Supporting Information

Catalytic Asymmetric Conjugate Addition and Sulfenylation of Diarylthiazolidin-2,4-Diones

Lihui Jiao,[†] Liwei Bu,[†] Xinyi Ye,[‡] Xiaowei Zhao,[†] and Zhiyong Jiang*[,†]

[†]*Key Laboratory of Natural Medicine and Immuno-Engineering of Henan Province, Henan University, Kaifeng, Henan, P. R. China, 475004*

[‡]*Division of Chemistry and Biological Chemistry, Nanyang Technological University, 21 Nanyang Link, 637371, Singapore*

E-mail: chmjzy@henu.edu.cn

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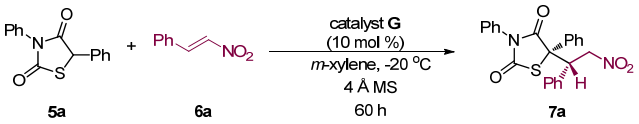
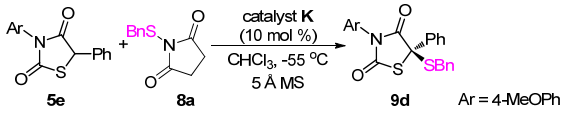
Table S1. Investigation on the effect of additives

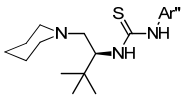


5a 6a 7a

entry	additive	*ee* (%)	dr
1	K_2HPO_4	77/1	87:13
2	Na_2HPO_4	73/7	85:15
3	KH_2PO_4	77/6	87:13
4	NaH_2PO_4	77/8	85:15
5	K_3PO_4	53/9	71:29
6	Na_3PO_4	17/21	62:38
7	$NaPF_6$	20/0	66:34
8	LiF	77/0	88:12
9	NaF	76/8	90:10
10	KF	73/6	88:12
11	NaBr	86/14	94:6
12	NaI	81/1	91:9
13	$PhSO_2Na$	80/2	93:7
14	NH_4Cl	62/0	77:23
15	LiCl	85/6	91:9
16	NaCl	89/4	90:10

Table S2. Optimization of the reaction conditions of sulfenylation[a]





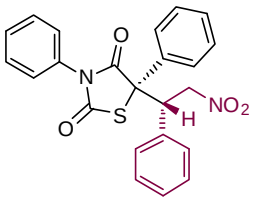
H: Ar" = 3,5-$(CF_3)_2$Ph
I: Ar" = 3,5-$(OCH_3)_2$Ph
J: Ar" = 3,5-F_2Ph
K: Ar" = 4-MeOPh
L: Ar" = 4-*t*BuPh

M: Ar" = 4-ClPh
N: Ar" = 3-ClPh
O: Ar" = 2-ClPh
P: Ar" = Ph

entry	cat.	solvent	additive	*T* (°C)	*ee* (%)
1	**H**	CH_2Cl_2	--	25	40
2	**H**	toluene	--	25	12
3	**H**	THF	--	25	12
4	**H**	Et_2O	--	25	20
5	**H**	DCE	--	25	42
6	**H**	$CHCl_3$	--	25	32
7	**H**	DCE	--	10	50
8	**H**	DCE	--	0	55
9	**H**	DCE	--	−10	64
10	**H**	DCE	--	−20	60
11	**I**	DCE	--	−10	73
12	**J**	DCE	--	−10	67
13	**K**	DCE	--	−10	74
14	**L**	DCE	--	−10	72
15	**M**	DCE	--	−10	73
16	**N**	DCE	--	−10	70
17	**O**	DCE	--	−10	69
18	**P**	DCE	--	−10	72
19	**K**	CH_2Cl_2	--	−10	68
20	**K**	THF	--	−10	59
21	**K**	DCE	--	−20	76
24	**K**	DCE	--	−30	78
25	**K**	DCE	--	−40	79
26	**K**	DCE	--	−50	79
27	**K**	DCE	--	−60	72
28	**K**	DCE	--	−70	67
29	**K**	CH_2Cl_2	--	−40	78
30	**K**	$CHCl_3$	--	−40	82
31	**K**	$CHCl_3$	5 Å MS	−40	86
32[b]	**K**	$CHCl_3$	5 Å MS	−55	91

[a]**5e**:**8a** = 1:1.2. [b]**5e**:**8a** = 1:2.0

2. Copies of HPLC spectra



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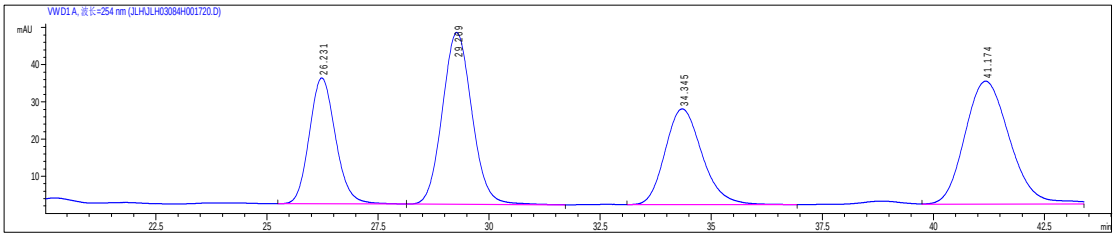
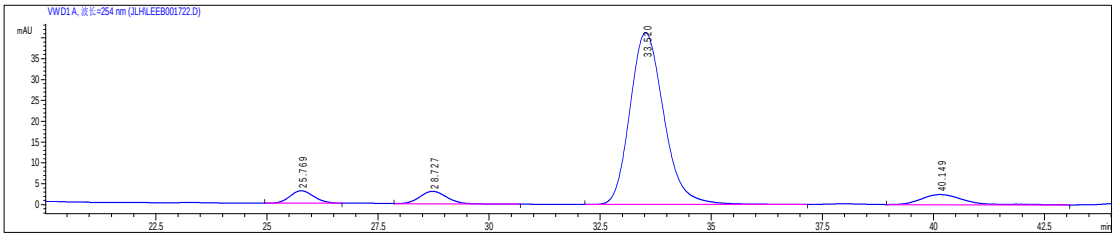
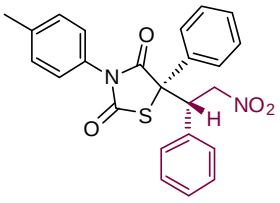


Entry	Retention Time	Area	Height	%Area
1	26.231	1386.2	33.8	19.281
2	29.269	2129.9	46.2	29.625
3	34.347	1455.8	25.5	20.249
4	41.174	2217.6	32.7	30.845



Entry	Retention Time	Area	Height	%Area
1	25.77	110	3	4.348
2	28.728	117.1	2.9	4.631
3	33.518	2169.4	41.2	85.775
4	40.16	132.7	2.3	5.247



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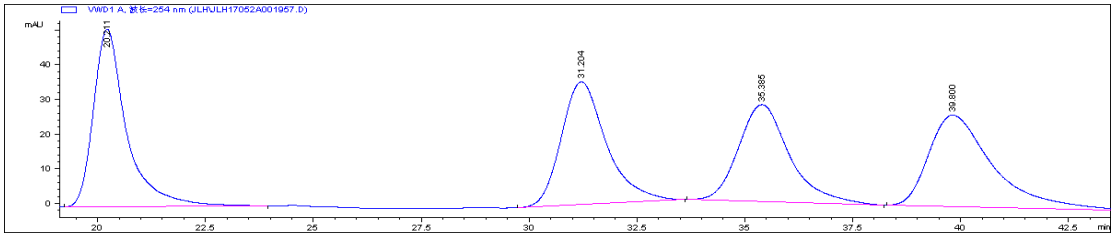
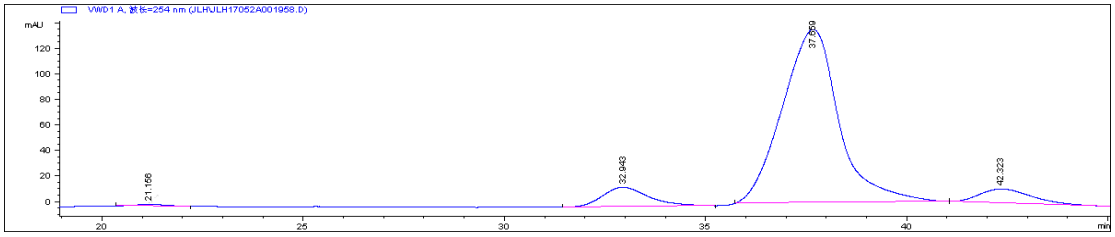
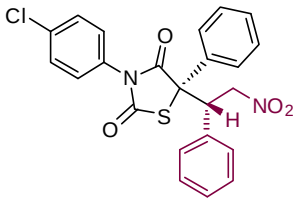


Entry	Retention Time	Area	Height	%Area
1	20.211	2740.1	51.2	26.411
2	31.204	2573.5	35.4	24.805
3	35.385	2305.2	28	22.220
4	39.8	2756	26.5	26.564



Entry	Retention Time	Area	Height	%Area
1	21.156	90.2	1.6	0.581
2	32.943	1206	15.2	7.762
3	37.659	13250.4	135.6	85.282
4	42.323	990.4	10.9	6.375



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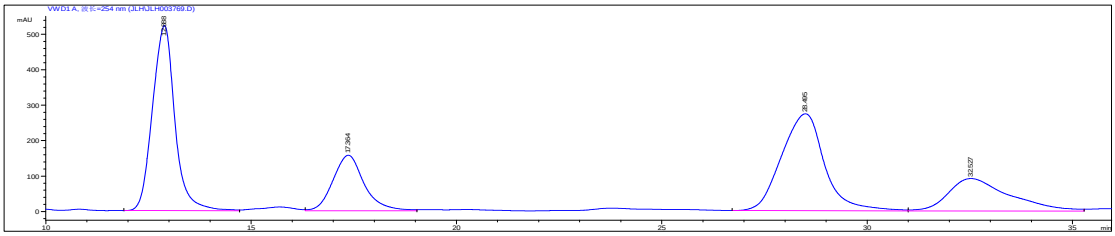
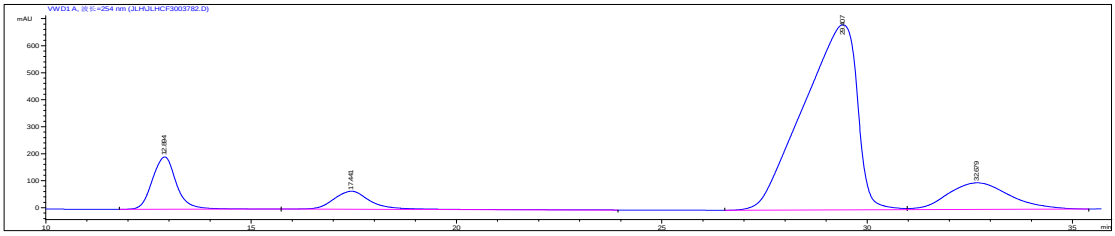


Entry	Retention Time	Area	Height	%Area
1	12.888	19735.9	522.3	35.504
2	17.365	7892.7	154.4	14.199
3	28.495	19554	272.5	35.177
4	32.527	8405.1	87.8	15.120



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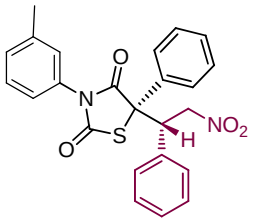
1	12.895	7571.7	192	9.110
2	17.443	3634.6	64.2	4.373
3	29.407	62218.8	685.2	74.860
4	32.68	9688.4	96.1	11.657



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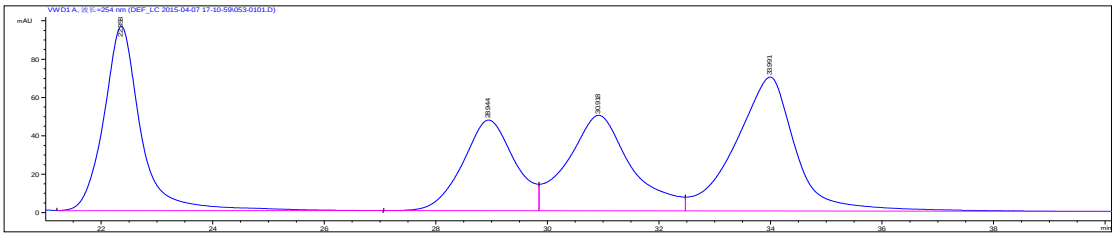
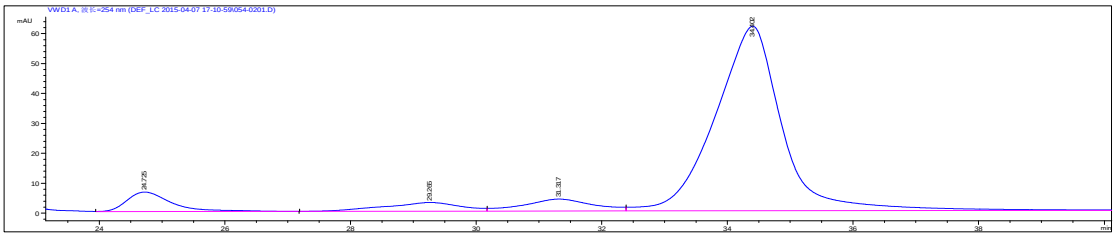
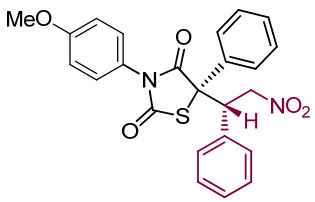


Entry	Retention Time	Area	Height	%Area
1	24.725	322	6.5	5.894
2	29.265	237.9	2.9	4.354
3	31.317	301.6	4	5.520
4	34.402	4601.7	61.7	84.231



Entry	Retention Time	Area	Height	%Area
1	22.358	4436.1	96.2	26.579
2	28.944	2725.2	44.2	20.438
3	30.918	3023.8	43.7	22.678
4	33.991	5260.5	69.9	31.519



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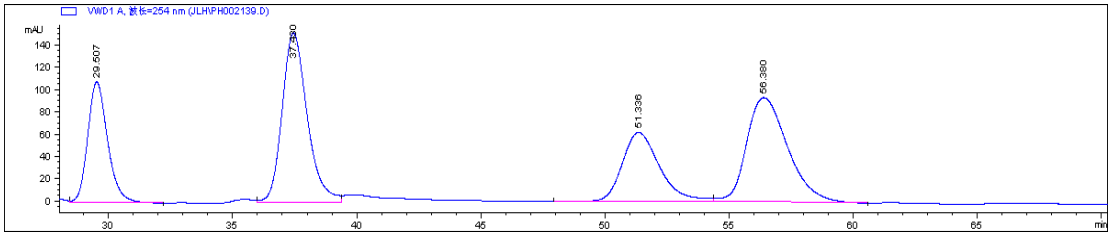
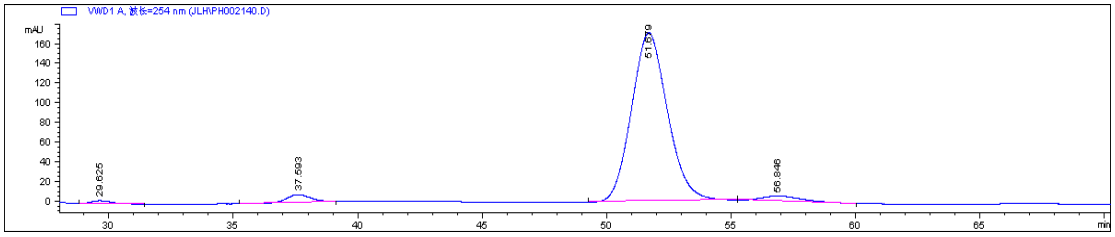


Entry	Retention Time	Area	Height	%Area
1	29.507	6093	108.6	17.689
2	37.43	10808.8	152.6	31.380
3	51.336	6618.3	62.3	19.214
4	56.38	10925	94.1	31.717



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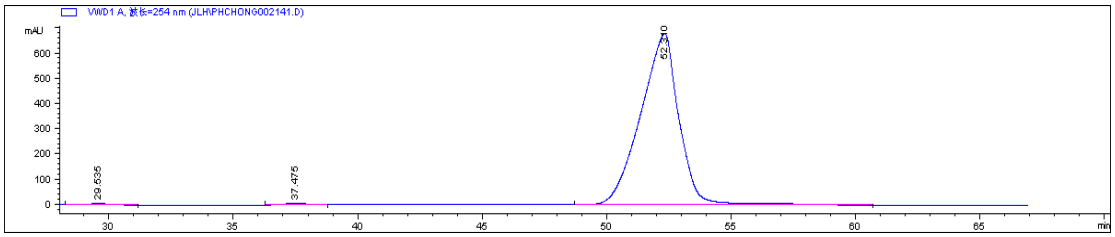
1	29.625	188.1	3.2	1.018
2	37.592	518	7.7	2.805
3	51.679	17181.8	170.9	93.044
4	56.845	578.5	5.2	3.133



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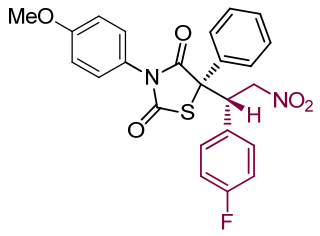
3	52.310	72596.9	678	100.000



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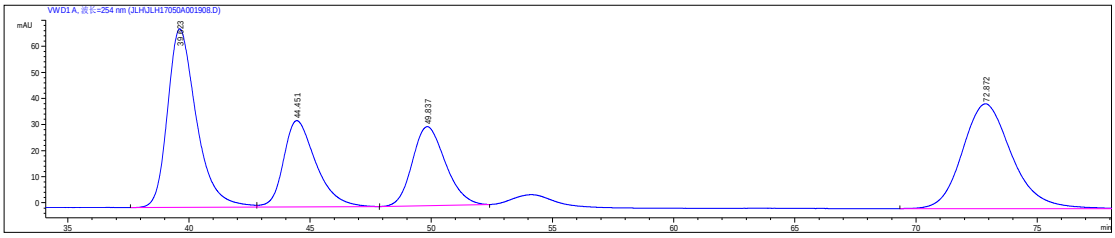
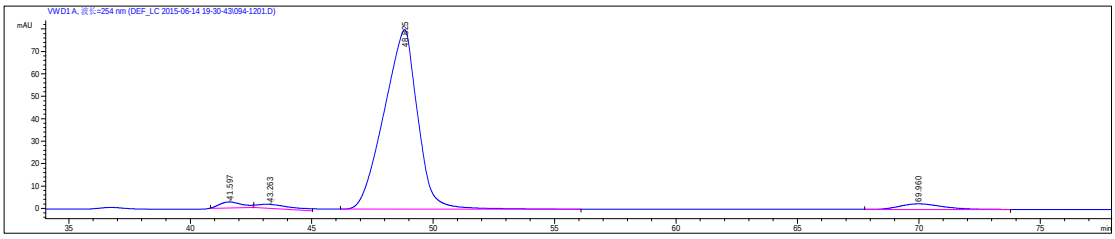
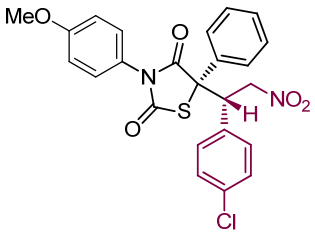


Entry	Retention Time	Area	Height	%Area
1	39.623	5648.9	68.4	32.688
2	44.451	3058.2	33.1	17.696
3	49.837	2871.2	30.3	16.615
4	72.872	5702.9	40.2	33.000



Entry	Retention Time	Area	Height	%Area
1	41.597	174.4	2.7	2.099
2	43.263	179.3	1.8	2.159
3	48.825	7653.3	80	92.126
4	69.96	300.5	2.5	3.617



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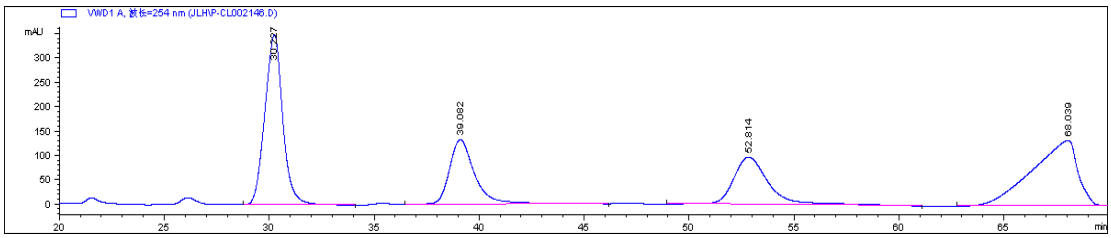
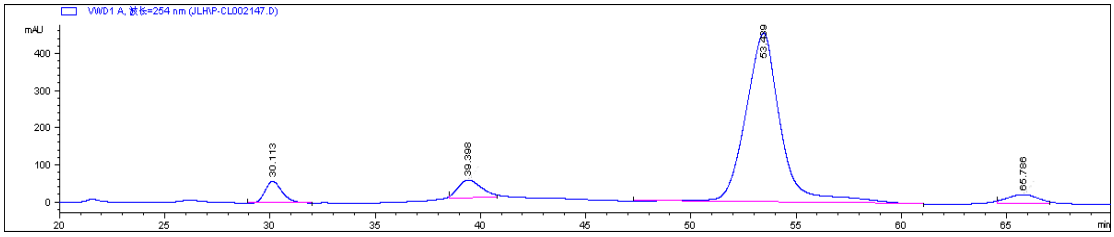
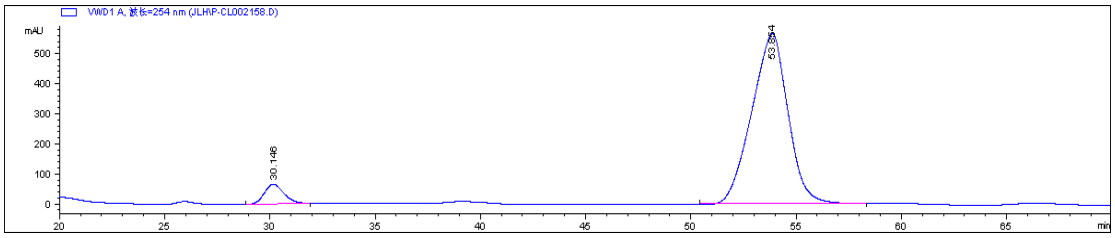


Entry	Retention Time	Area	Height	%Area
1	30.228	20752.4	349.5	32.266
2	39.081	11222.8	133.1	17.449
3	52.814	11684.8	97.8	18.168
4	68.044	20656.5	135.6	32.117



Entry	Retention Time	Area	Height	%Area
1	30.113	3321.6	58.3	5.299
2	39.398	3991.6	50.1	6.367
3	53.439	52753.1	455.8	84.153
4	65.788	2621.1	25.7	4.181



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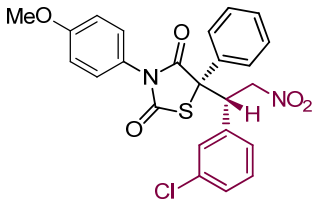
1	30.149	3781.7	61.7	5.276
2	53.855	67895.8	565.6	94.724



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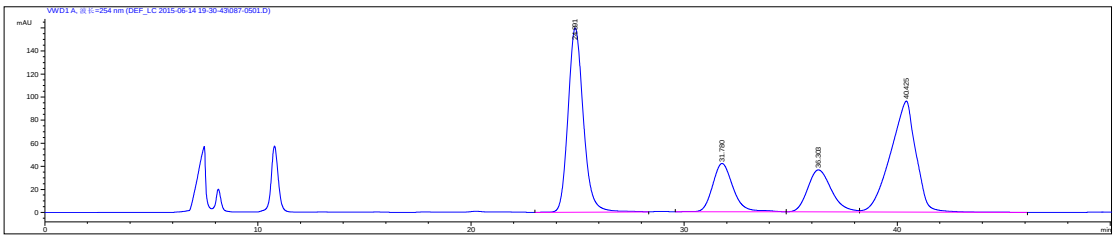
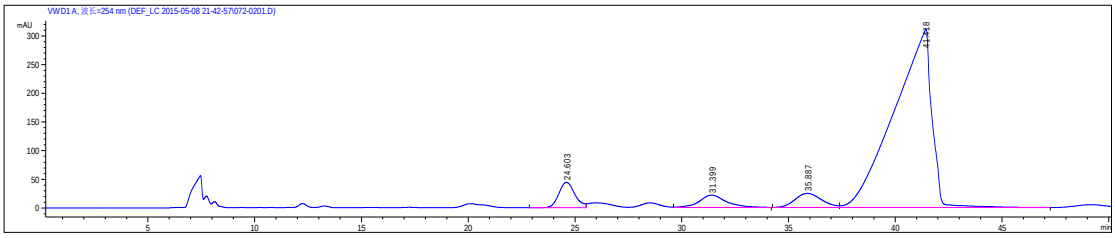
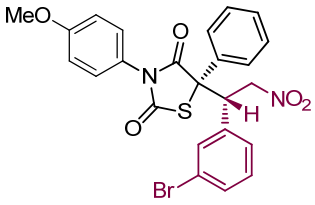


Entry	Retention Time	Area	Height	%Area
1	24.891	7968.6	159.6	36.971
2	31.78	2793	41.9	12.958
3	36.303	2811.5	36.4	13.044
4	40.425	7980.8	96.2	37.027



Entry	Retention Time	Area	Height	%Area
1	24.603	2291.4	44.1	5.183
2	31.399	1862.5	21.5	4.213
3	35.887	2083	24.4	4.712
4	41.418	37973.6	310	85.893



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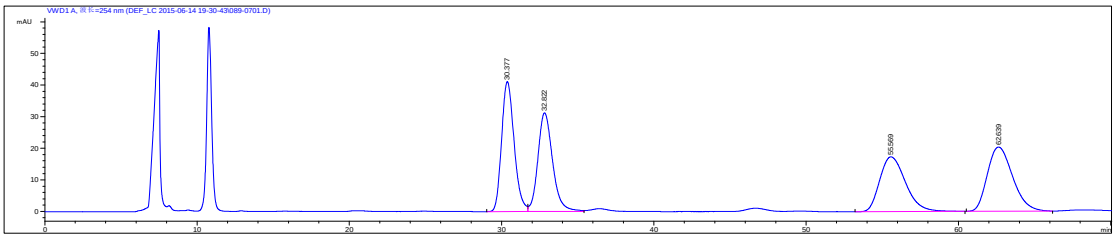
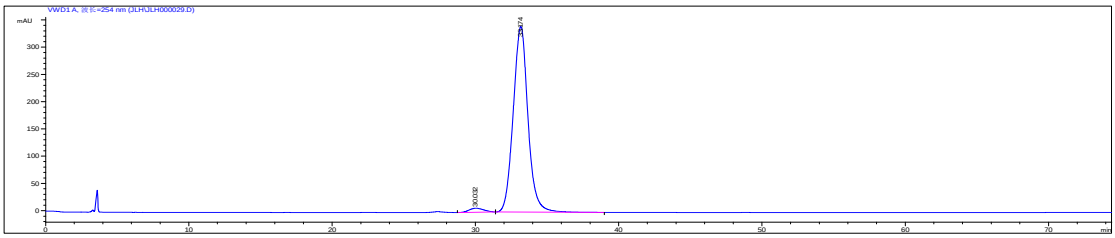


Entry	Retention Time	Area	Height	%Area
1	30.377	2352.3	41.1	26.673
2	32.822	2100.5	31.3	23.817
3	55.569	2031.1	17.3	23.031
4	62.639	2335.3	20.3	26.479



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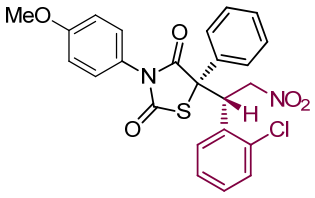
1	30.032	518.9	7.4	2.090
2	33.174	24315.8	340.4	97.910



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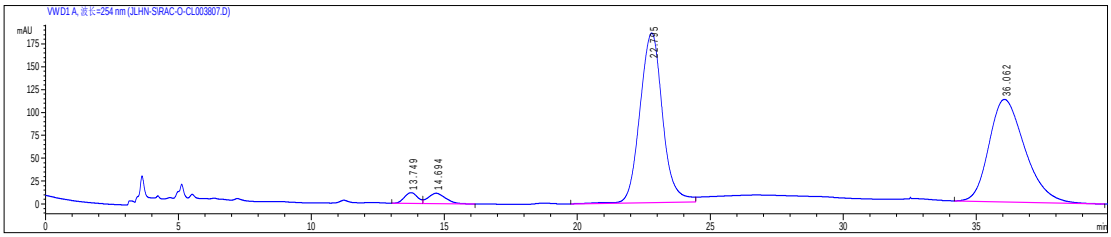
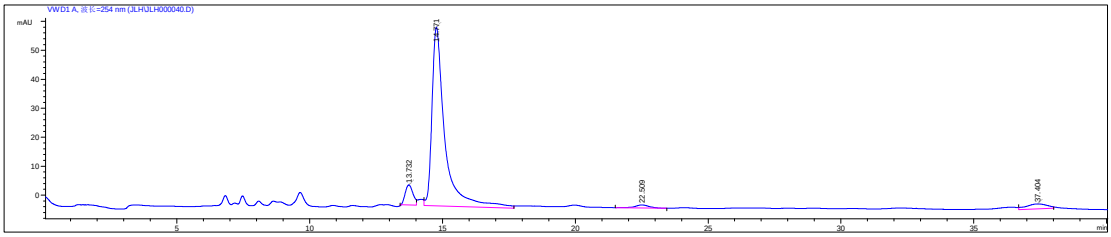
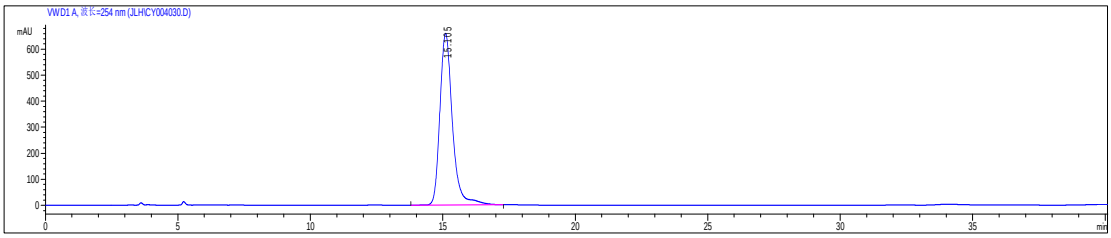


Entry	Retention Time	Area	Height	%Area
1	13.749	409.5	11.8	1.828
2	14.694	518.4	11.4	2.313
3	22.795	10979.8	185.4	48.998
4	36.062	10501	112	46.861



Entry	Retention Time	Area	Height	%Area
1	13.732	140.4	7	5.927
2	14.771	2091.9	61.7	88.338
3	22.509	40.1	1.1	1.694
4	37.404	95.7	1.7	4.041



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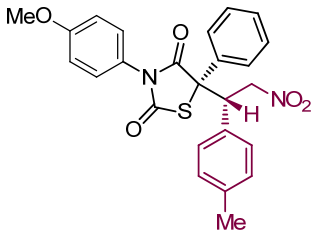

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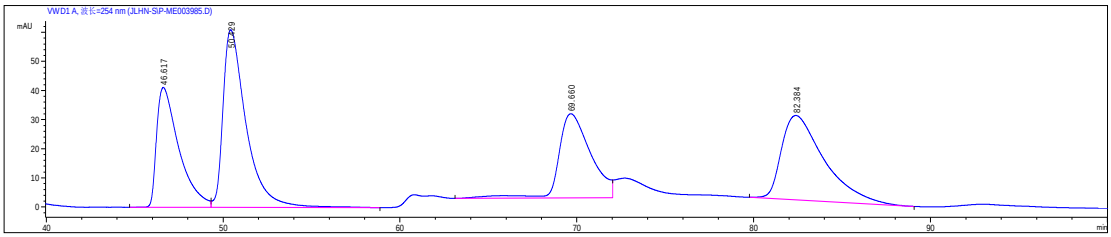
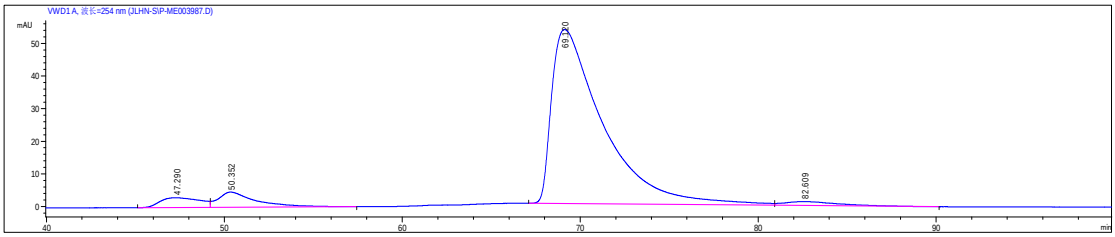
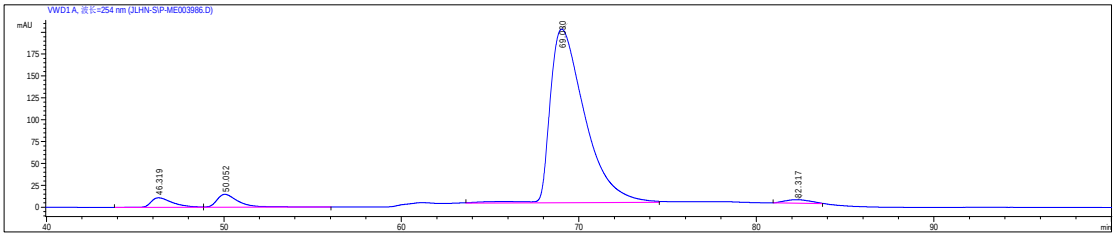


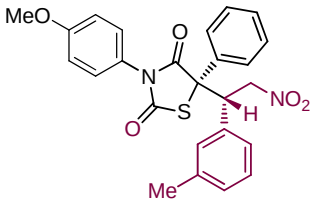
Entry	Retention Time	Area	Height	%Area
1	46.617	3605.8	41.2	20.753
2	50.429	5546.8	61	31.923
3	69.66	3345.3	28.4	19.253
4	82.385	4877.4	29	28.071



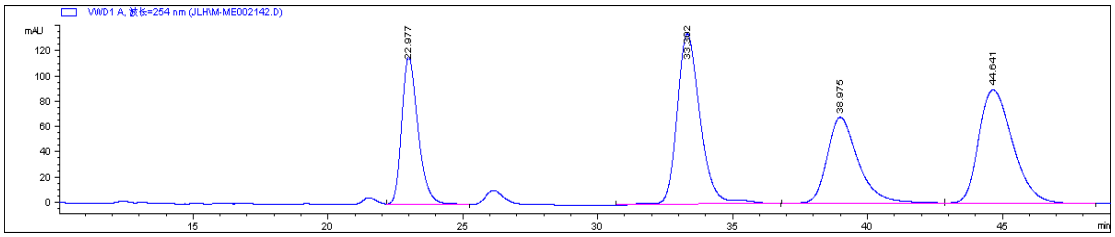
Entry	Retention Time	Area	Height	%Area
1	47.296	482.6	3	3.864
2	50.359	648.4	4.6	5.191
3	69.117	11103.3	53.9	88.890
4	82.662	256.7	1.2	2.055



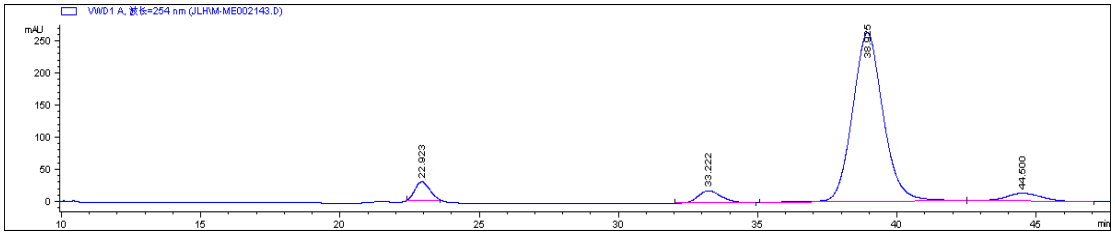
Entry	Retention Time	Area	Height	%Area
1	46.319	877.1	10.8	2.988
2	50.052	1214.8	14.6	4.139
3	69.03	26849.4	198.4	91.484
4	82.317	407.5	4	1.389



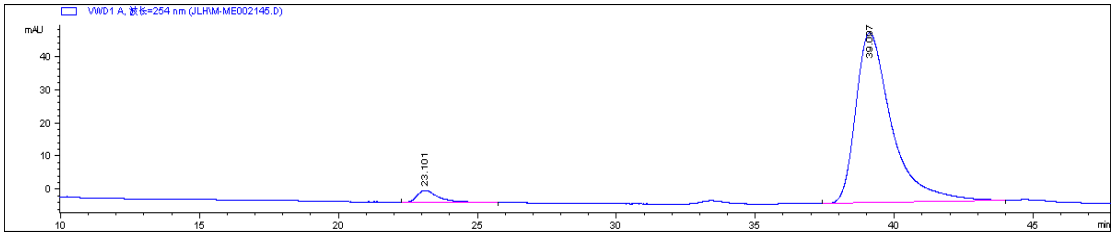
7m



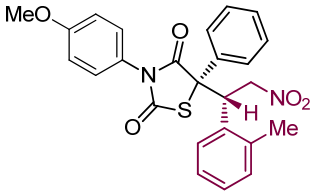
Entry	Retention Time	Area	Height	%Area
1	22.977	4972.2	117.3	19.287
2	33.302	7568.8	133.4	29.359
3	38.974	5405.4	68	20.967
4	44.641	7833.7	89.7	30.387



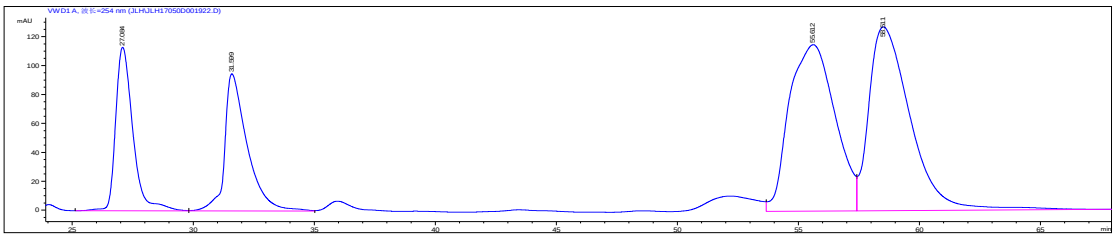
Entry	Retention Time	Area	Height	%Area
1	22.922	1111.4	29.3	4.756
2	33.225	1121.1	19	4.798
3	38.925	20090	262.8	85.974
4	44.499	1045	12	4.472



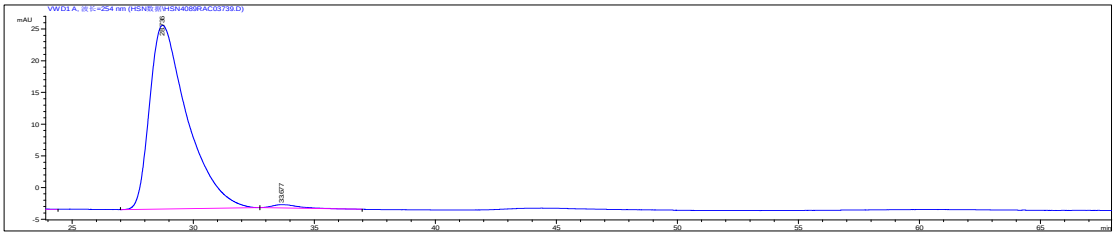
Entry	Retention Time	Area	Height	%Area
1	23.107	170.6	3.6	3.532
2	33.407	64.5	1.1	1.336
3	39.097	4595.1	51.2	95.132



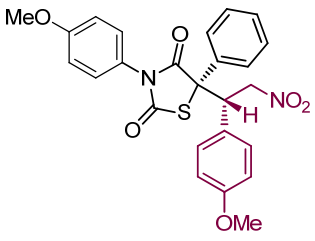
7n



Entry	Retention Time	Area	Height	%Area
1	27.083	5569	112.9	13.557
2	31.594	6027.9	94.5	14.674
3	55.612	15076	114.6	36.700
4	58.511	14406	126.3	35.069



Entry	Retention Time	Area	Height	%Area
1	28.737	3126.6	29	98.874
2	33.711	35.6	5.2E-1	1.126



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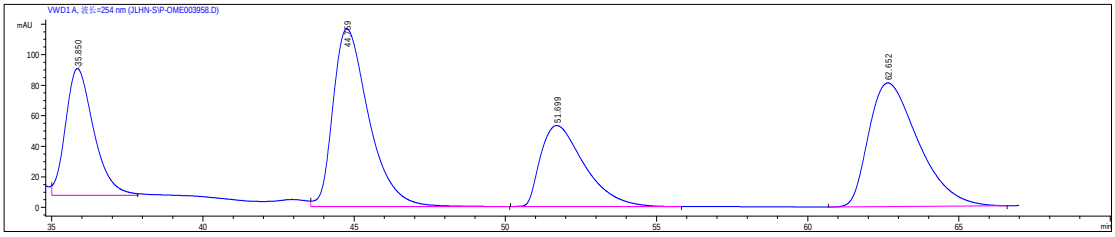
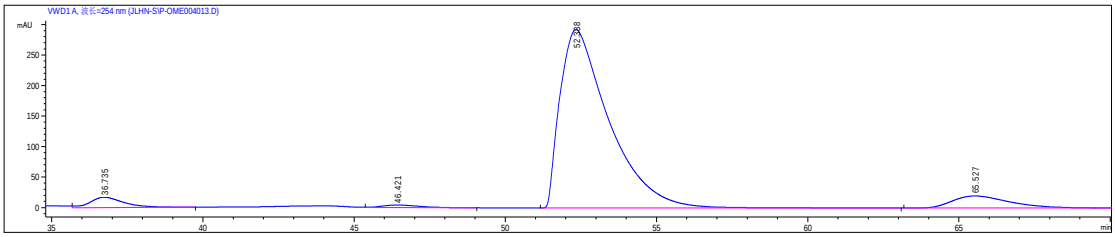
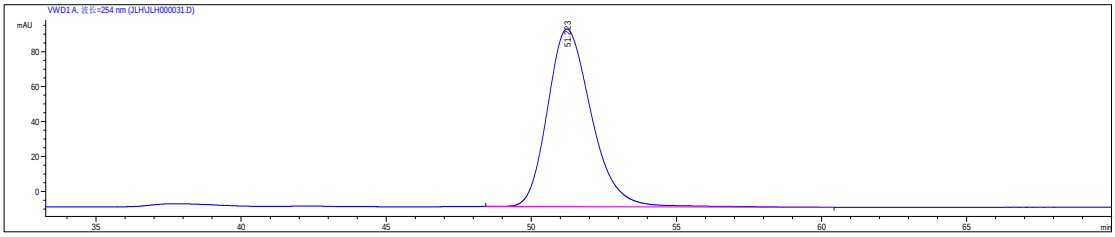


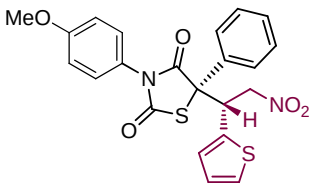
Entry	Retention Time	Area	Height	%Area
1	35.85	5476.4	84.8	18.778
2	44.759	9117.2	114.4	31.262
3	51.698	5344	53	18.324
4	62.651	9226.4	81	31.636



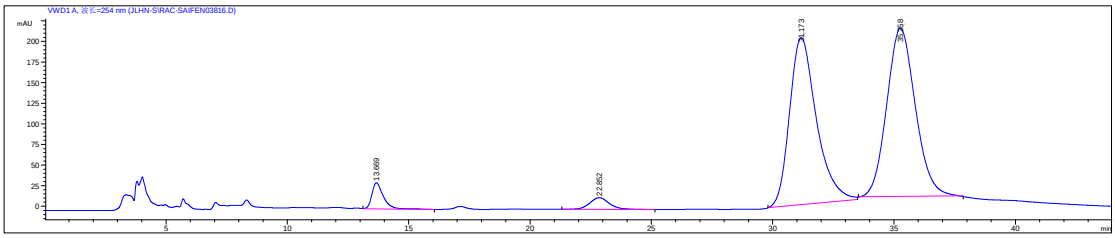
Entry	Retention Time	Area	Height	%Area
1	36.735	1293.1	16.9	3.488
2	46.425	374.4	4.3	1.010
3	52.337	32834	292.2	88.561
4	65.528	2573.7	19.7	6.942



