

Supplementary Materials

1. Crystal Data and Structures Refinement for Enantiopure 4a and 5a

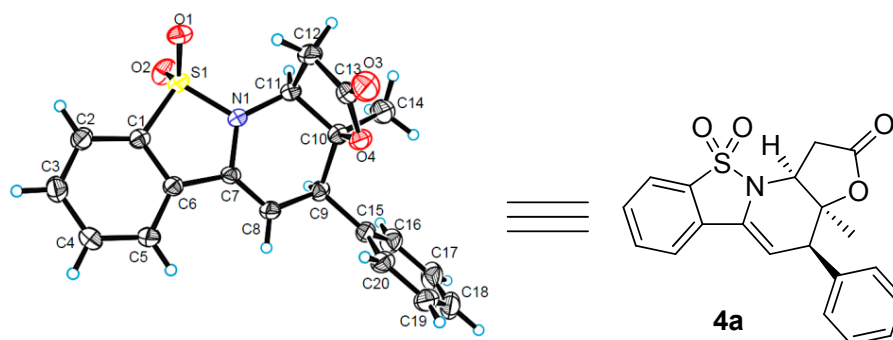


Figure 1. X-ray structure of enantiopure **4a**.

Table 1. Crystal data of enantiopure **4a**.

Identification code	4a
Empirical formula	C ₂₀ H ₁₇ NO ₄ S
Formula weight	367.40
Temperature/K	290(2)
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	10.0540(3)
b/Å	12.0824(5)
c/Å	14.5627(4)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	1769.03(10)
Z	4
ρ _{calc} /cm ³	1.379
μ/mm ⁻¹	0.209
F(000)	768.0
Crystal size/mm ³	0.42 × 0.32 × 0.3
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	6.534 to 52.732
Index ranges	-9 ≤ h ≤ 12, -9 ≤ k ≤ 15, -18 ≤ l ≤ 18
Reflections collected	9168
Independent reflections	3620 [R _{int} = 0.0210, R _{sigma} = 0.0289]
Data/restraints/parameters	3620/0/235
Goodness-of-fit on F ²	1.065
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0369, wR ₂ = 0.0840
Final R indexes [all data]	R ₁ = 0.0446, wR ₂ = 0.0886
Largest diff. peak/hole / e Å ⁻³	0.14/-0.31
Flack parameter	-0.05(3)

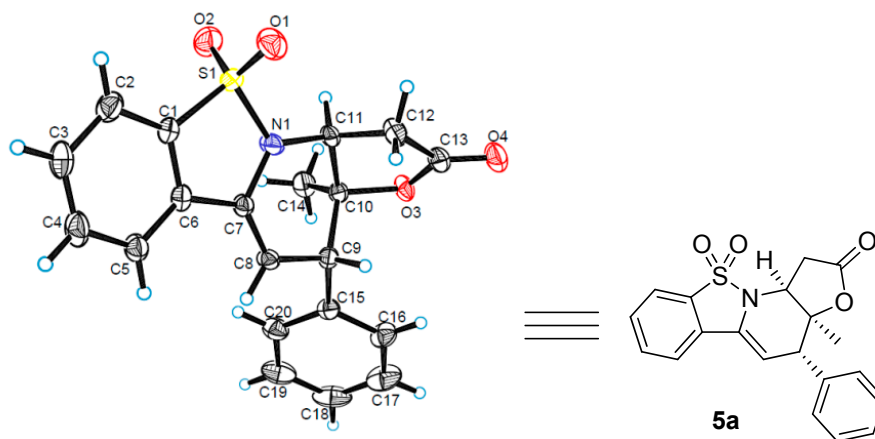
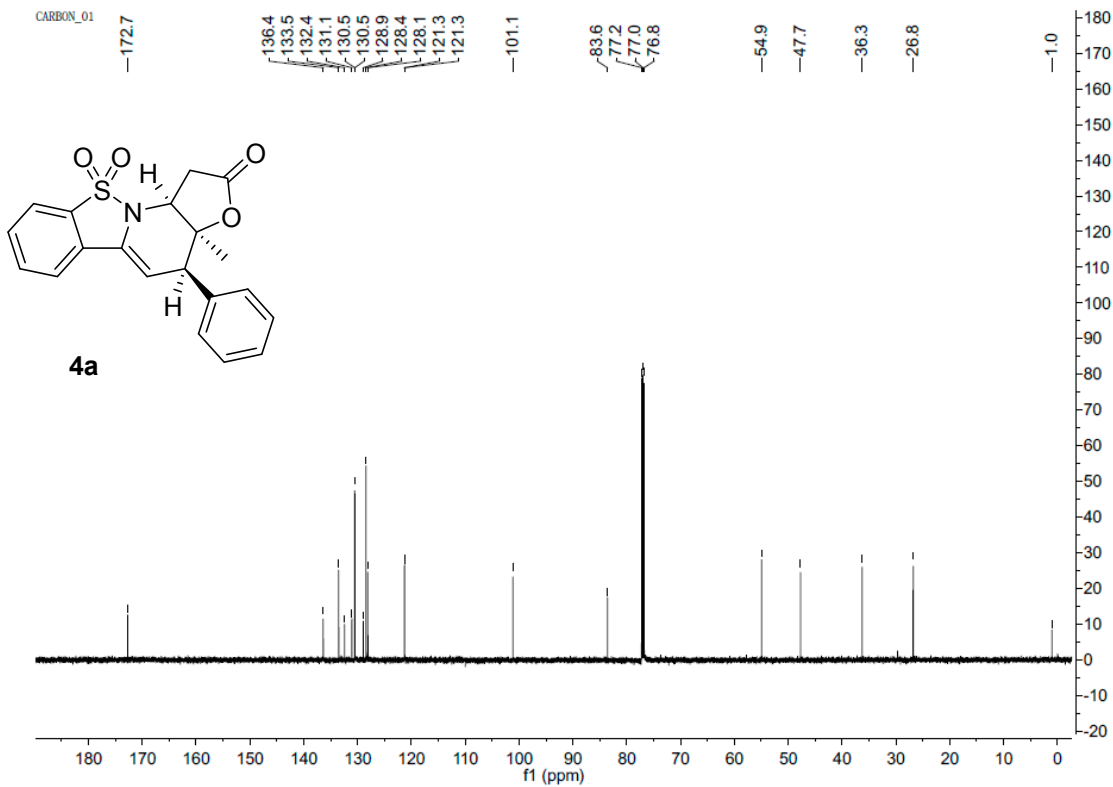
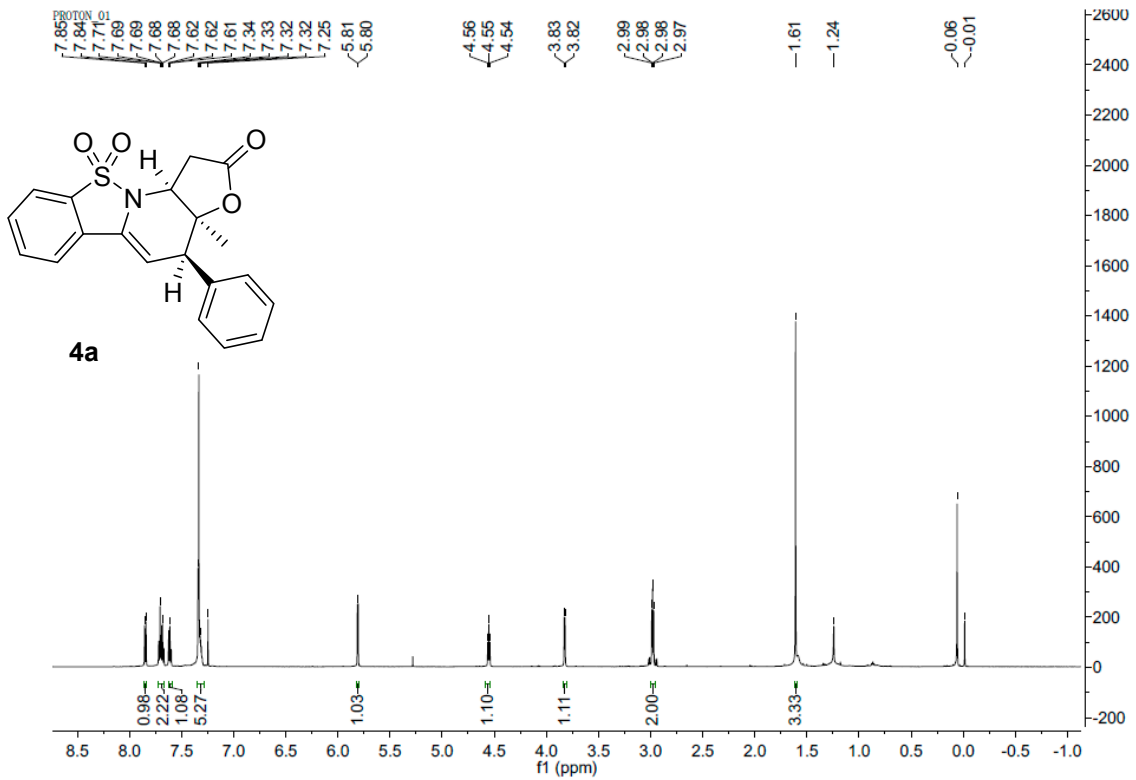


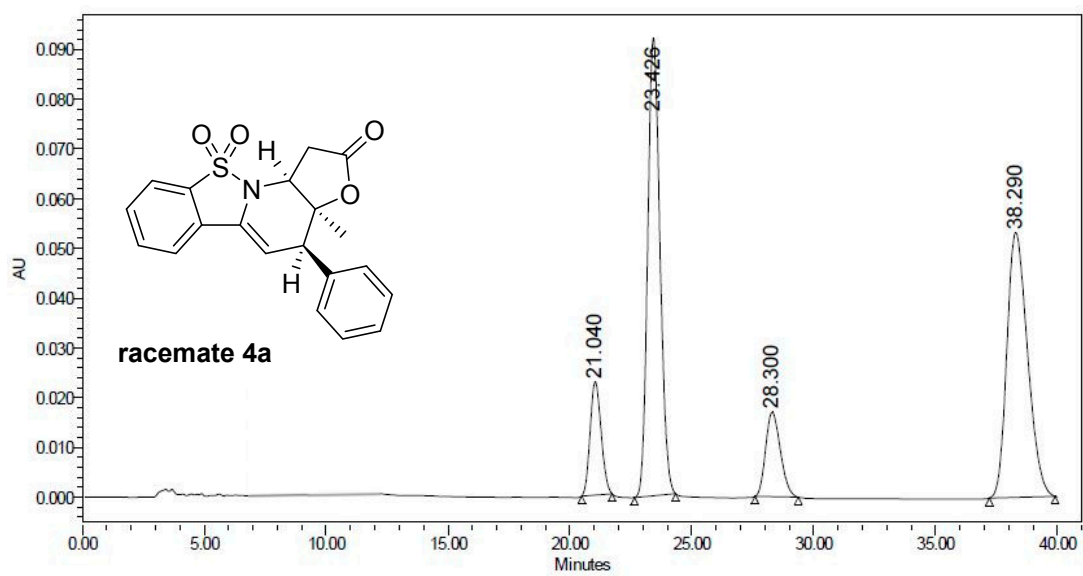
Figure 2. X-ray structure of enantiopure **5a**.

Table 2. Crystal data of enantiopure **5a**.

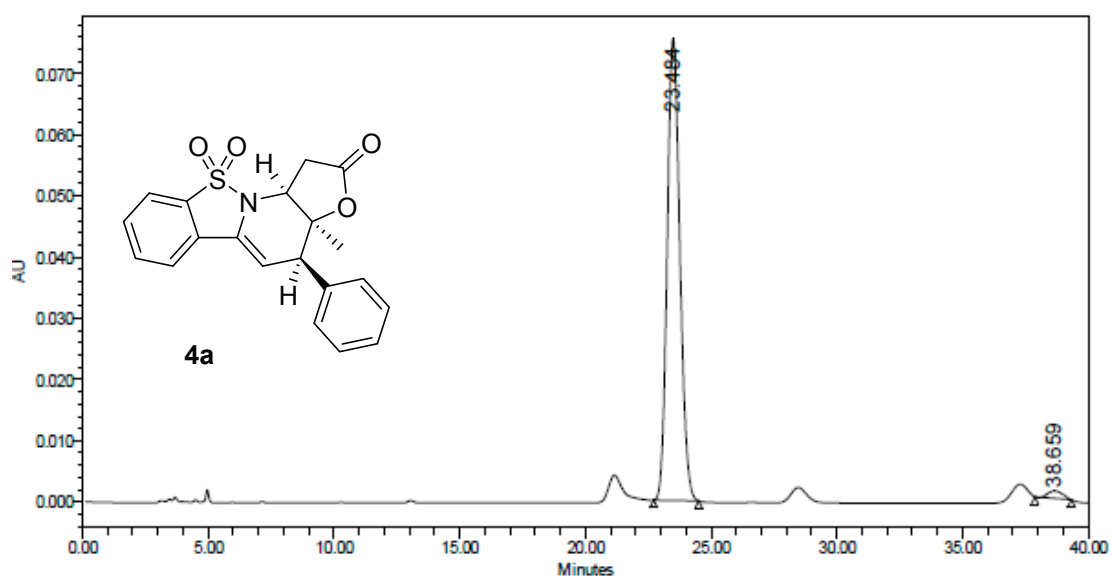
Identification code	5a
Empirical formula	C ₂₀ H ₁₇ NO ₄ S
Formula weight	367.40
Temperature/K	291(2)
Crystal system	monoclinic
Space group	P2 ₁
a/Å	8.3275(5)
b/Å	6.8178(4)
c/Å	15.4042(8)
α/°	90
β/°	95.886(5)
γ/°	90
Volume/Å ³	869.97(8)
Z	2
ρ _{calc} /cm ³	1.403
μ/mm ⁻¹	0.212
F(000)	384.0
Crystal size/mm ³	0.32 × 0.3 × 0.25
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	6.54 to 52.744
Index ranges	-10 ≤ h ≤ 10, -8 ≤ k ≤ 8, -19 ≤ l ≤ 19
Reflections collected	8527
Independent reflections	3483 [R _{int} = 0.0265, R _{sigma} = 0.0295]
Data/restraints/parameters	3483/1/235
Goodness-of-fit on F ²	1.060
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0709, wR ₂ = 0.1873
Final R indexes [all data]	R ₁ = 0.0730, wR ₂ = 0.1886
Largest diff. peak/hole/e Å ⁻³	0.90/-0.32
Flack parameter	0.08(6)

2. NMR Spectra and HPLC Chromatograms

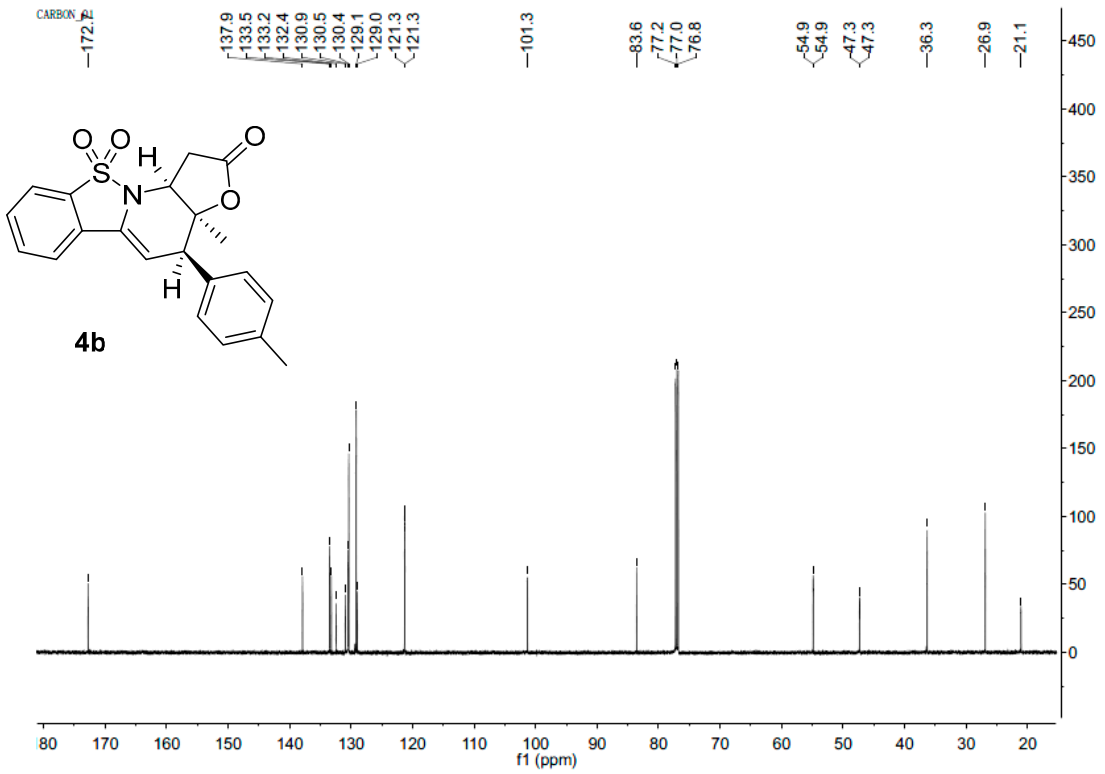
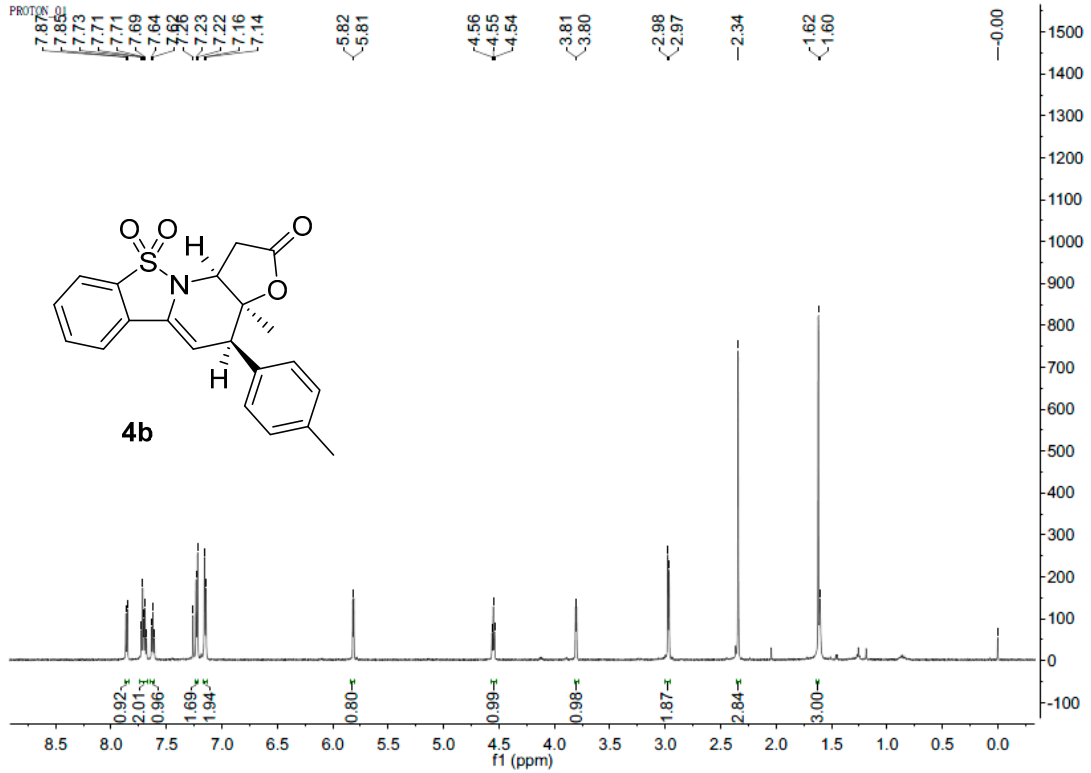


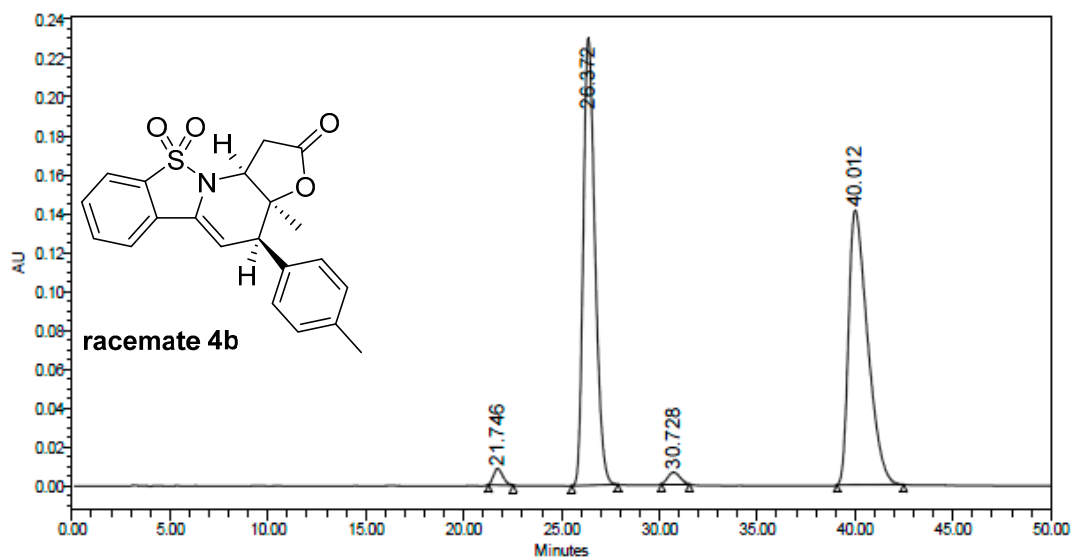


	RT	Area	% Area	Height
1	21.040	715013	9.18	22797
2	23.426	3212990	41.27	92060
3	28.300	716262	9.20	16994
4	38.290	3141649	40.35	53265

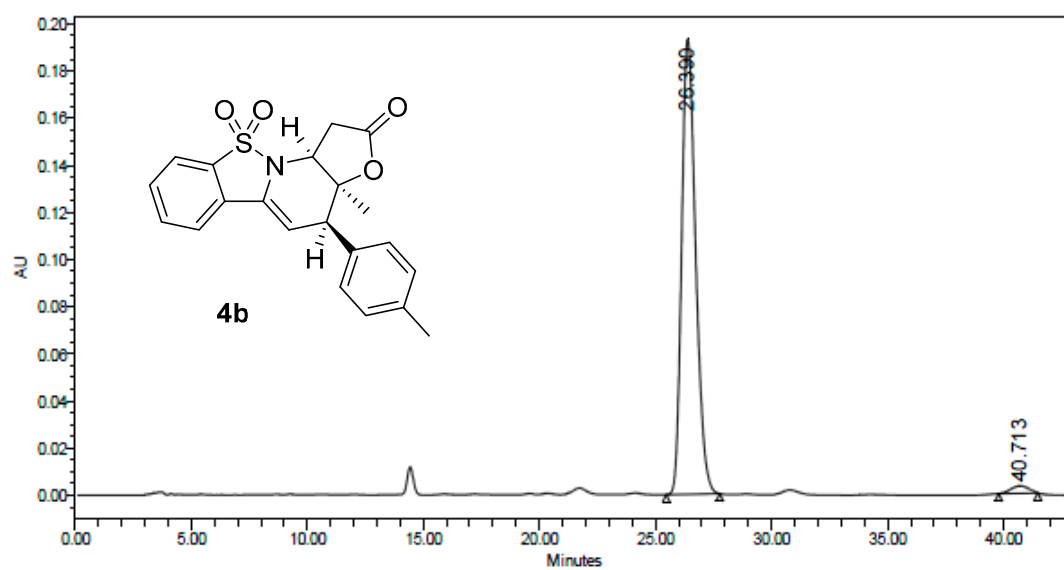


	RT	Area	% Area	Height
1	23.484	2635687	98.09	75481
2	38.659	51335	1.91	1217

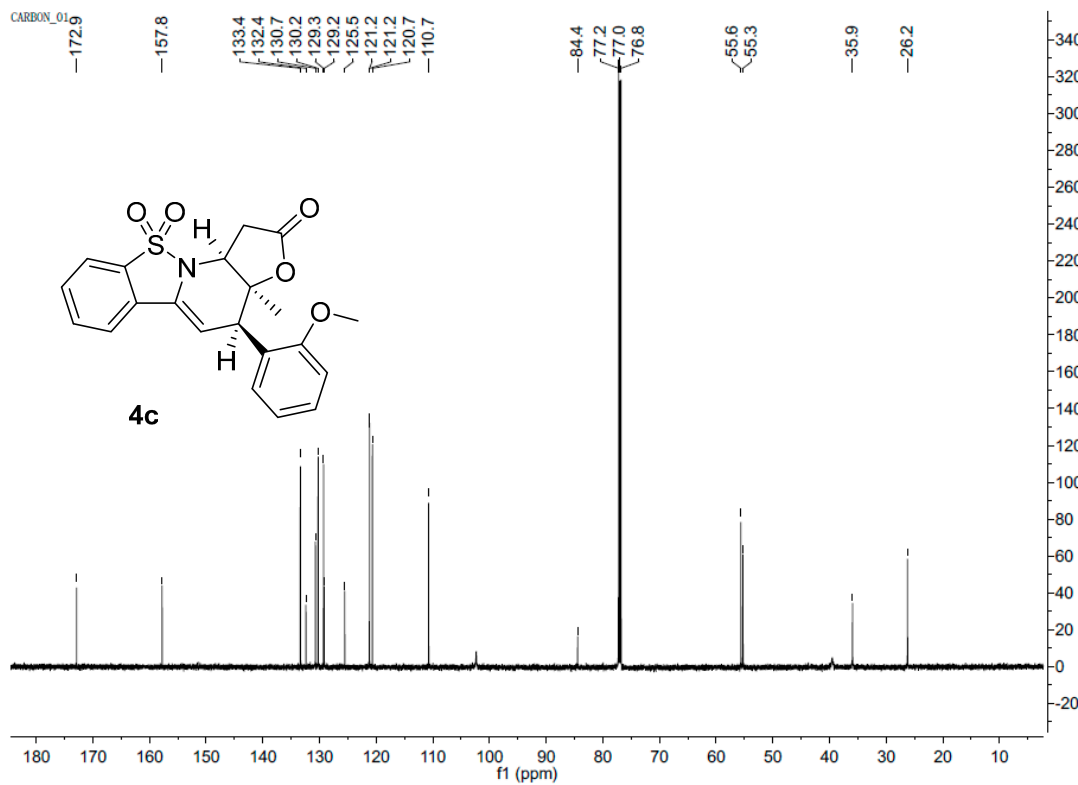
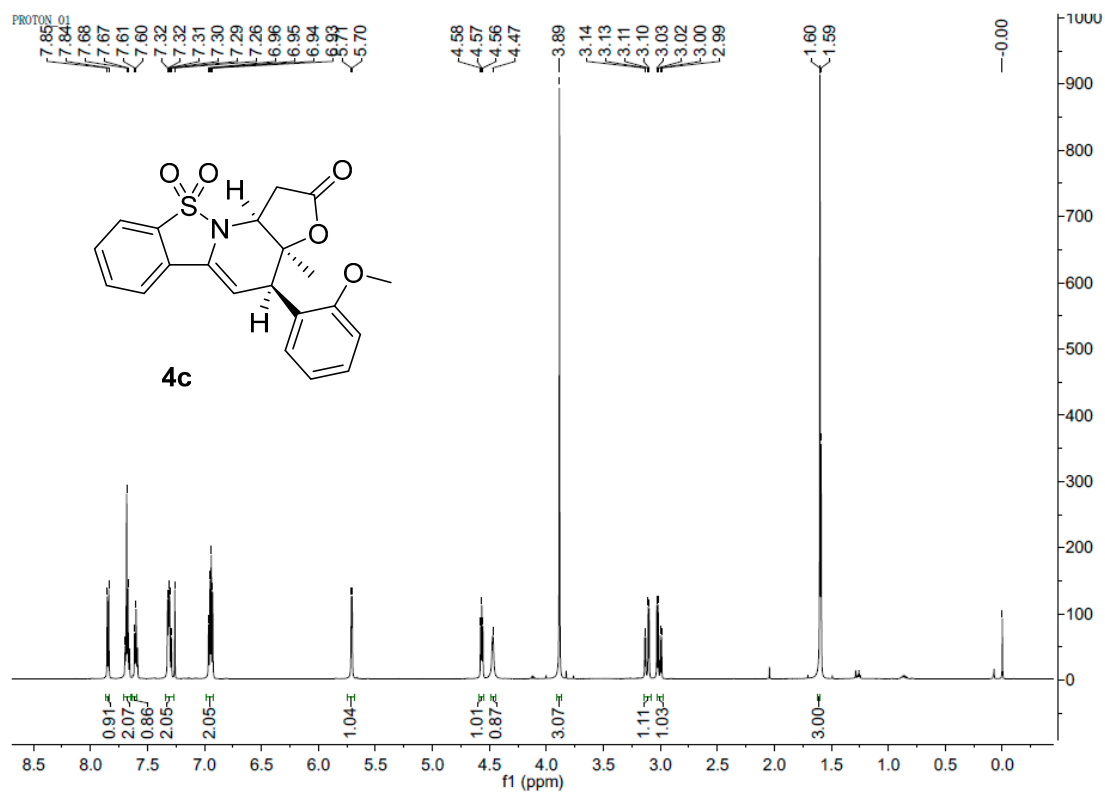


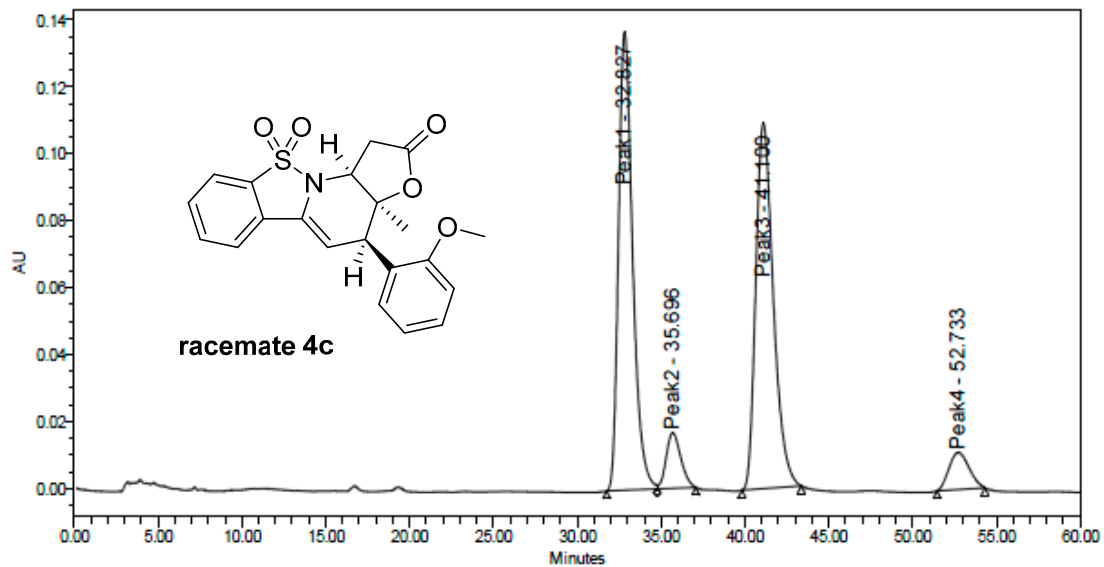


	RT	Area	% Area	Height
1	21.746	276315	1.41	8224
2	26.372	9562954	48.75	229757
3	30.728	258665	1.32	6046
4	40.012	9517600	48.52	140945

