

Supporting Information

Organocatalytic Asymmetric Mannich/aza-Michael Cascade Reaction of δ -Formyl- α,β -unsaturated Ketones with Cyclic *N*-Sulfinamines: Enantioselective Synthesis of Benzosulfamidate-fused Pyrrolidines

Hanna Kim, Yerin Kim, and Sung-Gon Kim*

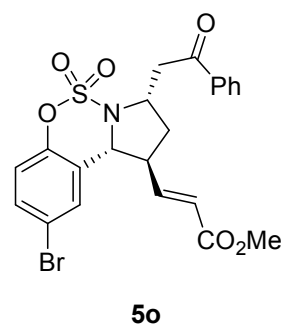
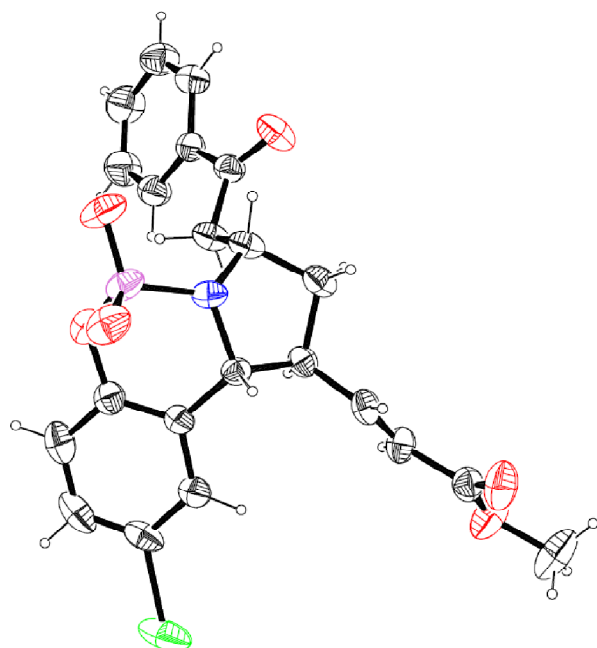
Department of Chemistry, Kyonggi University, 154-42, Gwanggyosan-ro, Yeongtong-gu, Suwon-si, Gyeonggi-do 443-760, Republic of Korea

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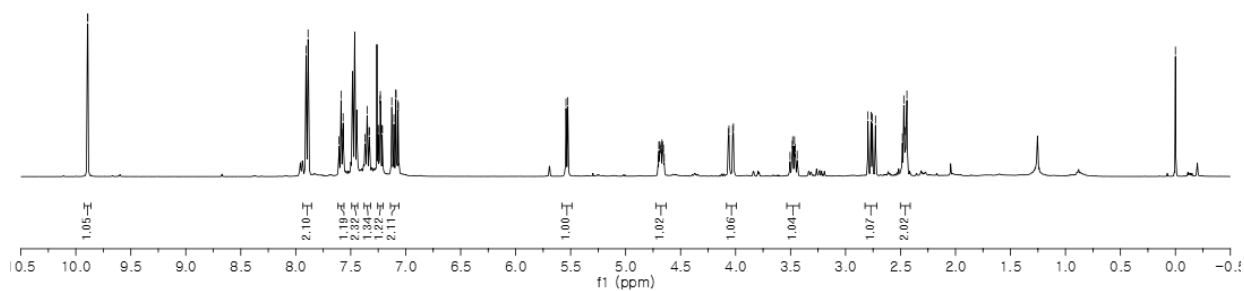
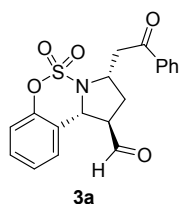
Crystallography Data for Compound 5o

The ellipsoid contour % probability level is 50.

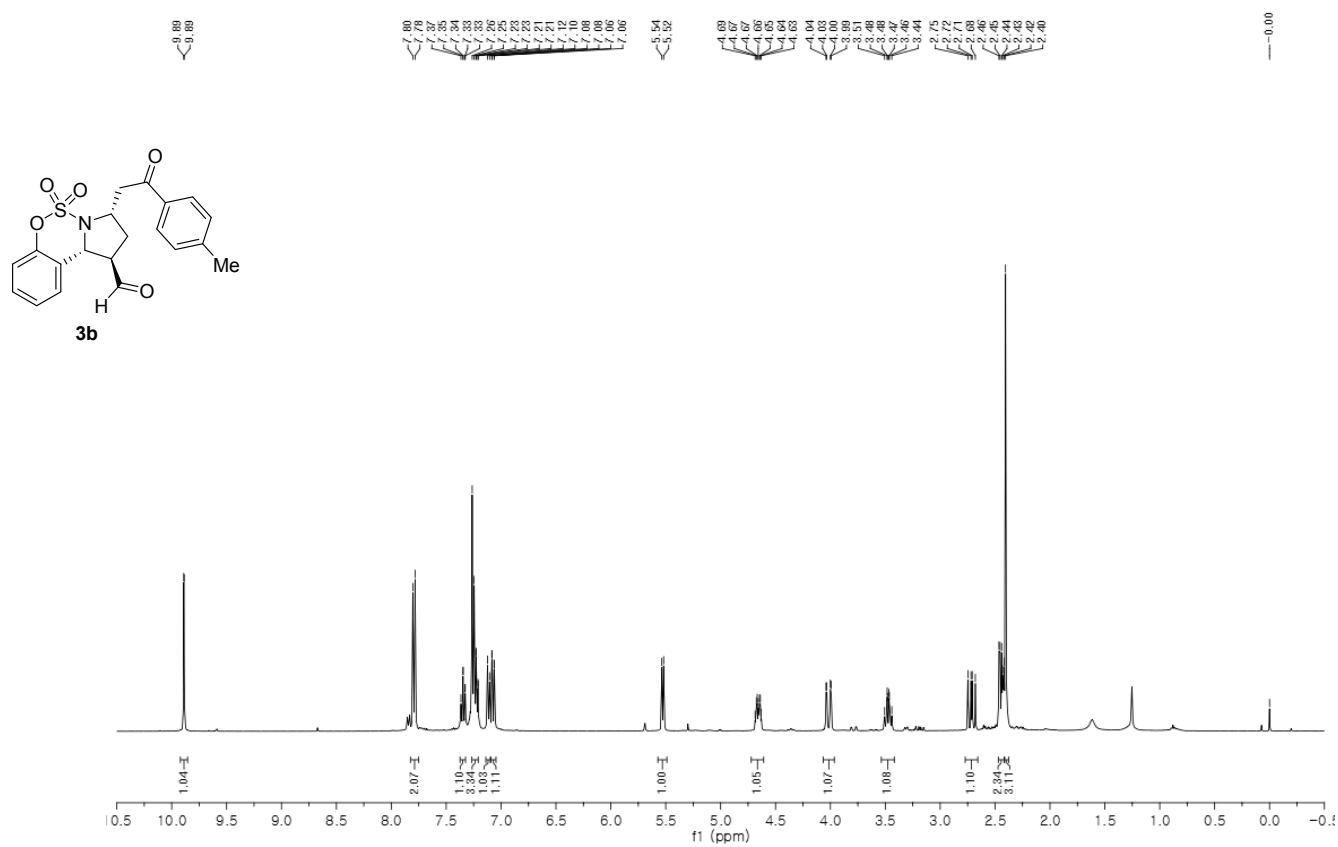
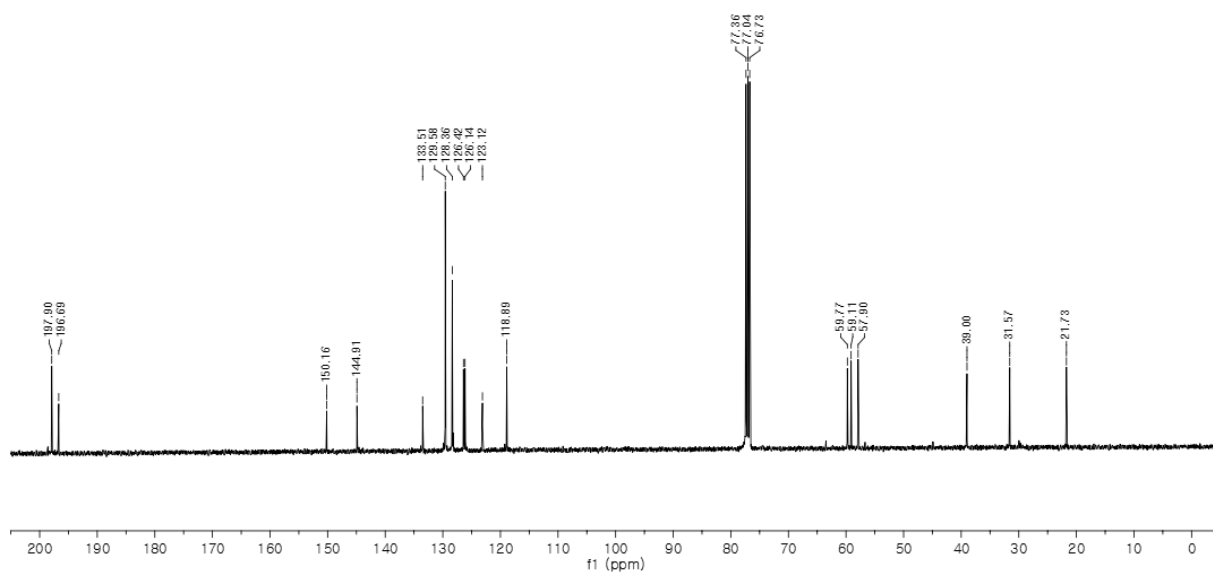
Identification code	SGK0701	
Empirical formula	C ₂₂ H ₂₀ Br N O ₆ S	
Formula weight	506.36	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Hexagonal	
Space group	P6 ₅	
Unit cell dimensions	a = 11.4848(5) Å	α = 90°.
	b = 11.4848(5) Å	β = 90°.
	c = 28.4095(15) Å	γ = 120°.
Volume	3245.2(3) Å ³	
Z	6	
Density (calculated)	1.555 Mg/m ³	
Absorption coefficient	2.036 mm ⁻¹	
F(000)	1548	
Crystal size	0.220 x 0.180 x 0.120 mm ³	
Theta range for data collection	2.048 to 28.336°.	

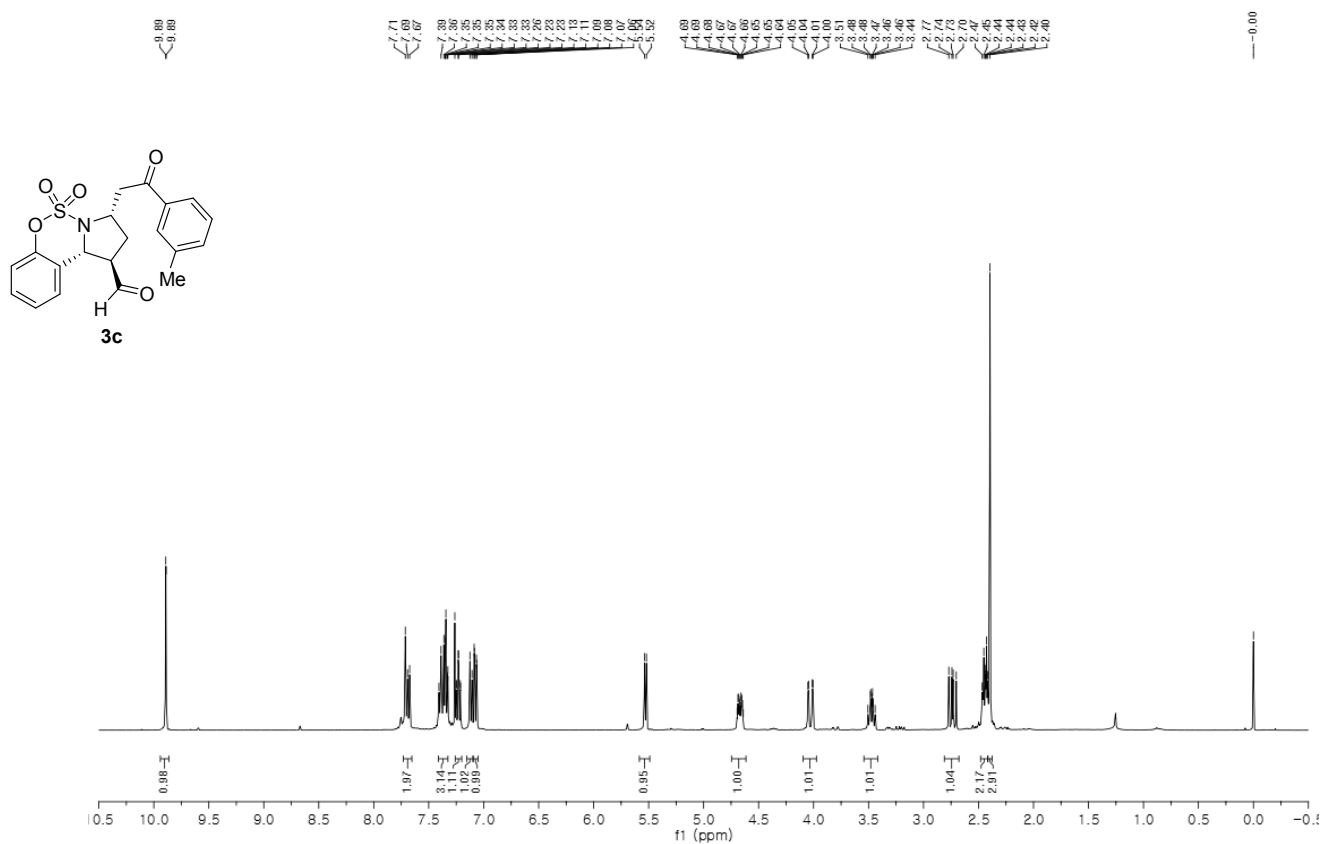
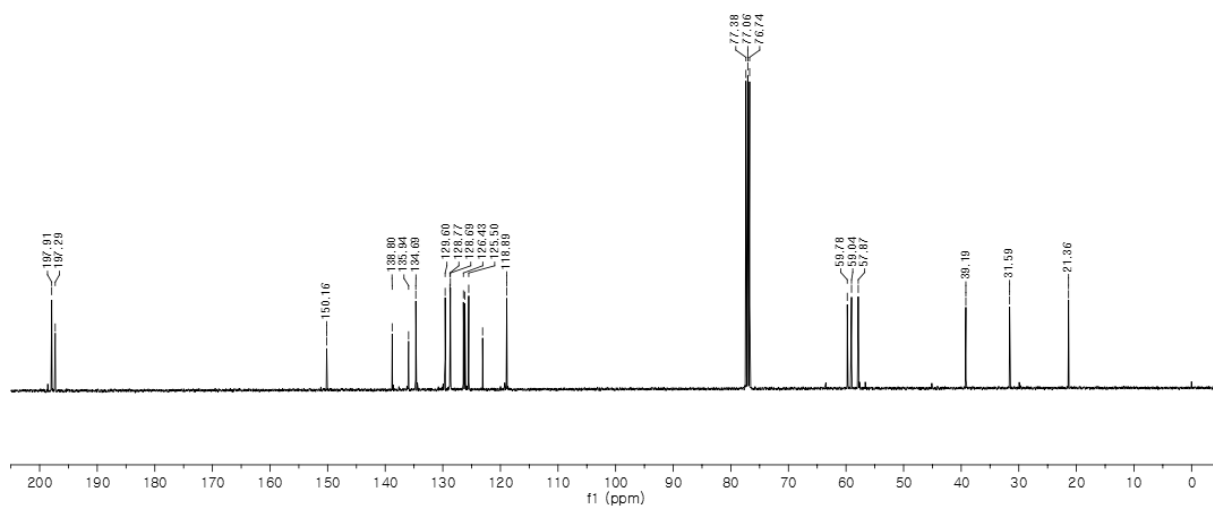
Index ranges	-15<=h<=15, -15<=k<=15, -37<=l<=37
Reflections collected	204302
Independent reflections	5402 [R(int) = 0.1036]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7457 and 0.6684
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5402 / 1 / 281
Goodness-of-fit on F ²	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0303, wR2 = 0.0554
R indices (all data)	R1 = 0.0542, wR2 = 0.0616
Absolute structure parameter	-0.004(2)
Extinction coefficient	n/a
Largest diff. peak and hole	0.252 and -0.224 e.Å ⁻³

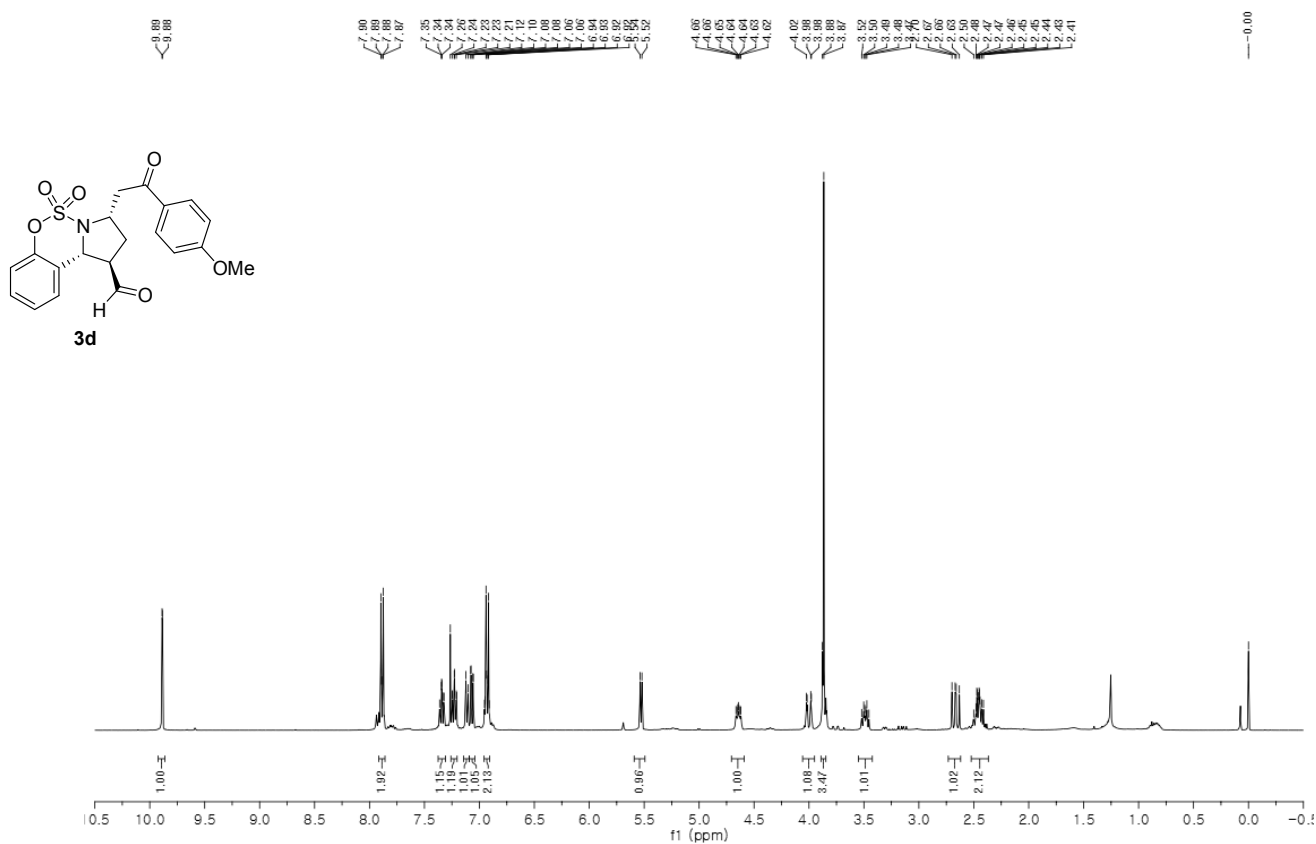
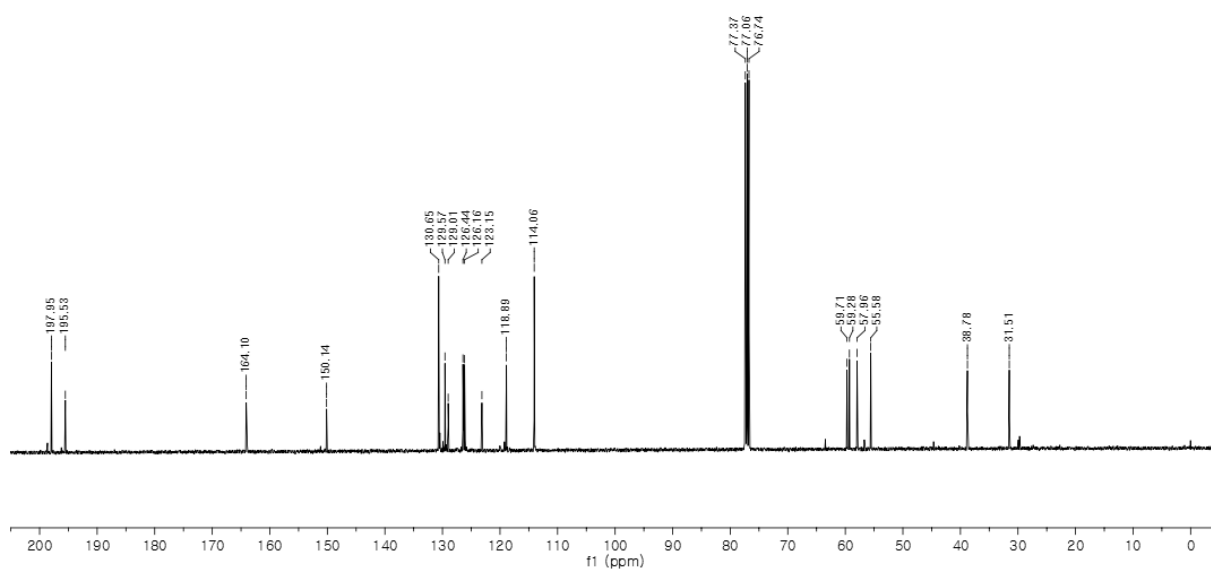
Number of nodes	Frequency
1	7.91
2	7.60
3	7.58
4	7.57
5	7.57
6	7.37
7	7.33
8	7.33
9	7.25
10	7.25
11	7.23
12	7.23
13	7.11
14	7.11
15	7.09
16	7.09
17	5.94
18	5.53
19	4.70
20	4.70
21	4.69
22	4.68
23	4.68
24	4.67
25	4.66
26	4.66
27	4.67
28	4.06
29	4.06
30	4.03
31	4.03
32	3.50
33	3.46
34	3.46
35	3.46
36	3.44
37	2.89
38	2.77
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40	2.73
41	2.73
42	2.48
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44	2.46
45	2.46
46	2.44