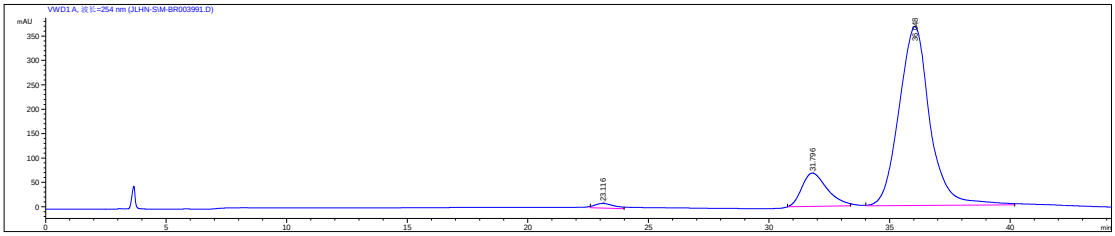
Entry	Retention Time	Area	Height	%Area
1	51.222	10654.8	101.5	100.000



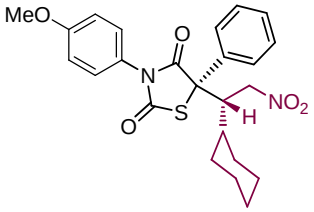
7p



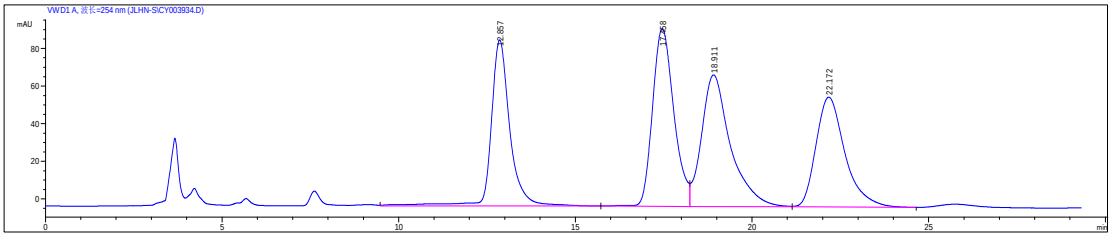
Entry	Retention Time	Area	Height	%Area
1	13.669	1047.7	31.7	3.069
2	22.852	796.8	14.1	2.334
3	31.173	15624.2	202.8	45.769
4	35.258	16668	204.3	48.827



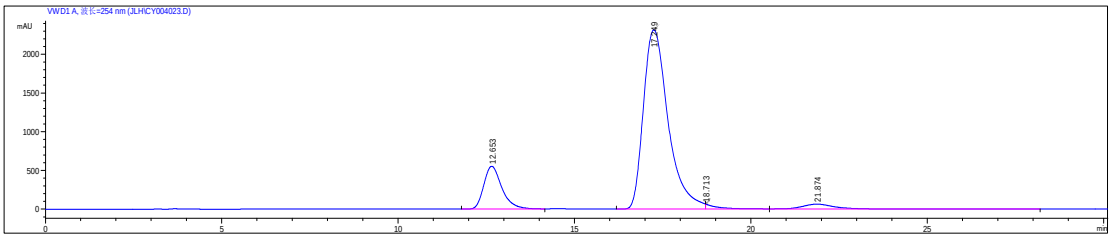
Entry	Retention Time	Area	Height	%Area
1	23.116	506.3	9.5	1.328
2	31.796	4976	68.2	13.052
3	36.048	32641.1	366.9	85.619



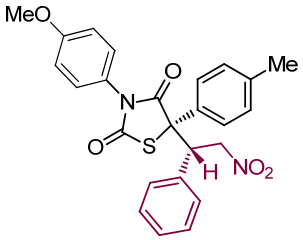
7q



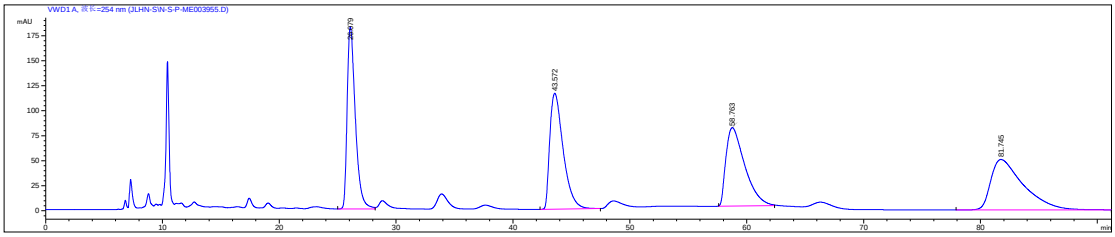
Entry	Retention Time	Area	Height	%Area
1	12.857	3269.1	88.2	22.492
2	17.458	3966.3	94.4	27.288
3	18.911	3969.5	70	27.310
4	22.172	3329.9	58.4	22.910



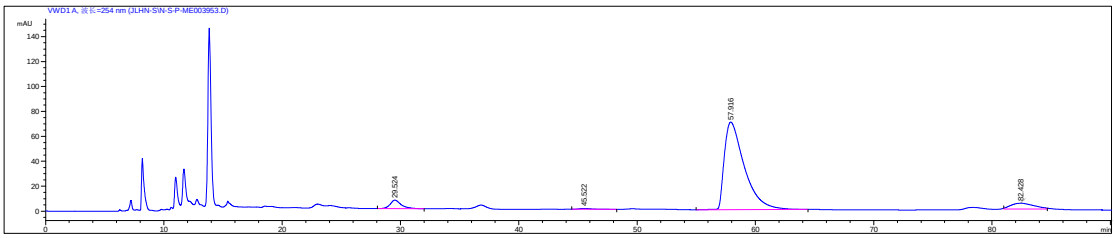
Entry	Retention Time	Area	Height	%Area
1	12.653	19690.8	552.4	14.272
2	17.249	112721.4	2315.1	81.703
3	18.713	1494.2	65.3	1.083
4	21.874	4057.9	63.3	2.941



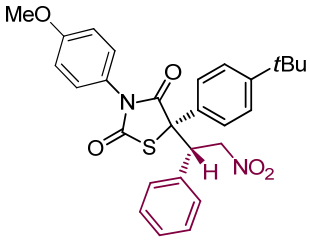
7r



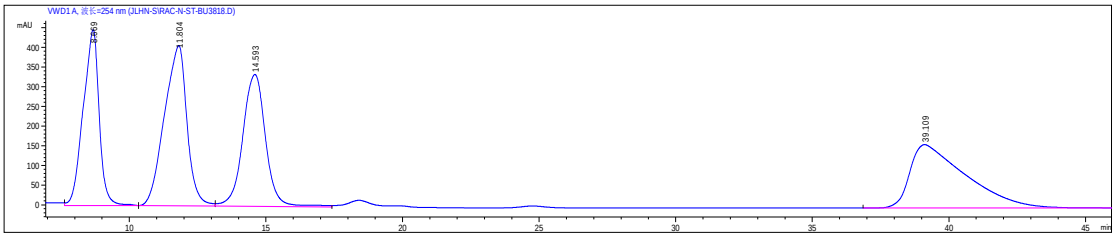
Entry	Retention Time	Area	Height	%Area
1	26.079	8863.5	181.9	24.246
2	43.572	9218.6	115.8	25.217
3	58.763	8777.6	78.5	24.011
4	81.745	9697.4	50.3	26.527



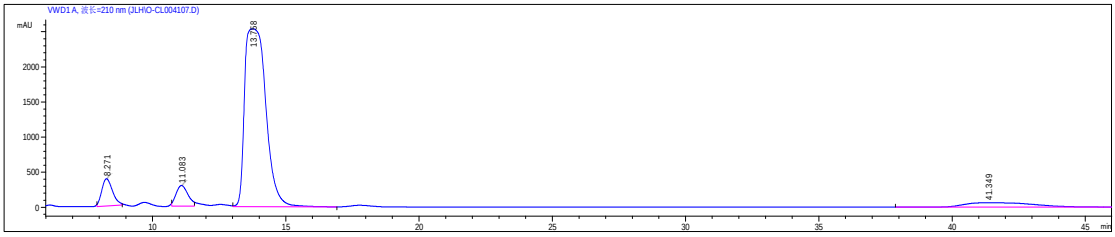
Entry	Retention Time	Area	Height	%Area
1	29.524	443.8	6.8	4.753
2	45.522	58.1	6.6E-1	0.622
3	57.916	8235.2	70.3	88.209
4	82.428	598.9	4.5	6.415



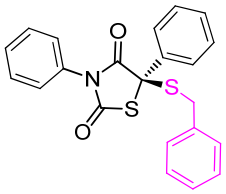
7s



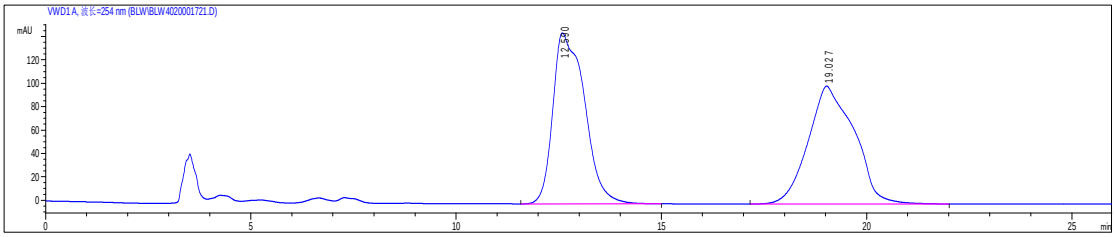
Entry	Retention Time	Area	Height	%Area
1	8.673	18117.9	446.4	21.873
2	11.808	23205.4	405.9	28.015
3	14.595	18778	332.5	22.670
4	39.107	22731.3	160.7	27.443



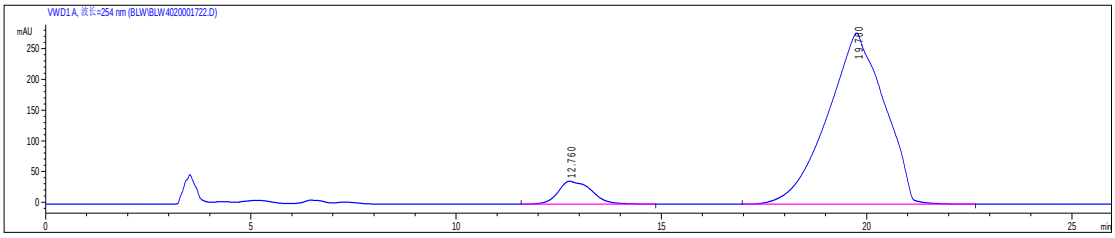
Entry	Retention Time	Area	Height	%Area
1	8.271	10861.8	388.5	6.616
2	11.083	9052.5	292.7	5.514
3	13.752	140428.5	2535	85.540
4	41.334	3823.8	31.5	2.329



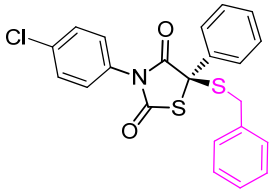
9a



Entry	Retention Time	Area	Height	%Area
1	12.59	7846.6	146.2	49.911
2	19.027	7874.4	100.8	50.089



Entry	Retention Time	Area	Height	%Area
1	12.76	1874.8	37.3	6.533
2	19.76	26823.1	278.9	93.467



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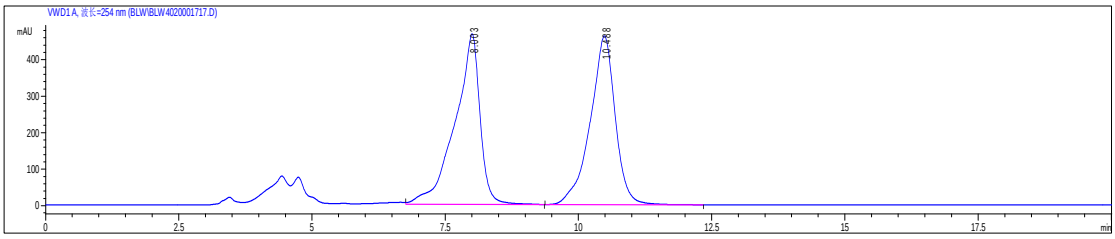
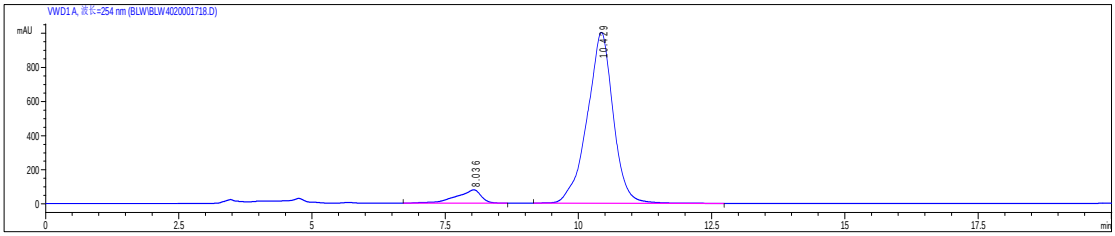
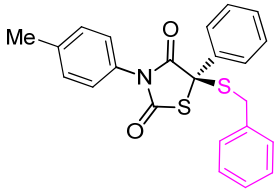


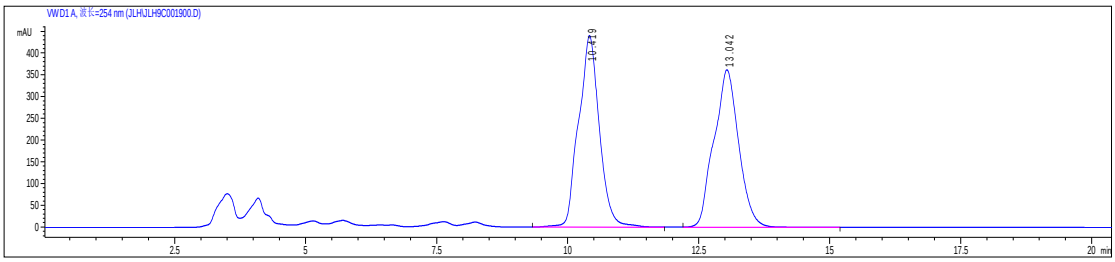
Entry	Retention Time	Area	Height	%Area
1	8.003	15242.3	467.3	50.247
2	10.488	15092.6	462.5	49.753



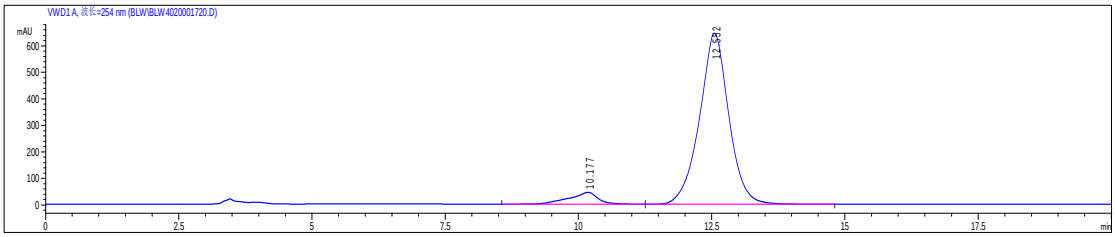
Entry	Retention Time	Area	Height	%Area
1	8.036	2110.9	78.9	5.862
2	10.429	33897.5	1001.9	94.138



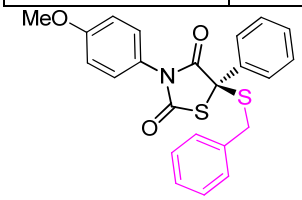
9c



Entry	Retention Time	Area	Height	%Area
1	10.419	12155.5	440.4	50.579
2	13.042	11877.2	361.9	49.421



Entry	Retention Time	Area	Height	%Area
1	10.177	1278.9	45.1	4.945
2	12.552	24585.1	646.1	95.055



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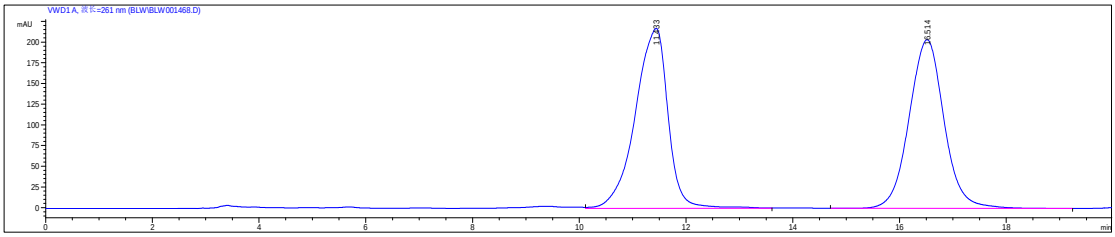
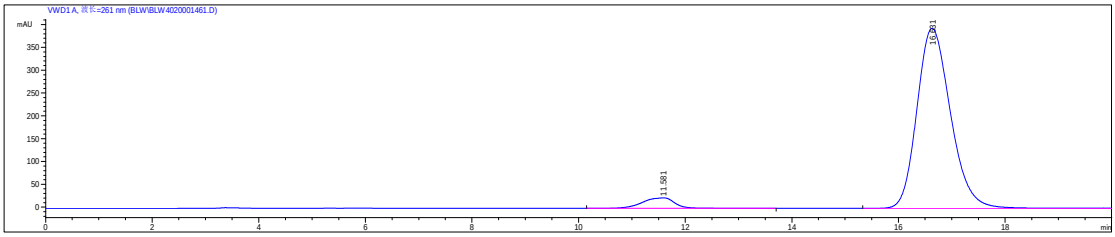
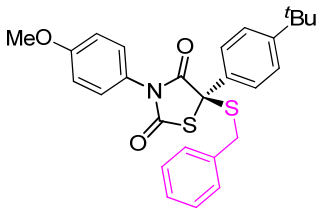


Entry	Retention Time	Area	Height	%Area
1	11.433	9246.7	217.4	50.000
2	16.514	9246.8	203.6	50.000



Entry	Retention Time	Area	Height	%Area
1	11.589	806	21.7	4.480
2	16.631	17186.6	394.2	95.520



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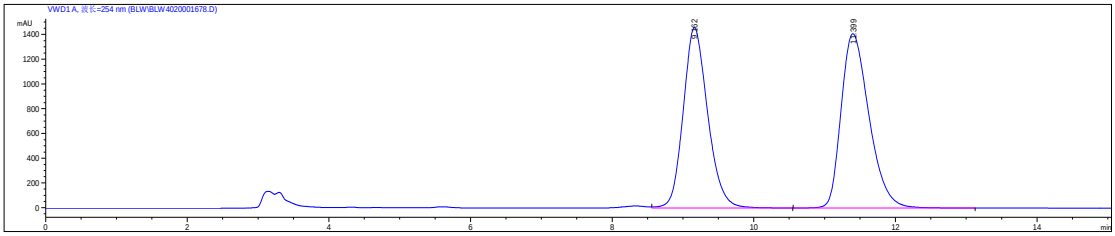
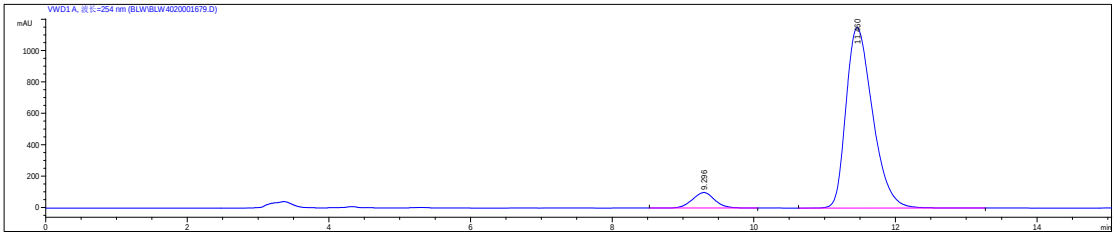
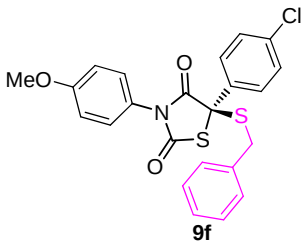


Entry	Retention Time	Area	Height	%Area
1	9.162	11501	342.4	50.431
2	11.399	11304.4	285.5	49.569



Entry	Retention Time	Area	Height	%Area
1	9.296	2150	98.5	6.713
2	11.46	29877.9	1149.8	93.287



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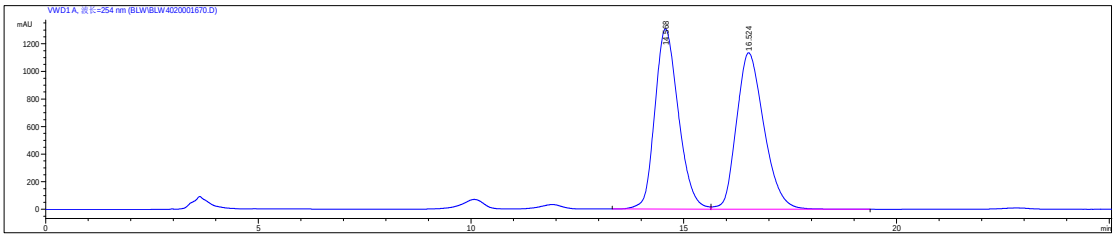
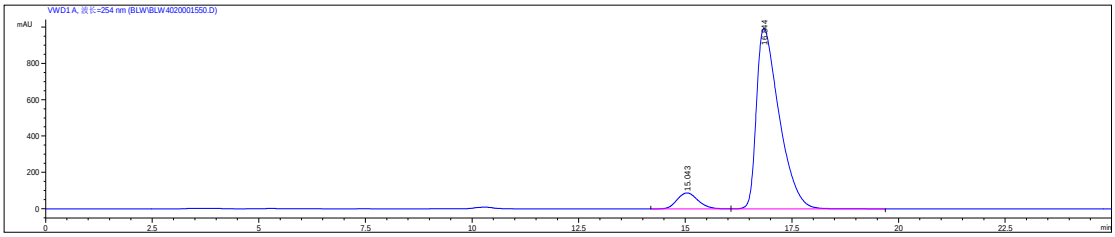
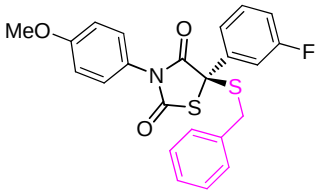


Entry	Retention Time	Area	Height	%Area
1	14.568	50132.8	1306.6	49.719
2	16.524	50700	1134.2	50.281



Entry	Retention Time	Area	Height	%Area
1	15.043	2494.2	81	6.359
2	16.844	36728.1	993.5	93.641



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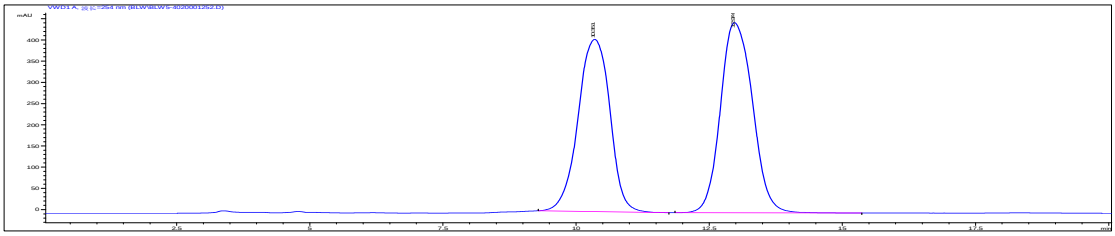
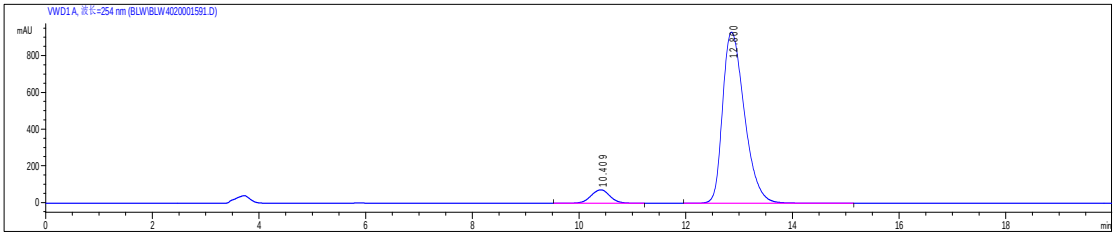
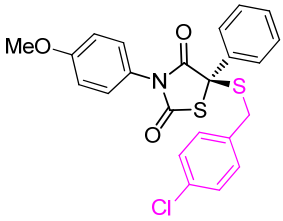


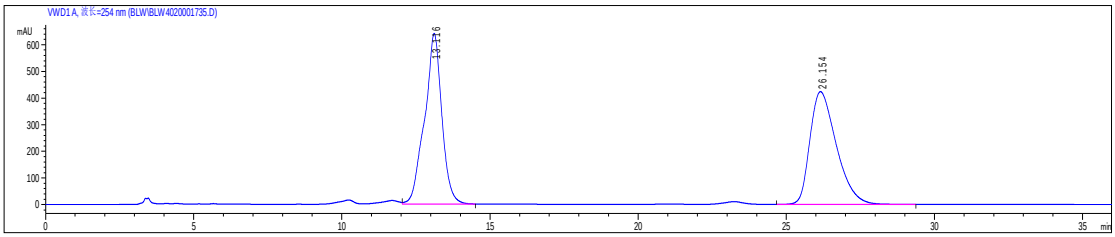
Entry	Retention Time	Area	Height	%Area
1	10.351	16888.9	406.2	47.298
2	12.974	18818.3	448.5	52.702



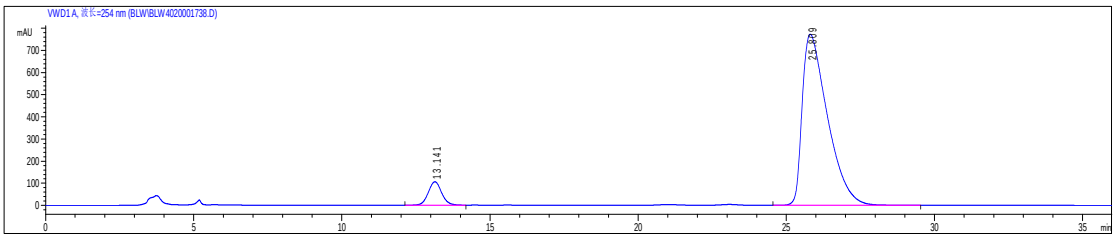
Entry	Retention Time	Area	Height	%Area
1	10.409	1596.2	73.9	5.676
2	12.86	26526.6	933	94.324



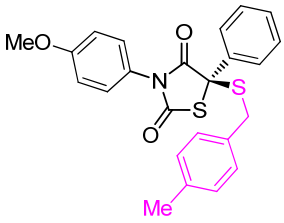
9h



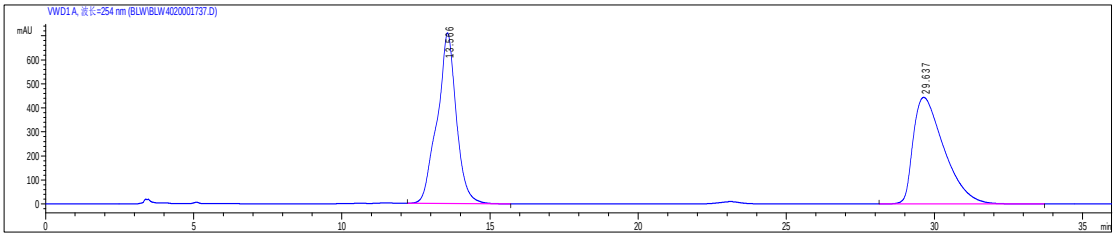
Entry	Retention Time	Area	Height	%Area
1	13.116	25873.7	641.1	49.593
2	26.154	26298	423.7	50.407



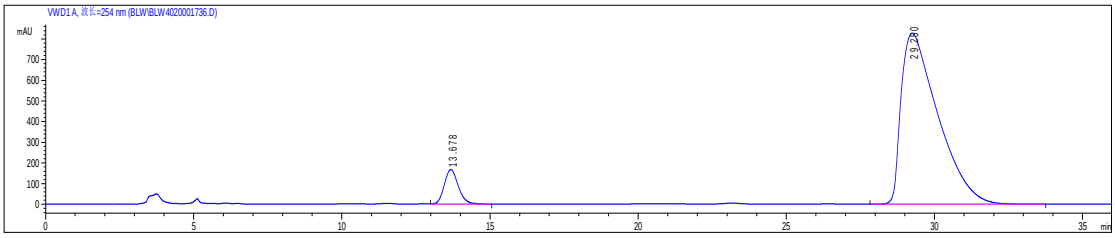
Entry	Retention Time	Area	Height	%Area
1	13.141	3003.9	106.4	6.159
2	25.809	45767	773.3	93.841



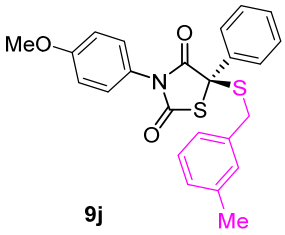
9i



Entry	Retention Time	Area	Height	%Area
1	13.566	31740.1	710.4	49.688
2	29.637	32138.4	443.8	50.312



Entry	Retention Time	Area	Height	%Area
1	13.678	4848.7	167.4	6.374
2	29.25	71225.2	828.3	93.626



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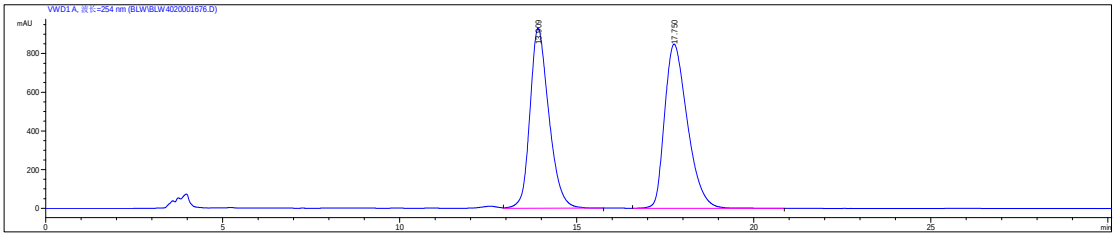
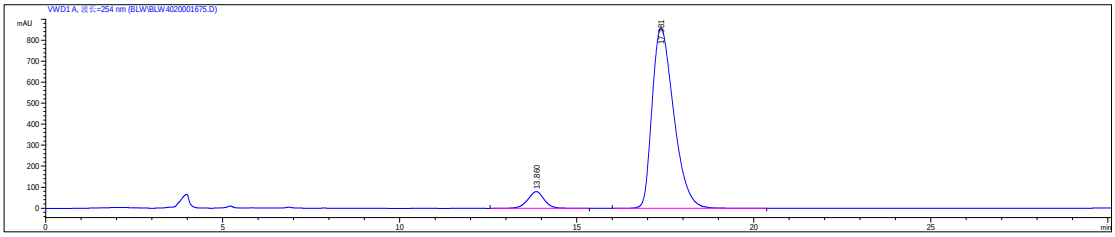
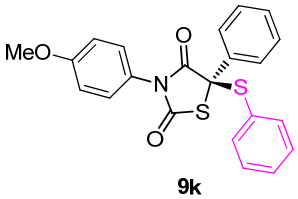


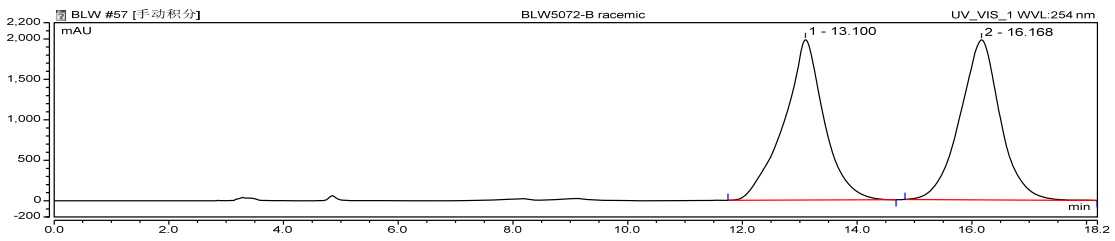
Entry	Retention Time	Area	Height	%Area
1	13.909	34482.1	931.7	47.614
2	17.75	37937.8	848.7	52.386



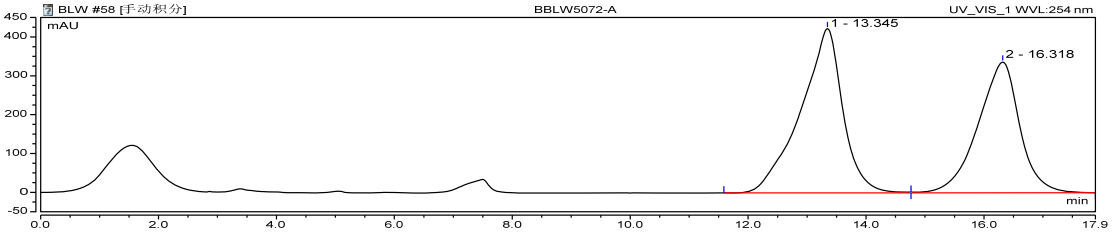
Entry	Retention Time	Area	Height	%Area
1	13.86	2170.4	74.7	5.629
2	17.381	36384.9	859	94.371



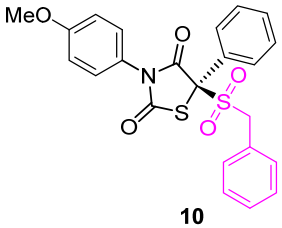
9k



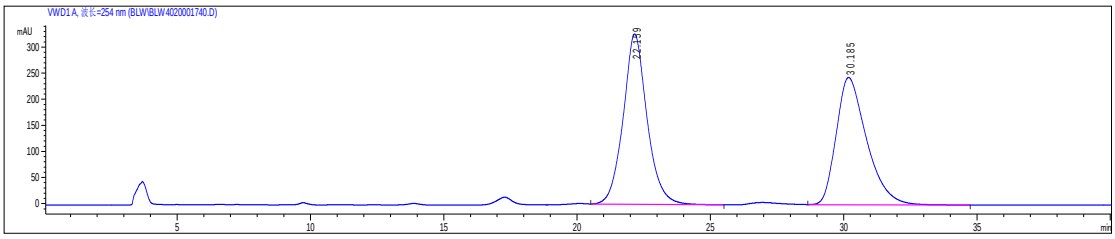
Entry	Retention Time	Area	Height	%Area
1	13.100	1607.3926	1980.46	50.02
2	16.168	1606.1558	1976.27	49.98



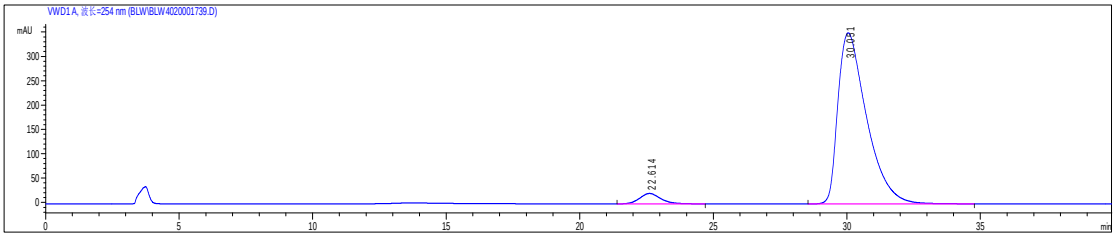
Entry	Retention Time	Area	Height	%Area
1	13.345	349.7697	422.62	55.96
2	16.318	275.3053	336.15	44.04



10



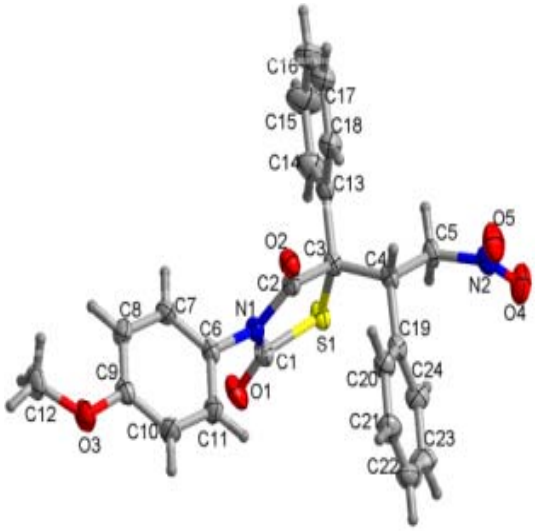
Entry	Retention Time	Area	Height	%Area
1	22.159	5794.9	96.5	52.668
2	30.185	5207.7	82.7	47.332



Entry	Retention Time	Area	Height	%Area
1	22.614	1179.6	21.4	4.309
2	30.051	26198.3	351.9	95.691

3.Determination of the absolute configuration by *X*-ray crystallography

1) Absolute configurations of **7** and the derivative **10** are determined by X-ray structure analysis of the product **7f** (CCDC1430350).



Displacement ellipsoids are drawn at the 30% probability level.

Table 1 Crystal data and structure refinement for JLH06047.

Identification code	JLH06047
Empirical formula	$C_{24}H_{20}N_2O_5S$
Formula weight	448.48
Temperature/K	291.15
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	8.6723(2)
b/Å	16.0081(4)
c/Å	16.3709(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2272.72(9)
Z	4
ρ_{calc}g/cm^3	1.311
μ/mm^{-1}	1.585
F(000)	936.0
Crystal size/mm^3	0.19 × 0.17 × 0.16
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.724 to 134.158
Index ranges	-5 ≤ h ≤ 10, -19 ≤ k ≤ 19, -19 ≤ l ≤ 19
Reflections collected	8203

Independent reflections	4076 [R_{int} = 0.0282, R_{sigma} = 0.0382]
Data/restraints/parameters	4076/0/290
Goodness-of-fit on F^2	1.017
Final R indexes [I>=2σ (I)]	R_1 = 0.0378, wR_2 = 0.0914
Final R indexes [all data]	R_1 = 0.0447, wR_2 = 0.0958
Largest diff. peak/hole / e Å^{-3}	0.15/-0.15
Flack parameter	0.025(14)

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for JLH06047. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	2572(4)	5049(2)	1720.3(18)	48.7(7)
C2	3862(3)	3907.4(18)	2327.8(18)	40.5(6)
C3	3347(4)	4359.9(19)	3112.3(17)	40.8(7)
C4	4812(4)	4571(2)	3627.1(17)	41.9(7)
C5	4318(4)	4980(2)	4423.6(19)	50.6(8)
C6	3619(4)	3929.4(19)	835.0(17)	43.6(7)
C7	2674(5)	3303(2)	565.3(19)	52.2(8)
C8	2909(5)	2942(2)	-197(2)	54.6(9)
C9	4124(5)	3218(2)	-671.6(19)	50.1(8)
C10	5074(5)	3849(3)	-396(2)	60.3(10)
C11	4825(5)	4206(3)	363(2)	58.5(9)
C12	3435(7)	2334(3)	-1786(2)	82.7(15)
C13	2242(4)	3776(2)	3581.9(17)	45.7(7)
C14	729(5)	3979(3)	3738(3)	73.1(12)
C15	-221(6)	3429(4)	4152(3)	98.8(18)
C16	326(6)	2667(4)	4403(3)	88.1(15)
C17	1826(6)	2459(3)	4255(2)	71.0(11)
C18	2780(5)	3005(2)	3844(2)	56.2(9)
C19	6014(4)	5064.5(19)	3157.8(17)	41.8(7)
C20	7131(4)	4637(2)	2724(2)	52.6(8)
C21	8234(4)	5056(3)	2268(3)	65.1(10)
C22	8261(5)	5906(3)	2261(3)	69.6(11)
C23	7180(5)	6346(2)	2699(3)	71.0(11)
C24	6051(4)	5934(2)	3144(2)	55.8(9)
N1	3344(3)	4294.8(16)	1626.9(15)	44.0(6)
N2	5682(4)	5125(2)	4963.8(17)	55.8(7)
O1	2072(4)	5467.6(17)	1173.9(14)	71.8(8)
O2	4618(3)	3277.5(14)	2327.7(13)	51.7(6)
O3	4464(4)	2909.1(17)	-1424.9(15)	67.8(8)
O4	5797(4)	5792(2)	5298(2)	89.6(10)

O5		6611(4)	4566(2)	5045.2(18)	82.9(9)
S1		2394.4(10)	5313.8(5)	2758.0(5)	48.0(2)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for JLH06047. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	53.2(18)	55.3(17)	37.7(14)	-2.2(13)	-4.3(15)	2.7(16)
C2	43.4(15)	43.6(16)	34.4(14)	-1.8(13)	-0.3(13)	-3.9(13)
C3	44.4(17)	45.5(16)	32.4(14)	-1.0(12)	-1.0(13)	4.4(14)
C4	47.0(17)	46.8(17)	31.9(13)	-1.9(13)	-2.4(13)	5.6(14)
C5	51.9(18)	64(2)	35.7(15)	-8.7(14)	-1.0(14)	1.7(17)
C6	50.3(17)	48.7(17)	31.9(14)	-2.2(13)	-3.5(13)	3.1(15)
C7	61(2)	54.1(18)	41.6(15)	-0.8(14)	7.3(16)	-8.2(18)
C8	68(2)	48.6(18)	47.7(18)	-7.2(14)	-6.7(17)	-9.3(17)
C9	67(2)	48.0(18)	35.4(15)	-3.3(13)	-4.8(16)	6.3(16)
C10	62(2)	74(2)	45.4(18)	-6.0(18)	9.0(17)	-14(2)
C11	63(2)	66(2)	46.9(18)	-11.7(17)	2.2(17)	-16.4(19)
C12	135(4)	65(2)	48(2)	-20.1(19)	-10(3)	-5(3)
C13	48.0(18)	58.7(18)	30.3(13)	-3.5(12)	0.8(13)	-3.3(15)
C14	62(2)	88(3)	69(3)	11(2)	15(2)	10(2)
C15	64(3)	130(5)	102(4)	33(4)	33(3)	3(3)
C16	86(3)	106(4)	73(3)	21(3)	19(3)	-23(3)
C17	88(3)	69(3)	57(2)	10.2(19)	1(2)	-15(2)
C18	59(2)	57.2(19)	52.4(19)	4.3(15)	0.5(17)	-4.6(18)
C19	44.5(16)	47.7(16)	33.1(13)	0.9(12)	-2.9(12)	4.2(14)
C20	50.1(17)	55.1(17)	52.6(17)	-5.5(17)	4.0(16)	1.1(16)
C21	50.1(19)	87(3)	58(2)	-5(2)	7.6(18)	-2.9(19)
C22	57(2)	87(3)	65(2)	19(2)	2(2)	-11(2)
C23	76(3)	52.5(19)	85(3)	23(2)	-8(3)	-5.9(19)
C24	55(2)	52.0(19)	61(2)	1.4(16)	-1.7(17)	4.9(17)
N1	50.3(15)	48.3(14)	33.2(12)	-2.9(11)	-2.8(11)	2.0(12)
N2	66.5(19)	66.3(19)	34.6(13)	-5.6(13)	-5.3(13)	-0.2(16)
O1	98(2)	73.8(17)	43.4(13)	5.2(12)	-14.8(13)	27.1(16)
O2	64.4(14)	48.1(12)	42.6(11)	-3.7(10)	0.1(11)	12.3(11)
O3	91(2)	71.6(17)	41.2(13)	-16.0(12)	4.9(14)	2.3(16)
O4	101(2)	82(2)	86(2)	-32.2(18)	-28.0(19)	-1.2(19)
O5	89(2)	89(2)	70.8(18)	-5.9(17)	-31.4(16)	21.9(19)
S1	54.4(4)	50.7(4)	38.8(3)	-4.4(3)	-4.4(4)	13.2(4)

Table 4 Bond Lengths for JLH06047.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	N1	1.390(4)	C9	O3	1.361(4)

C1	O1	1.199(4)	C10	C11	1.385(5)
C1	S1	1.758(3)	C12	O3	1.411(5)
C2	C3	1.541(4)	C13	C14	1.376(5)
C2	N1	1.379(4)	C13	C18	1.388(5)
C2	O2	1.203(4)	C14	C15	1.383(6)
C3	C4	1.562(4)	C15	C16	1.373(8)
C3	C13	1.544(4)	C16	C17	1.365(7)
C3	S1	1.831(3)	C17	C18	1.378(5)
C4	C5	1.521(4)	C19	C20	1.382(4)
C4	C19	1.517(4)	C19	C24	1.392(5)
C5	N2	1.494(4)	C20	C21	1.387(5)
C6	C7	1.367(5)	C21	C22	1.361(6)
C6	C11	1.373(5)	C22	C23	1.375(6)
C6	N1	1.442(4)	C23	C24	1.387(5)
C7	C8	1.391(5)	N2	O4	1.204(4)
C8	C9	1.381(5)	N2	O5	1.211(4)
C9	C10	1.379(5)			

Table 5 Bond Angles for JLH06047.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	C1	S1	111.0(2)	C6	C11	C10	119.3(3)
O1	C1	N1	125.3(3)	C14	C13	C3	122.8(3)
O1	C1	S1	123.7(3)	C14	C13	C18	118.3(4)
N1	C2	C3	112.8(2)	C18	C13	C3	118.9(3)
O2	C2	C3	123.5(3)	C13	C14	C15	120.6(5)
O2	C2	N1	123.6(3)	C16	C15	C14	120.5(5)
C2	C3	C4	108.4(2)	C17	C16	C15	119.5(5)
C2	C3	C13	108.1(2)	C16	C17	C18	120.3(5)
C2	C3	S1	105.00(19)	C17	C18	C13	120.8(4)
C4	C3	S1	111.0(2)	C20	C19	C4	118.9(3)
C13	C3	C4	111.6(2)	C20	C19	C24	118.0(3)
C13	C3	S1	112.5(2)	C24	C19	C4	123.1(3)
C5	C4	C3	109.1(2)	C19	C20	C21	121.4(3)
C19	C4	C3	113.5(2)	C22	C21	C20	120.0(4)
C19	C4	C5	113.8(3)	C21	C22	C23	119.7(4)
N2	C5	C4	110.6(3)	C22	C23	C24	120.8(4)
C7	C6	C11	120.7(3)	C23	C24	C19	120.1(4)
C7	C6	N1	119.2(3)	C1	N1	C6	122.1(3)
C11	C6	N1	120.0(3)	C2	N1	C1	117.1(2)
C6	C7	C8	120.5(3)	C2	N1	C6	120.8(3)
C9	C8	C7	118.9(3)	O4	N2	C5	118.1(3)

C10	C9	C8	120.4(3)	O4	N2	O5	123.4(3)
O3	C9	C8	123.9(3)	O5	N2	C5	118.5(3)
O3	C9	C10	115.7(3)	C9	O3	C12	118.7(3)
C9	C10	C11	120.2(4)	C1	S1	C3	93.77(14)

Table 6 Torsion Angles for JLH06047.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C2	C3	C4	C5	-177.3(3)	C13	C3	S1	C1	-113.3(2)
C2	C3	C4	C19	54.8(3)	C13	C14	C15	C16	-0.9(8)
C2	C3	C13	C14	-117.9(4)	C14	C13	C18	C17	-0.4(5)
C2	C3	C13	C18	60.7(4)	C14	C15	C16	C17	1.2(9)
C2	C3	S1	C1	4.0(2)	C15	C16	C17	C18	-1.1(8)
C3	C2	N1	C1	5.1(4)	C16	C17	C18	C13	0.7(6)
C3	C2	N1	C6	-175.6(3)	C18	C13	C14	C15	0.5(7)
C3	C4	C5	N2	175.2(3)	C19	C4	C5	N2	-57.1(4)
C3	C4	C19	C20	-89.5(3)	C19	C20	C21	C22	2.0(6)
C3	C4	C19	C24	90.7(4)	C20	C19	C24	C23	0.5(5)
C3	C13	C14	C15	179.1(4)	C20	C21	C22	C23	-0.8(6)
C3	C13	C18	C17	-179.0(3)	C21	C22	C23	C24	-0.5(6)
C4	C3	C13	C14	123.0(4)	C22	C23	C24	C19	0.7(6)
C4	C3	C13	C18	-58.4(4)	C24	C19	C20	C21	-1.8(5)
C4	C3	S1	C1	120.9(2)	N1	C1	S1	C3	-1.6(3)
C4	C5	N2	O4	134.9(4)	N1	C2	C3	C4	-124.4(3)
C4	C5	N2	O5	-45.3(4)	N1	C2	C3	C13	114.6(3)
C4	C19	C20	C21	178.4(3)	N1	C2	C3	S1	-5.7(3)
C4	C19	C24	C23	-179.8(3)	N1	C6	C7	C8	179.8(3)
C5	C4	C19	C20	145.0(3)	N1	C6	C11	C10	180.0(4)
C5	C4	C19	C24	-34.8(4)	O1	C1	N1	C2	178.9(4)
C6	C7	C8	C9	0.9(6)	O1	C1	N1	C6	-0.3(5)
C7	C6	C11	C10	0.5(6)	O1	C1	S1	C3	177.7(4)
C7	C6	N1	C1	-99.7(4)	O2	C2	C3	C4	56.5(4)
C7	C6	N1	C2	81.1(4)	O2	C2	C3	C13	-64.6(4)
C7	C8	C9	C10	-0.8(6)	O2	C2	C3	S1	175.1(3)
C7	C8	C9	O3	179.8(3)	O2	C2	N1	C1	-175.7(3)
C8	C9	C10	C11	0.6(6)	O2	C2	N1	C6	3.6(5)
C8	C9	O3	C12	6.8(5)	O3	C9	C10	C11	180.0(4)
C9	C10	C11	C6	-0.4(6)	S1	C1	N1	C2	-1.8(4)
C10	C9	O3	C12	-172.6(4)	S1	C1	N1	C6	178.9(3)
C11	C6	C7	C8	-0.7(6)	S1	C3	C4	C5	67.9(3)
C11	C6	N1	C1	80.8(4)	S1	C3	C4	C19	-60.0(3)
C11	C6	N1	C2	-98.5(4)	S1	C3	C13	C14	-2.5(4)

C13	C3	C4	C5	-58.4(3)	S1	C3	C13 C18	176.1(2)
C13	C3	C4	C19	173.7(3)				

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for JLH06047.

