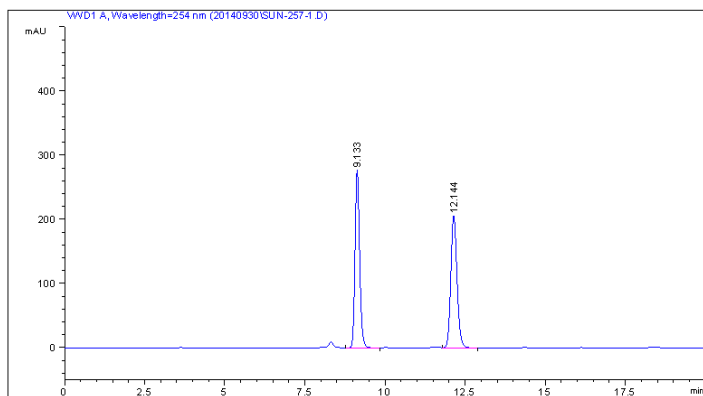
^1H NMR of **2g**



^{13}C NMR of **2g**



Racemate of 2g



Area Percent Report

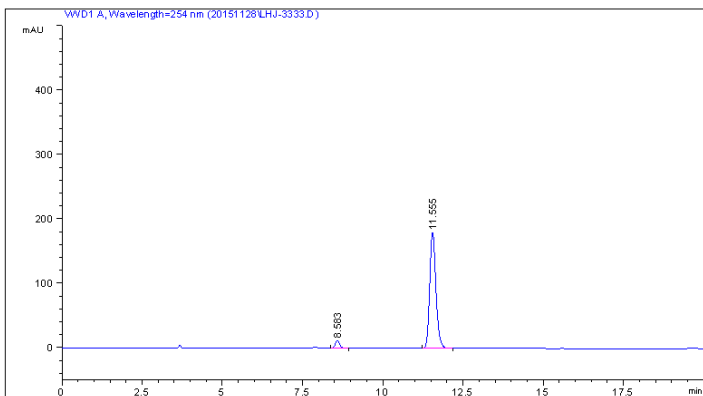
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: VMD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	9.133	VB	0.1552	2783.09058		276.70059	49.9497
2	12.144	VV	0.2104	2788.69458		205.91554	50.0503

Totals : 5571.78516 482.61613

Enantiomeric excess of 2g: 91%



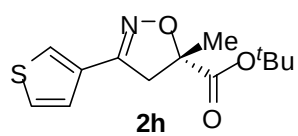
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Use Multiplier & Dilution Factor with ISTDs

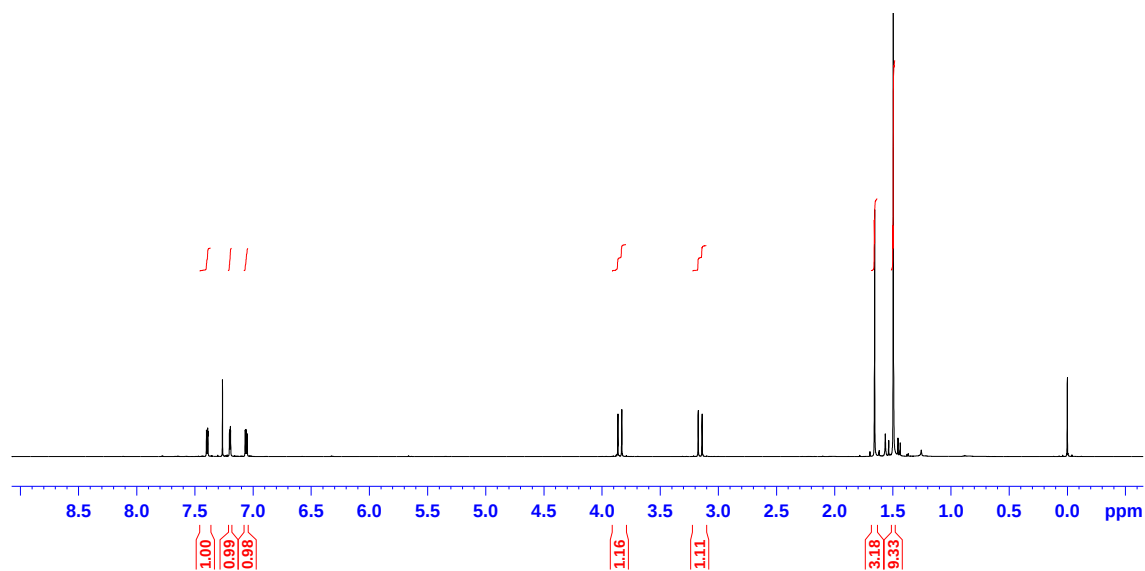
Signal 1: VMD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	8.583	BB	0.1480	112.42895		11.60137	4.4422
2	11.555	BB	0.2061	2418.47681		180.18913	95.5578

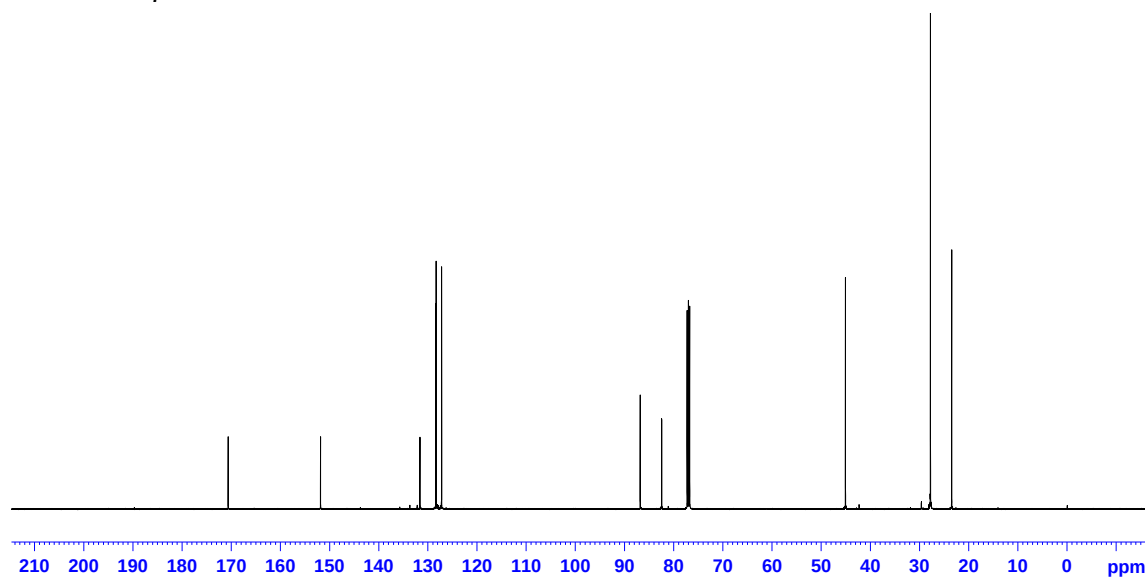
Totals : 2530.90575 191.79050



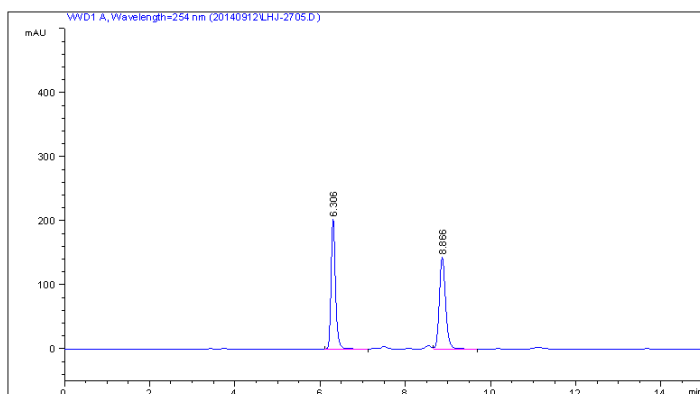
^1H NMR of **2h**



^{13}C NMR of **2h**



Racemate of **2h**



Area Percent Report

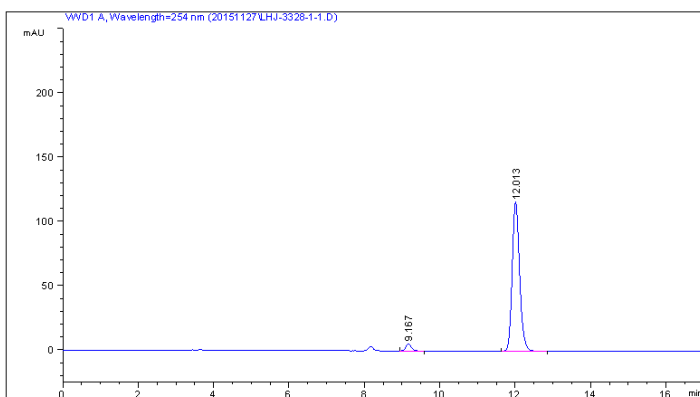
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	6.306	VV	0.1083	1450.21460		202.49289	50.0351
2	8.866	VB	0.1559	1448.18237		143.16666	49.9649

Totals : 2898.39697 345.65955

Enantiomeric excess of **2h**: 93%



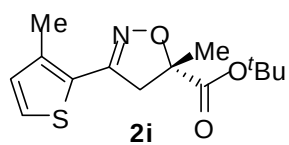
Area Percent Report

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Use Multiplier & Dilution Factor with ISTDs

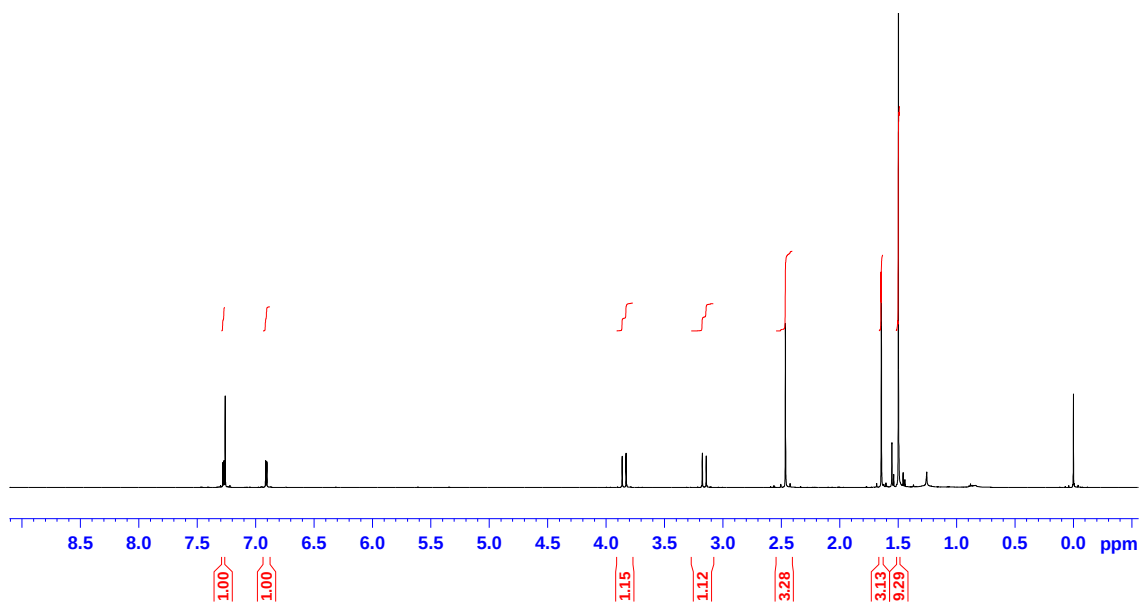
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	9.167	BB	0.1574	57.24918		5.58578	3.4908
2	12.013	BB	0.2106	1582.75513		115.68507	96.5092