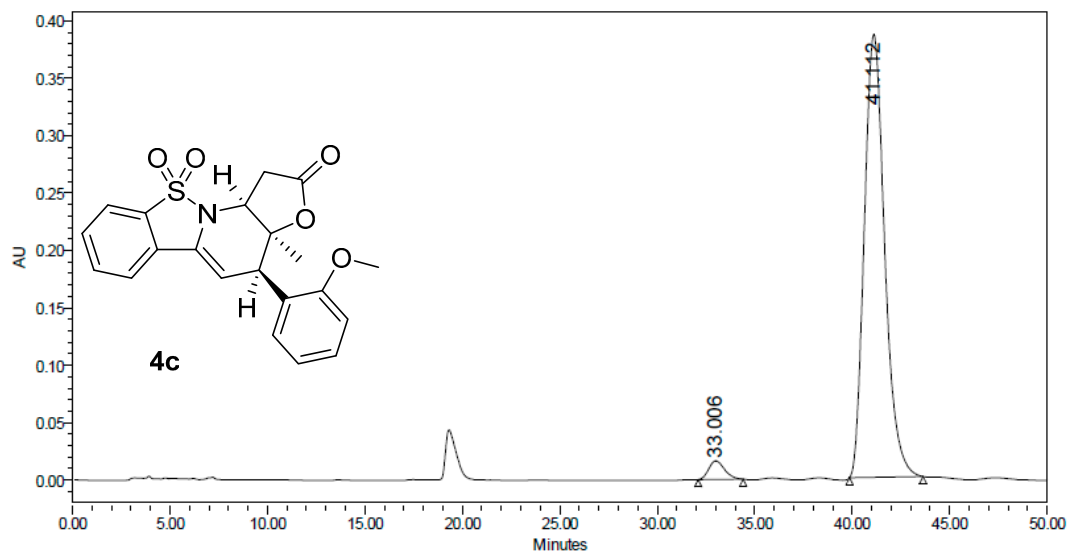


	RT	Area	% Area	Height
1	26.390	8054746	97.99	193261
2	40.713	165058	2.01	3145

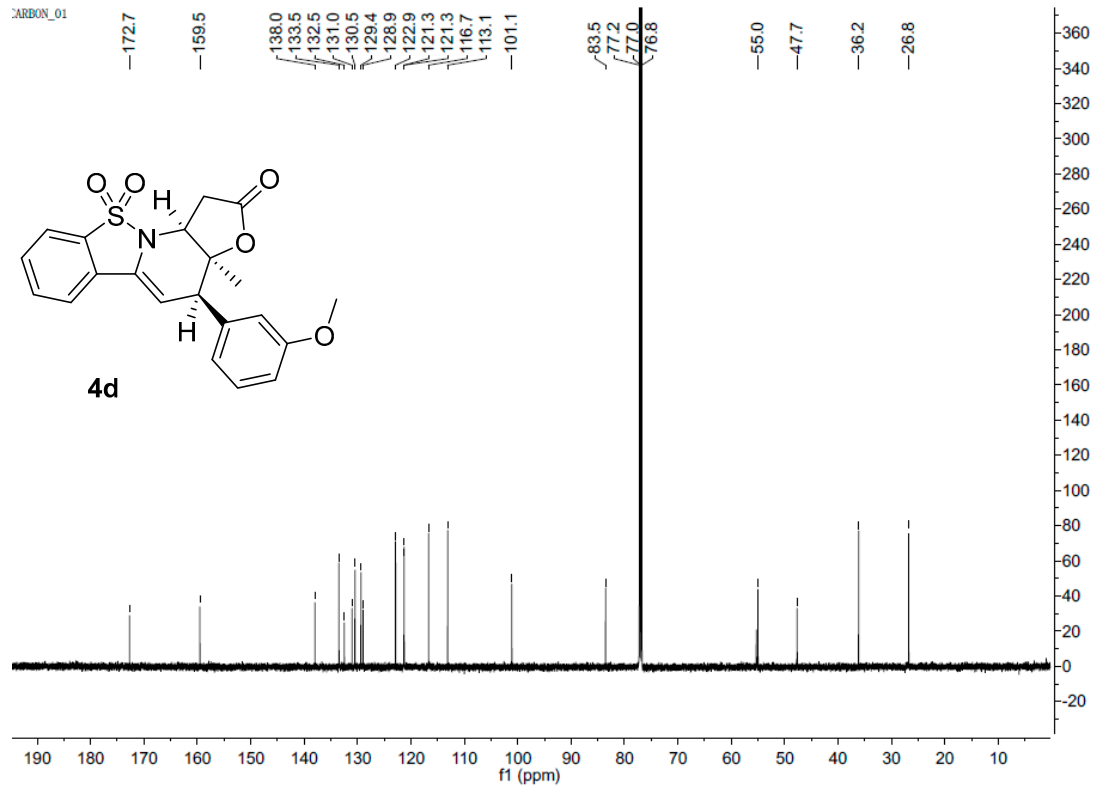
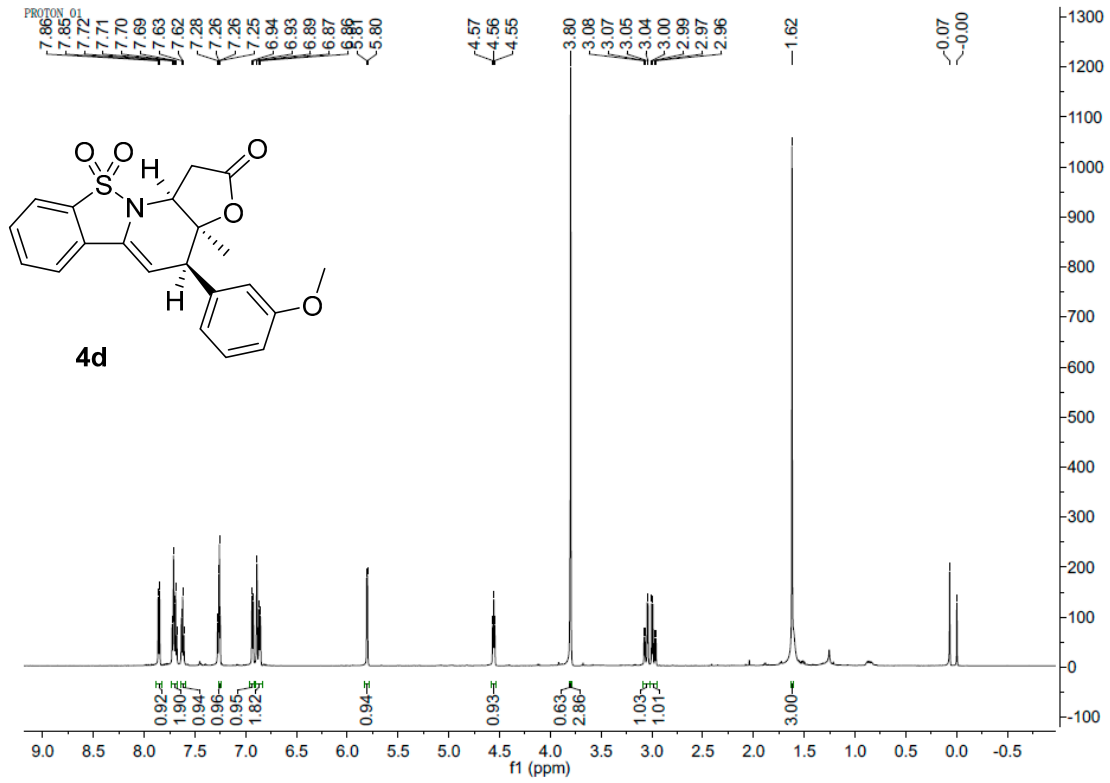


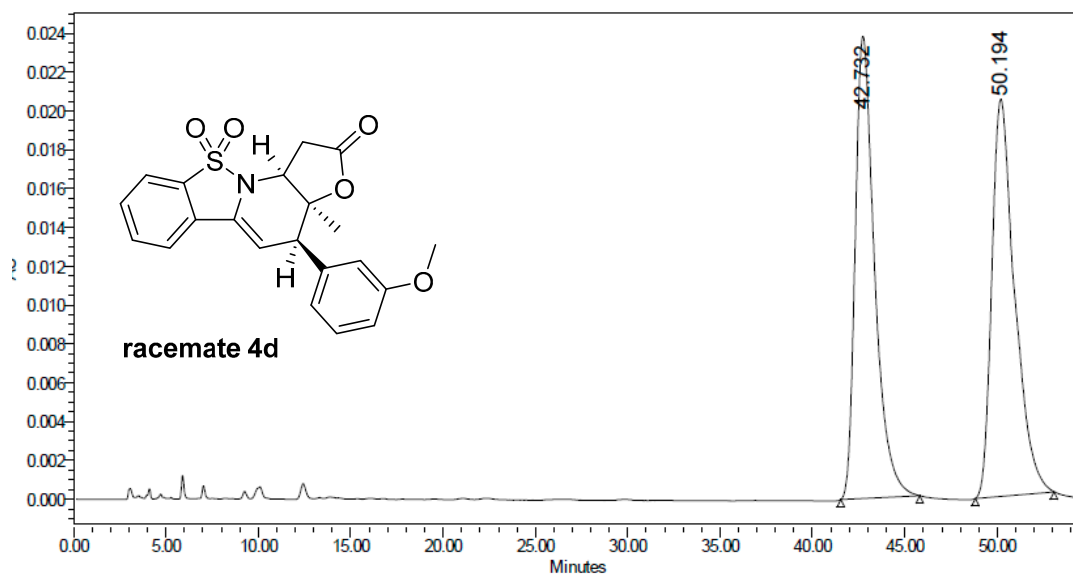


	Peak Name	RT	Area	% Area	Height
1	Peak1	32.827	7971683	44.73	136870
2	Peak2	35.696	1003578	5.63	16577
3	Peak3	41.100	7924881	44.47	109220
4	Peak4	52.733	921693	5.17	11076

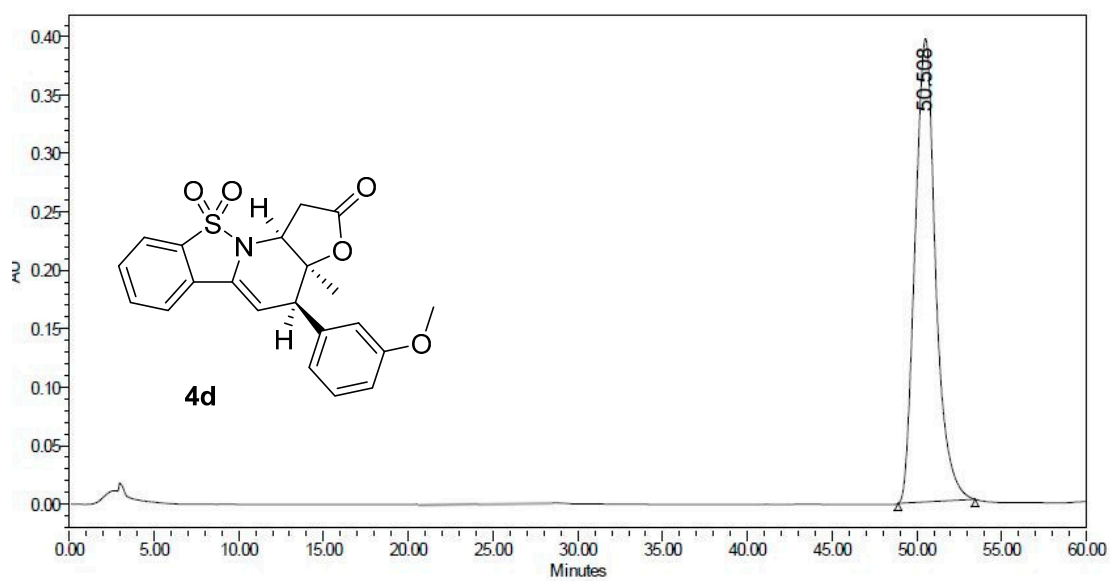


	RT	Area	% Area	Height
1	33.006	912001	3.16	16169
2	41.112	27950441	96.84	385884

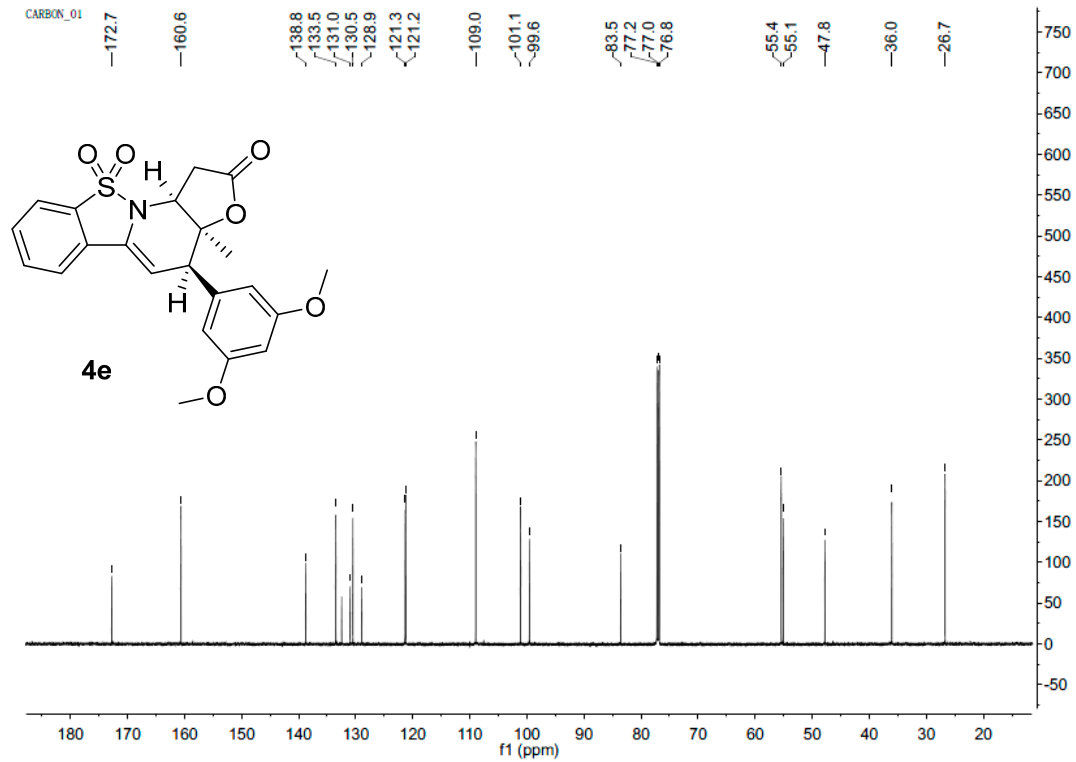
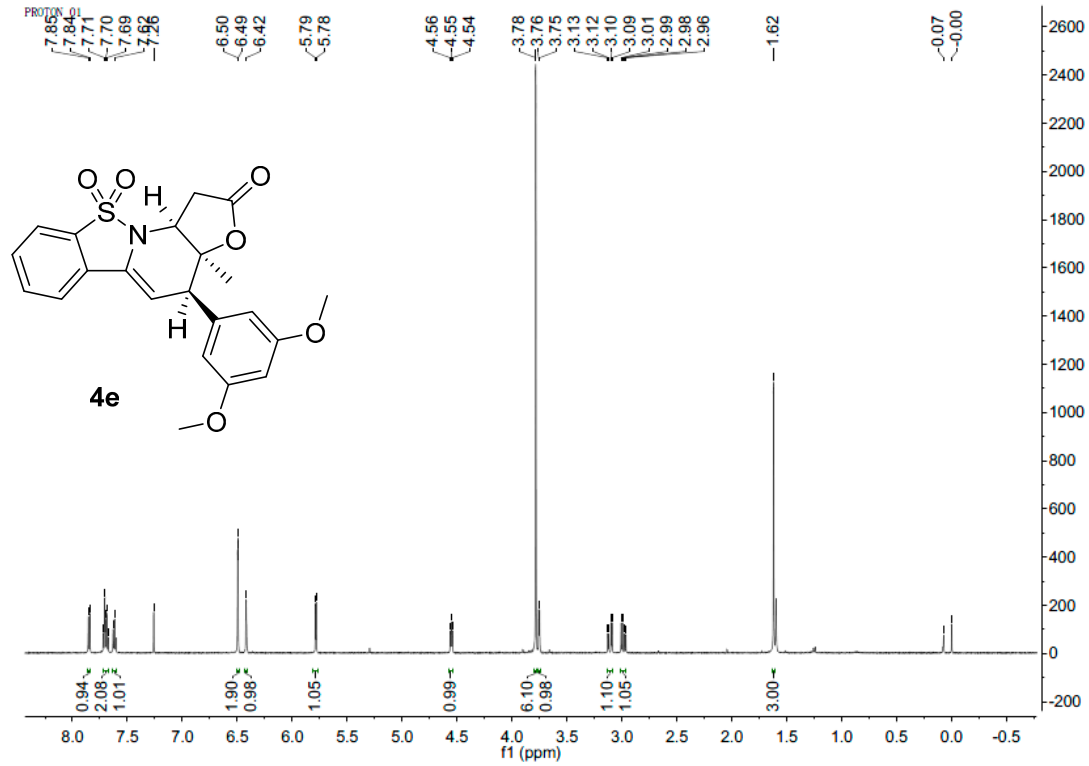


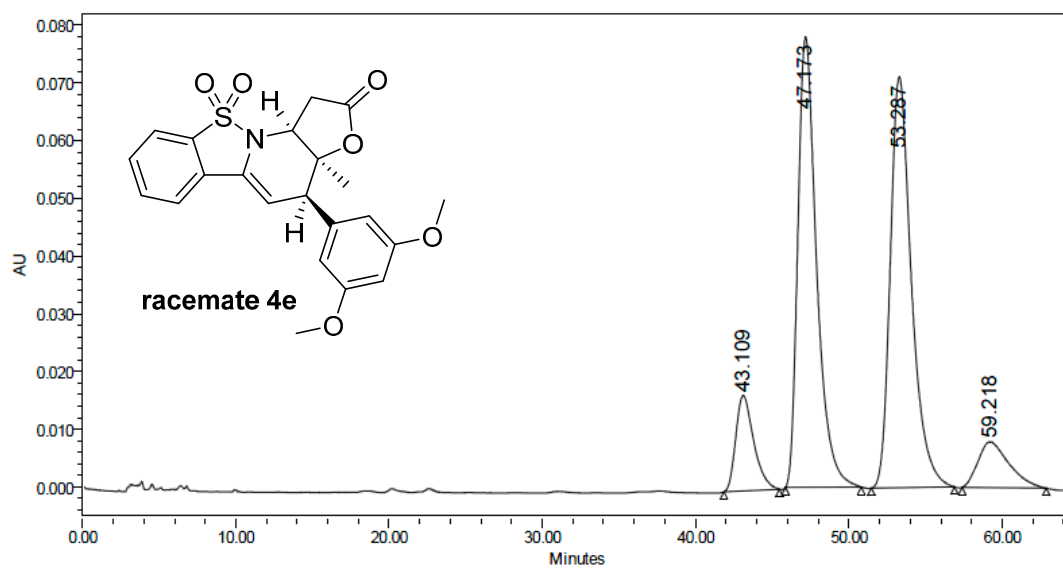


	RT	Area	% Area	Height
1	42.732	1734197	49.58	23804
2	50.194	1763332	50.42	20459

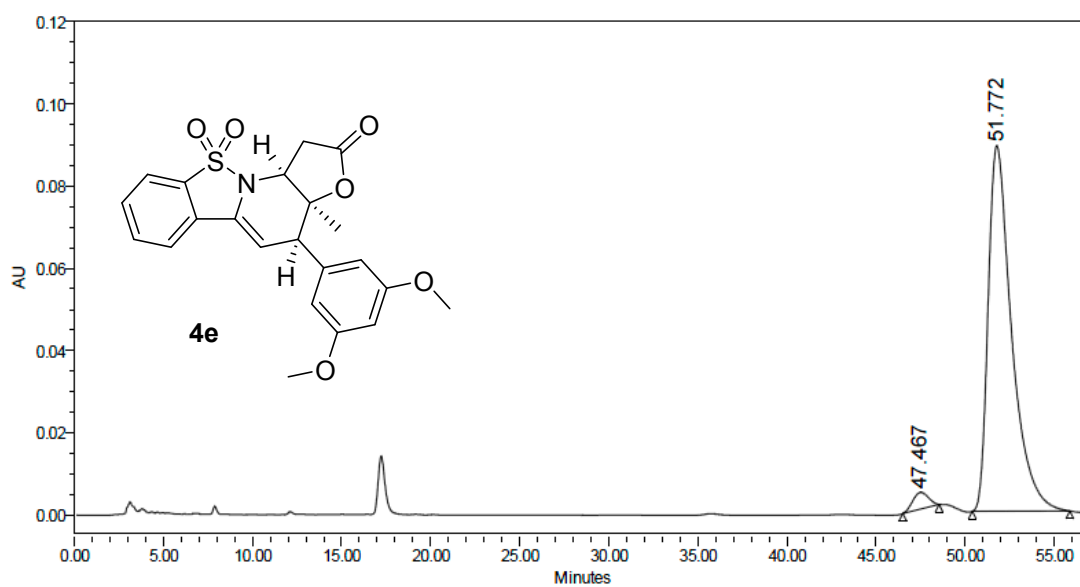


	RT	Area	% Area	Height
1	50.508	33483180	100.00	396374

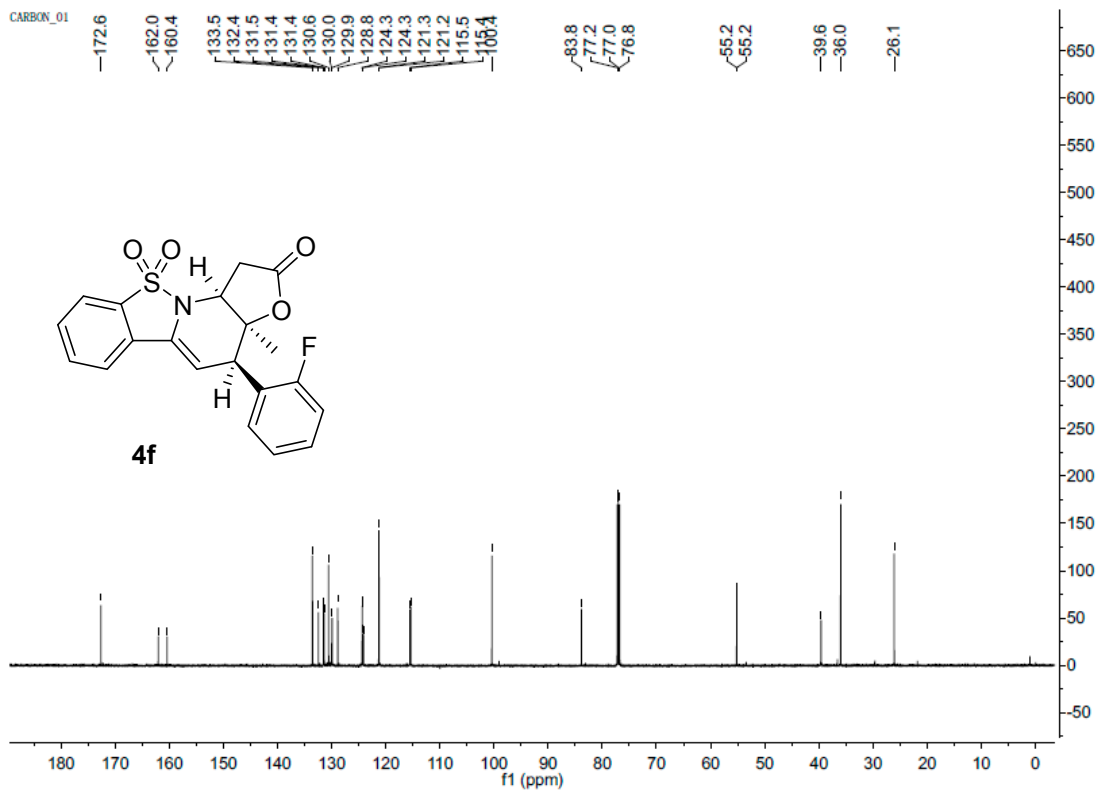
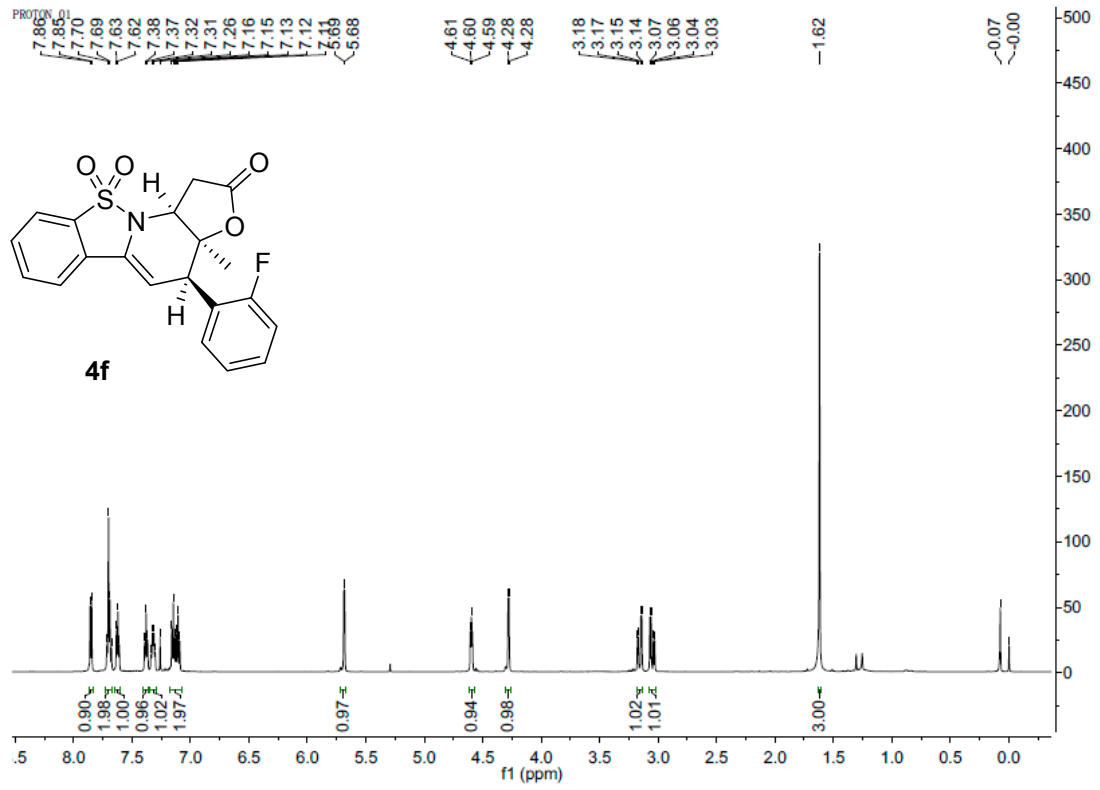


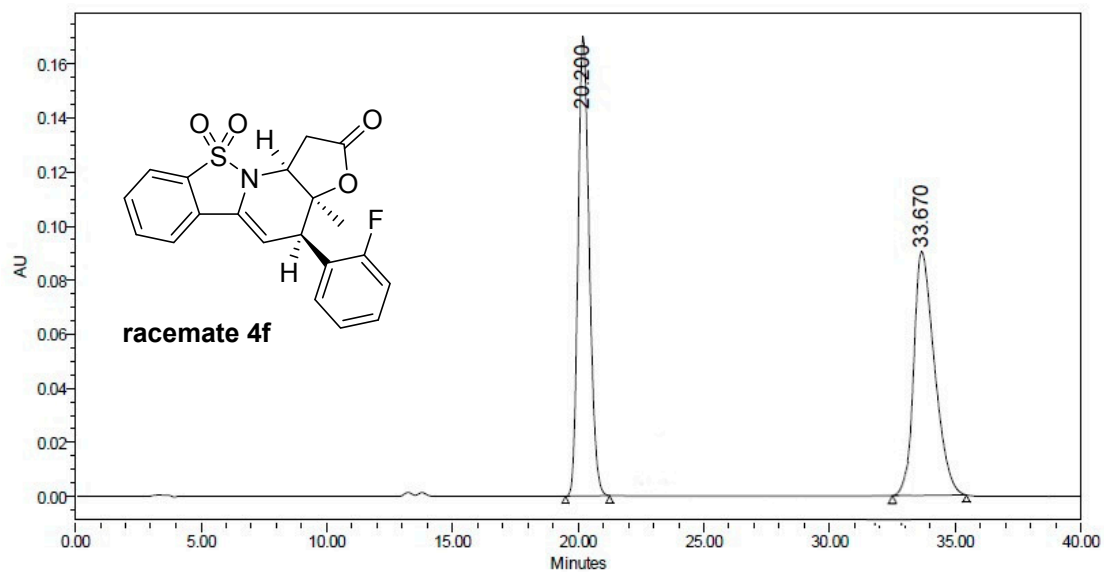


	RT	Area	% Area	Height
1	43.109	1346765	8.47	16496
2	47.173	6611212	41.58	78021
3	53.287	6823393	42.92	71199
4	59.218	1118237	7.03	7953