Atom	*x*	*y*	*z*	U(eq)
H4	5291	4037	3773	50
H5A	3818	5509	4308	61
H5B	3582	4624	4702	61
H7	1869	3118	894	63
H8	2260	2521	-385	66
H10	5883	4036	-721	72
H11	5468	4629	552	70
H12A	3802	2185	-2320	124
H12B	2432	2584	-1831	124
H12C	3371	1842	-1452	124
H14	342	4491	3564	88
H15	-1238	3577	4261	119
H16	-322	2294	4672	106
H17	2207	1947	4433	85
H18	3798	2854	3742	67
H20	7142	4056	2738	63
H21	8956	4756	1967	78
H22	9008	6189	1961	84
H23	7205	6927	2697	85
H24	5319	6238	3433	67

Experimental

The crystal was kept at 291.15 K during data collection. Using Olex2 [1], the structure was solved with the Superflip [2] structure solution program using Charge Flipping and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Palatinus, L. & Chapuis, G. (2007). J. Appl. Cryst., 40, 786-790; Palatinus, L. & van der Lee, A. (2008). J. Appl. Cryst. 41, 975-984; Palatinus, L., Prathapa, S. J. & van Smaalen, S. (2012). J. Appl. Cryst. 45, 575-580.
3. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

Crystal Data for $C_{24}H_{20}N_2O_5S$ (M =448.48 g/mol): orthorhombic, space group $P2_12_12_1$ (no. 19), a = 8.6723(2) Å, b = 16.0081(4) Å, c = 16.3709(3) Å, V = 2272.72(9) Å^3, Z = 4, T = 291.15 K, μ(CuKα) = 1.585 mm^{-1}, *Dcalc* = 1.311 g/cm^3, 8203 reflections measured (7.724° ≤ 2Θ ≤ 134.158°), 4076 unique (R_{int} = 0.0282, R_{sigma} = 0.0382) which were used in all calculations. The final R_1 was 0.0378 (I > 2σ(I)) and wR_2 was 0.0958 (all data).

Refinement model description

Number of restraints -0, number of constraints - unknown.

Details:

1. Fixed Uiso

At 1.2 times of:

All C(H) groups, All C(H,H) groups

At 1.5 times of:

All C(H,H,H) groups

2.a Ternary CH refined with riding coordinates:

C4(H4)

2.b Secondary CH2 refined with riding coordinates:

C5(H5A,H5B)

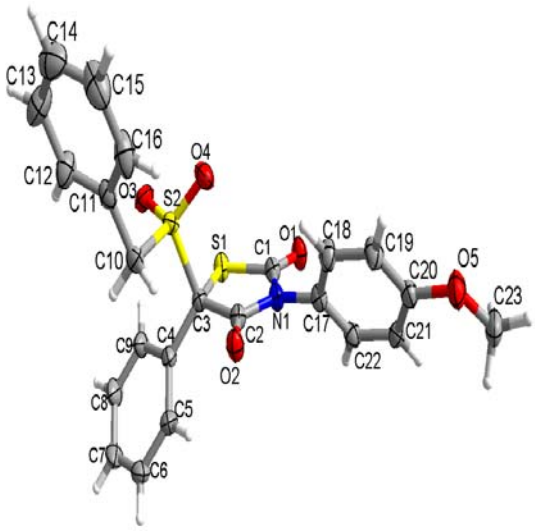
2.c Aromatic/amide H refined with riding coordinates:

C7(H7), C8(H8), C10(H10), C11(H11), C14(H14), C15(H15), C16(H16), C17(H17), C18(H18), C20(H20), C21(H21), C22(H22), C23(H23), C24(H24)

2.d Idealised Me refined as rotating group:

C12(H12A,H12B,H12C)

2) Absolute configurations of **9** and the derivative **11** are determined by X-ray structure analysis of the product **11** (CCDC1489694).



Displacement ellipsoids are drawn at the 30% probability level.

Table 1 Crystal data and structure refinement for BLWyanghua.

Identification code	BLWyanghua
Empirical formula	$C_{23}H_{19}NO_5S_2$
Formula weight	453.51
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	8.62184(14)

b/Å	15.2120(3)
c/Å	16.4772(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2161.08(6)
Z	4
ρ_{calc}g/cm^3	1.394
μ/mm^{-1}	2.538
F(000)	944.0
Crystal size/mm^3	0.15 × 0.1 × 0.08
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.91 to 141.83
Index ranges	-9 ≤ h ≤ 10, -18 ≤ k ≤ 17, -19 ≤ l ≤ 19
Reflections collected	8178
Independent reflections	4097 [R_{int} = 0.0294, R_{sigma} = 0.0385]
Data/restraints/parameters	4097/0/281
Goodness-of-fit on F^2	1.033
Final R indexes [I>=2σ (I)]	R_1 = 0.0348, wR_2 = 0.0886
Final R indexes [all data]	R_1 = 0.0381, wR_2 = 0.0913
Largest diff. peak/hole / e Å^{-3}	0.19/-0.23
Flack parameter	0.015(10)

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for BLWyanghua. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	8116(4)	4308(2)	6808.4(19)	44.1(6)
C2	5946(3)	3396(2)	6516.0(17)	40.7(6)
C3	5095(3)	4240.9(19)	6762.5(16)	38.8(6)
C4	3893(3)	4596(2)	6181.9(17)	42.4(6)
C5	3396(4)	4140(2)	5499.6(18)	51.9(7)
C6	2311(5)	4519(3)	4983(2)	62(1)
C7	1706(5)	5326(3)	5138(2)	65.5(10)
C8	2158(5)	5776(3)	5825(2)	66.9(10)
C9	3262(5)	5420(2)	6335(2)	56.4(8)
C10	2521(4)	3356(2)	7540(2)	51.0(7)
C11	1771(4)	3079(2)	8319(2)	47.1(7)
C12	705(5)	3621(3)	8696(3)	66.0(9)
C13	37(6)	3360(4)	9421(3)	86.1(14)

C14	401(6)	2578(4)	9767(3)	89.0(16)
C15	1442(6)	2043(4)	9400(4)	91.6(17)
C16	2137(5)	2286(3)	8675(3)	73.5(12)
C17	8582(3)	2759.6(19)	6486.9(18)	40.9(6)
C18	8438(4)	2045(2)	7007(2)	52.2(7)
C19	9454(4)	1353(2)	6940(2)	55.7(8)
C20	10639(4)	1371(2)	6371.2(18)	45.7(6)
C21	10795(4)	2089(2)	5857.7(18)	45.4(6)
C22	9750(4)	2779(2)	5920.5(19)	44.7(6)
C23	12837(6)	634(3)	5808(3)	80.8(14)
N1	7547(3)	3490.2(16)	6571.1(15)	41.7(5)
O1	9445(3)	4499.4(16)	6872.2(19)	59.9(6)
O2	5307(3)	2733.0(14)	6317.3(16)	52.2(5)
O3	3756(3)	4814.5(17)	8118.2(14)	60.3(6)
O4	5326(3)	3468.4(19)	8203.9(15)	62.1(6)
O5	11568(3)	646.8(18)	6352.8(18)	67.4(7)
S1	6579.5(9)	5054.1(5)	6980.8(5)	50.0(2)
S2	4219.3(8)	3992.5(5)	7772.9(4)	42.79(18)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for BLWyanghua. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	40.0(16)	43.7(14)	48.8(15)	2.4(12)	-1.1(13)	0.1(12)
C2	37.2(14)	43.2(15)	41.8(13)	-0.8(11)	0.8(12)	1.6(12)
C3	37.6(13)	41.3(14)	37.5(12)	-2.8(11)	-0.7(11)	1.6(11)
C4	39.3(15)	52.4(16)	35.5(12)	3.8(11)	2.3(11)	5.2(12)
C5	51.5(17)	65(2)	38.7(13)	-6.4(13)	-0.3(13)	5.8(17)
C6	57(2)	92(3)	36.7(15)	-0.1(16)	-5.5(14)	-1(2)
C7	57(2)	92(3)	47.6(17)	18.8(17)	-4.4(17)	16(2)
C8	69(2)	70(2)	62(2)	4.7(18)	-4.5(18)	25.8(19)
C9	64(2)	56.4(18)	48.5(16)	-5.2(14)	-6.7(16)	18.3(17)
C10	41.8(16)	65.9(19)	45.4(14)	-6.9(14)	-5.6(13)	-7.2(15)
C11	39.3(15)	50.6(16)	51.4(15)	-2.6(13)	-3.9(13)	-6.2(13)
C12	65(2)	63(2)	70(2)	6.4(18)	15(2)	0(2)
C13	85(3)	92(3)	81(3)	-7(3)	36(3)	-14(3)
C14	83(3)	116(4)	67(2)	23(3)	2(2)	-45(3)
C15	66(3)	85(3)	123(4)	57(3)	-12(3)	-23(3)
C16	52(2)	57(2)	111(3)	11(2)	-1(2)	-4.3(17)
C17	36.2(13)	40.2(14)	46.3(14)	2.2(11)	-2.7(12)	0.8(12)

C18	45.2(15)	54.3(17)	57.1(17)	10.6(14)	11.1(14)	4.6(14)
C19	56.0(18)	50.7(16)	60.3(17)	16.0(15)	4.9(16)	8.7(15)
C20	41.3(14)	47.1(15)	48.7(14)	-0.3(12)	-6.2(13)	8.0(13)
C21	40.4(14)	53.7(16)	42.2(13)	0.6(12)	4.0(13)	1.6(14)
C22	43.6(15)	46.5(15)	43.9(14)	6.8(12)	-0.9(12)	-1.2(13)
C23	73(3)	94(3)	76(3)	4(2)	11(2)	46(3)
N1	35.0(12)	40.6(12)	49.6(12)	1.8(10)	-1.2(10)	0.8(10)
O1	38.5(12)	54.7(12)	86.5(17)	-4.7(12)	-2.4(12)	-6.9(10)
O2	42.4(11)	45.6(12)	68.5(13)	-10.8(10)	-4.6(10)	-1.2(9)
O3	68.0(16)	68.2(15)	44.6(11)	-13.8(11)	9.3(11)	-3.9(12)
O4	49.9(13)	81.7(17)	54.8(12)	16.8(13)	-12.9(10)	-5.1(12)
O5	62.8(15)	63.2(15)	76.3(16)	12.2(13)	7.6(14)	25.0(13)
S1	42.6(4)	39.9(3)	67.5(5)	-7.8(3)	-1.3(3)	-1.0(3)
S2	39.6(3)	55.3(4)	33.5(3)	-1.1(3)	-3.9(3)	-3.1(3)

Table 4 Bond Lengths for BLWyanghua.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	N1	1.394(4)	C11	C12	1.382(5)
C1	O1	1.186(4)	C11	C16	1.377(5)
C1	S1	1.767(3)	C12	C13	1.385(6)
C2	C3	1.534(4)	C13	C14	1.356(8)
C2	N1	1.391(4)	C14	C15	1.355(9)
C2	O2	1.195(4)	C15	C16	1.387(8)
C3	C4	1.510(4)	C17	C18	1.390(4)
C3	S1	1.816(3)	C17	C22	1.373(4)
C3	S2	1.867(3)	C17	N1	1.432(4)
C4	C5	1.389(4)	C18	C19	1.374(5)
C4	C9	1.389(5)	C19	C20	1.386(5)
C5	C6	1.389(5)	C20	C21	1.388(4)
C6	C7	1.358(6)	C20	O5	1.362(4)
C7	C8	1.379(6)	C21	C22	1.387(4)
C8	C9	1.381(5)	C23	O5	1.416(5)
C10	C11	1.498(5)	O3	S2	1.431(3)
C10	S2	1.797(3)	O4	S2	1.432(3)

Table 5 Bond Angles for BLWyanghua.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°

N1	C1	S1	110.7(2)	C14	C13	C12	121.2(5)
O1	C1	N1	125.7(3)	C15	C14	C13	119.5(4)
O1	C1	S1	123.5(3)	C14	C15	C16	120.7(5)
N1	C2	C3	111.8(3)	C11	C16	C15	120.1(5)
O2	C2	C3	124.0(3)	C18	C17	N1	119.5(3)
O2	C2	N1	124.2(3)	C22	C17	C18	120.1(3)
C2	C3	S1	106.6(2)	C22	C17	N1	120.4(3)
C2	C3	S2	105.06(19)	C19	C18	C17	119.6(3)
C4	C3	C2	117.4(2)	C18	C19	C20	120.6(3)
C4	C3	S1	111.4(2)	C19	C20	C21	119.9(3)
C4	C3	S2	111.1(2)	O5	C20	C19	115.6(3)
S1	C3	S2	104.25(14)	O5	C20	C21	124.5(3)
C5	C4	C3	123.1(3)	C22	C21	C20	119.1(3)
C9	C4	C3	118.5(3)	C17	C22	C21	120.7(3)
C9	C4	C5	118.5(3)	C1	N1	C17	120.0(2)
C4	C5	C6	119.8(3)	C2	N1	C1	117.4(3)
C7	C6	C5	121.2(3)	C2	N1	C17	122.2(3)
C6	C7	C8	119.6(3)	C20	O5	C23	118.6(3)
C7	C8	C9	120.0(4)	C1	S1	C3	93.40(13)
C8	C9	C4	120.9(3)	C10	S2	C3	104.36(14)
C11	C10	S2	108.7(2)	O3	S2	C3	106.90(14)
C12	C11	C10	120.3(3)	O3	S2	C10	109.16(16)
C16	C11	C10	120.8(4)	O3	S2	O4	118.39(17)
C16	C11	C12	118.9(4)	O4	S2	C3	106.60(14)
C11	C12	C13	119.5(4)	O4	S2	C10	110.44(16)

Table 6 Torsion Angles for BLWyanghua.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C2	C3	C4	C5	8.4(4)	C18	C19	C20	O5	-179.4(3)
C2	C3	C4	C9	-171.3(3)	C19	C20	C21	C22	-0.3(5)
C2	C3	S1	C1	-2.6(2)	C19	C20	O5	C23	-177.7(4)
C2	C3	S2	C10	-78.7(2)	C20	C21	C22	C17	0.6(5)
C2	C3	S2	O3	165.7(2)	C21	C20	O5	C23	3.7(6)
C2	C3	S2	O4	38.2(2)	C22	C17	C18	C19	-1.2(5)
C3	C2	N1	C1	-1.7(4)	C22	C17	N1	C1	-62.9(4)
C3	C2	N1	C17	170.8(2)	C22	C17	N1	C2	124.7(3)
C3	C4	C5	C6	-178.5(3)	N1	C1	S1	C3	1.8(2)
C3	C4	C9	C8	-180.0(4)	N1	C2	C3	C4	128.6(3)
C4	C3	S1	C1	-131.9(2)	N1	C2	C3	S1	2.9(3)

C4	C3	S2	C10	49.2(2)	N1	C2	C3	S2	-107.4(2)
C4	C3	S2	O3	-66.4(2)	N1	C17	C18	C19	-178.4(3)
C4	C3	S2	O4	166.1(2)	N1	C17	C22	C21	177.4(3)
C4	C5	C6	C7	-1.0(6)	O1	C1	N1	C2	-178.8(3)
C5	C4	C9	C8	0.3(6)	O1	C1	N1	C17	8.5(5)
C5	C6	C7	C8	-0.8(6)	O1	C1	S1	C3	-179.7(3)
C6	C7	C8	C9	2.3(6)	O2	C2	C3	C4	-52.8(4)
C7	C8	C9	C4	-2.1(6)	O2	C2	C3	S1	-178.5(3)
C9	C4	C5	C6	1.2(5)	O2	C2	C3	S2	71.2(3)
C10	C11	C12	C13	-179.1(4)	O2	C2	N1	C1	179.7(3)
C10	C11	C16	C15	179.4(4)	O2	C2	N1	C17	-7.7(5)
C11	C10	S2	C3	177.0(2)	O5	C20	C21	C22	178.3(3)
C11	C10	S2	O3	-69.0(3)	S1	C1	N1	C2	-0.4(3)
C11	C10	S2	O4	62.8(3)	S1	C1	N1	C17	-173.1(2)
C11	C12	C13	C14	-0.5(8)	S1	C3	C4	C5	131.7(3)
C12	C11	C16	C15	-0.1(6)	S1	C3	C4	C9	-48.0(4)
C12	C13	C14	C15	0.3(8)	S1	C3	S2	C10	169.29(16)
C13	C14	C15	C16	0.0(8)	S1	C3	S2	O3	53.71(18)
C14	C15	C16	C11	-0.1(7)	S1	C3	S2	O4	-73.82(18)
C16	C11	C12	C13	0.3(6)	S2	C3	C4	C5	-112.5(3)
C17	C18	C19	C20	1.4(6)	S2	C3	C4	C9	67.8(3)
C18	C17	C22	C21	0.1(5)	S2	C3	S1	C1	108.19(16)
C18	C17	N1	C1	114.4(3)	S2	C10	C11	C12	87.4(4)
C18	C17	N1	C2	-58.0(4)	S2	C10	C11	C16	-92.1(4)
C18	C19	C20	C21	-0.7(5)					

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for BLWyanghua.

Atom	***x***	***y***	***z***	**U(eq)**
H5	3787	3583	5389	62
H6	1994	4214	4523	74
H7	990	5573	4783	79
H8	1720	6320	5944	80
H9	3586	5736	6788	68
H10A	1802	3706	7222	61
H10B	2807	2843	7225	61
H12	438	4157	8464	79
H13	-675	3728	9675	103
H14	-61	2410	10253	107

H15	1694	1506	9636	110
H16	2851	1914	8428	88
H18	7660	2035	7397	63
H19	9346	868	7279	67
H21	11590	2107	5477	54
H22	9841	3260	5575	54
H23A	12460	670	5261	121
H23B	13410	99	5877	121
H23C	13502	1127	5916	121

Experimental

The crystal was kept at 293(2) K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal Data for $C_{23}H_{19}NO_5S_2$ (M =453.51 g/mol): orthorhombic, space group $P2_12_12_1$ (no. 19), a = 8.62184(14) Å, b = 15.2120(3) Å, c = 16.4772(2) Å, V = 2161.08(6) Å^3, Z = 4, T = 293(2) K, μ(CuKα) = 2.538 mm^{-1}, *Dcalc* = 1.394 g/cm^3, 8178 reflections measured (7.91° ≤ 2Θ ≤ 141.83°), 4097 unique (R_{int} = 0.0294, R_{sigma} = 0.0385) which were used in all calculations. The final R_1 was 0.0348 (I > 2σ(I)) and wR_2 was 0.0913 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

1. Fixed Uiso

 At 1.2 times of:

  All C(H) groups, All C(H,H) groups

 At 1.5 times of:

  All C(H,H,H) groups

2.a Secondary CH2 refined with riding coordinates:

 C10(H10A,H10B)

2.b Aromatic/amide H refined with riding coordinates:

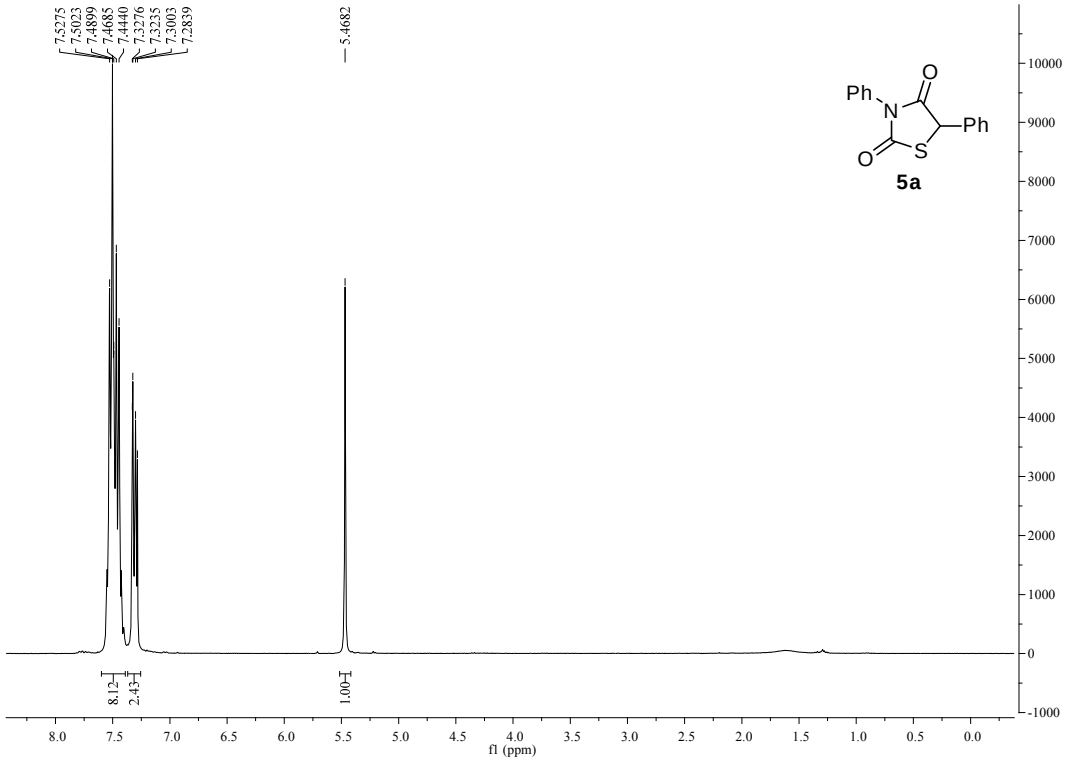
 C5(H5), C6(H6), C7(H7), C8(H8), C9(H9), C12(H12), C13(H13), C14(H14),

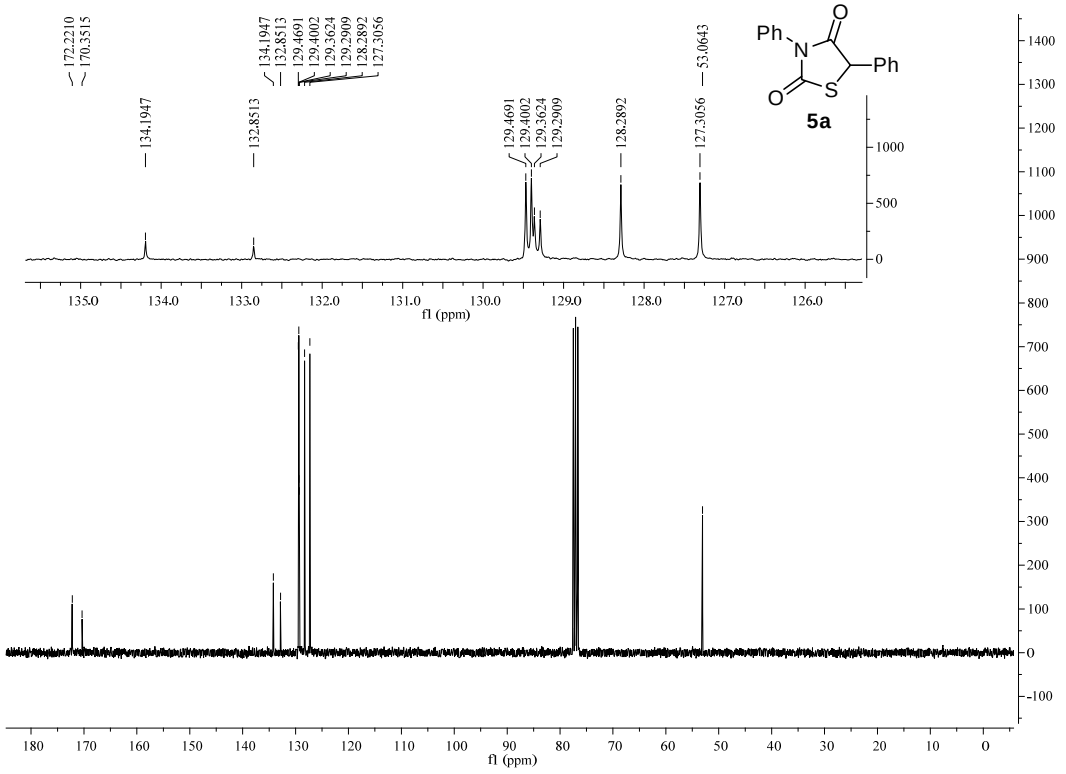
 C15(H15), C16(H16), C18(H18), C19(H19), C21(H21), C22(H22)

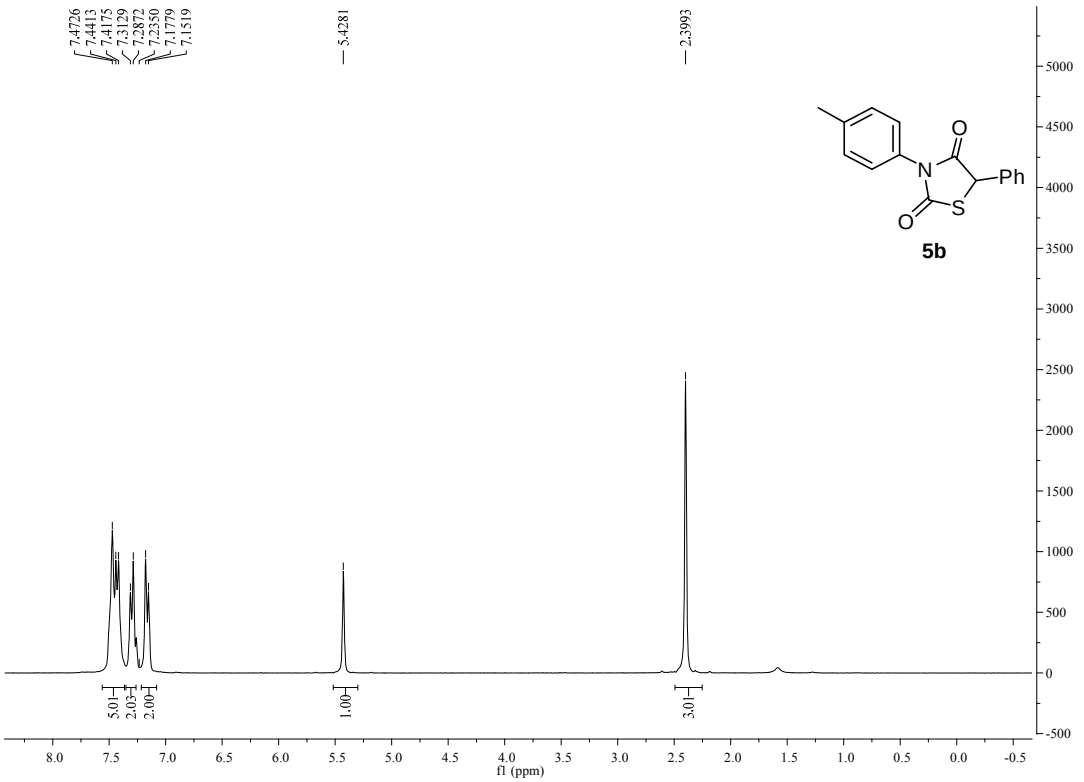
2.c Idealised Me refined as rotating group:

 C23(H23A,H23B,H23C)