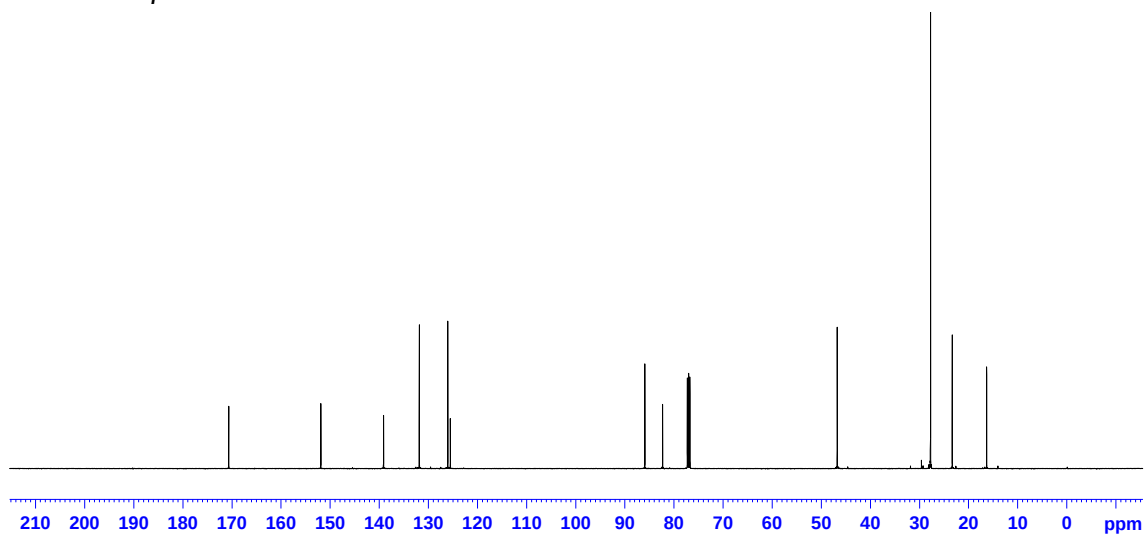
Totals : 1640.00431 121.27085



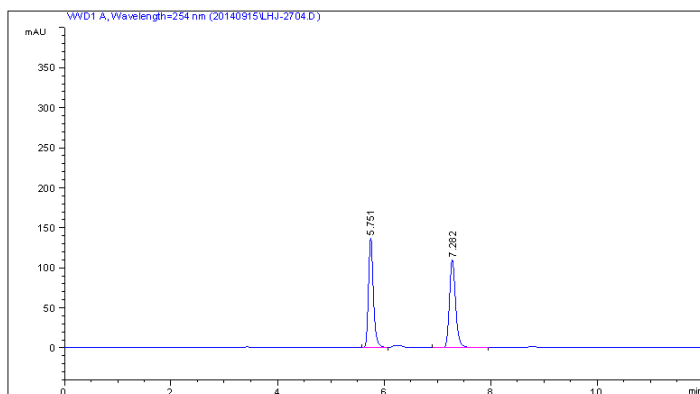
^1H NMR of **2i**



^{13}C NMR of **2i**



Racemate of **2i**



Area Percent Report

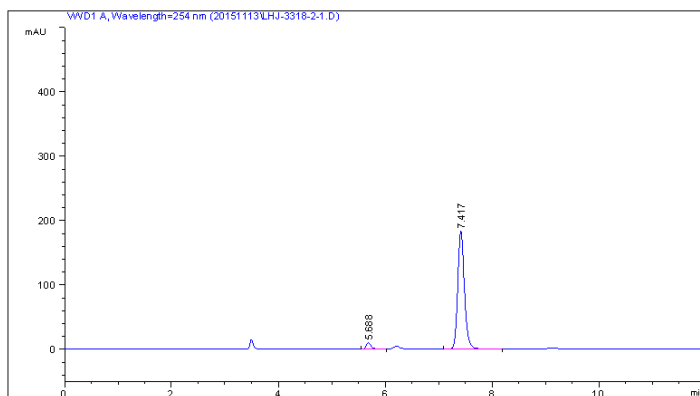
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	5.751	BV	0.0982	879.98999	137.01599	49.9310	
2	7.282	VB	0.1228	882.42261	109.88358	50.0690	

Totals : 1762.41260 246.89957

Enantiomeric excess of **2i**: 93%



Area Percent Report

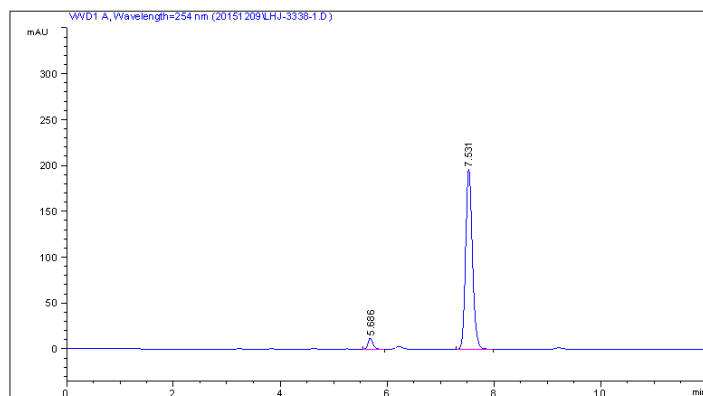
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Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	5.688	BV	0.1015	61.02224	9.27376	3.7224	
2	7.417	VB	0.1329	1578.30933	182.47626	96.2776	

Totals : 1639.33156 191.75002

Enantiomeric excess of 2i: 91% (Large-scale reaction in Scheme 2)



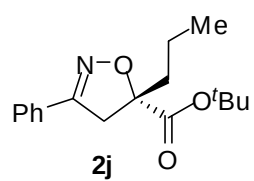
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Area Percent Report
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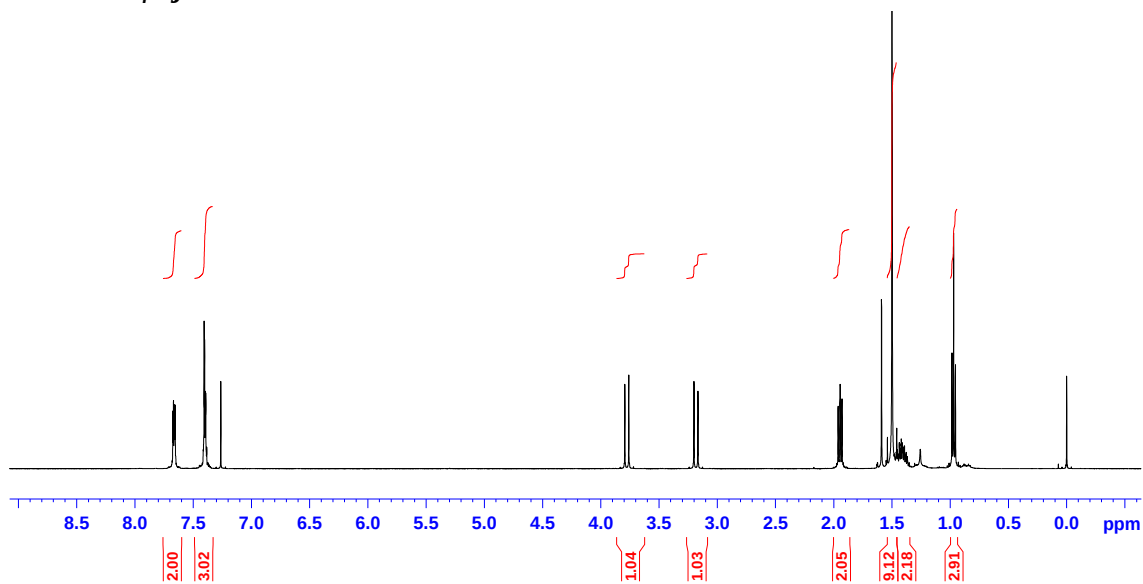
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]
1	5.686	BB	0.1002	79.51534	4.3919	12.06533
2	7.531	BB	0.1350	1730.99976	95.6081	196.19098

