

**Supporting Information for**

**Thiophene-Core Estrogen Receptor Ligands Having Superagonist Activity**

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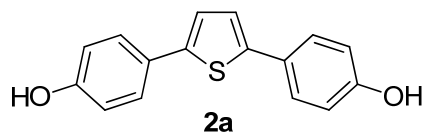
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## PART I. SUMMARY OF HPLC RESULTS

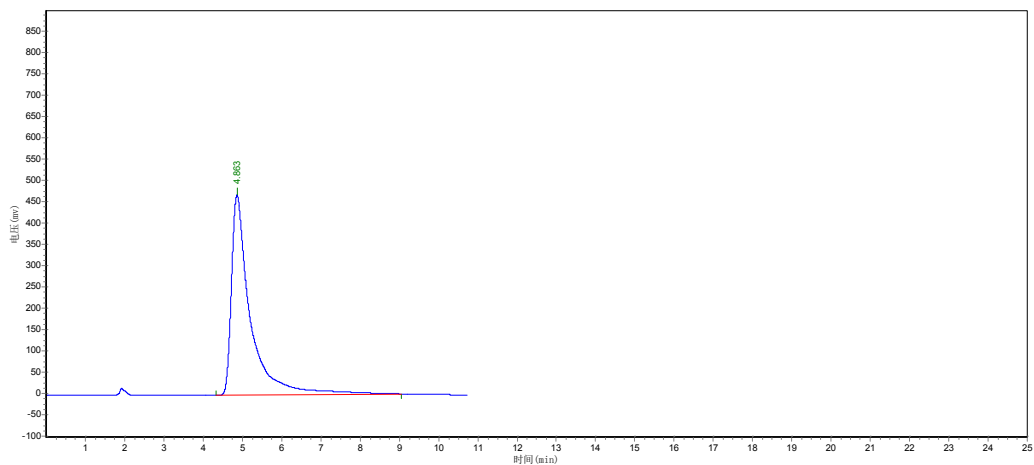
Cmpd	Normal Phase	Ret. Time	%Purity	Reverse Phase	Ret. Time	%Purity
2a	30:70 EtOAc:Hex	4.863	100.0000	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.217	100.0000
2b	30:70 EtOAc:Hex	3.763	97.7655	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.515	98.1484
2c	30:70 EtOAc:Hex	3.120	96.8973	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	5.618	96.6949
2d	30:70 EtOAc:Hex	3.248	98.1529	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	5.968	98.9121
2e	30:70 EtOAc:Hex	5.498	98.5124	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.347	100.0000
2f	30:70 EtOAc:Hex	4.990	100.0000	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.007	100.0000
2g	30:70 EtOAc:Hex	4.797	99.3402	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	5.975	96.8976
2h	30:70 EtOAc:Hex	4.790	98.1834	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	5.343	97.7597
2i	30:70 EtOAc:Hex	3.747	99.0071	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	5.200	95.8788
2j	30:70 EtOAc:Hex	4.805	100.0000	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.298	100.0000
2k	30:70 EtOAc:Hex	4.298	98.9884	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.518	100.0000
2l	30:70 EtOAc:Hex	3.223	97.7352	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	5.802	98.2713
2m	30:70 EtOAc:Hex	3.838	95.6289	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	5.127	100.0000
4a	30:70 EtOAc:Hex	3.435	95.6272	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	3.858	98.0512
4b	30:70 EtOAc:Hex	3.670	96.6890	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	5.147	99.7345
4c	30:70 EtOAc:Hex	4.508	97.3305	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	5.138	99.4313
4d	30:70 EtOAc:Hex	3.435	95.0513	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	7.262	98.1410
4e	30:70 EtOAc:Hex	4.797	99.3787	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.518	100.0000
4f	30:70 EtOAc:Hex	5.802	99.2925	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.502	100.0000
6a	30:70 EtOAc:Hex	5.653	99.7312	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.368	100.0000
6b	30:70 EtOAc:Hex	5.392	100.0000	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.312	99.0518
8a	30:70 EtOAc:Hex	5.598	99.5308	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.332	100.0000
8b	30:70 EtOAc:Hex	4.625	98.6786	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.590	100.0000
10a	30:70 EtOAc:Hex	4.848	100.0000	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.217	100.0000
10b	30:70 EtOAc:Hex	4.442	97.4312	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.258	98.9578
10c	30:70 EtOAc:Hex	4.417	100.0000	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.522	100.0000
10d	30:70 EtOAc:Hex	5.582	100.0000	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.893	100.0000

Cmpd	Normal Phase	Ret. Time	%Purity	Reverse Phase	Ret. Time	%Purity
12a	30:70 EtOAc:Hex	5.037	100.0000	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.243	100.0000
12b	30:70 EtOAc:Hex	4.920	100.0000	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.097	100.0000
14a	30:70 EtOAc:Hex	5.542	95.2782	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	3.575	98.0363
14b	30:70 EtOAc:Hex	6.112	98.0220	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.138	98.0481
14c	30:70 EtOAc:Hex	7.123	97.9189	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	3.665	100.0000
16a	30:70 EtOAc:Hex	3.748	97.8027	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.768	97.7940
16b	30:70 EtOAc:Hex	4.625	99.5229	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.238	100.0000
16c	30:70 EtOAc:Hex	5.612	96.3286	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.787	95.6711
16d	30:70 EtOAc:Hex	3.223	97.2168	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.525	96.9878
18a	30:70 EtOAc:Hex	4.205	97.6740	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.398	99.0805
18b	30:70 EtOAc:Hex	5.710	100.0000	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	3.815	100.0000
18c	30:70 EtOAc:Hex	4.403	98.1523	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.220	96.1641
18d	30:70 EtOAc:Hex	5.103	100.0000	70:30 CH <sub>3</sub> CN:H <sub>2</sub> O	4.245	100.0000