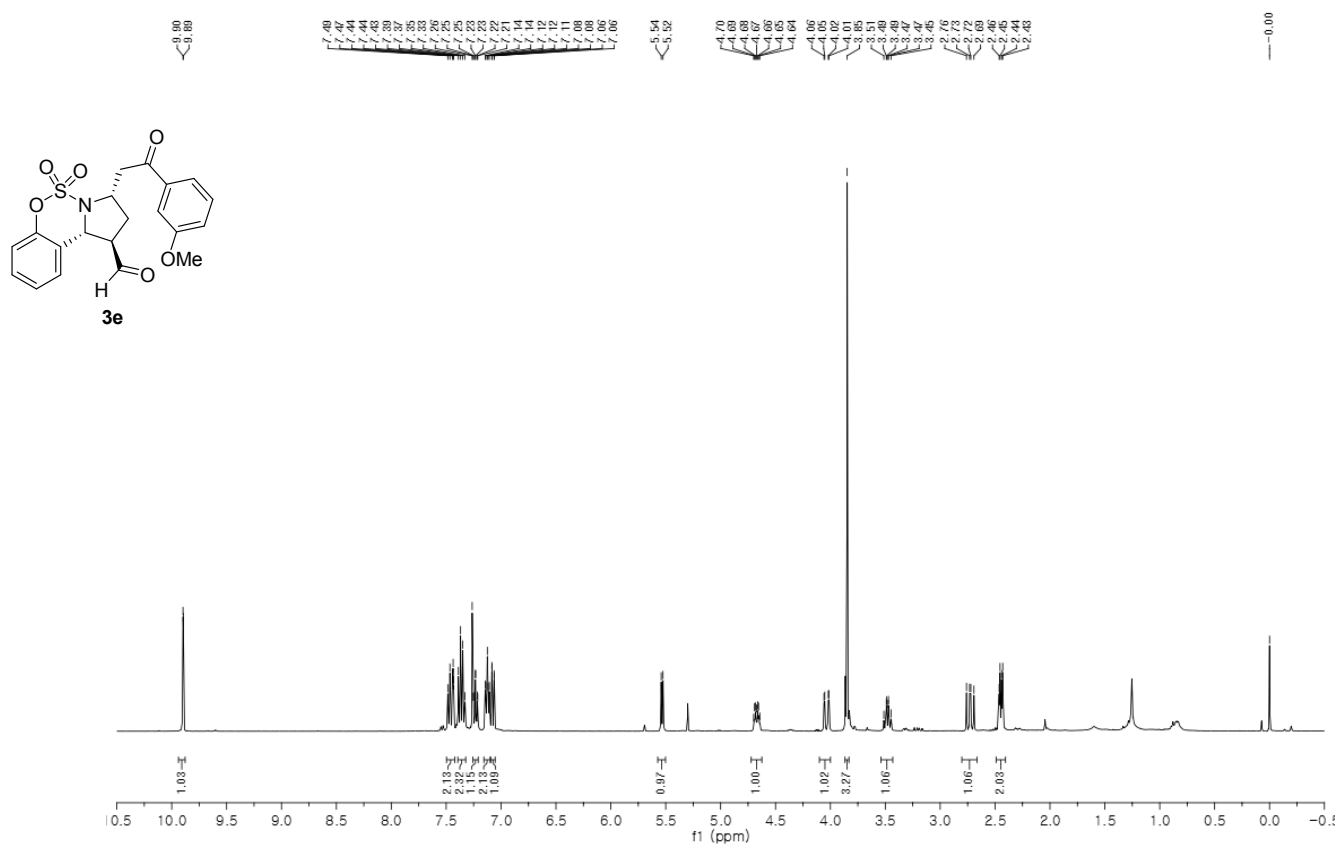
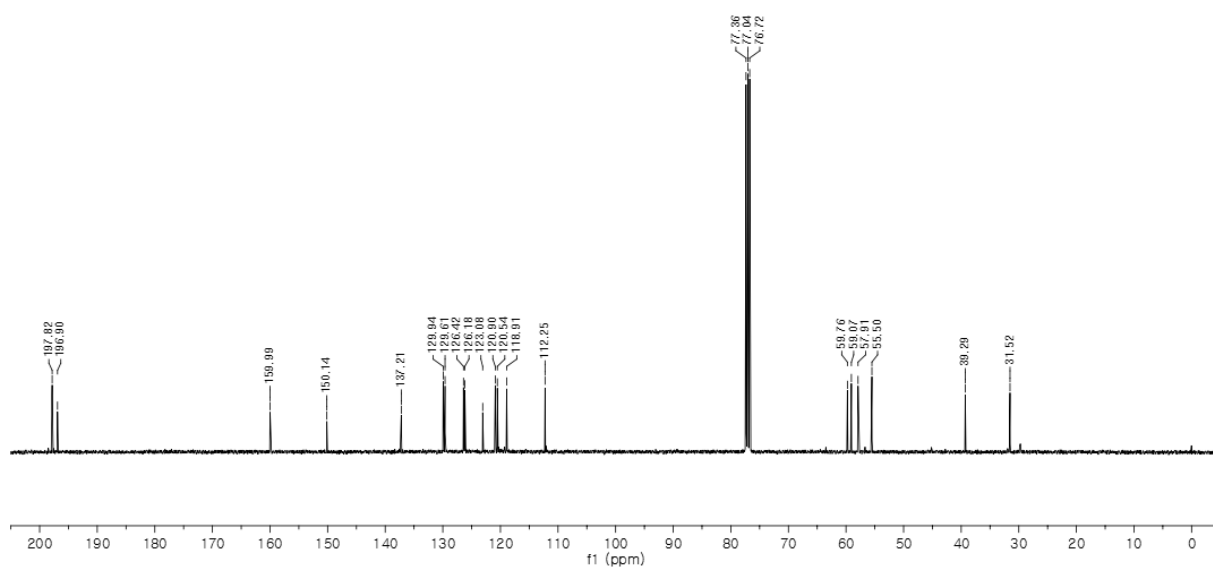


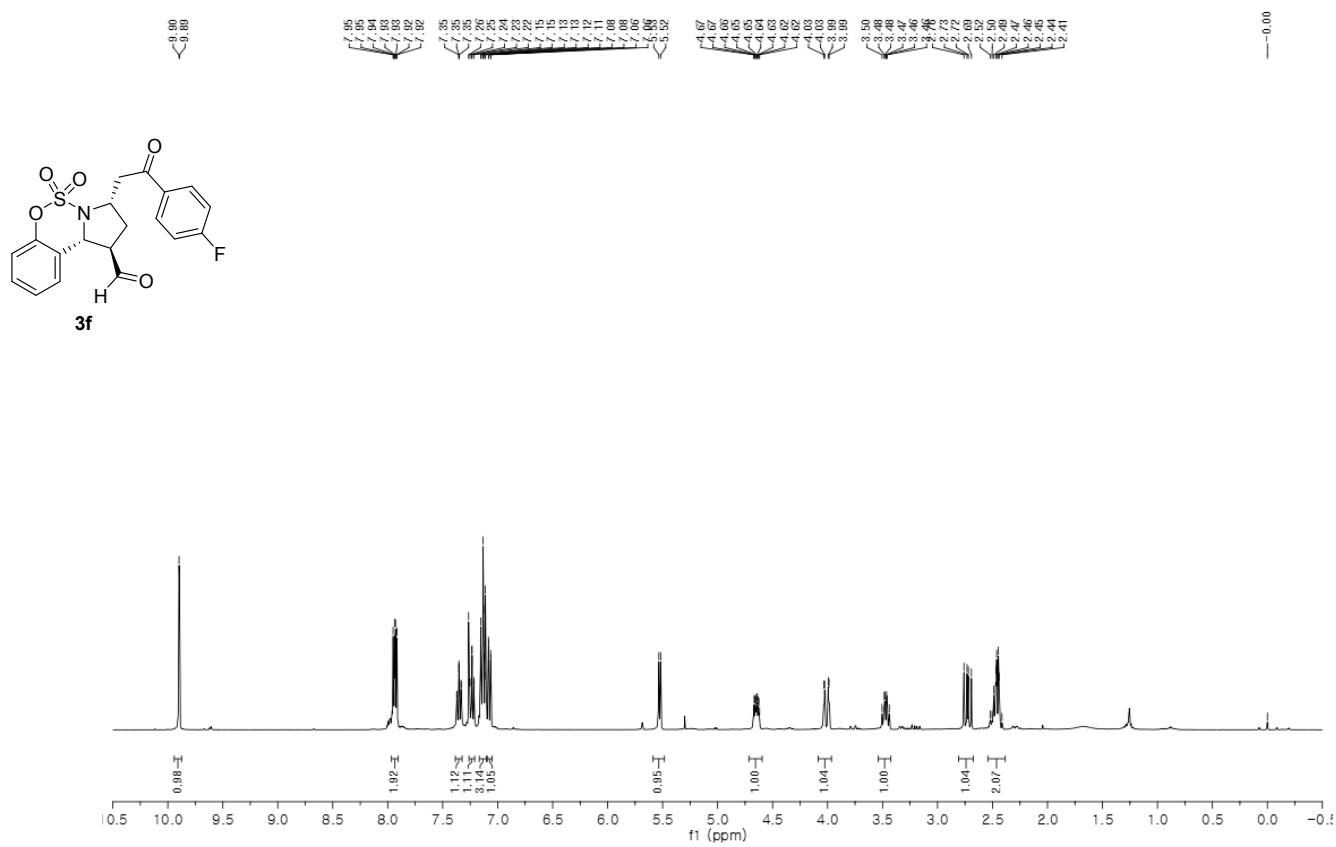
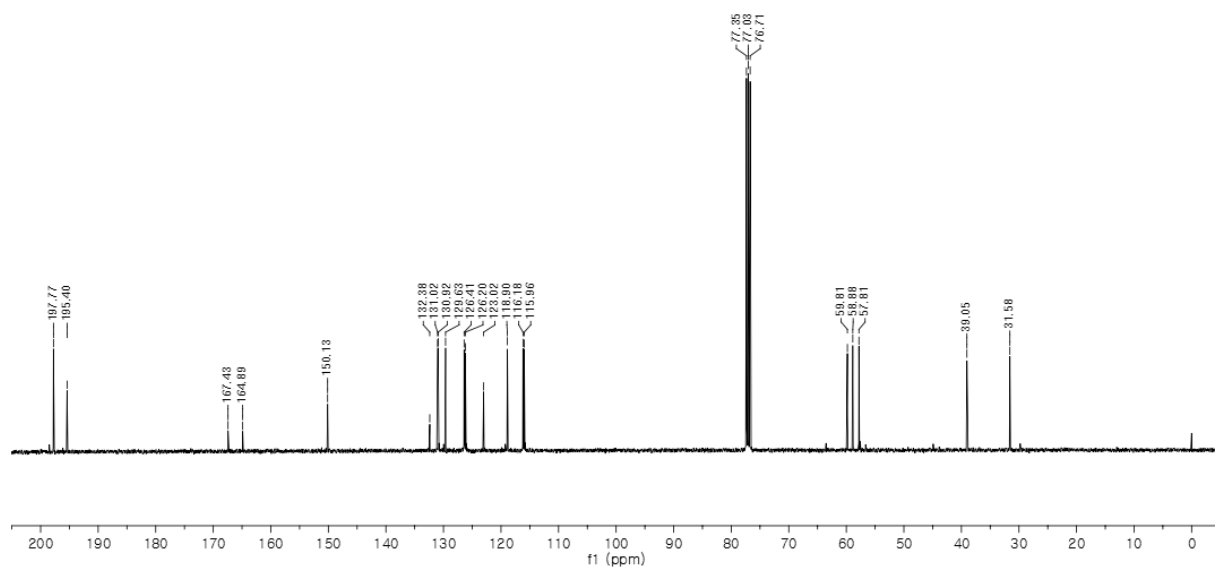
¹³C NMR spectrum (CDCl₃) of compound 10a. The x-axis is labeled 'f1 (ppm)' and ranges from 0 to 200. The spectrum shows several peaks with the following chemical shifts labeled: 197.05, 197.05, 150.15, 135.92, 133.92, 128.62, 128.91, 128.22, 128.22, 126.18, 126.09, 118.92, 77.37, 77.37, 77.37, 76.74, 59.79, 59.98, 59.69, 39.04, and 31.62. A solvent triplet for CDCl₃ is visible around 77 ppm.

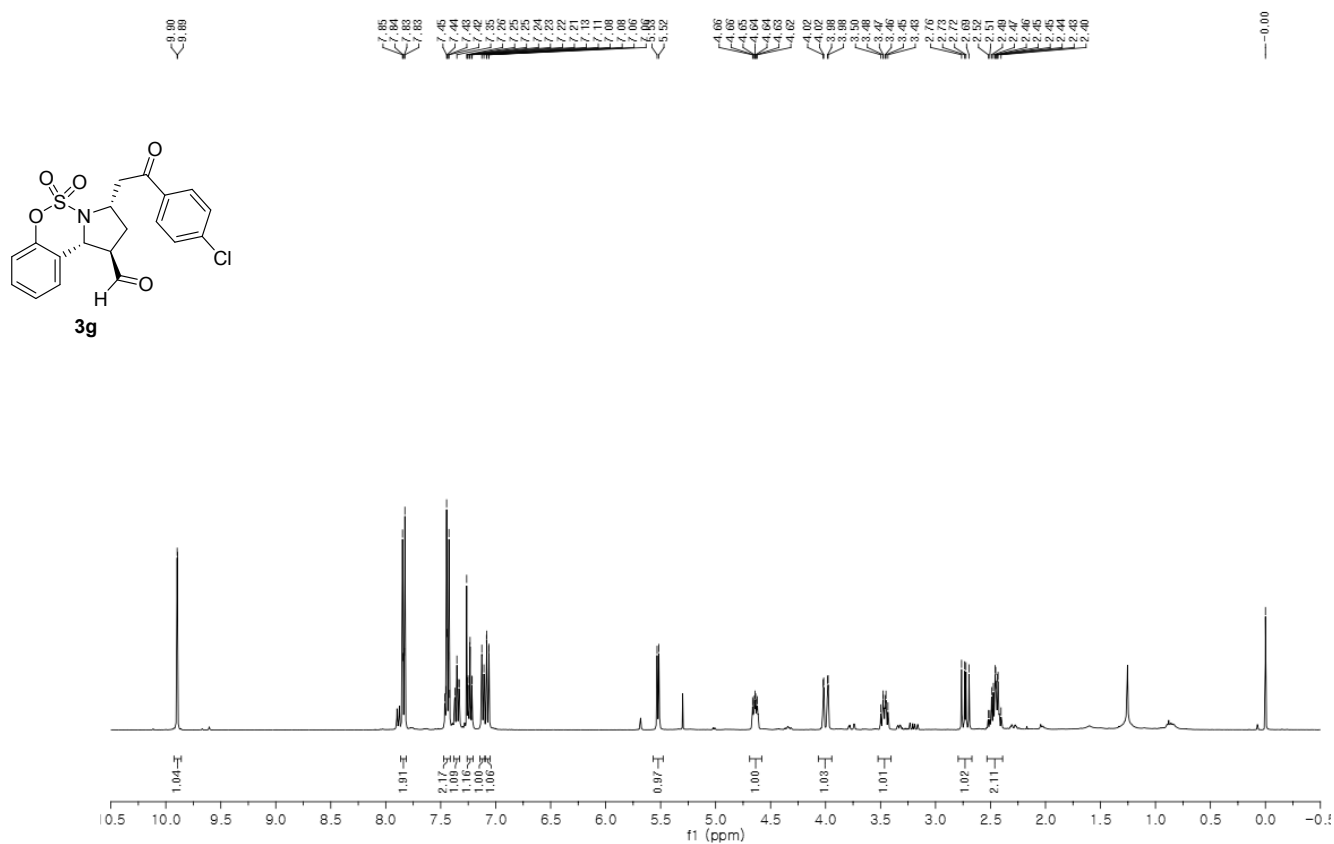
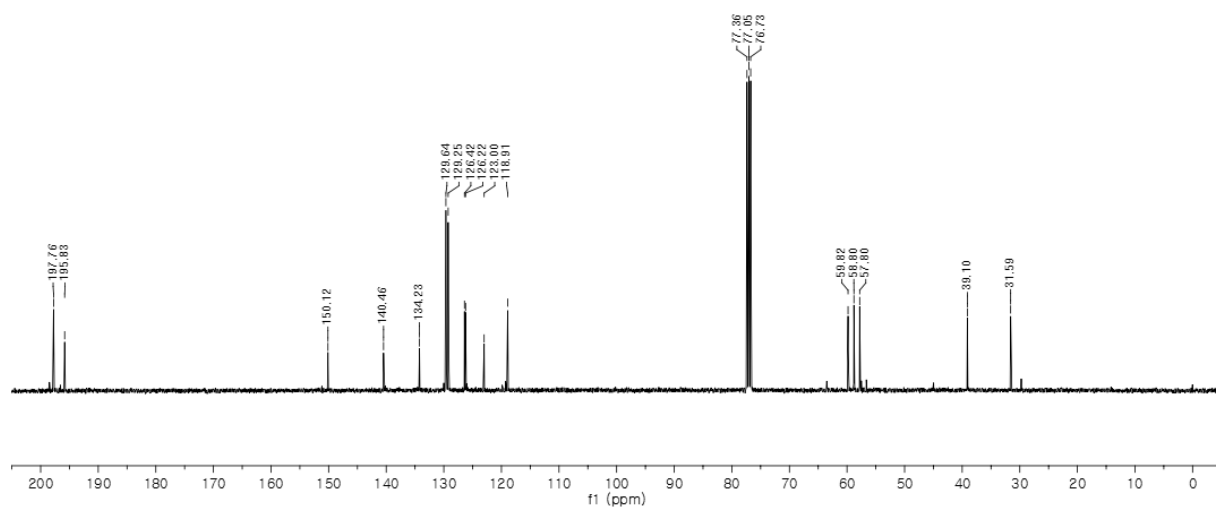
^1H NMR (400 MHz) in CDCl_3  **^{13}C NMR (100 MHz) in CDCl_3** 