4. Copies of NMR spectra.



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7.2872
7.2350
7.1779
7.1519
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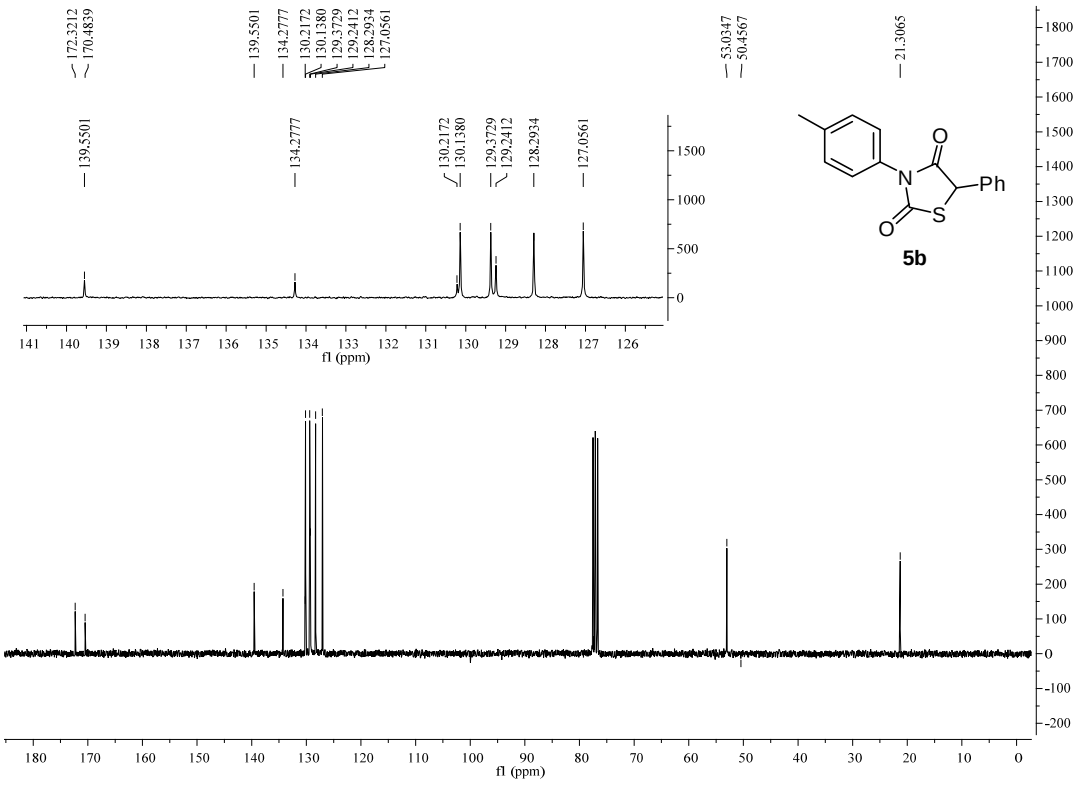
2.3993
5.01
2.03
2.00
1.00
3.01
fl (ppm)
O
N
Ph
S
O
5b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129.3729
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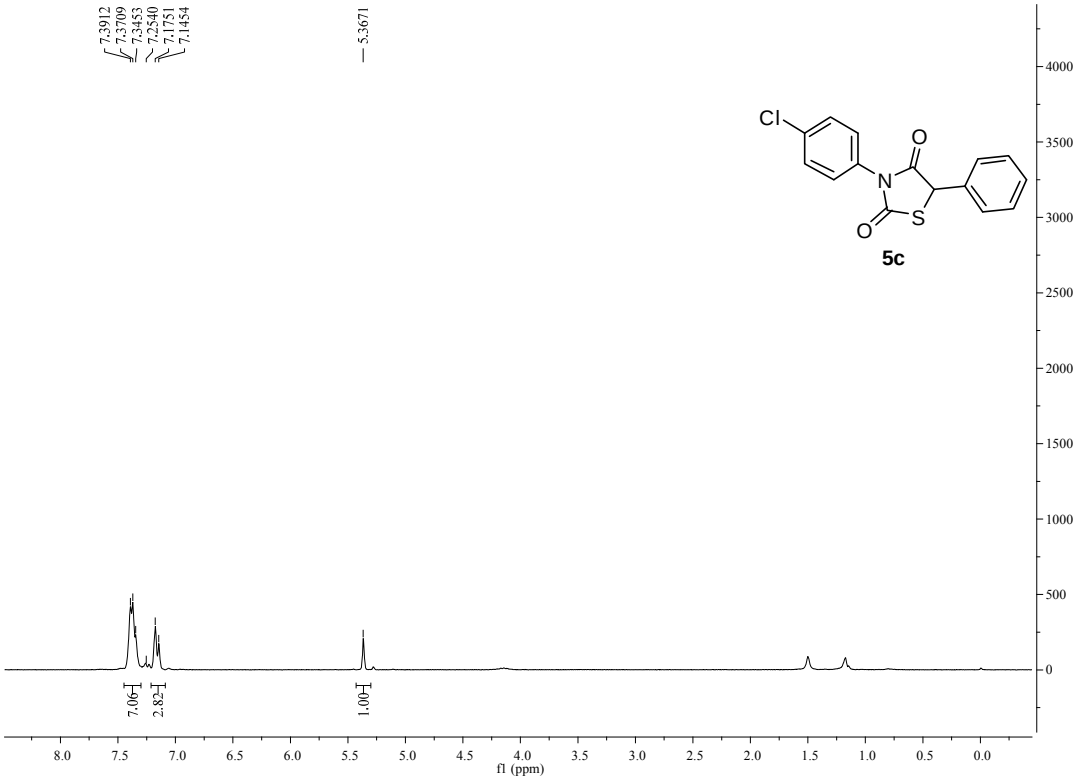
53.0347
50.4567
21.3065
fl (ppm)
O
N
Ph
S
O
5b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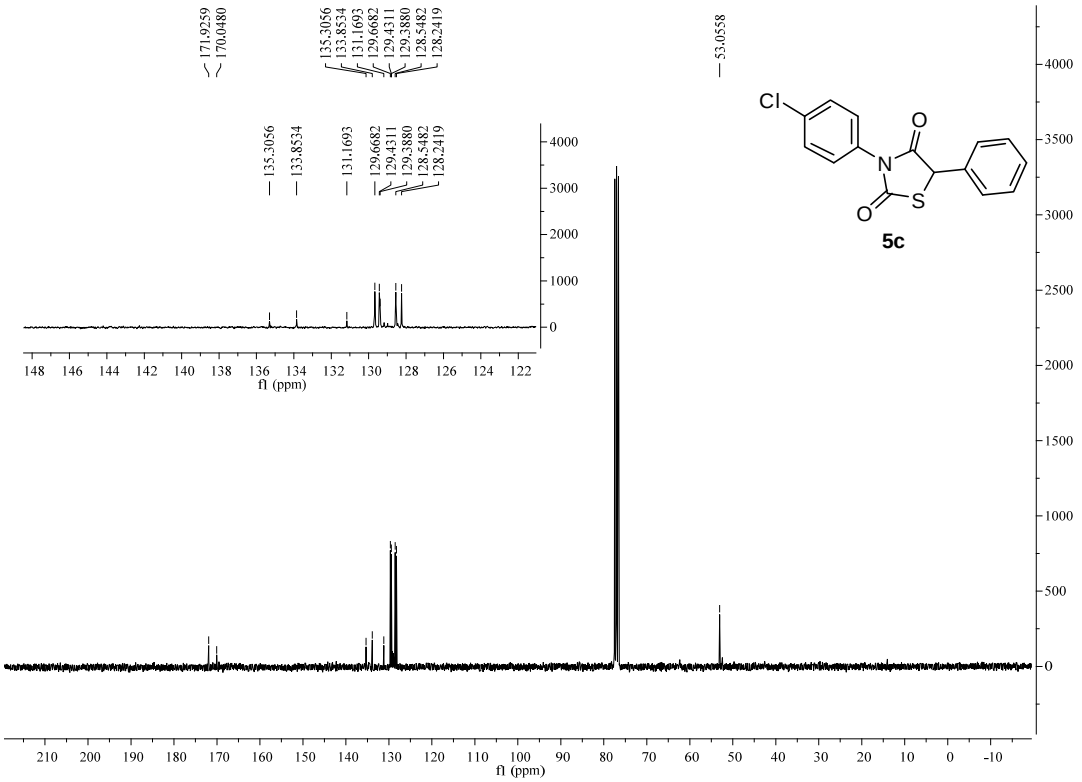
N
S
O
5c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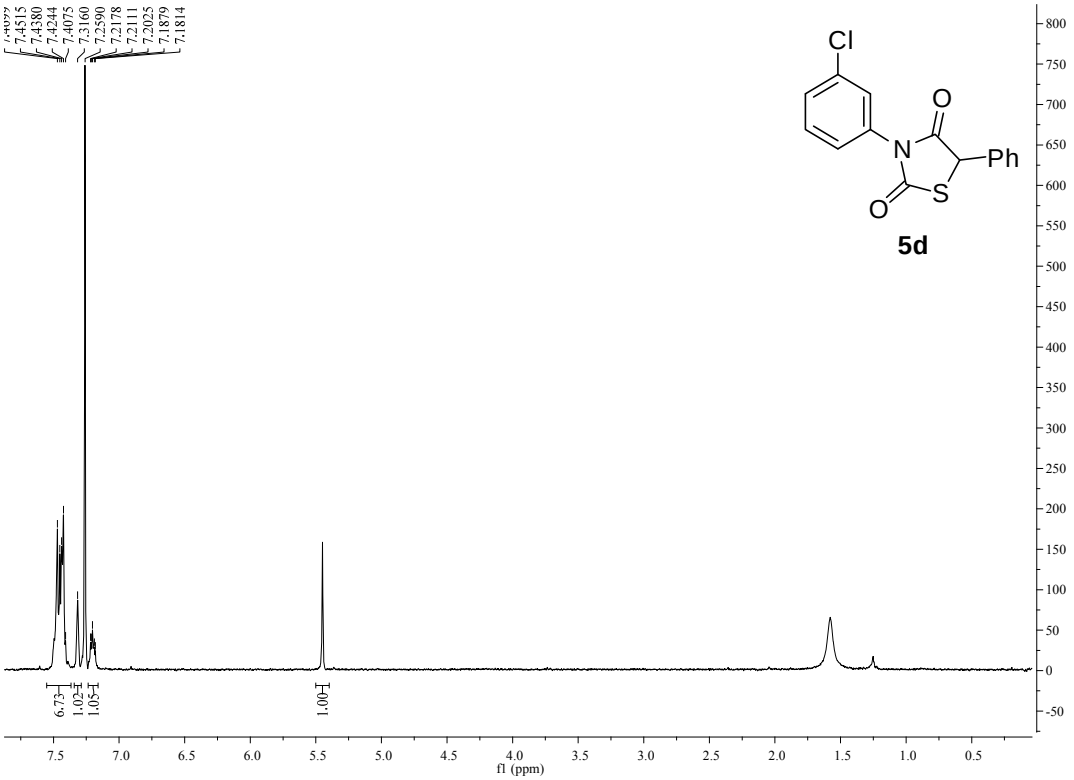
f1 (ppm)
Cl
O
N
S
O
5c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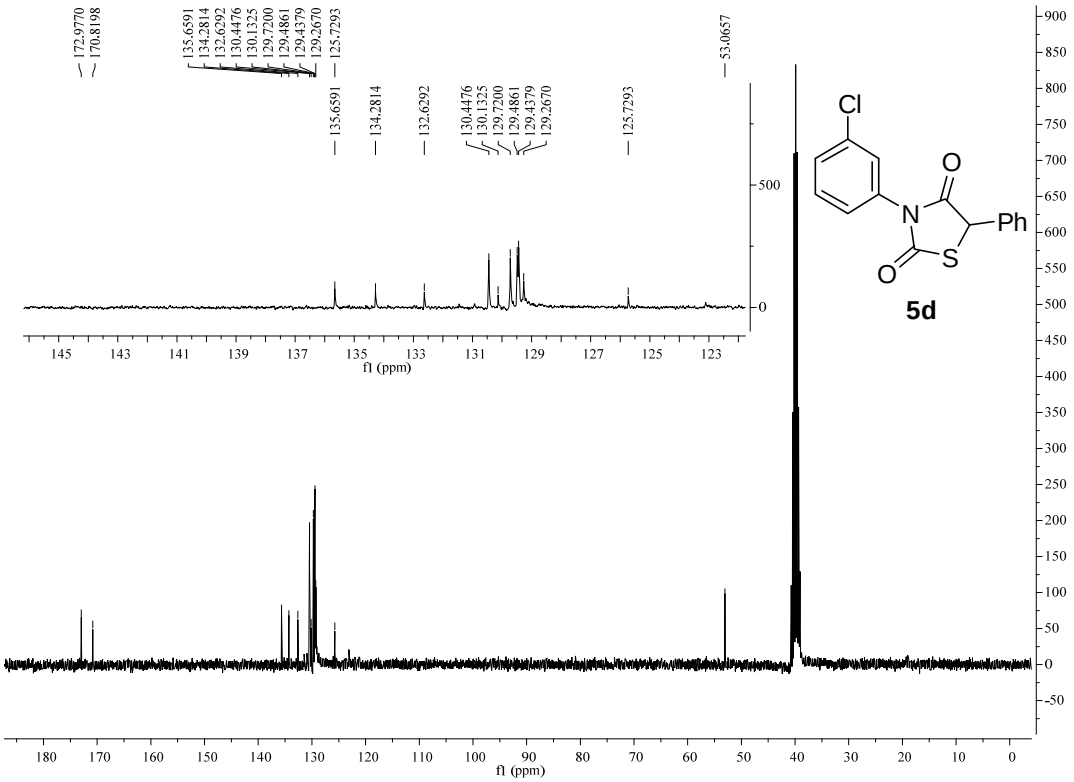
6.73
1.02
1.05
1.00
f1 (ppm)
Cl
O
N
Ph
S
O
5d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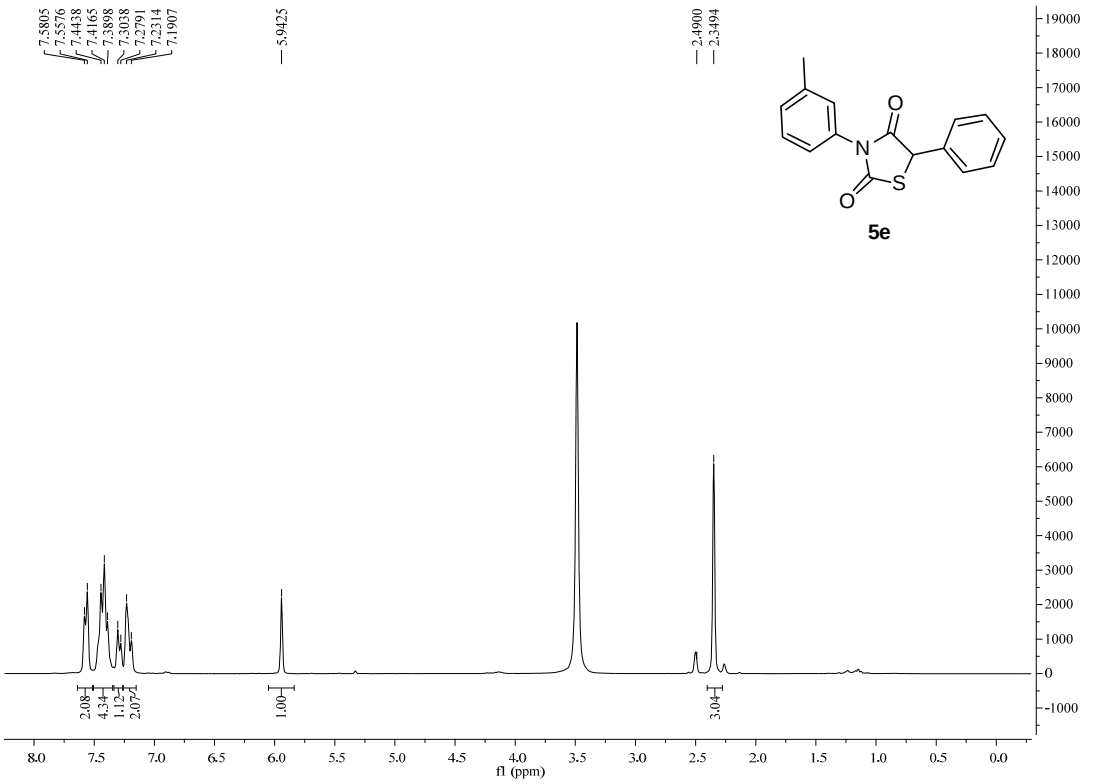
f1 (ppm)
Cl
O
N
Ph
S
O
5d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7.2791
7.2314
7.1907
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1.12
2.07
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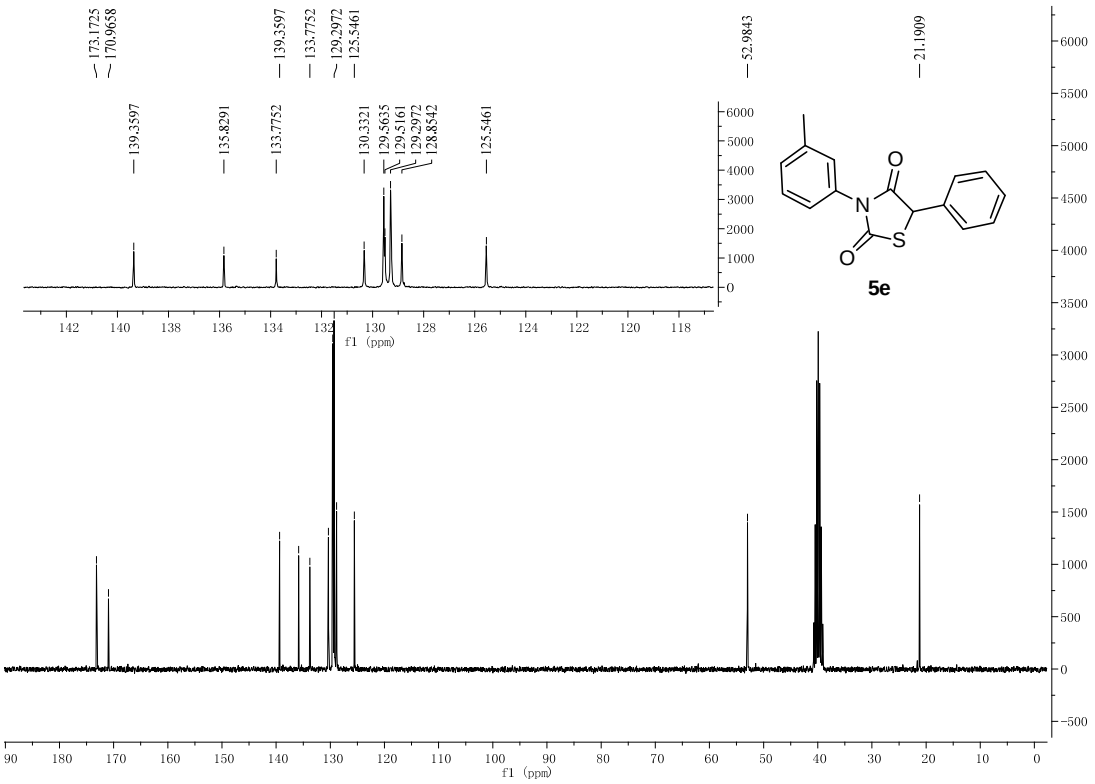
f1 (ppm)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128.8542
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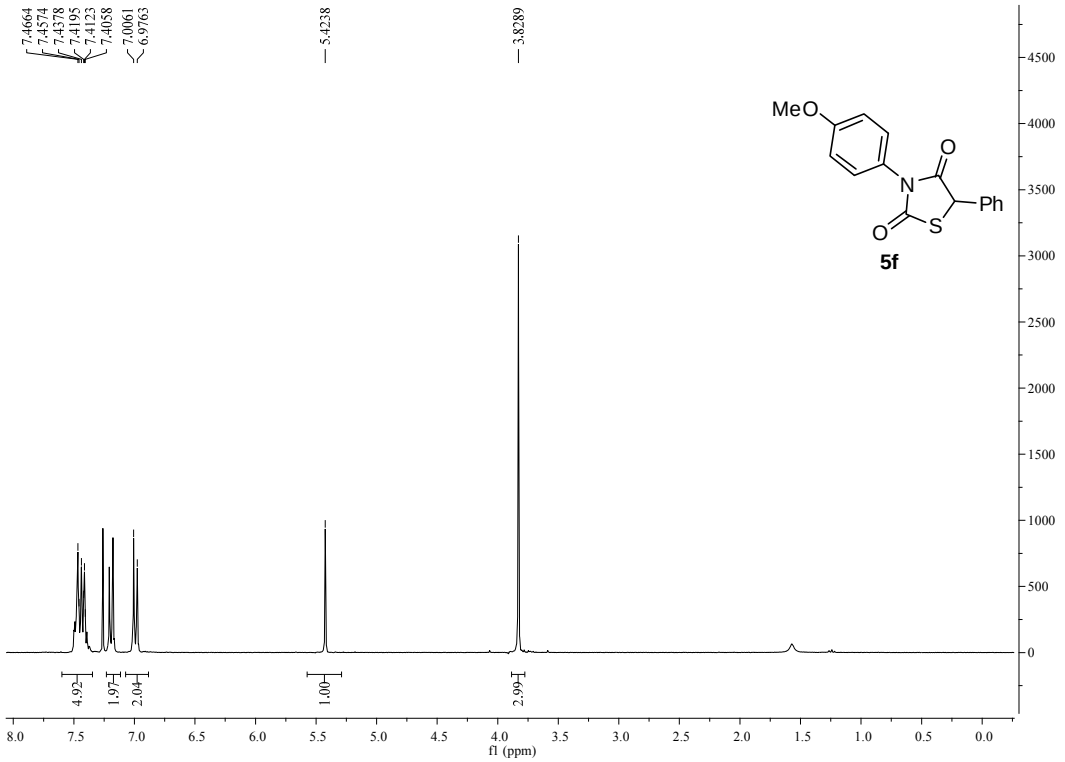
5e
f1 (ppm)
f1 (ppm)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Ph
O
S
5f
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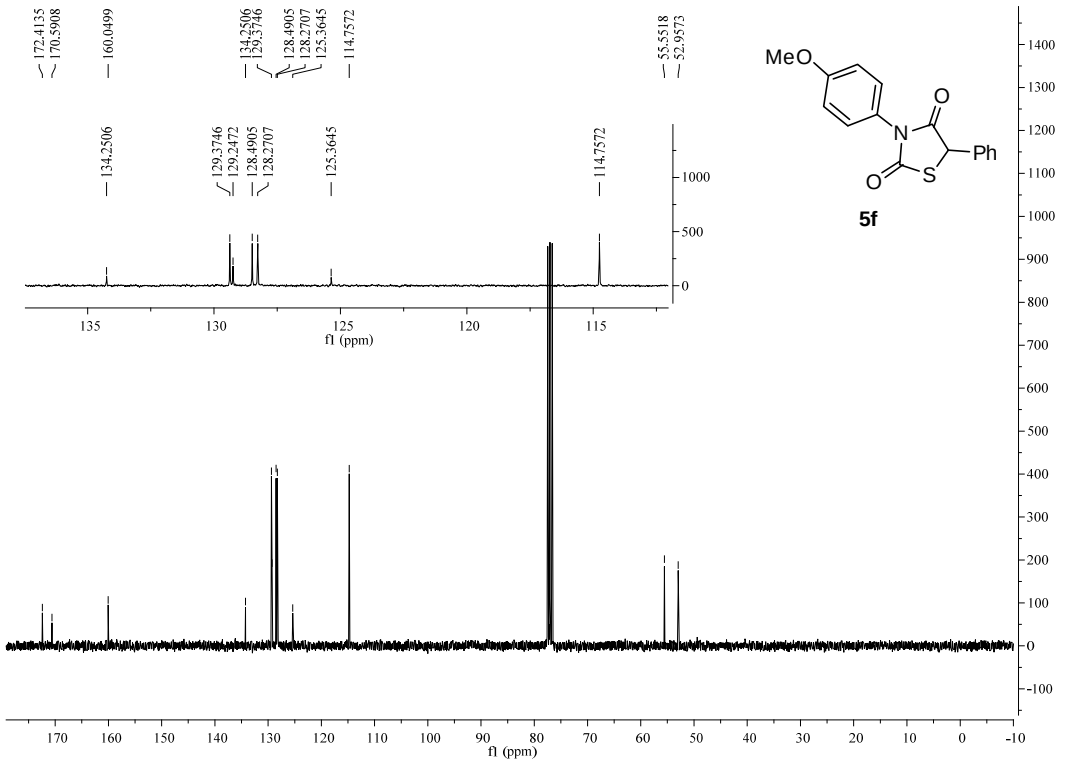
2.99
fl (ppm)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Ph
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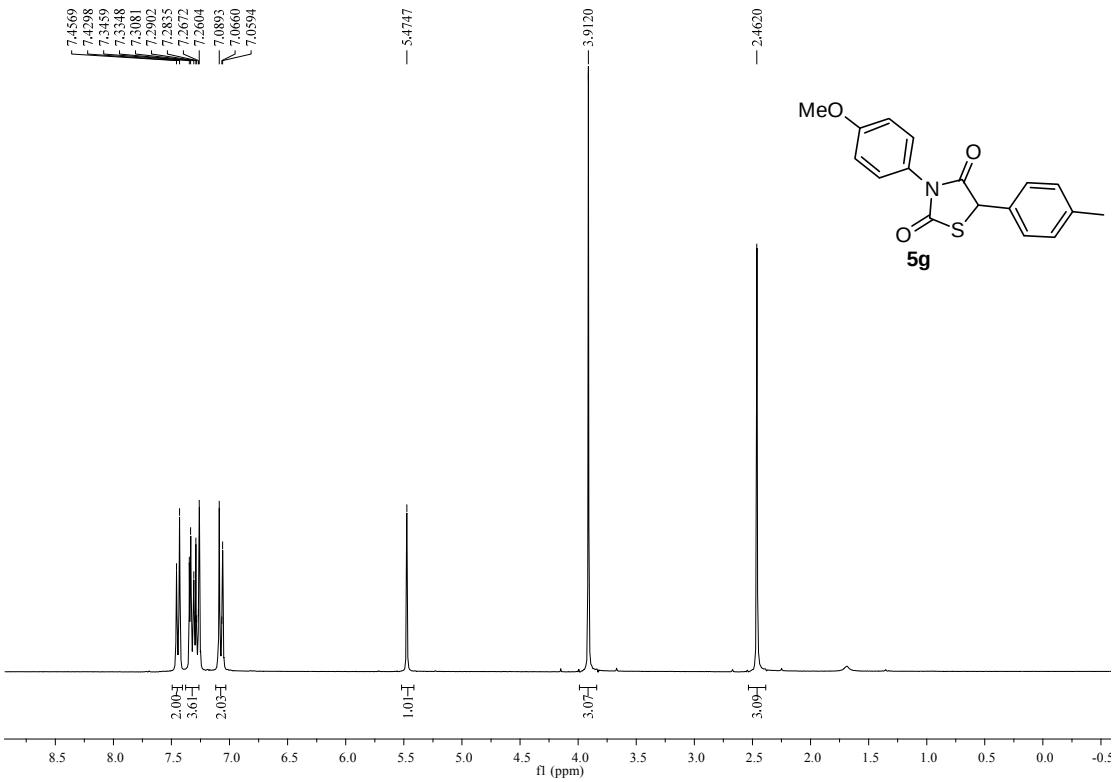
S
5f
fl (ppm)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S
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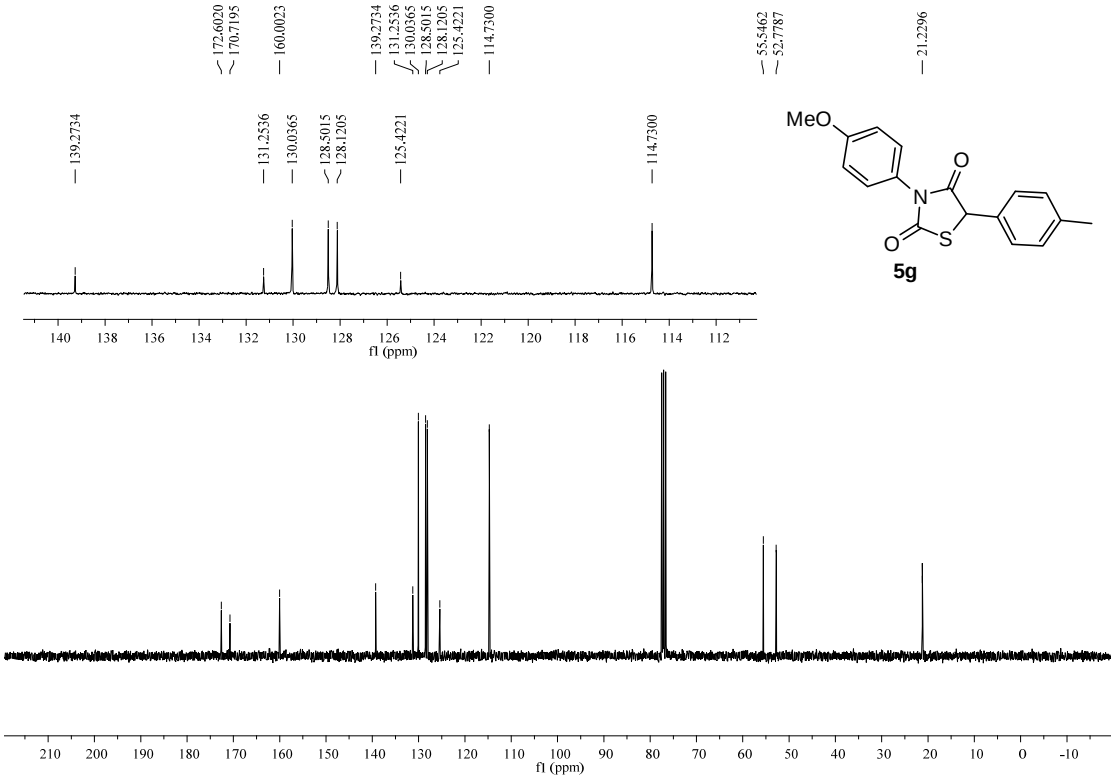
f1 (ppm)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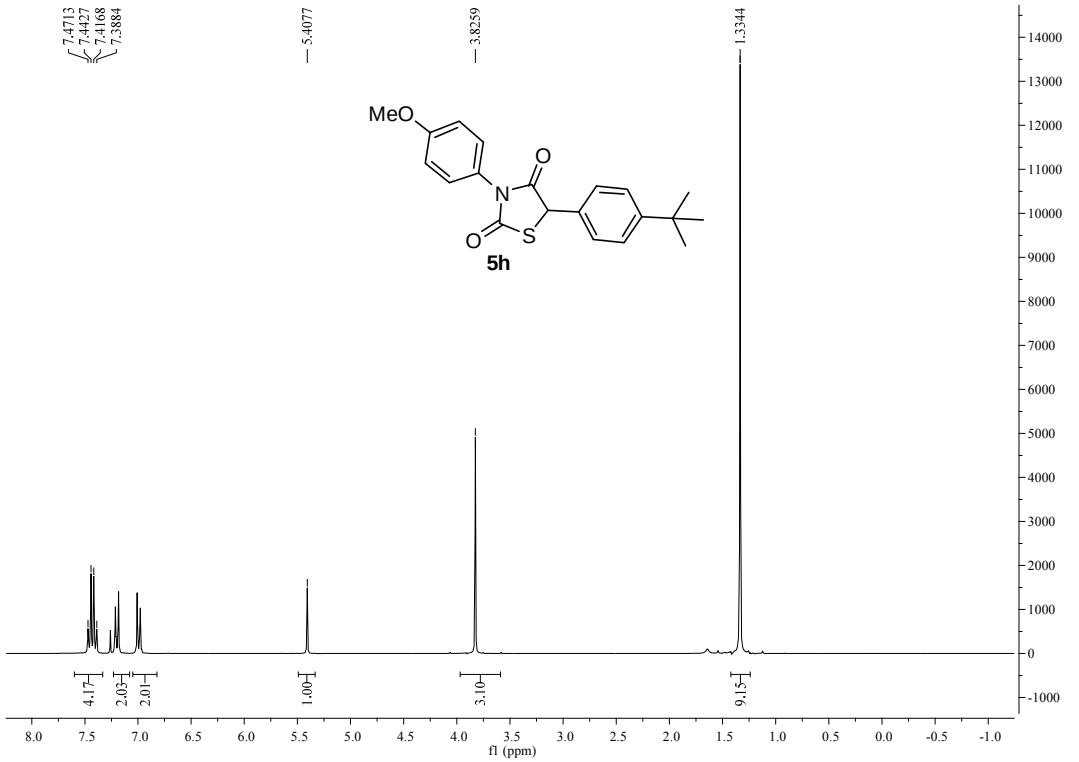
5g
f1 (ppm)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5.4077
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N
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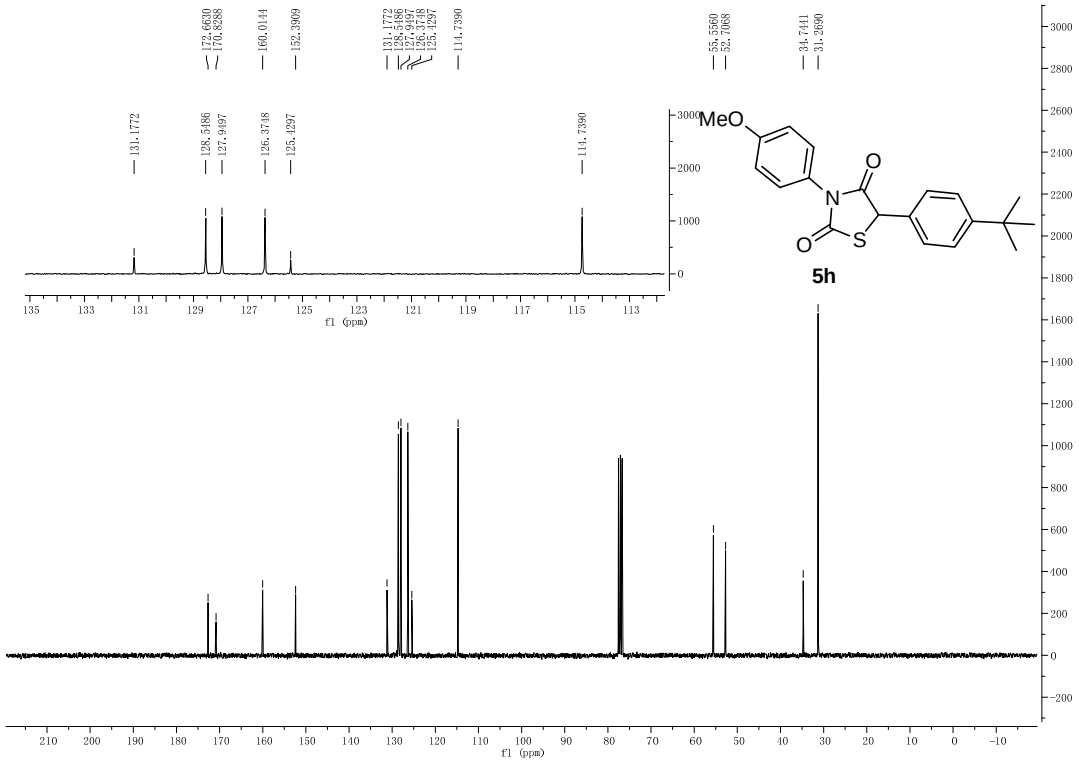
f1 (ppm)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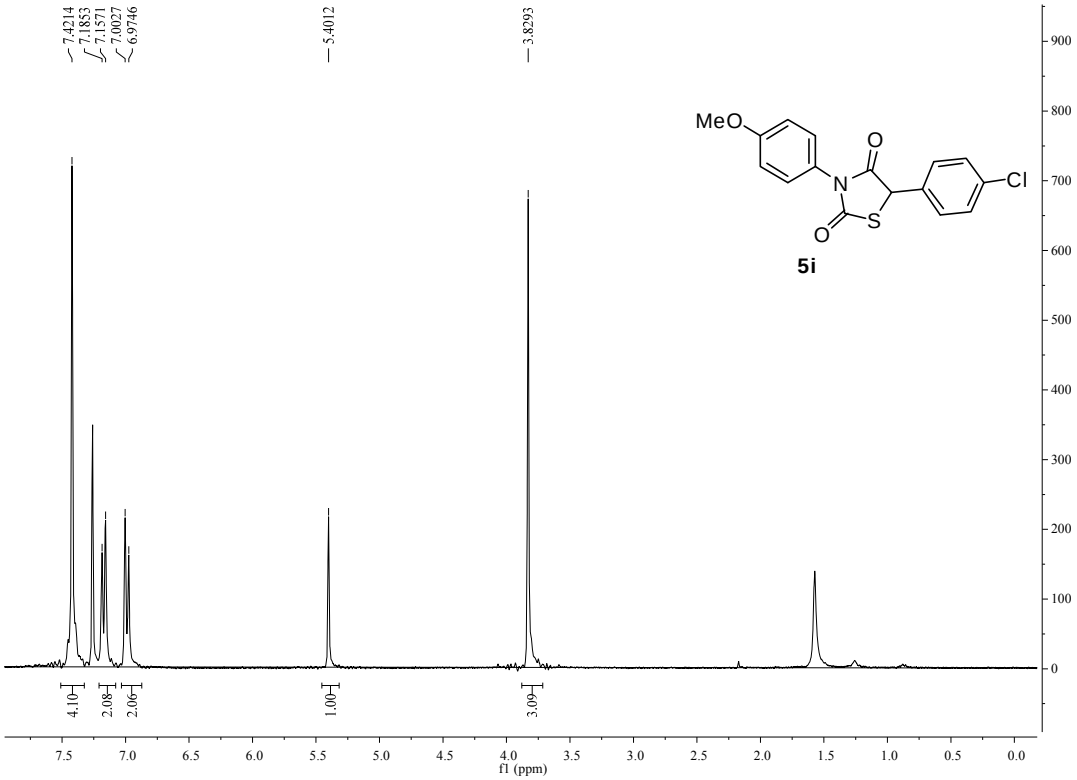
S
5h
f1 (ppm)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2.06
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3.09
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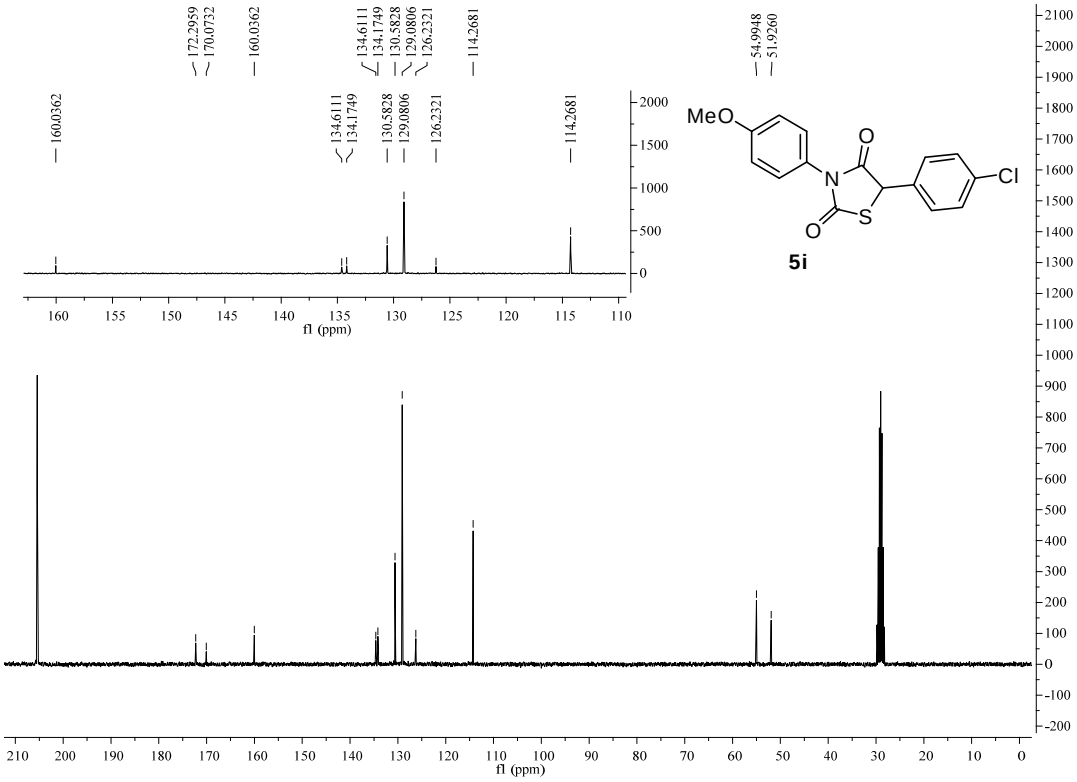
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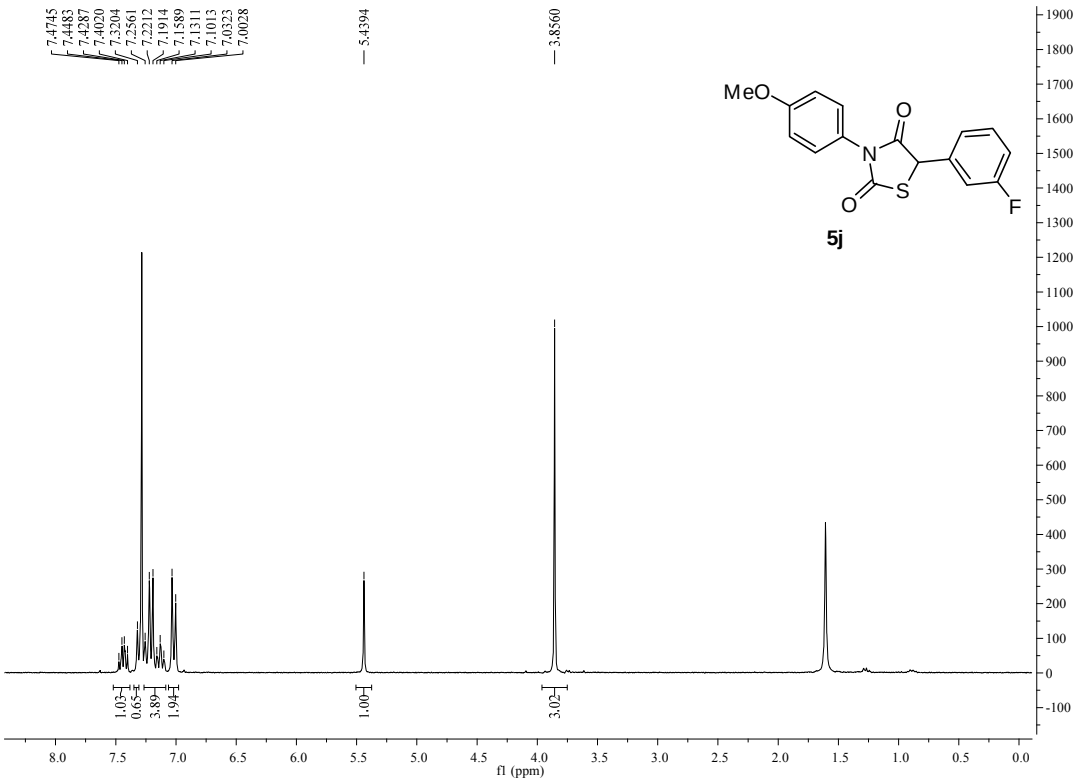
f1 (ppm)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7.1013
7.0323
7.0028
5.4394
3.8560
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S
O
F
5j
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1.94
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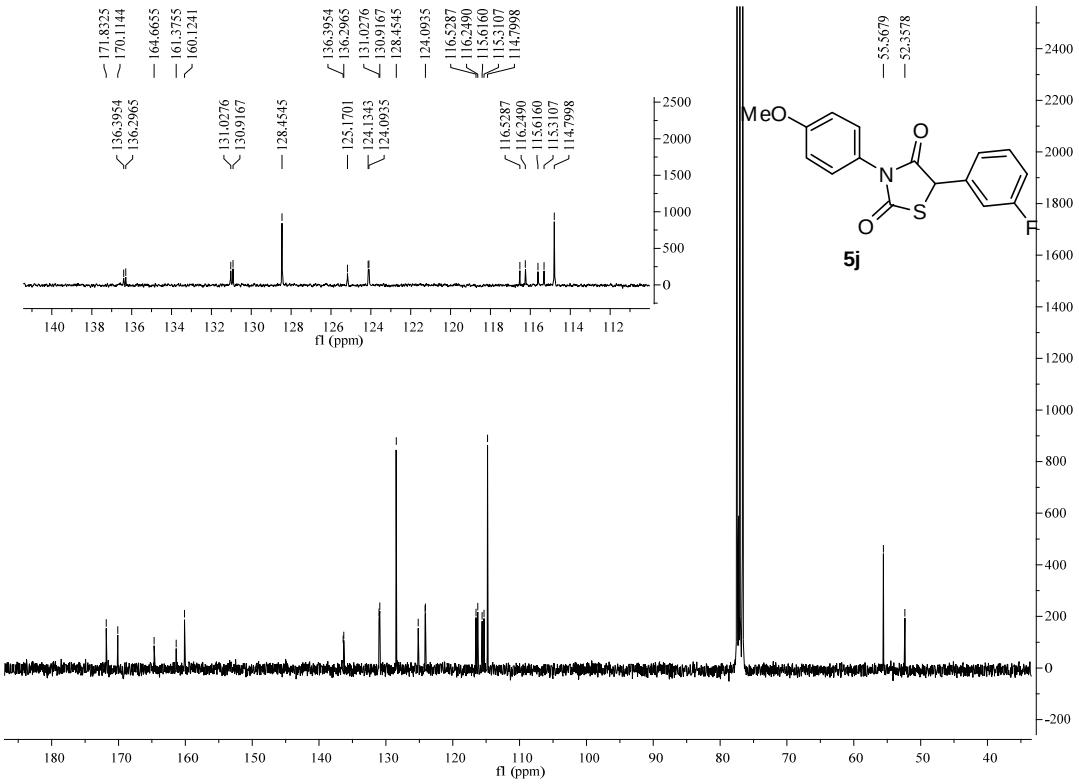
3.02
f1 (ppm)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124.1343
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S
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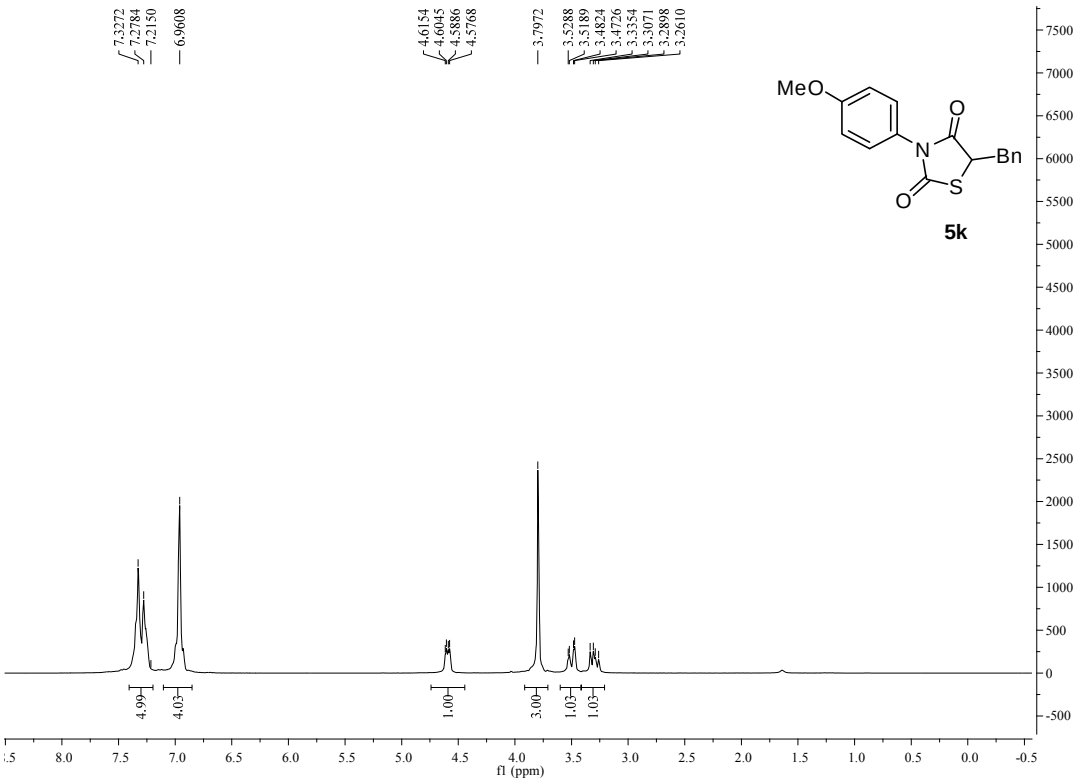
F
5j
f1 (ppm)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3.5189
3.4824
3.4726
3.3354
3.3071
3.2898
3.2610
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Bn
S
O
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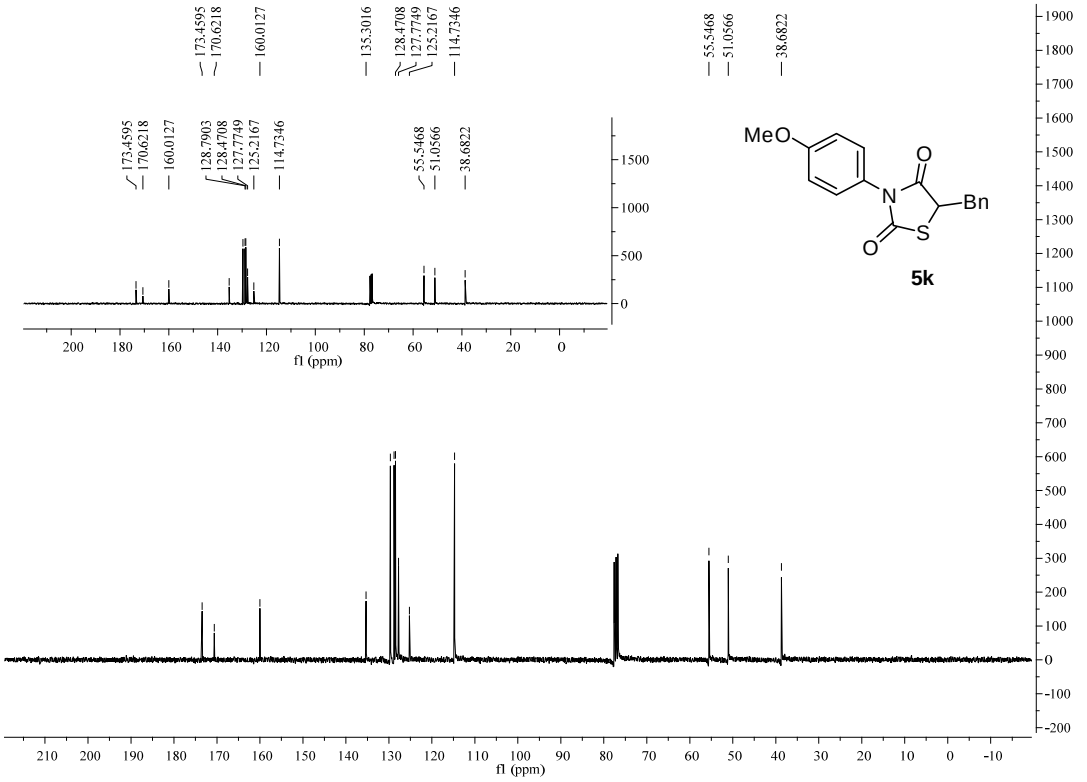
4.99
4.03
1.00
3.00
1.03
1.03
f1 (ppm)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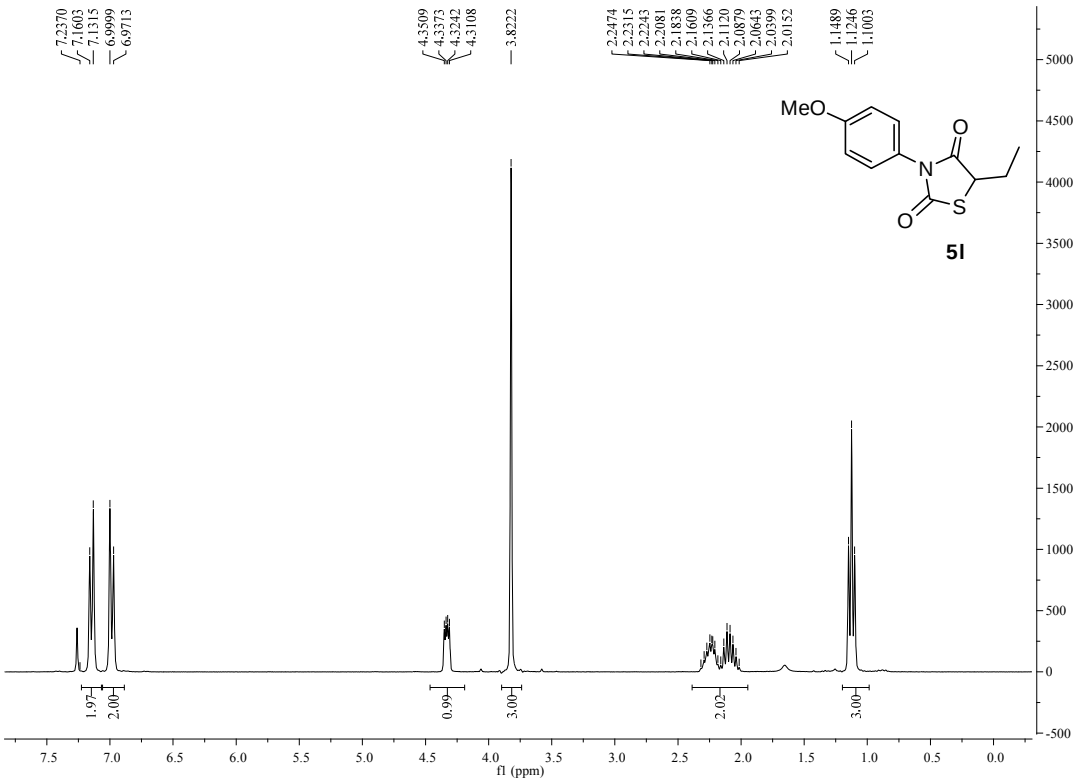
O
5k
f1 (ppm)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2.1609
2.1366
2.1120
2.0879
2.0643
2.0399
2.0152
1.1489
1.1246
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3.00
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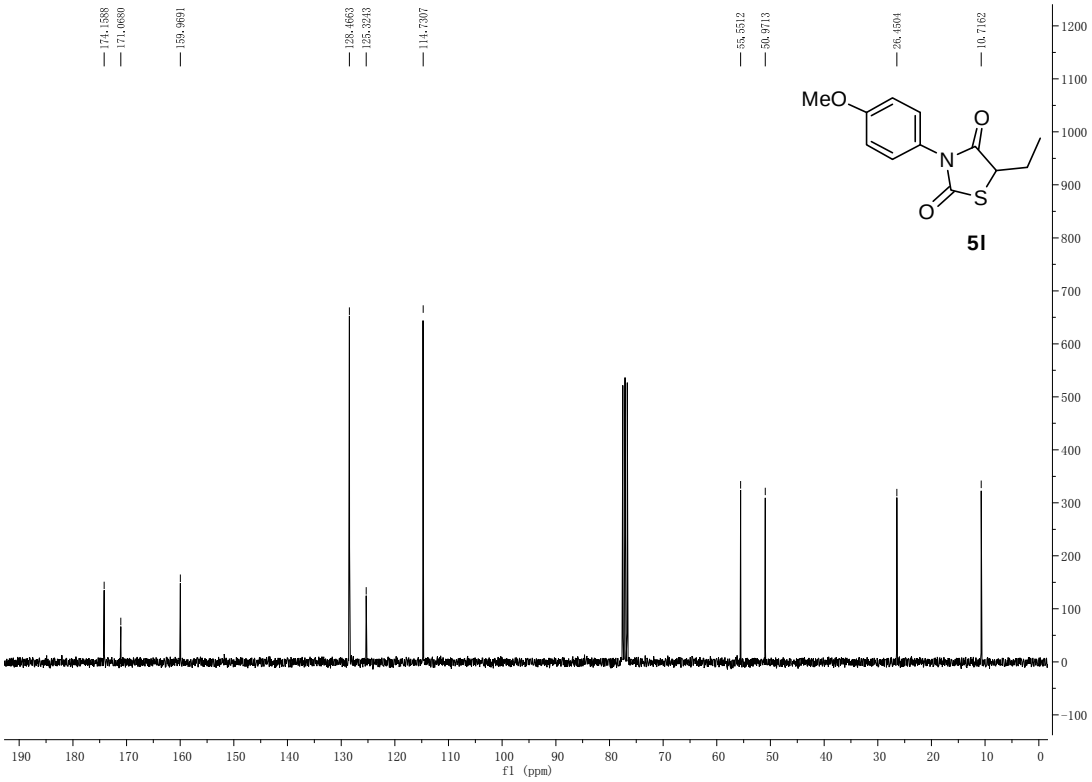
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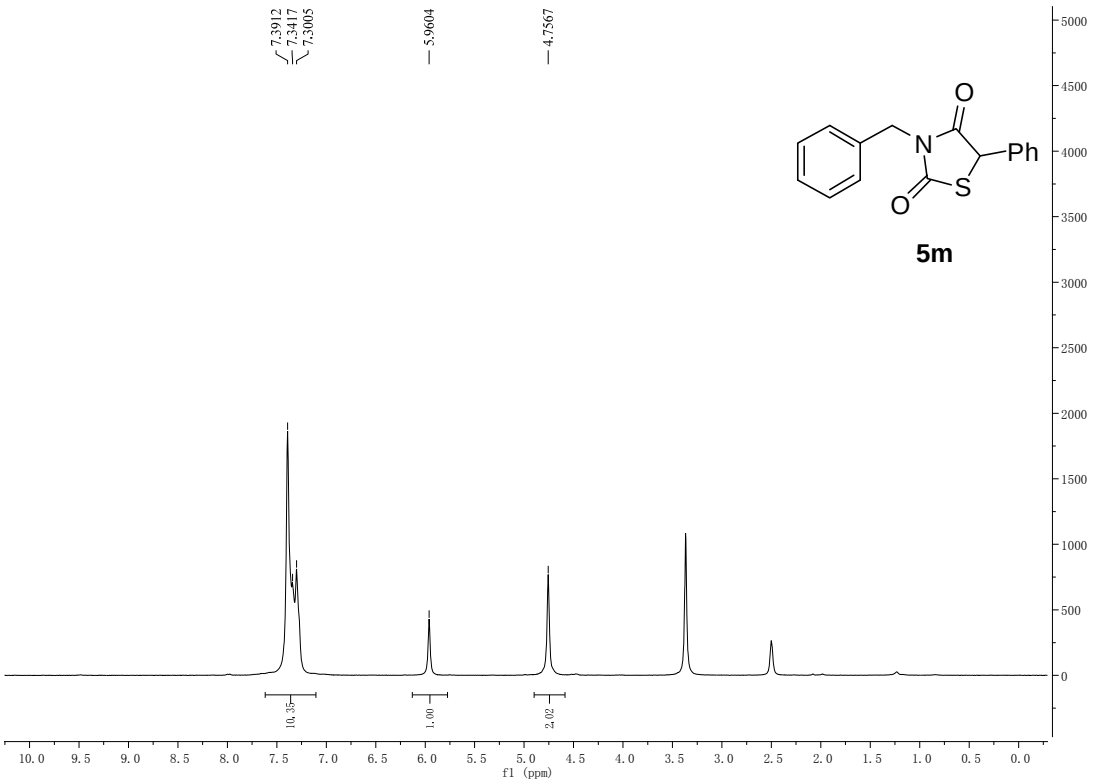
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S
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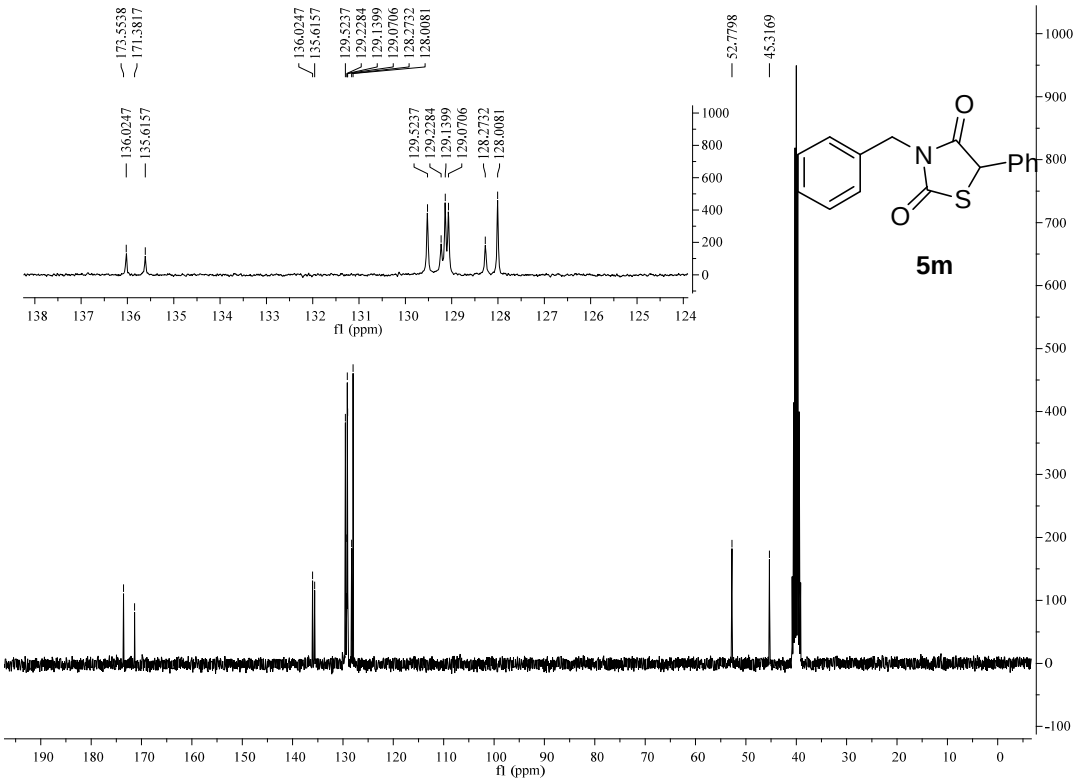
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Ph
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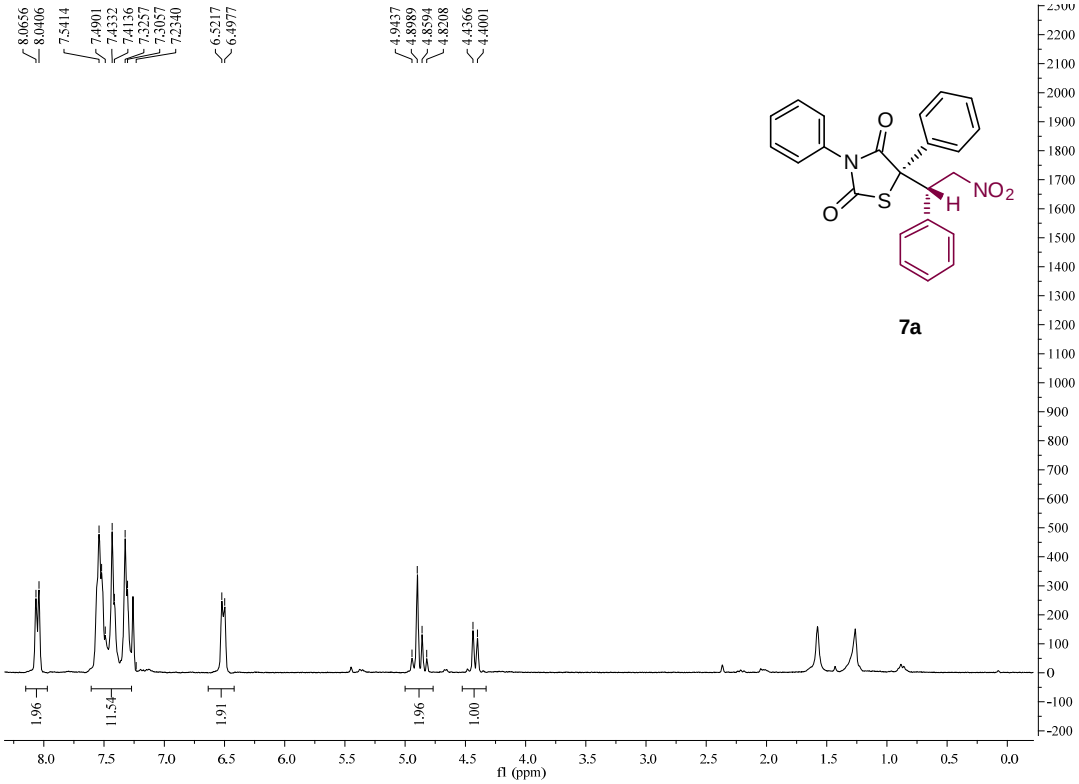
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1.91
1.96
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fl (ppm)
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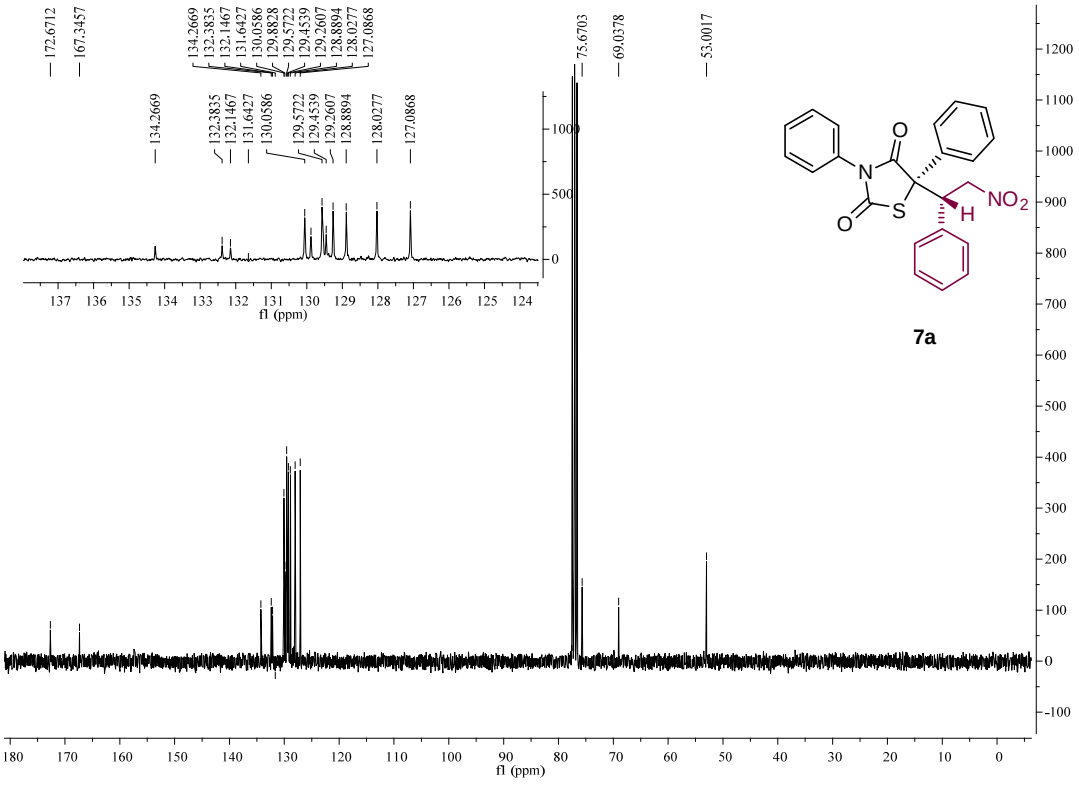
S
O
H
NO2