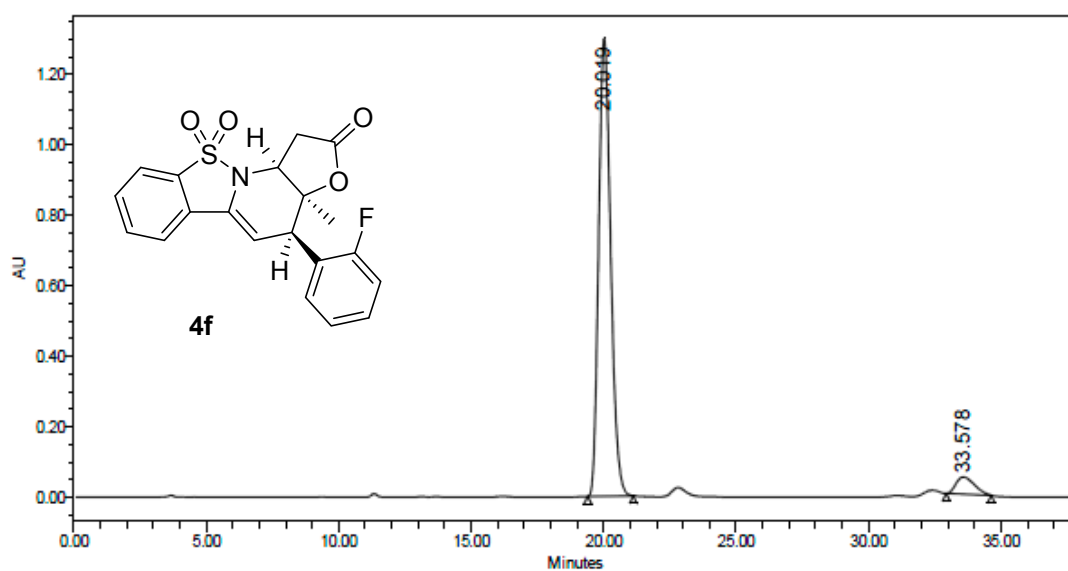


	RT	Area	% Area	Height
1	47.467	246945	2.95	4059
2	51.772	8132592	97.05	88859

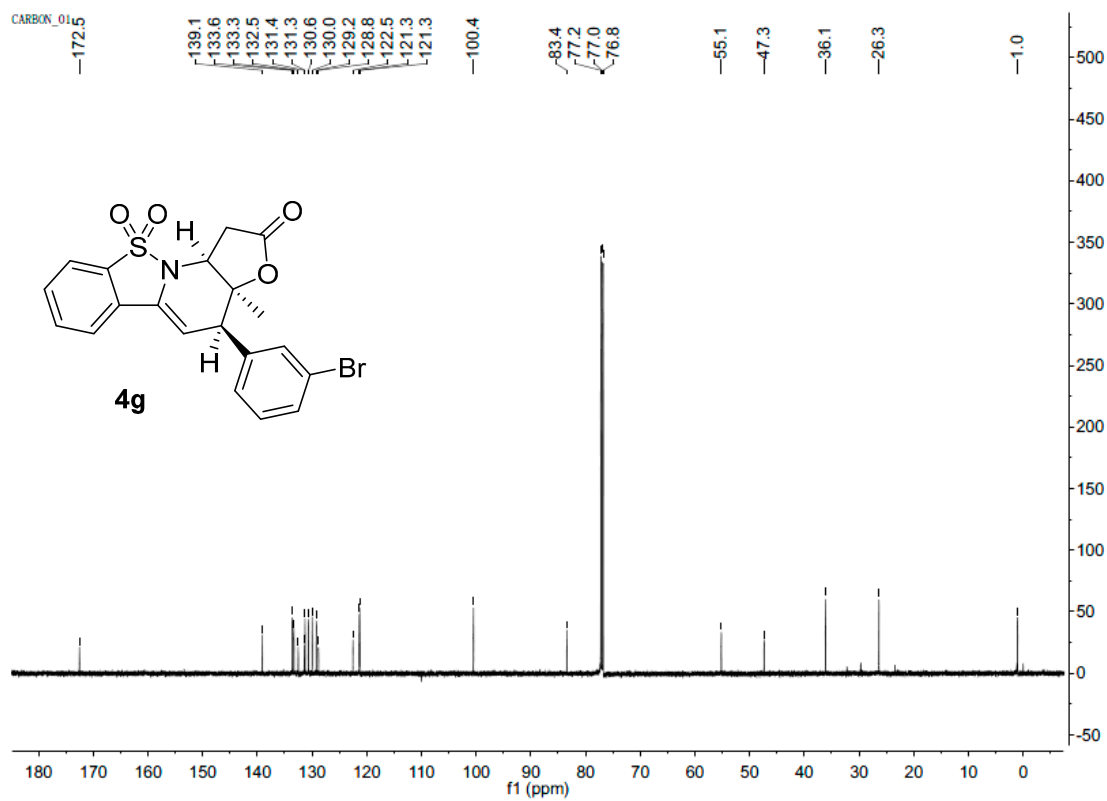
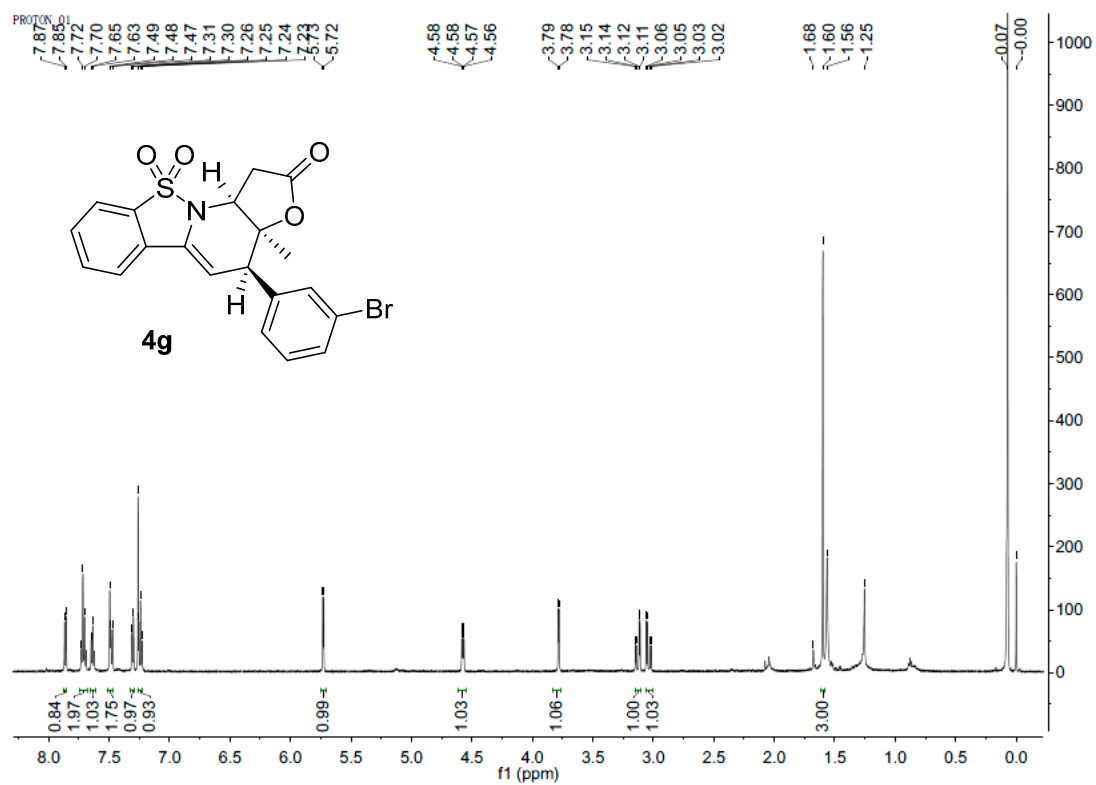


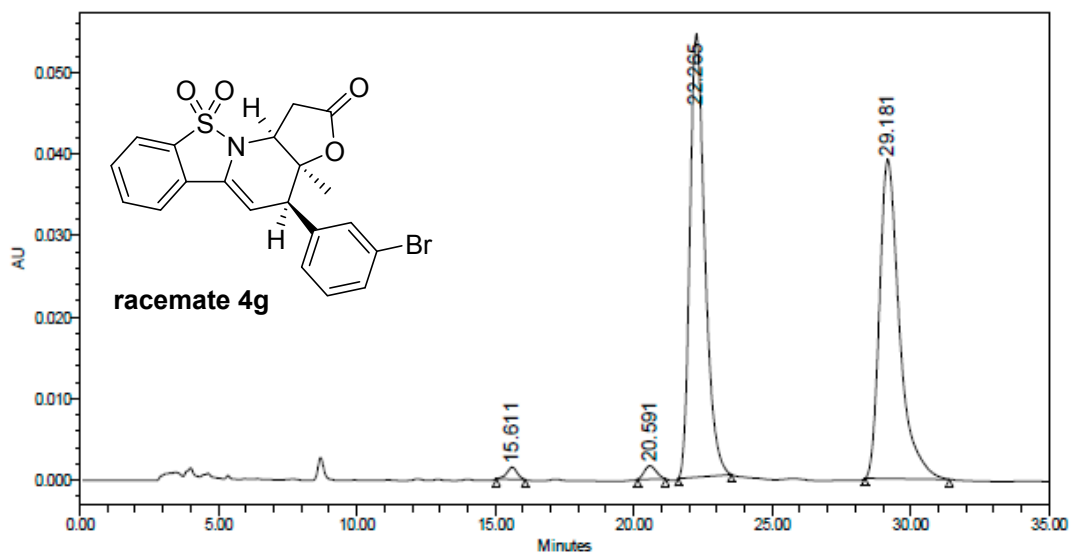


	RT	Area	% Area	Height
1	20.200	5250167	50.43	170013
2	33.670	5160455	49.57	90352

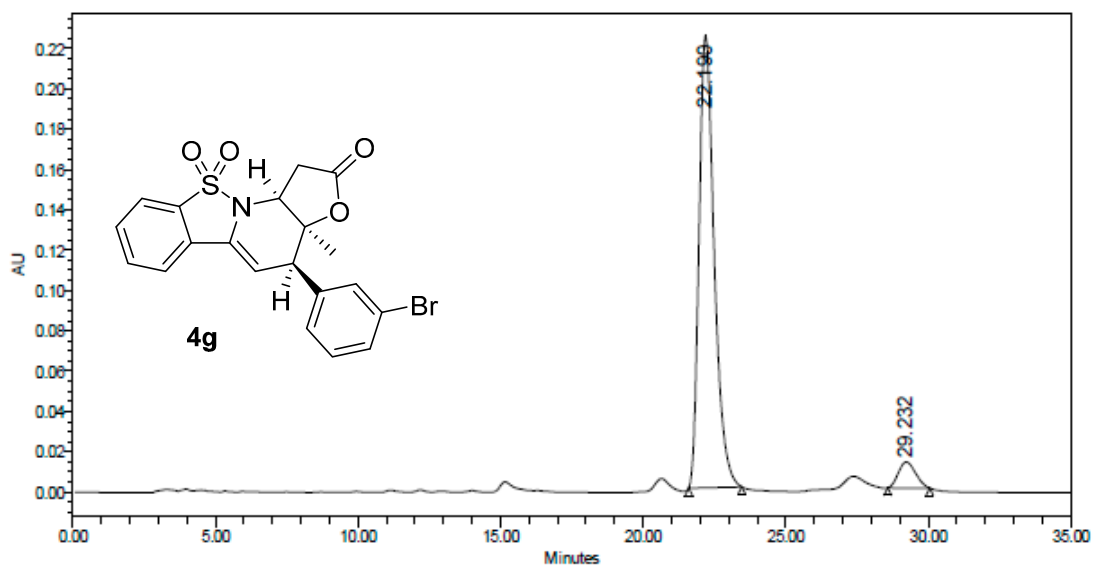


	RT	Area	% Area	Height
1	20.019	40831708	94.51	1299700
2	33.578	2371705	5.49	49007

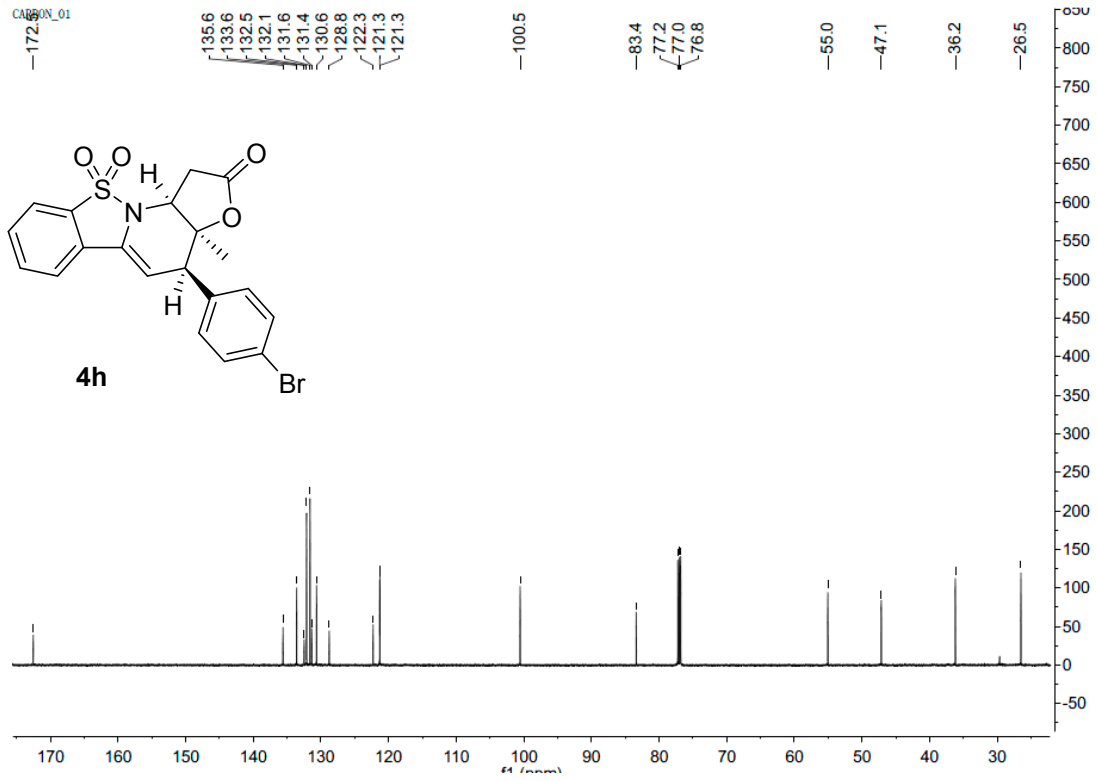
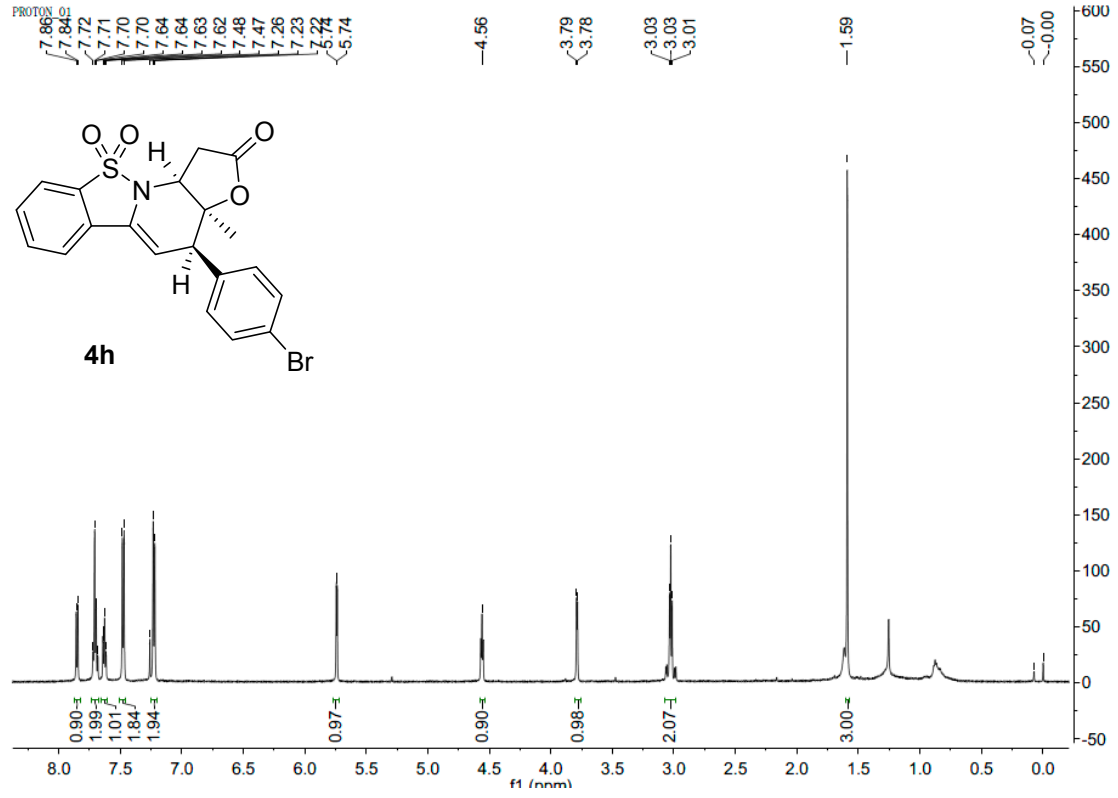


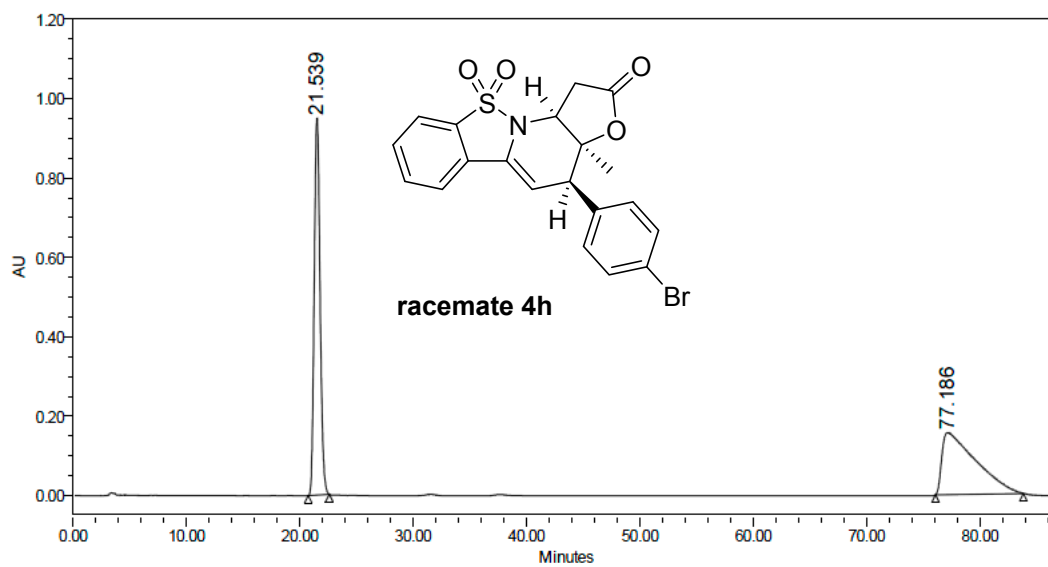


	RT	Area	% Area	Height
1	15.611	38976	0.95	1475
2	20.591	48658	1.19	1636
3	22.265	2040259	49.93	54265
4	29.181	1958268	47.92	39116

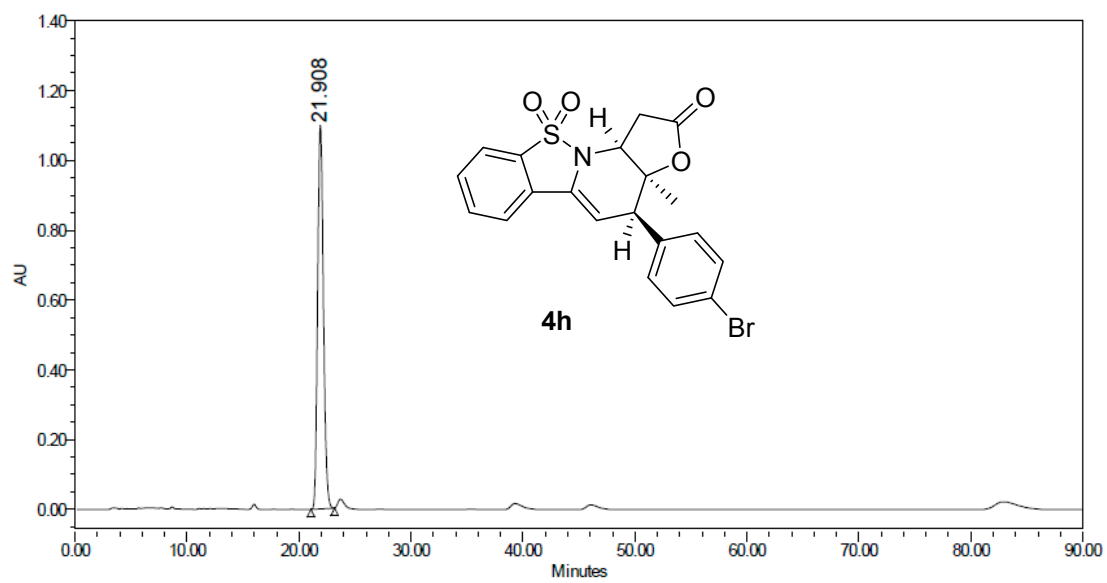


	RT	Area	% Area	Height
1	22.190	8284859	93.87	224216
2	29.232	540744	6.13	12918

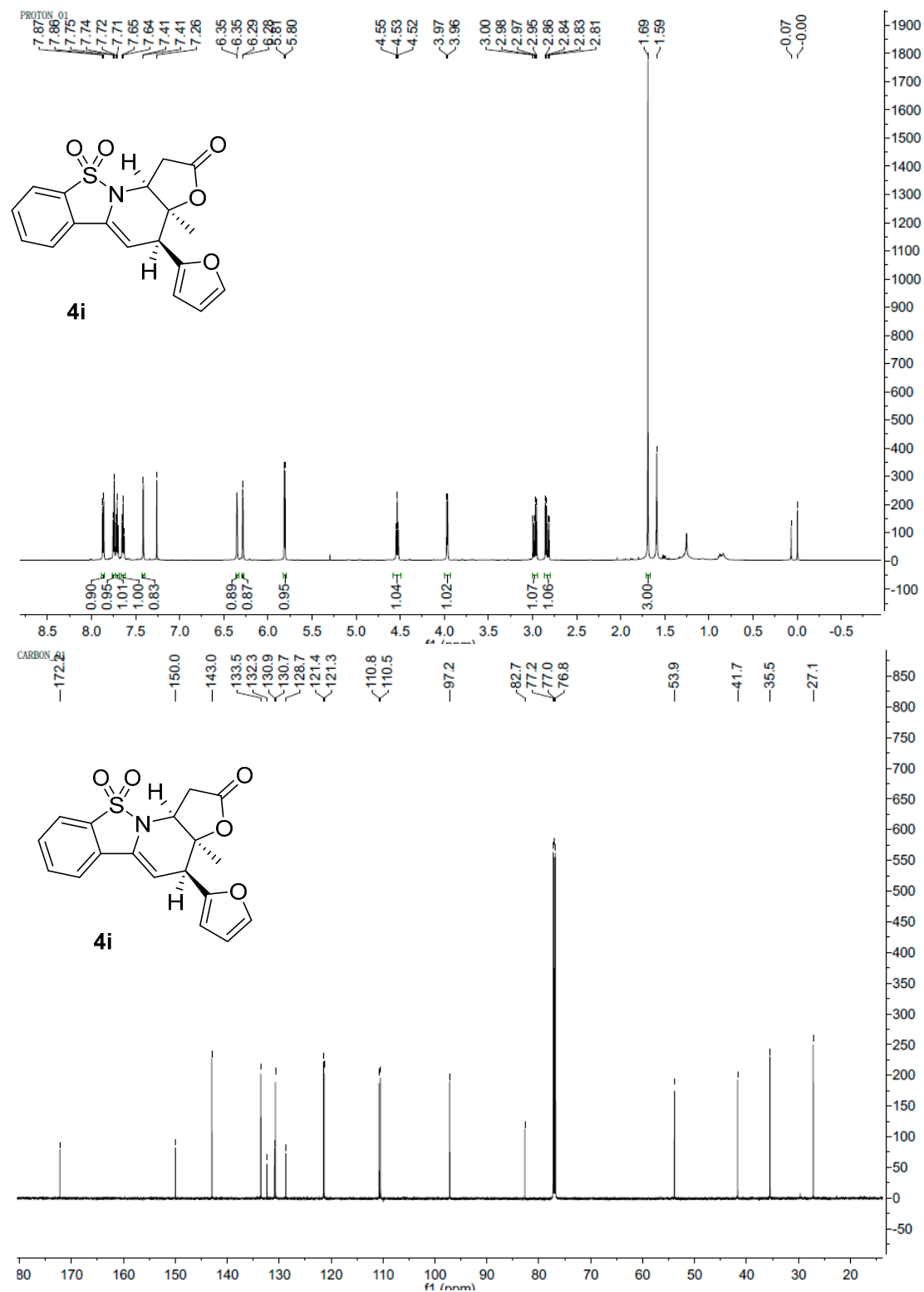


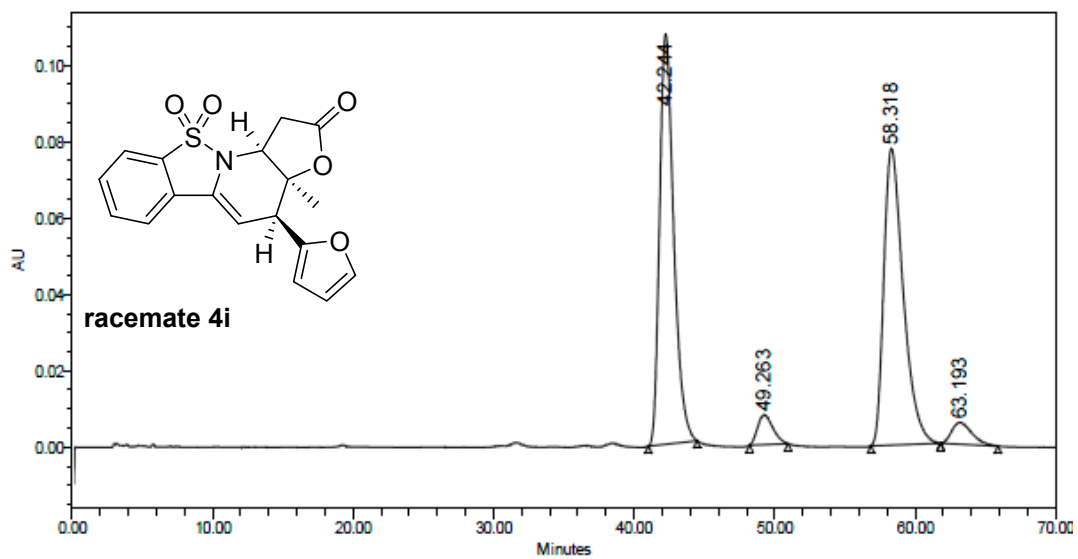


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1	21.539	33943648	51.20	949857
2	77.186	32347438	48.80	156180

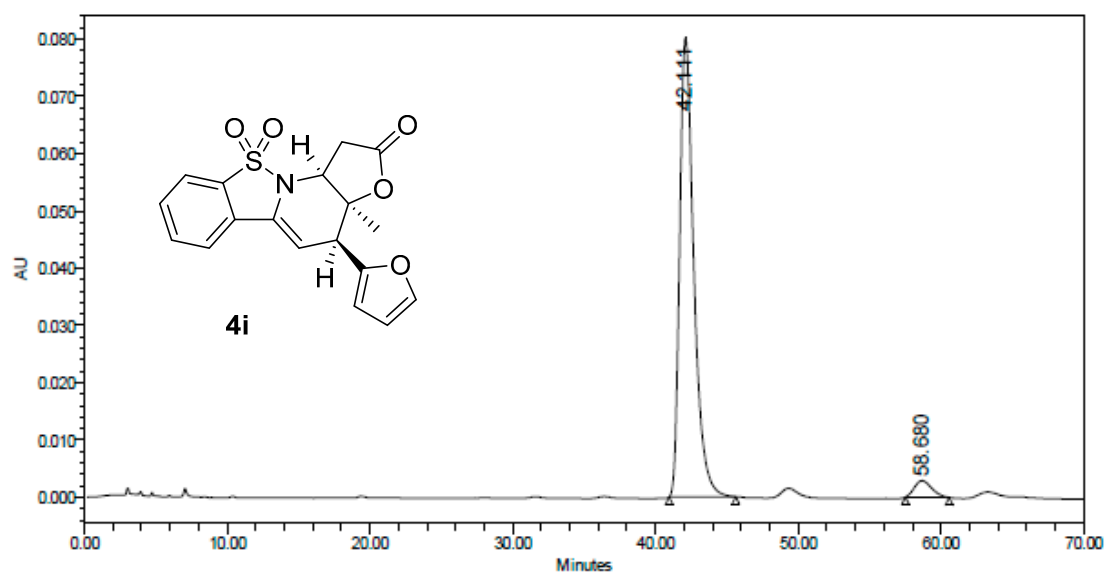


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1	21.908	39559832	100.00	1098527