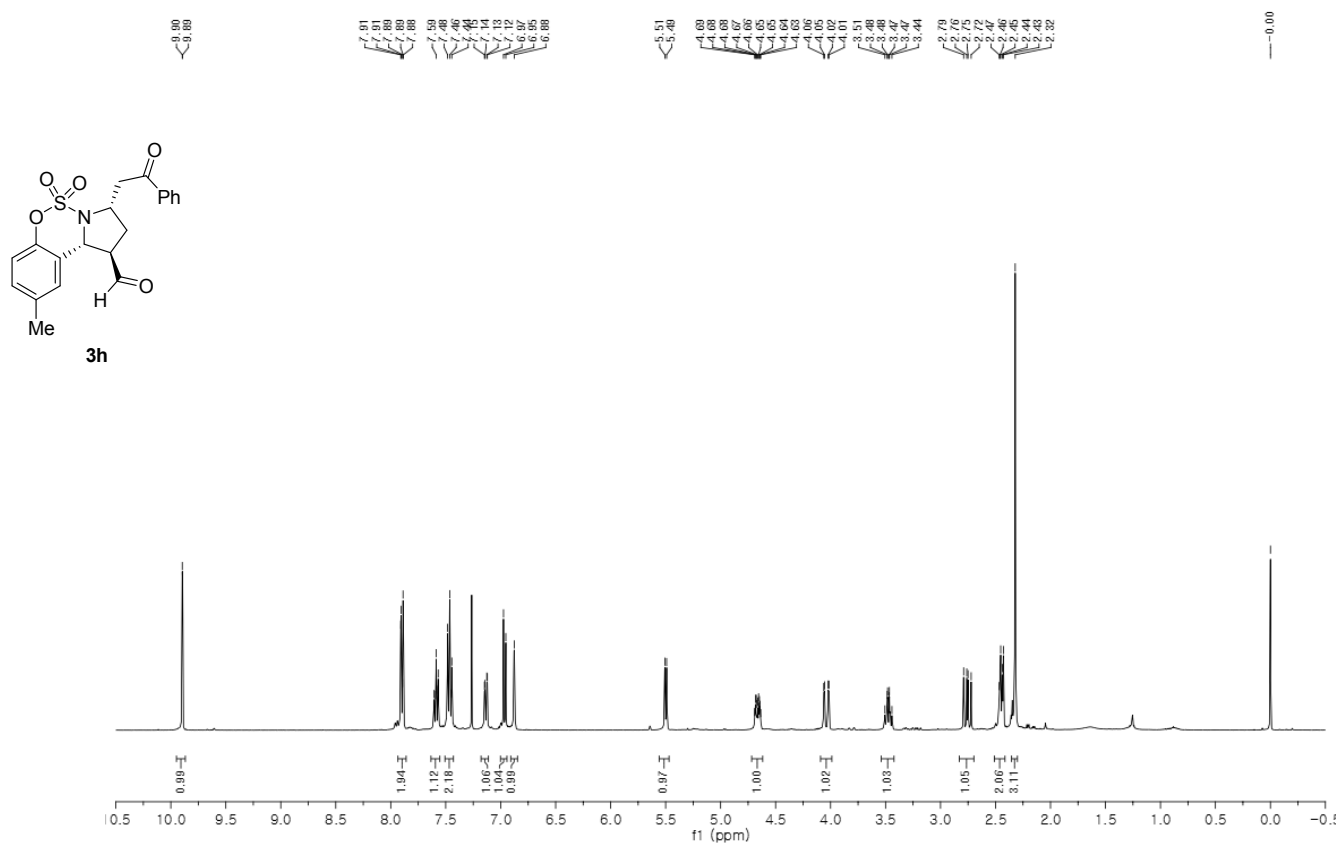
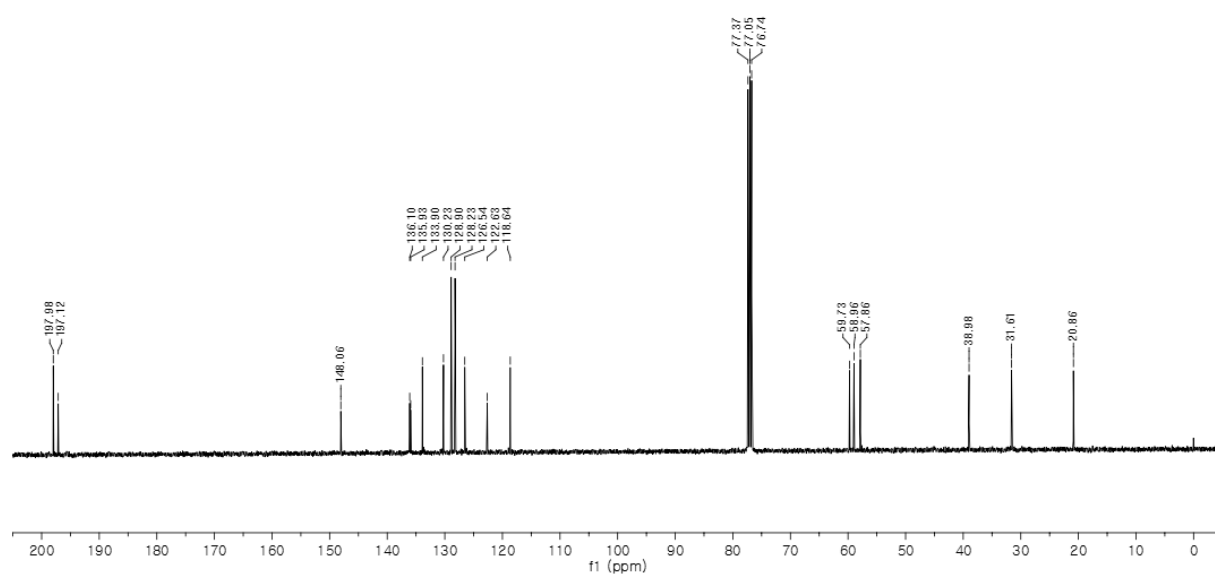
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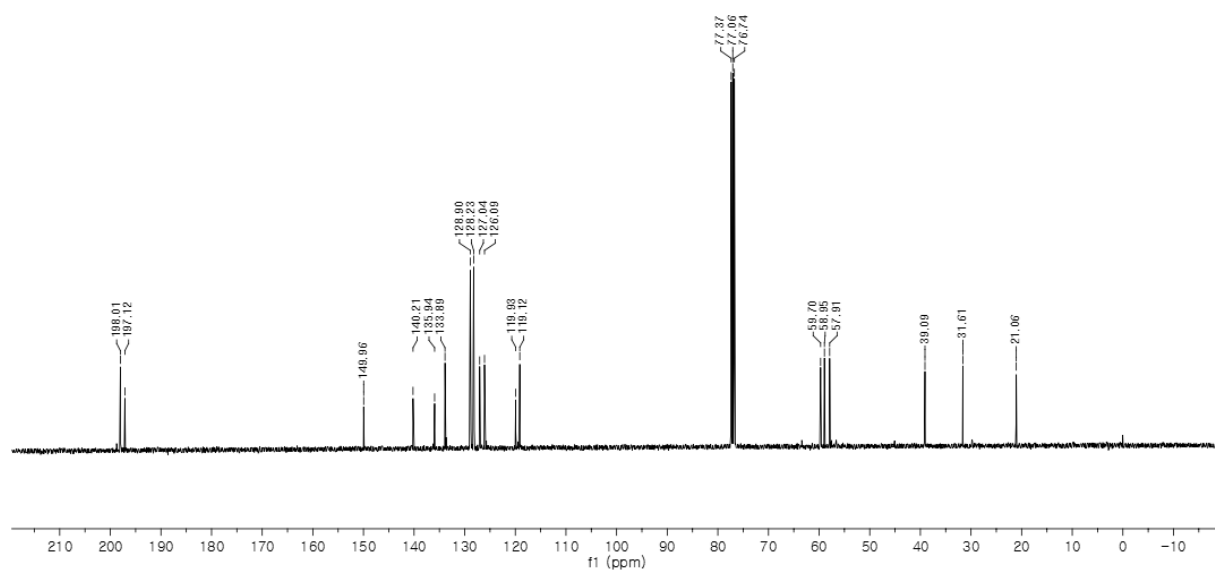
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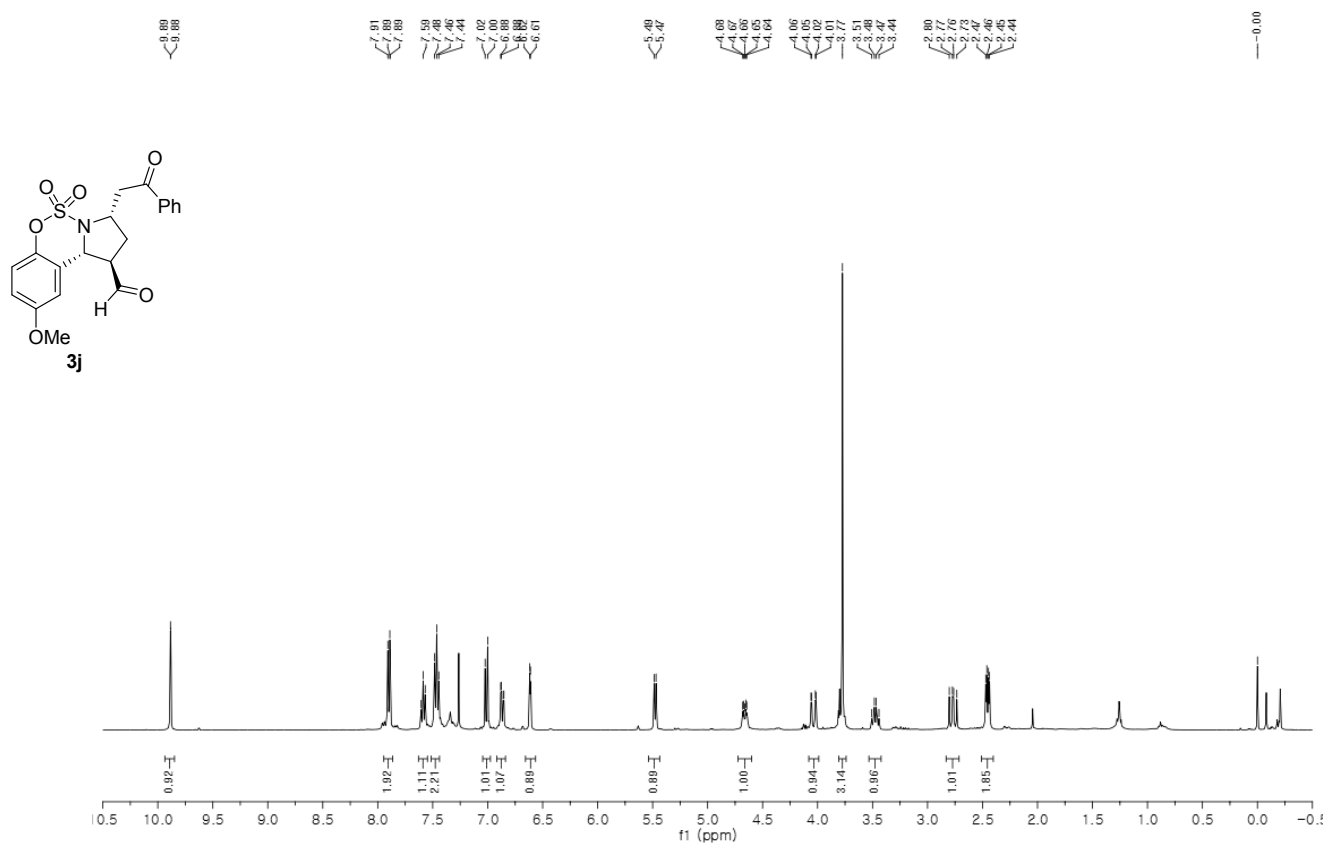
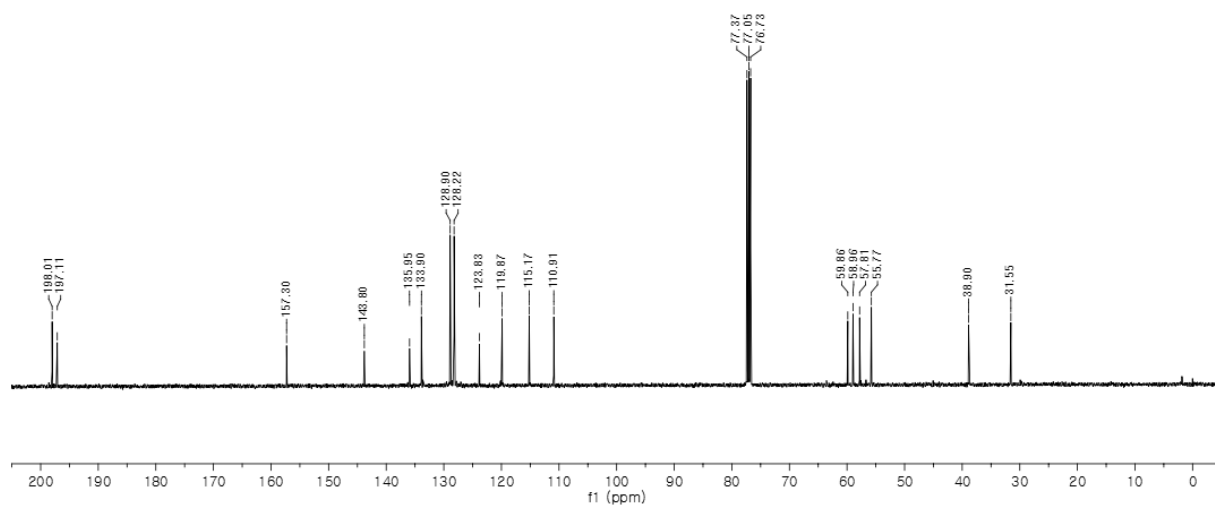
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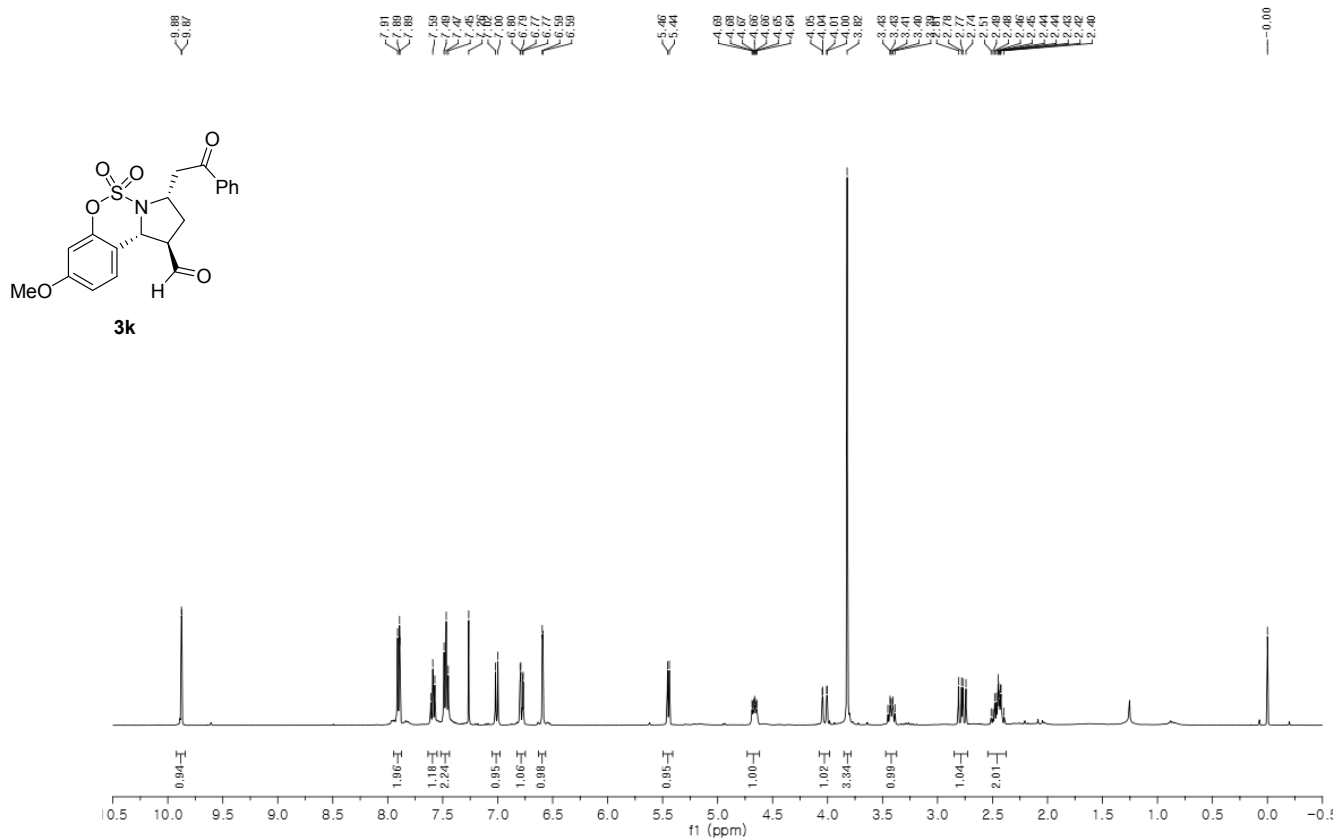
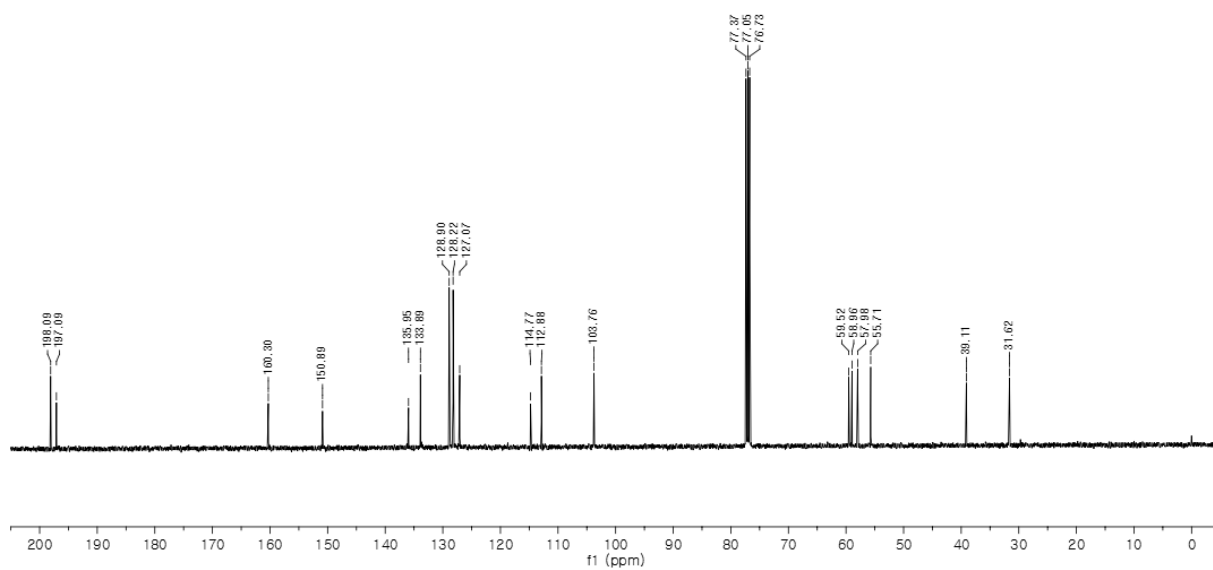
^1H NMR (400 MHz) in CDCl_3  **^{13}C NMR (100 MHz) in CDCl_3** 

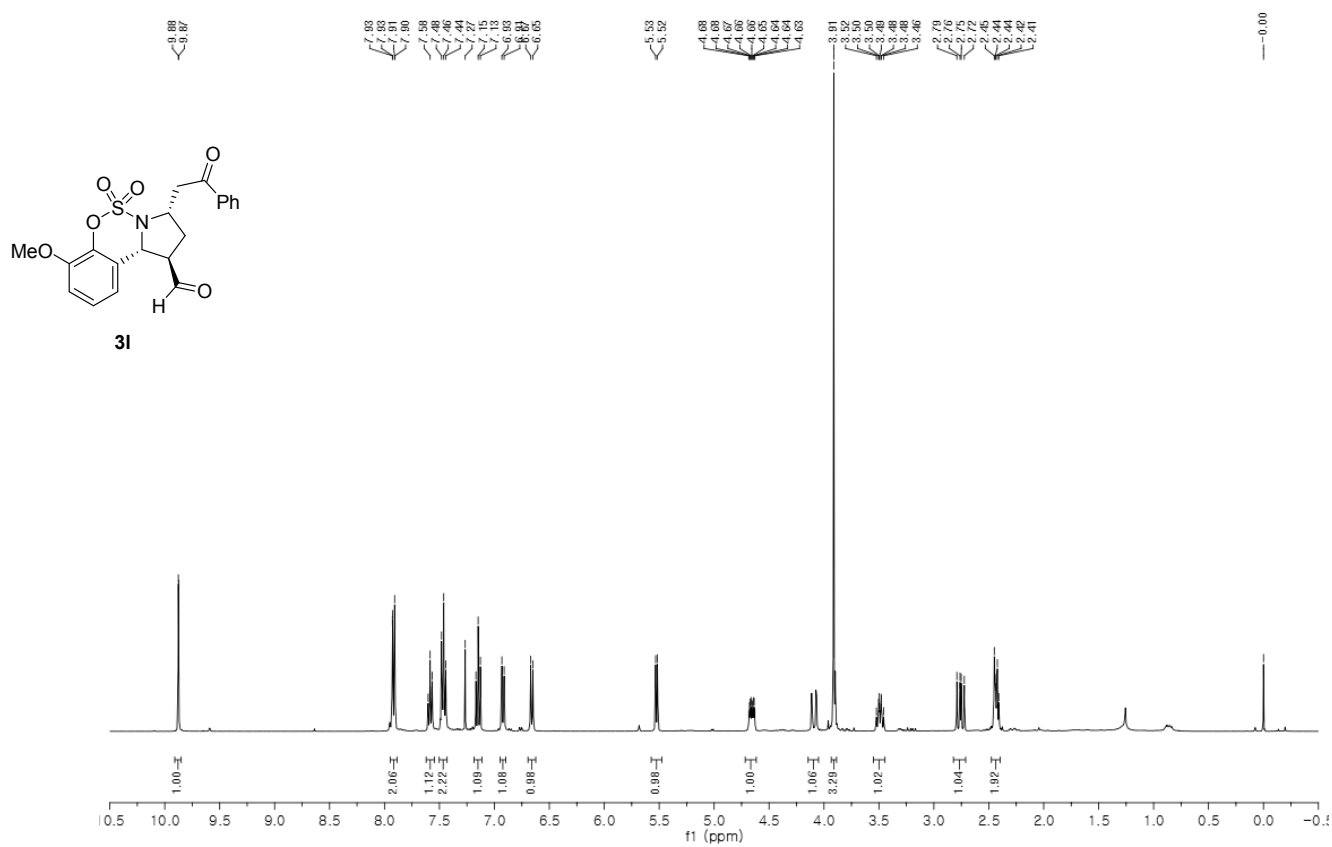
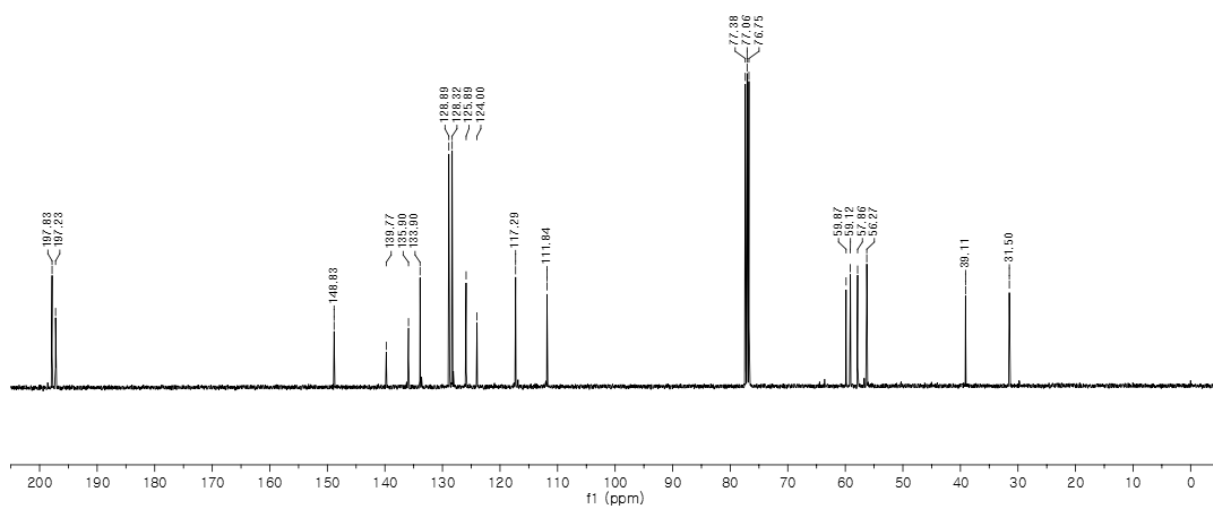
^1H NMR (400 MHz) in CDCl_3  **^{13}C NMR (100 MHz) in CDCl_3** 

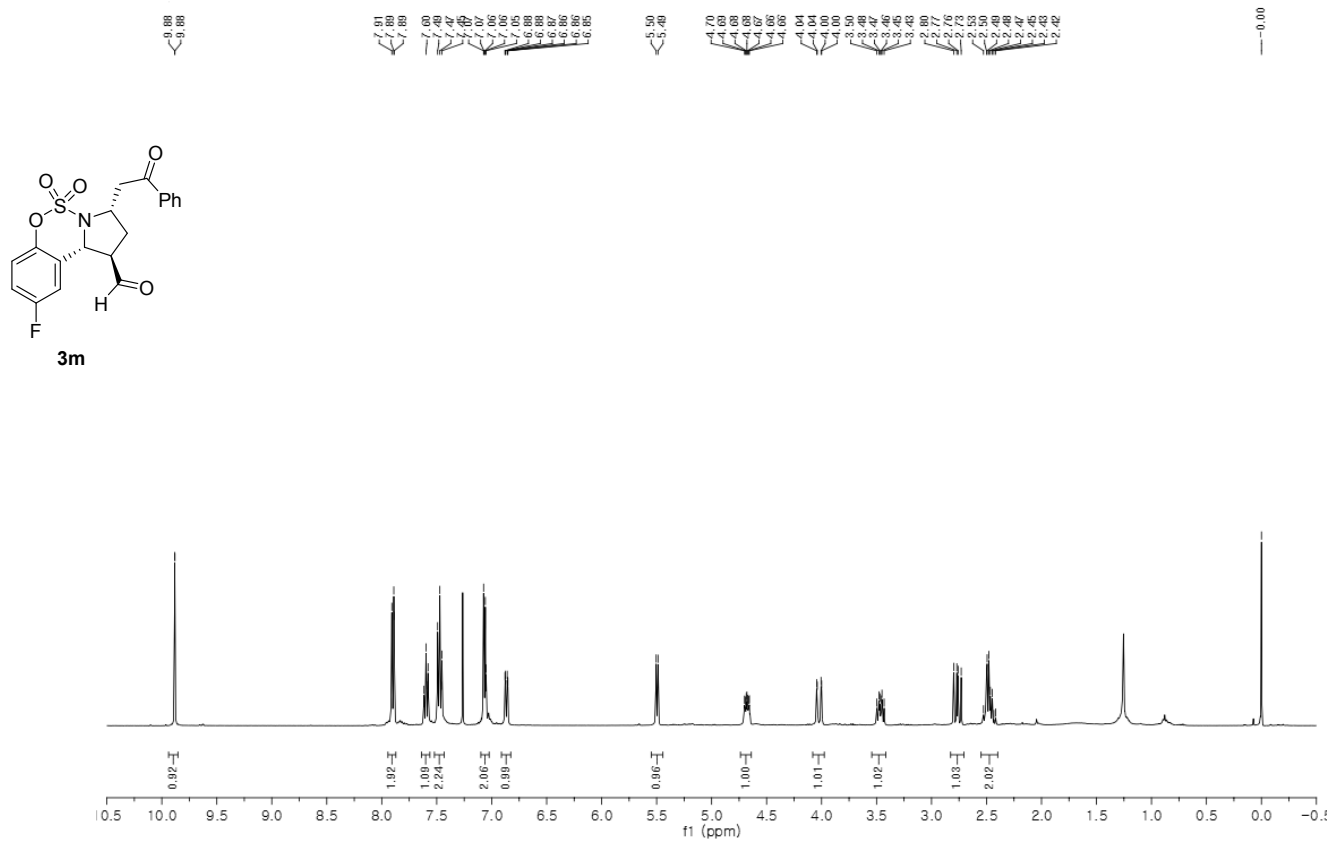
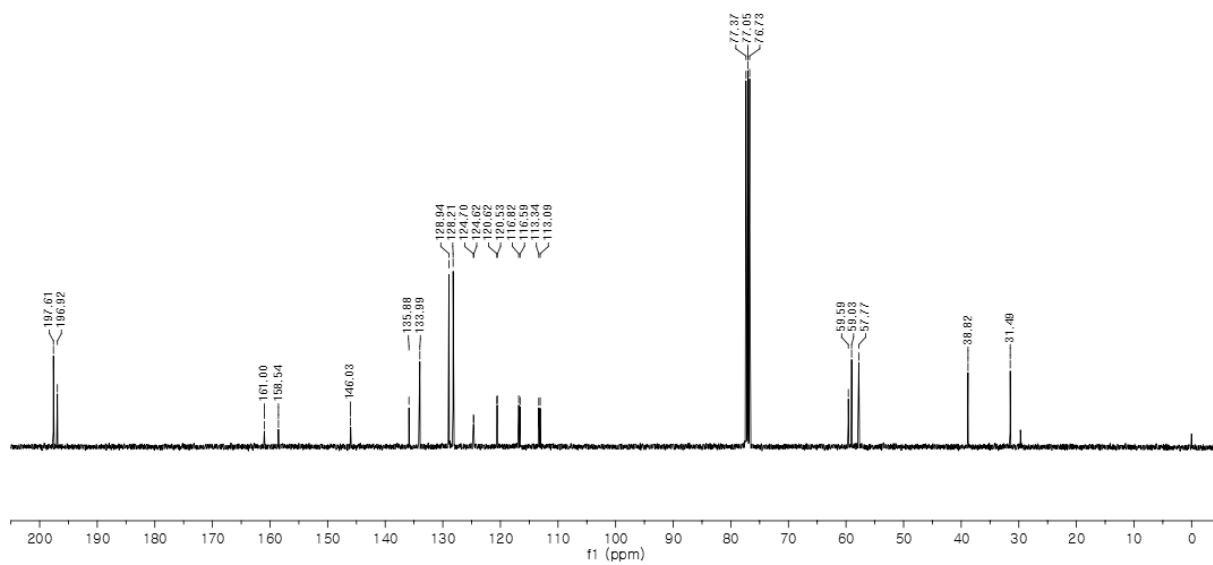
^1H NMR (400 MHz) in CDCl_3  **^{13}C NMR (100 MHz) in CDCl_3** 