7a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fl (ppm)
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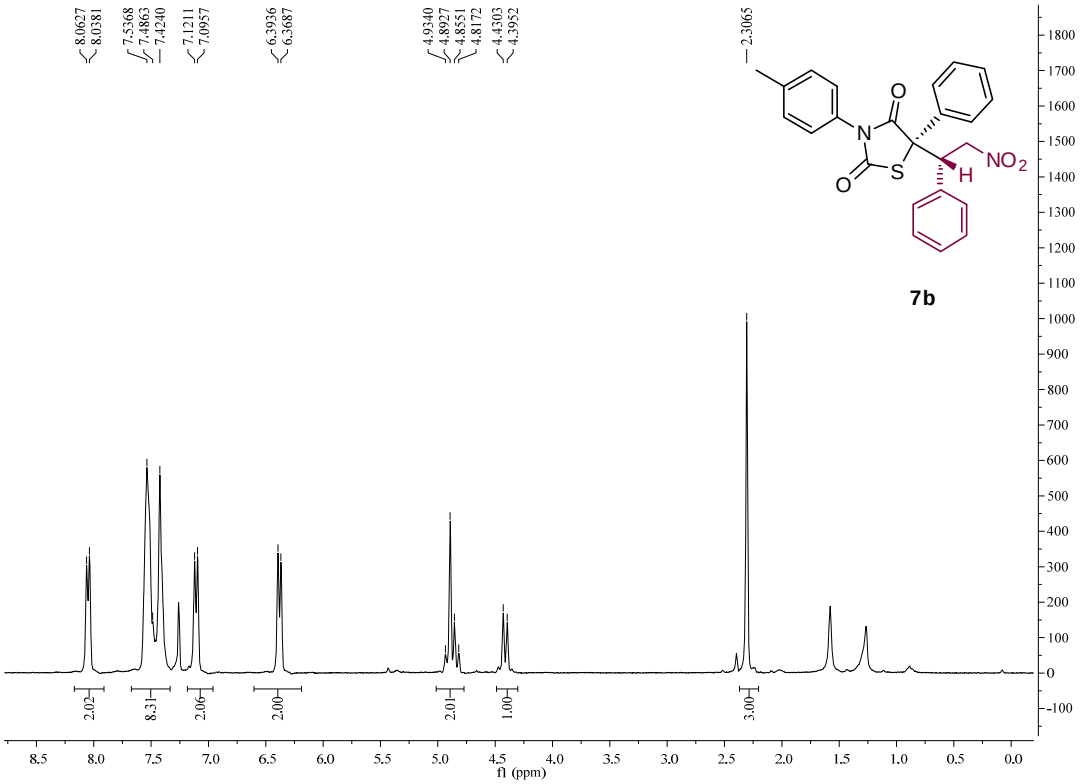
S
O
H
NO2

7a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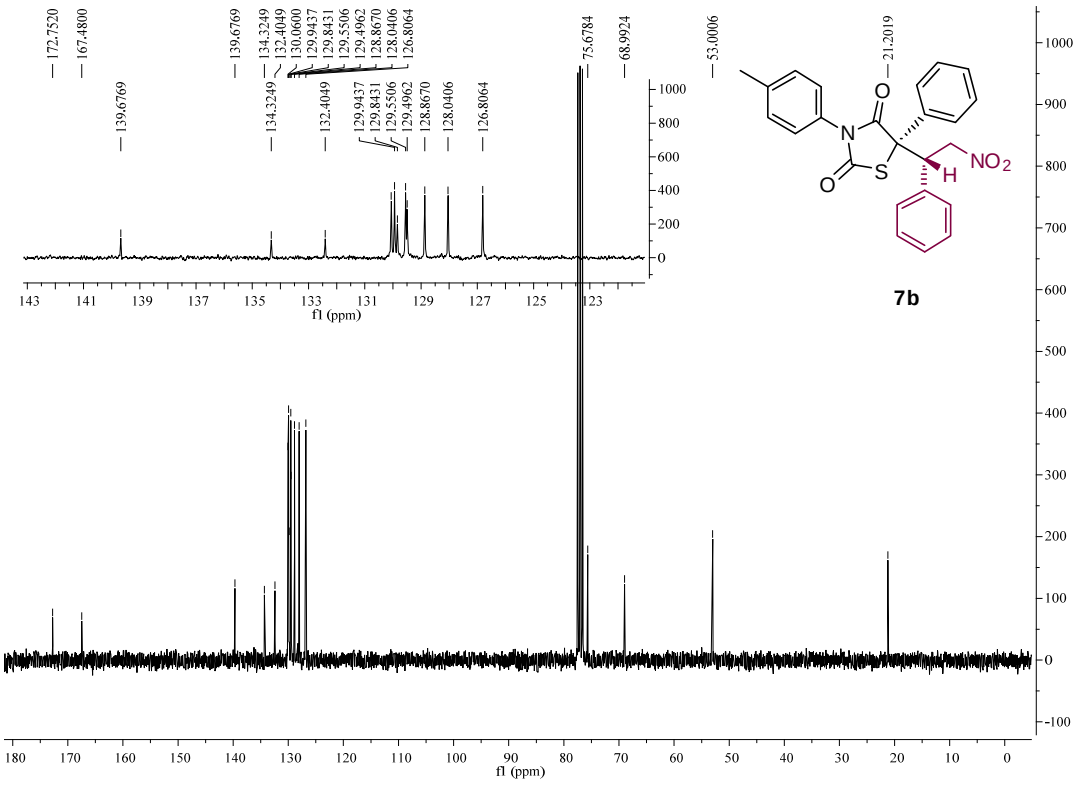
4.8927
4.8551
4.8172
4.4303
4.3952
2.3065
2.02
8.31
2.06
2.00
2.01
1.00
3.00
f1 (ppm)
O
N
S
O
NO2
H
7b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128.0406
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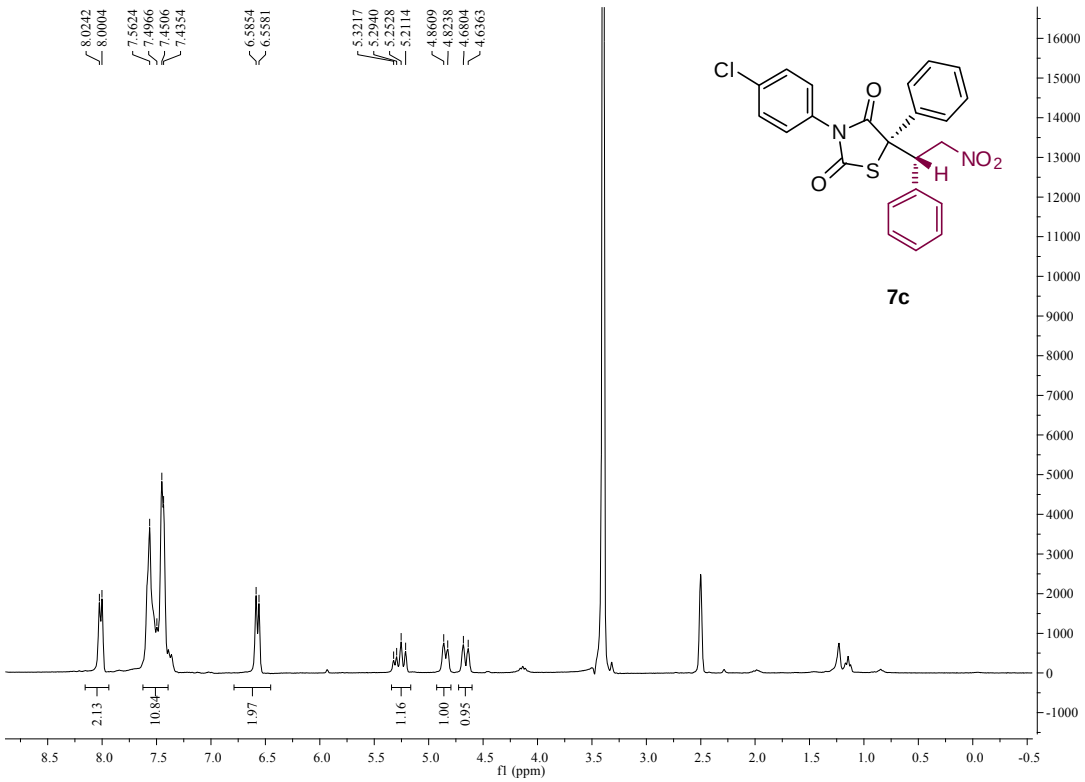
53.0006
21.2019
f1 (ppm)
O
N
S
O
NO2
H
7b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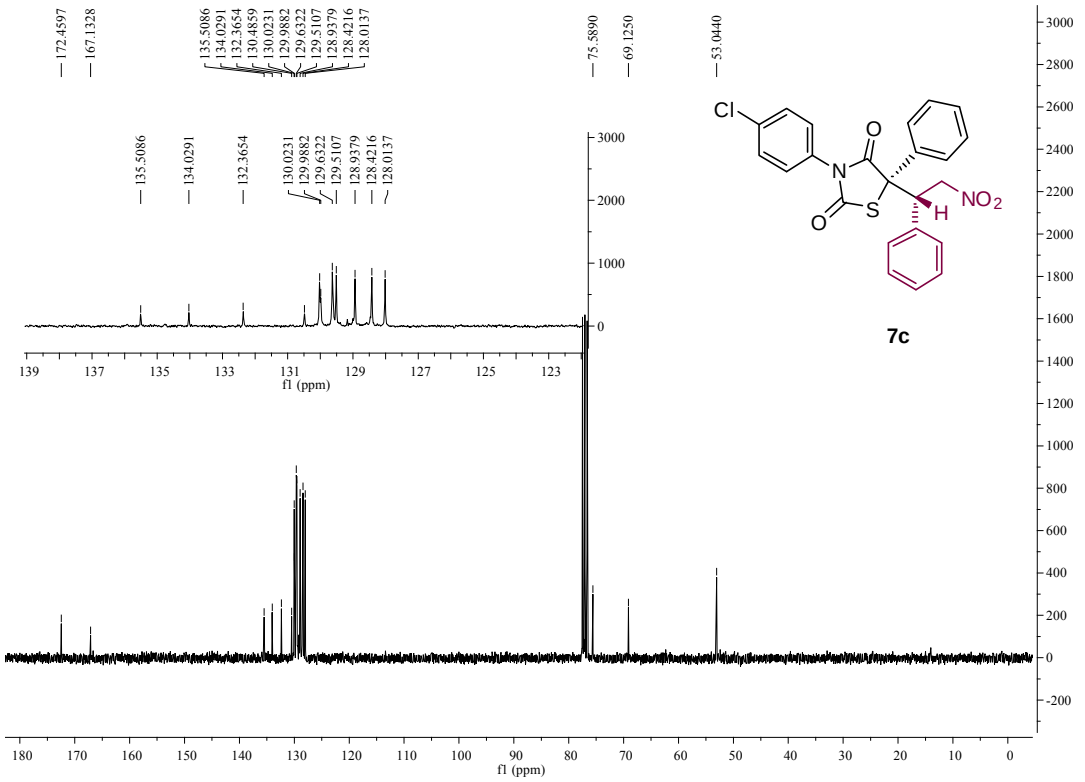
5.2528
5.2114
4.8609
4.8238
4.6804
4.6363
2.13
10.84
1.97
1.16
1.00
0.95
f1 (ppm)
Cl
O
N
S
O
NO2
H
7c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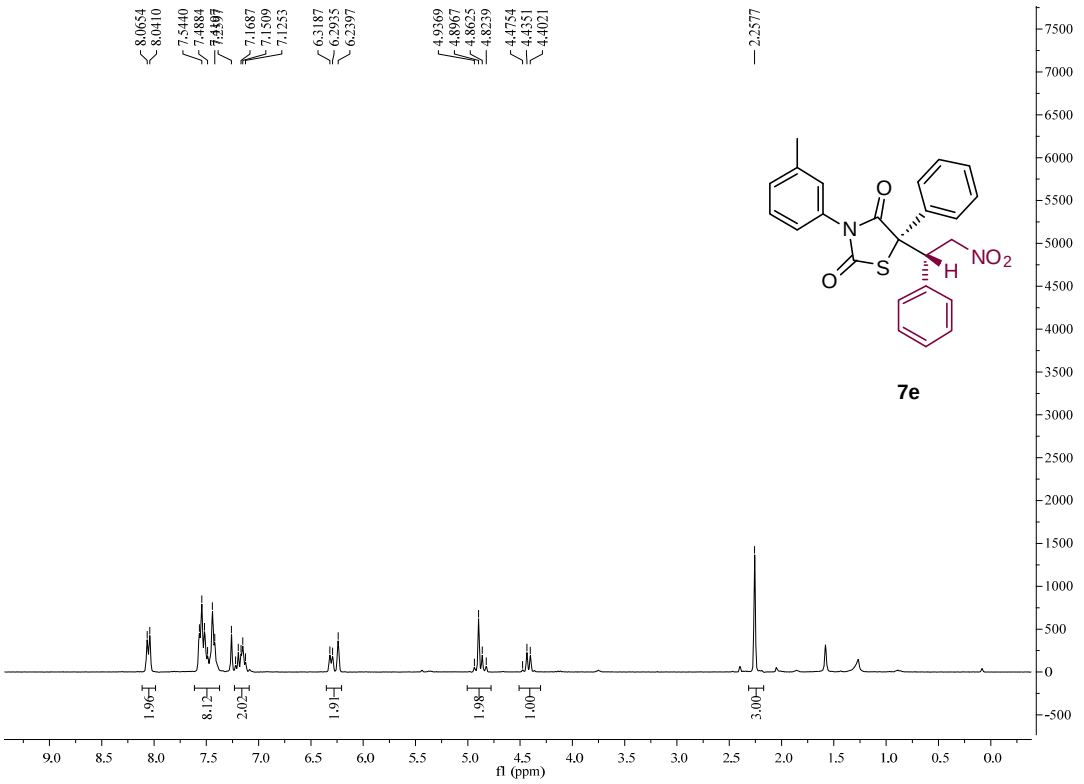
128.9379
128.4216
128.0137
75.5890
69.1250
53.0440
f1 (ppm)
Cl
O
N
S
O
NO2
H
7c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7.1687
7.1509
7.1253
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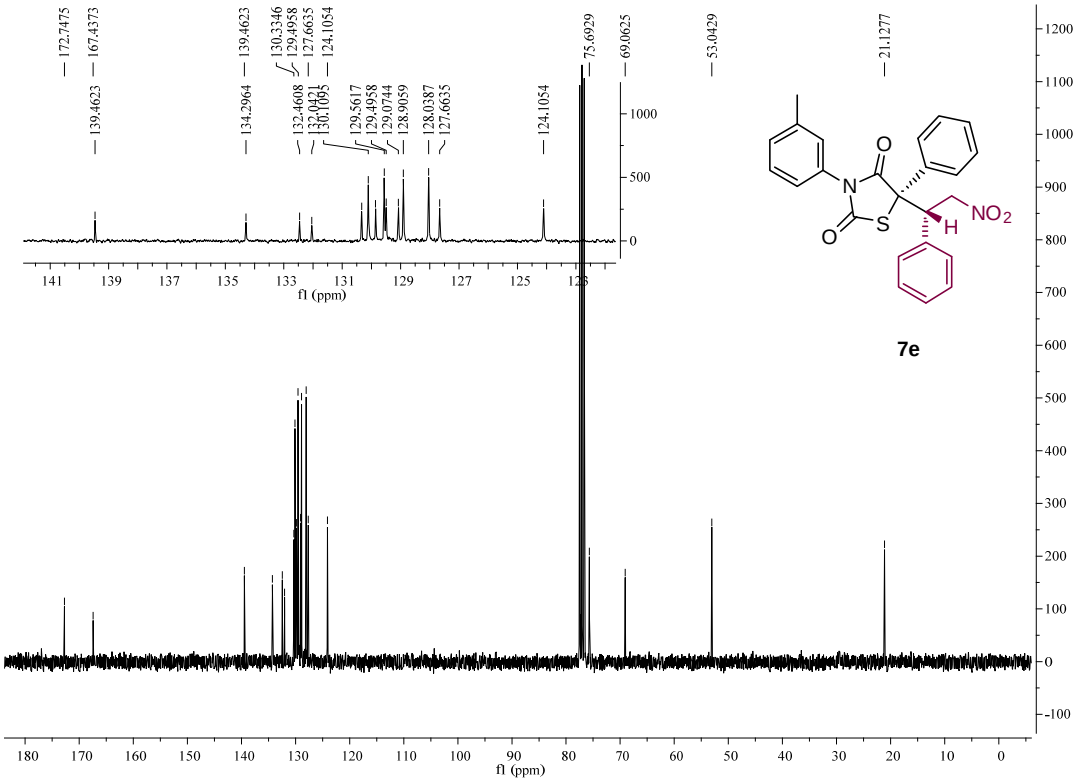
6.2935
6.2397
4.9369
4.8967
4.8625
4.8239
4.4754
4.4351
4.4021
2.2577
1.96
8.12
2.02
1.91
1.98
1.00
3.00
fl (ppm)
O
N
S
O
H
NO2

7e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129.4958
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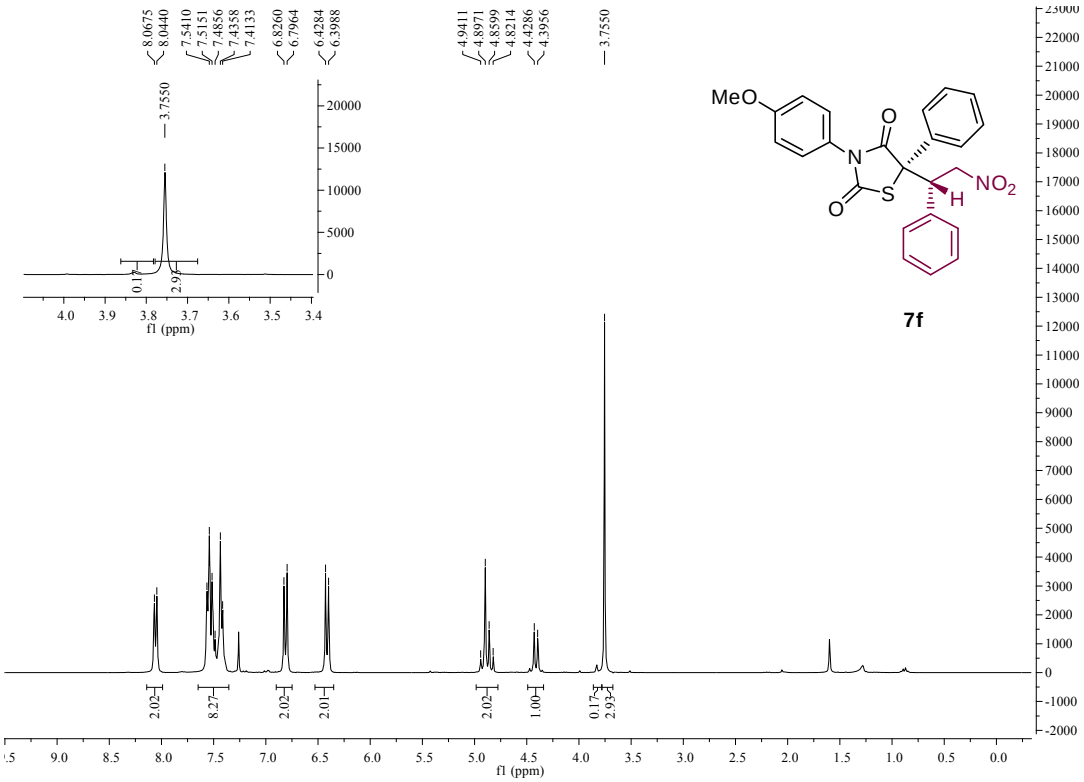
129.0744
128.9059
128.0387
127.6635
124.1054
75.6929
69.0625
53.0429
21.1277
fl (ppm)
O
N
S
O
H
NO2