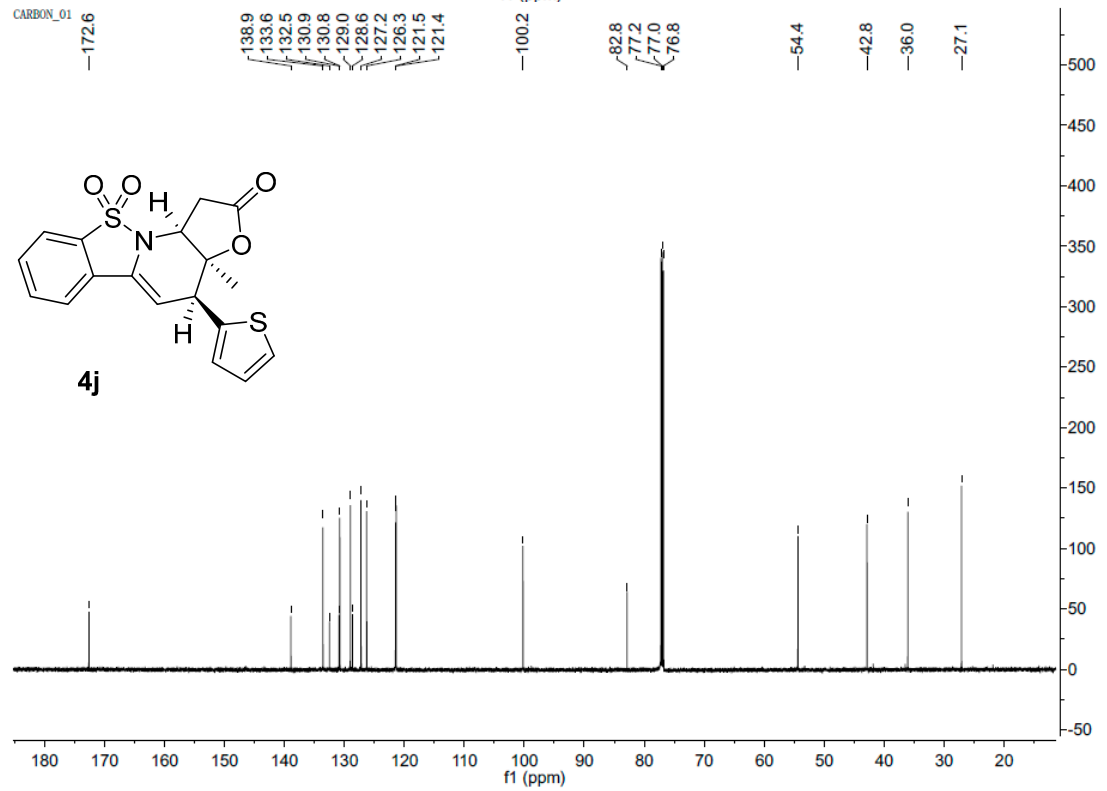
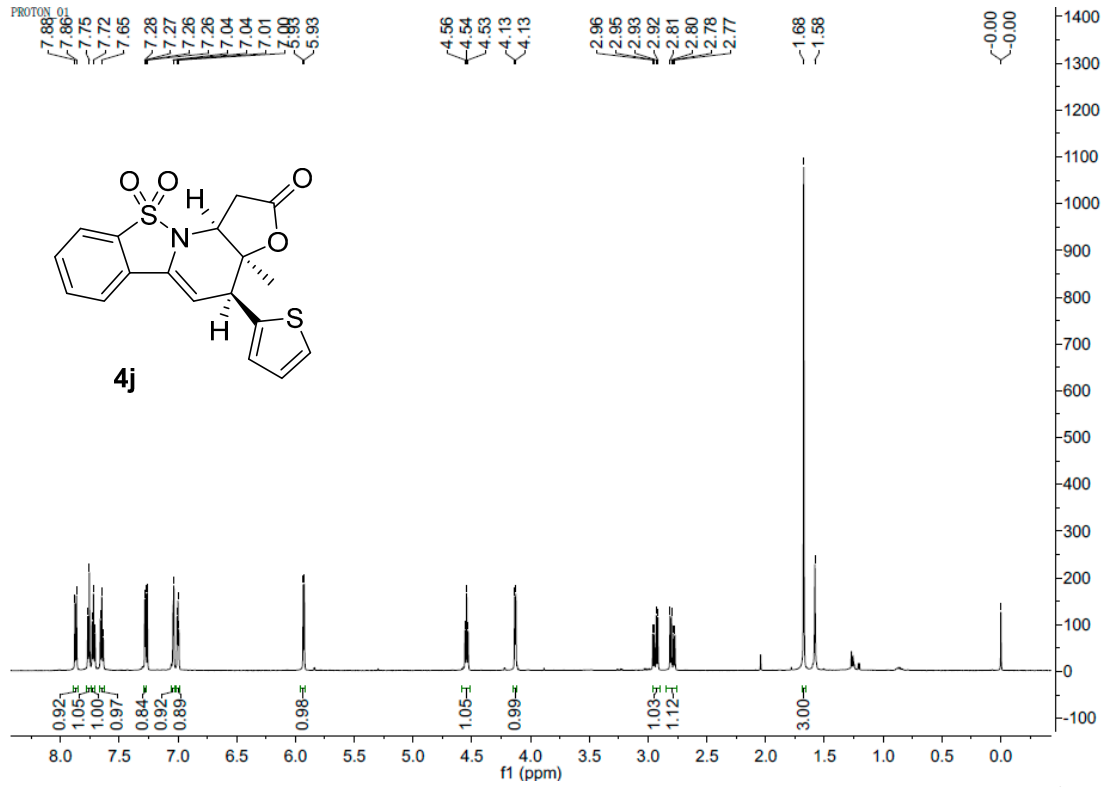


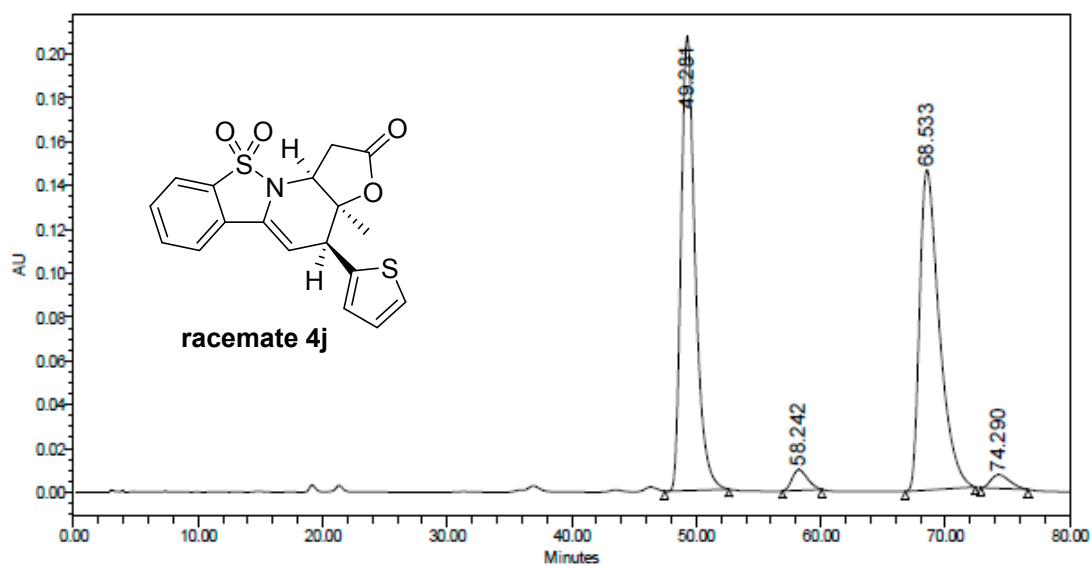


	RT	Area	% Area	Height
1	42.244	7482839	46.43	107305
2	49.263	584841	3.63	7774
3	58.318	7482430	46.43	77582
4	63.193	566023	3.51	5687

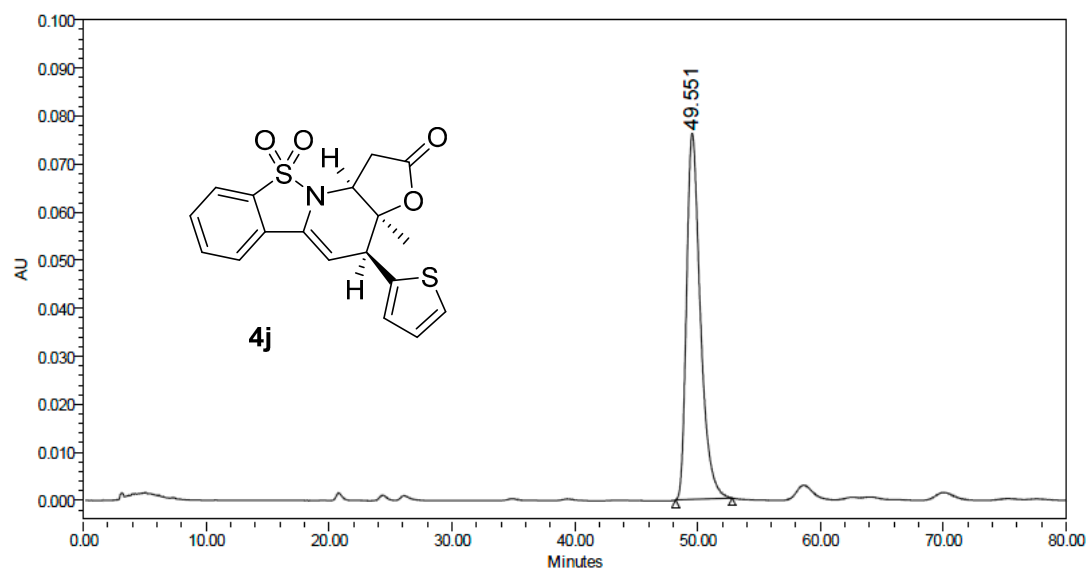


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1	42.111	5506236	95.74	80189
2	58.680	245288	4.26	2895

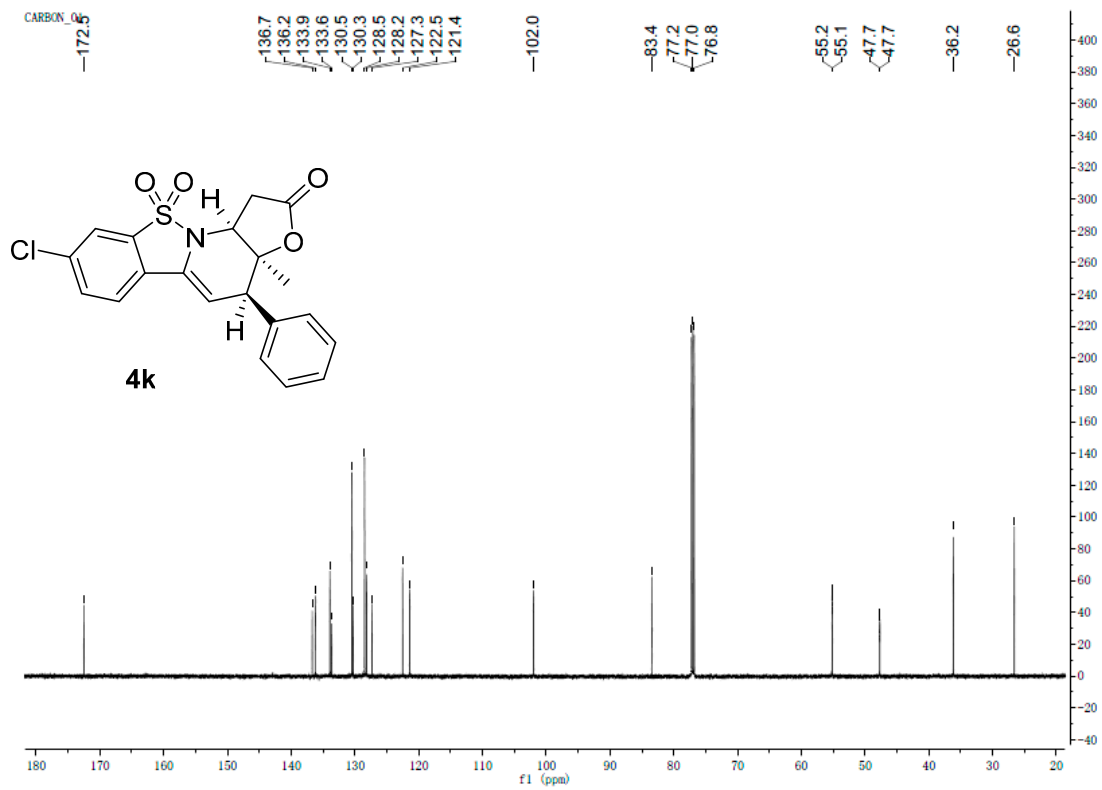
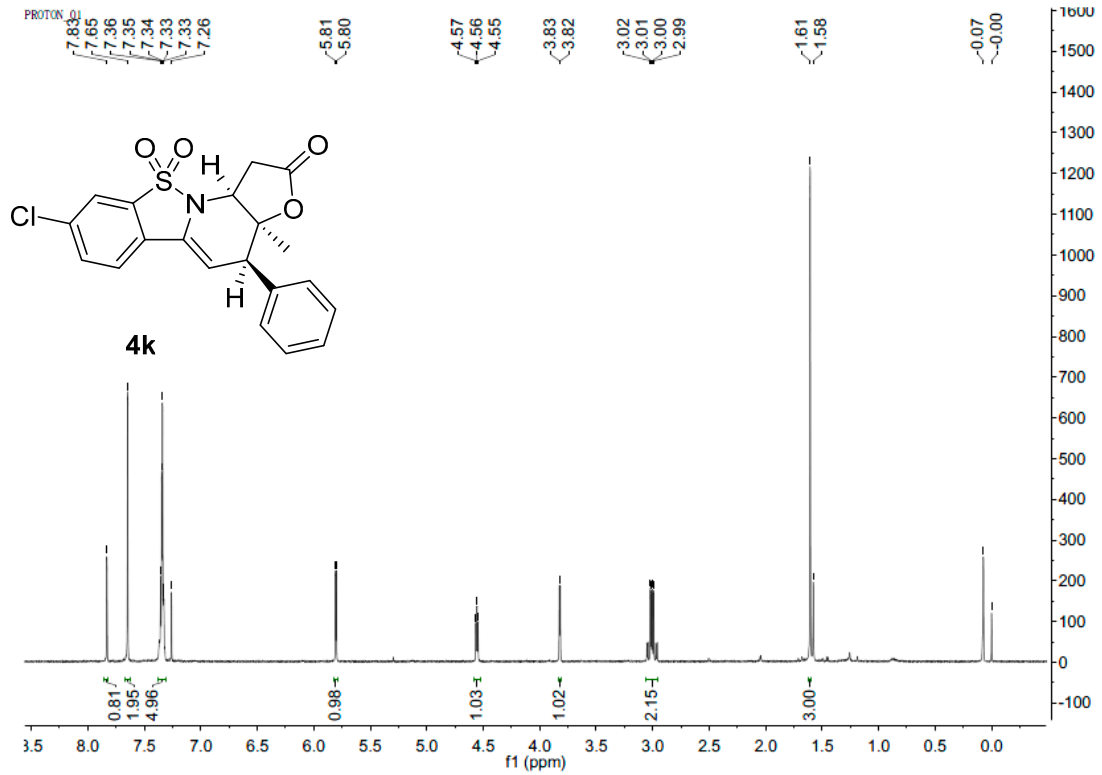


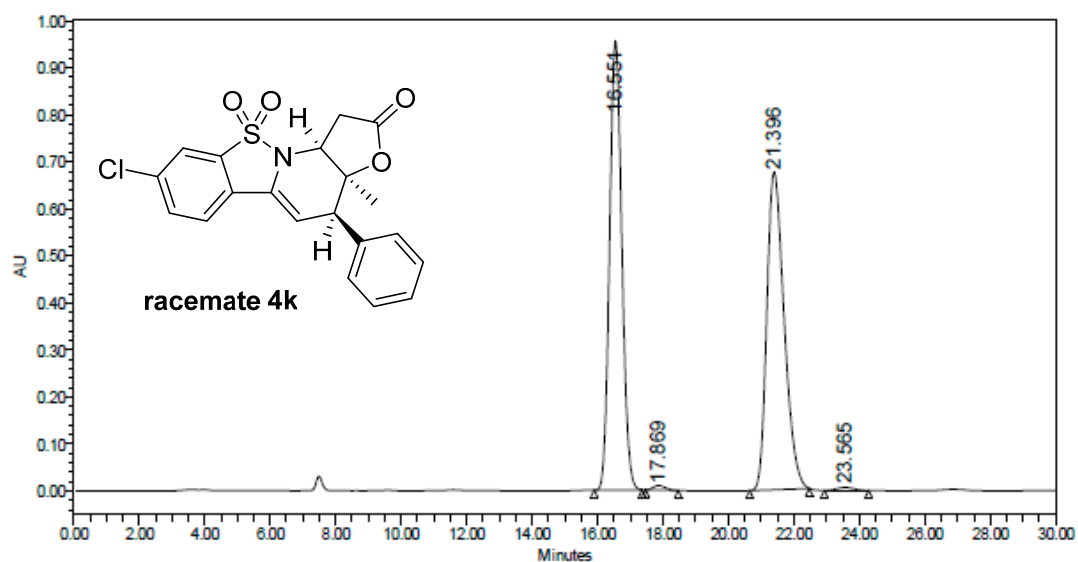


	RT	Area	% Area	Height
1	49.281	16380653	48.23	207160
2	58.242	808300	2.38	9421
3	68.533	16107054	47.43	146183
4	74.290	666806	1.96	6305

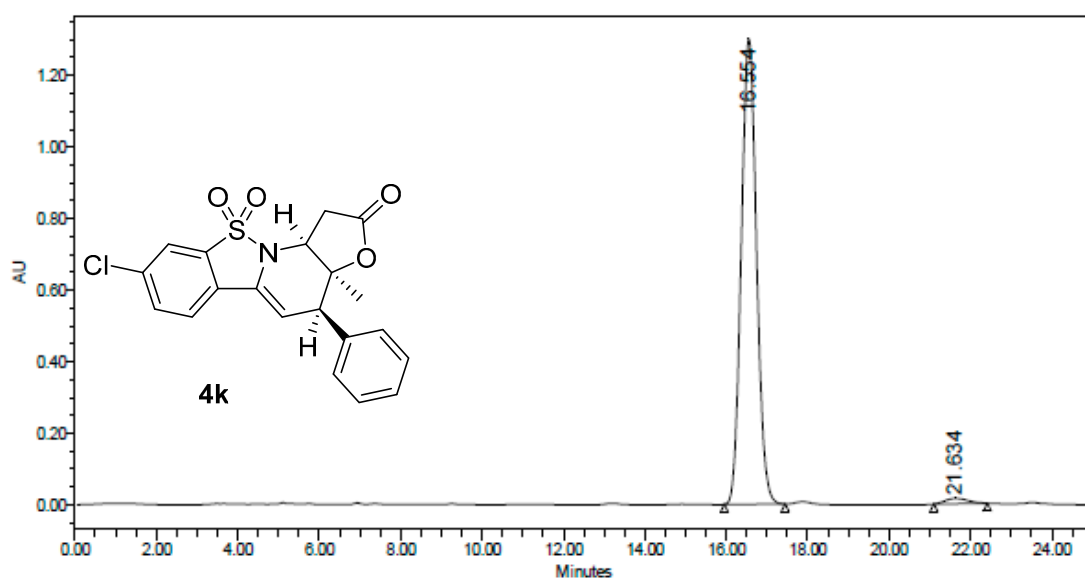


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1	49.551	5961579	100.00	76135

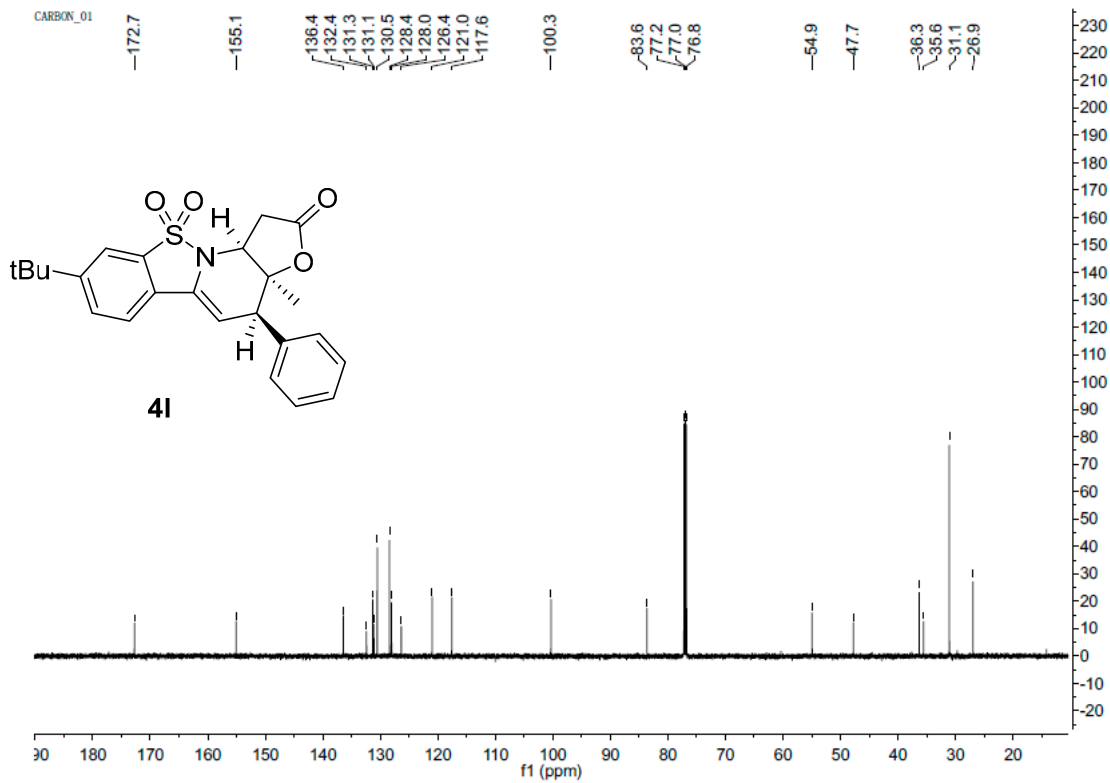
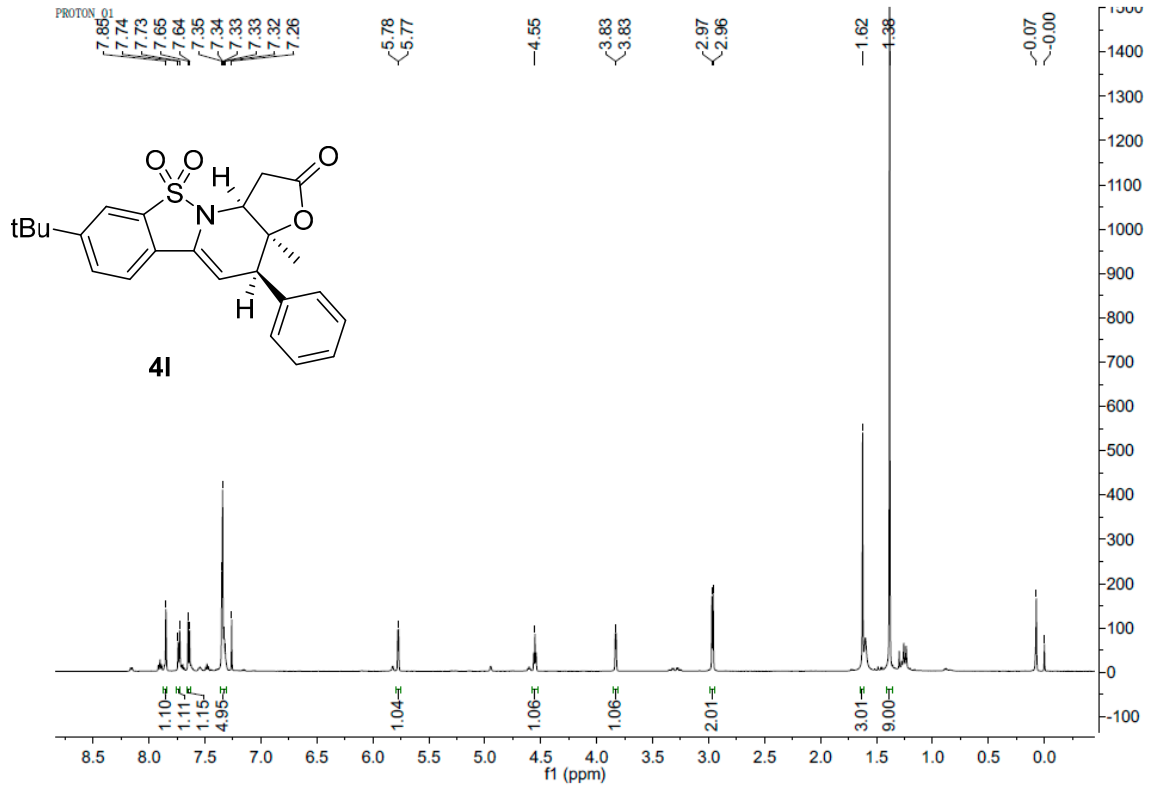


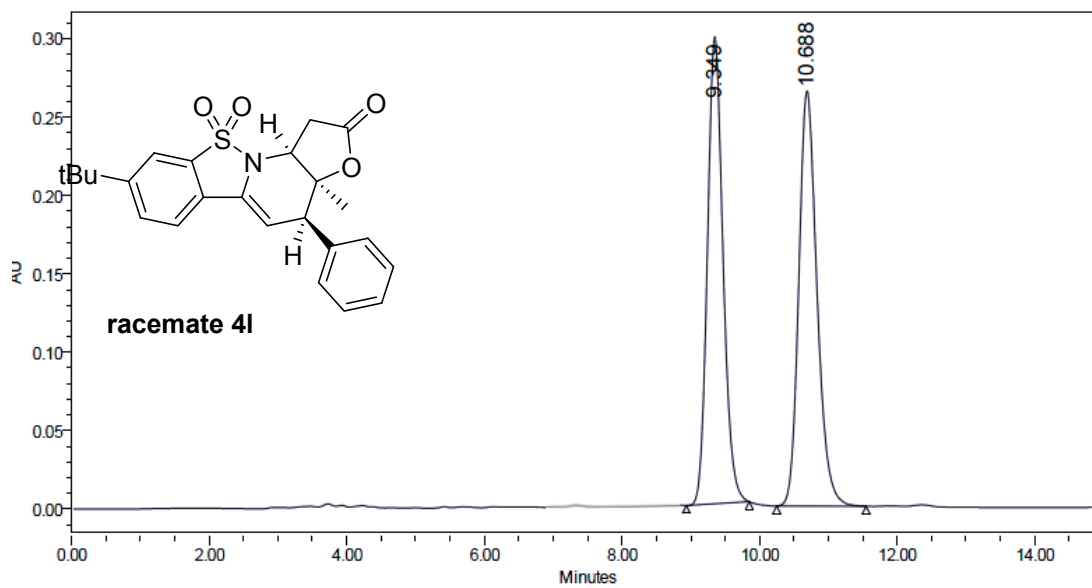


	RT	Area	% Area	Height
1	16.551	24740656	49.45	954355
2	17.869	255013	0.51	9600
3	21.396	24802676	49.57	675931
4	23.565	232287	0.46	6382

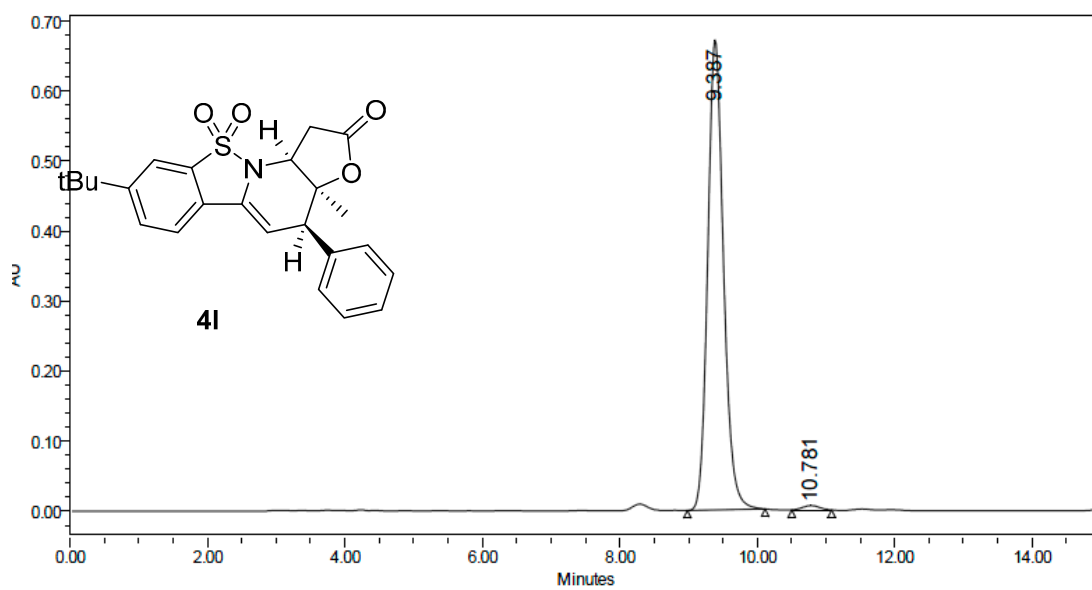


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1	16.554	33957861	98.34	1301504
2	21.634	574111	1.66	14976

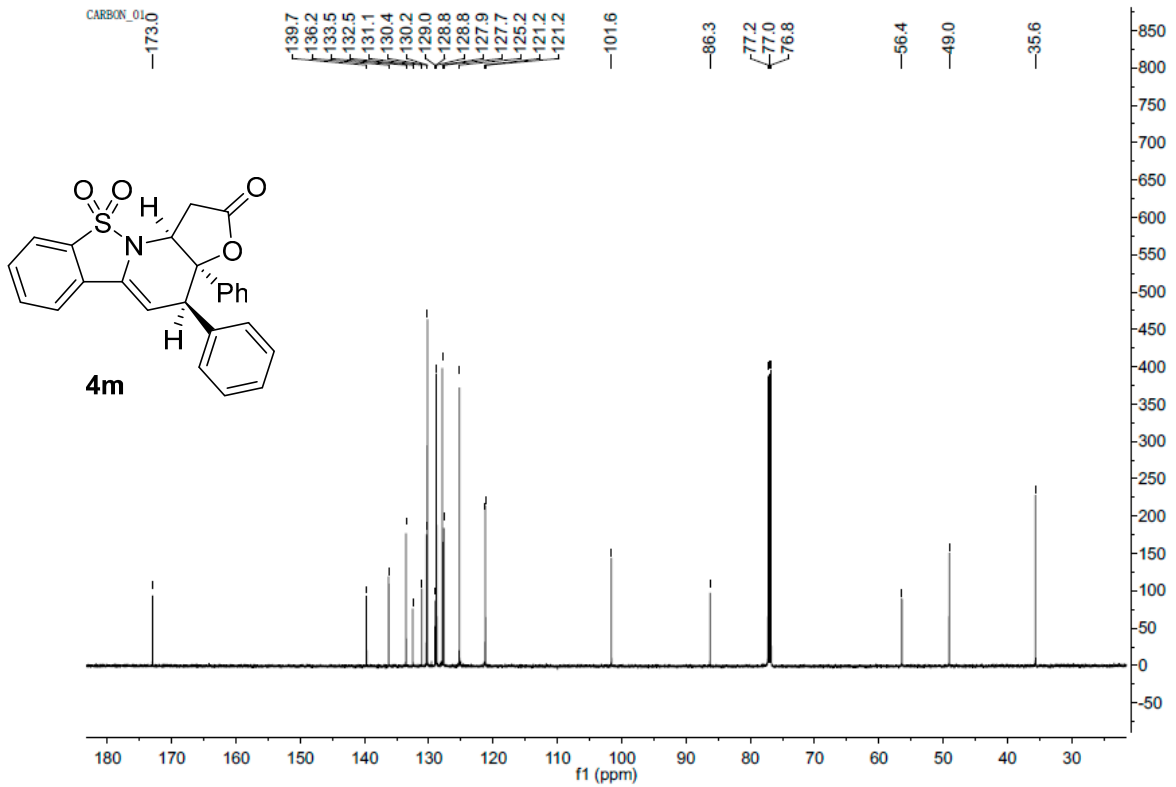
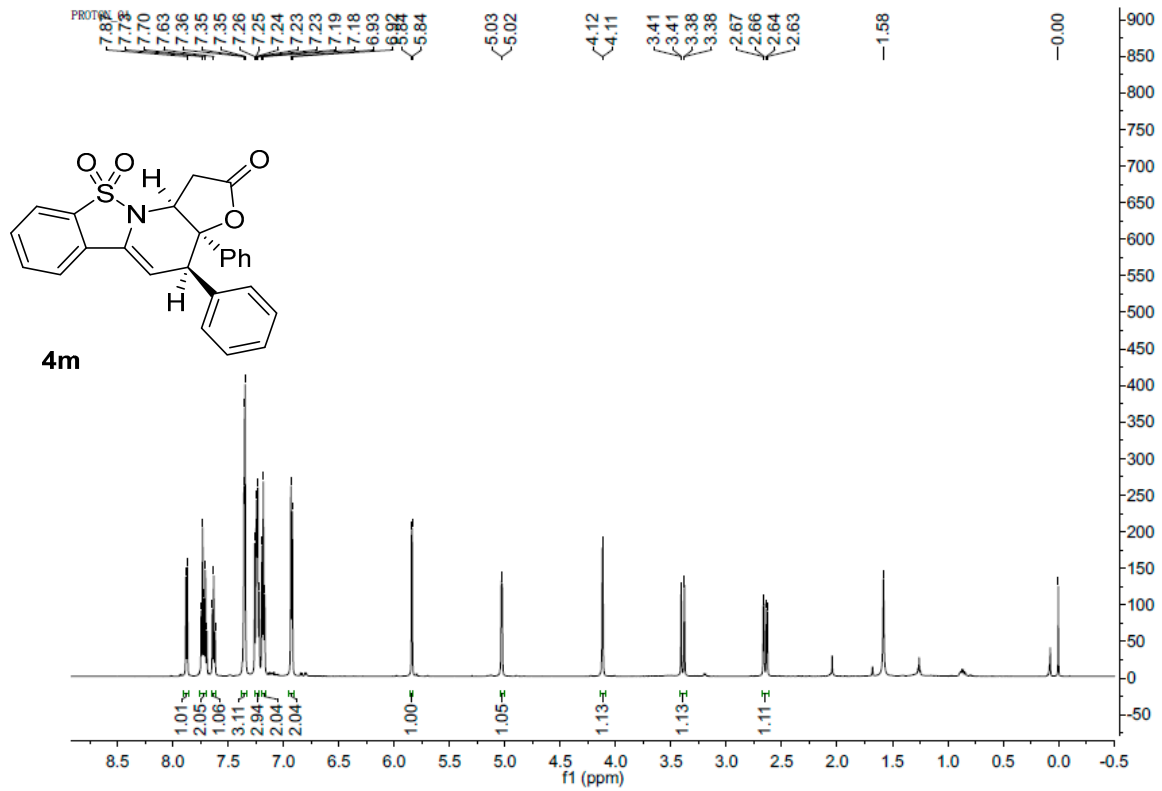