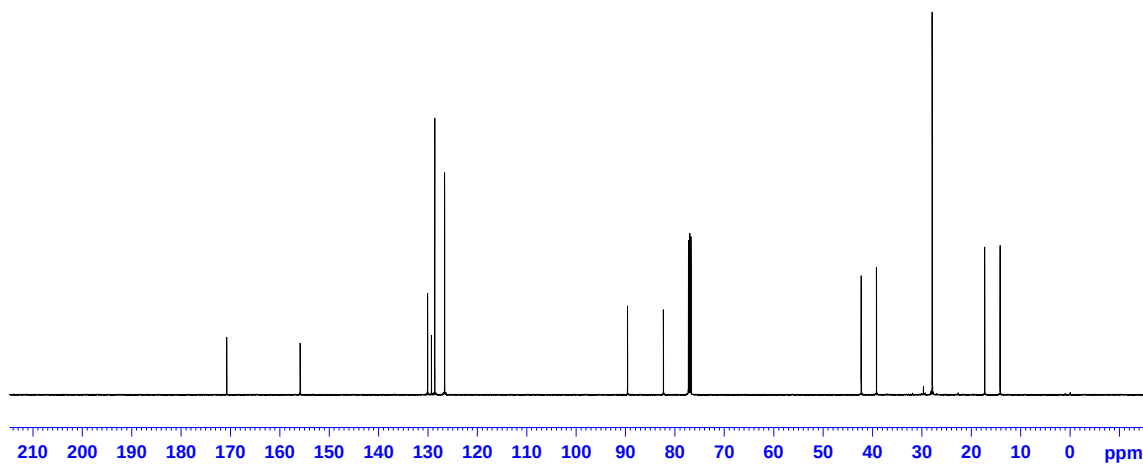
Totals : 1810.51509 208.25631



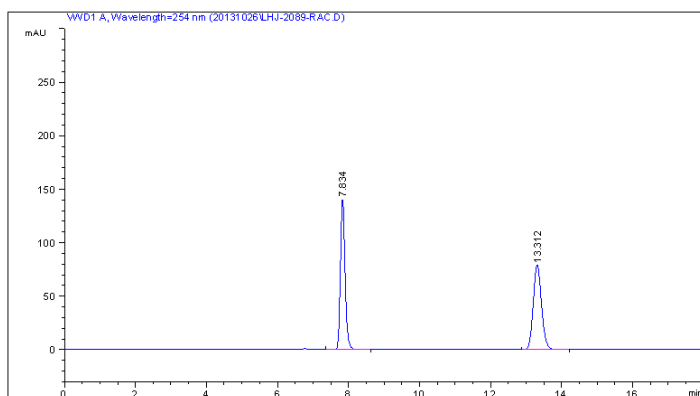
^1H NMR of **2j**



^{13}C NMR of **2j**



Racemate of 2j



Area Percent Report

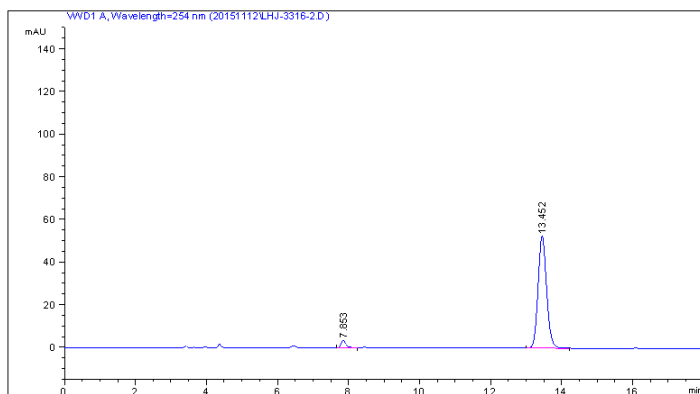
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]
1	7.834	VB	0.1404	1286.46912	49.8572	140.44131
2	13.312	BB	0.2517	1293.83630	50.1428	79.23025

Totals : 2580.30542 219.67156

Enantiomeric excess of 2j: 92%



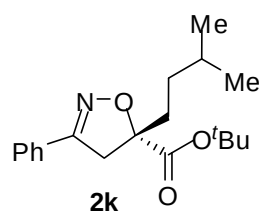
Area Percent Report

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

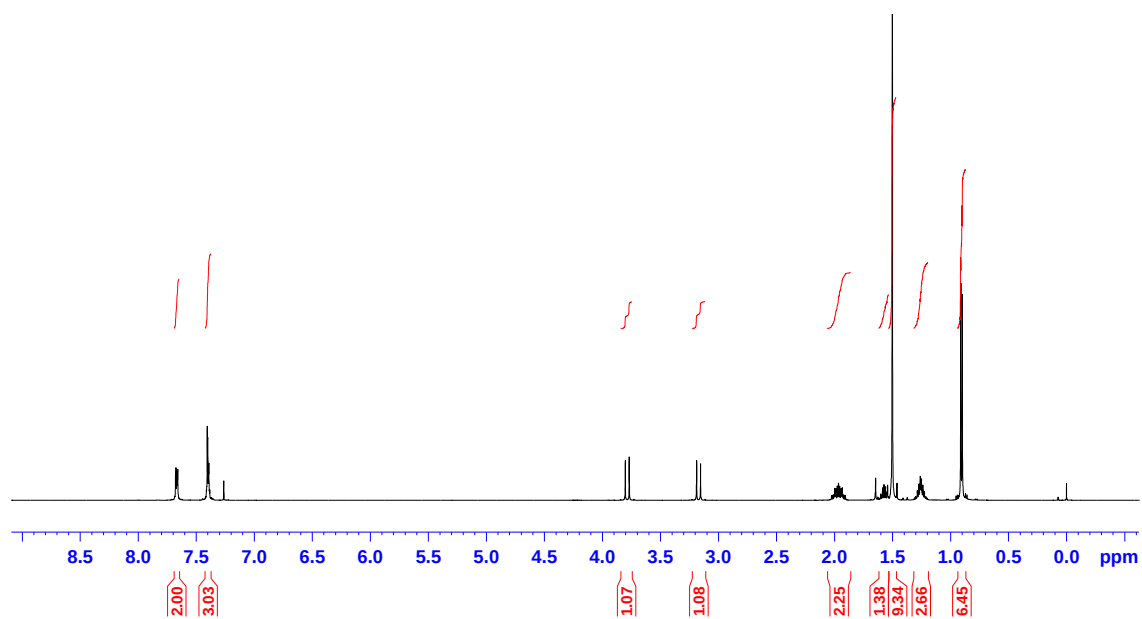
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]
1	7.853	VB	0.1517	34.99219	3.8433	3.49650
2	13.452	BB	0.2585	875.47357	96.1567	52.53211

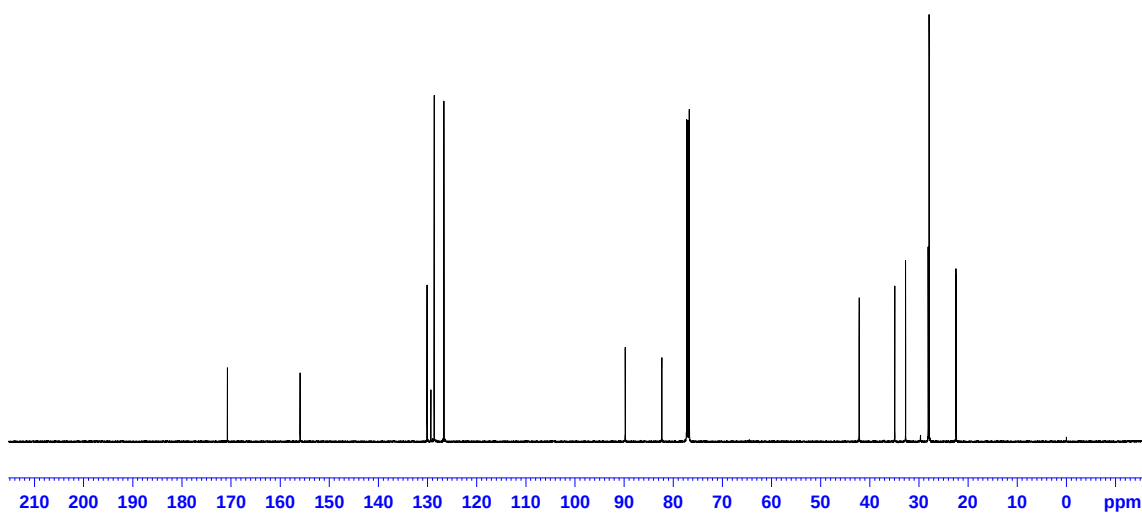
Totals : 910.46576 56.02861



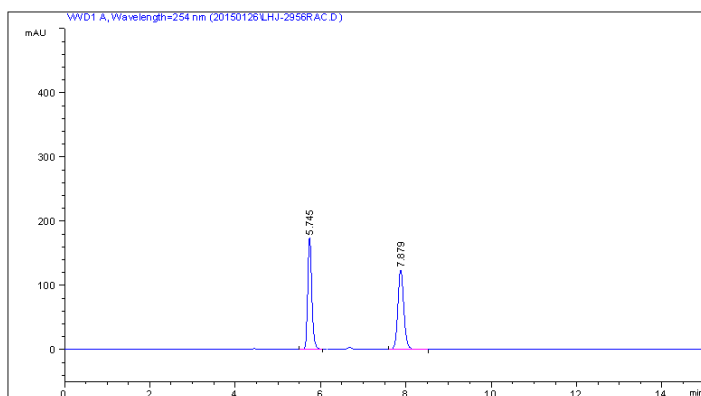
^1H NMR of **2k**



^{13}C NMR of **2k**



Racemate of **2k**



Area Percent Report

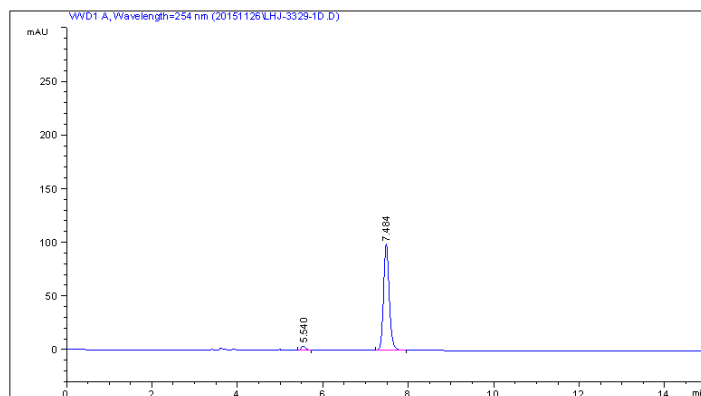
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VMD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	5.745	VV	0.1031	1168.26074	173.99263	49.3966
2	7.879	VB	0.1476	1196.80054	123.91225	50.6034

Totals : 2365.06128 297.90488

Enantiomeric excess of **2k**: 94%



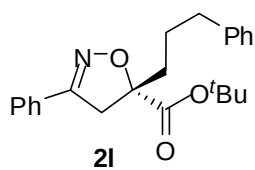
Area Percent Report

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

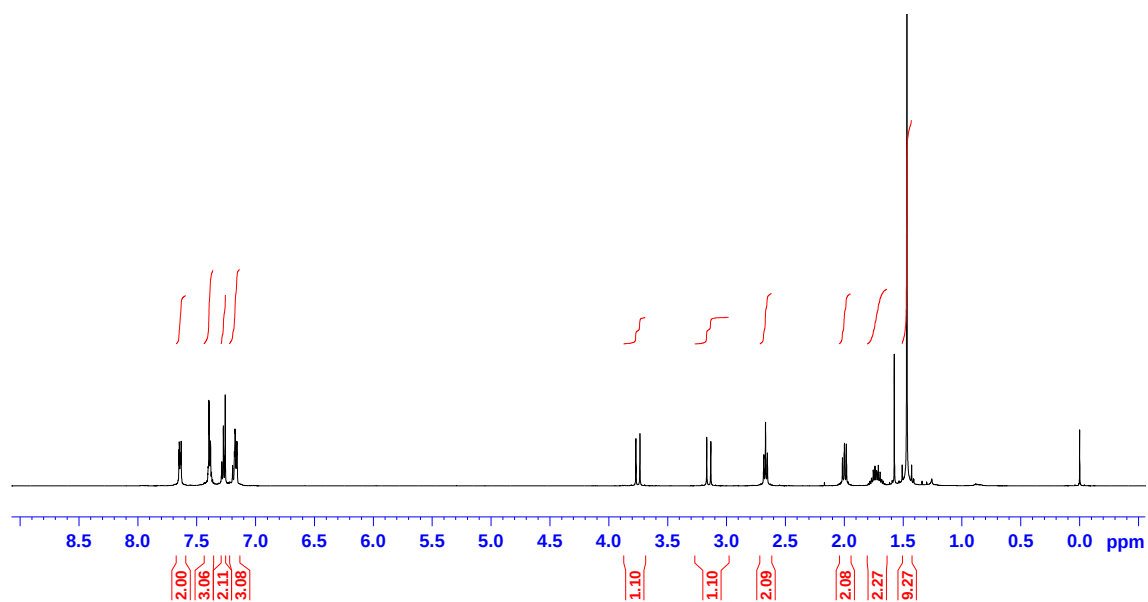
Signal 1: VMD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	5.540	VB	0.1023	26.53551	3.92065	2.7993
2	7.484	BB	0.1420	921.39496	99.05399	97.2007