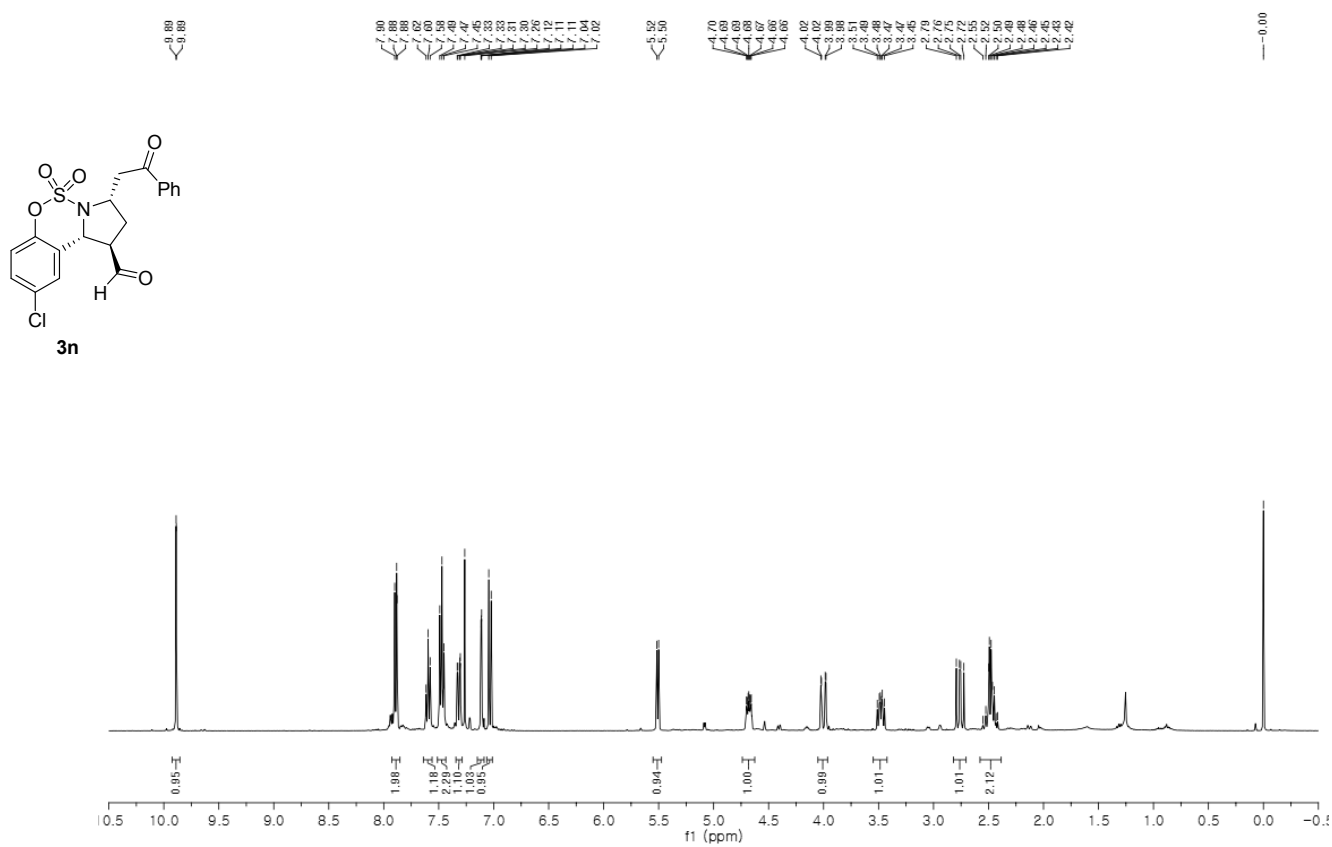
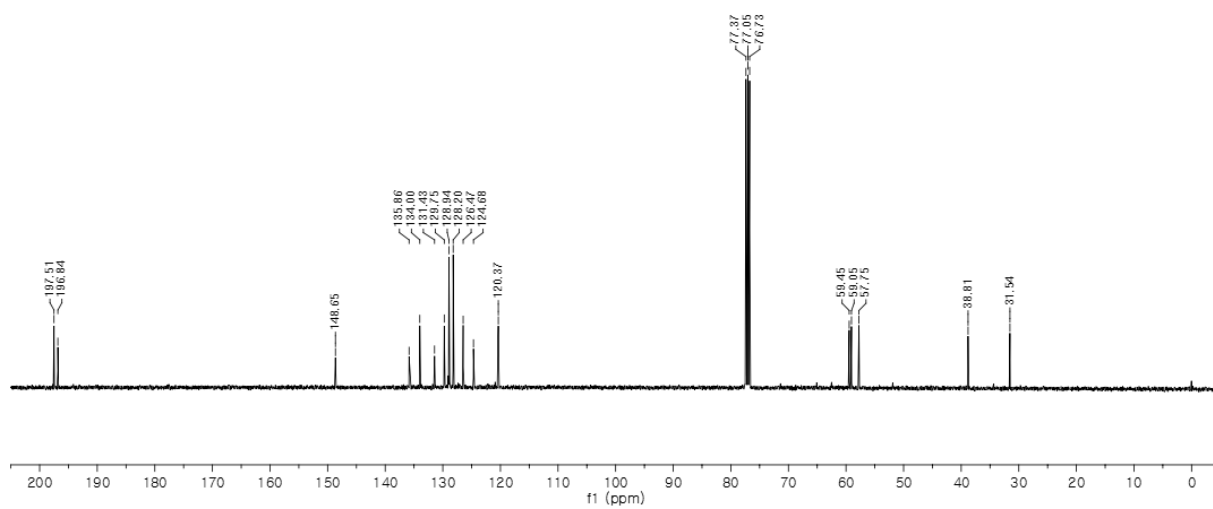


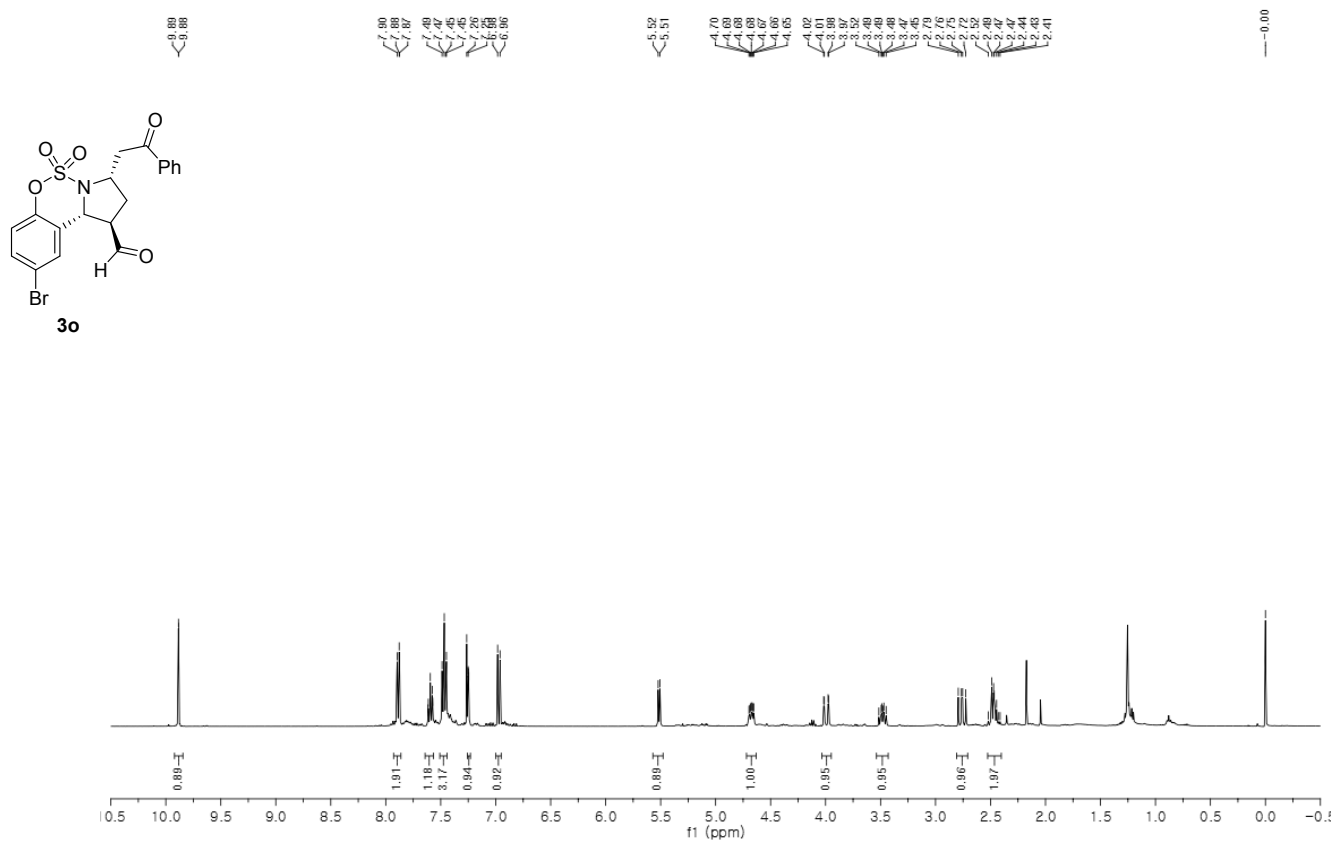
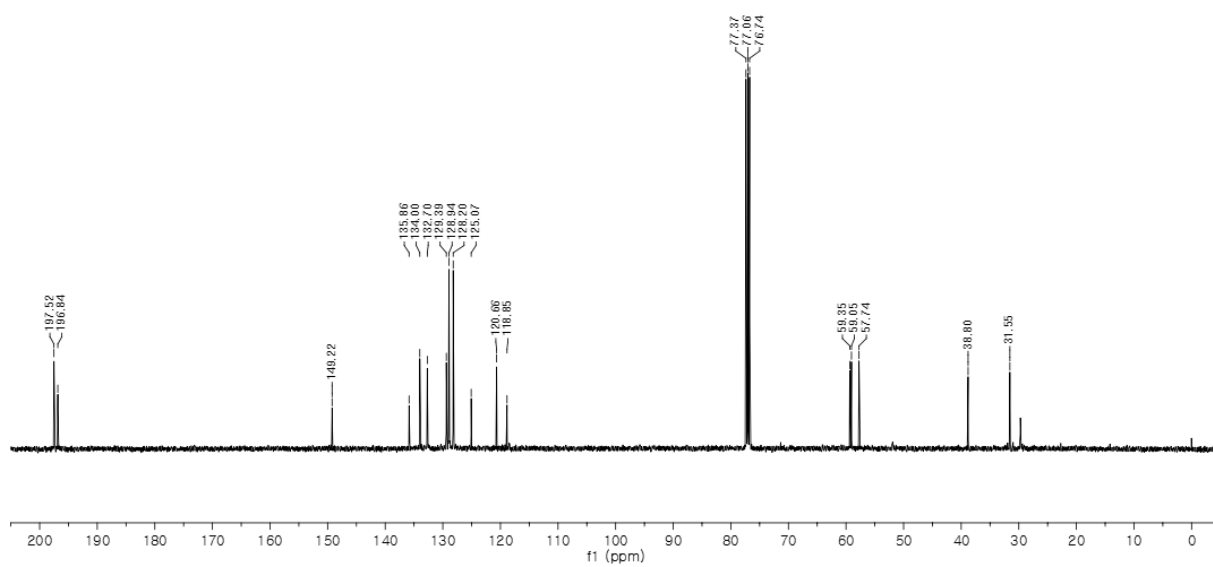
^1H NMR (400 MHz) in CDCl_3  **^{13}C NMR (100 MHz) in CDCl_3** 

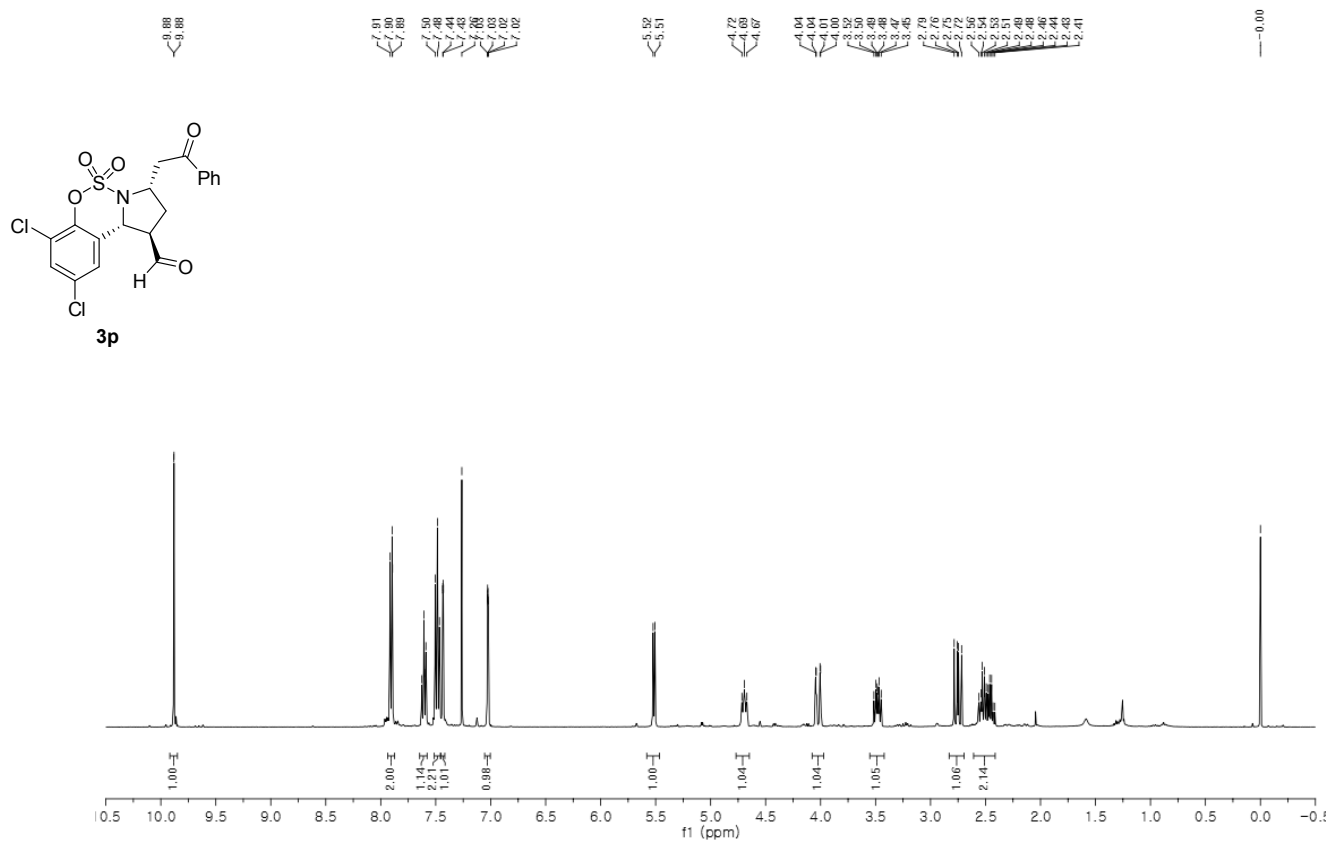
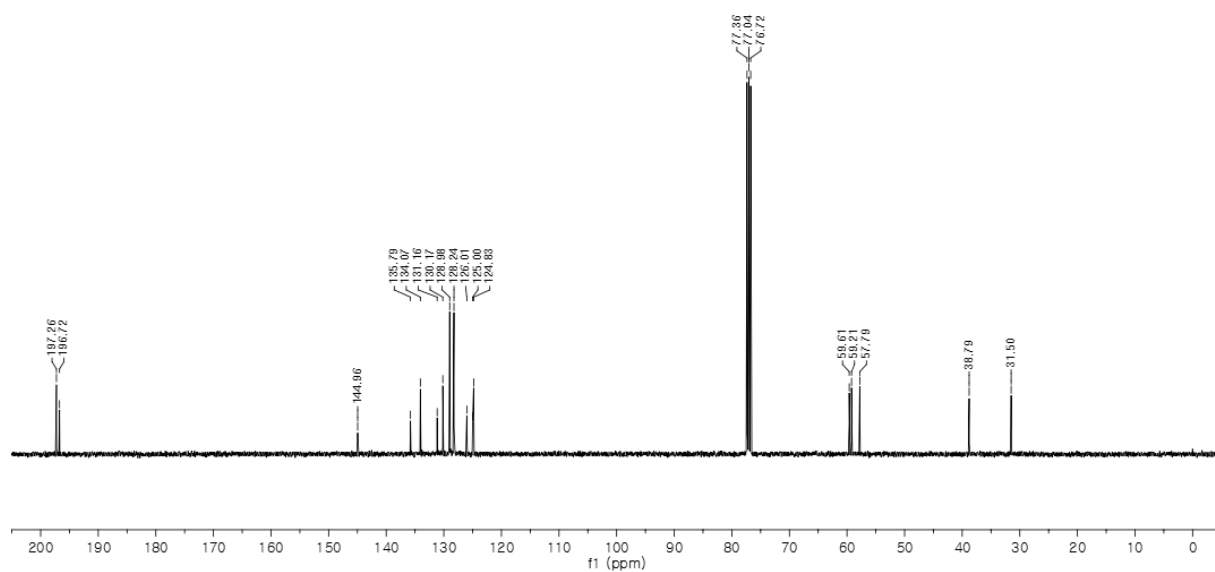
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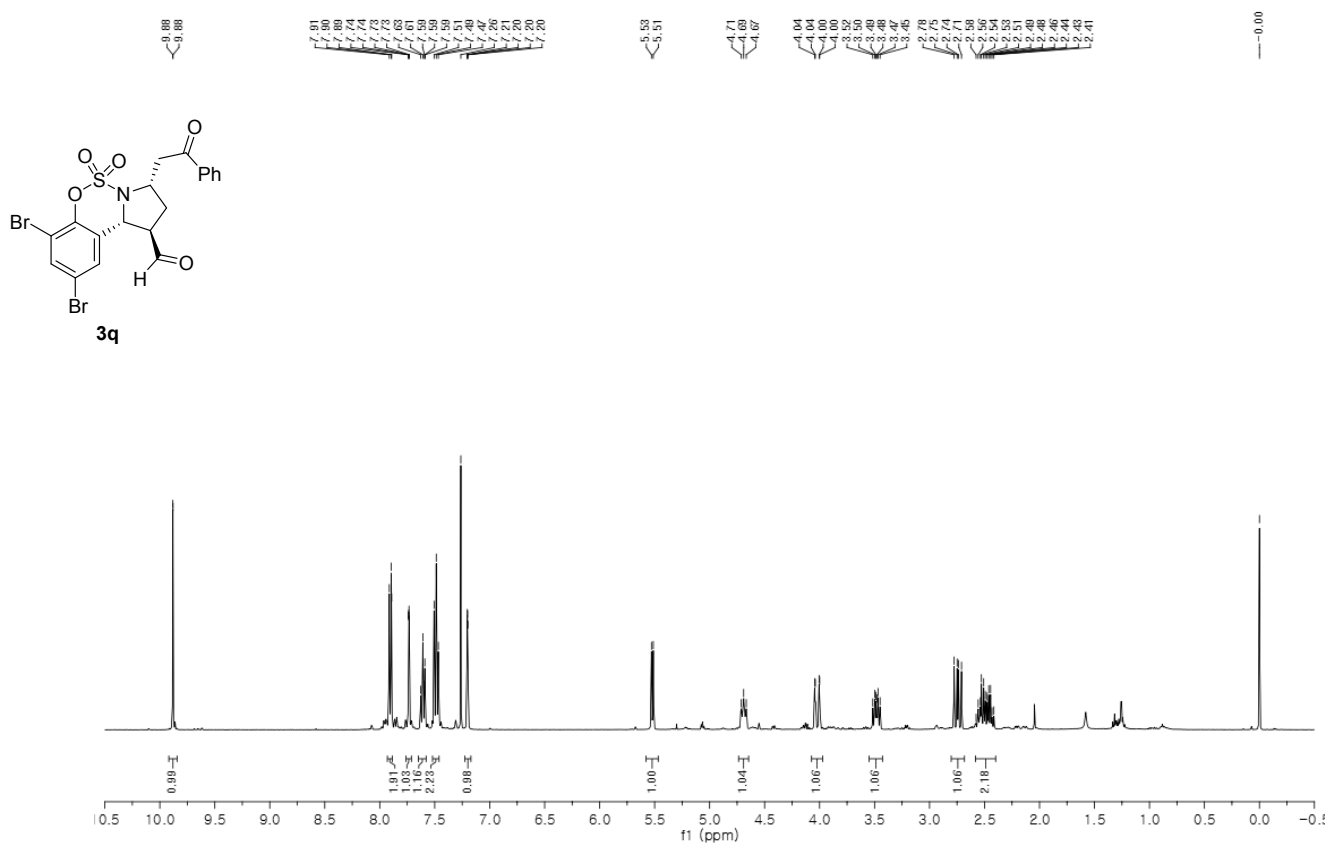
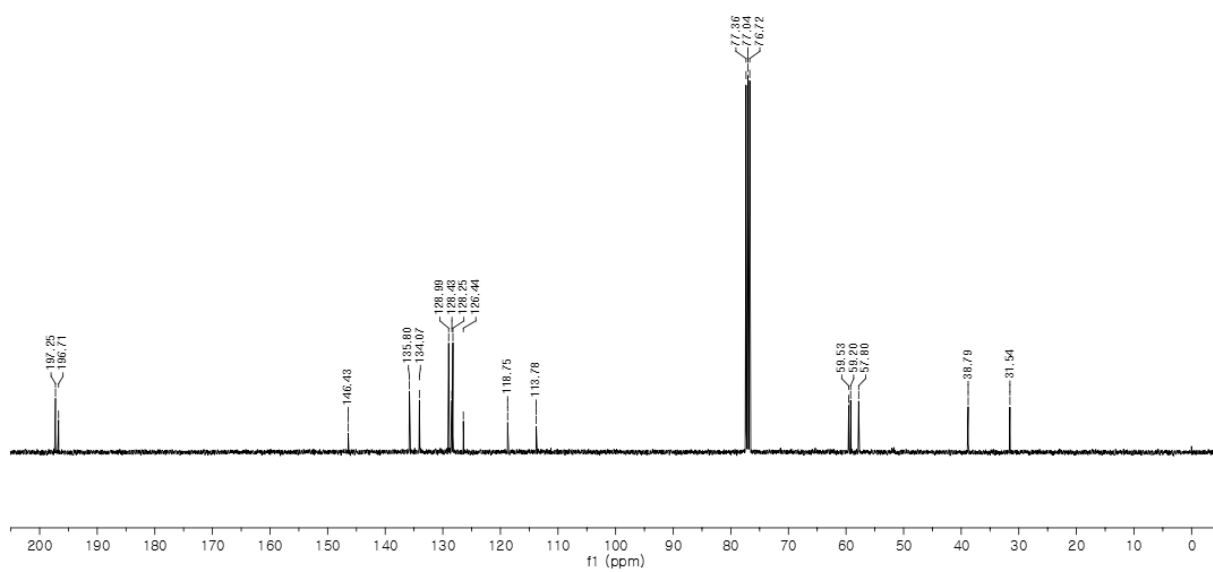
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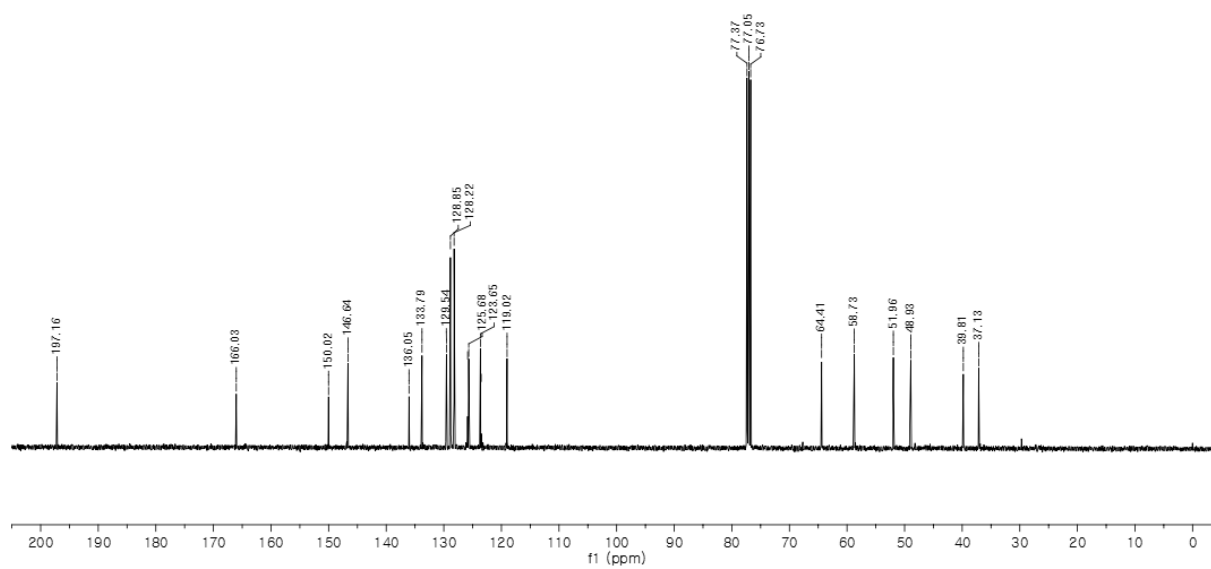
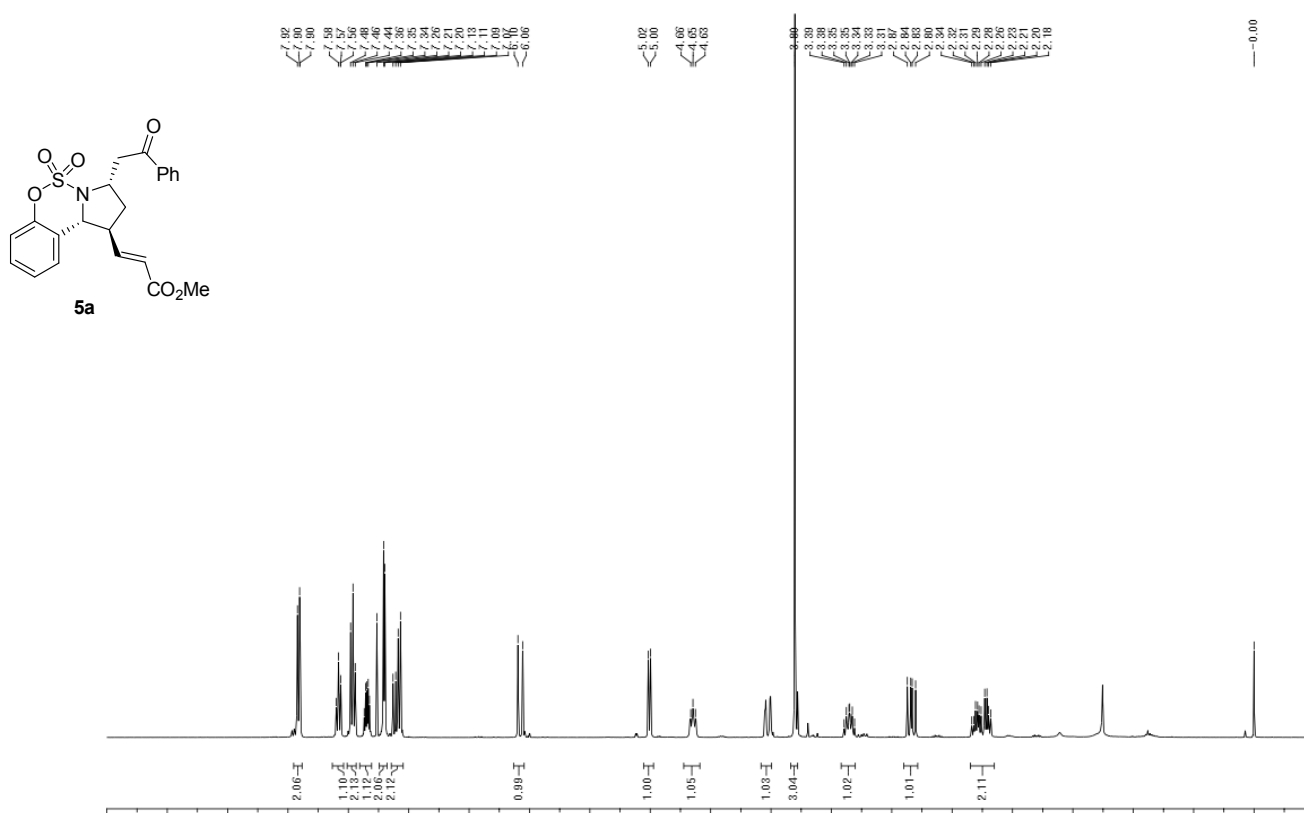
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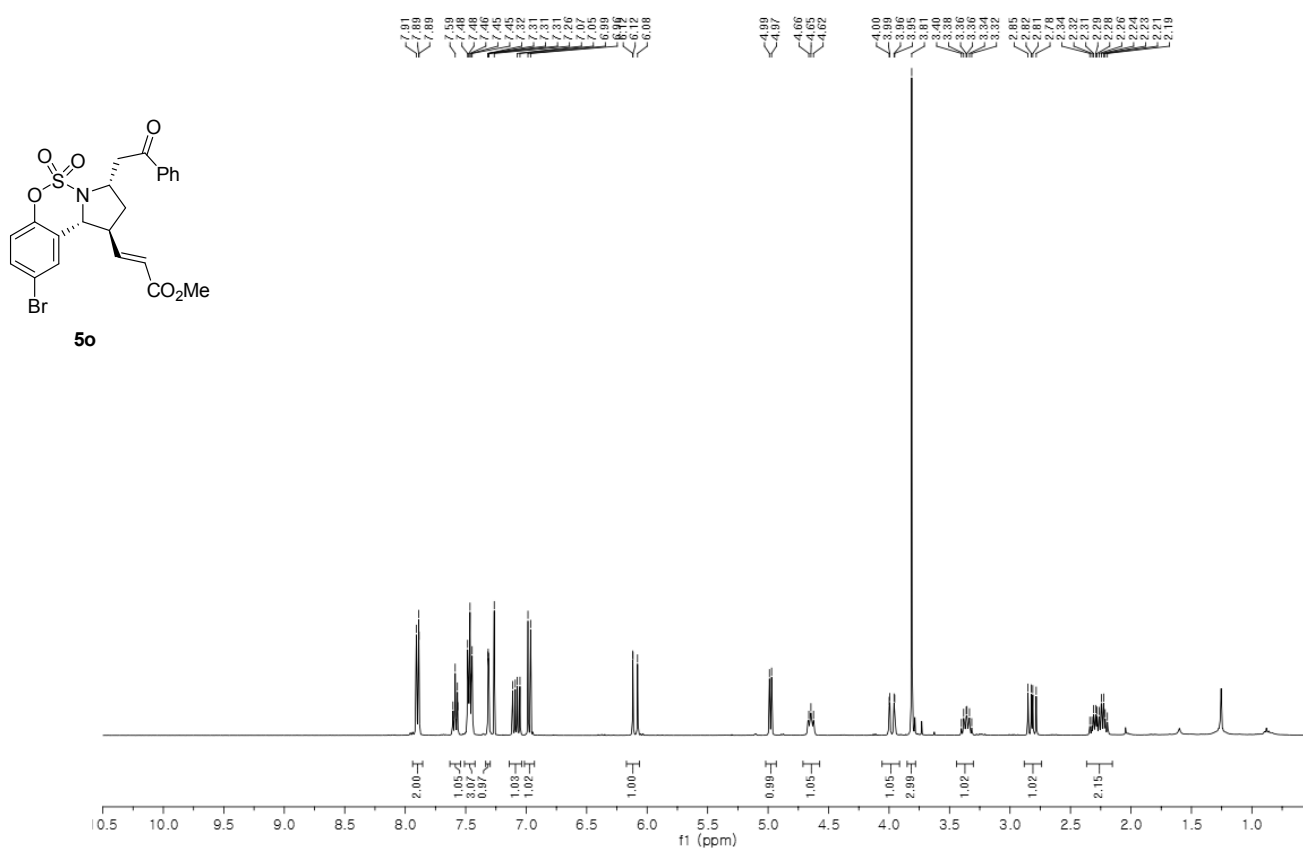
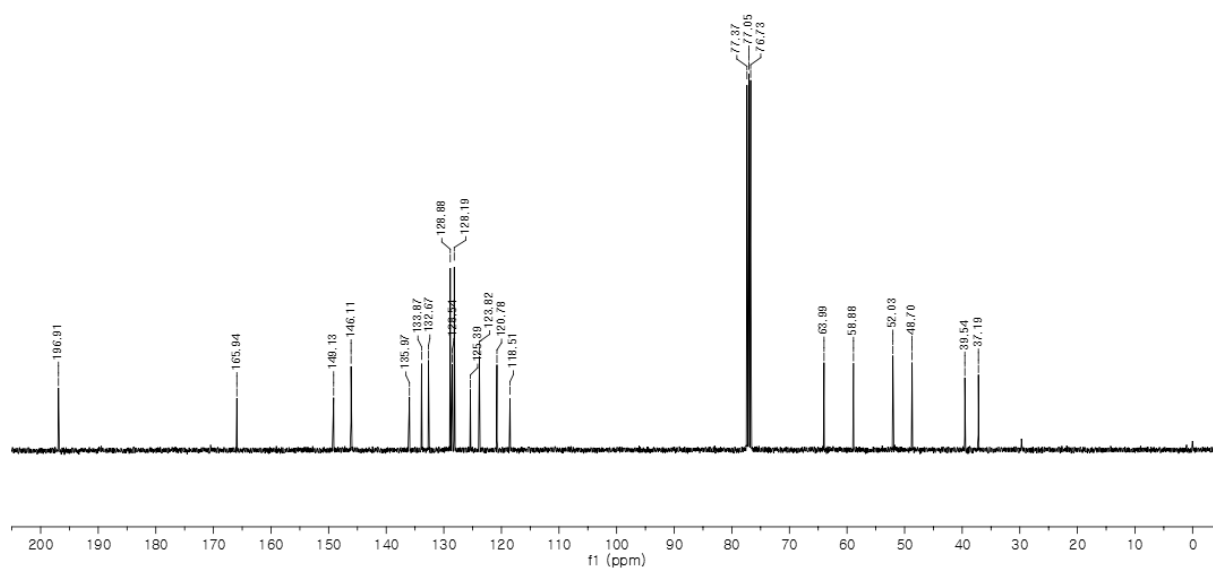
^1H NMR (400 MHz) in CDCl_3  **^{13}C NMR (100 MHz) in CDCl_3** 