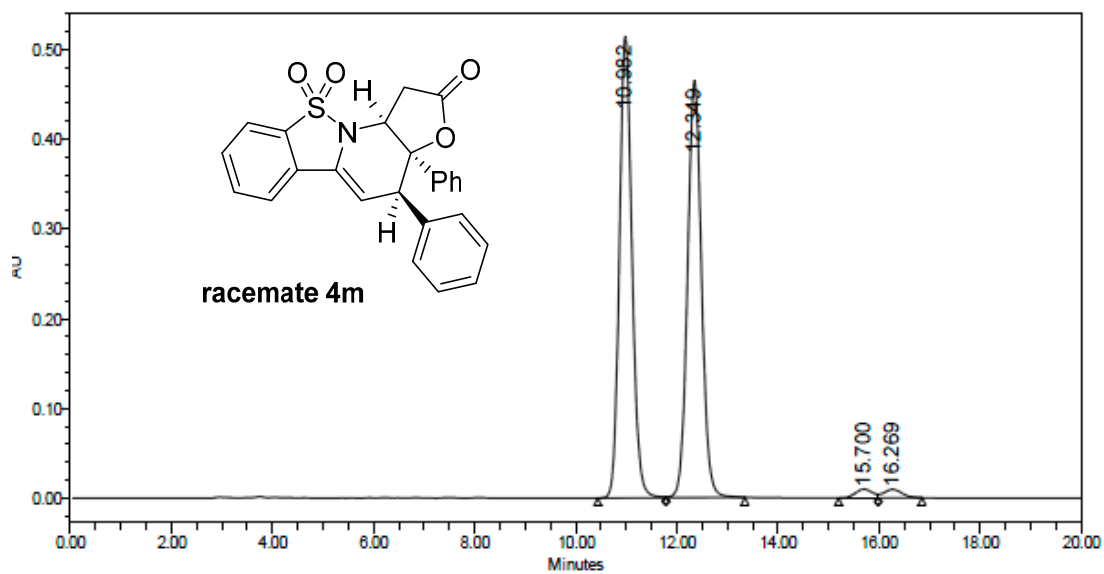


	RT	Area	% Area	Height
1	9.349	4698821	49.10	298266
2	10.688	4871030	50.90	265172

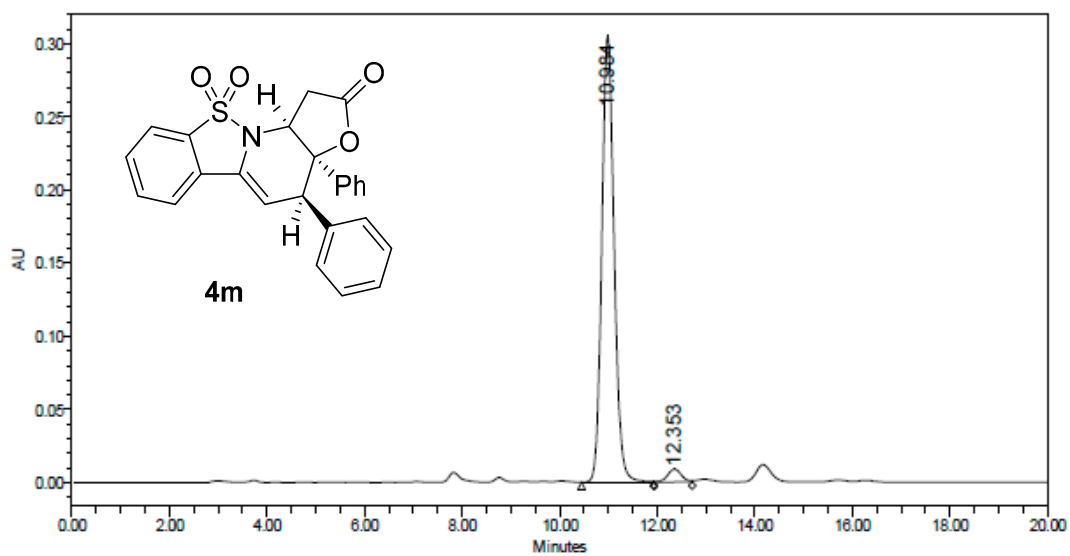


	RT	Area	% Area	Height
1	9.387	10755950	99.01	672355
2	10.781	107179	0.99	6236

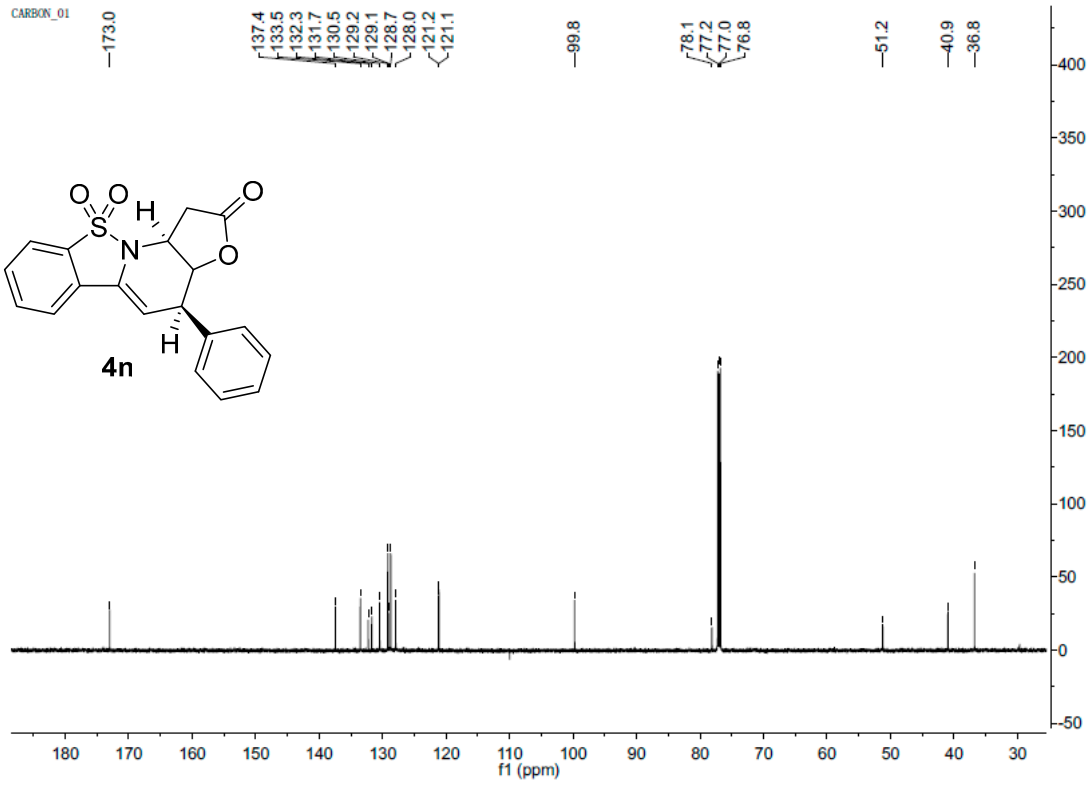
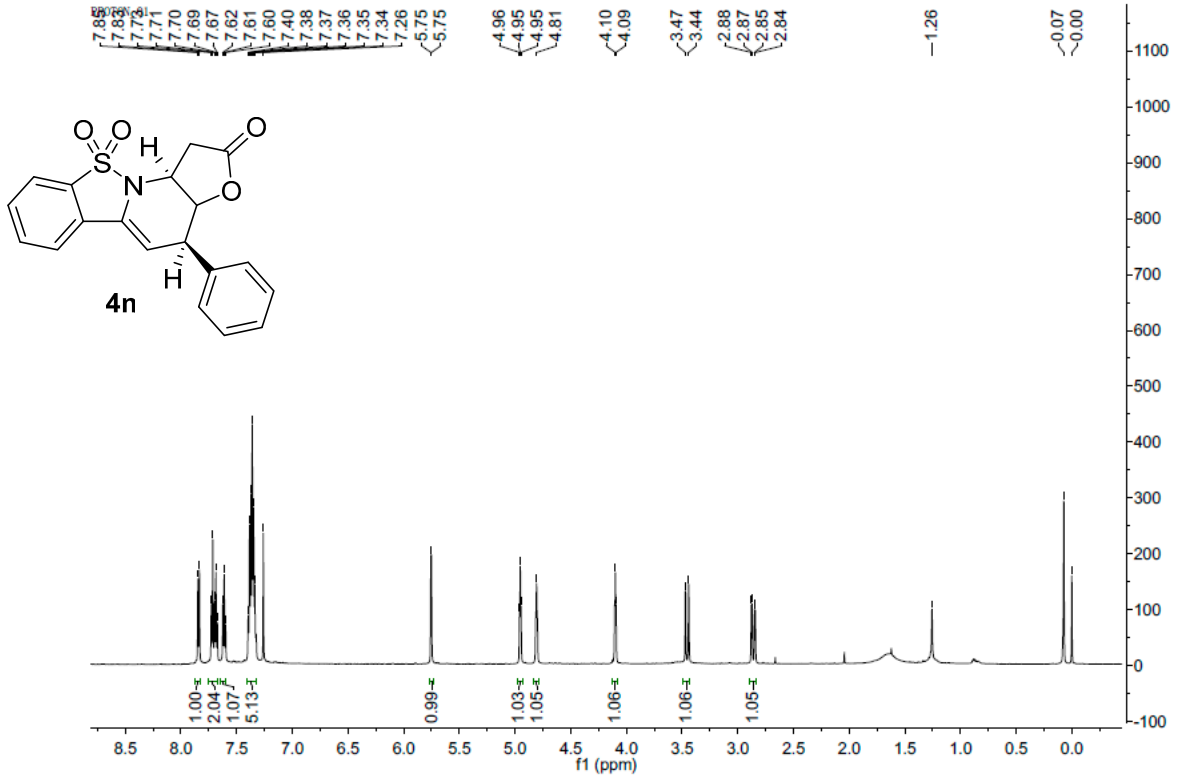


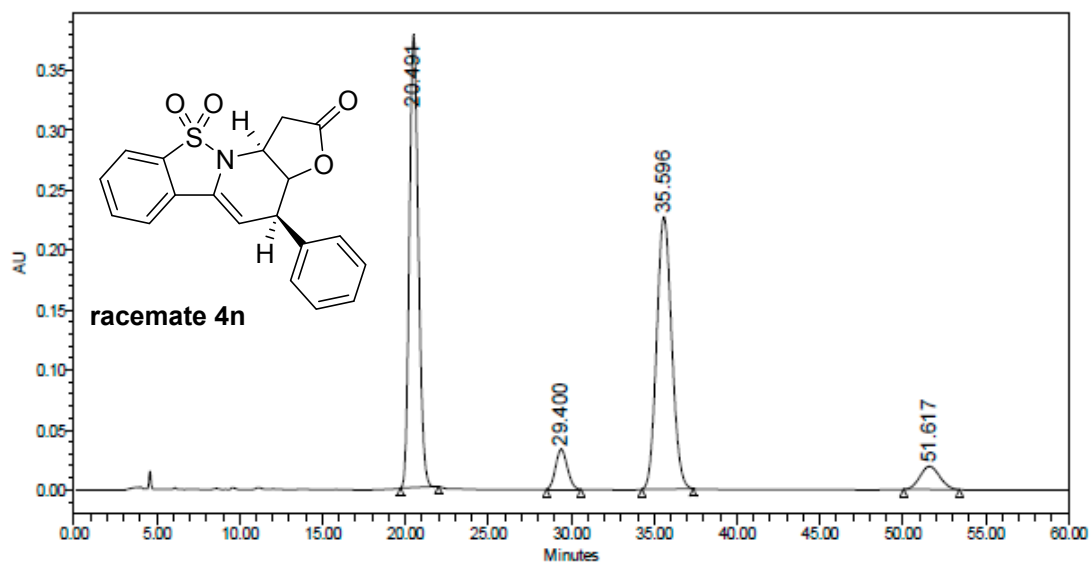


	RT	Area	% Area	Height
1	10.982	8871416	48.66	514878
2	12.349	8896318	48.80	464827
3	15.700	227038	1.25	9658
4	16.269	235925	1.29	9316

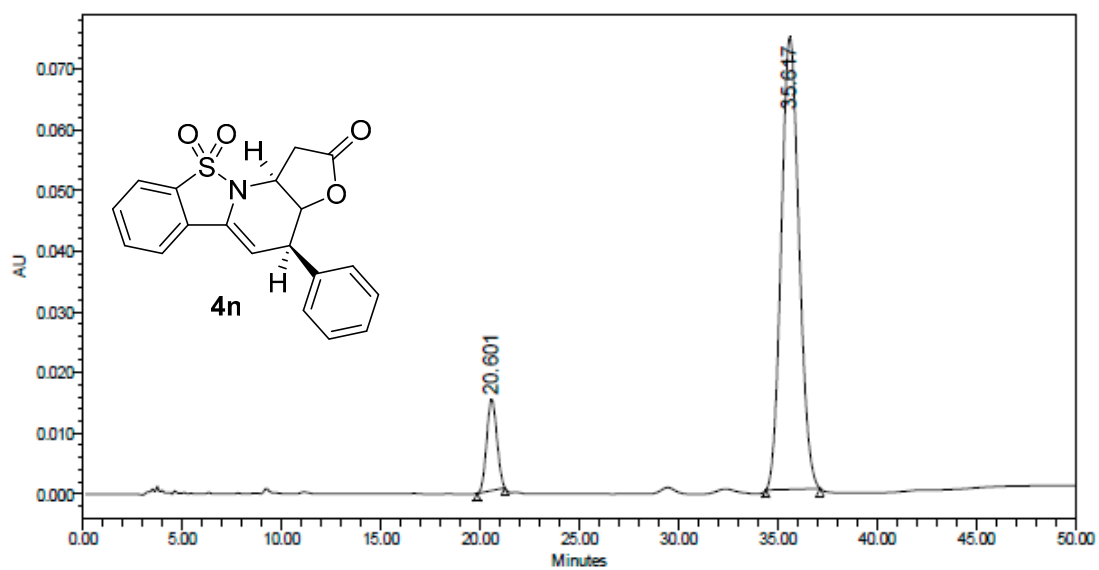


	RT	Area	% Area	Height
1	10.984	5320336	96.83	305045
2	12.353	174016	3.17	8846

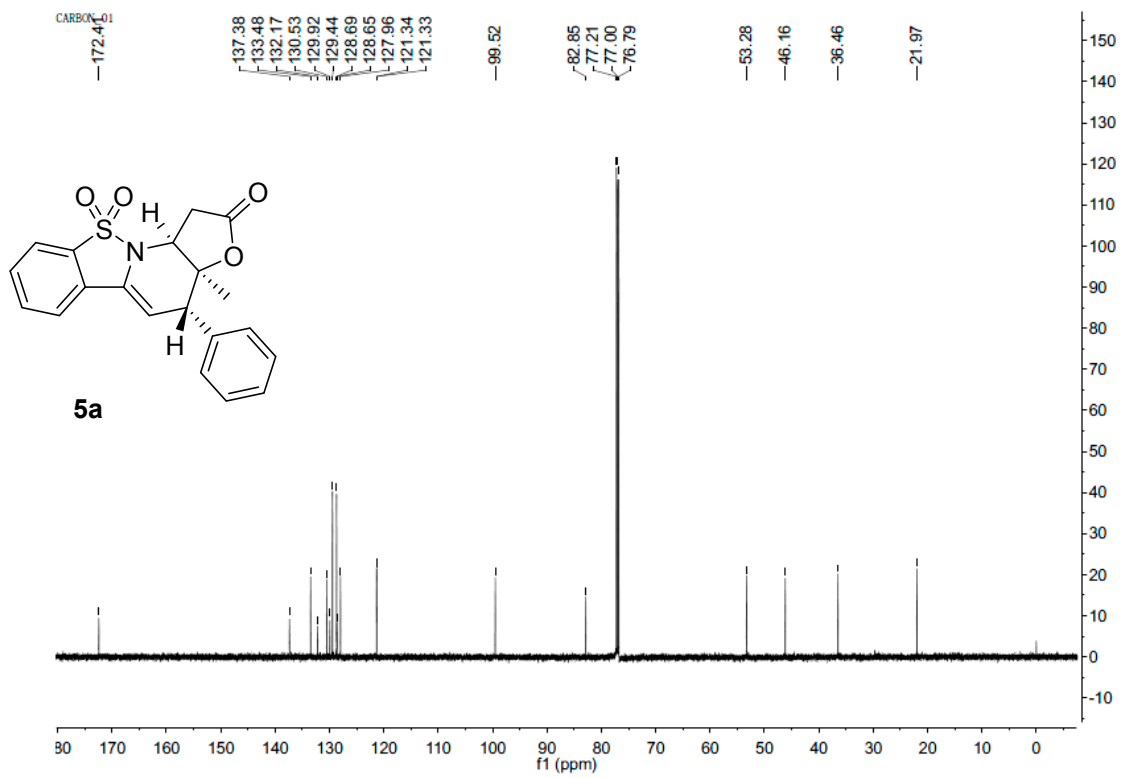
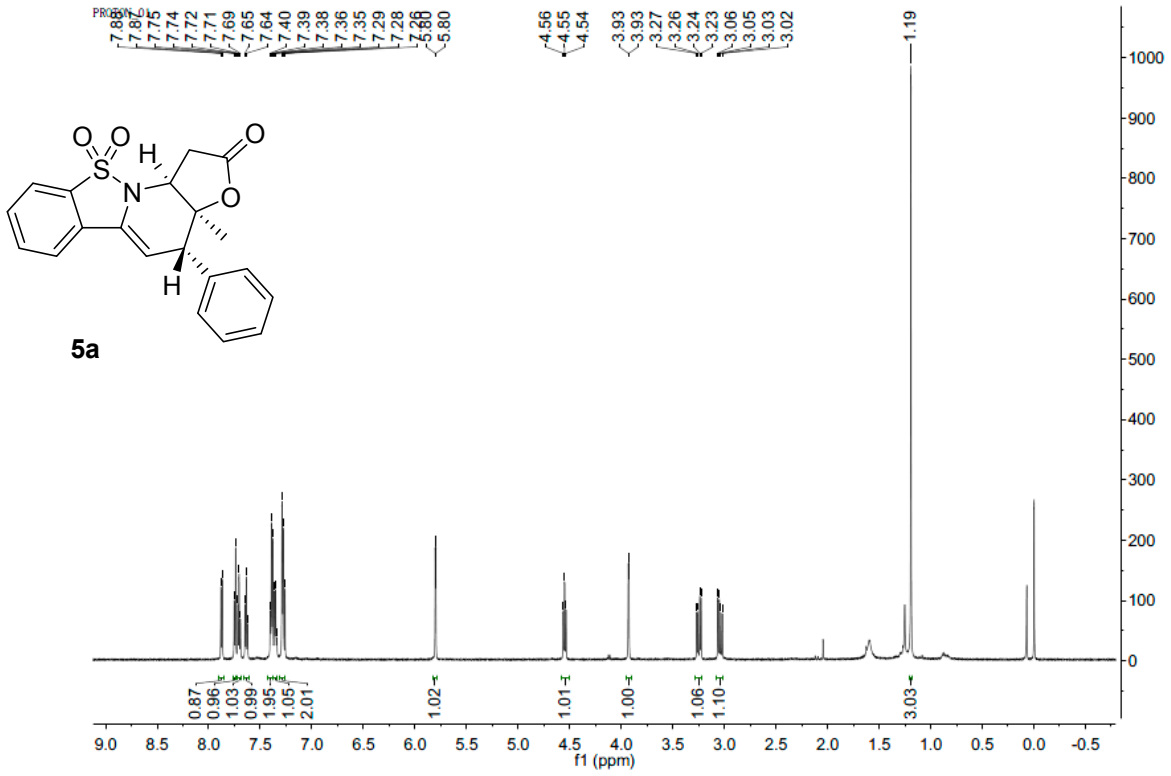


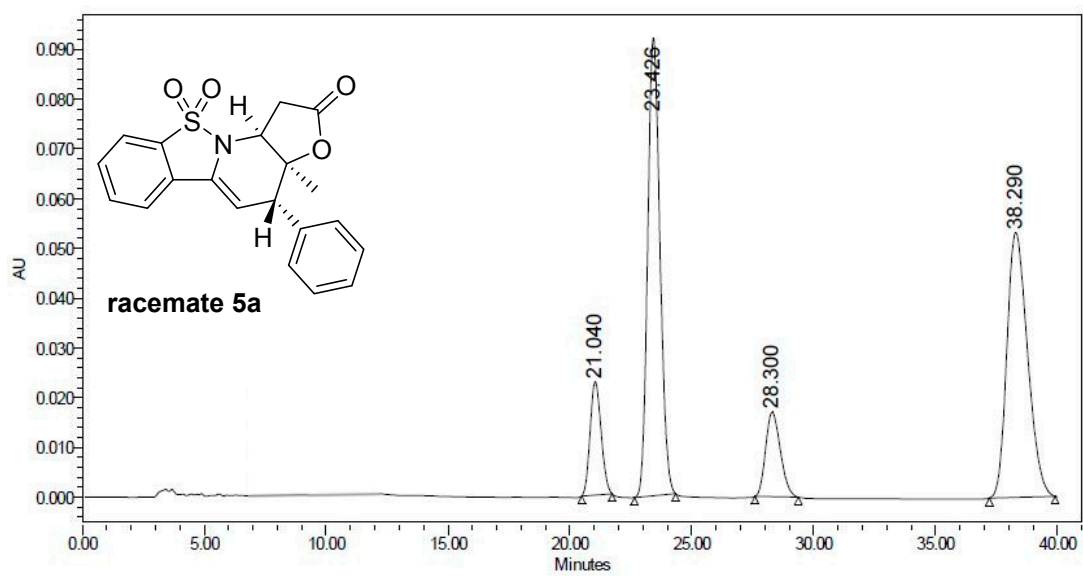


	RT	Area	% Area	Height
1	20.491	14232480	44.84	377691
2	29.400	1630739	5.14	33314
3	35.596	14277406	44.98	227085
4	51.617	1603183	5.05	19330

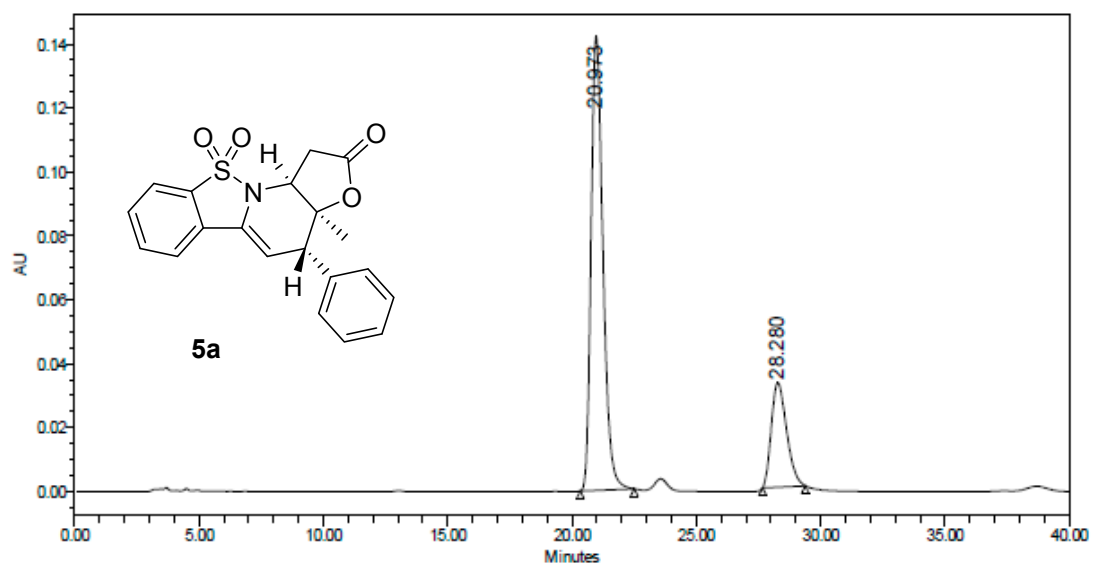


	RT	Area	% Area	Height
1	20.601	536588	10.35	15013
2	35.617	4650127	89.65	74588

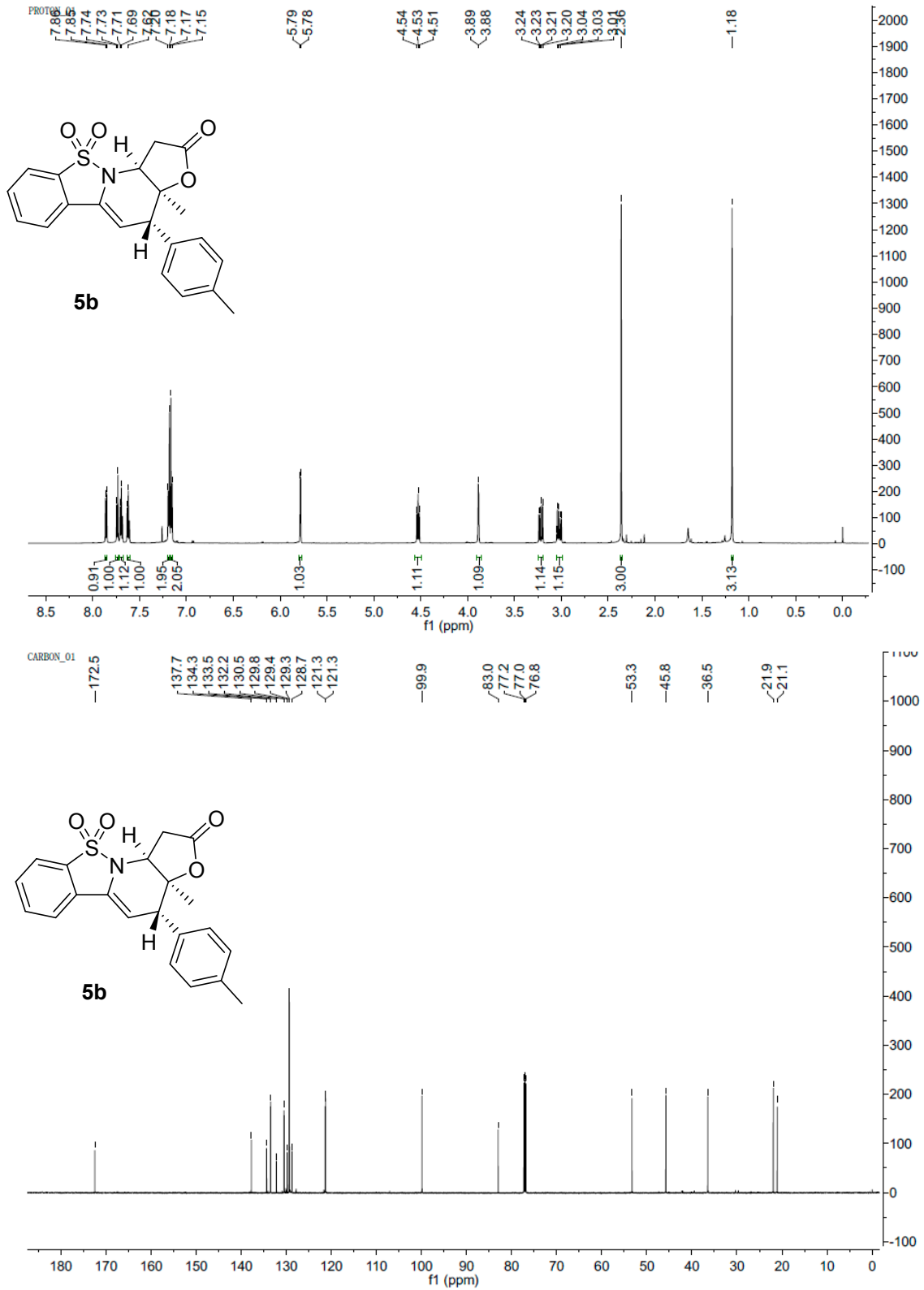


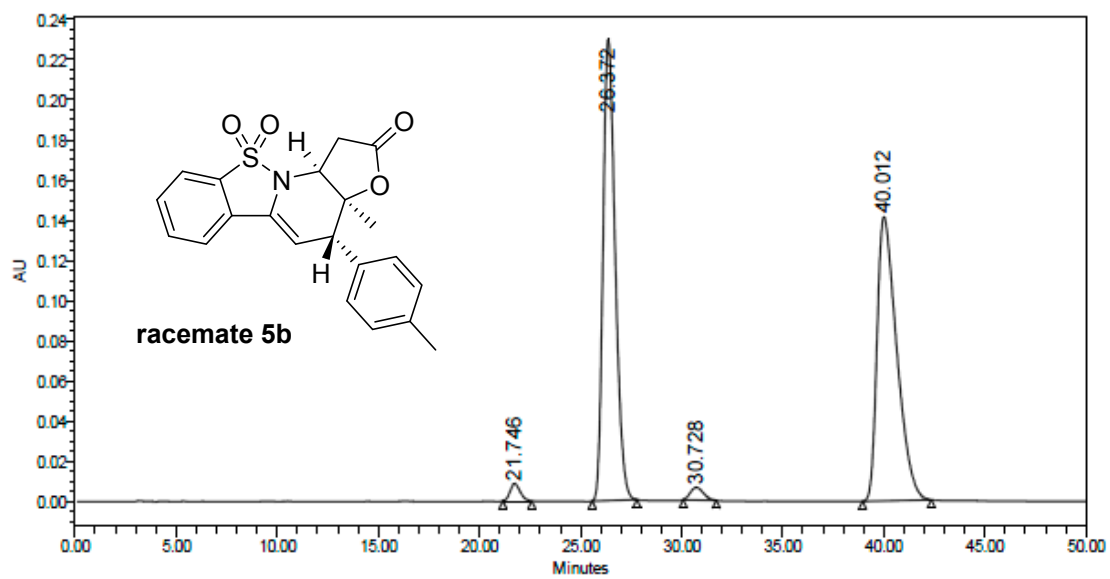


	RT	Area	% Area	Height
1	21.040	715013	9.18	22797
2	23.426	3212990	41.27	92060
3	28.300	716262	9.20	16994
4	38.290	3141649	40.35	53265