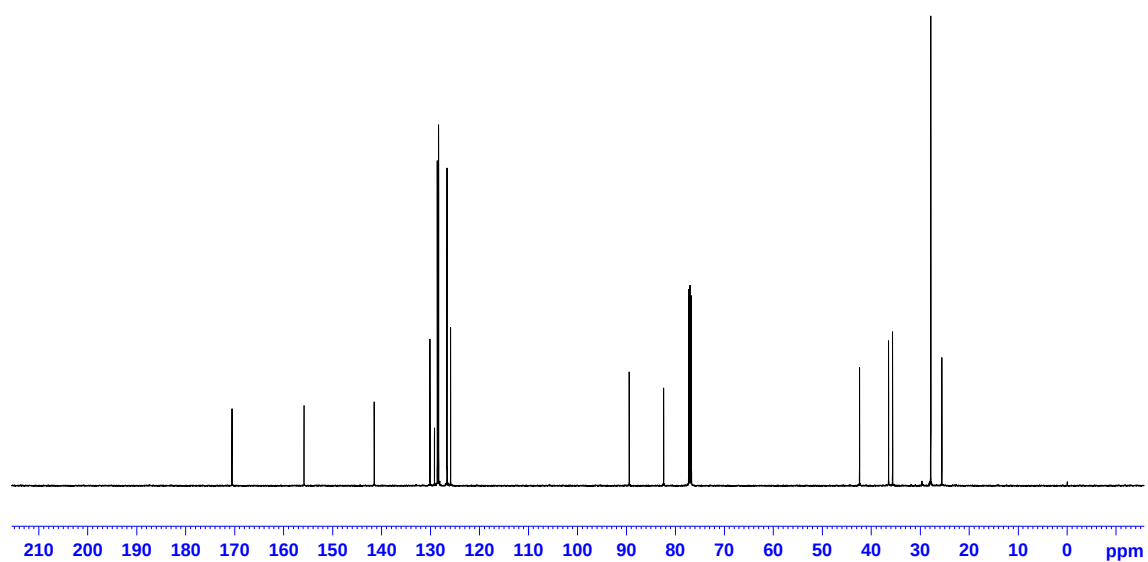
Totals : 947.93046 102.97464



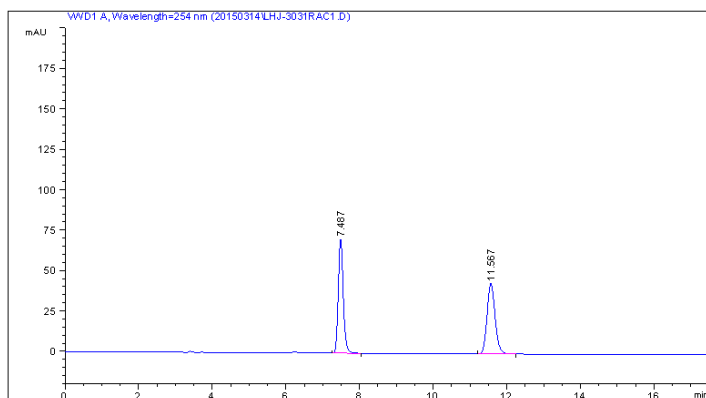
^1H NMR of **2l**



^{13}C NMR of **2l**



Racemate of **2l**



Area Percent Report

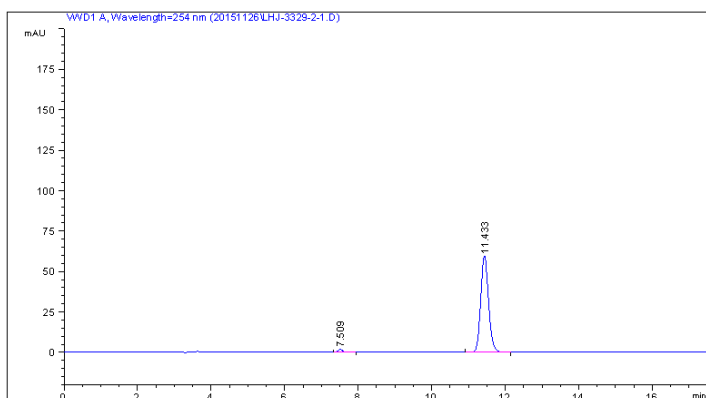
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]
1	7.487	BB	0.1447	663.16943	50.0487	70.46494
2	11.567	BB	0.2338	661.87988	49.9513	43.62590

Totals : 1325.04932 114.09084

Enantiomeric excess of **2l**: 96%



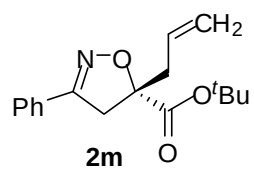
Area Percent Report

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

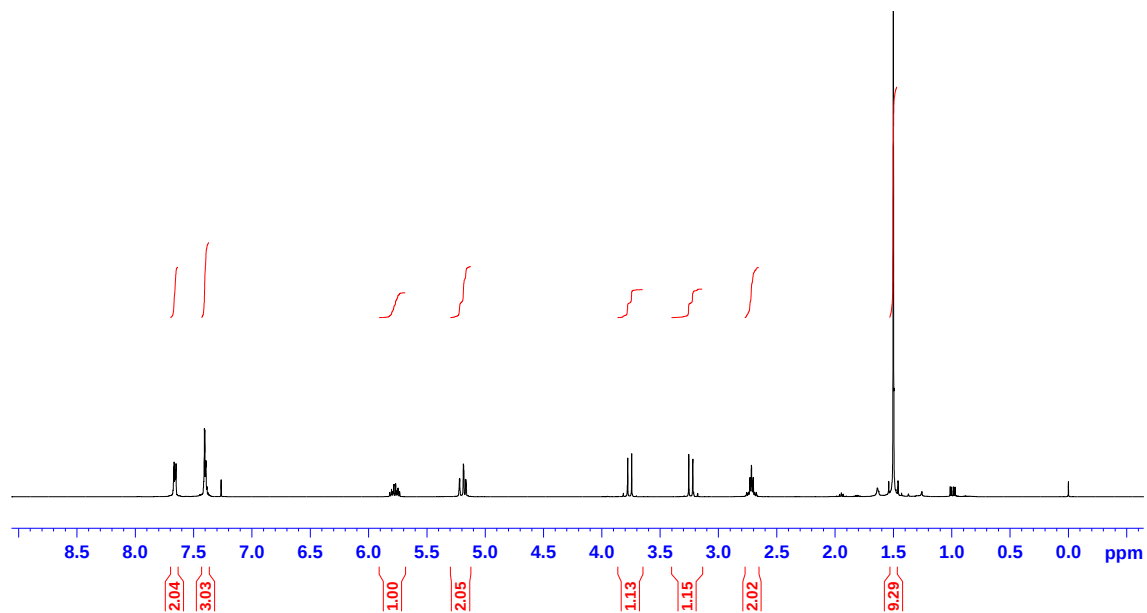
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]
1	7.509	BB	0.1490	18.81346	2.0726	1.92525
2	11.433	BB	0.2323	888.92828	97.9274	59.59748

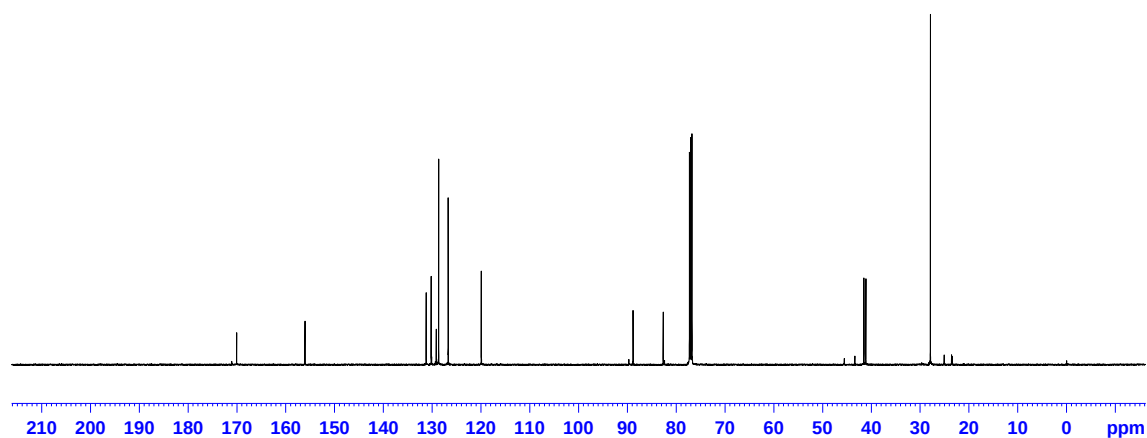
Totals : 907.74174 61.52273



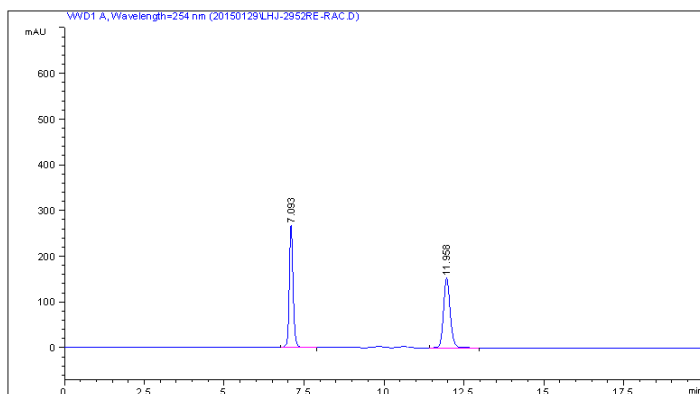
^1H NMR of **2m**



^{13}C NMR of **2m**



Racemate of 2m



Area Percent Report

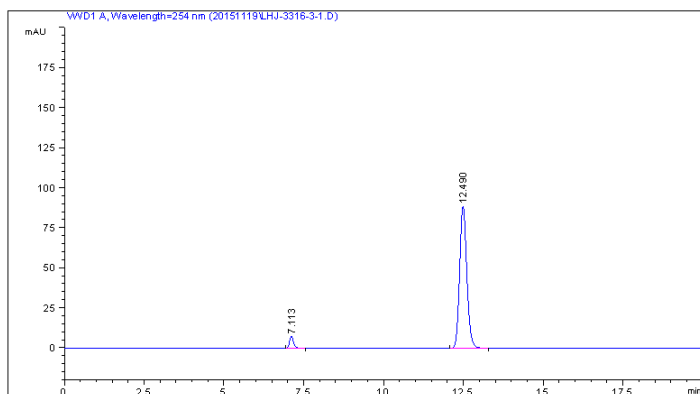
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	7.093	VB	0.1266	2235.71045		267.53488	50.4578
2	11.958	VB	0.2206	2195.14136		152.27338	49.5422