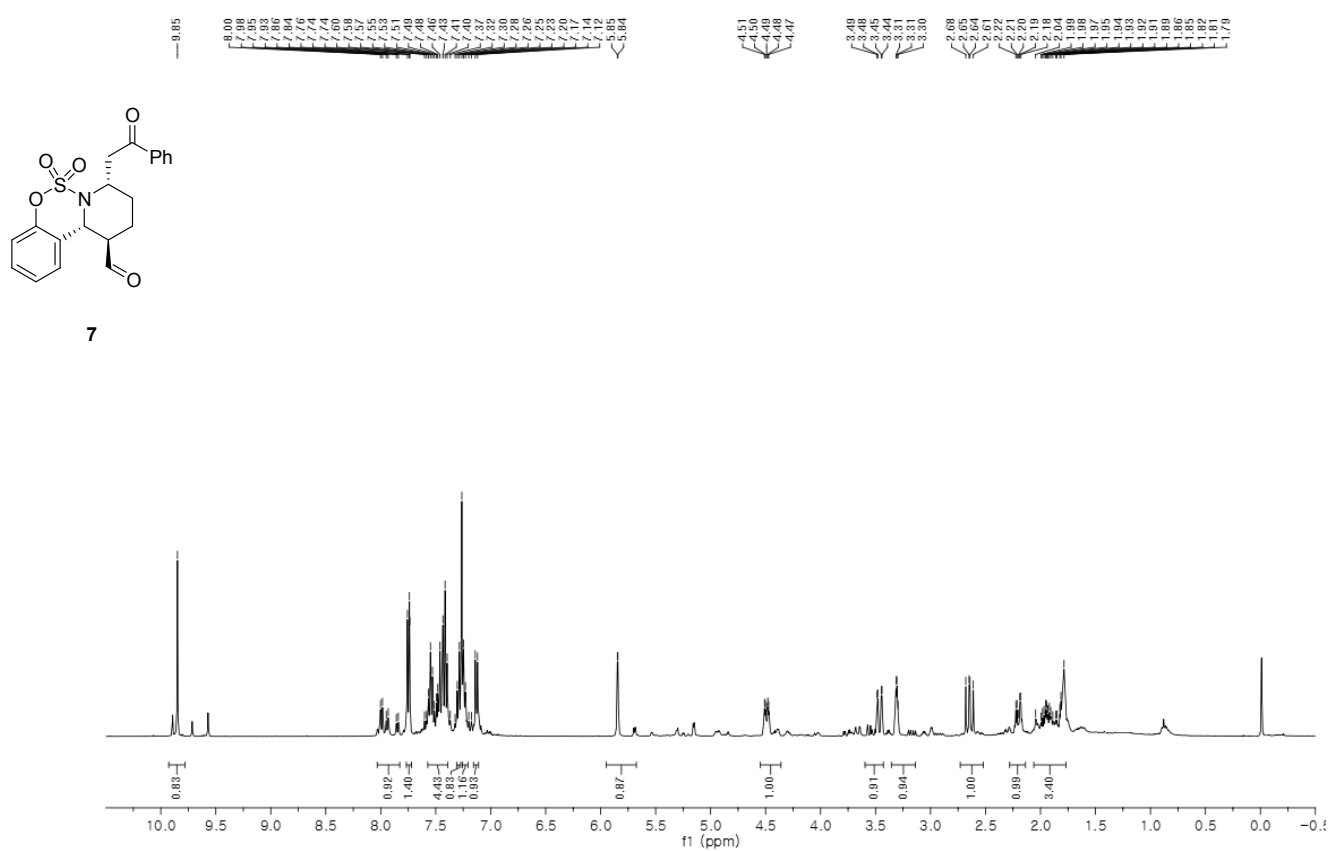
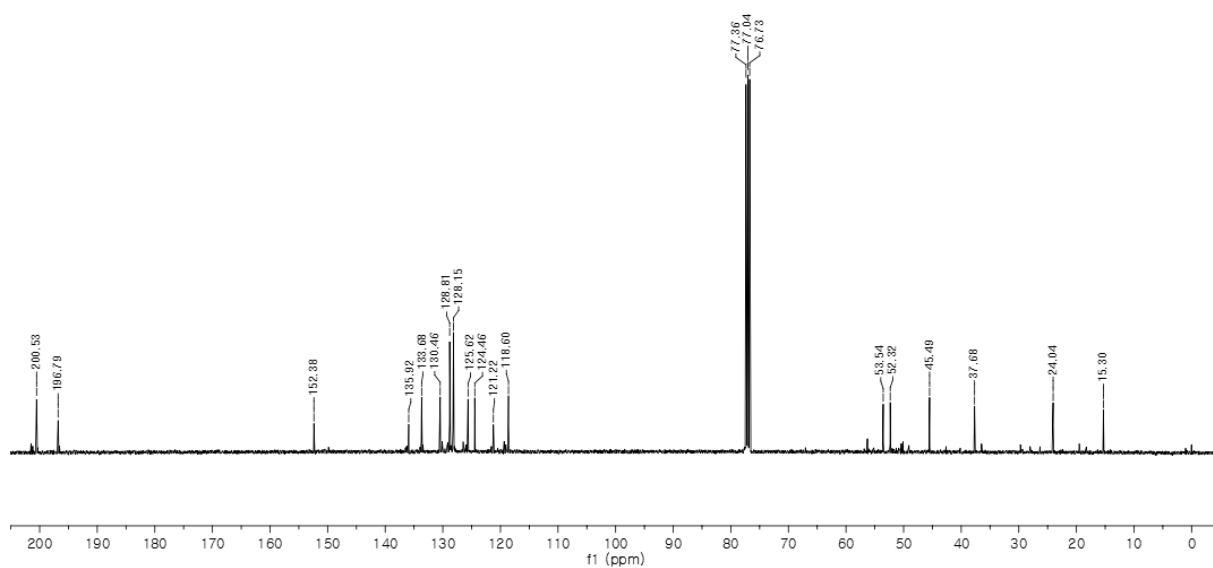
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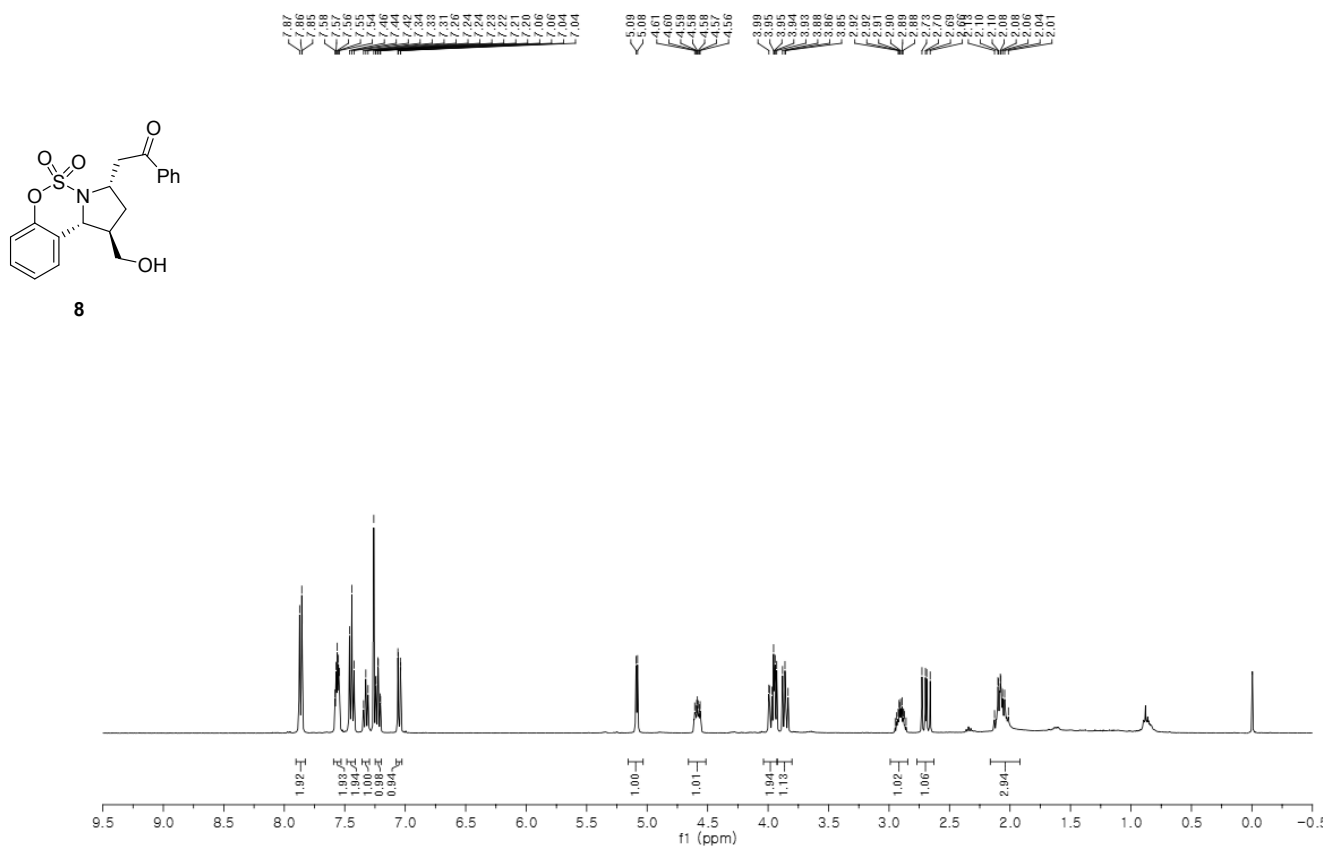
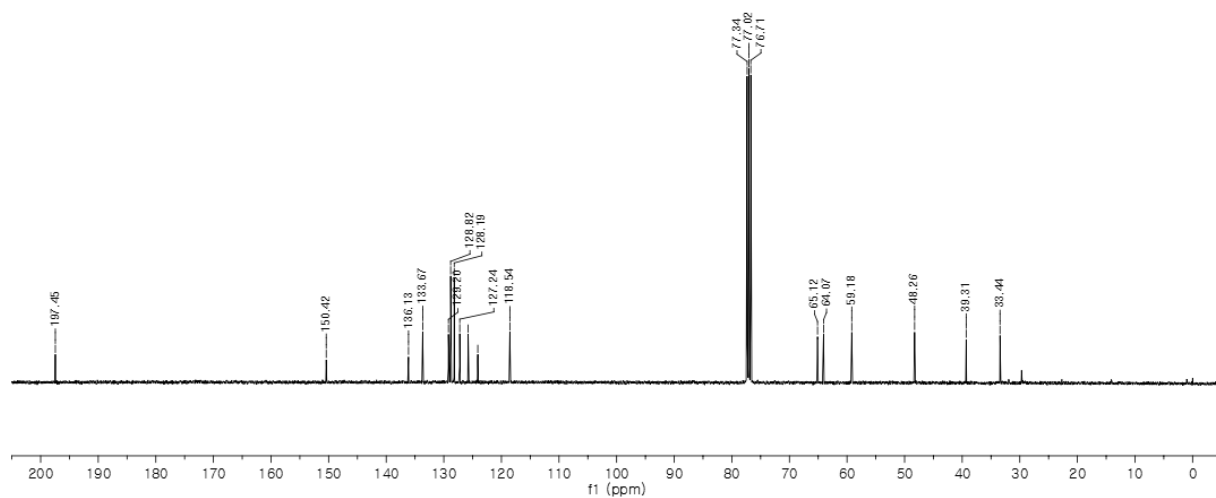
^1H NMR (400 MHz) in CDCl_3  **^{13}C NMR (100 MHz) in CDCl_3** 

^1H NMR (400 MHz) in CDCl_3  **^{13}C NMR (100 MHz) in CDCl_3** 



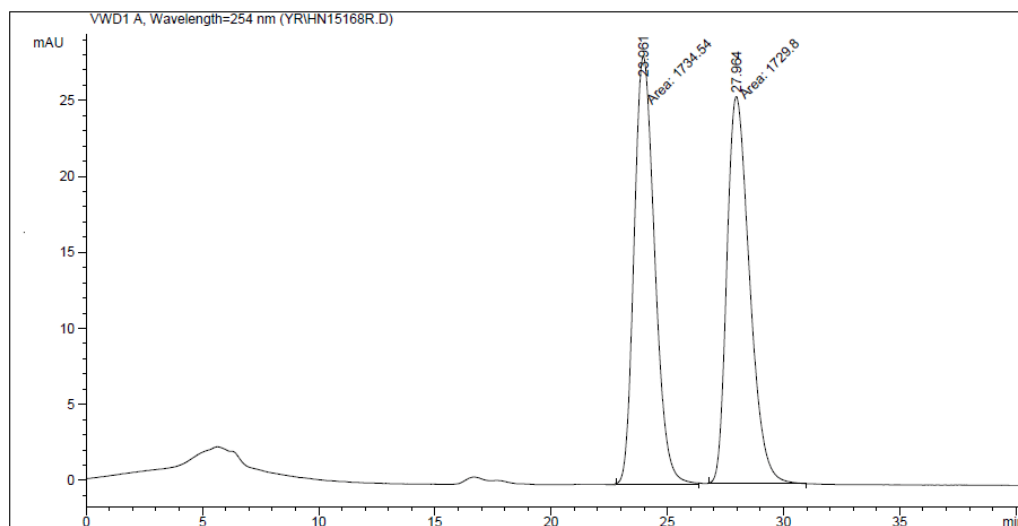
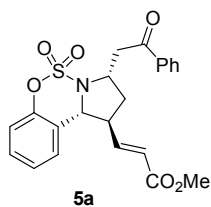
^1H NMR (400 MHz) in CDCl_3  **^{13}C NMR (100 MHz) in CDCl_3** 