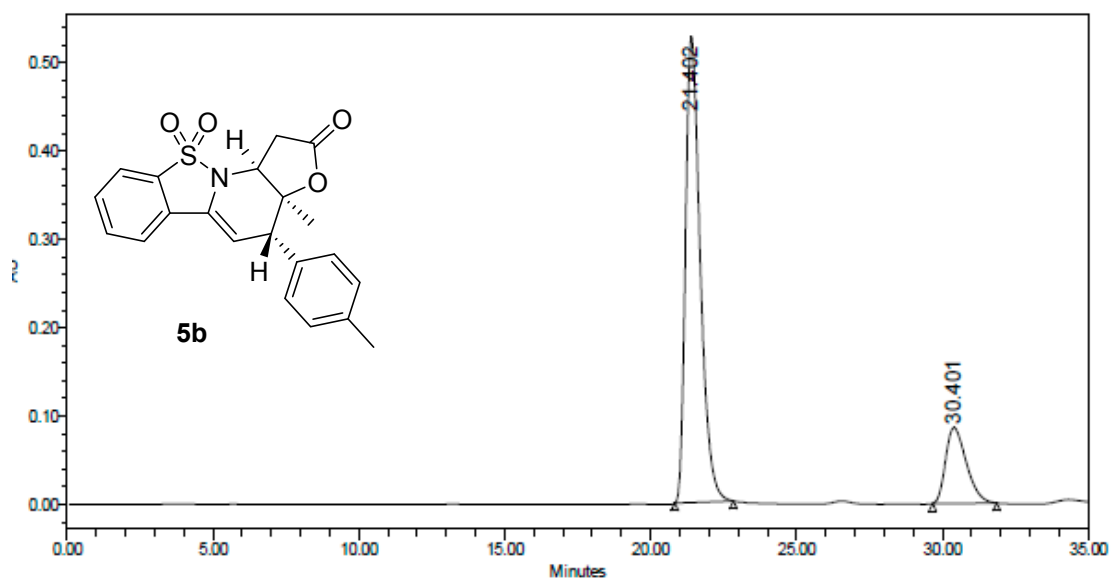


	RT	Area	% Area	Height
1	20.973	4706598	77.12	142165
2	28.280	1396014	22.88	32668

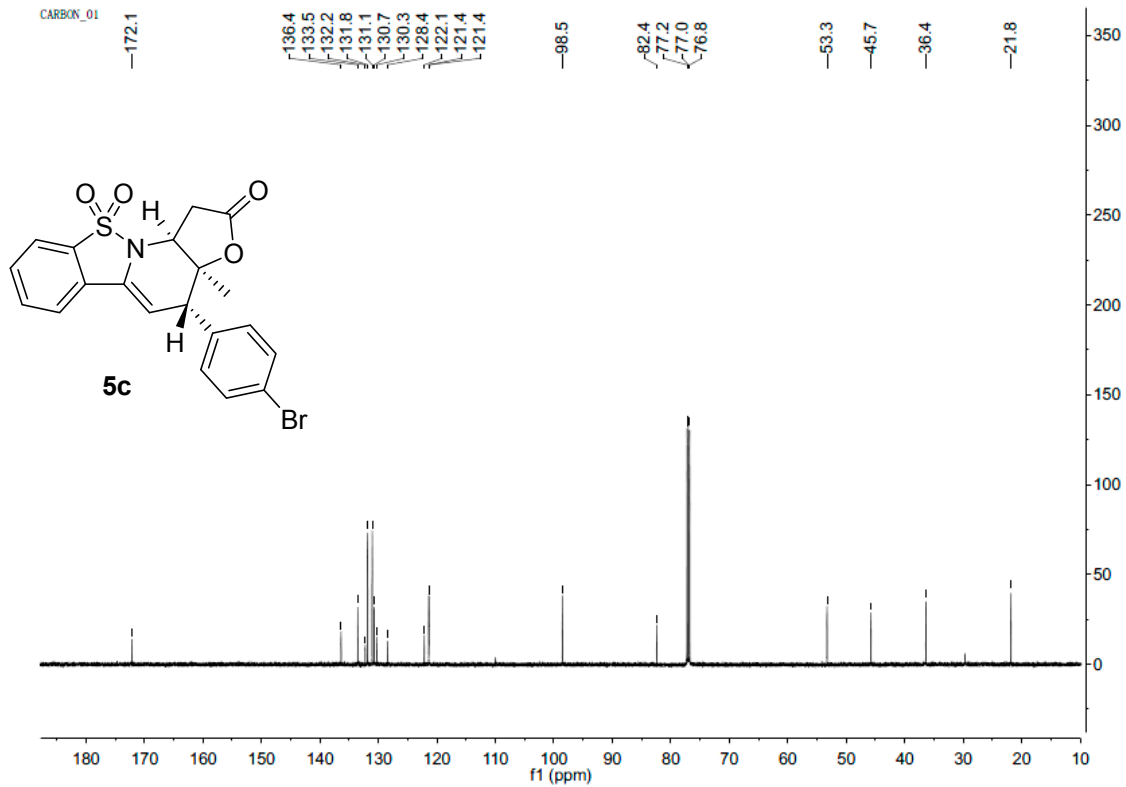
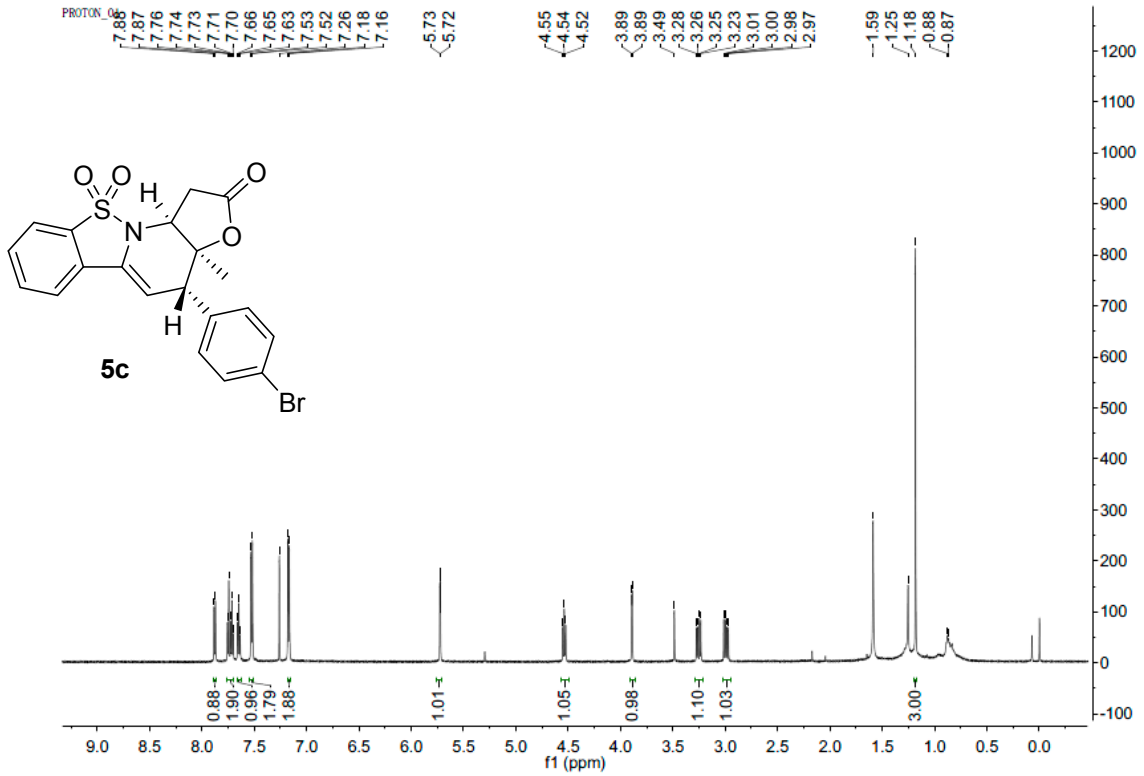


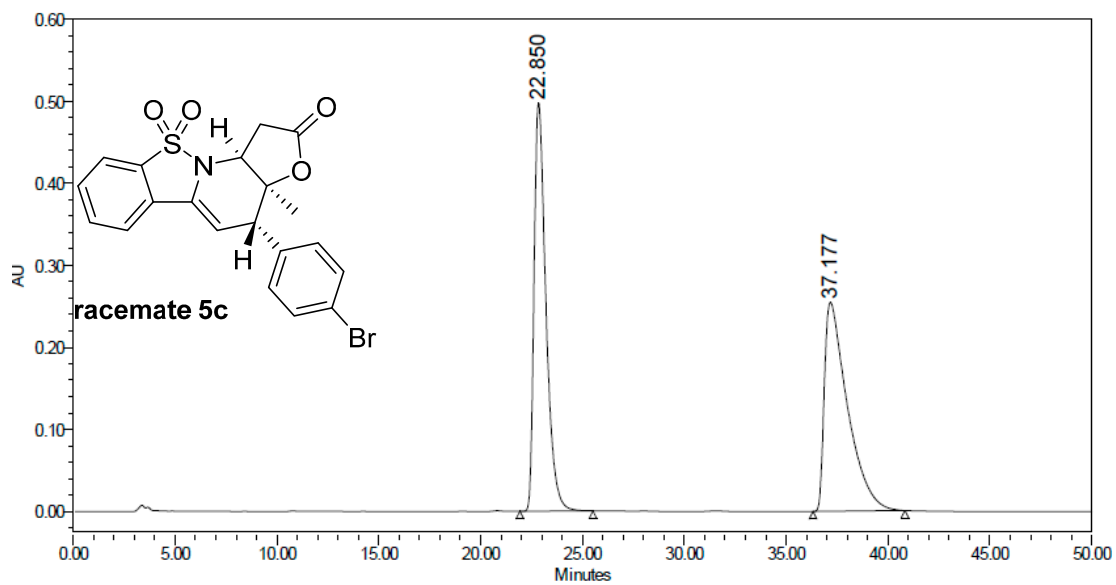


	RT	Area	% Area	Height
1	21.746	298751	1.52	8549
2	26.372	9539691	48.49	229589
3	30.728	283220	1.44	6299
4	40.012	9550840	48.55	141247

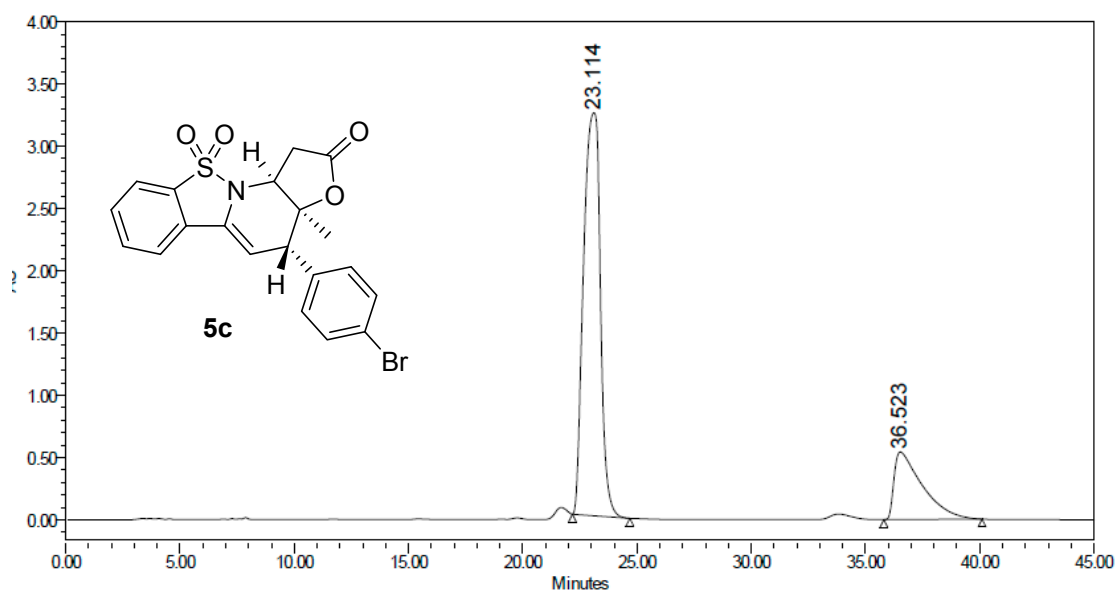


	RT	Area	% Area	Height
1	21.402	18484106	81.34	527128
2	30.401	4239659	18.66	85597

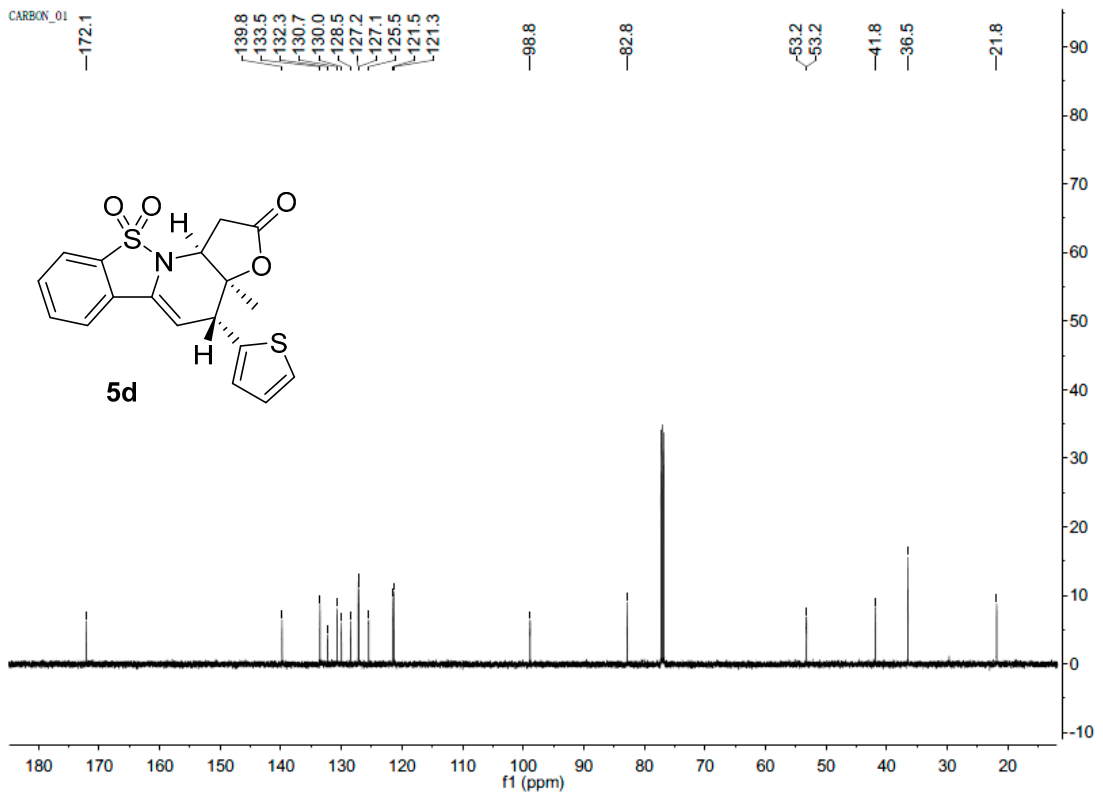
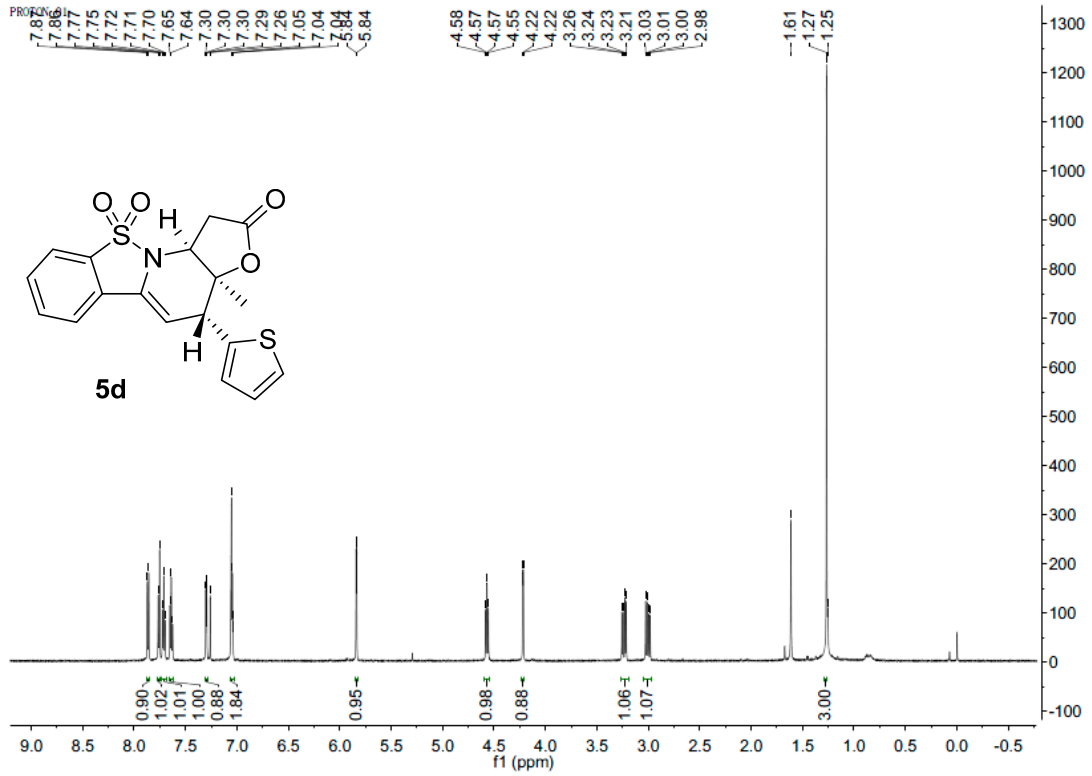


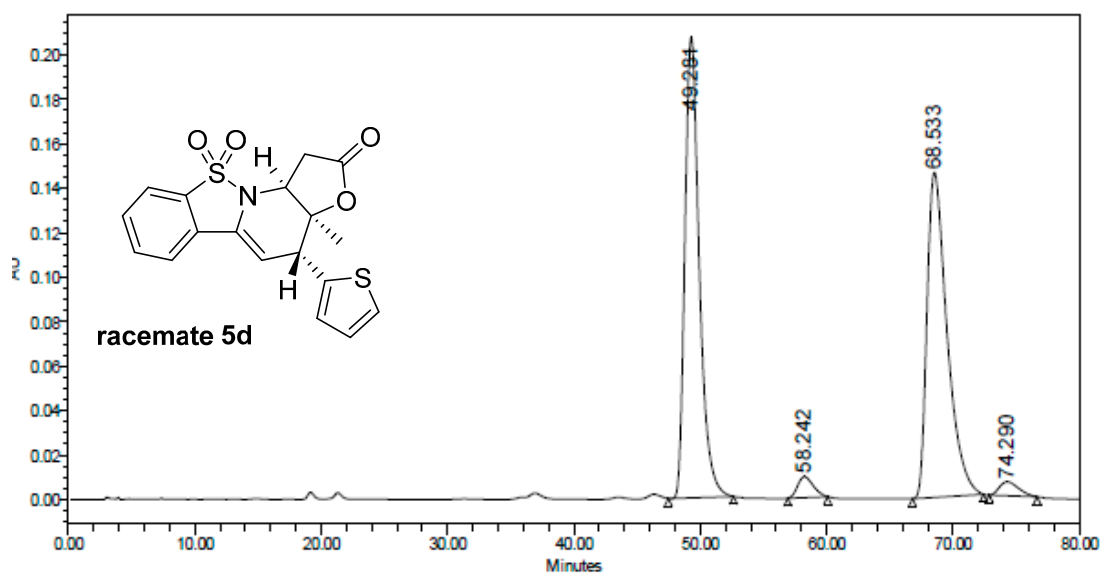


	RT	Area	% Area	Height
1	22.850	20133558	50.05	497551
2	37.177	20091897	49.95	254692

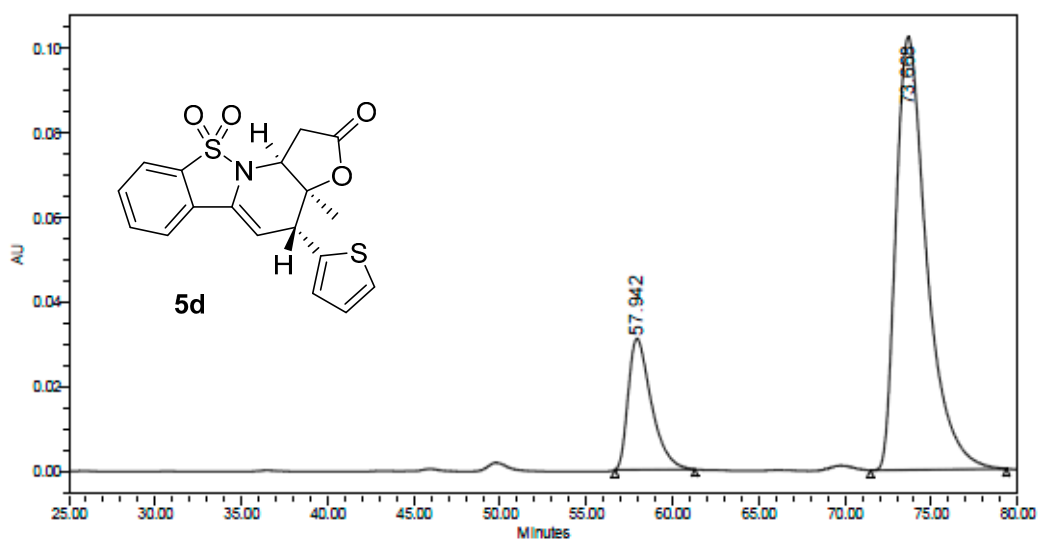


	RT	Area	% Area	Height
1	23.114	165666082	78.00	3237204
2	36.523	46722257	22.00	543690

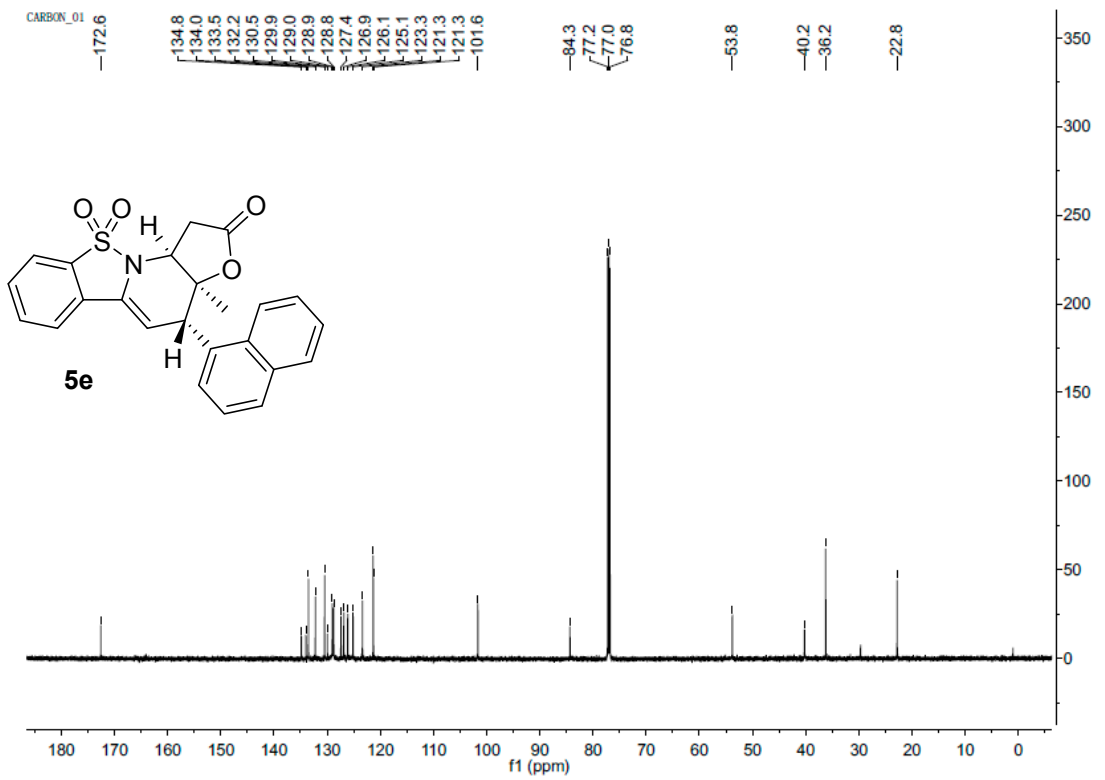
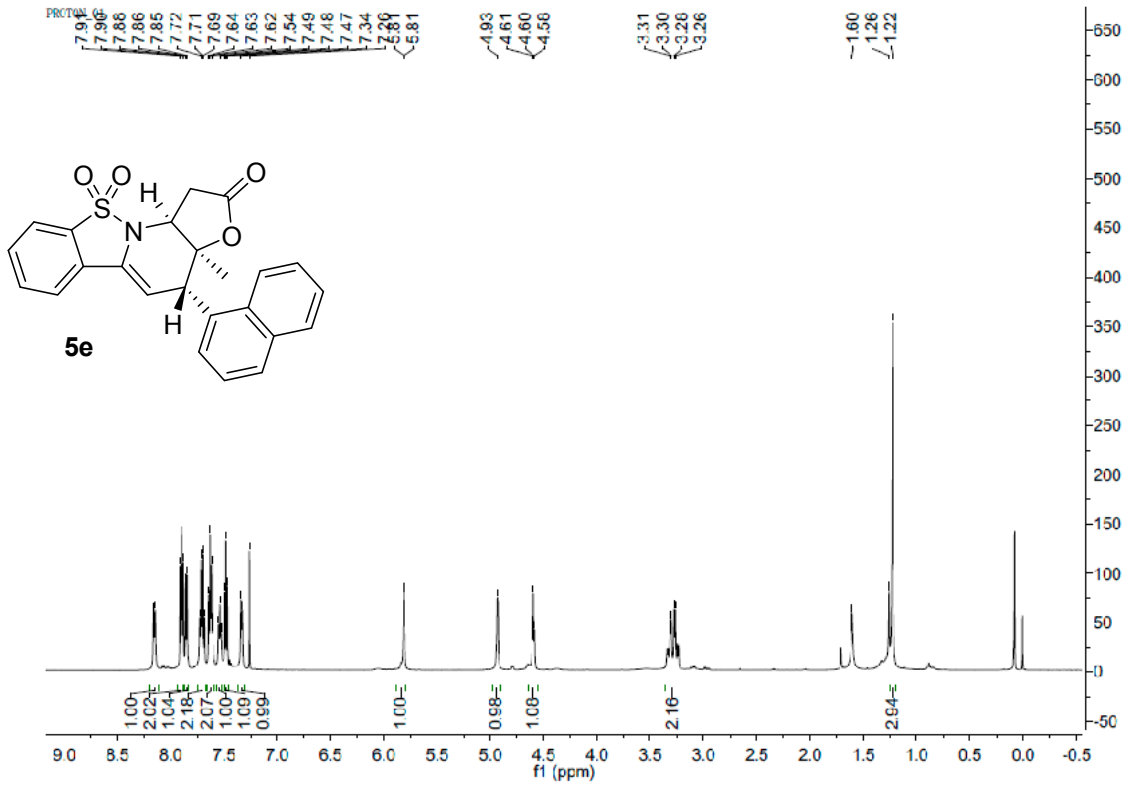


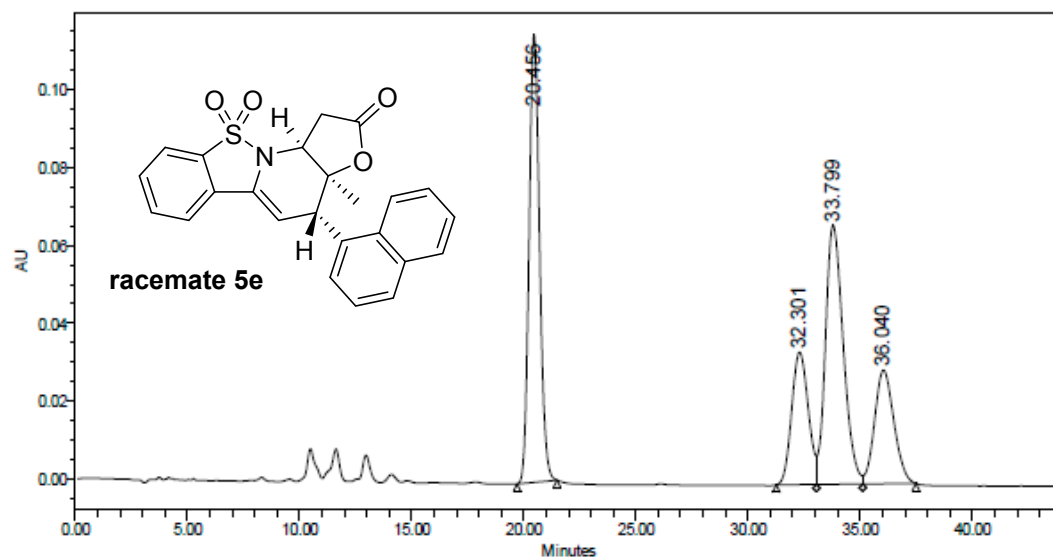


Peak	RT	Area	% Area	Height
1	49.281	16380653	48.23	207160
2	58.242	808300	2.38	9421
3	68.533	16107054	47.43	146183
4	74.290	666806	1.96	6305