7e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6.3988
4.9411
4.8971
4.8599
4.8214
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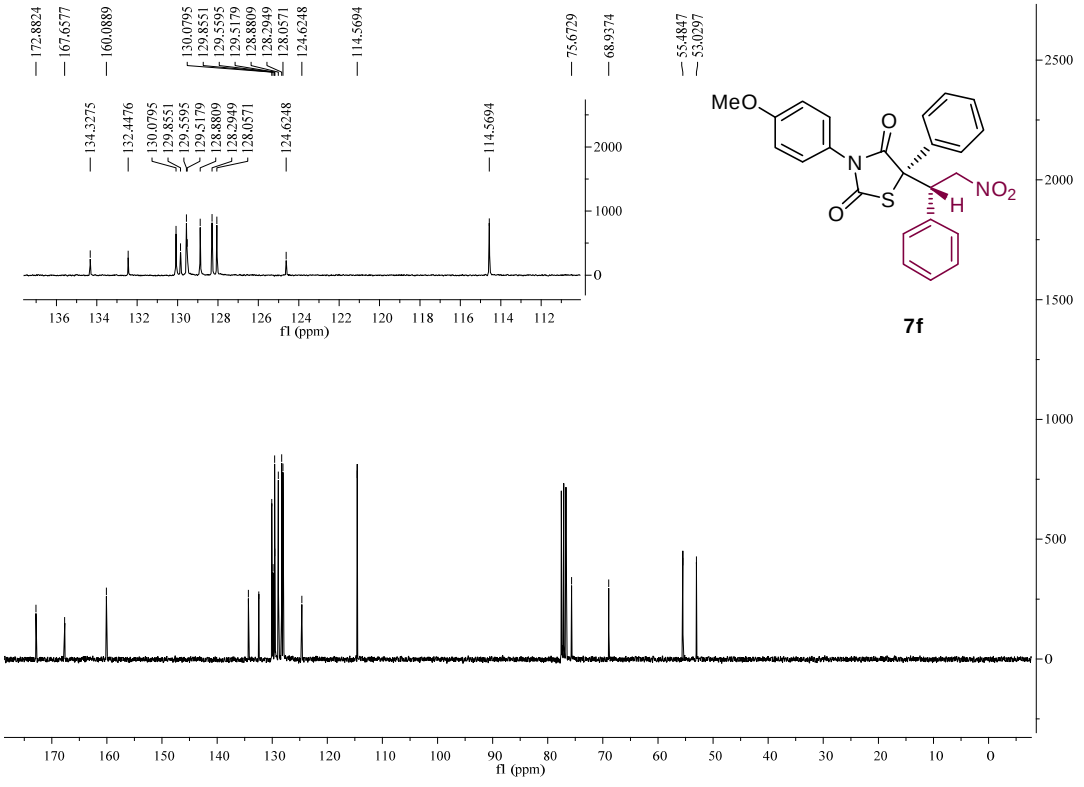
4.3956
3.7550
MeO
O
N
S
O
NO2
H
7f
fl (ppm)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124.6248
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55.4847
53.0297
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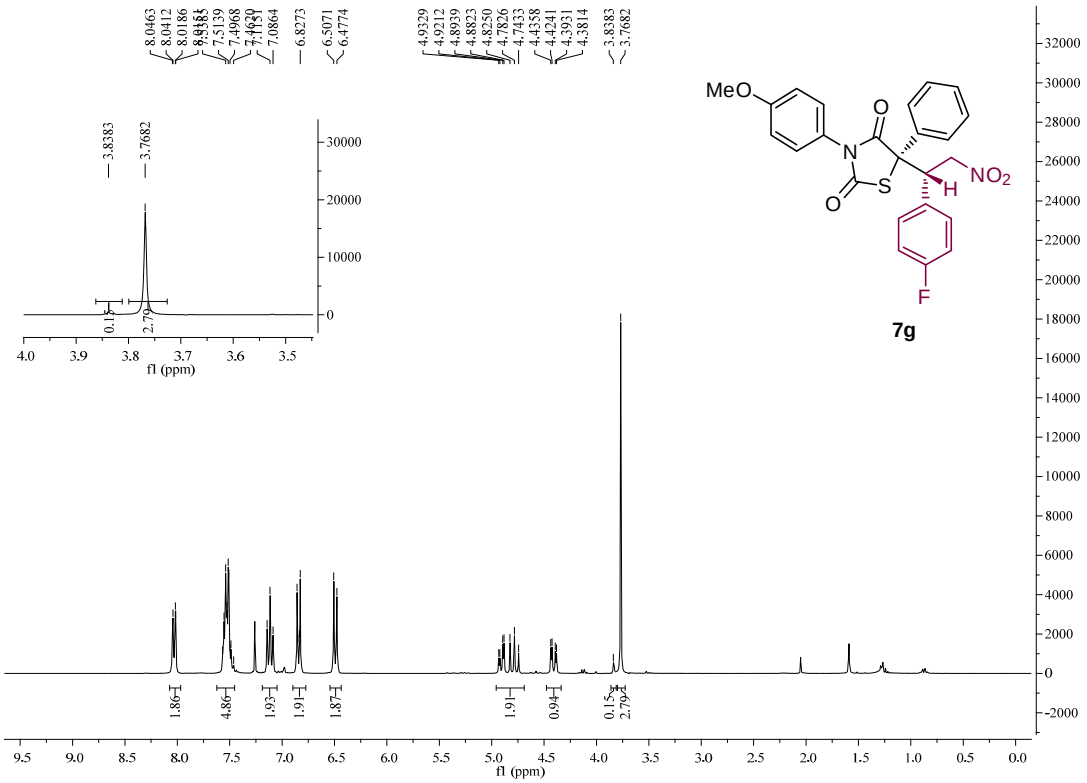
N
S
O
NO2
H
7f
fl (ppm)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8.0186
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7.4968
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7.1151
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6.5071
6.4774
4.9329
4.9212
4.8939
4.8823
4.8250
4.7826
4.7433
4.4358
4.4241
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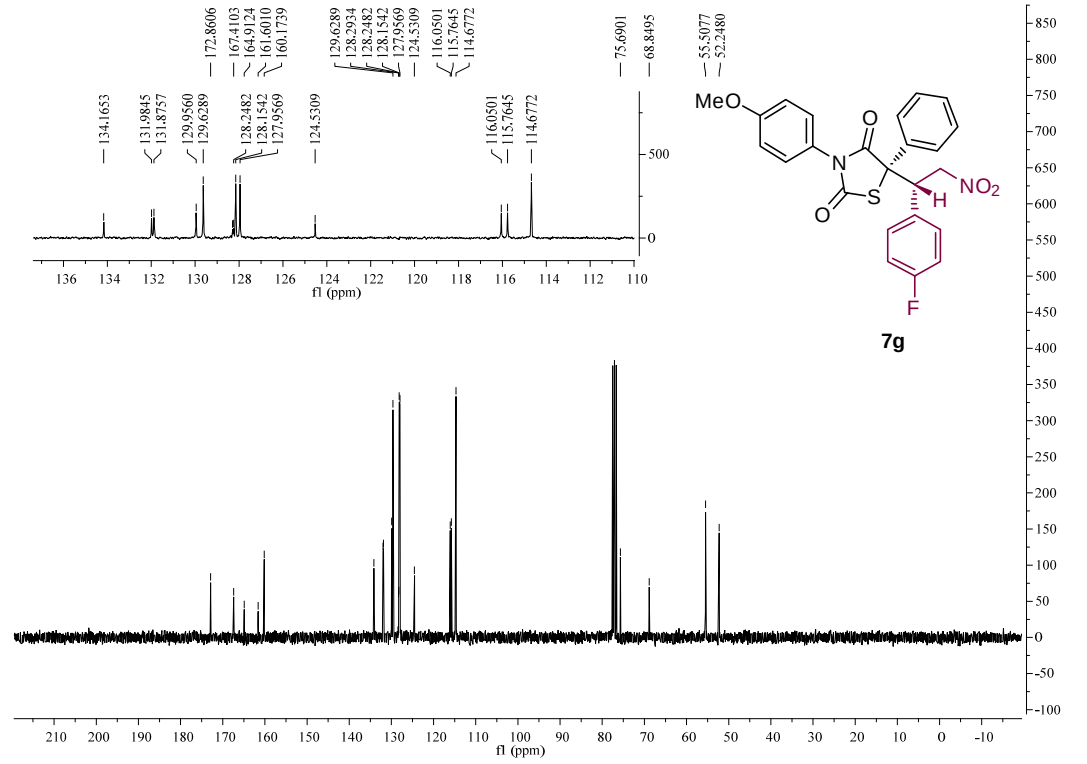
3.8383
3.7682
MeO
O
N
S
O
H
NO2
F
7g
fl (ppm)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131.8757
129.9560
129.6289
128.2934
128.2482
128.1542
127.9569
124.5309
116.0501
115.7645
114.6772
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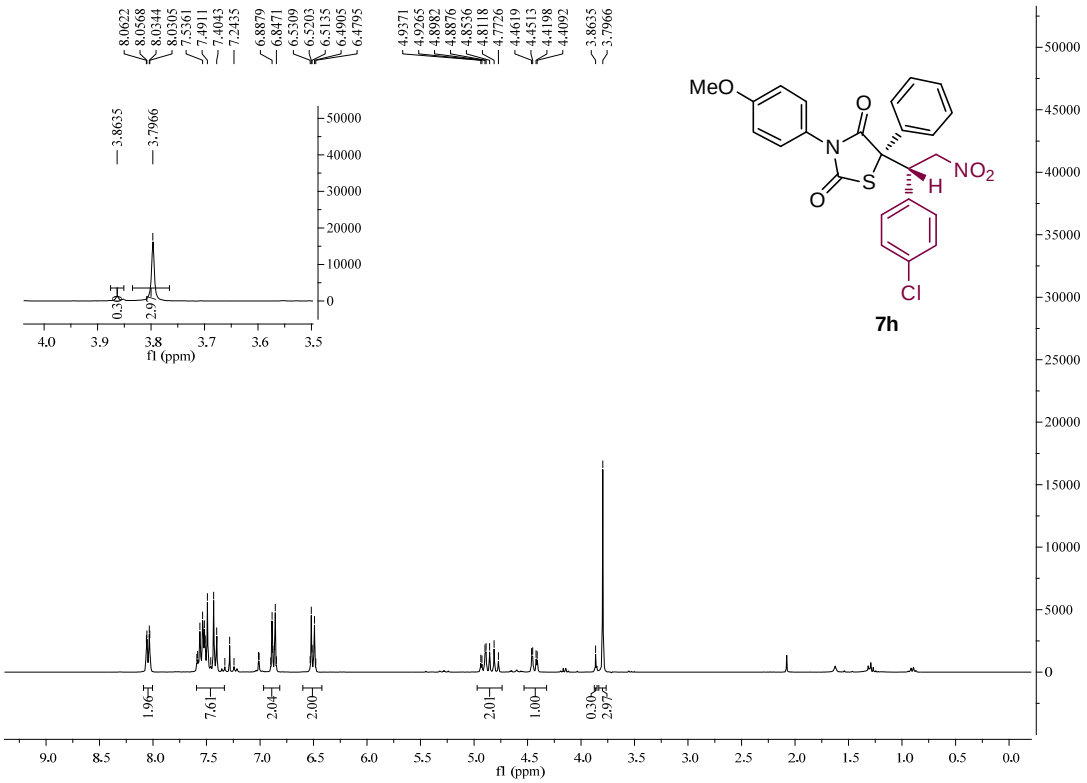
55.5077
52.2480
MeO
O
N
S
O
H
NO2
F
7g
fl (ppm)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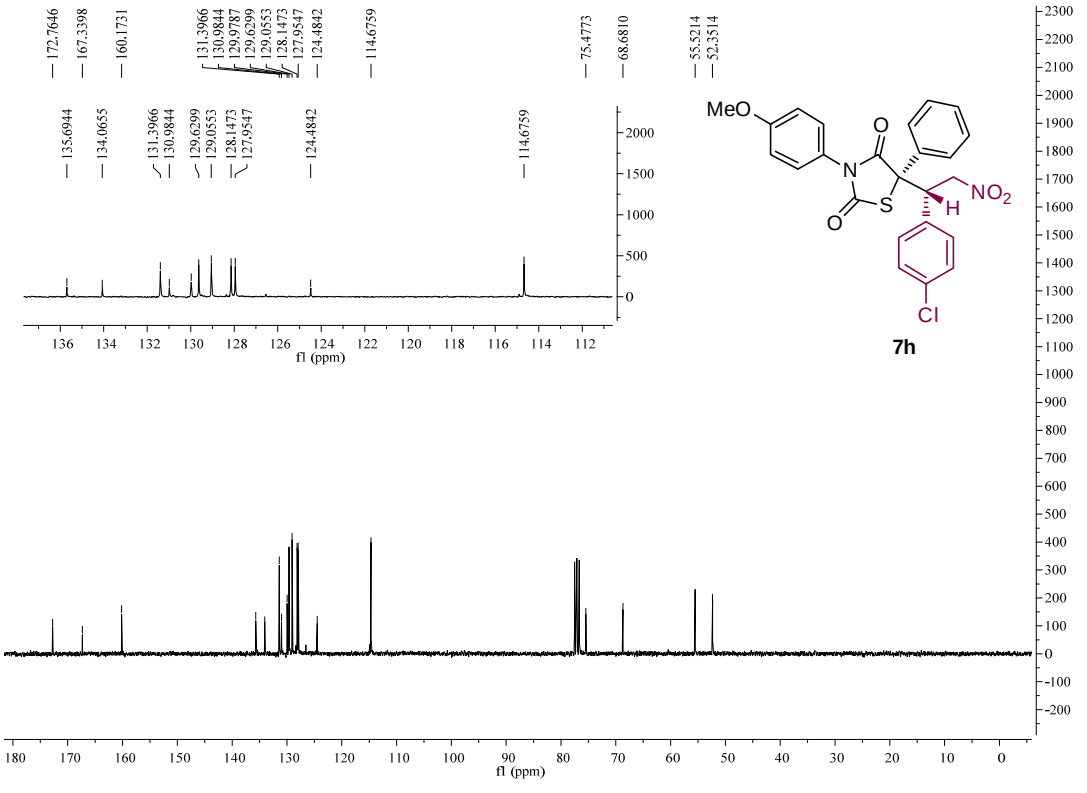
7.4911
7.4043
7.2435
6.8879
6.8471
6.5309
6.5203
6.5135
6.4905
6.4795
4.9371
4.9265
4.8982
4.8876
4.8536
4.8118
4.7726
4.4619
4.4513
4.4198
4.4092
3.8635
3.7966
MeO
O
N
S
O
H
NO2
Cl
7h
f1 (ppm)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130.9844
129.9787
129.6299
129.0553
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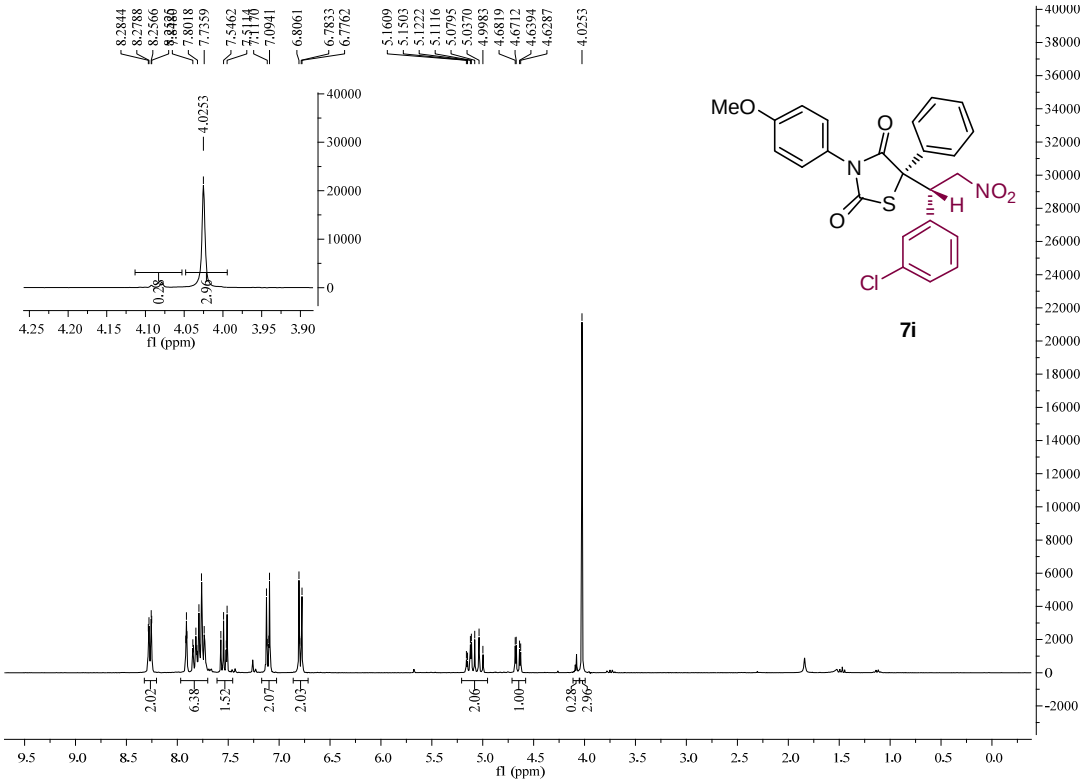
127.9547
124.4842
114.6759
75.4773
68.6810
55.5214
52.3514
MeO
O
N
S
O
H
NO2
Cl
7h
f1 (ppm)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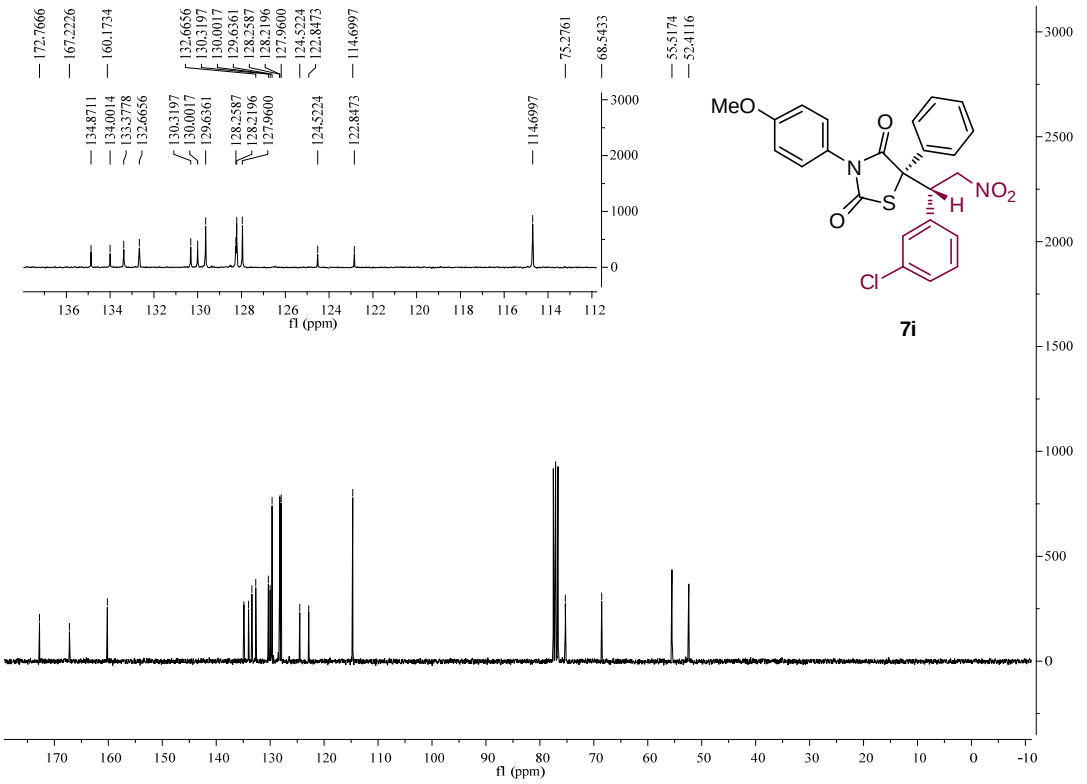
O
N
S
O
NO2
H
Cl
7i
f1 (ppm)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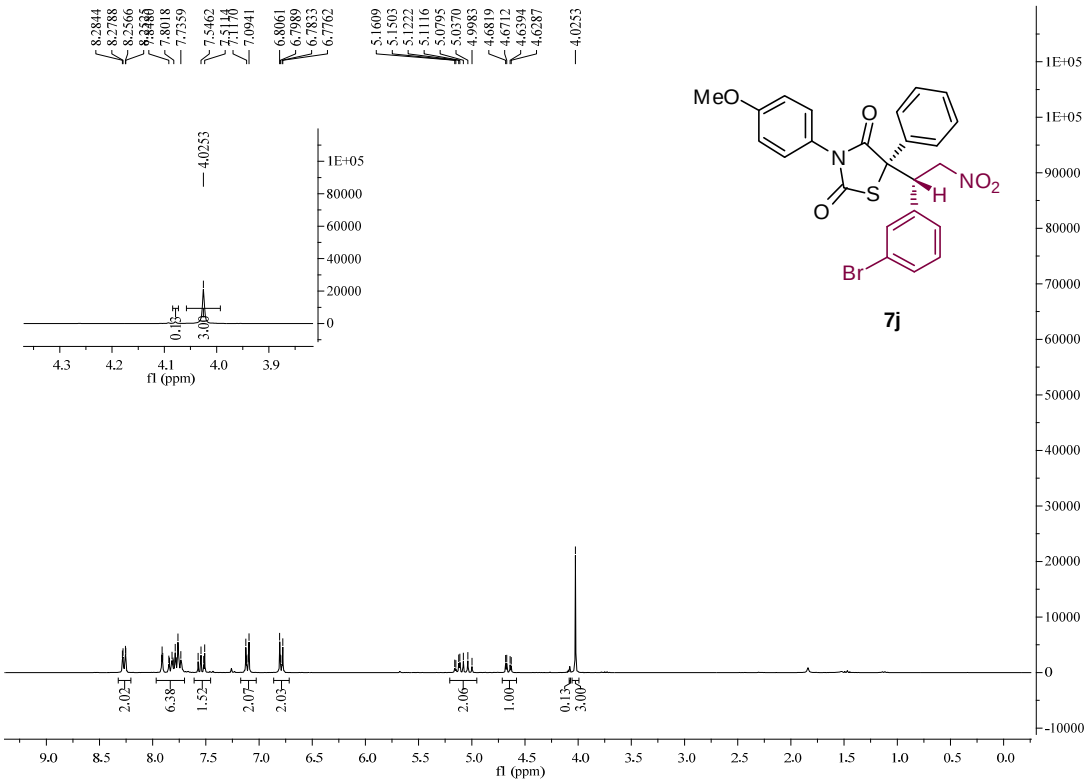
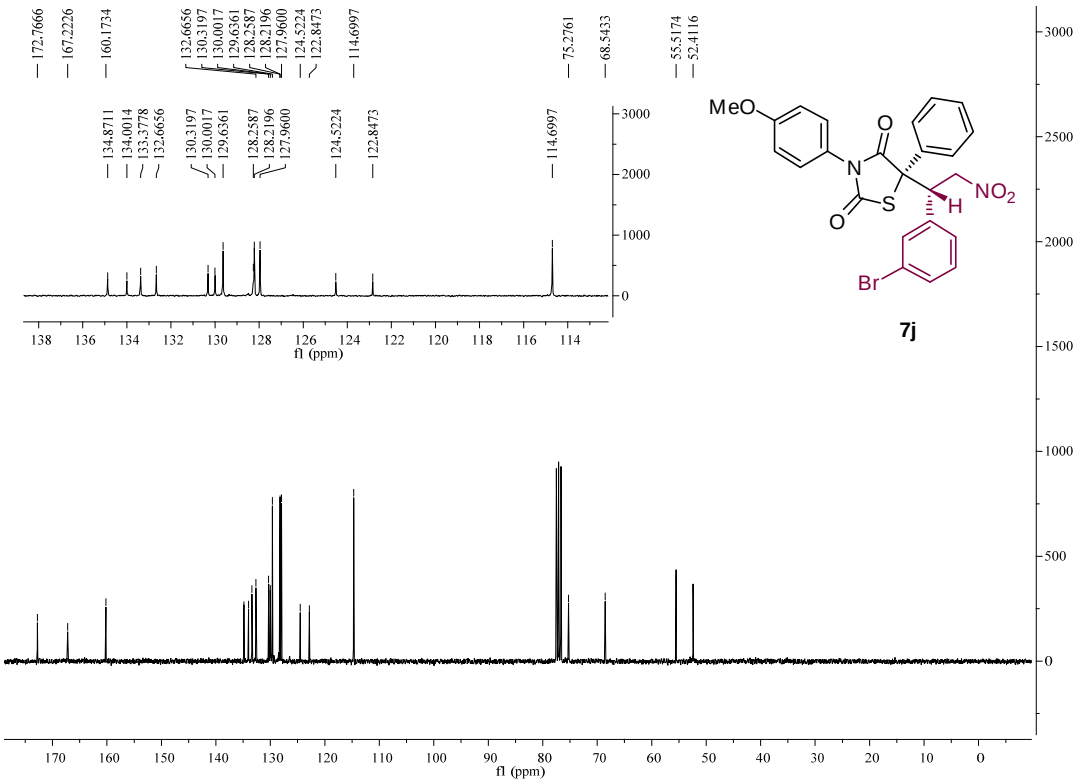
O
N
S
O
NO2
H
Cl
7i
f1 (ppm)


MeO
O
N
S
O
NO2
H
Br
7j
f1 (ppm)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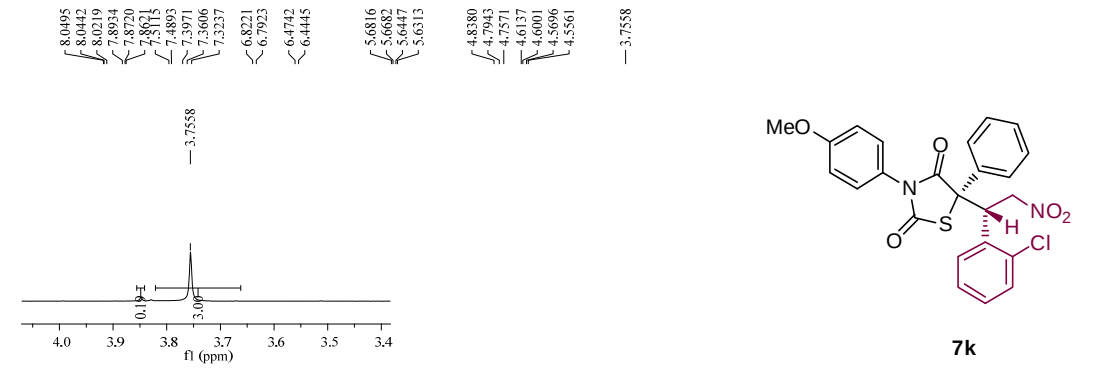
O
N
S
O
NO2
H
Br
7j
f1 (ppm)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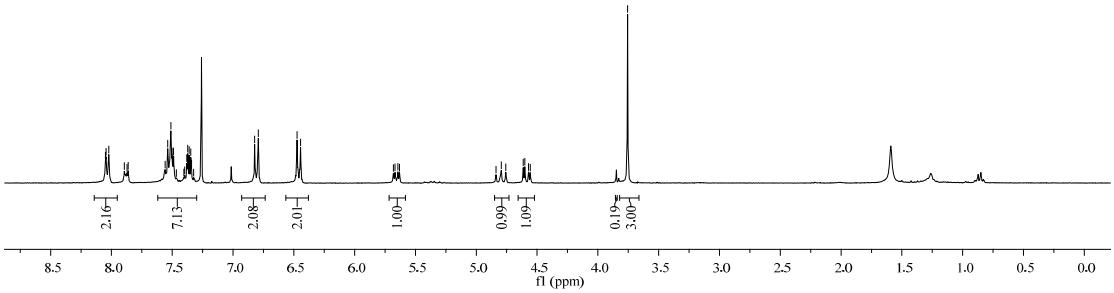
7.3237
6.8221
6.7923
6.4742
6.4445
5.6816
5.6682
5.6447
5.6313
4.8380
4.7943
4.7571
4.6137
4.6001
4.5696
4.5561
3.7558
MeO
O
N
S
O
NO2
H
Cl

3.7558
0.19
3.00
4.0 3.9 3.8 3.7 3.6 3.5 3.4
f1 (ppm)

7k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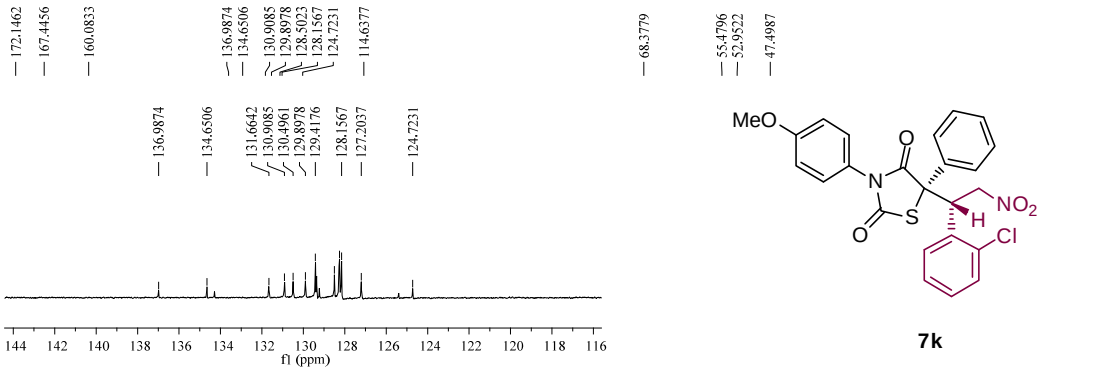
7.13
2.08
2.01
1.00
0.99
1.09
0.19
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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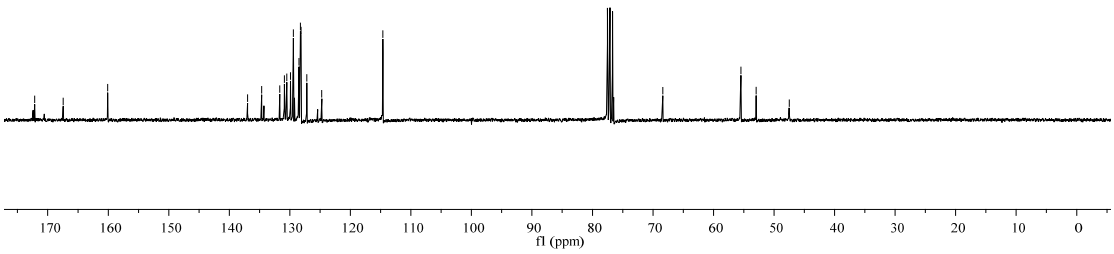
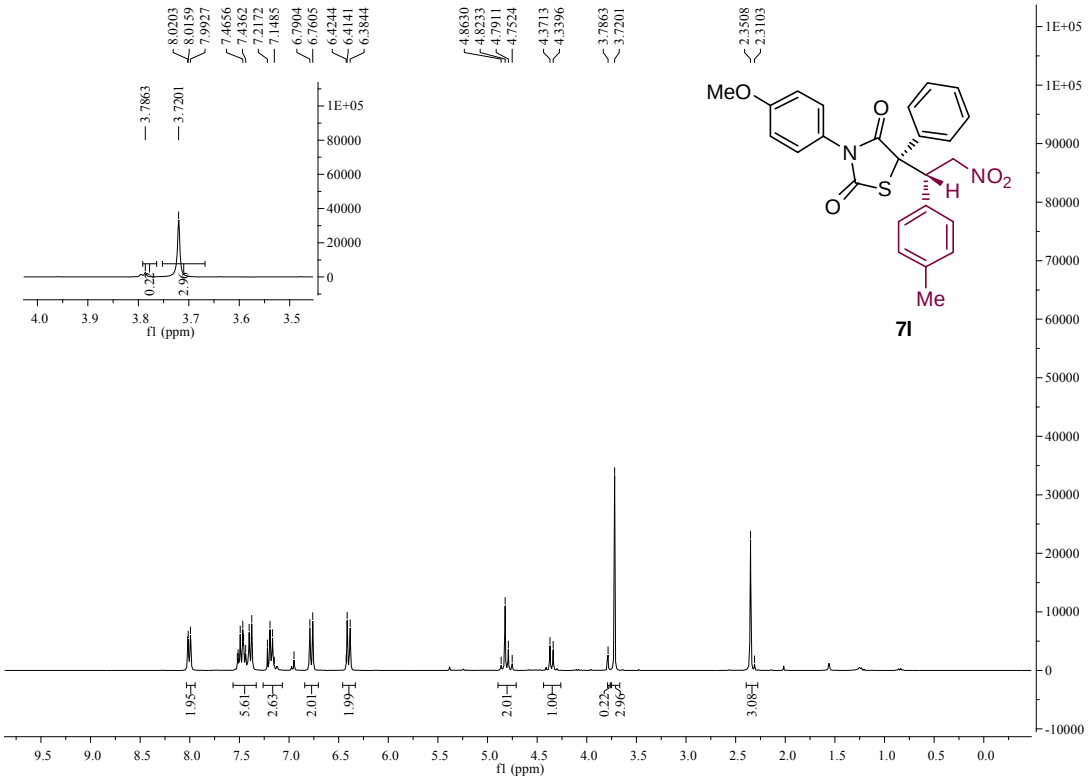
130.9085
129.8978
128.5023
128.1567
124.7231
114.6377
68.3779
55.4796
52.9522
47.4987
136.9874
134.6506
131.6642
130.9085
130.4961
129.8978
129.4176
128.1567
127.2037
124.7231
144 142 140 138 136 134 132 130 128 126 124 122 120 118 116
f1 (ppm)