¹H NMR (400 MHz) in CDCl₃**¹³C NMR (100 MHz) in CDCl₃**

^1H NMR (400 MHz) in CDCl_3  **^{13}C NMR (100 MHz) in CDCl_3** 

HPLC analysis

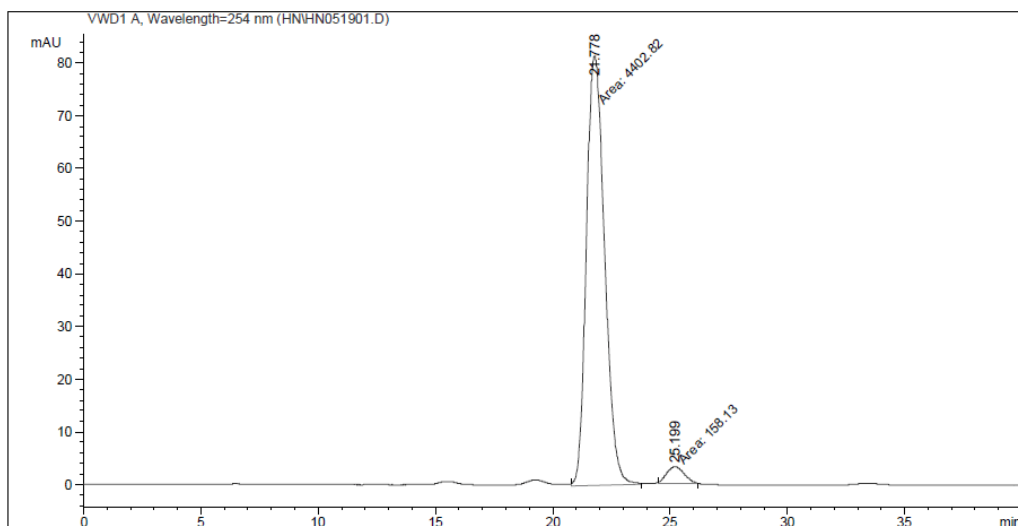
racemic



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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	23.961	MM	1.0263	1734.53796		28.16921	50.0684
2	27.964	MM	1.1312	1729.79736		25.48506	49.9316
Totals :				3464.33533		53.65427	

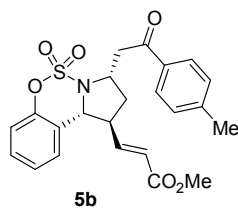
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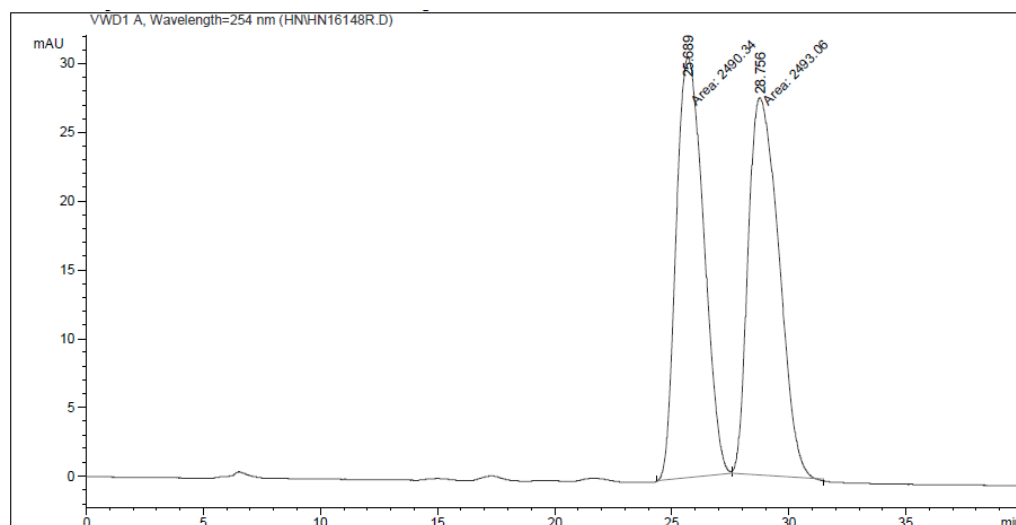
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Area Percent Report
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1	21.778	MM	0.9002	4402.82031		81.51640	96.5330
2	25.199	MM	0.8588	158.12971		3.06876	3.4670
Totals :				4560.95003		84.58515	

HPLC analysis



racemic

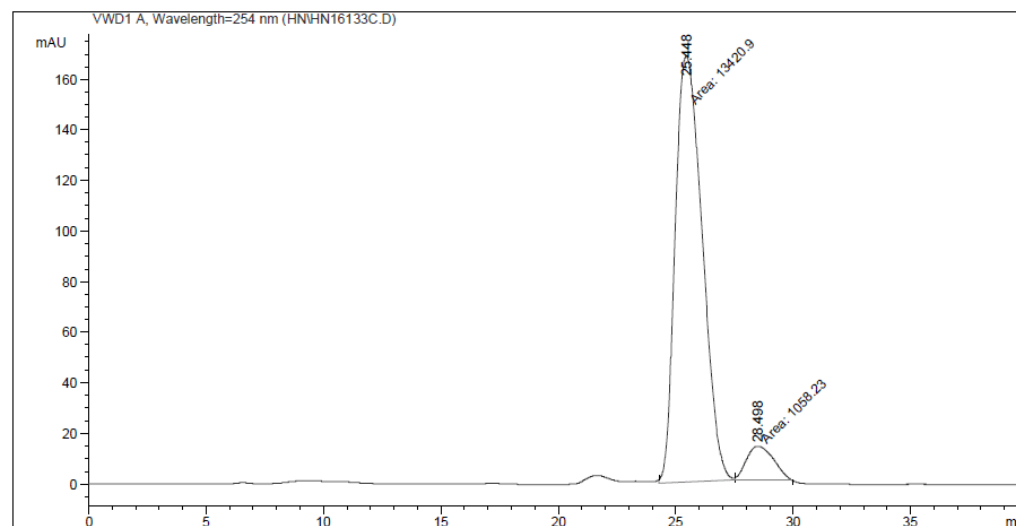


Area Percent Report

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	25.689	MM	1.3561	2490.33618		30.60761	49.9727
2	28.756	MM	1.5133	2493.05518		27.45744	50.0273

Totals : 4983.39136 58.06505

chiral



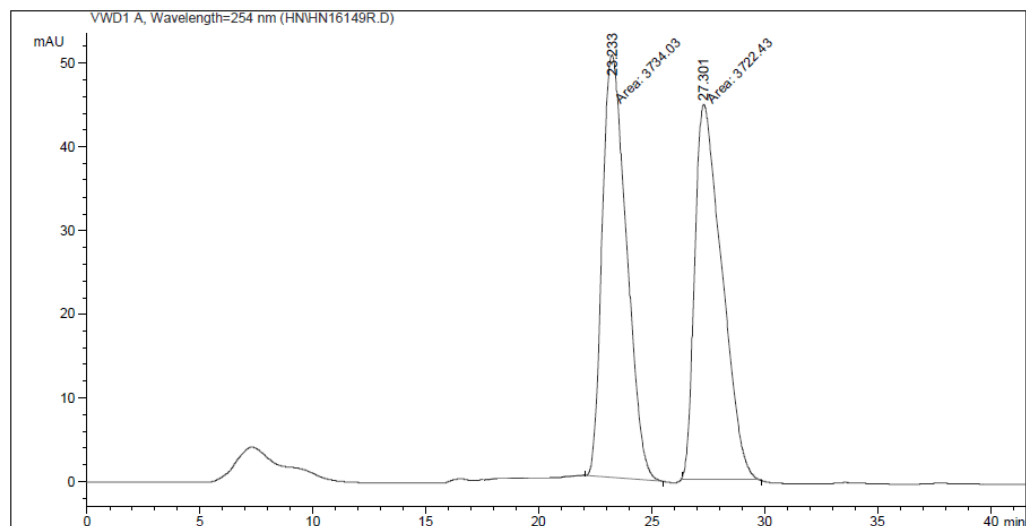
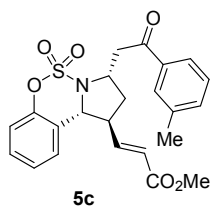
Area Percent Report

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
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2	28.498	MM	1.3351	1058.23267		13.21062	7.3087

Totals : 1.44791e4 181.64680

HPLC analysis

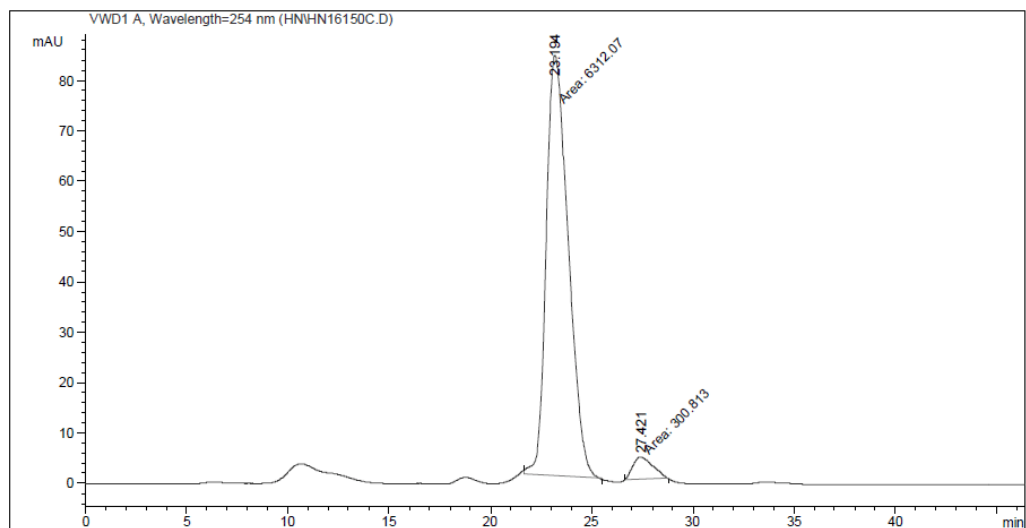
racemic



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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	23.233	MM	1.2342	3734.03369	50.42253	50.0778
2	27.301	MM	1.3835	3722.42700	44.84376	49.9222
Totals :				7456.46069	95.26629	

chiral

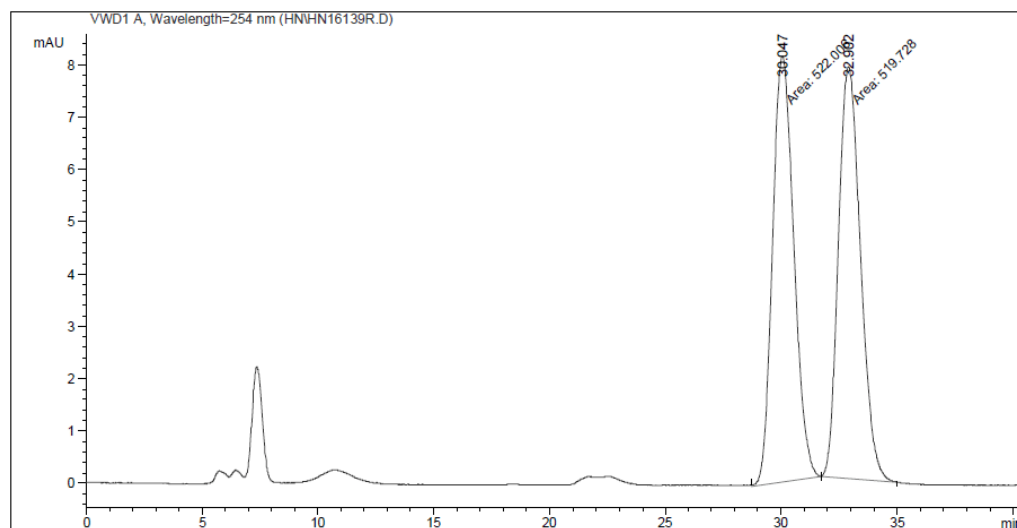
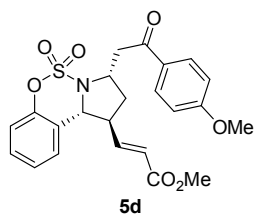


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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	23.194	MM	1.2610	6312.06836	83.42616	95.4511
2	27.421	MM	1.1445	300.81262	4.38066	4.5489
Totals :				6612.88098	87.80681	

HPLC analysis

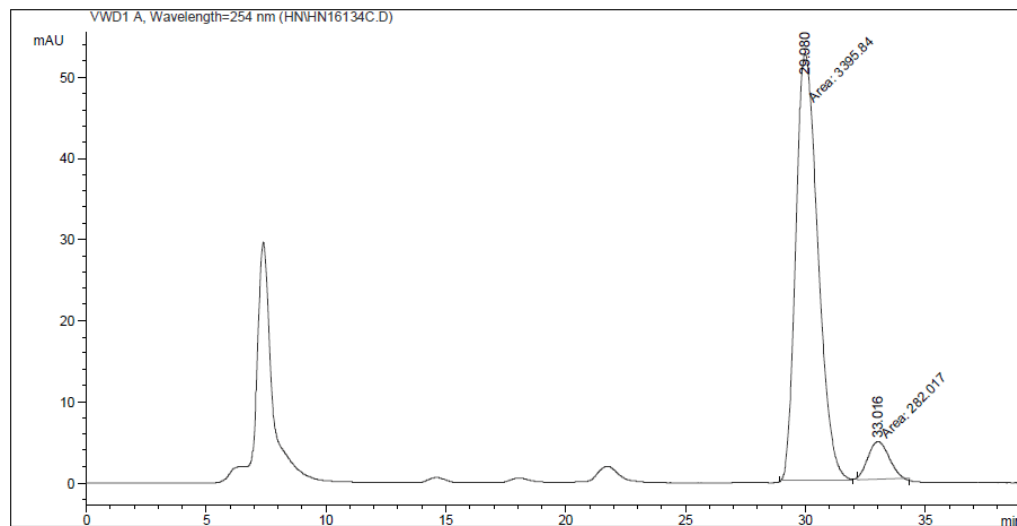
racemic



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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	30.047	MM	1.0683	522.00592		8.14361	50.1094
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Totals :				1041.73352		16.01267	

chiral

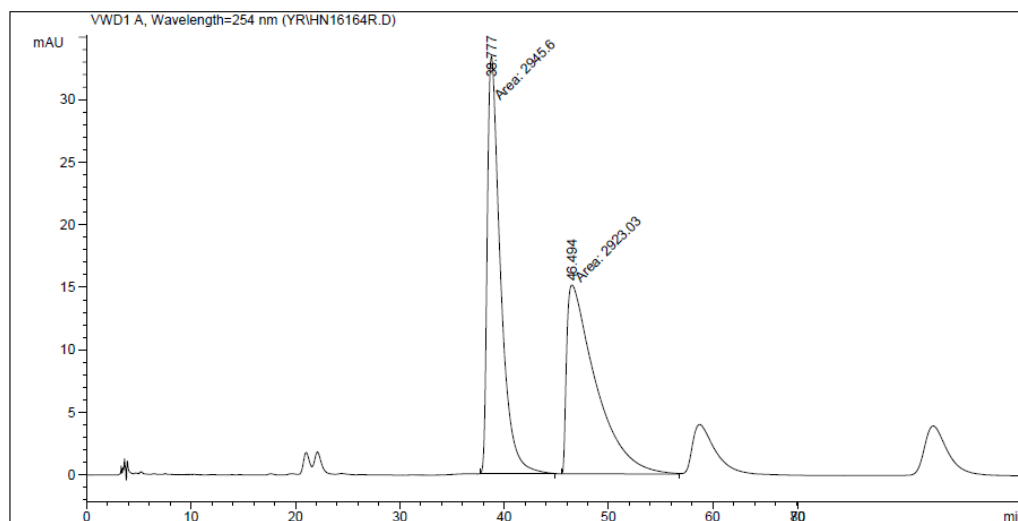
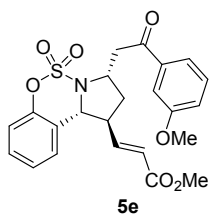


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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	29.980	MM	1.0742	3395.83643		52.68742	92.3320
2	33.016	MM	1.0146	282.01706		4.63265	7.6680
Totals :				3677.85349		57.32008	

HPLC analysis

racemic

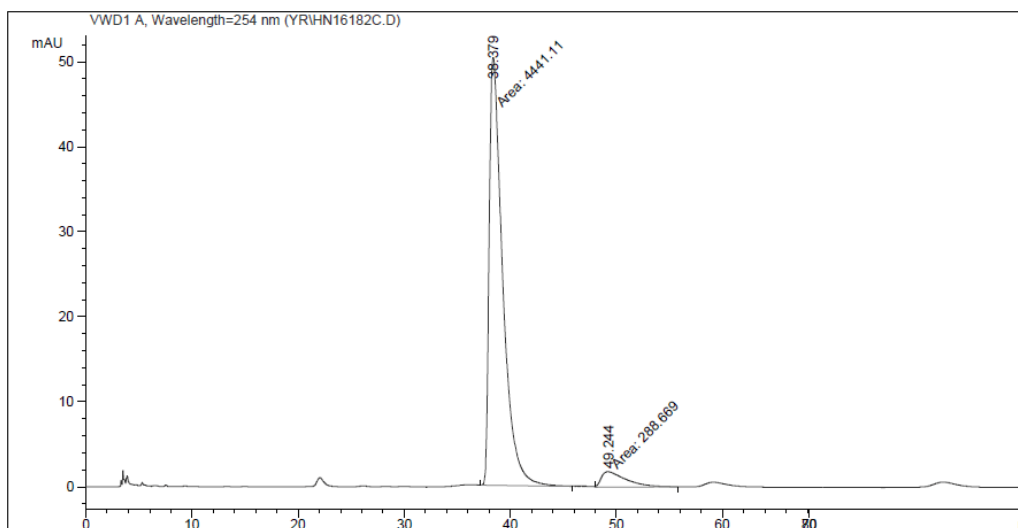


Area Percent Report

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]	Area %
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Totals : 5868.62109 48.44855

chiral



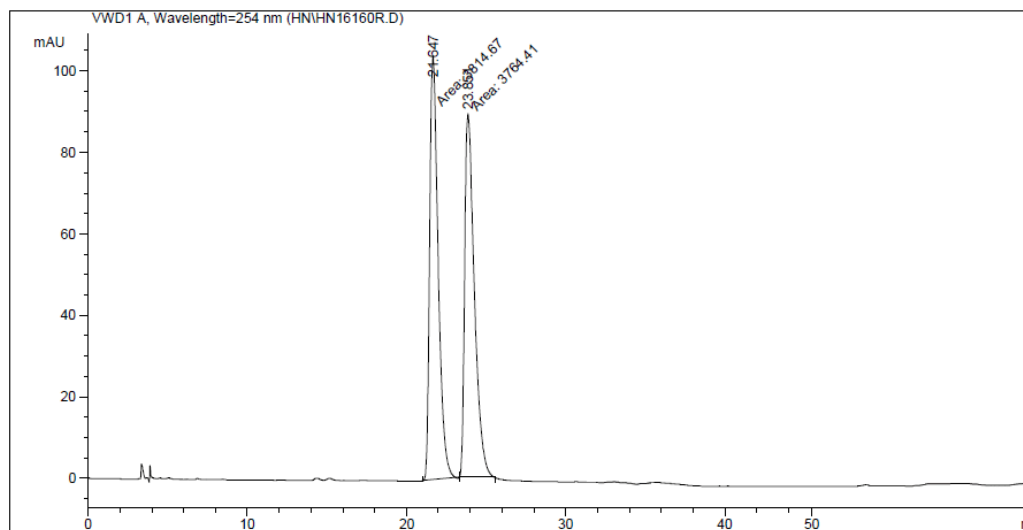
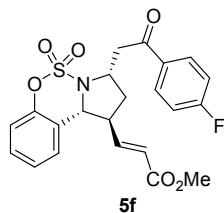
Area Percent Report

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Totals : 4729.78180 52.12272

HPLC analysis

racemic

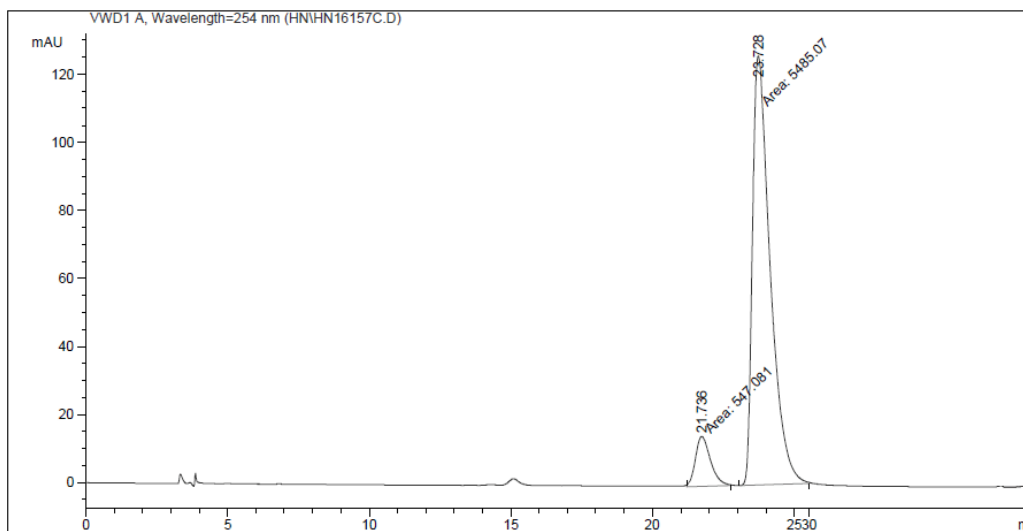


Area Percent Report

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]	Area %
1	21.647	MM	0.6114	3814.66675	50.3316	103.98962	
2	23.851	MM	0.7039	3764.40894	49.6684	89.12949	

Totals : 7579.07568 193.11912

chiral



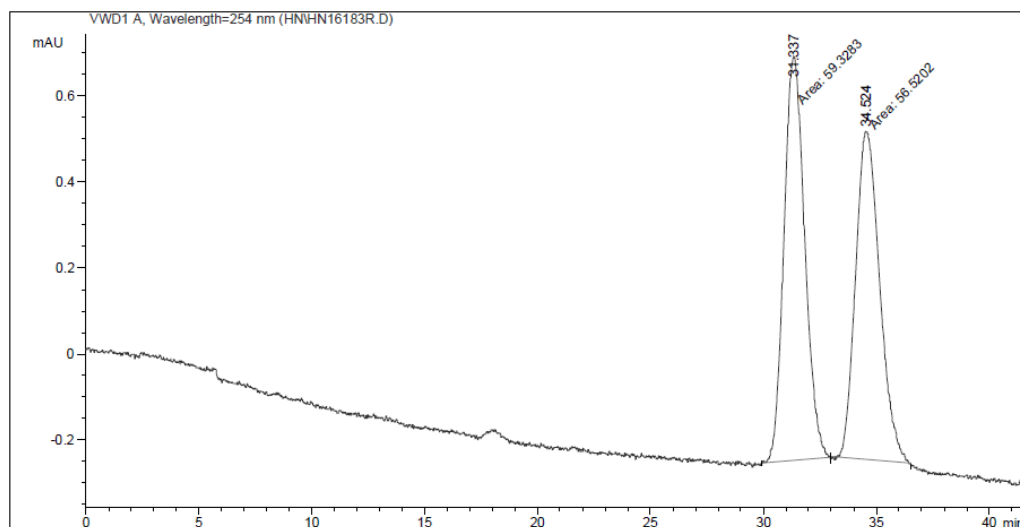
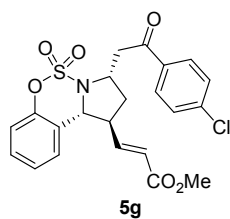
Area Percent Report