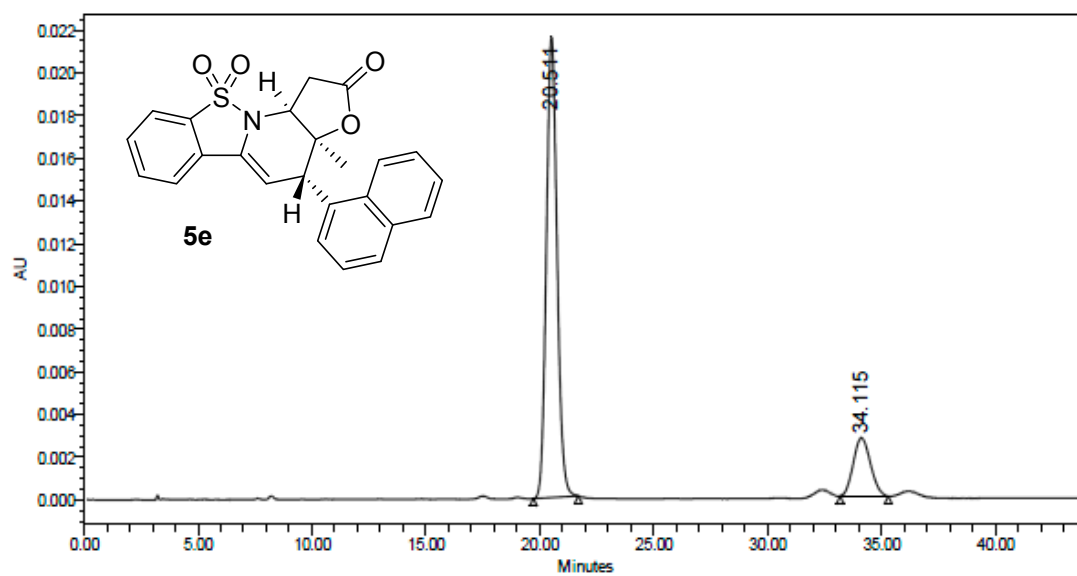


Peak	RT	Area	% Area	Height
1	57.942	2894642	18.58	30941
2	73.668	12687729	81.42	102286

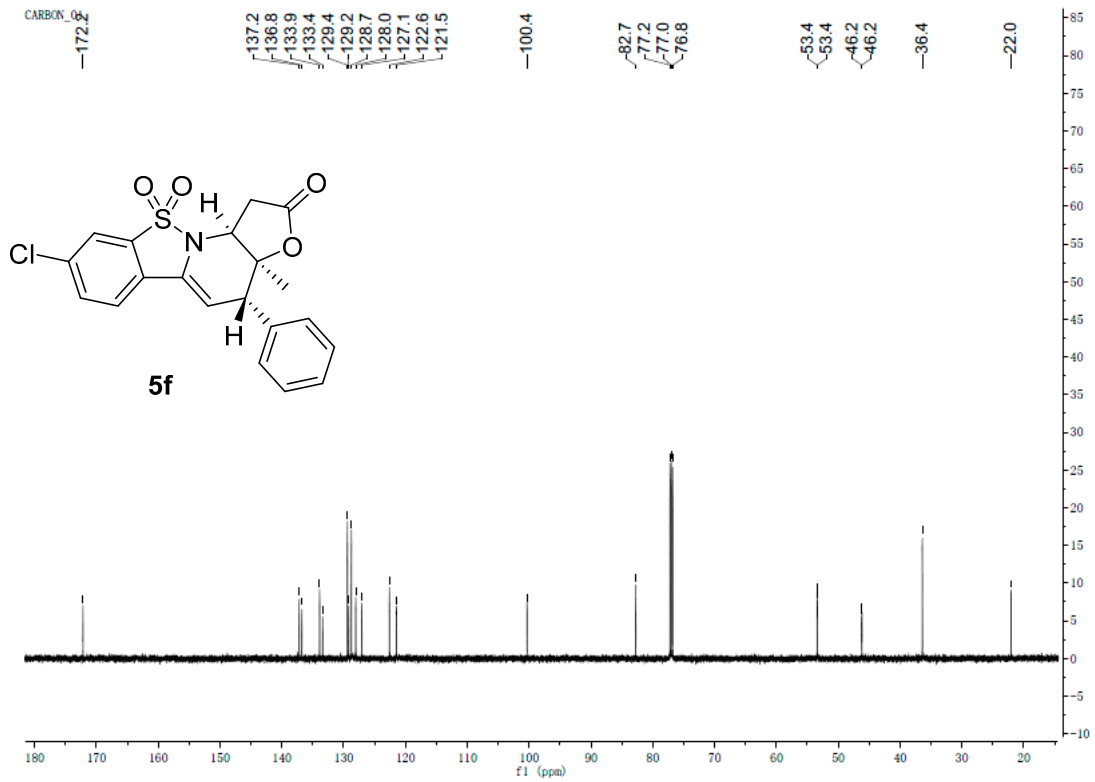
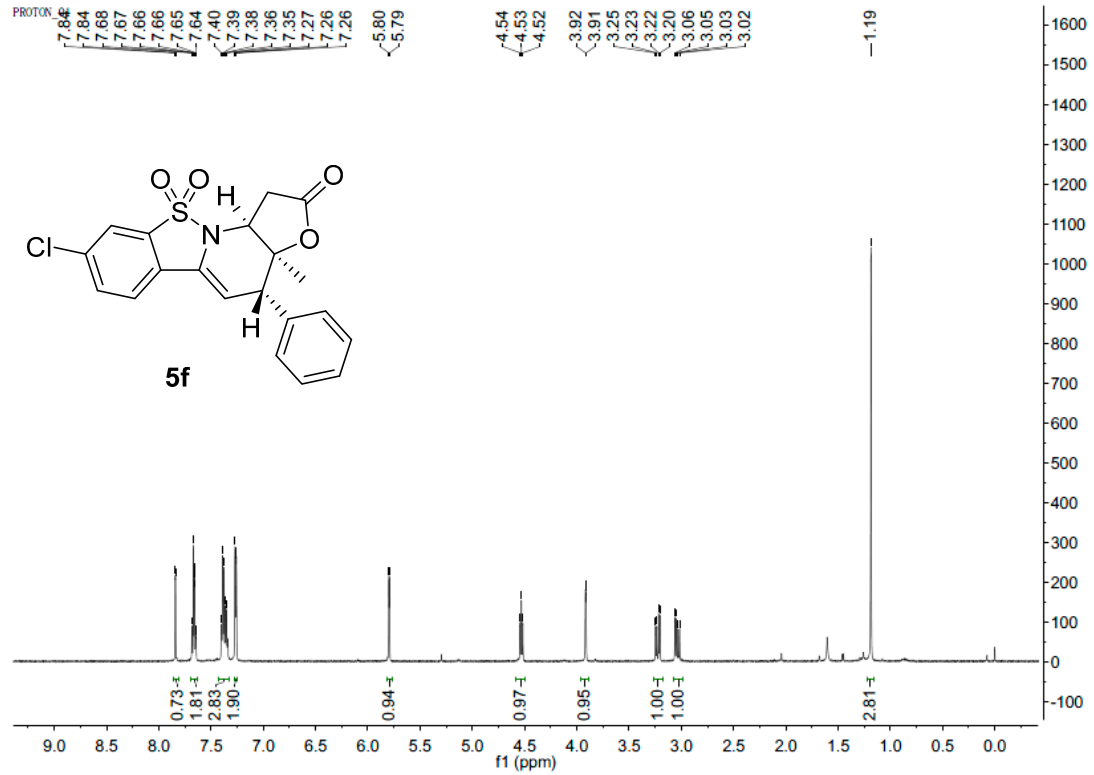


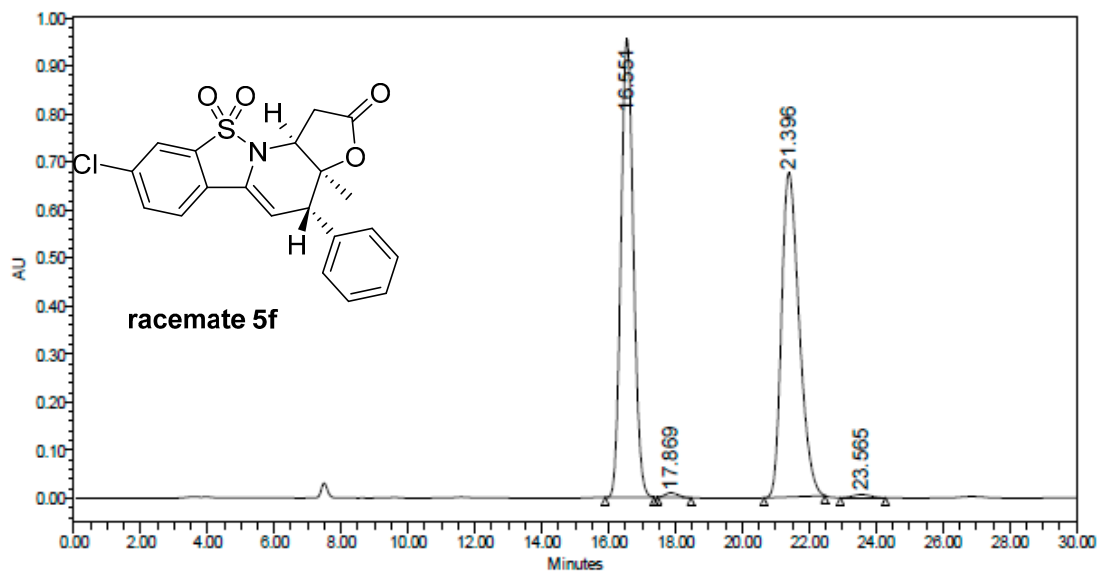


	RT	Area	% Area	Height
1	20.456	3723779	34.19	114965
2	32.301	1744441	16.02	34017
3	33.799	3670741	33.70	66507
4	36.040	1752980	16.09	29183

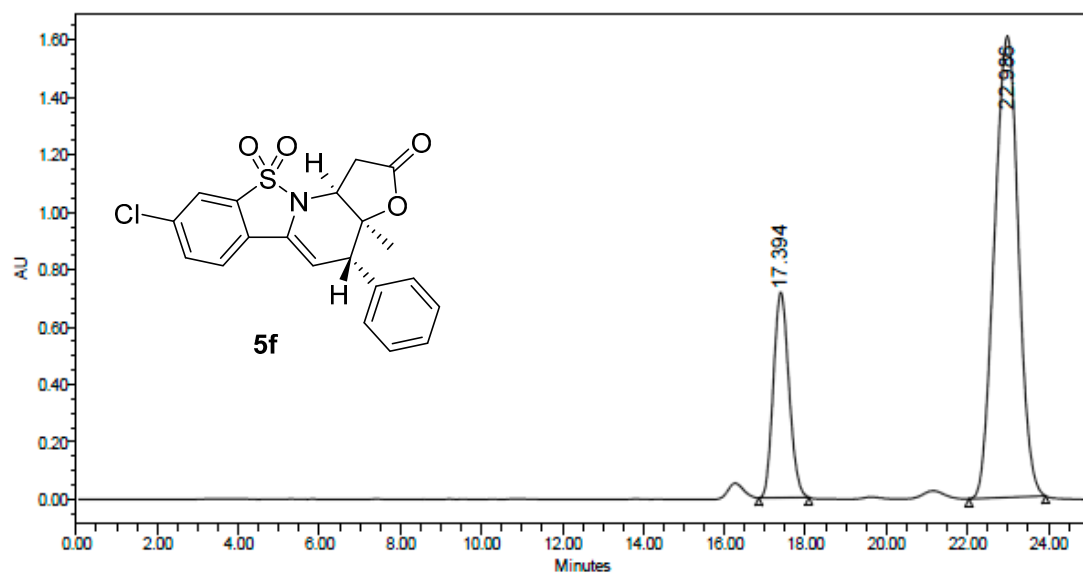


	RT	Area	% Area	Height
1	20.511	705440	83.11	21595
2	34.115	143350	16.89	2729

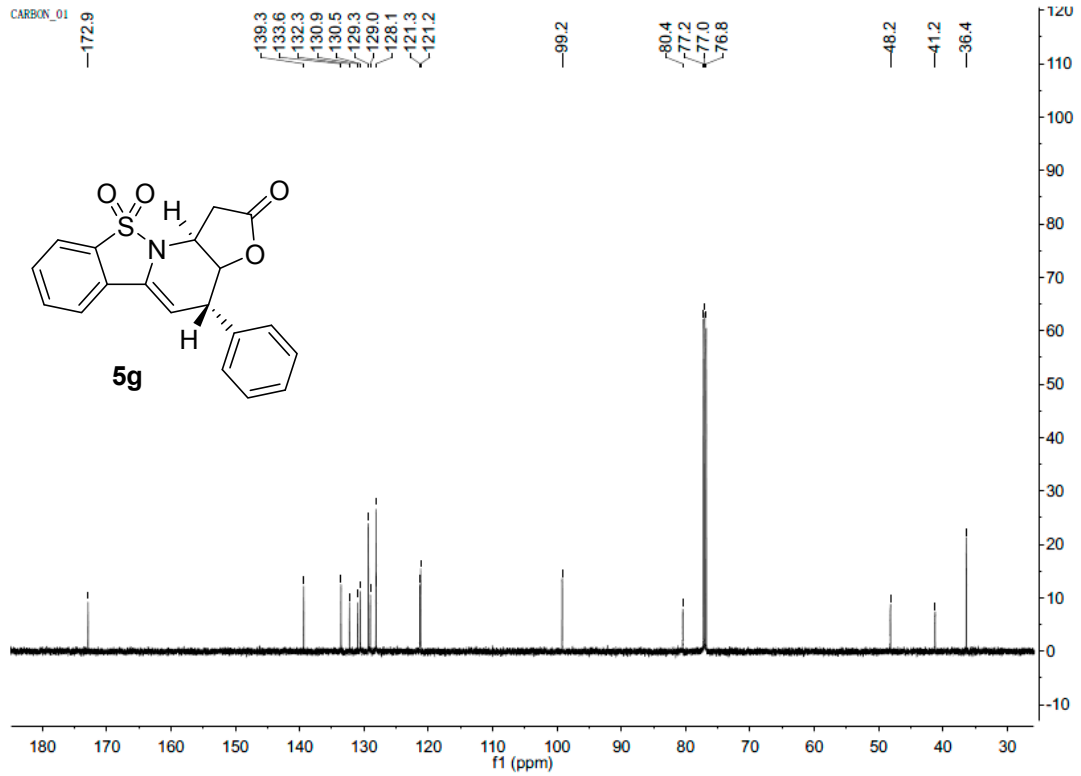
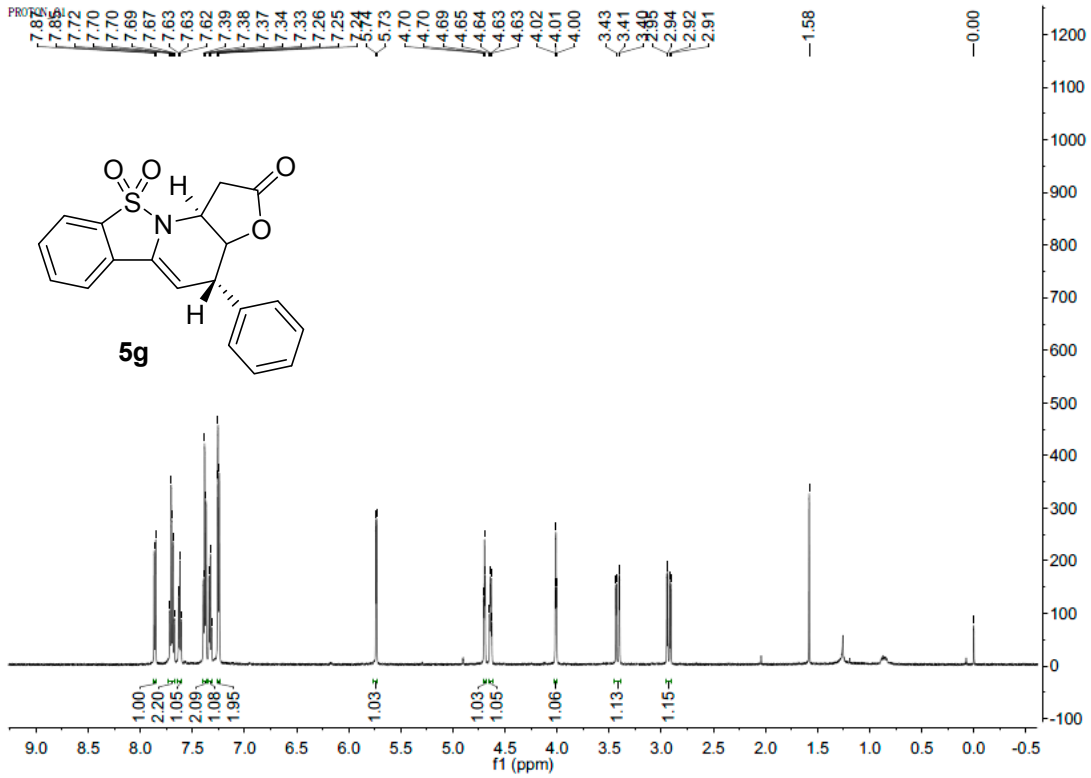


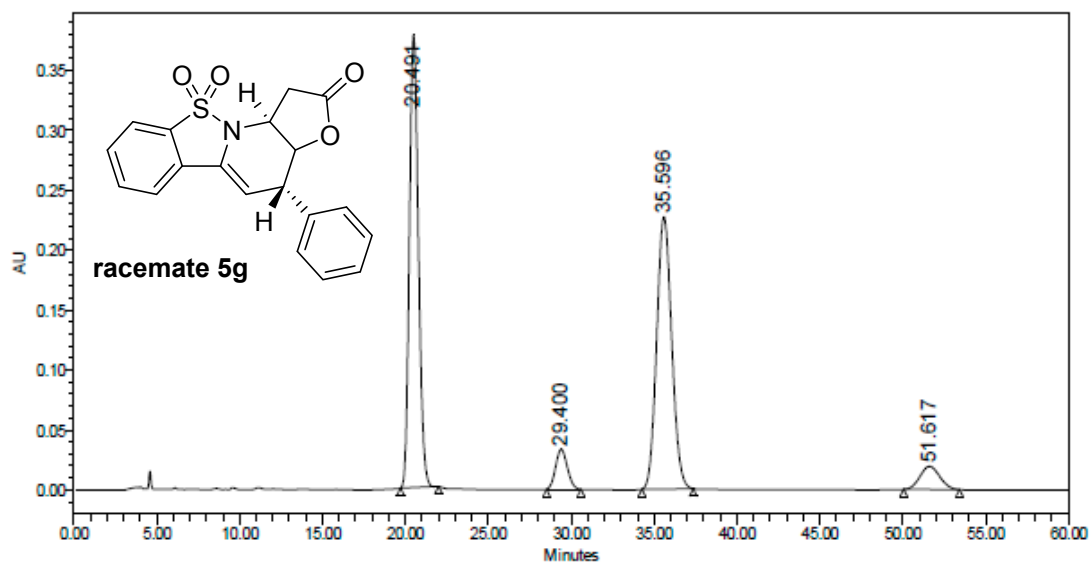


	RT	Area	% Area	Height
1	16.551	24740656	49.45	954355
2	17.869	255013	0.51	9600
3	21.396	24802676	49.57	675931
4	23.565	232287	0.46	6382

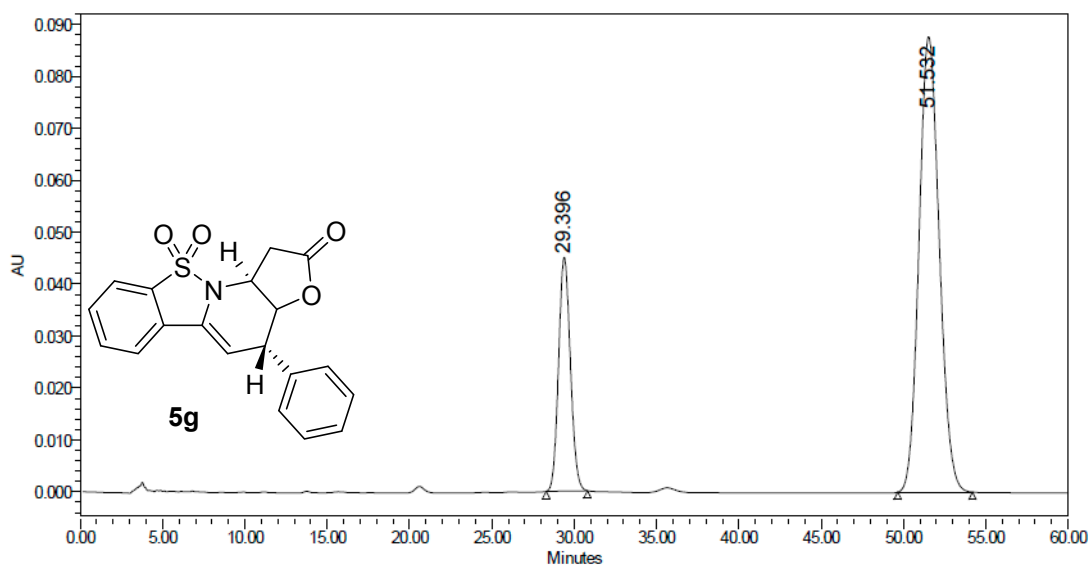


	RT	Area	% Area	Height
1	17.394	19144128	22.51	714822
2	22.986	65888719	77.49	1605184

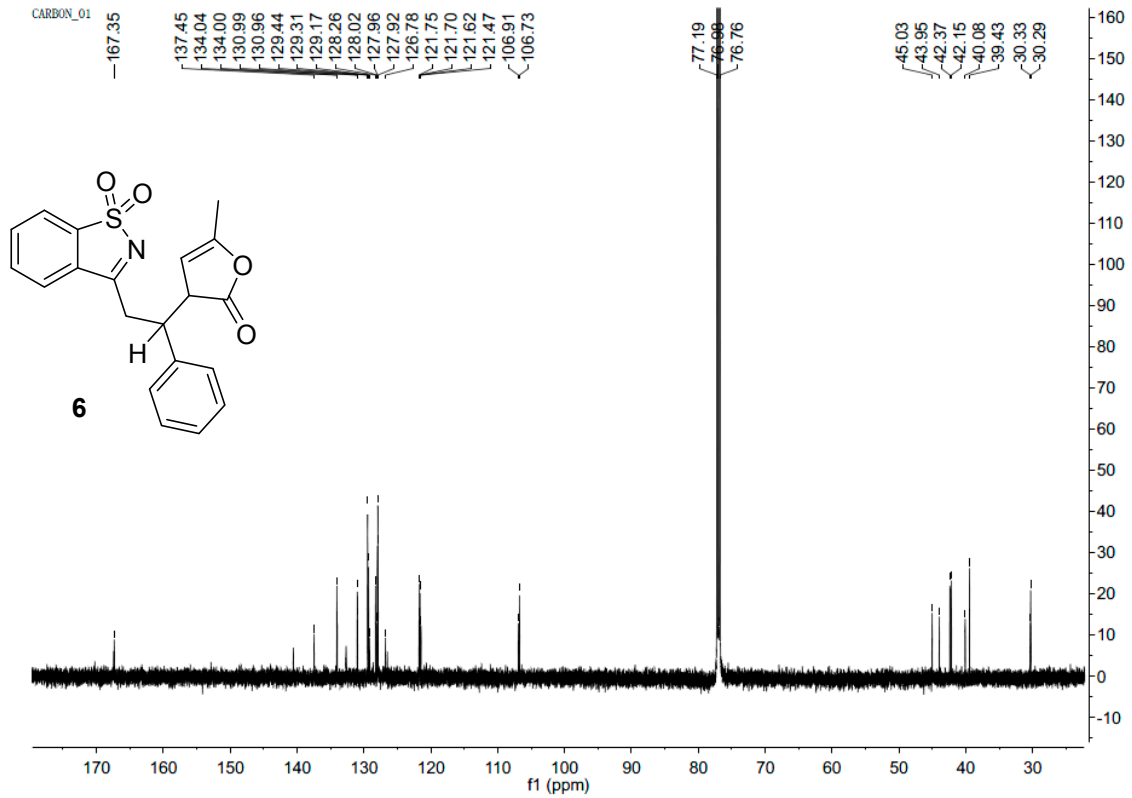
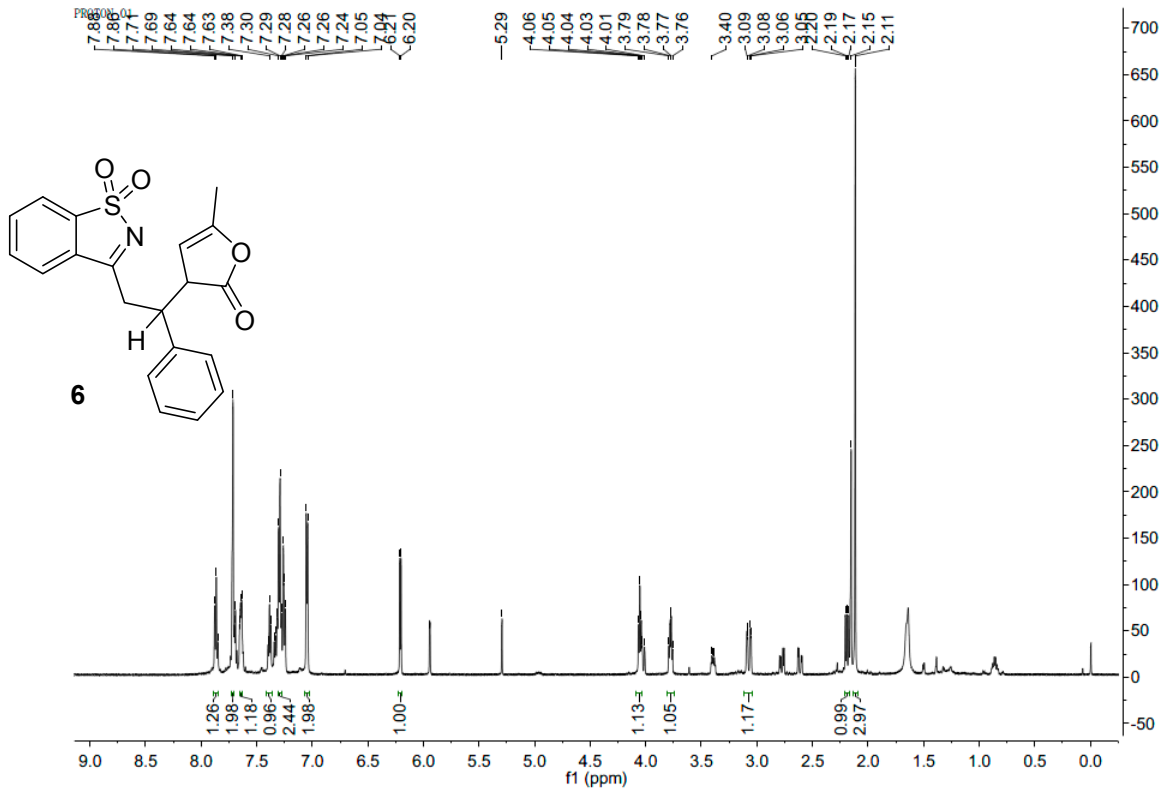


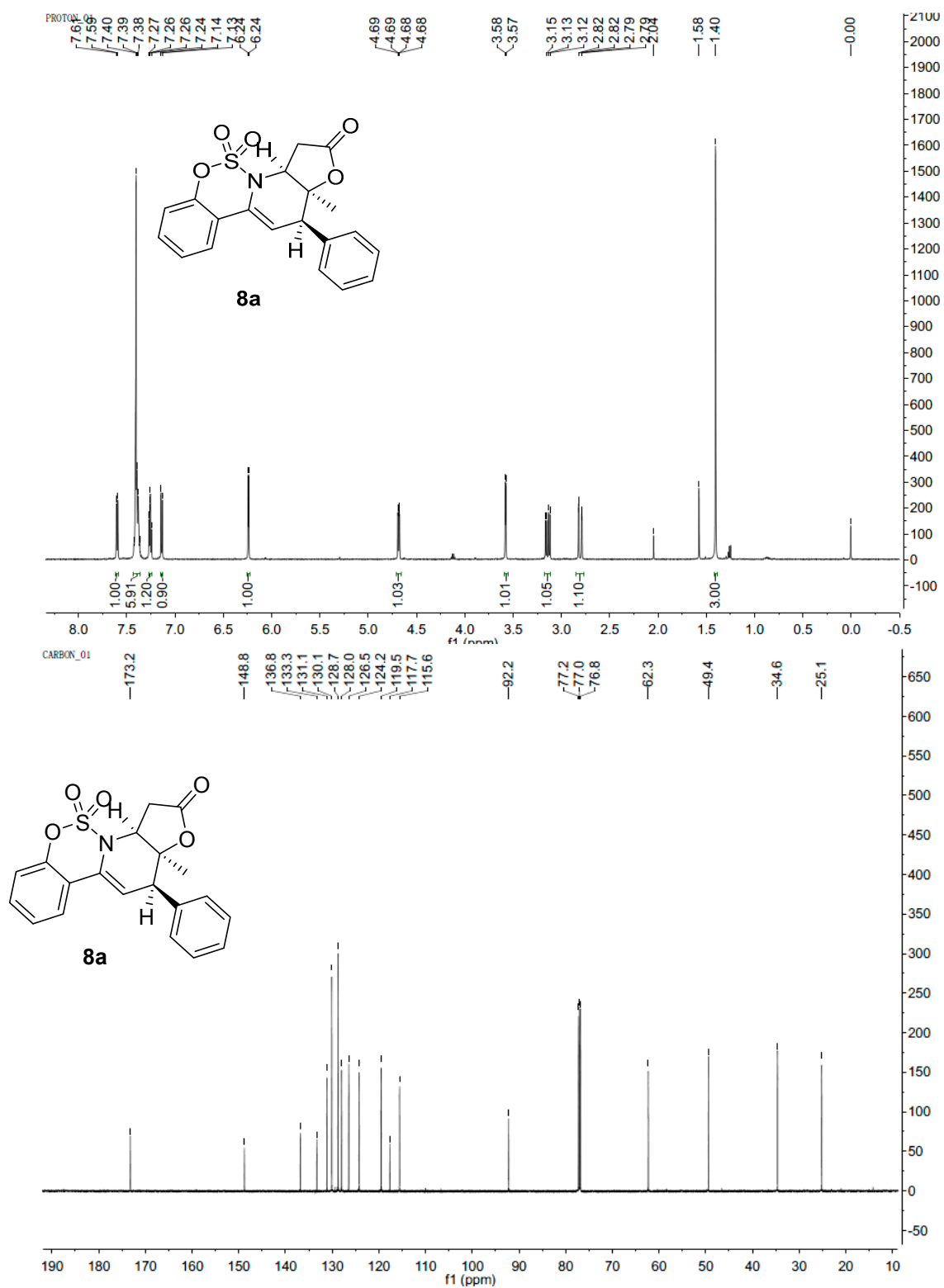


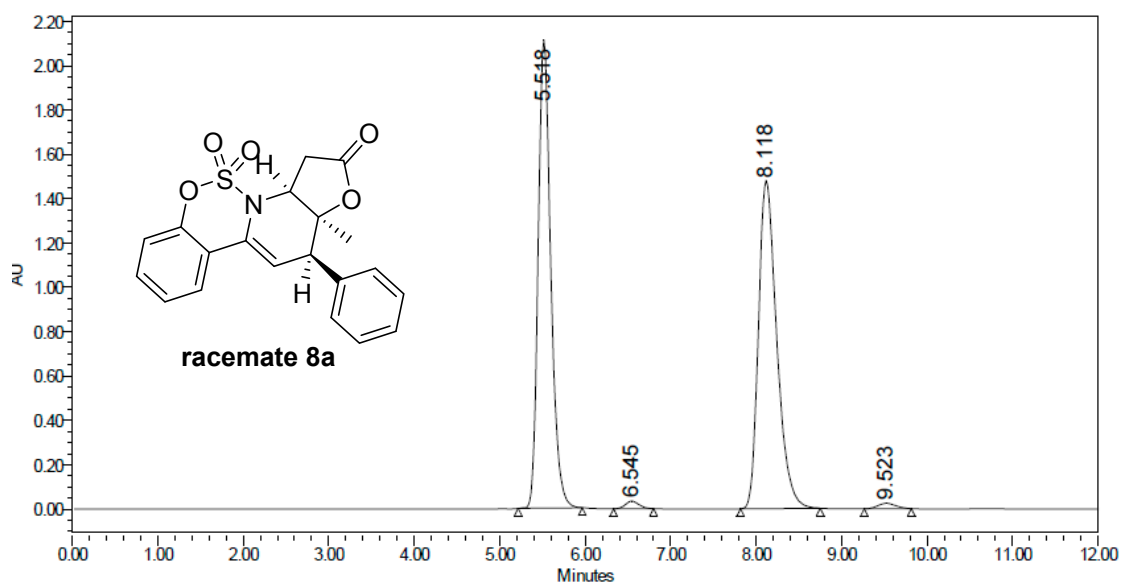
	RT	Area	% Area	Height
1	20.491	14232480	44.84	377691
2	29.400	1630739	5.14	33314
3	35.596	14277406	44.98	227085
4	51.617	1603183	5.05	19330