Totals : 4430.85181 419.80826

Enantiomeric excess of 2m: 91%



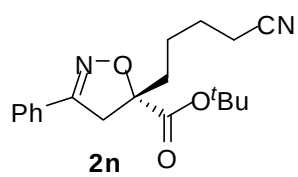
Area Percent Report

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

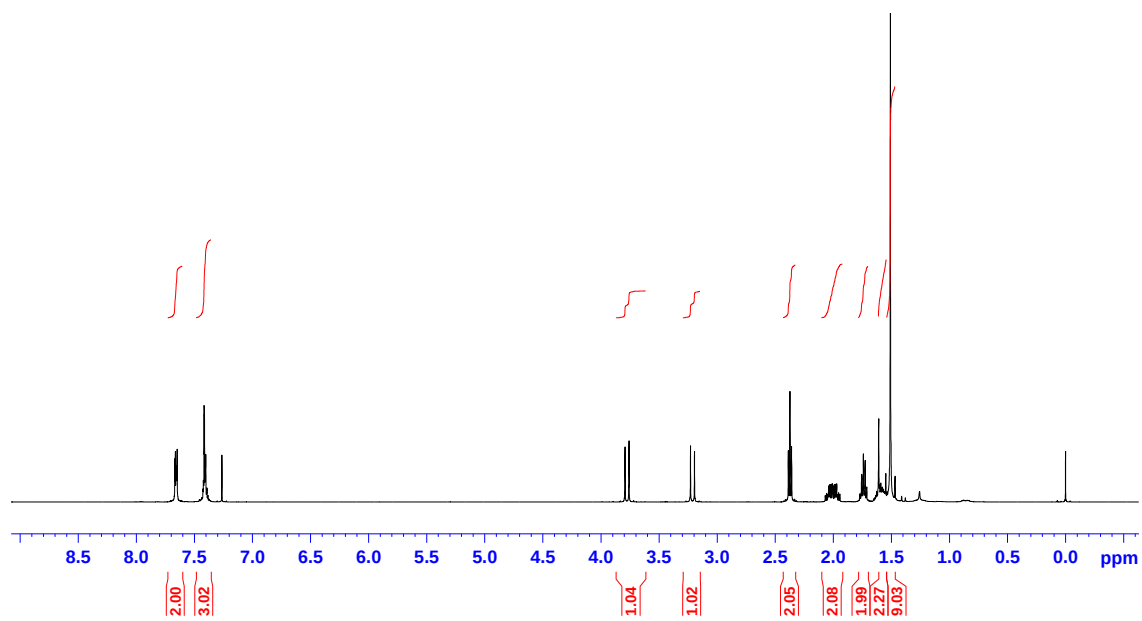
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	7.113	BB	0.1319	64.44812		7.52940	4.4245
2	12.490	BB	0.2414	1392.17041		88.66624	95.5755

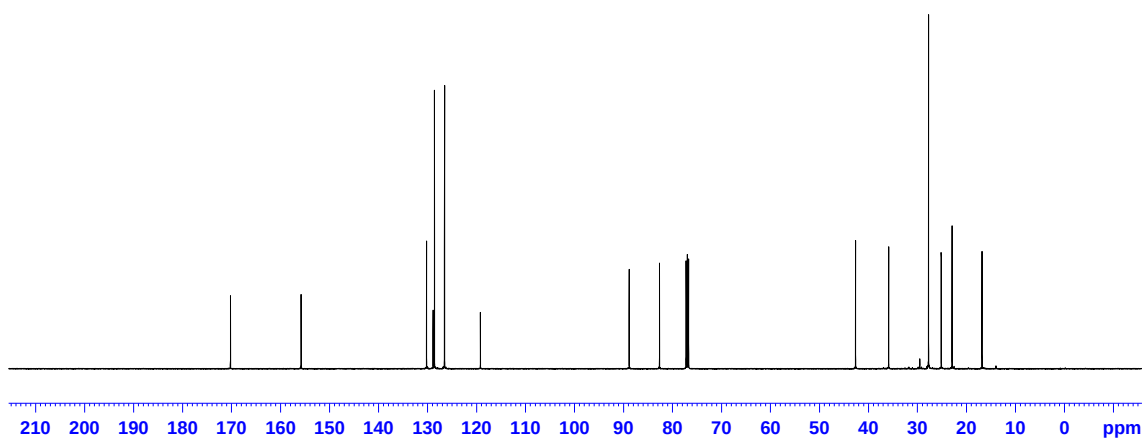
Totals : 1456.61853 96.19564



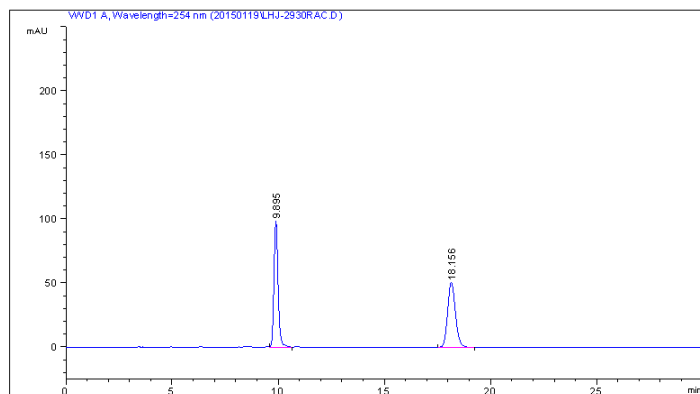
^1H NMR of **2n**



^{13}C NMR of **2n**



Racemate of **2n**



Area Percent Report

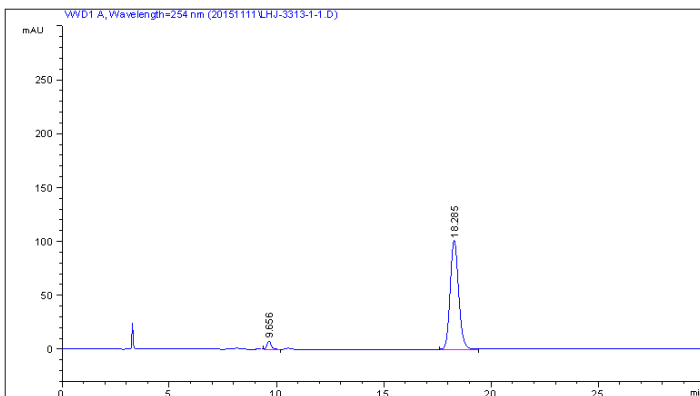
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	9.895	VV	0.2056	1314.25891		98.19707	50.3551
2	18.156	BB	0.3946	1295.72314		50.64198	49.6449

Totals : 2609.98206 148.83905

Enantiomeric excess of **2n**: 93%



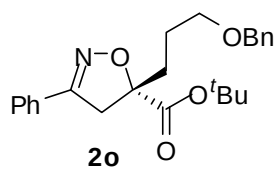
Area Percent Report

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

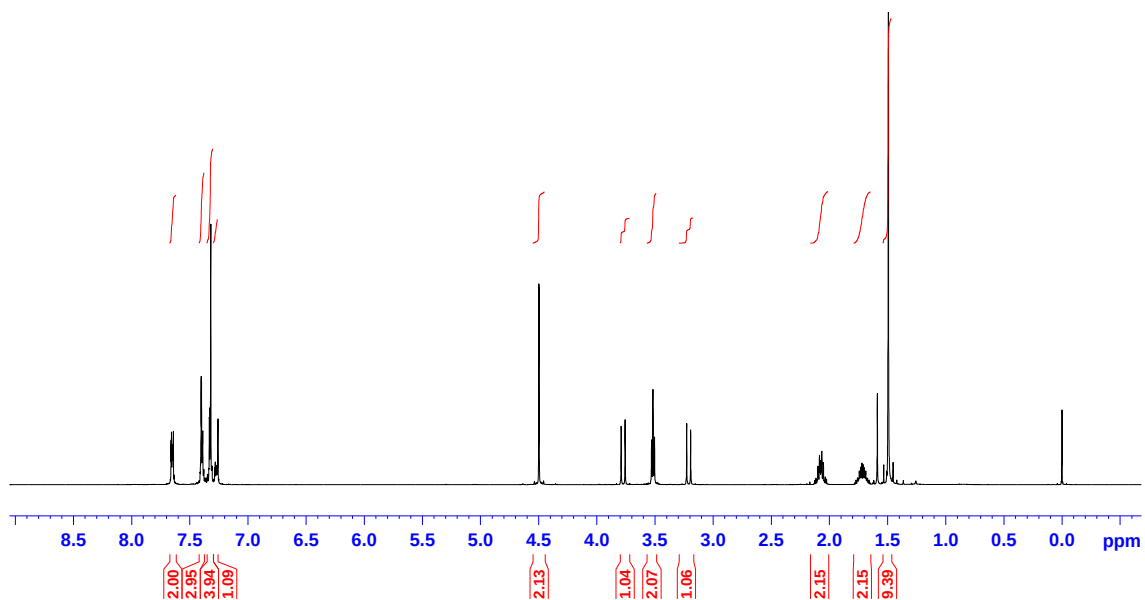
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	9.656	VB	0.2076	105.75453		7.80311	3.6889
2	18.285	BB	0.4234	2761.07886		101.12555	96.3111