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]	Area %
1	21.736	MM	0.6209	547.08136	9.0694	14.68570	
2	23.728	MM	0.7245	5485.06689	90.9306	126.18525	

Totals : 6032.14825 140.87095

HPLC analysis

racemic

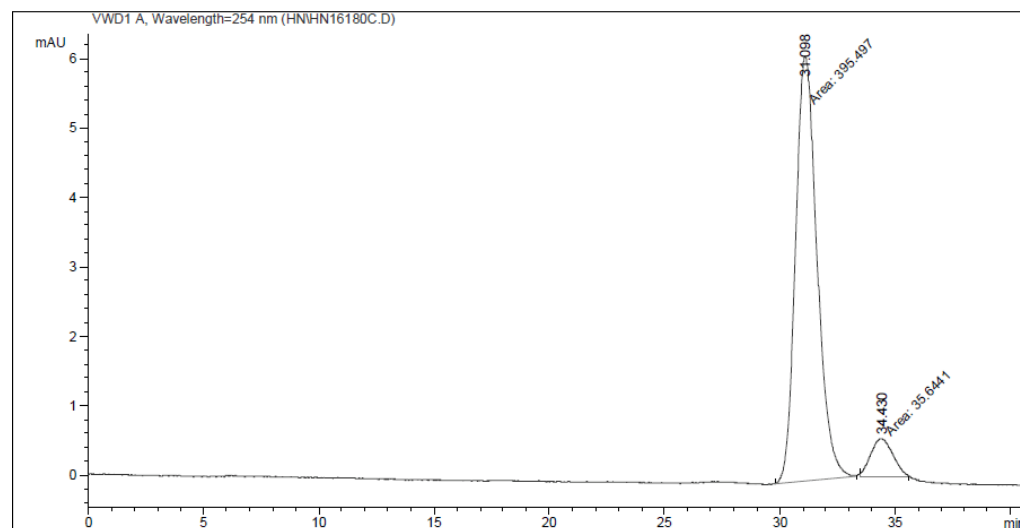


Area Percent Report

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	31.337	MM	1.0533	59.32825		9.38794e-1	51.2120
2	34.524	MM	1.2353	56.52019		7.62546e-1	48.7880

Totals : 115.84844 1.70134

chiral



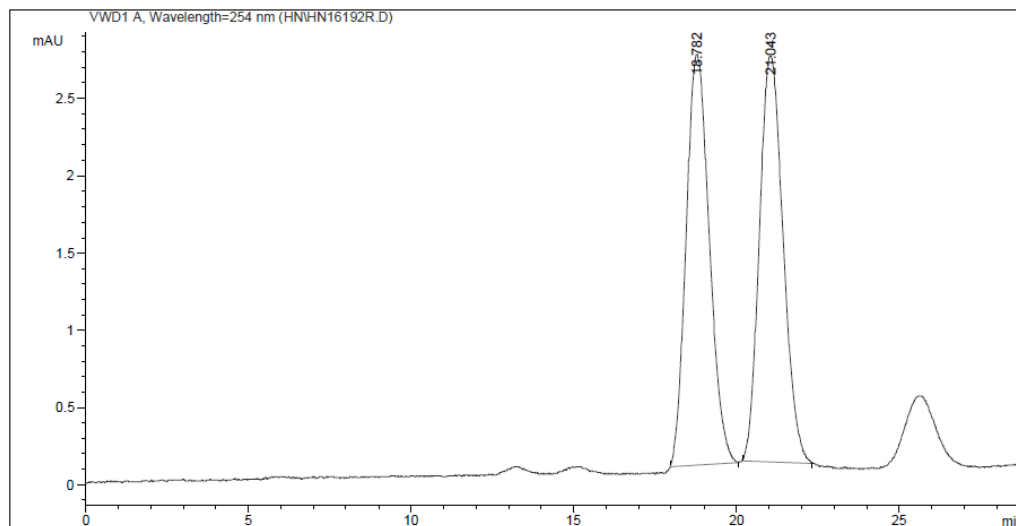
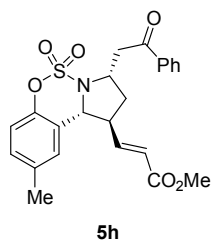
Area Percent Report

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	31.098	MM	1.0774	395.49719		6.11826	91.7326
2	34.430	MM	1.1040	35.64413		5.38125e-1	8.2674

Totals : 431.14132 6.65638

HPLC analysis

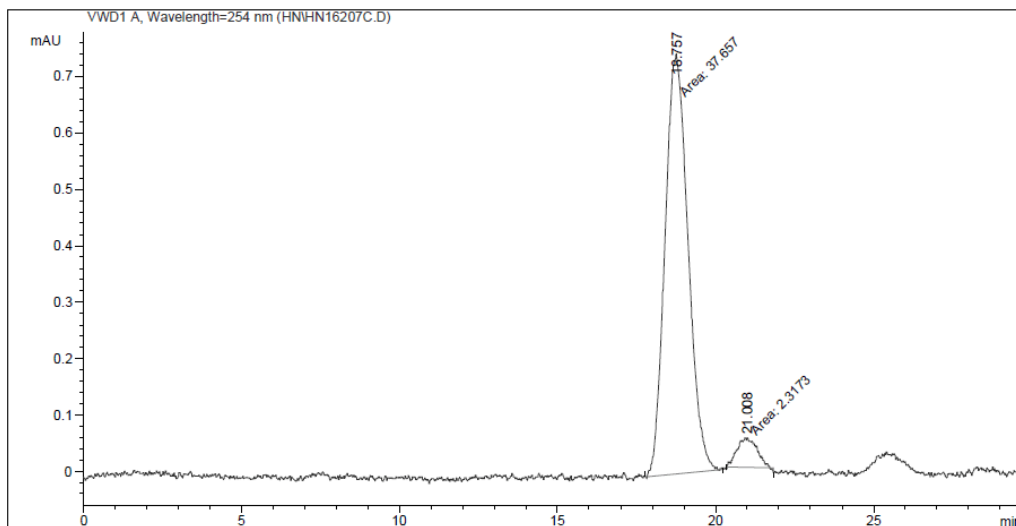
racemic



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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	18.782	BP	0.6681	132.05234		2.65933	49.8427
2	21.043	BB	0.6974	132.88559		2.62910	50.1573
Totals :				264.93793		5.28843	

chiral

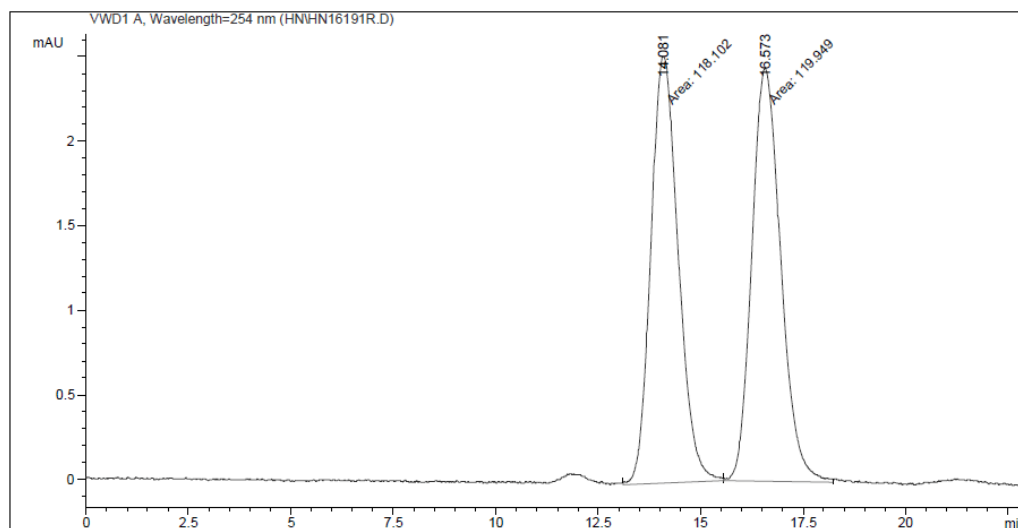
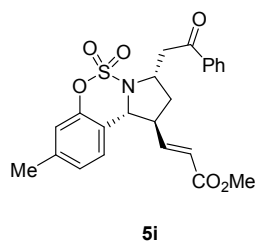


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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	18.757	MM	0.8428	37.65699		7.44645e-1	94.2030
2	21.008	MM	0.7341	2.31730		5.26099e-2	5.7970
Totals :				39.97429		7.97255e-1	

HPLC analysis

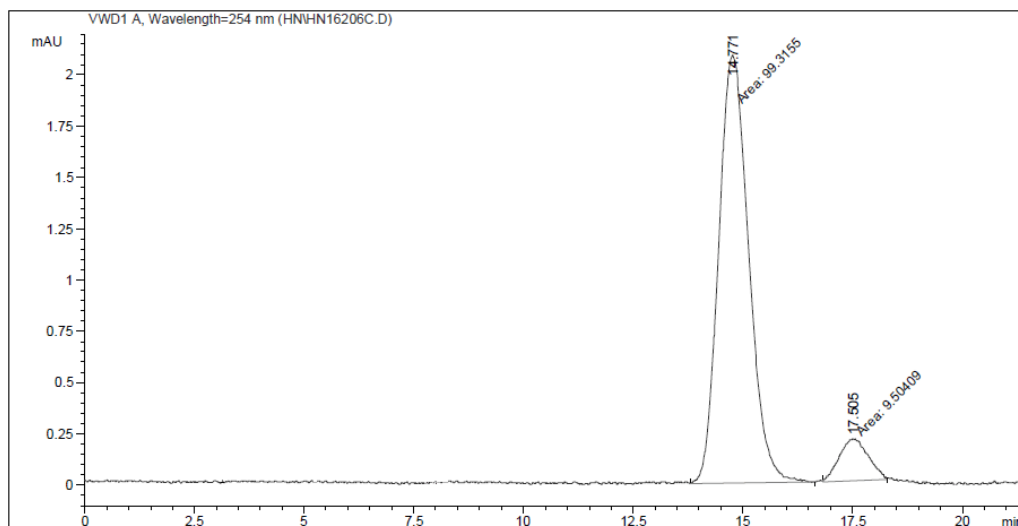
racemic



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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.081	MM	0.7791	118.10217	2.52653	49.6122
2	16.573	MM	0.8183	119.94852	2.44306	50.3878
Totals :				238.05070	4.96960	

chiral

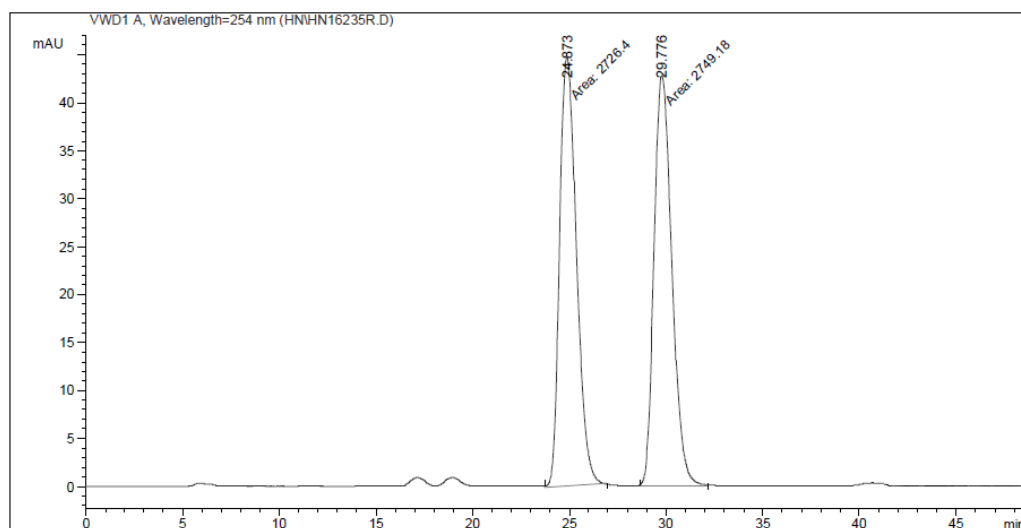
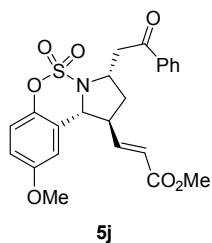


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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.771	MM	0.7927	99.31549	2.08820	91.2662
2	17.505	MM	0.7690	9.50409	2.05972e-1	8.7338
Totals :				108.81958	2.29418	

HPLC analysis

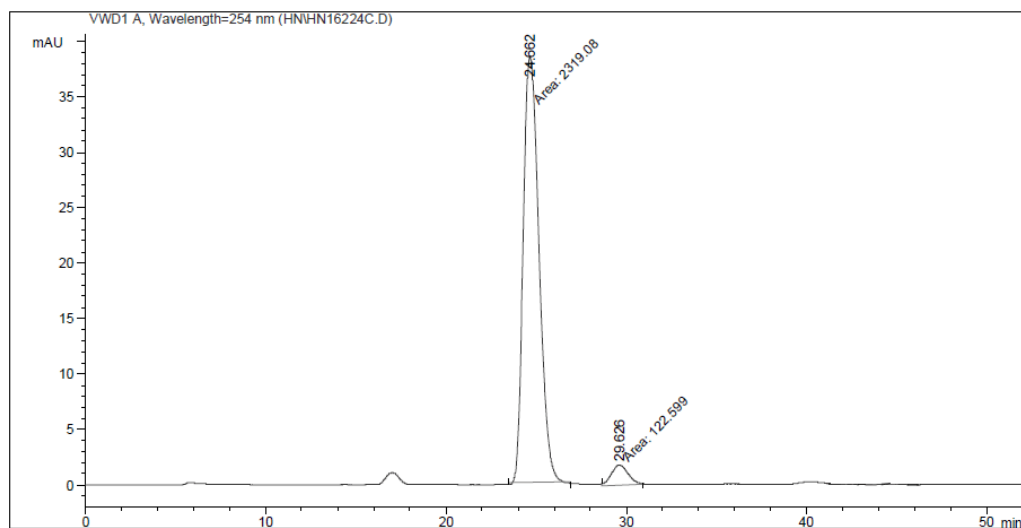
racemic



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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	24.873	MM	1.0165	2726.39819		44.70028	49.7920
2	29.776	MM	1.0709	2749.18018		42.78686	50.2080
Totals :				5475.57837		87.48713	

chiral

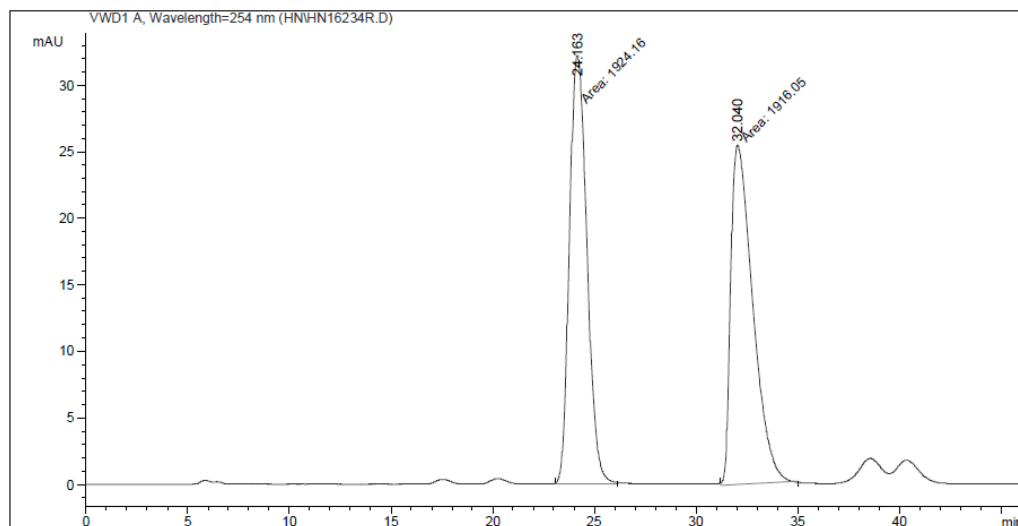
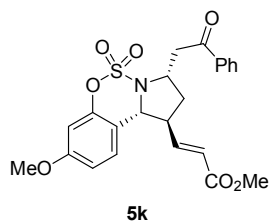


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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	24.662	MM	1.0056	2319.07886		38.43563	94.9789
2	29.626	MM	1.1135	122.59909		1.83500	5.0211
Totals :				2441.67795		40.27063	

HPLC analysis

racemic

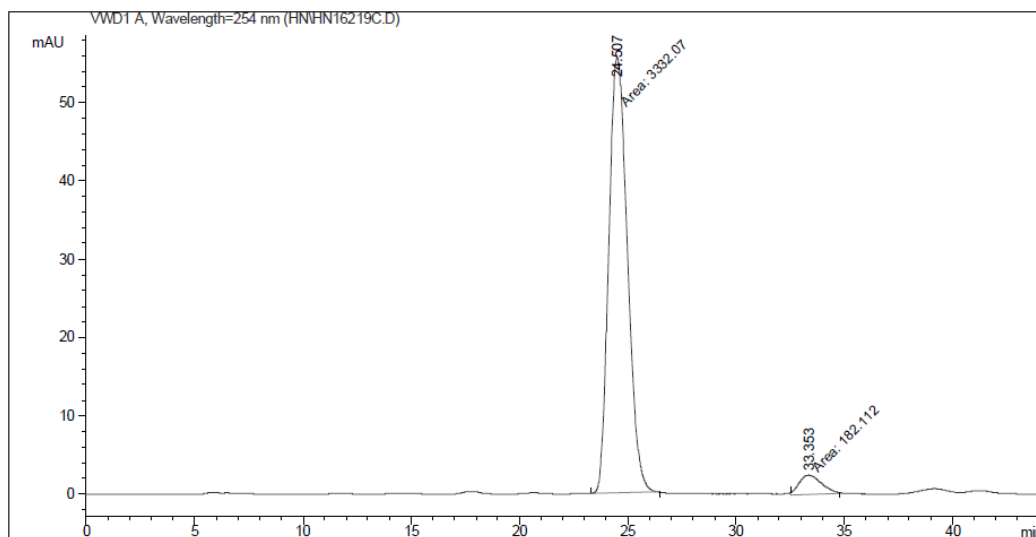


Area Percent Report

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	24.163	MM	0.9932	1924.16321		32.28959	50.1057
2	32.040	MM	1.2503	1916.04785		25.54020	49.8943

Totals : 3840.21106 57.82979

chiral



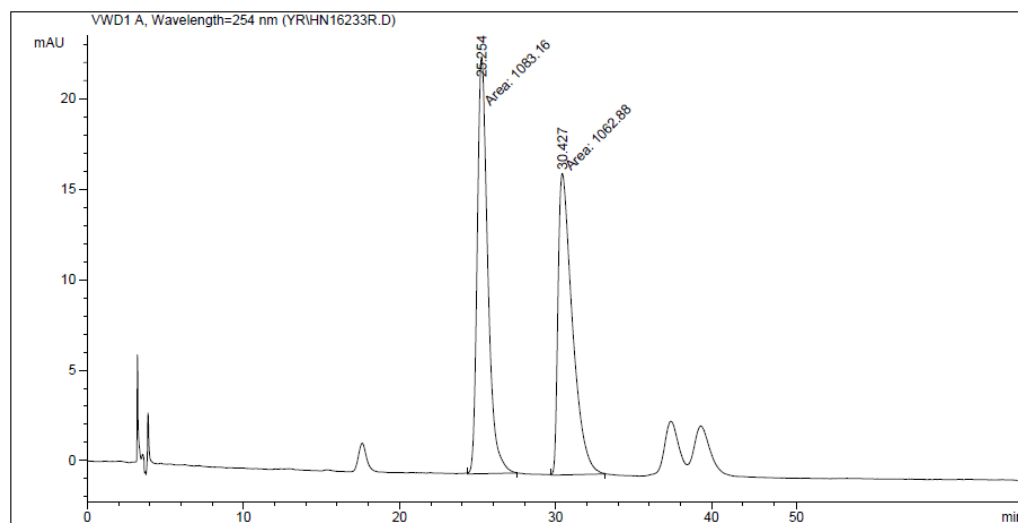
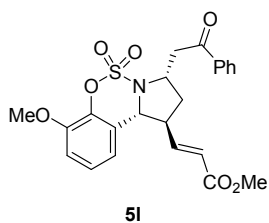
Area Percent Report

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	24.507	MM	0.9969	3332.07397		55.70707	94.8178
2	33.353	MM	1.2107	182.11192		2.50694	5.1822

Totals : 3514.18590 58.21400

HPLC analysis

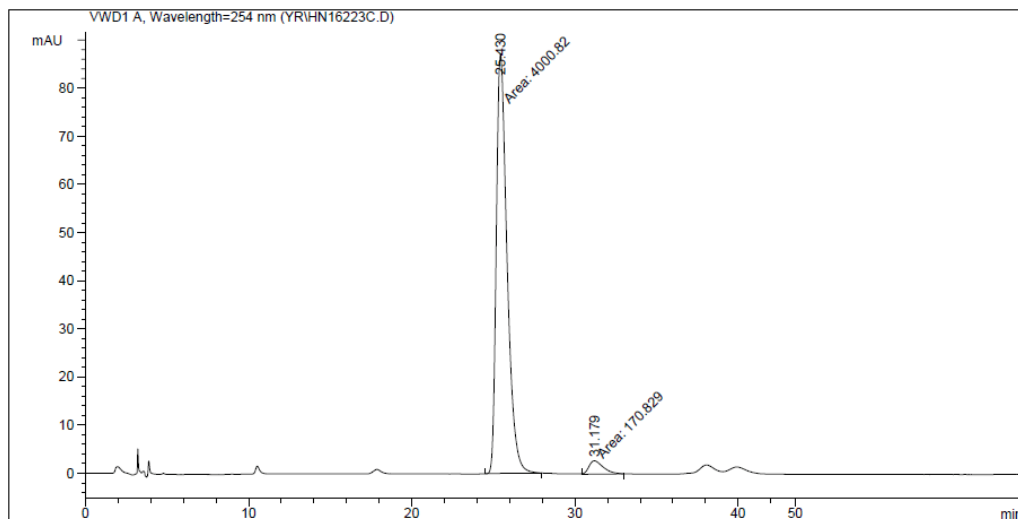
racemic



Area Percent Report

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]	Area %
1	25.254	MM	0.7826	1083.15979	50.4726	23.06693	50.4726
2	30.427	MM	1.0628	1062.87720	49.5274	16.66723	49.5274
Totals :				2146.03699	39.73415		

chiral

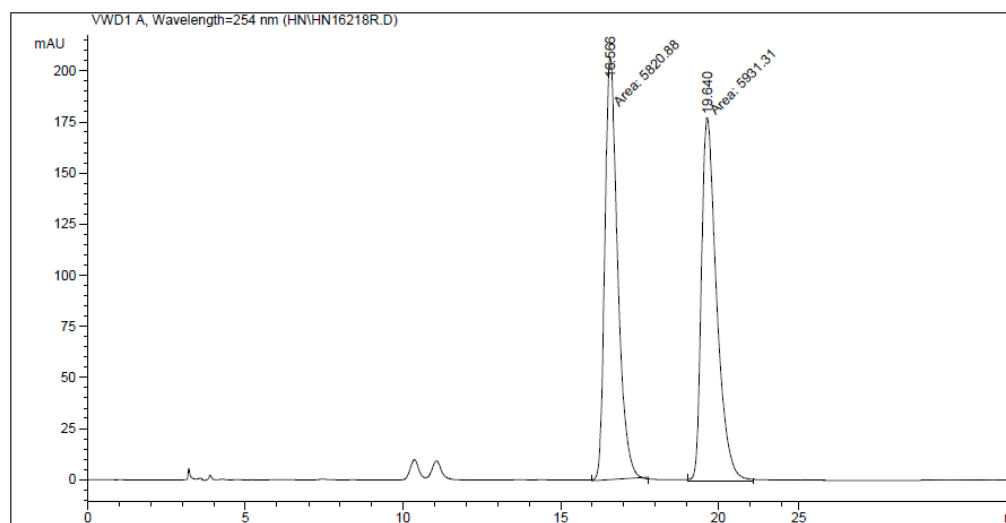
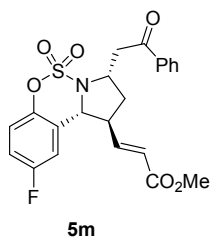