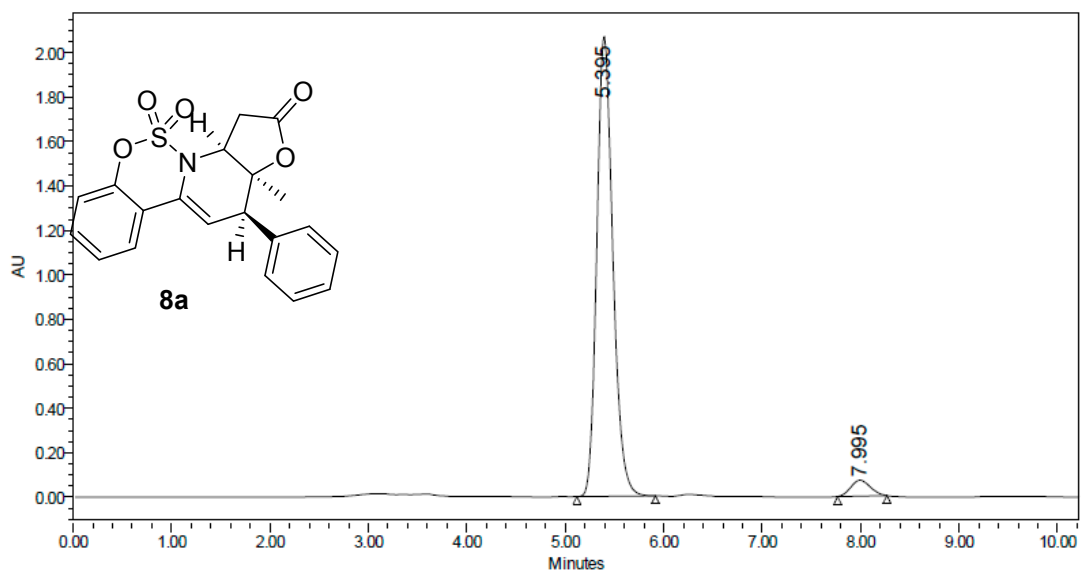
	RT	Area	% Area	Height
1	29.396	2245952	23.02	45059
2	51.532	7511547	76.98	87662



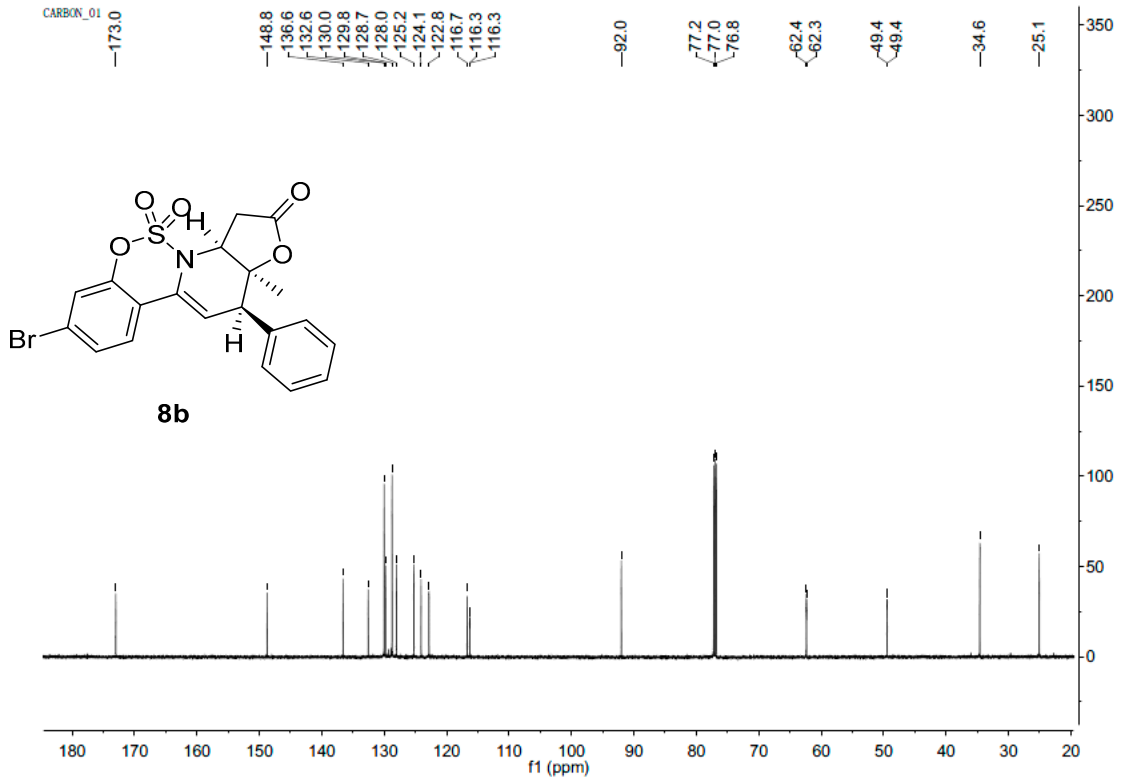
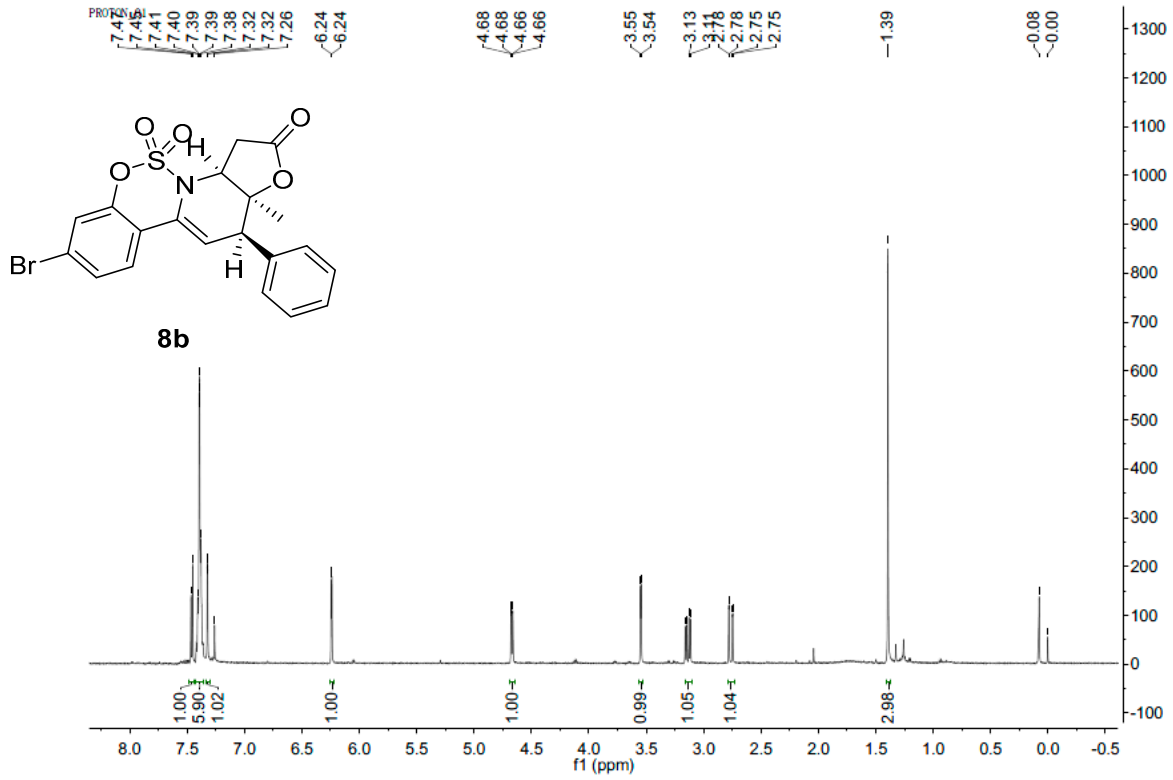


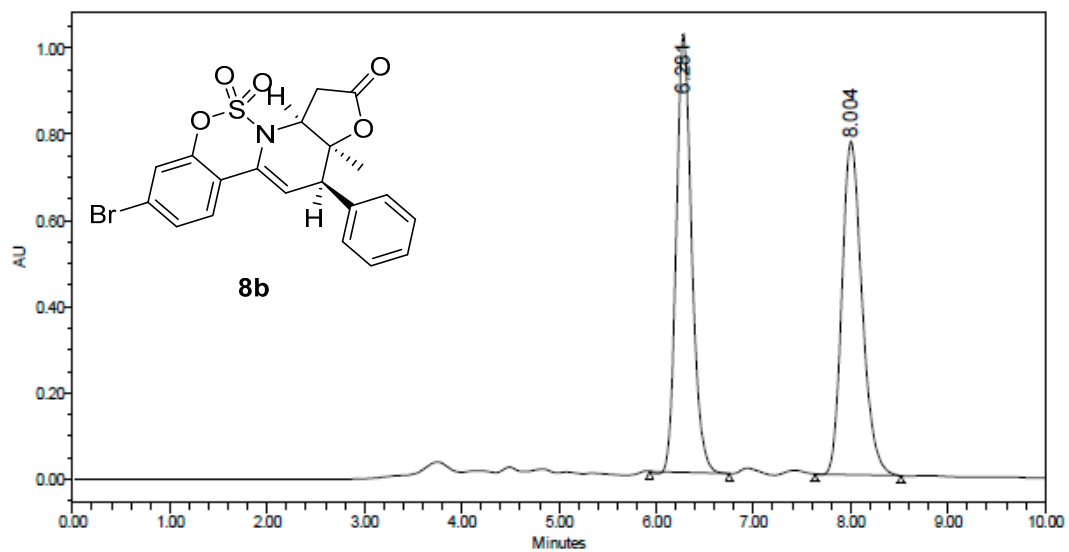


	RT	Area	% Area	Height
1	5.518	21616060	48.75	2109293
2	6.545	375747	0.85	34296
3	8.118	21988883	49.60	1479843
4	9.523	355988	0.80	24360

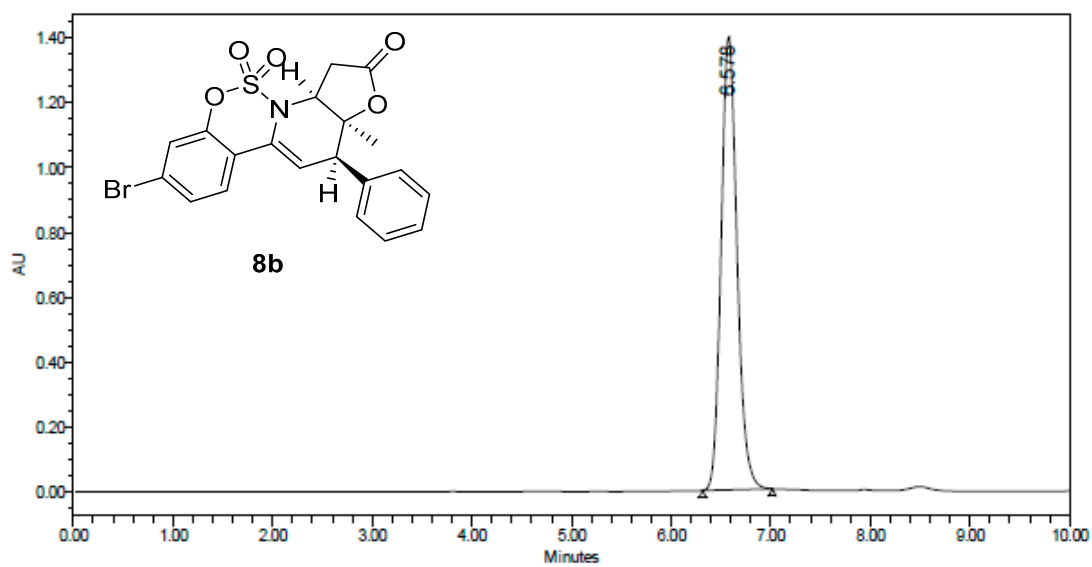


	RT	Area	% Area	Height
1	5.395	23545750	96.00	2072733
2	7.995	982185	4.00	71523

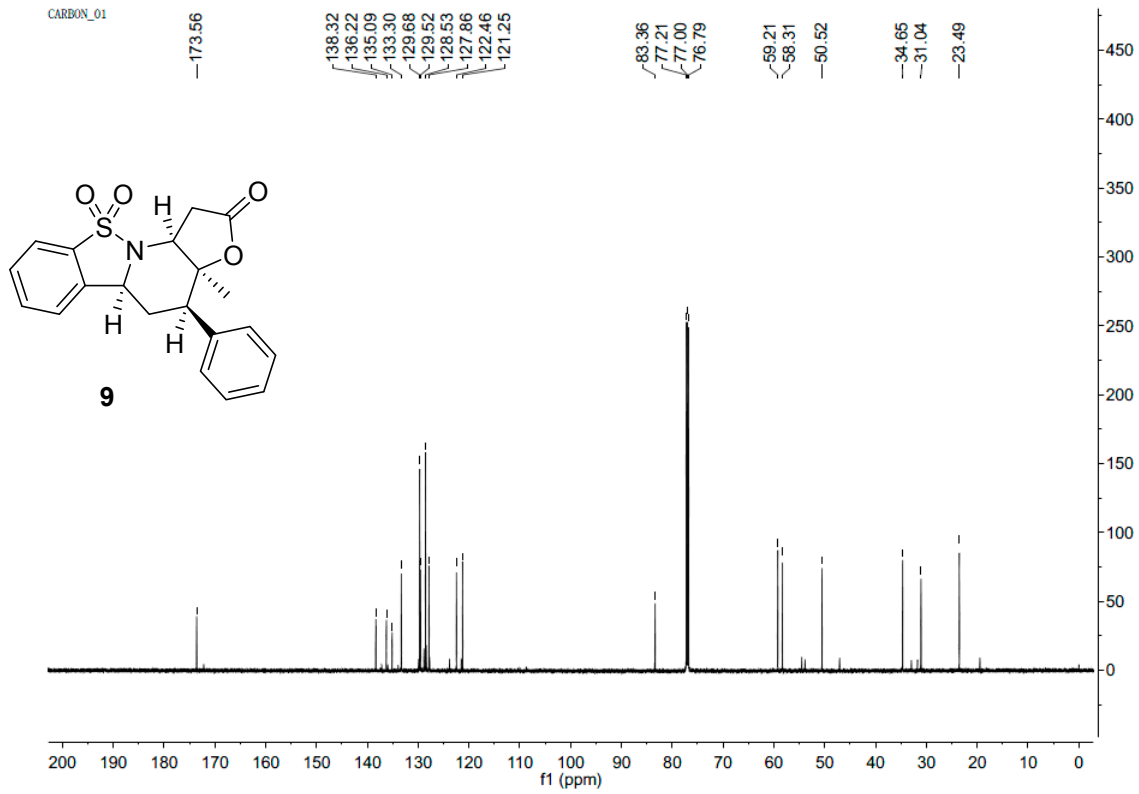
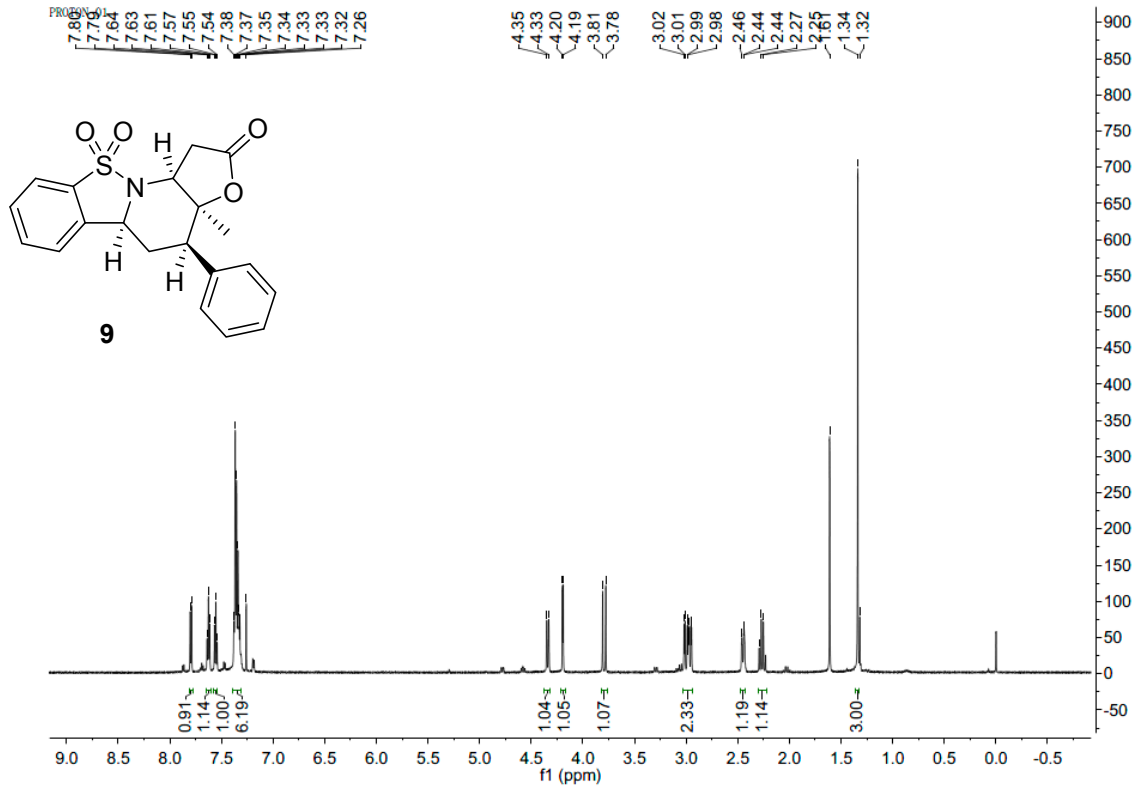




	RT	Area	% Area	Height
1	6.281	11217136	50.29	1016752
2	8.004	11087754	49.71	774545



	RT	Area	% Area	Height
1	6.578	15501566	100.00	1401323

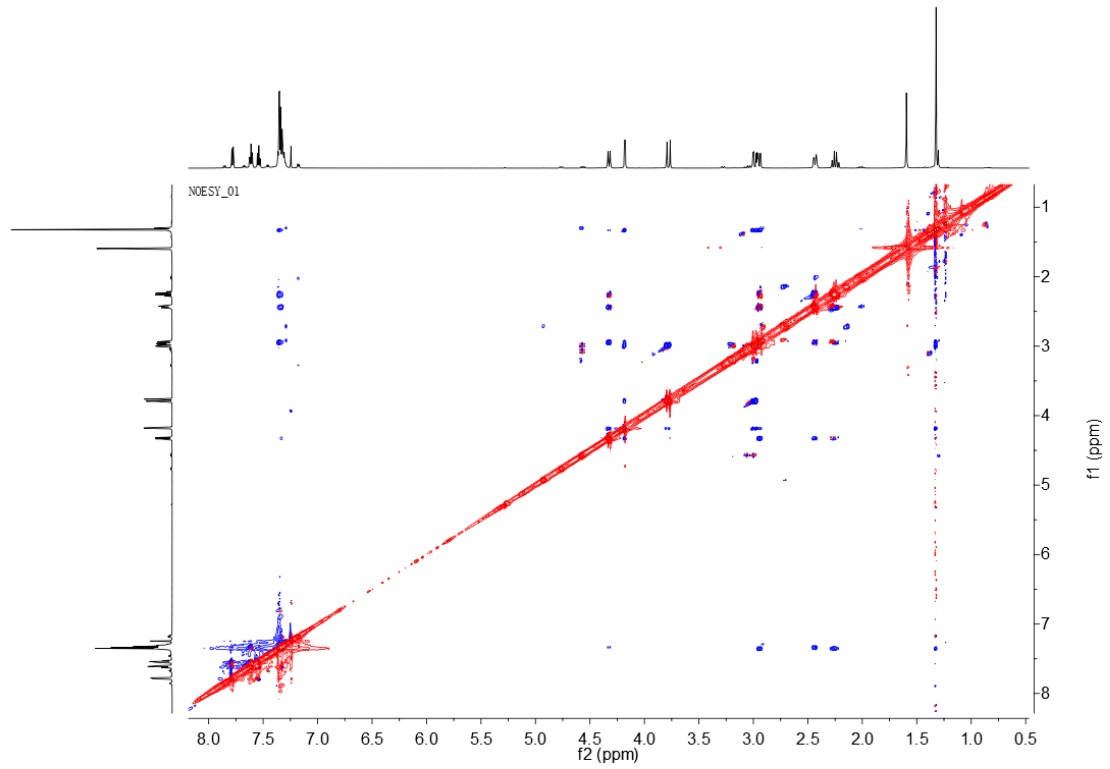
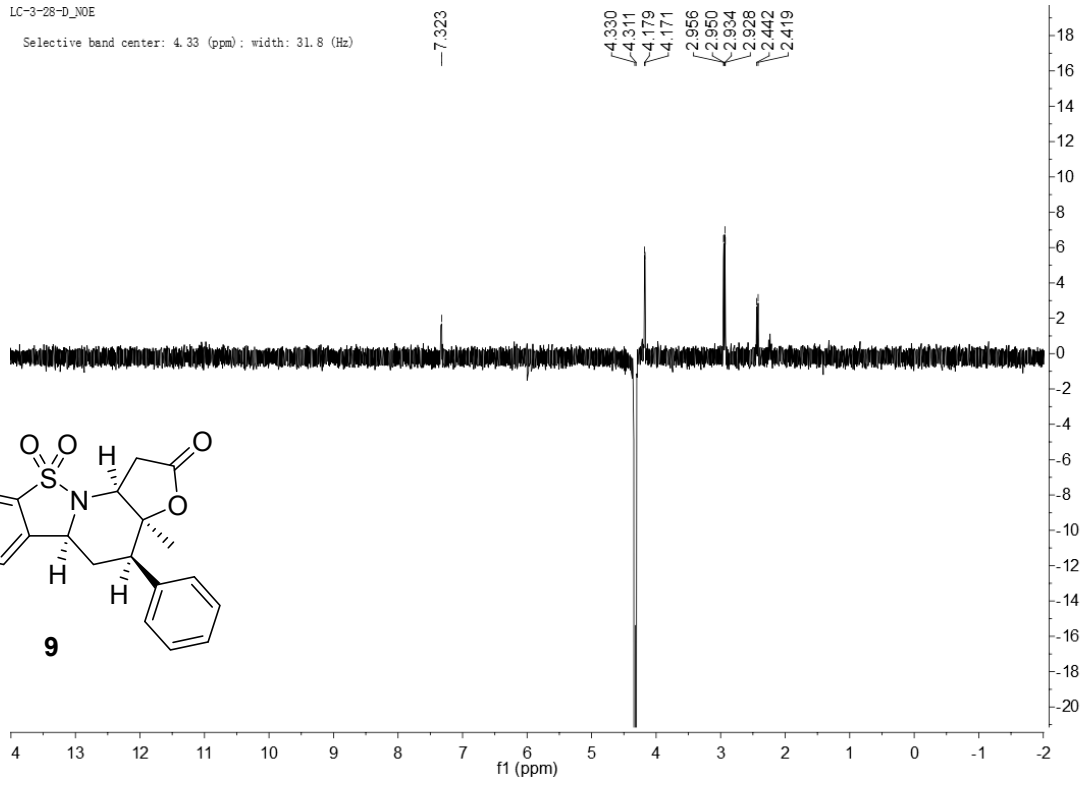
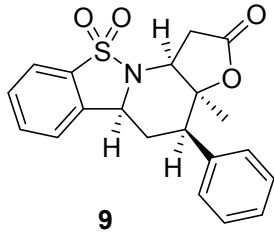


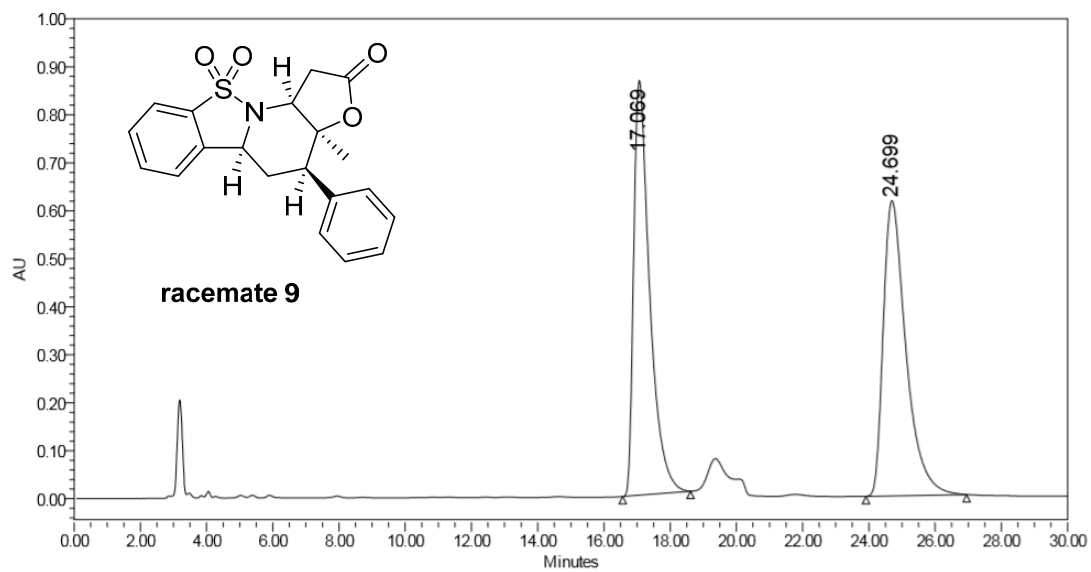
LC-3-28-D_NOE

Selective band center: 4.33 (ppm) : width: 31.8 (Hz)

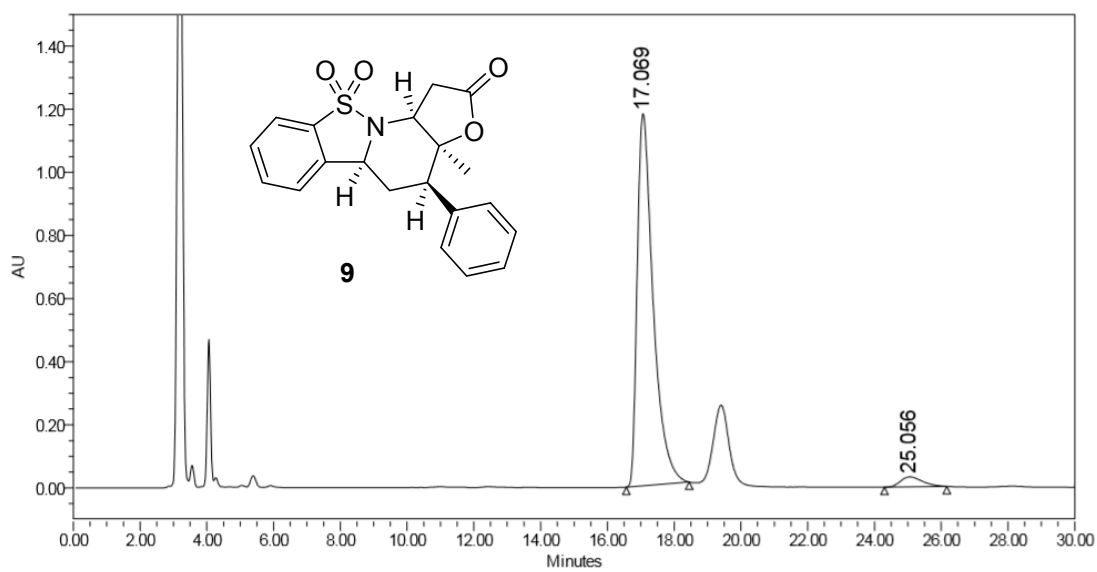
-7.323

4.330
4.311
4.179
4.171
2.966
2.950
2.934
2.928
2.442
2.419





	RT	Area	% Area	Height
1	17.069	28990104	49.74	864370
2	24.699	29298930	50.26	614975



	RT	Area	% Area	Height
1	17.069	39112459	96.40	1179202
2	25.056	1460920	3.60	31697