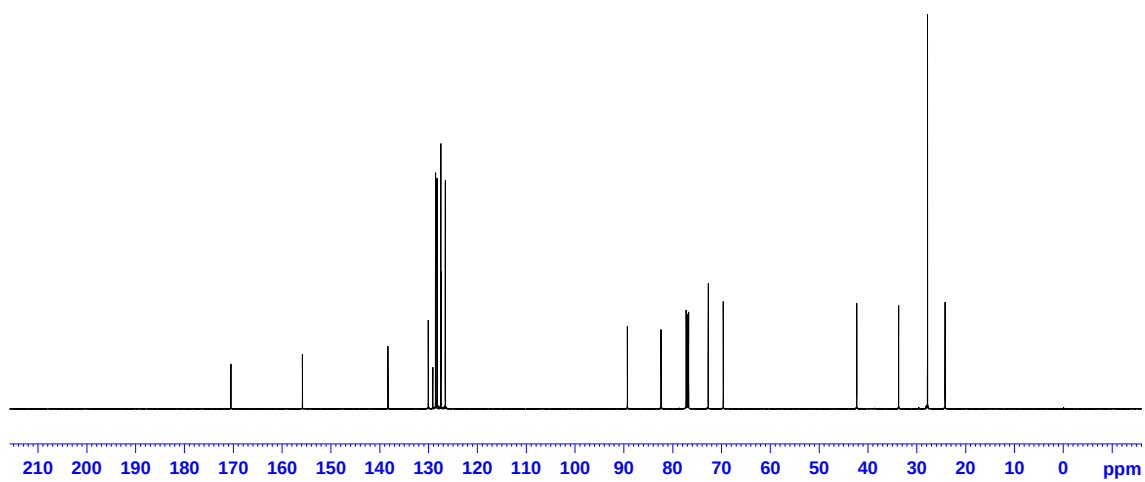
Totals : 2866.83339 108.92866



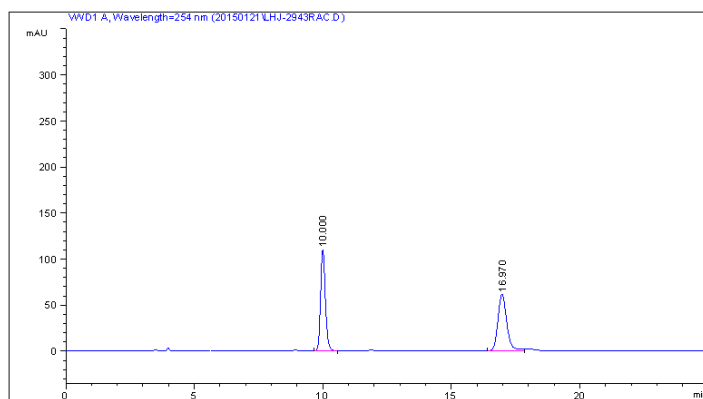
^1H NMR of **2o**



^{13}C NMR of **2o**



Racemate of **2o**



Area Percent Report

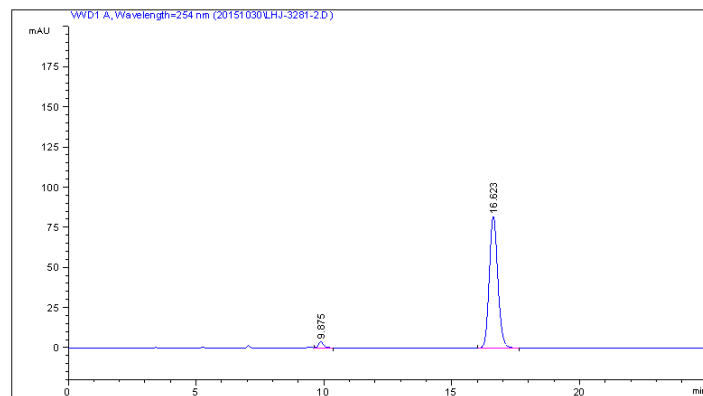
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.000	VV	0.1991	1425.52075	110.09648	49.3976
2	16.970	EV	0.3653	1460.28796	61.29941	50.6024

Totals : 2885.80872 171.39589

Enantiomeric excess of **2o**: 94%



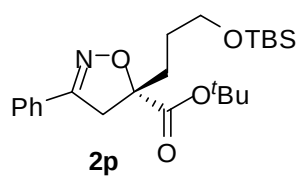
Area Percent Report

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

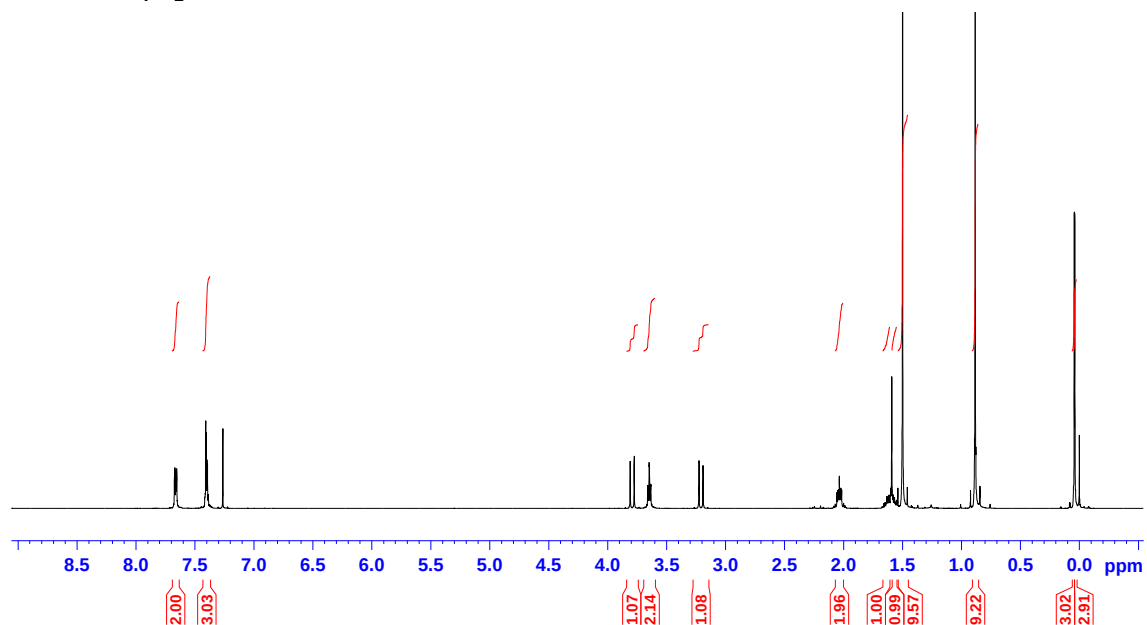
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.875	VV	0.2112	54.19002	3.91111	2.7729
2	16.623	BB	0.3577	1900.10962	81.99715	97.2271

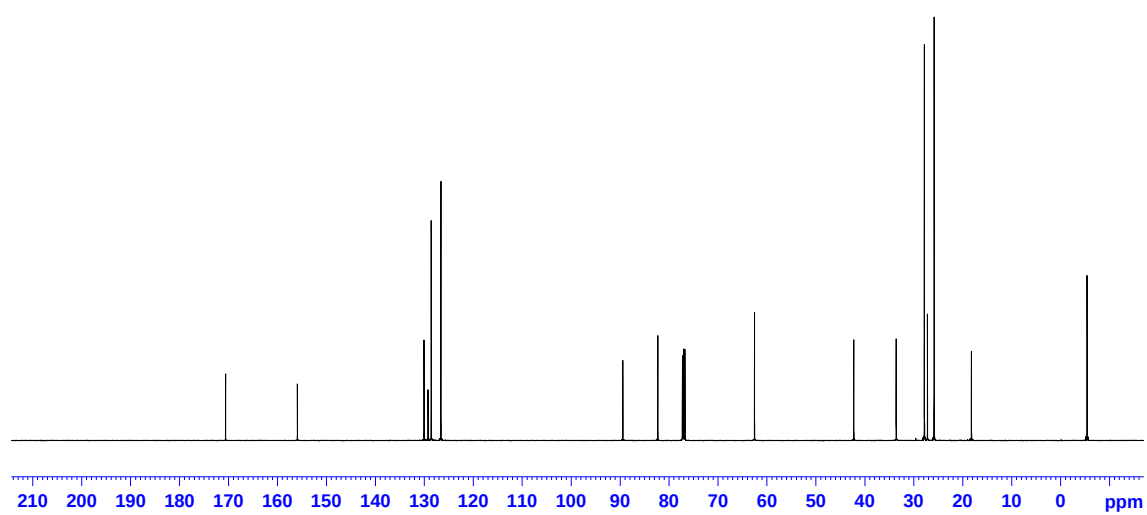
Totals : 1954.29964 85.90826



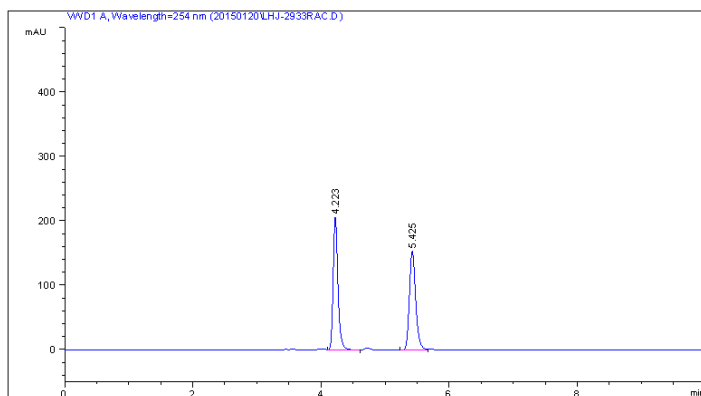
^1H NMR of **2p**



^{13}C NMR of **2p**



Racemate of 2p



Area Percent Report

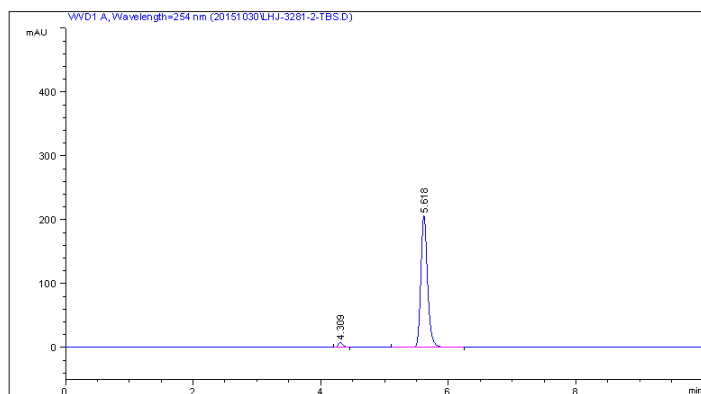
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s [mAU]	Area %
1	4.223	VV	0.0801	1083.11707	206.66322	50.6224
2	5.425	VV	0.1064	1056.48389	153.77689	49.3776