MeO
O
N
S
O
NO2
H
Cl

7k


170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.4362
7.2172
7.1485
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6.7605
6.4244
6.4141
6.3844
4.8630
4.8233
4.7911
4.7524
4.3713
4.3396
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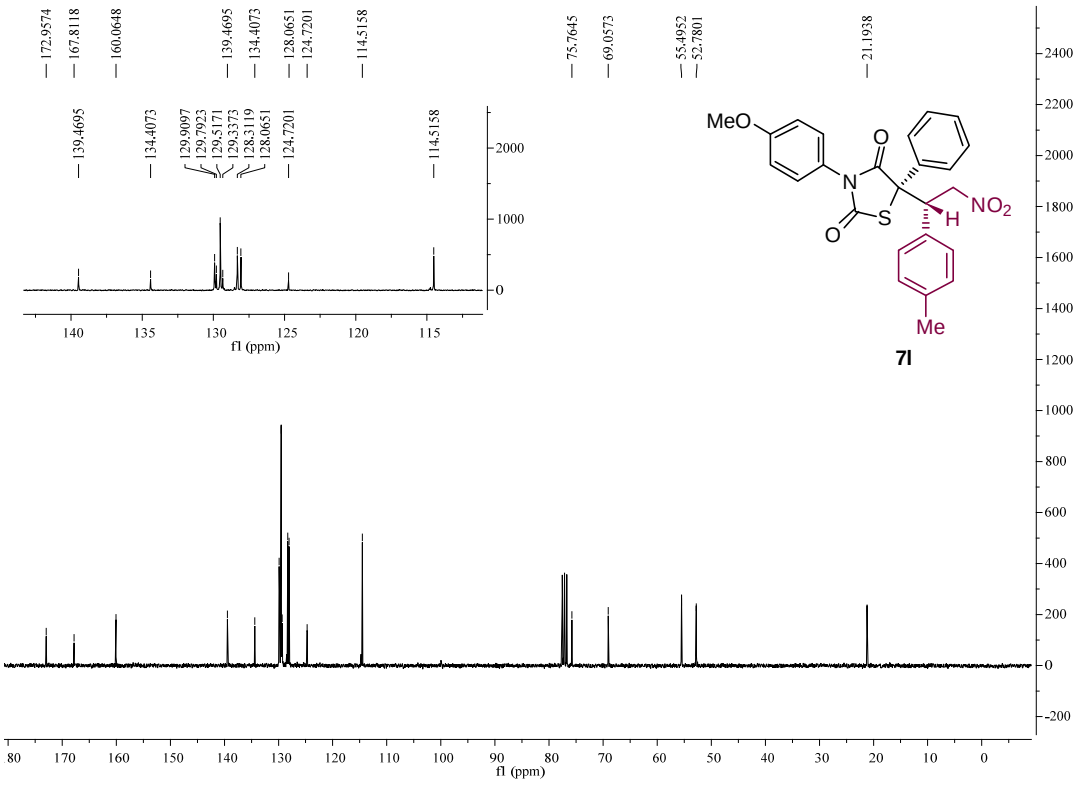
3.7201
2.3508
2.3103
MeO
O
N
S
O
H
NO2
Me
7l
fl (ppm)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124.7201
114.5158
75.7645
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52.7801
21.1938
MeO
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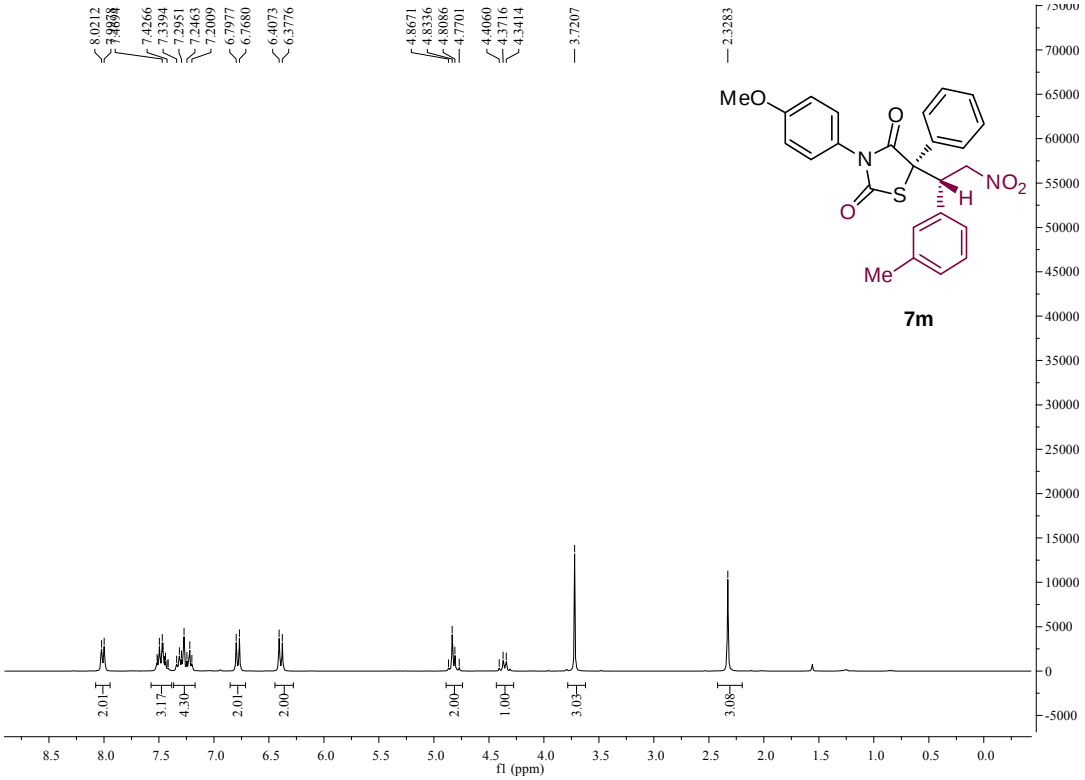
N
S
O
H
NO2
Me
7l
fl (ppm)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6.4073
6.3776
4.8671
4.8336
4.8086
4.7701
4.4060
4.3716
4.3414
3.7207
2.3283
MeO
O
N
S
O
NO2
H
Me
7m
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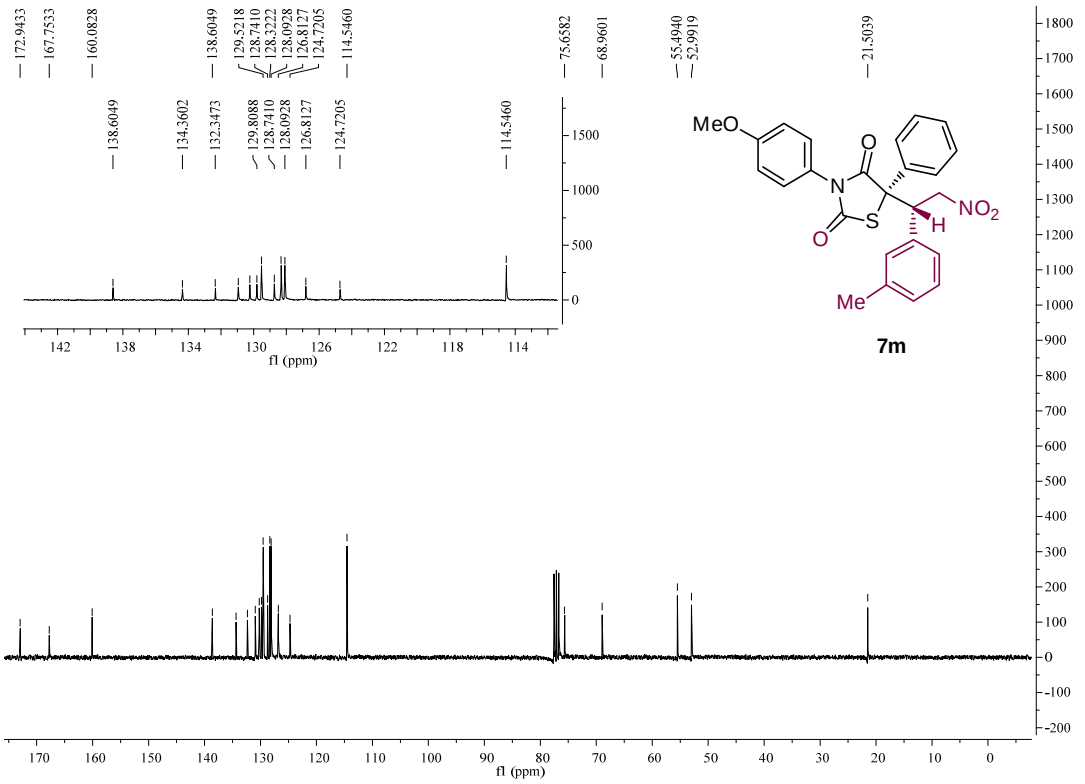
3.17
4.30
2.01
2.00
2.00
1.00
3.03
3.08
fl (ppm)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126.8127
124.7205
114.5460
75.6582
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52.9919
21.5039
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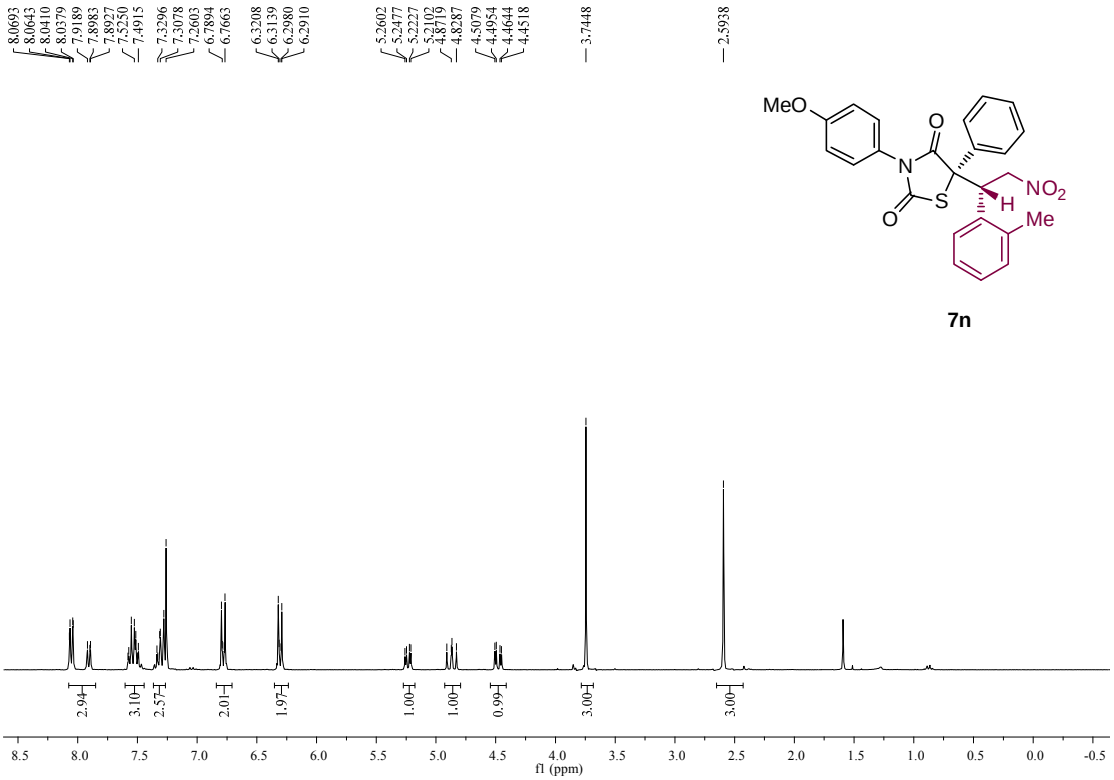
O
N
S
O
NO2
H
Me
7m
fl (ppm)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7.3078
7.2603
6.7894
6.7663
6.3208
6.3139
6.2980
6.2910
5.2602
5.2477
5.2227
5.2102
4.8719
4.8287
4.5079
4.4954
4.4644
4.4518
3.7448
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MeO
O
N
S
O
NO2
H
Me
7n
2.94
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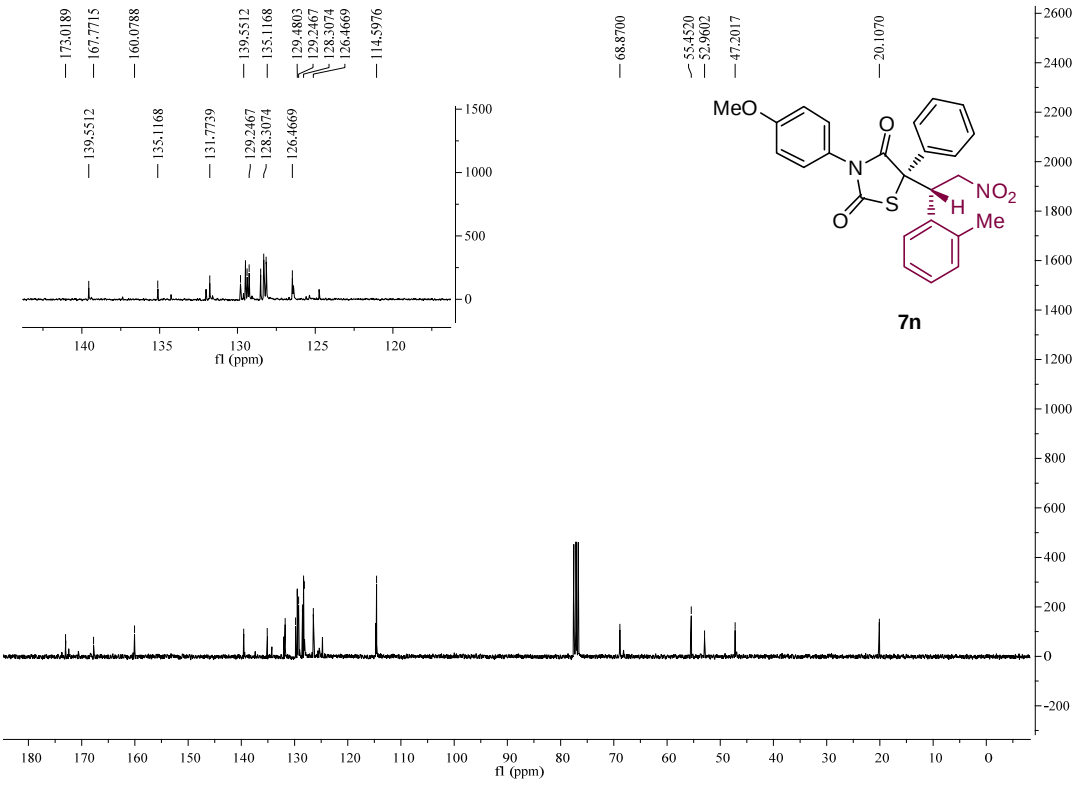
2.57
2.01
1.97
1.00
1.00
0.99
3.00
3.00
fl (ppm)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129.2467
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126.4669
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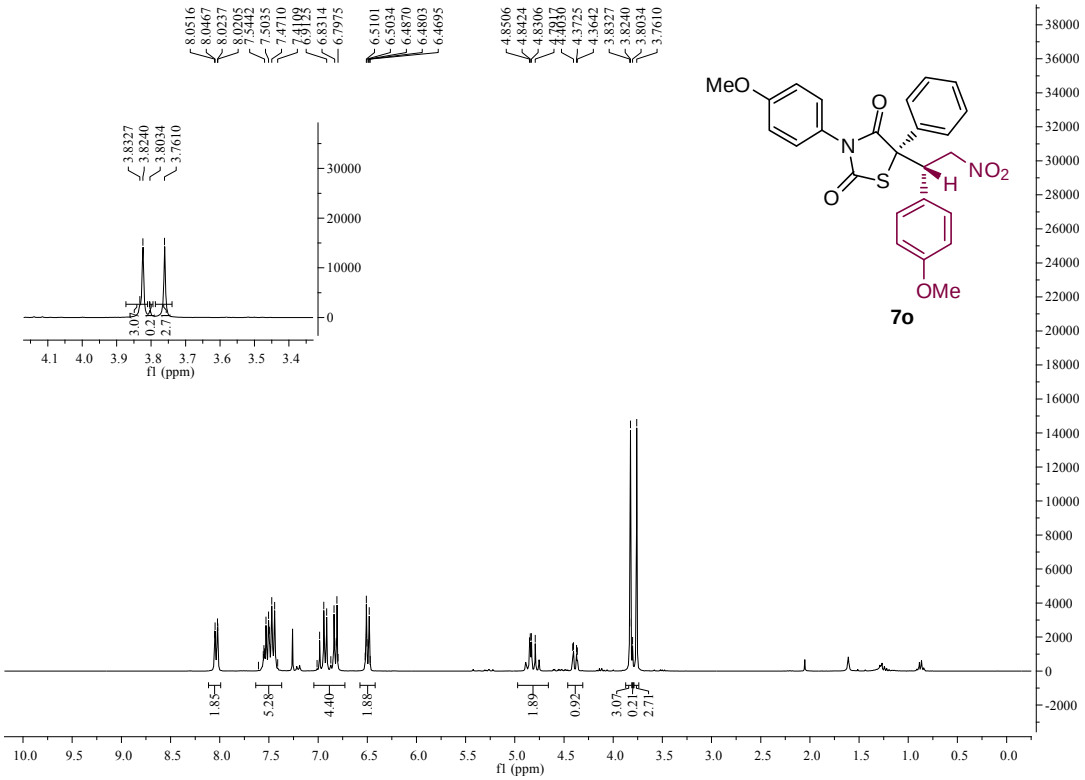
52.9602
47.2017
20.1070
131.7739
MeO
NO2
Me
7n
fl (ppm)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8.0205
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6.5034
6.4870
6.4803
6.4695
4.8506
4.8424
4.8306
4.4250
4.3725
4.3642
3.8327
3.8240
3.8034
3.7610
MeO
O
N
S
O
NO2
H
OMe
7o
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5.28
4.40
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1.89
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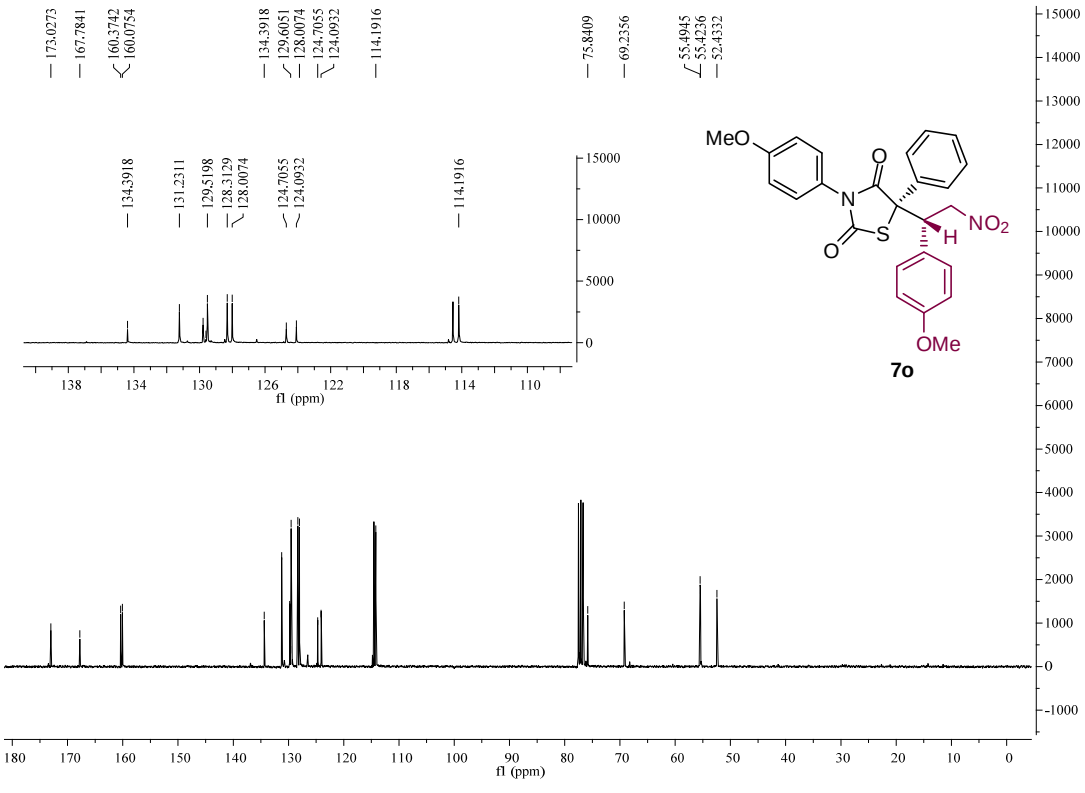
3.07
0.21
2.71
f1 (ppm)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75.8409
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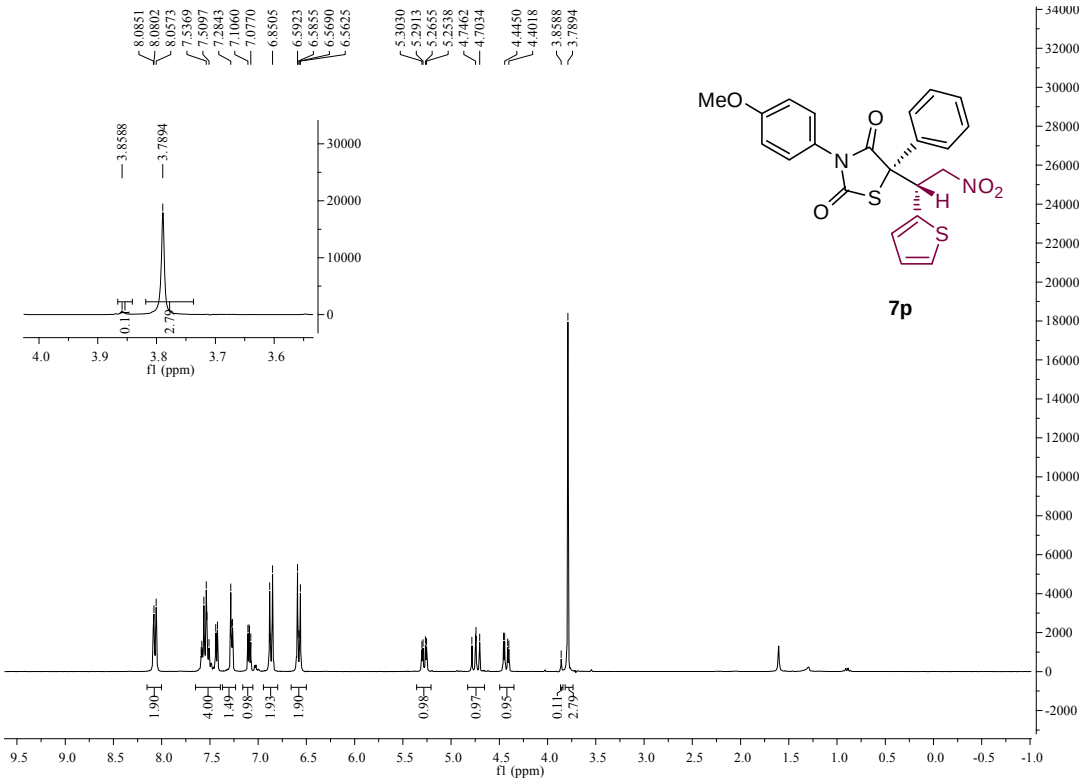
55.4236
52.4332
MeO
O
N
S
O
NO2
H
OMe
7o
f1 (ppm)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6.5690
6.5625
5.3030
5.2913
5.2655
5.2538
4.7462
4.7034
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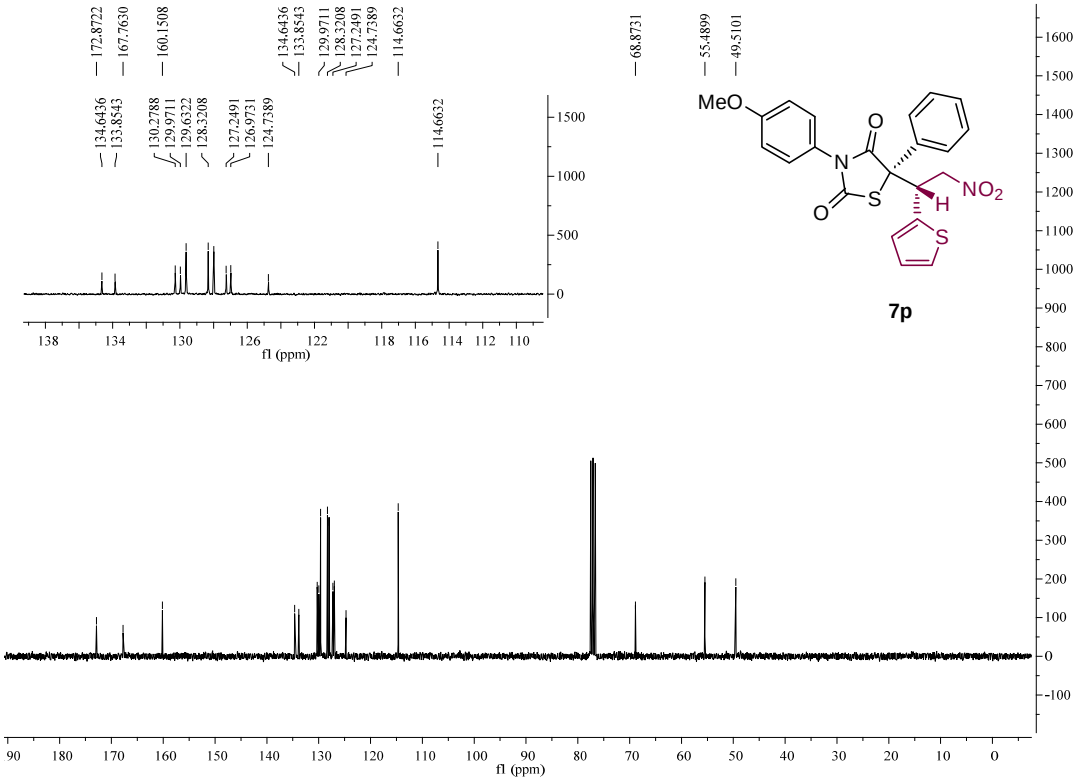
3.8588
3.7894
MeO
O
N
S
O
NO2
H
S
7p
fl (ppm)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55.4899
49.5101
MeO
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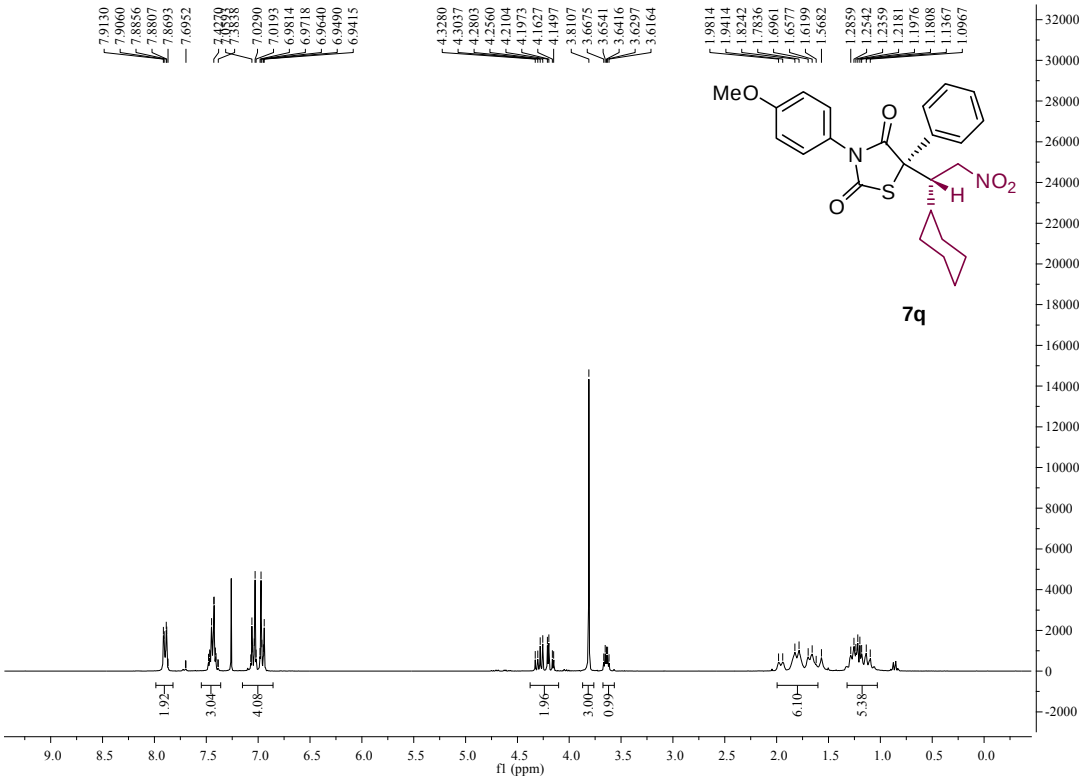
N
S
O
NO2
H
S
7p
fl (ppm)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6.9718
6.9640
6.9490
6.9415
4.3280
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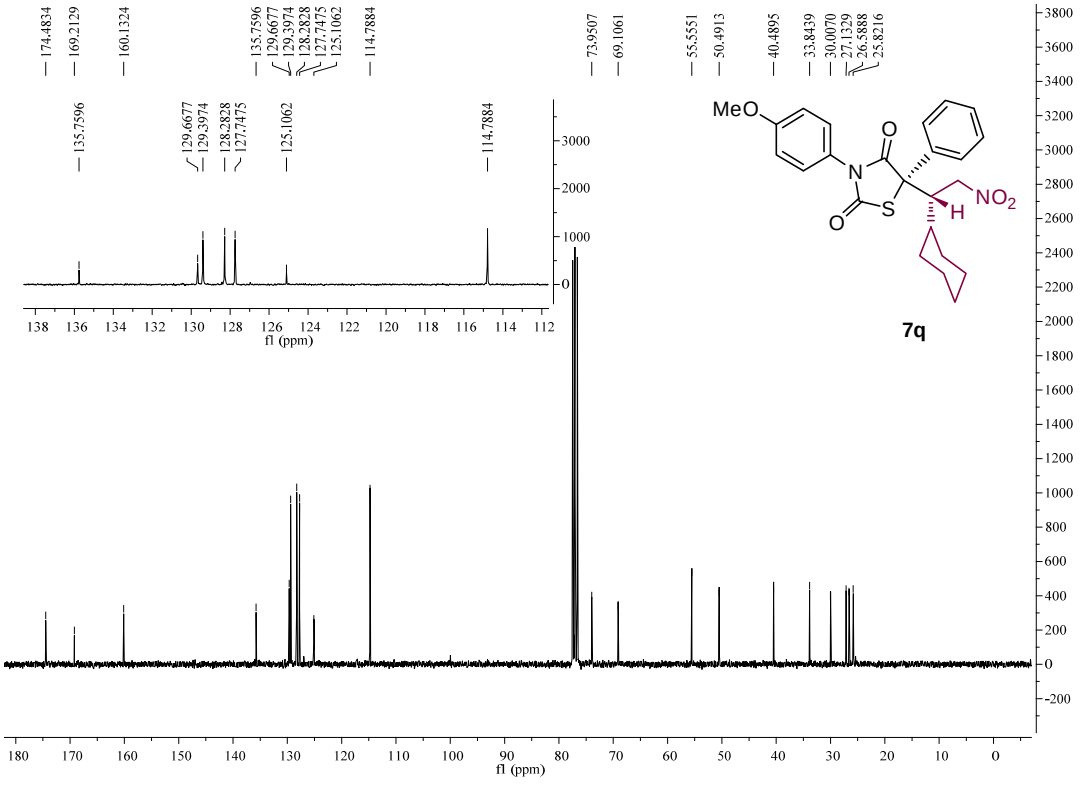
1.8242
1.7836
1.6961
1.6577
1.6199
1.5682
1.2859
1.2542
1.2359
1.2181
1.1976
1.1808
1.1367
1.0967
MeO
O
N
S
O
O
NO2
H
7q
1.92
3.04
4.08
1.96
3.00
0.99
6.10
5.38
f1 (ppm)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69.1061
55.5551
50.4913
40.4895
33.8439
30.0070
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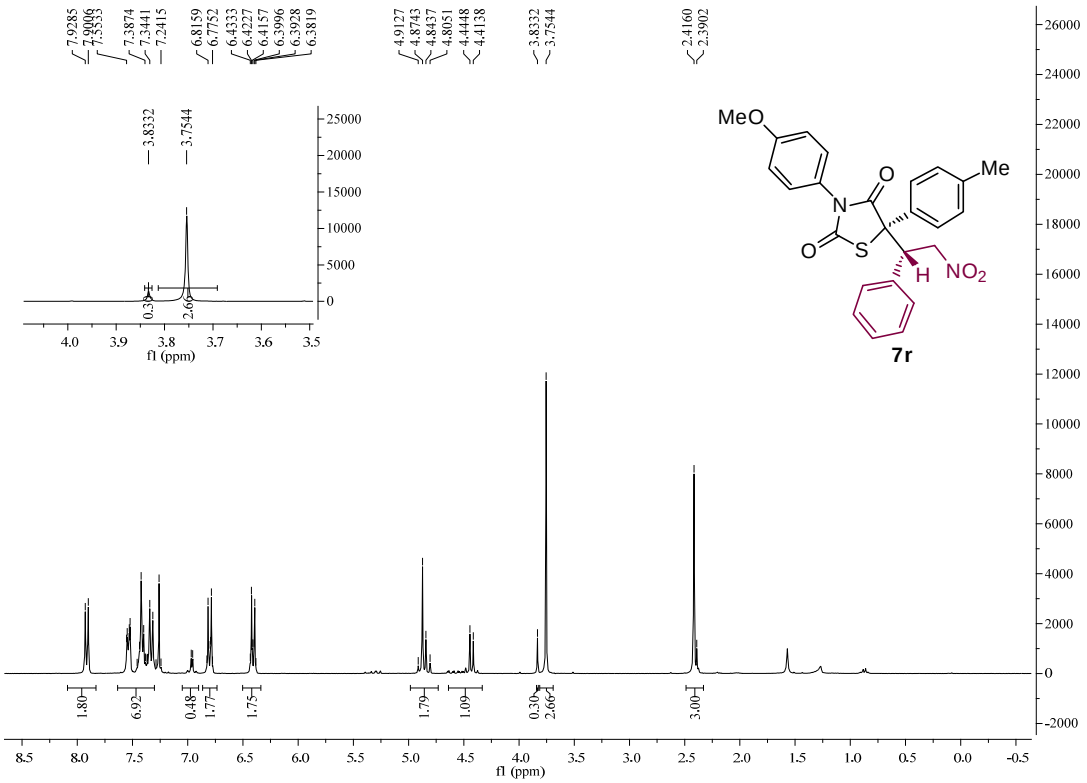
26.5888
25.8216
MeO
O
N
S
O
O
NO2
H
7q
f1 (ppm)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6.3996
6.3928
6.3819
4.9127
4.8743
4.8437
4.8051
4.4448
4.4138
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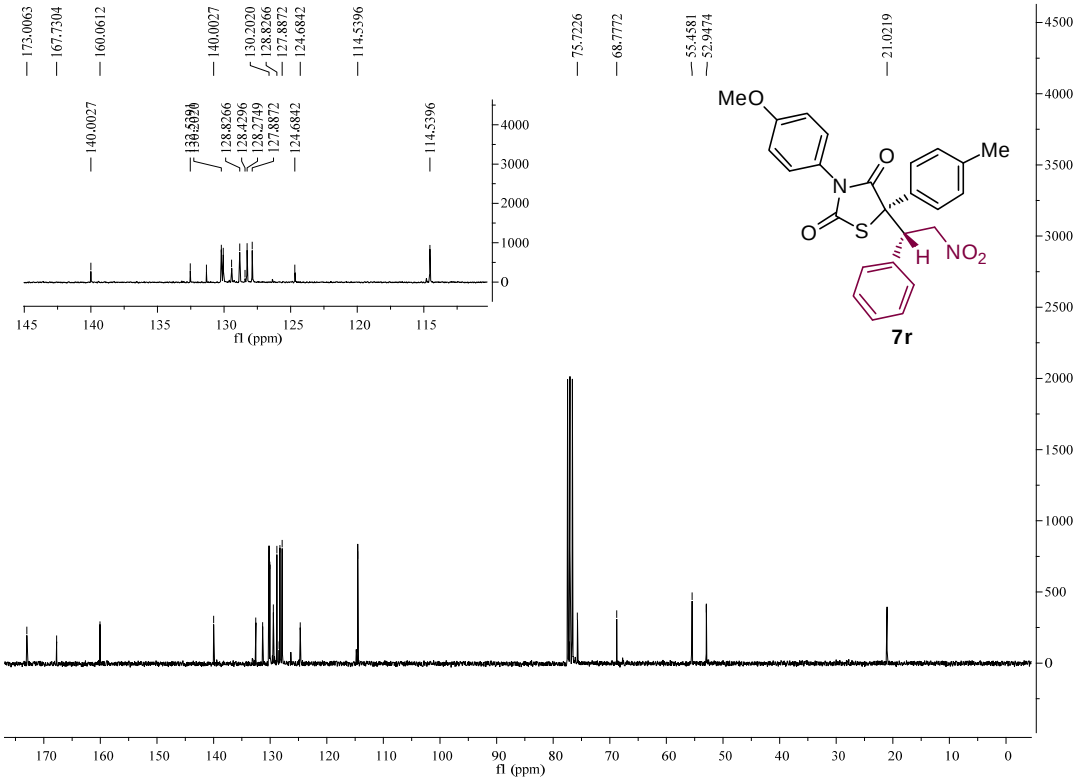
2.4160
2.3902
MeO
Me
O
N
S
O
H
NO2
7r
fl (ppm)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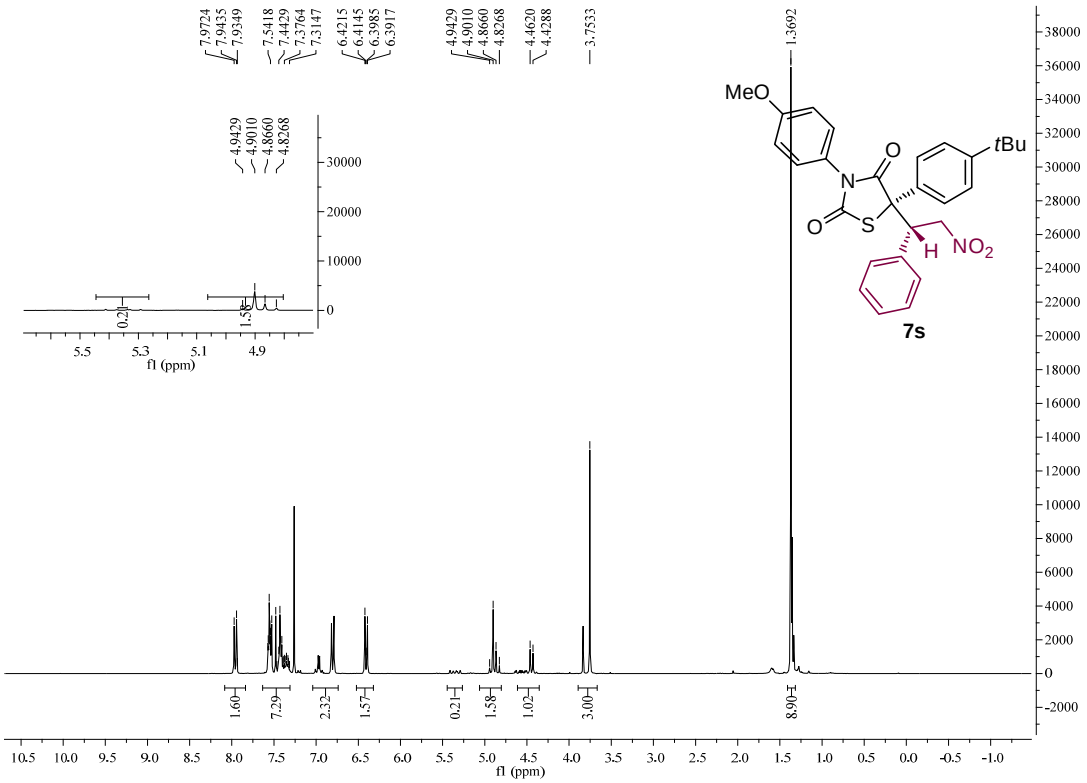
MeO
Me
O
N
S
O
H
NO2
7r
fl (ppm)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6.3917
4.9429
4.9010
4.8660
4.8268
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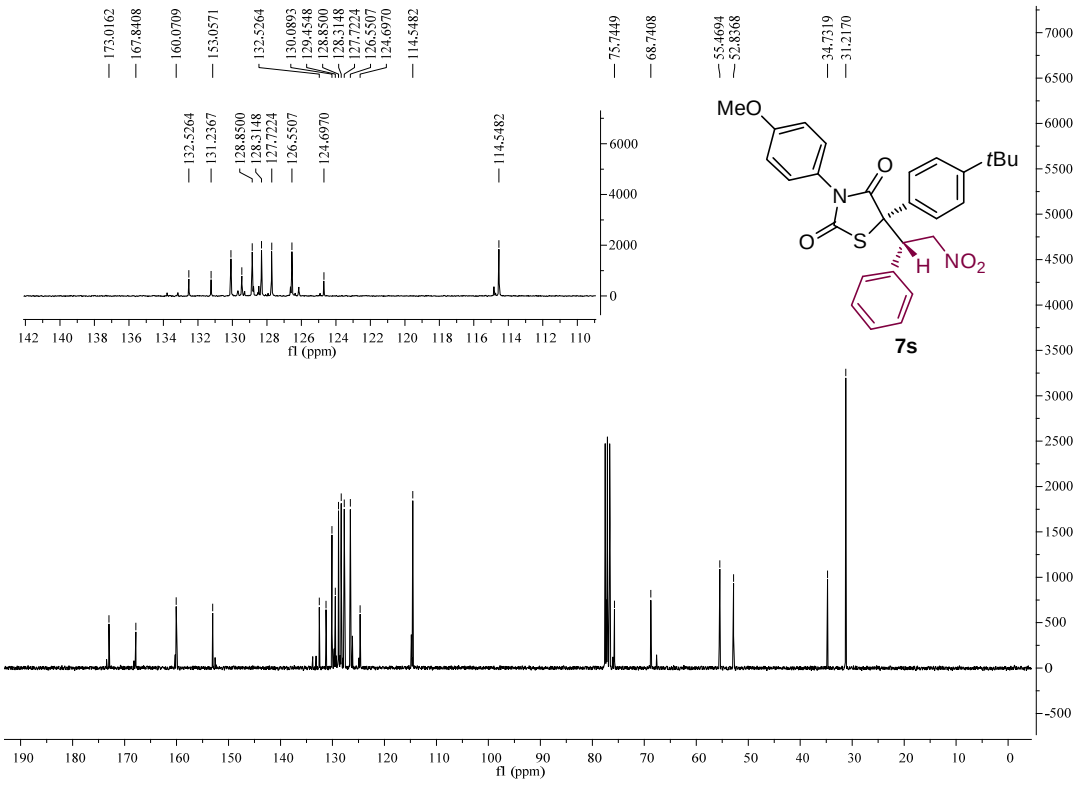
3.7533
1.3692
MeO
tBu
O
N
S
O
H
NO2
7s
fl (ppm)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68.7408
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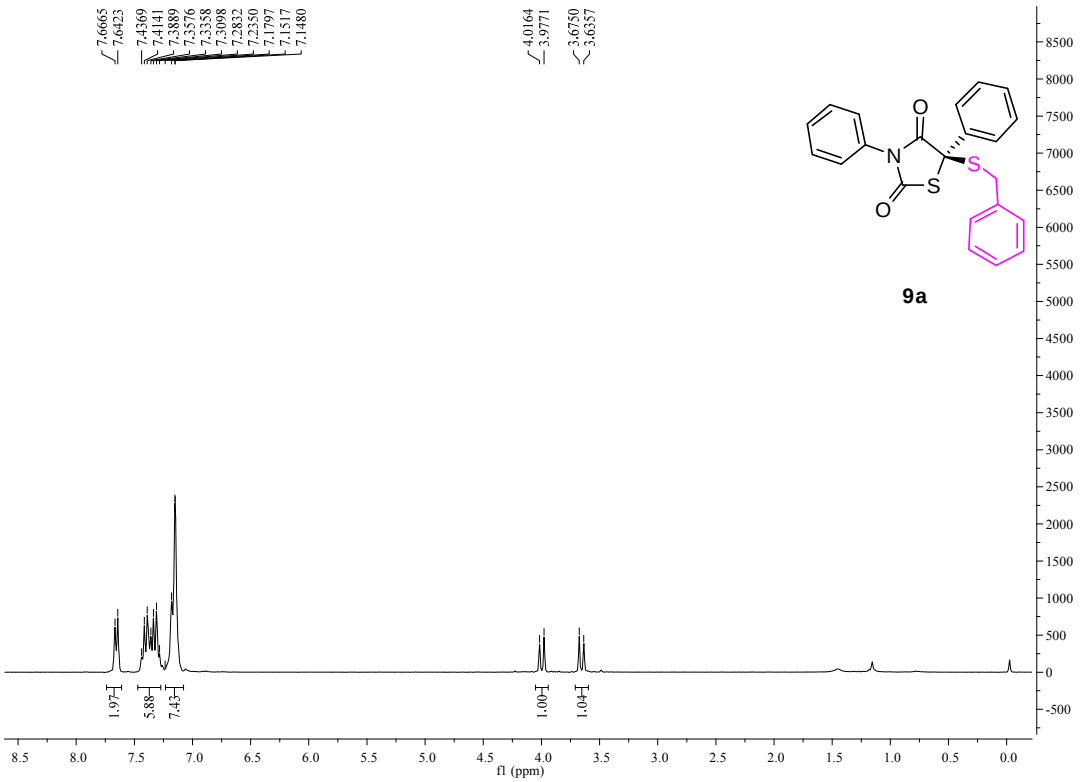
O
N
S
O
H
NO2
7s
fl (ppm)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7.2832
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7.1797
7.1517
7.1480
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3.6750
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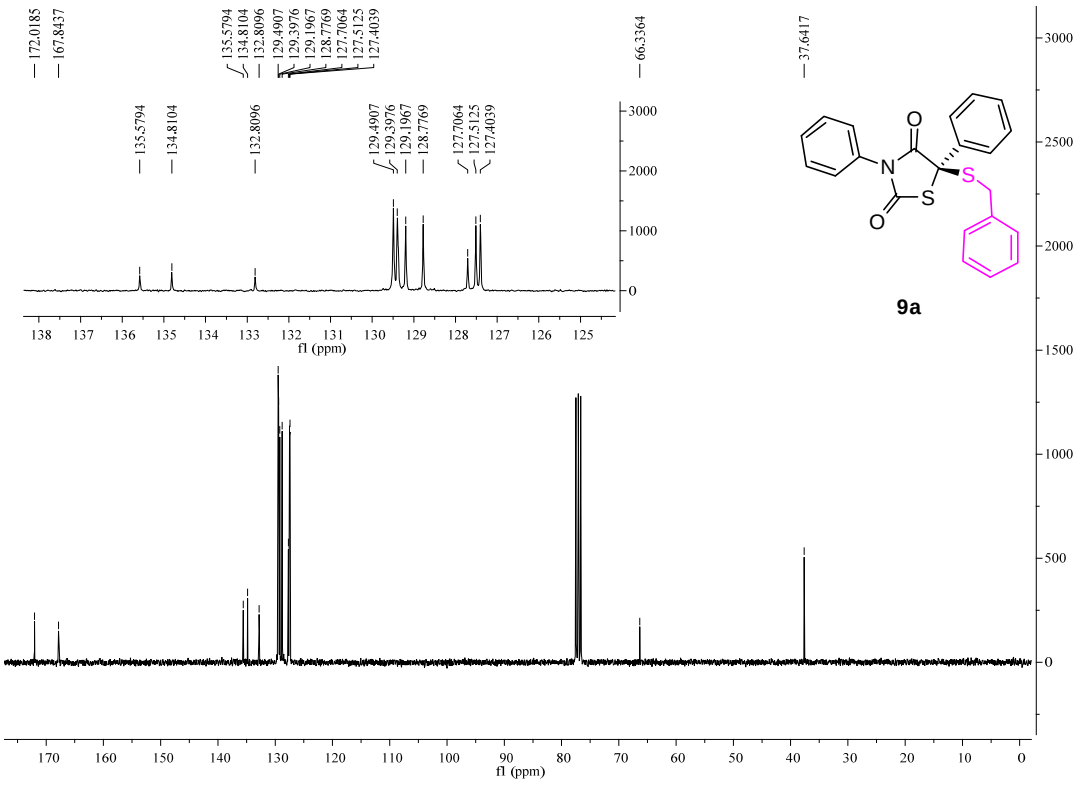
1.97
5.88
7.43
1.00
1.04
f1 (ppm)
9a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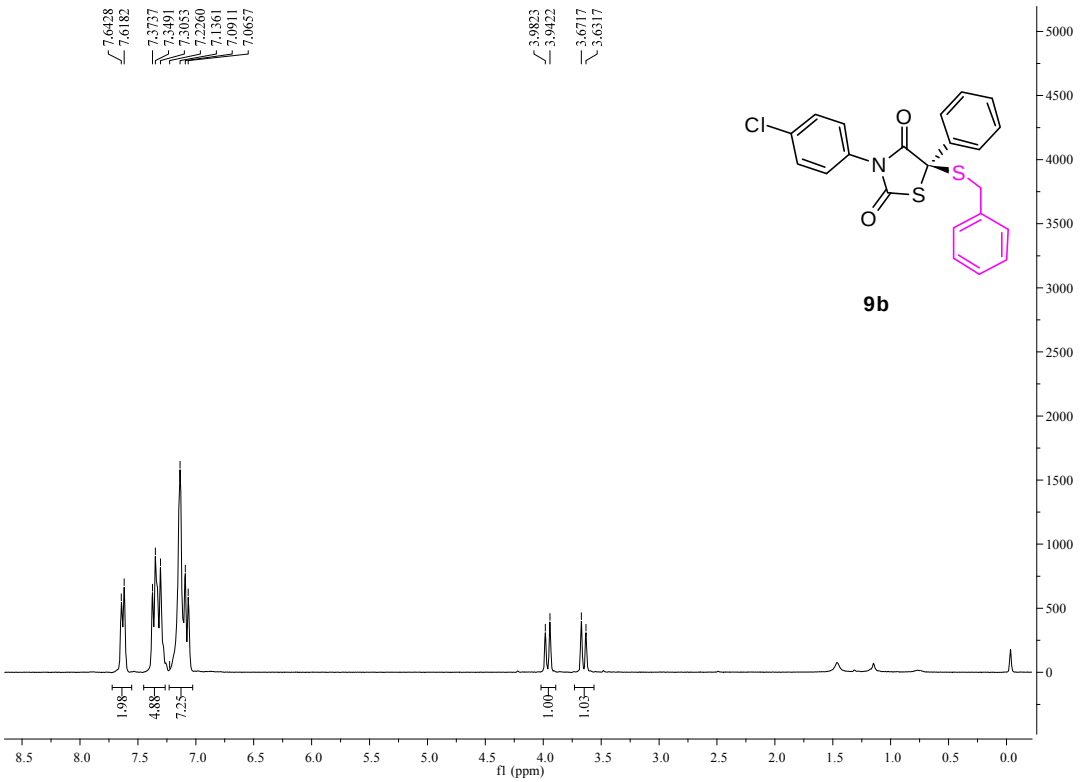
66.3364
37.6417
f1 (ppm)
9a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7.3737
7.3491
7.3053
7.2260
7.1361
7.0911
7.0657
3.9823
3.9422
3.6717
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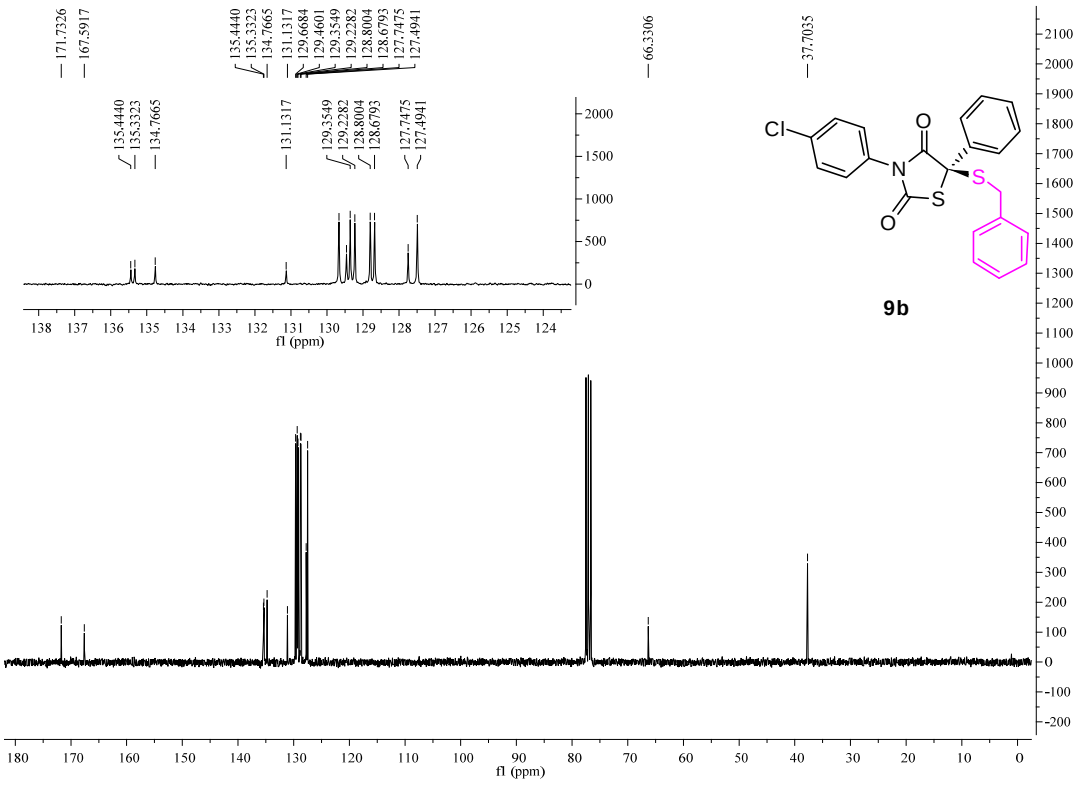
Cl
O
N
S
O
S
9b
1.98
4.88
7.25
1.00
1.03
fl (ppm)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128.8004
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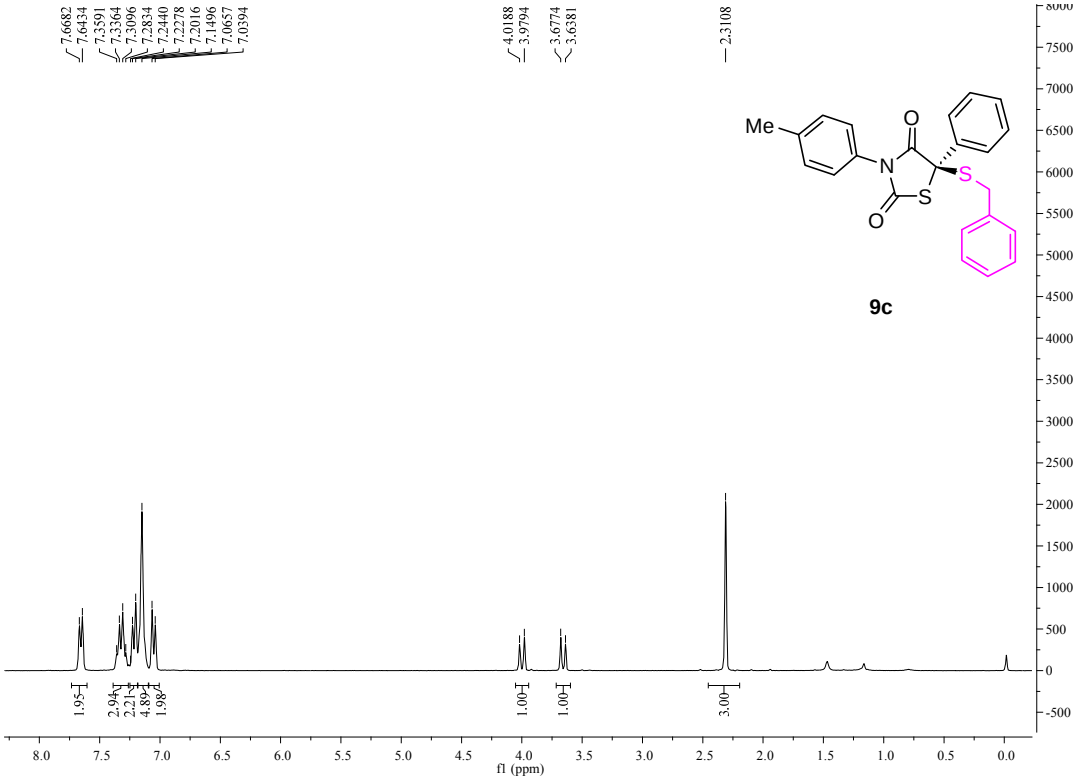
Cl
O
N
S
O
S
9b
fl (ppm)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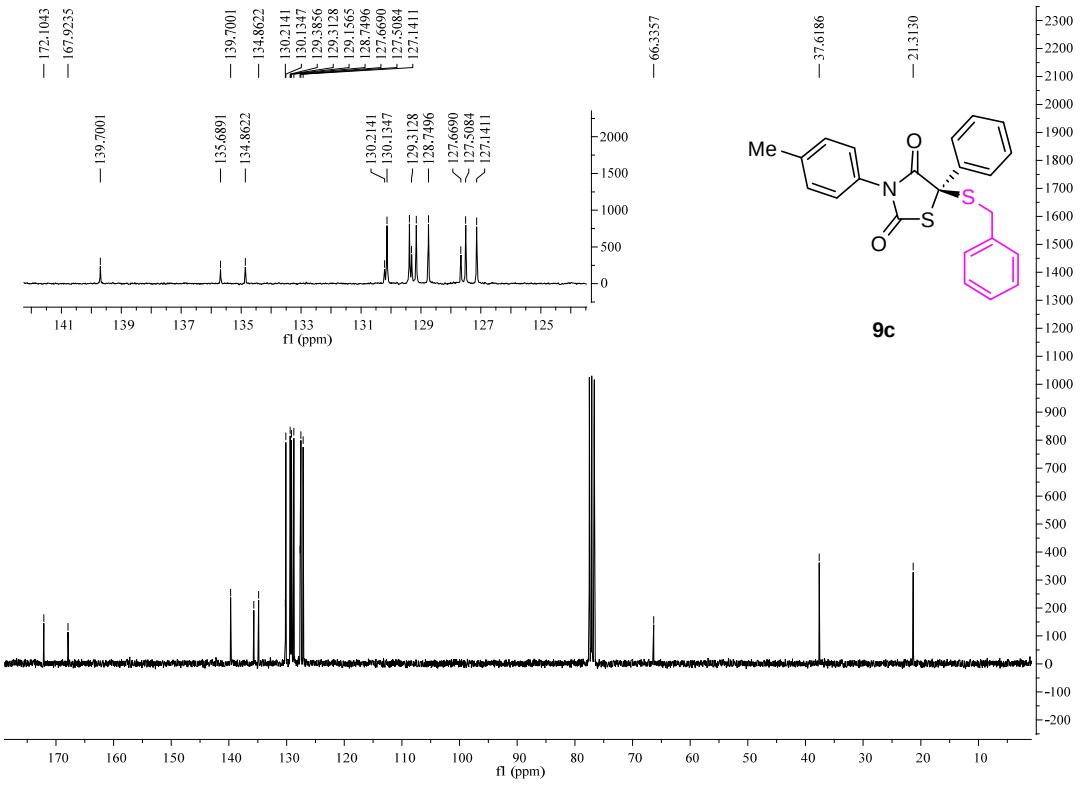
7.3096
7.2834
7.2440
7.2278
7.2016
7.1496
7.0657
7.0394
4.0188
3.9794
3.6774
3.6381
2.3108
Me
O
N
S
S
O
9c
1.95
2.94
2.21
4.89
1.98
1.00
1.00
3.00
f1 (ppm)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127.5084
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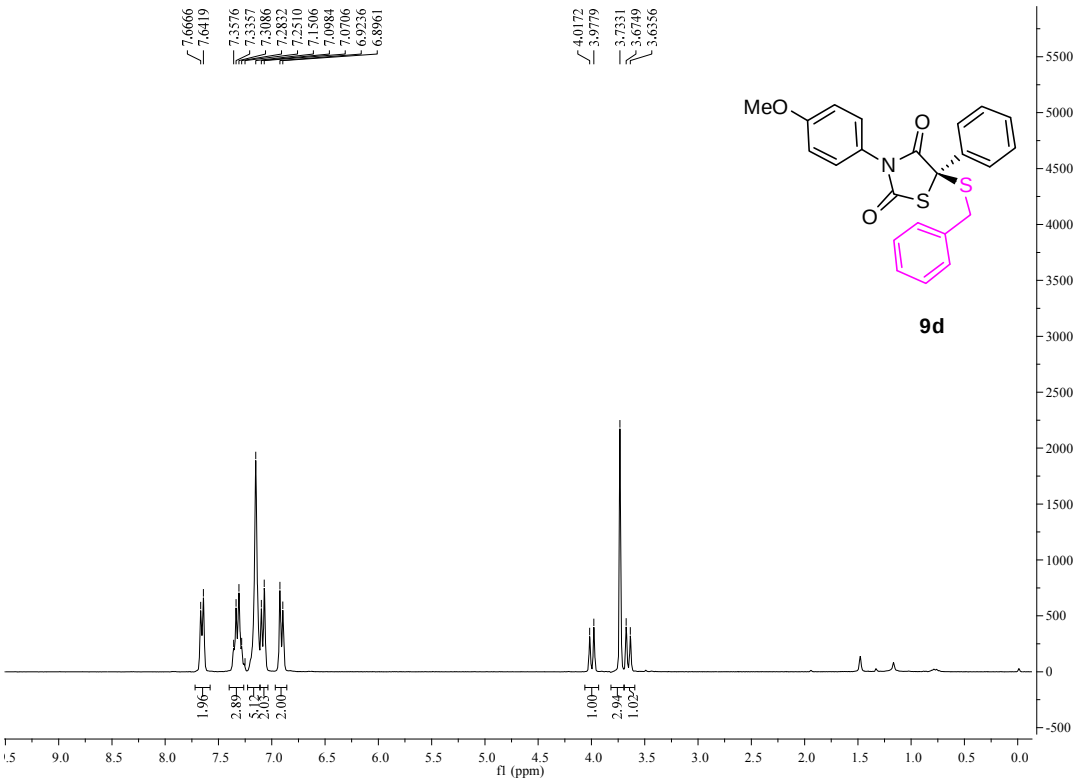
37.6186
21.3130
135.6891
Me
O
N
S
S
O
9c
f1 (ppm)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7.0984
7.0706
6.9236
6.8961
4.0172
3.9779
3.7331
3.6749
3.6356
MeO
O
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S
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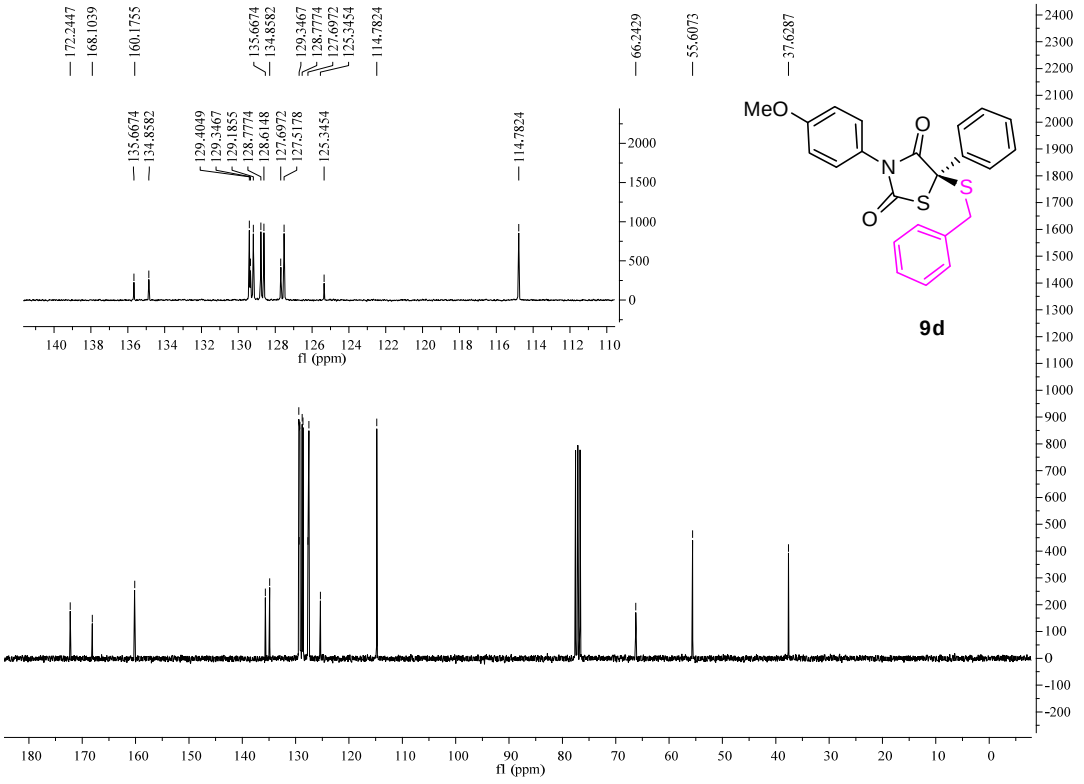
2.89
5.13
2.03
2.00
1.00
2.94
1.02
fl (ppm)