Area Percent Report

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]	Area %
1	25.430	MM	0.7650	4000.82349	95.9050	87.16438	95.9050
2	31.179	MM	1.0208	170.82895	4.0950	2.78900	4.0950
Totals :				4171.65244	89.95338		

HPLC analysis

racemic

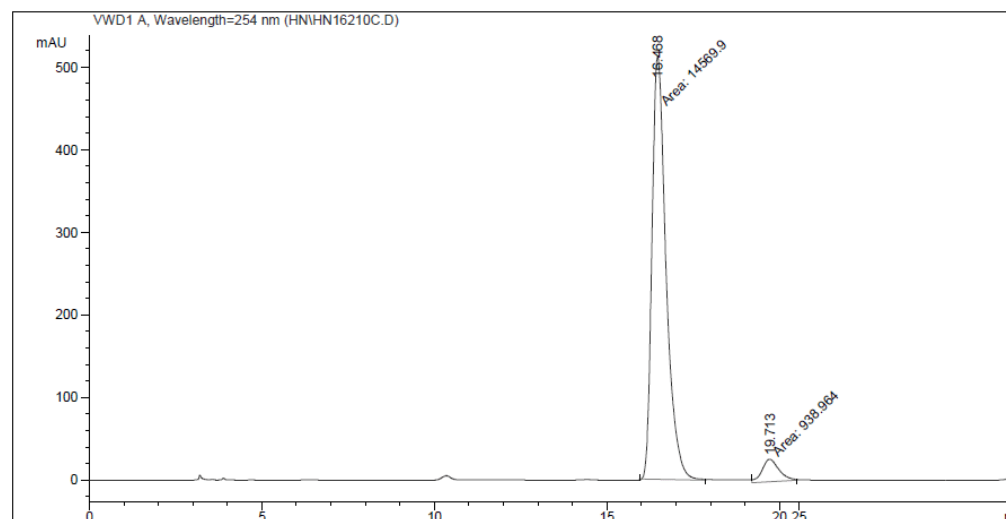


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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	16.566	MM	0.4692	5820.87500		206.75533	49.5301
2	19.640	MM	0.5565	5931.31152		177.62587	50.4699

Totals : 1.17522e4 384.38120

chiral



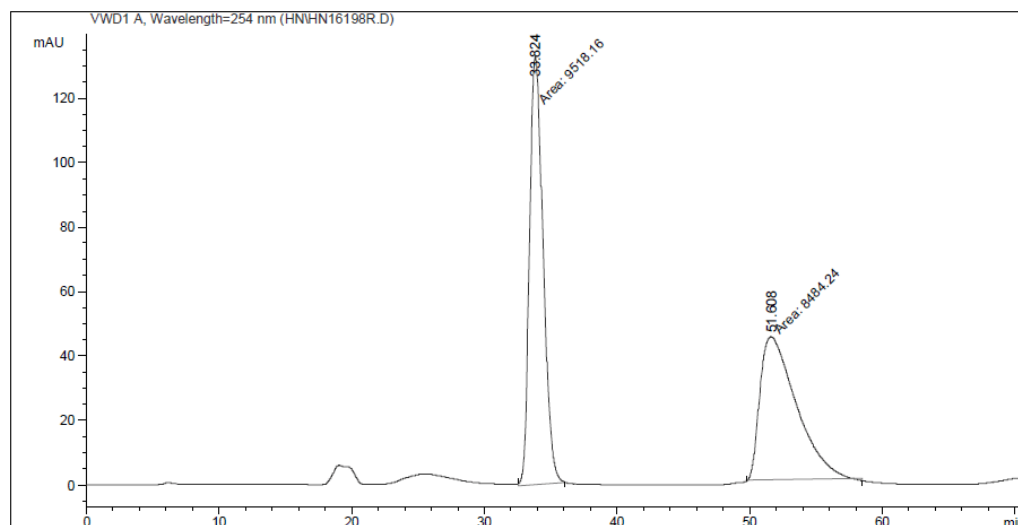
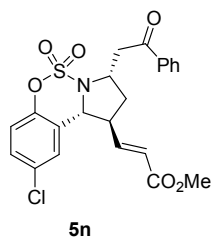
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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	16.468	MM	0.4740	1.45699e4		512.27533	93.9456
2	19.713	MM	0.5748	938.96405		27.22625	6.0544

Totals : 1.55088e4 539.50158

HPLC analysis

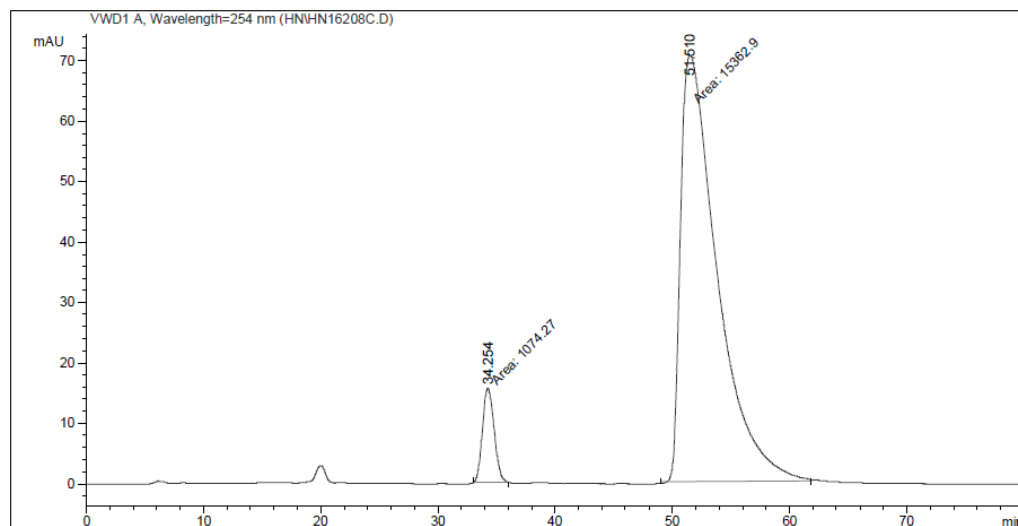
racemic



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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	33.824	MM	1.1914	9518.16016	133.14563	52.8716
2	51.608	MM	3.1858	8484.24023	44.38516	47.1284
Totals :				1.80024e4	177.53079	

chiral

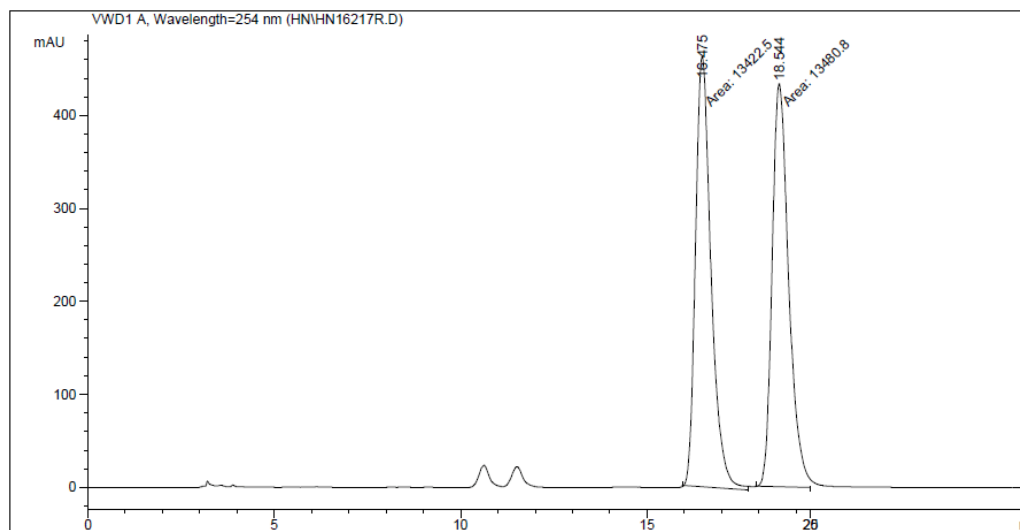
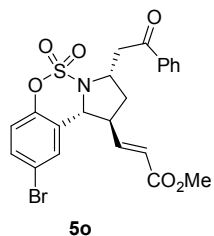


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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	34.254	MM	1.1497	1074.27258	15.57381	6.5356
2	51.510	MM	3.6300	1.53629e4	70.53585	93.4644
Totals :				1.64372e4	86.10966	

HPLC analysis

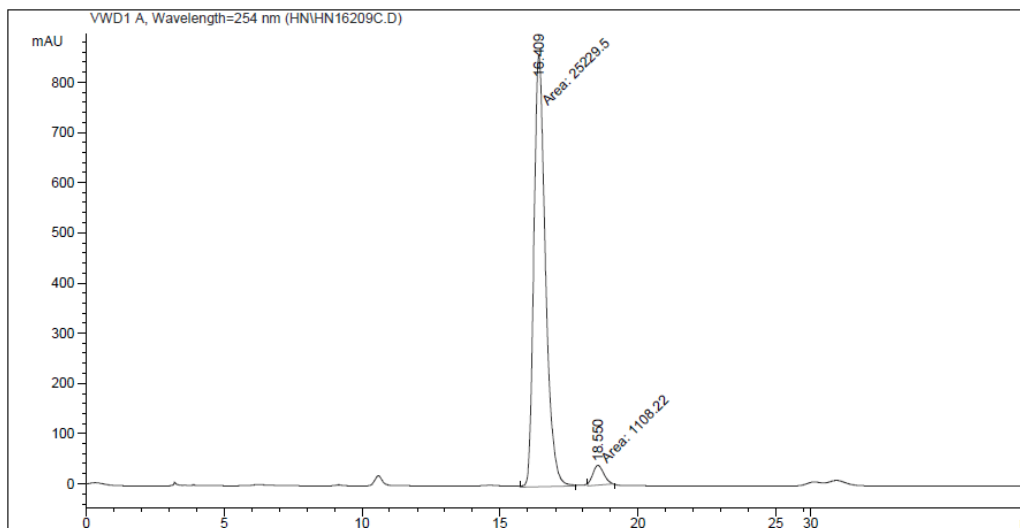
racemic



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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	16.475	MM	0.4833	1.34225e4		462.91742	49.8915
2	18.544	MM	0.5185	1.34808e4		433.29996	50.1085
Totals :				2.69033e4		896.21738	

chiral

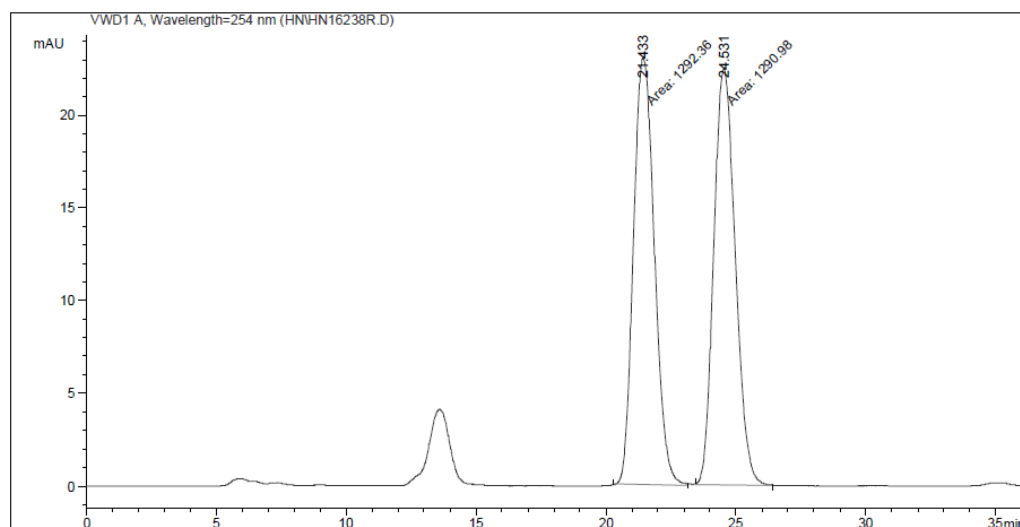
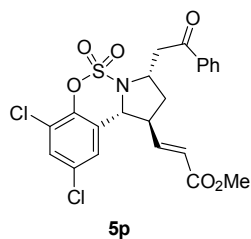


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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	16.409	MM	0.4889	2.52295e4		859.99896	95.7923
2	18.550	MM	0.4654	1108.22070		39.68834	4.2077
Totals :				2.63378e4		899.68730	

HPLC analysis

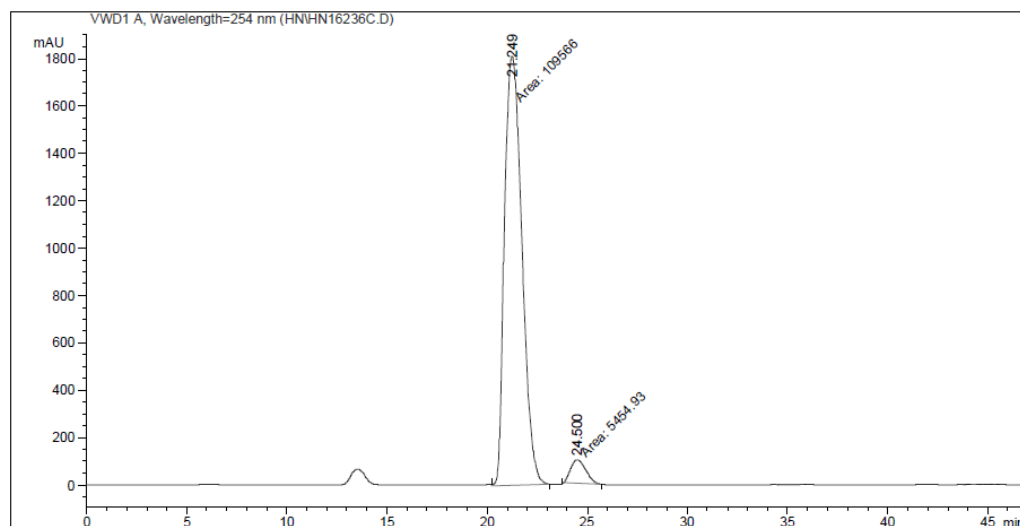
racemic



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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	21.433	MM	0.9334	1292.36169	23.07648	50.0268
2	24.531	MM	0.9591	1290.97632	22.43319	49.9732
Totals :				2583.33801	45.50967	

chiral

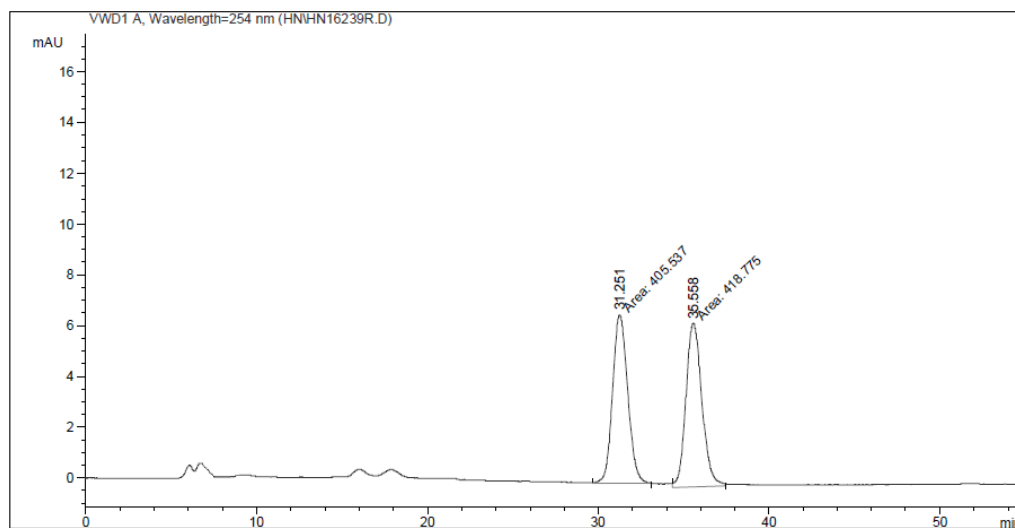
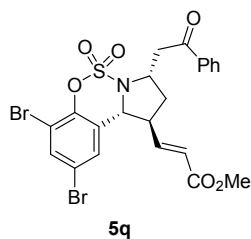


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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	21.249	MM	1.0079	1.09566e5	1811.83472	95.2574
2	24.500	MM	0.8991	5454.93359	101.11728	4.7426
Totals :				1.15021e5	1912.95200	

HPLC analysis

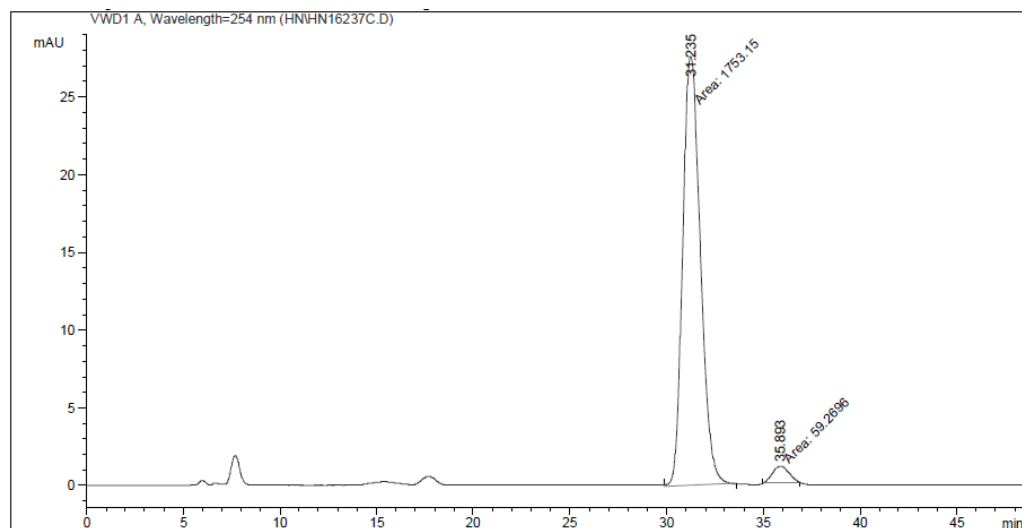
racemic



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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	31.251	MM	1.0193	405.53668		6.63088	49.1970
2	35.558	MM	1.0826	418.77460		6.44722	50.8030
Totals :				824.31128		13.07811	

chiral

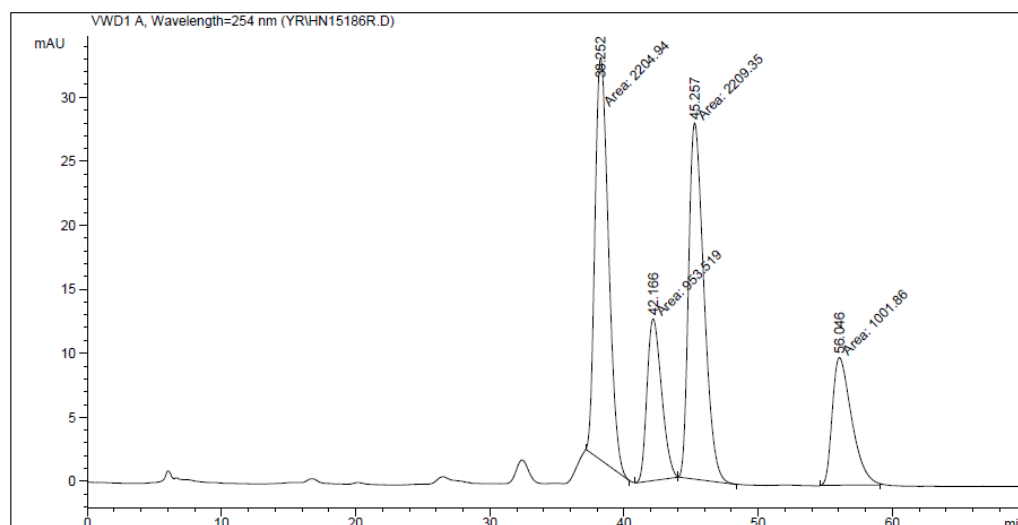
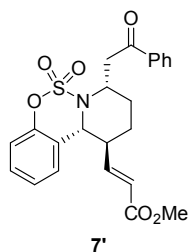


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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	31.235	MM	1.0564	1753.14709		27.65951	96.7298
2	35.893	MM	0.9531	59.26964		1.03646	3.2702
Totals :				1812.41674		28.69597	

HPLC analysis

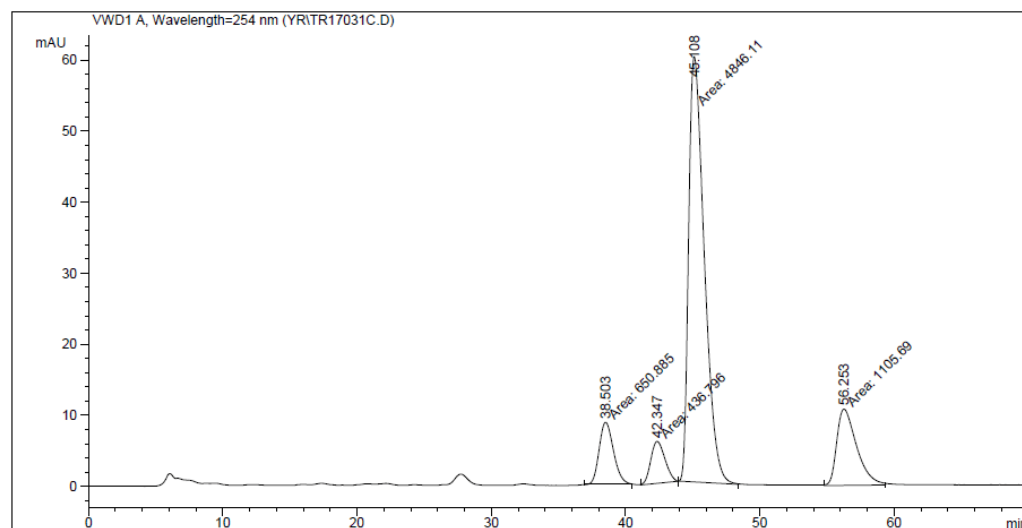
racemic



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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	38.252	MM	1.1691	2204.93848		31.43232	34.6163
2	42.166	MM	1.2563	953.51855		12.65013	14.9697
3	45.257	MM	1.3229	2209.34888		27.83367	34.6855
4	56.046	MM	1.6743	1001.85608		9.97259	15.7286
Totals :				6369.66199		81.88872	

chiral



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Area Percent Report
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Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	38.503	MM	1.2395	650.88489		8.75218	9.2462
2	42.347	MM	1.2268	436.79605		5.93392	6.2049
3	45.108	MM	1.3490	4846.11426		59.87284	68.8419
4	56.253	MM	1.7148	1105.68701		10.74623	15.7069
Totals :				7039.48221		85.30517	