Totals : 2139.60095 360.44011

Enantiomeric excess of 2p: 95%



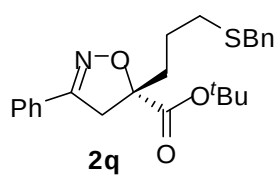
Area Percent Report

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

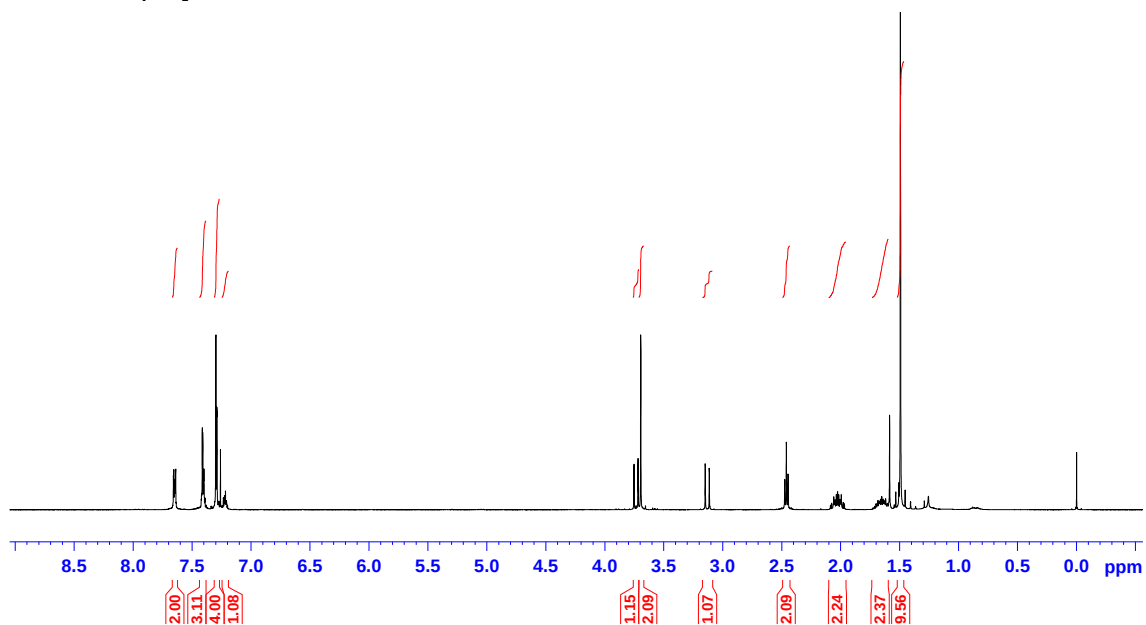
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s [mAU]	Area %
1	4.309	VV	0.0846	40.54492	7.36163	2.6342
2	5.618	BB	0.1112	1498.65222	205.82210	97.3658

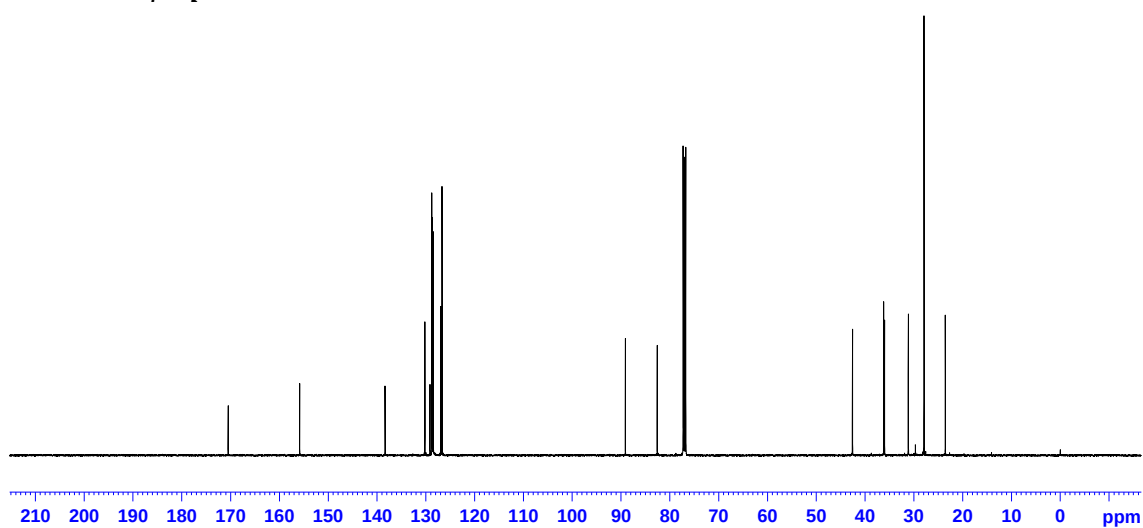
Totals : 1539.19714 213.18373



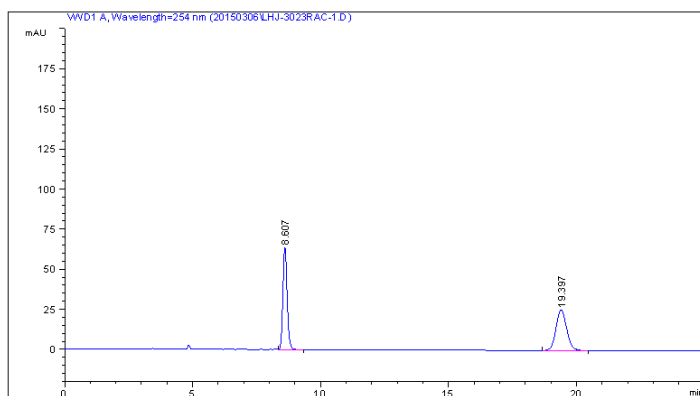
^1H NMR of **2q**



^{13}C NMR of **2q**



Racemate of 2q



Area Percent Report

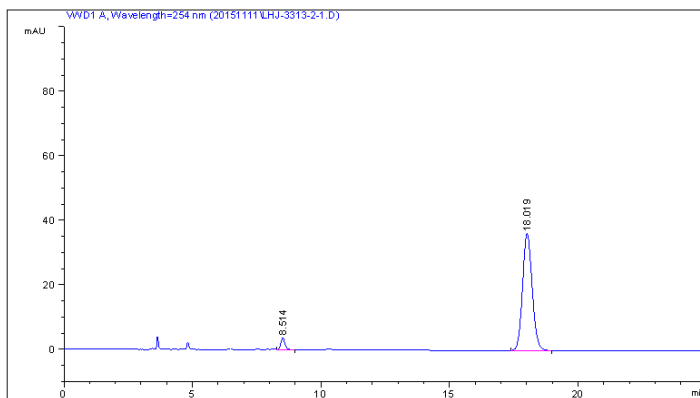
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	8.607	VB	0.1766	733.79401		63.71165	50.0692
2	19.397	BB	0.4471	731.76593		25.37792	49.9308

Totals : 1465.55994 89.08957

Enantiomeric excess of 2q: 92%



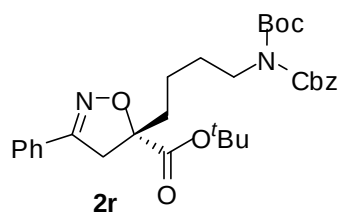
Area Percent Report

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

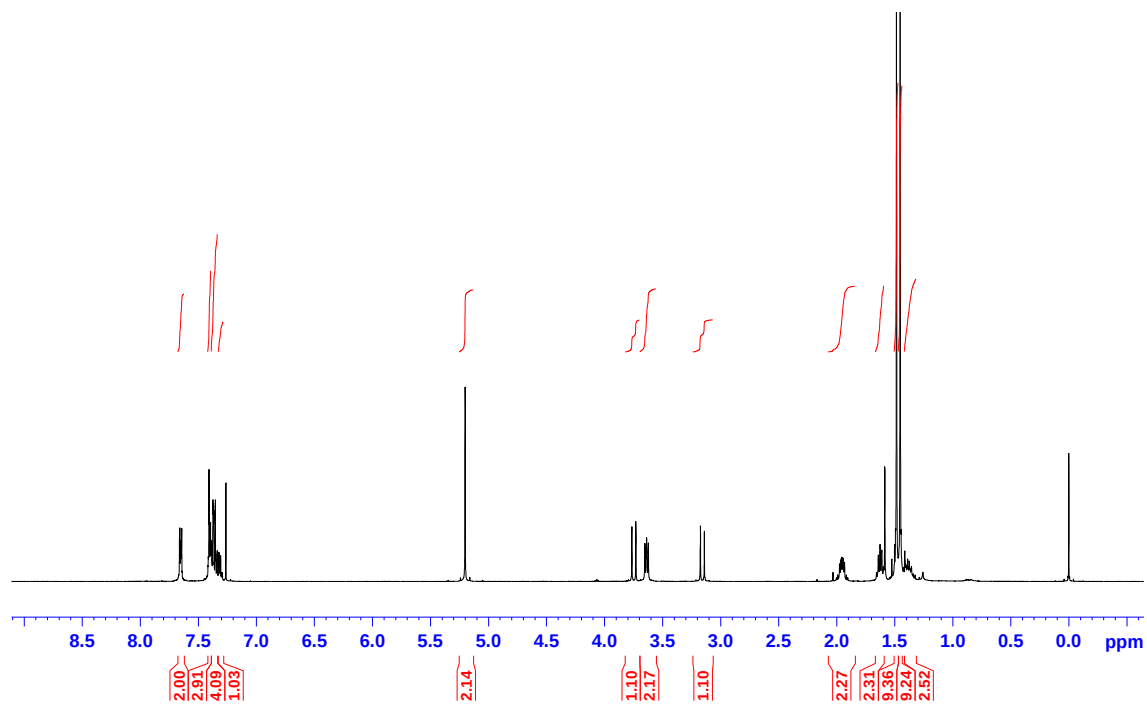
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	8.514	VB	0.1750	41.68641		3.66171	4.2372
2	18.019	BB	0.4021	942.13483		36.26045	95.7628