9d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127.6972
127.5178
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66.2429
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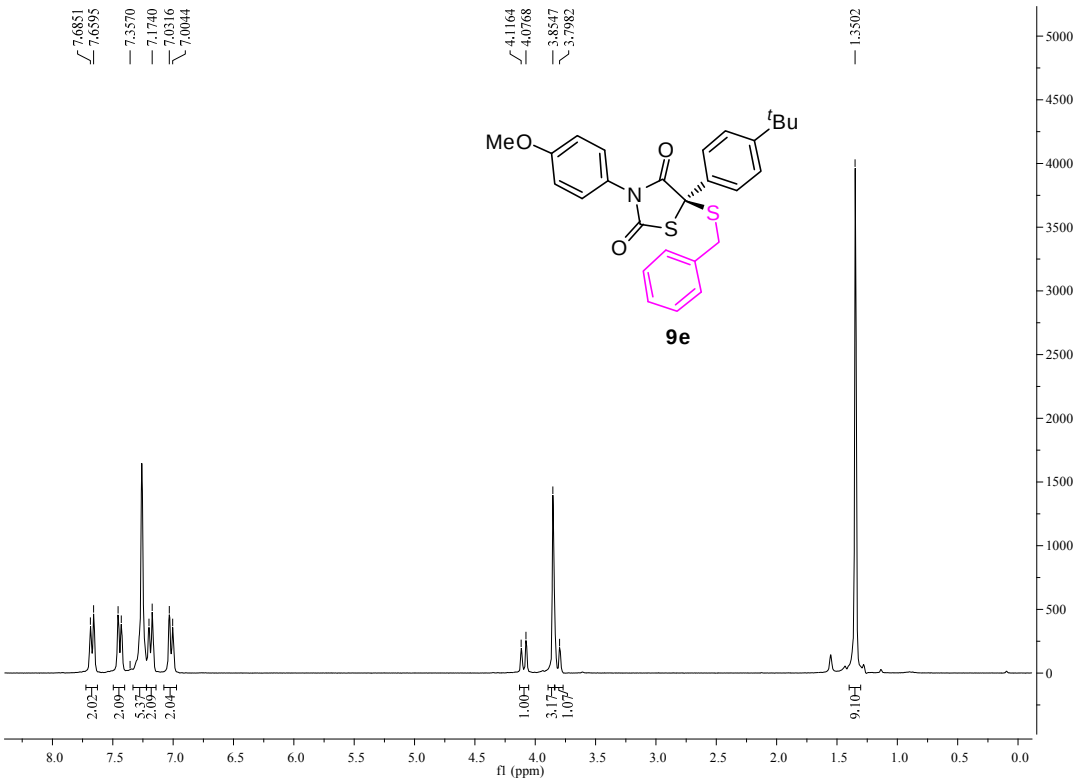
37.6287
MeO
O
N
O
S
S
fl (ppm)

9d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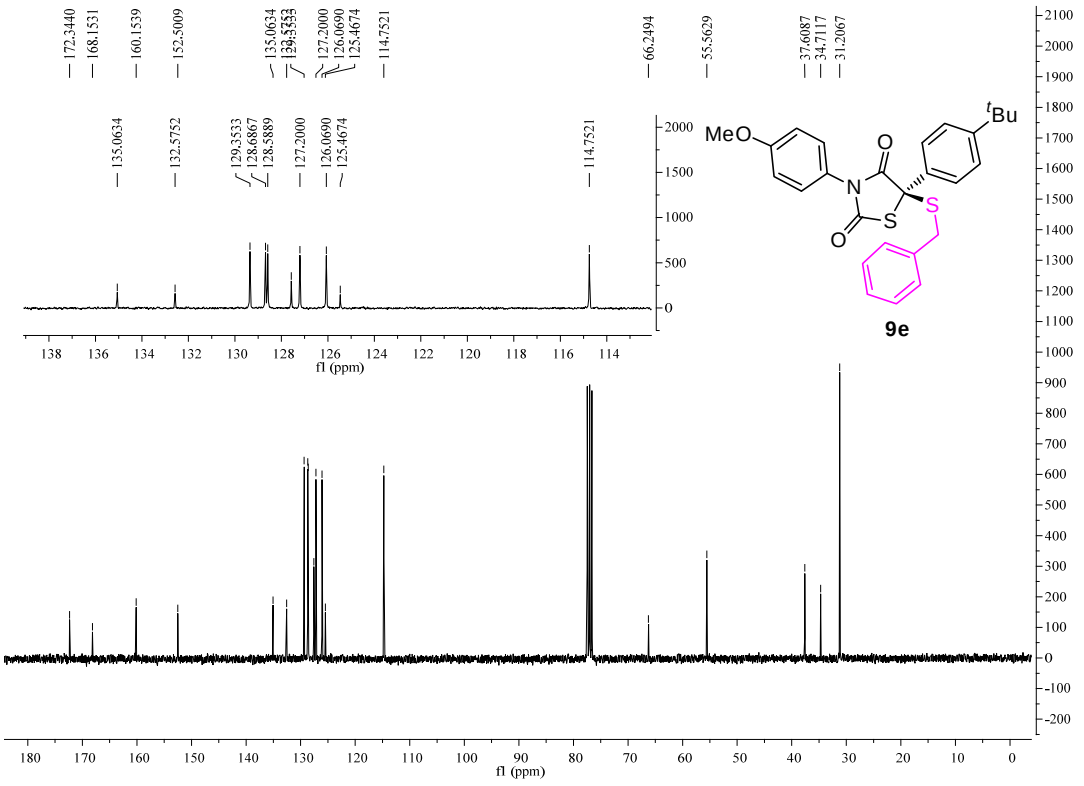
3.8547
3.7982
1.3502
MeO
O
N
S
O
S
tBu
9e
2.02
2.09
5.37
2.06
2.04
1.00
3.17
1.07
9.10
fl (ppm)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114.7521
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34.7117
31.2067
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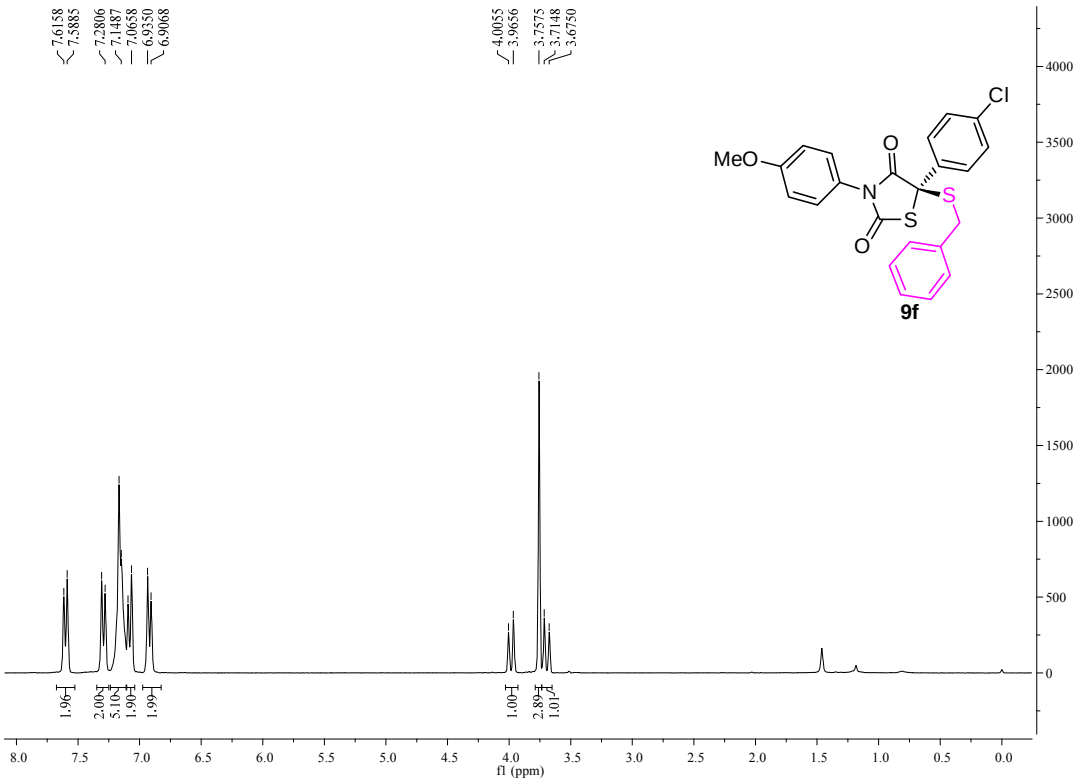
O
N
S
O
S
tBu
9e
fl (ppm)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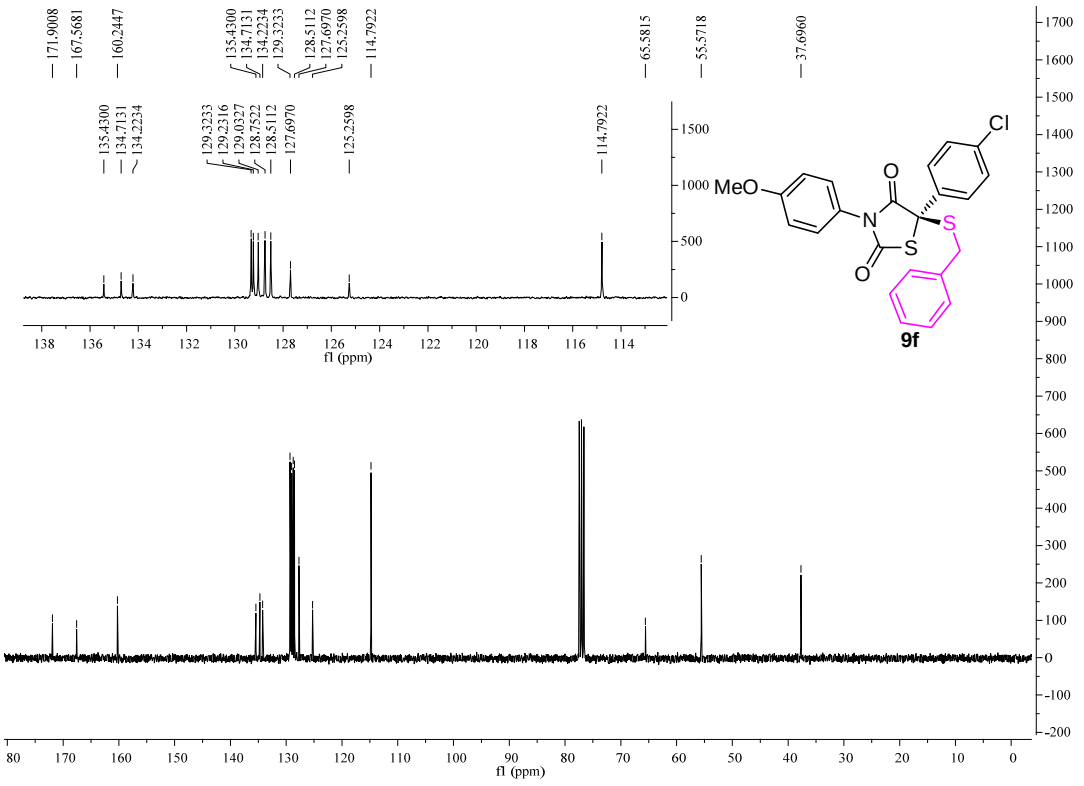
3.9656
3.7575
3.7148
3.6750
MeO
Cl
O
N
S
S
O
9f
1.96
2.00
5.10
1.90
1.99
1.00
2.89
1.01
fl (ppm)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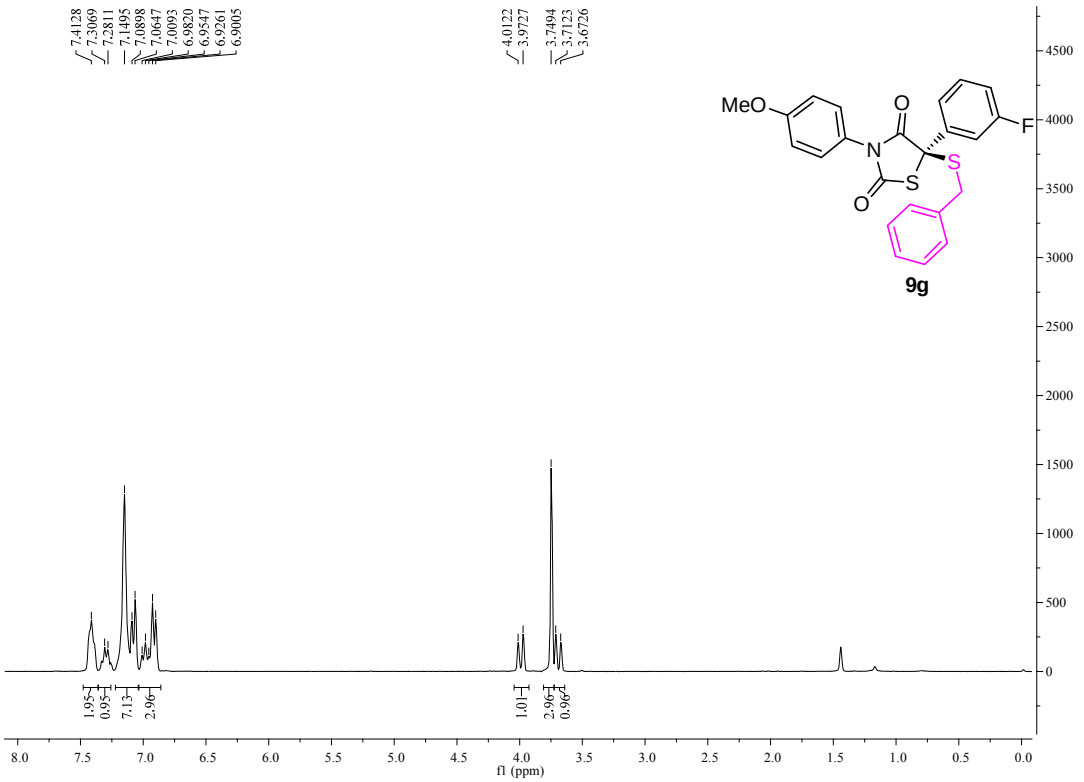
MeO
Cl
9f
fl (ppm)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6.9005
4.0122
3.9727
3.7494
3.7123
3.6726
MeO
O
N
S
O
S
F
9g
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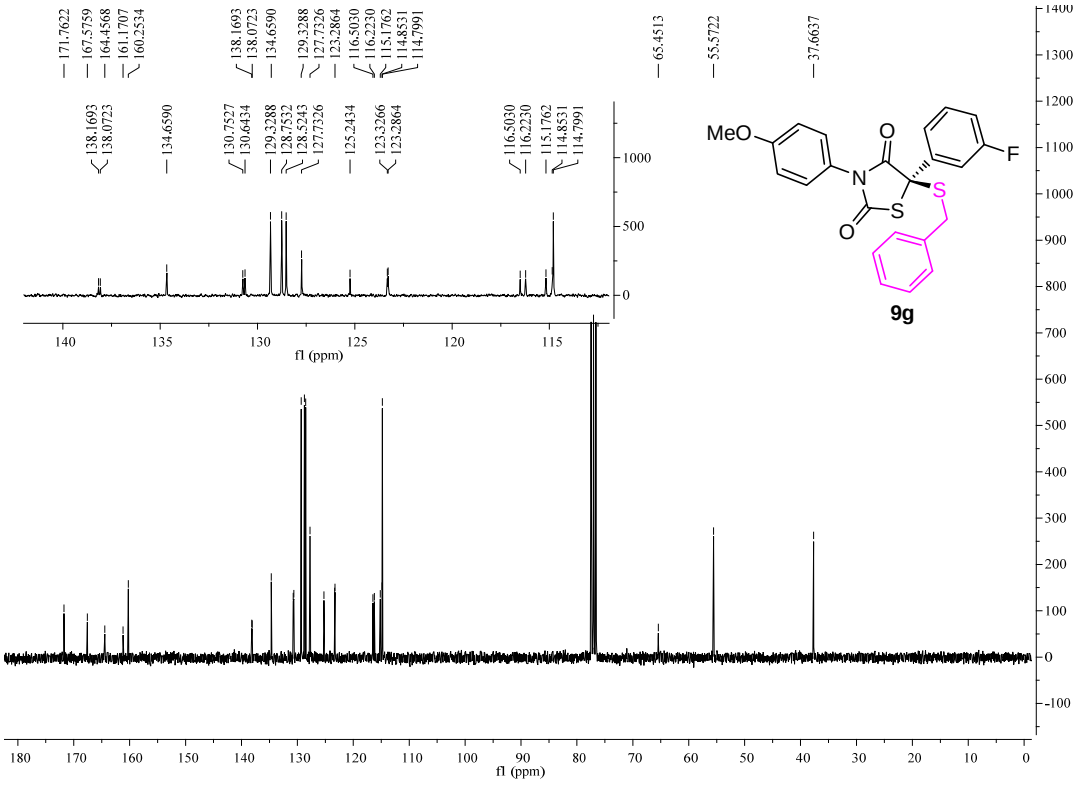
0.95
7.13
2.96
1.01
2.96
0.96
f1 (ppm)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128.7532
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127.7326
125.2434
123.3266
123.2864
116.5030
116.2230
115.1762
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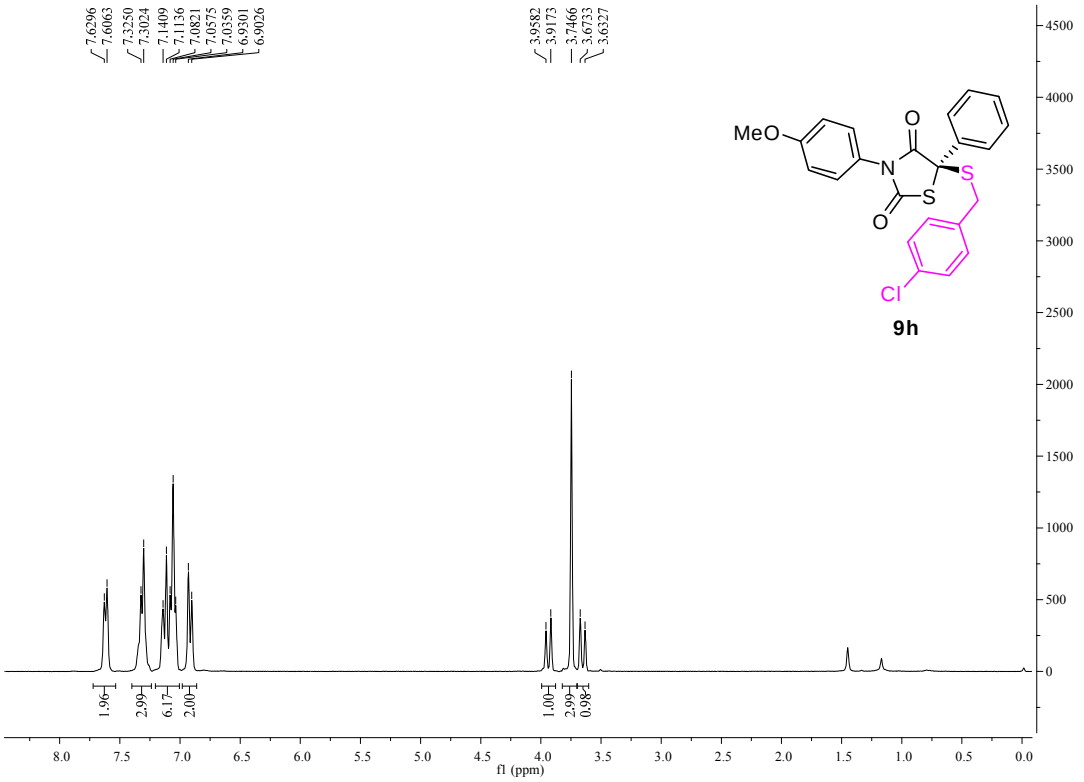
O
N
S
O
S
F
9g
f1 (ppm)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7.0359
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3.9582
3.9173
3.7466
3.6733
3.6327
MeO
O
N
S
O
S
Cl
9h
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2.99
6.17
2.00
1.00
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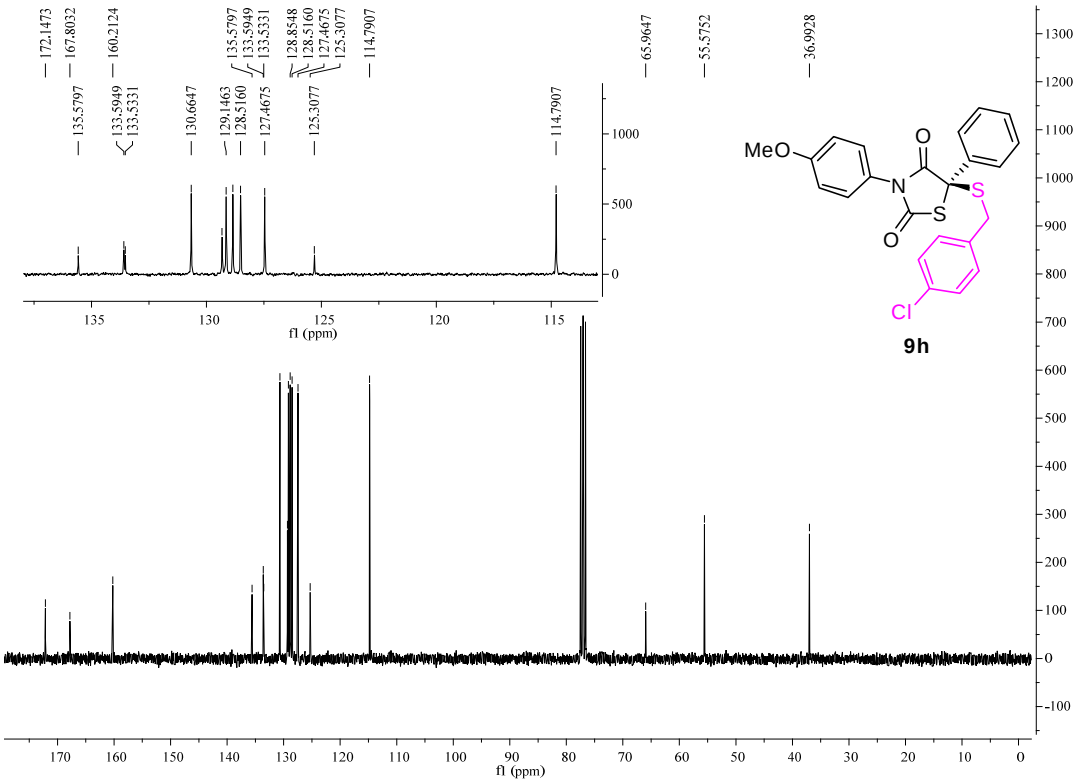
fl (ppm)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55.5752
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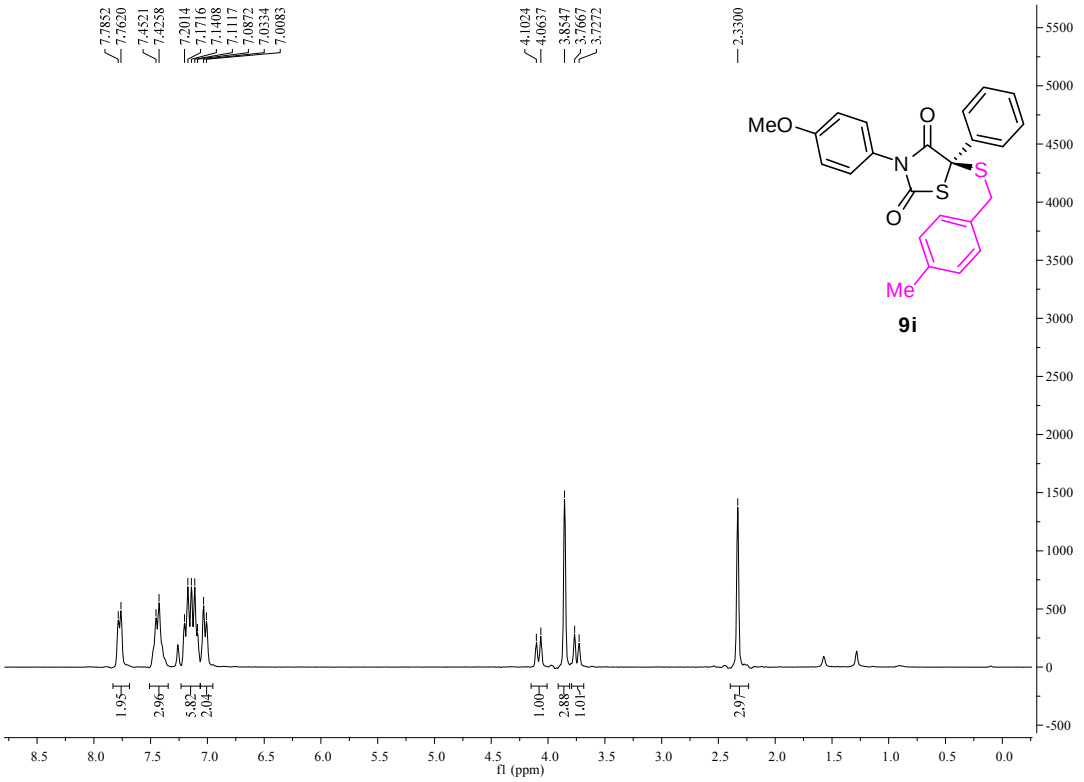
N
S
O
S
Cl
9h
fl (ppm)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4.0637
3.8547
3.7667
3.7272
2.3300
MeO
O
N
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S
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9i
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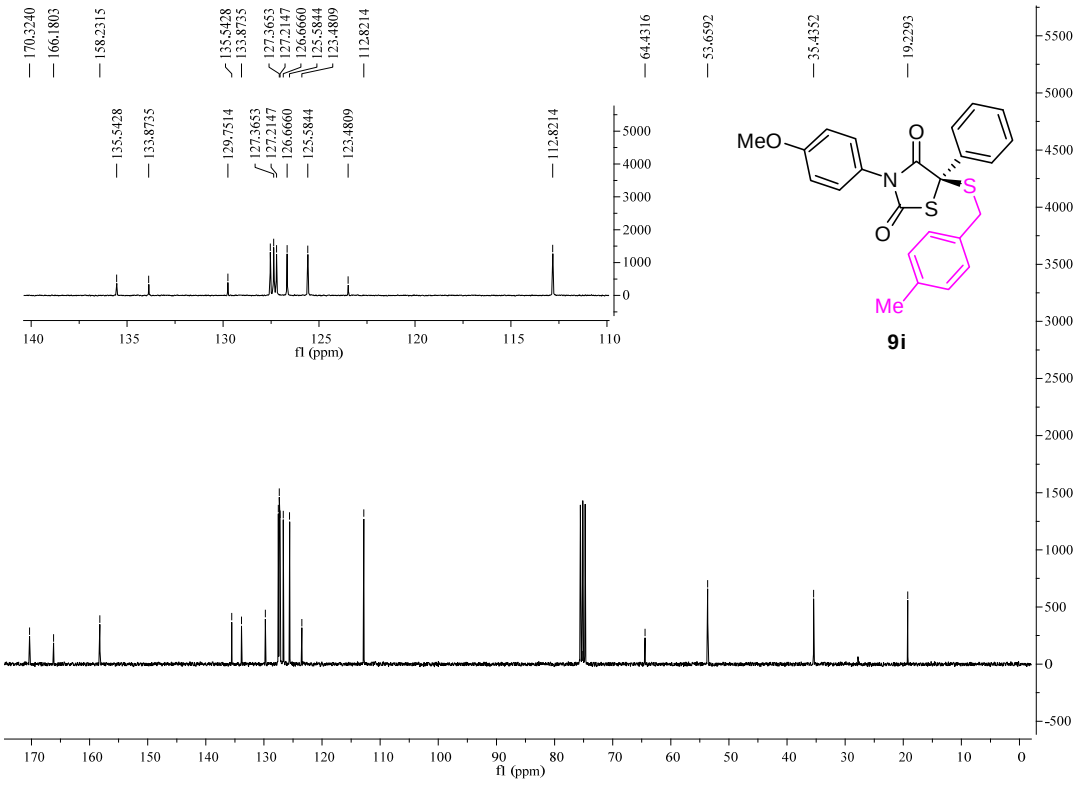
5.82
2.04
1.00
2.88
1.01
2.97
fl (ppm)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35.4352
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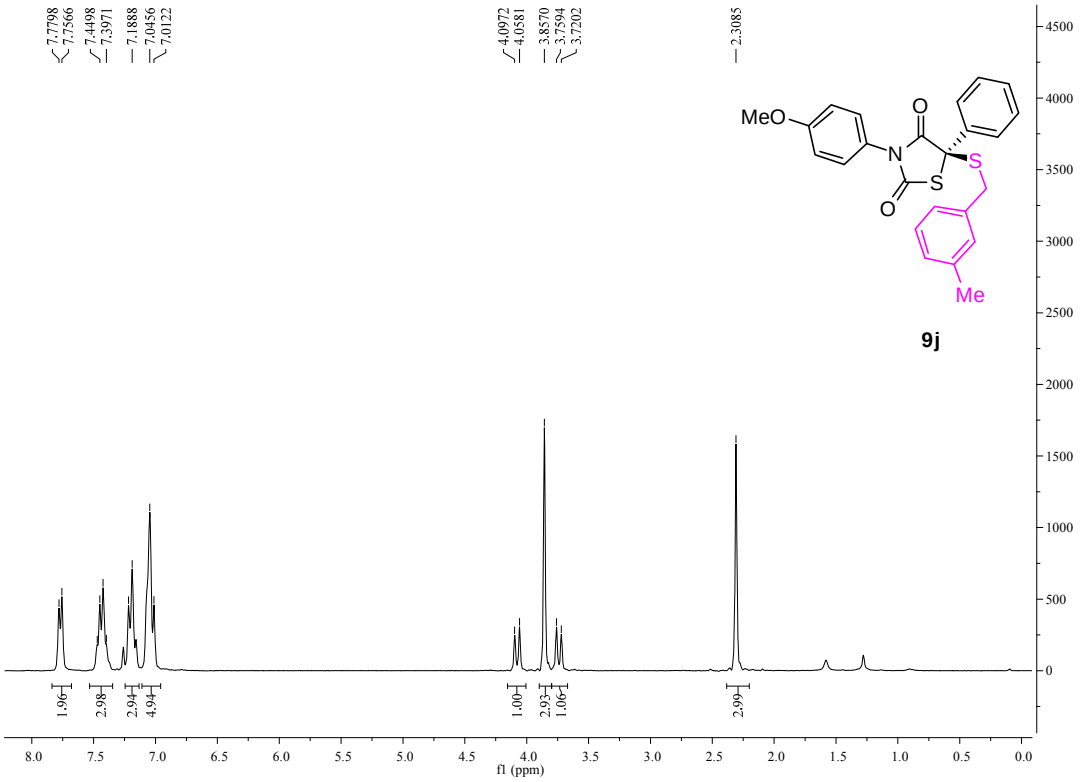
O
N
S
S
O
Me
9i
fl (ppm)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3.7594
3.7202
2.3085
MeO
N
O
S
O
S
Me
9j
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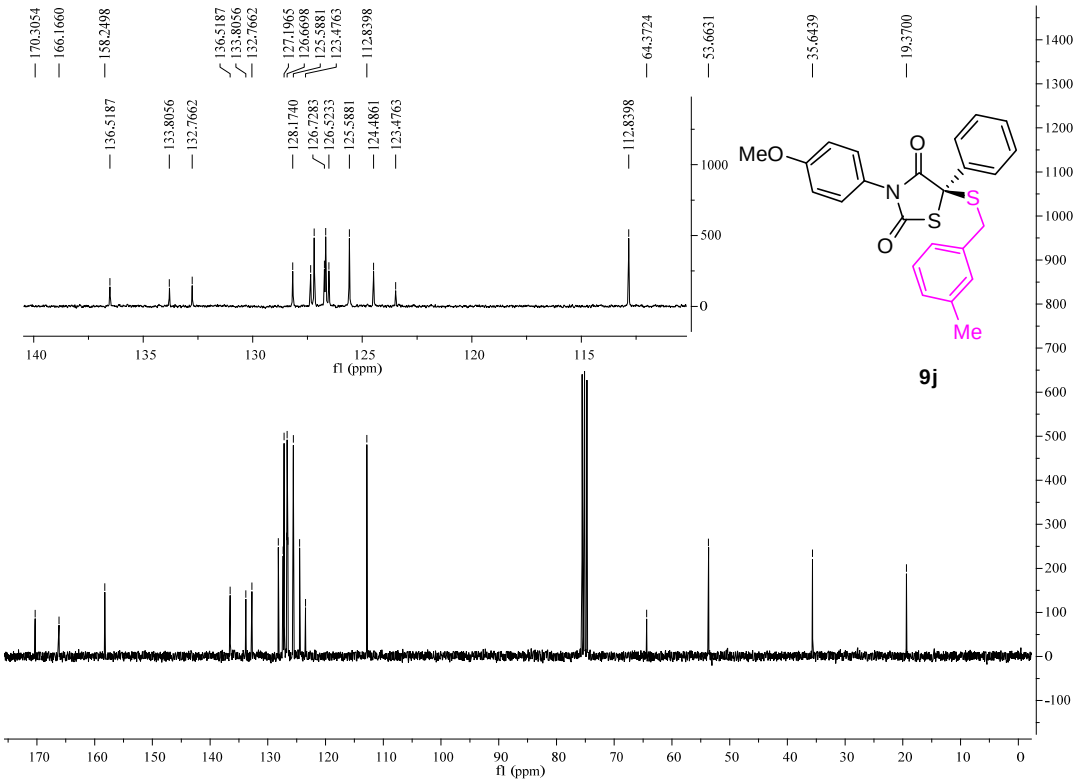
2.94
4.94
1.00
2.93
1.06
2.99
f1 (ppm)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123.4763
112.8398
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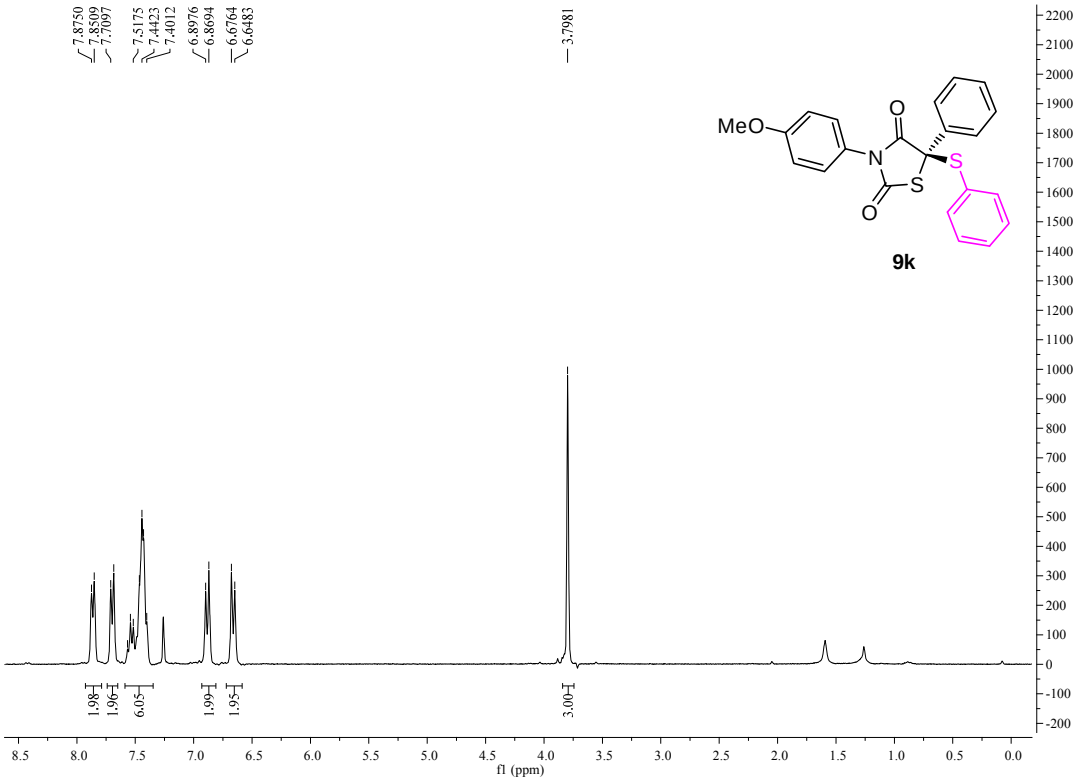
N
O
S
O
S
Me
9j
f1 (ppm)
f1 (ppm)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O
S
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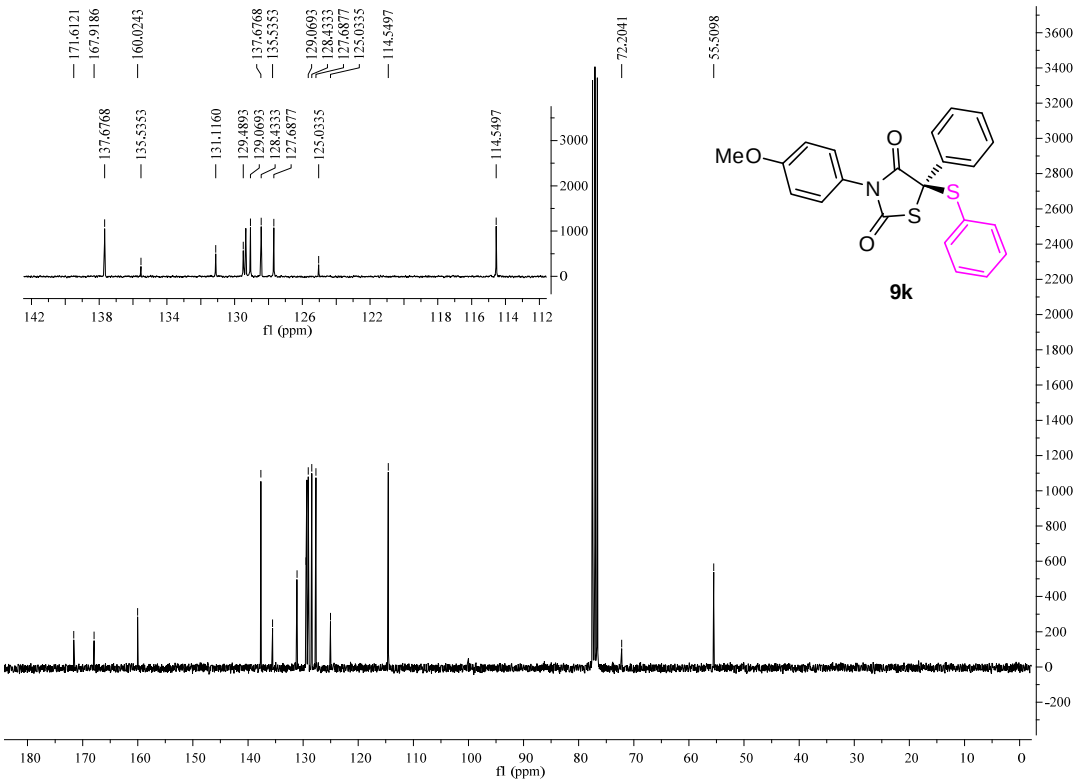
1.96
6.05
1.99
1.95
3.00
fl (ppm)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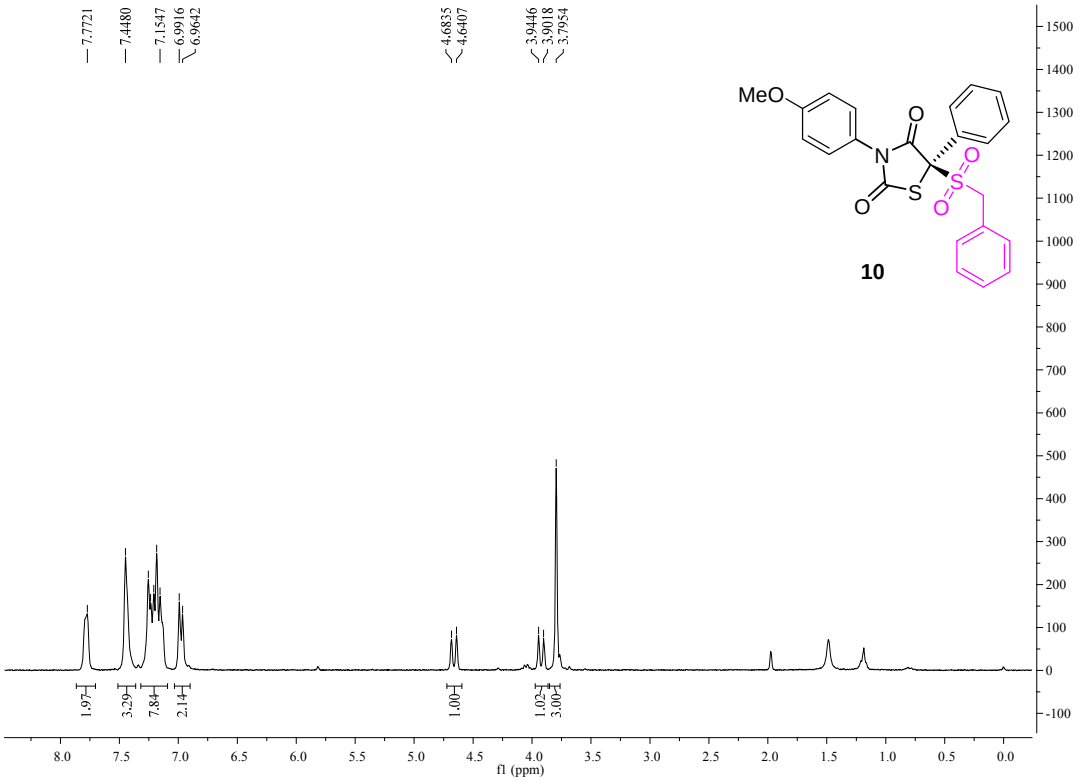
O
S
9k
fl (ppm)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4.6407
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3.9018
3.7954
MeO
O
N
O
S
O
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10
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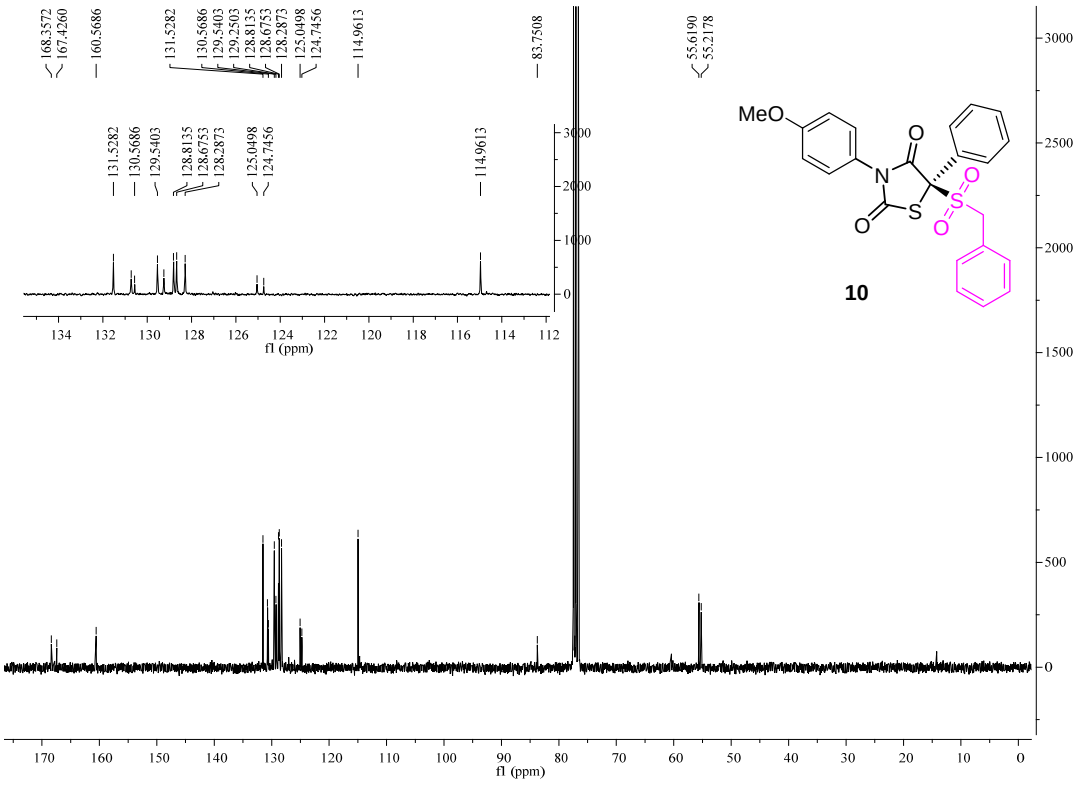
3.29
7.84
2.14
1.00
1.02
3.00
f1 (ppm)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124.7456
114.9613
83.7508
55.6190
55.2178
MeO
O
N
O
S
O
O=S=O
10
f1 (ppm)