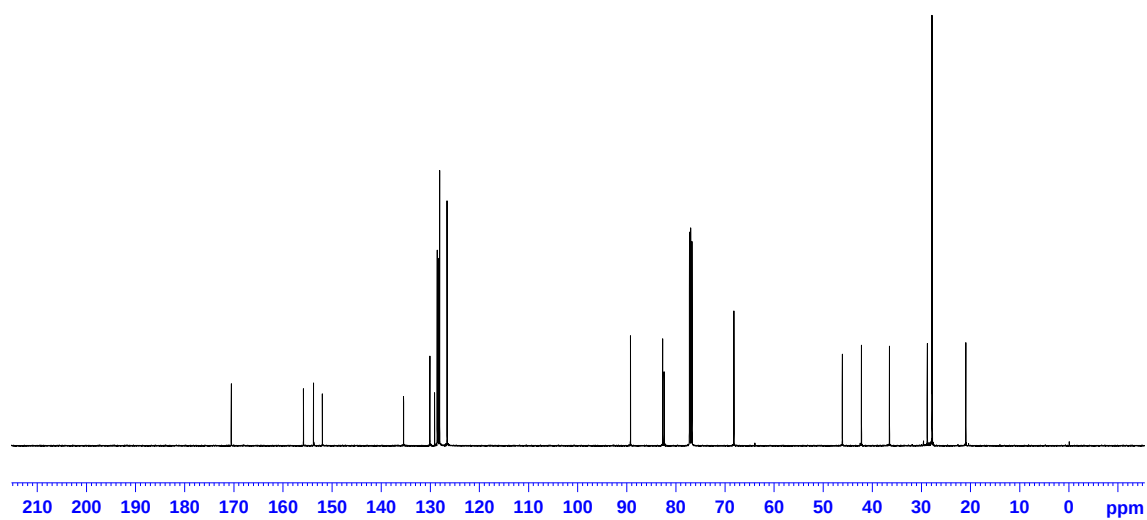
Totals : 983.82124 99.99997



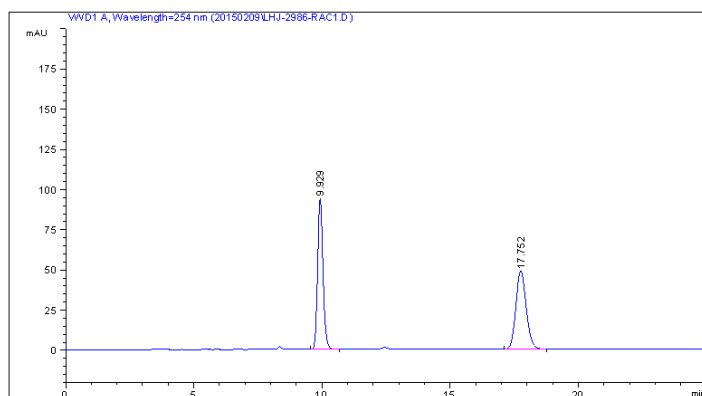
^1H NMR of **2r**



^{13}C NMR of **2r**



Racemate of 2r



Area Percent Report

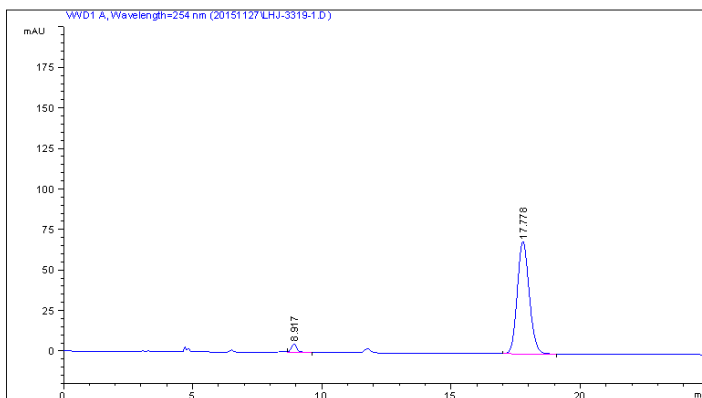
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VMD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	9.929	BB	0.2261	1372.83398		93.80367	50.1911
2	17.752	BB	0.4355	1362.38013		48.49714	49.8089

Totals : 2735.21411 142.30081

Enantiomeric excess of 2r: 93%



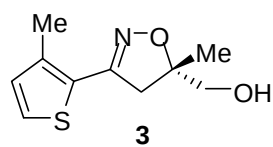
Area Percent Report

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

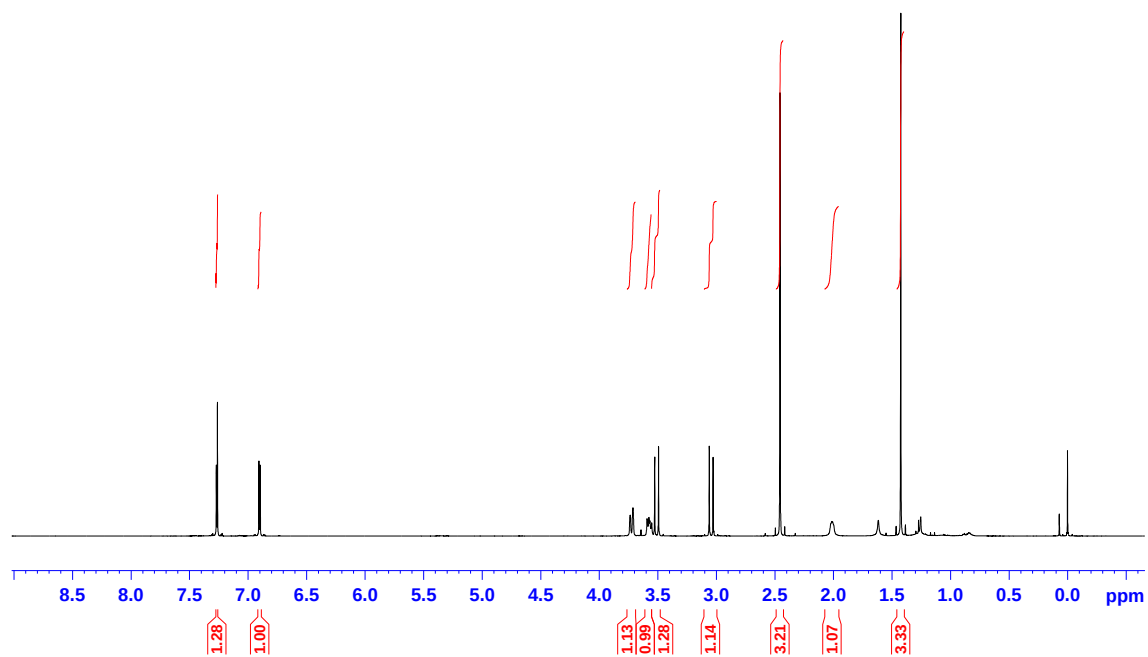
Signal 1: VMD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	8.917	VB	0.2351	80.92853		5.20856	3.5001
2	17.778	BB	0.5018	2231.26074		69.12740	96.4999

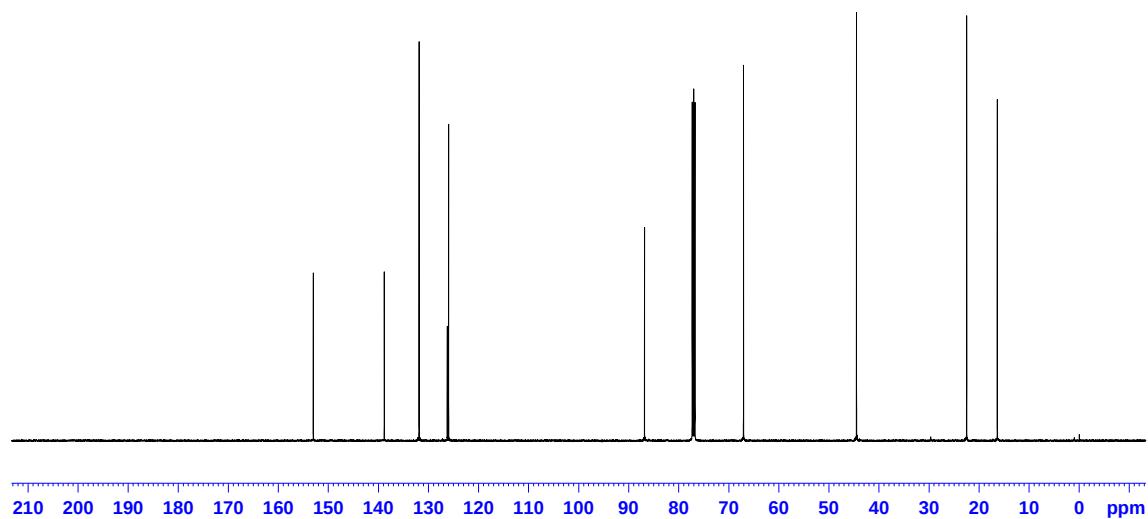
Totals : 2312.18927 74.33595

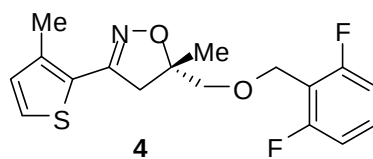


^1H NMR of **3**

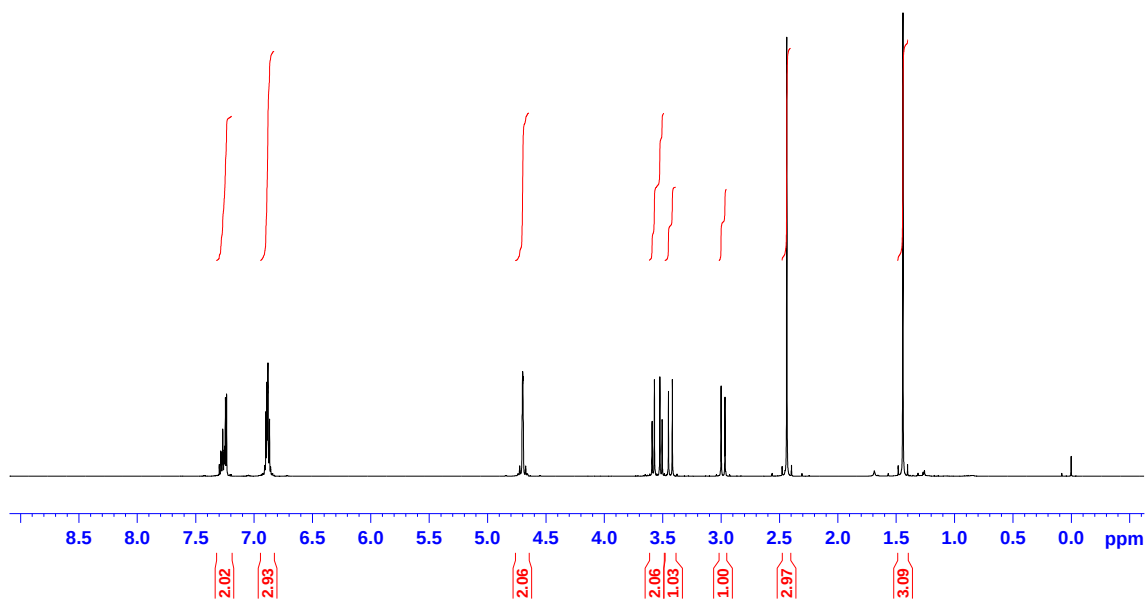


^{13}C NMR of **3**





^1H NMR of **4**



^{13}C NMR of **4**