## PART II. HPLC CHROMATOGRAMS

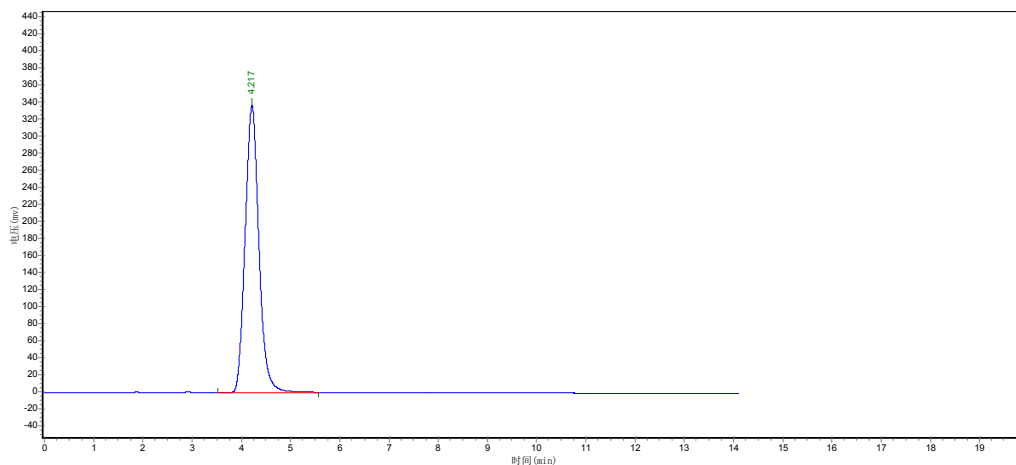


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

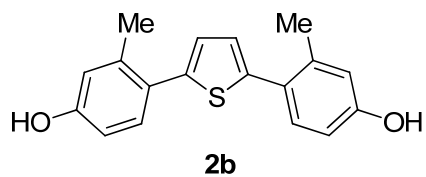


Name	Retention Time	Peak height	Area	Area Percent
Totals	4.863	469622.594	15815037.000	100.0000

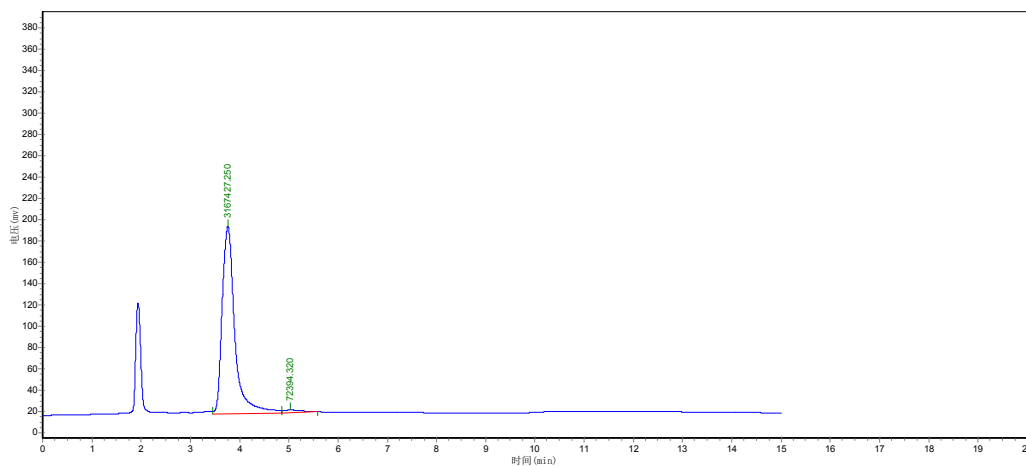
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
Totals	4.217	336381.563	6547481.000	100.0000

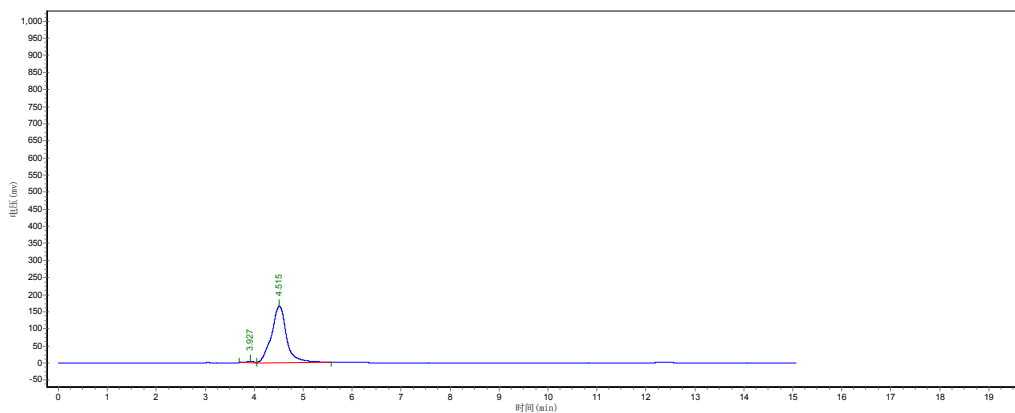


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

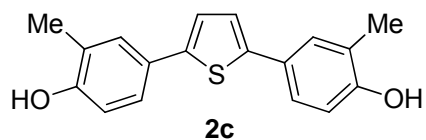


Name	Retention Time	Peak height	Area	Area Percent
	3.763	175996.281	3167427.250	97.7655
	5.035	2725.632	72394.320	2.2345
Totals		178721.913	3239821.570	100.0000

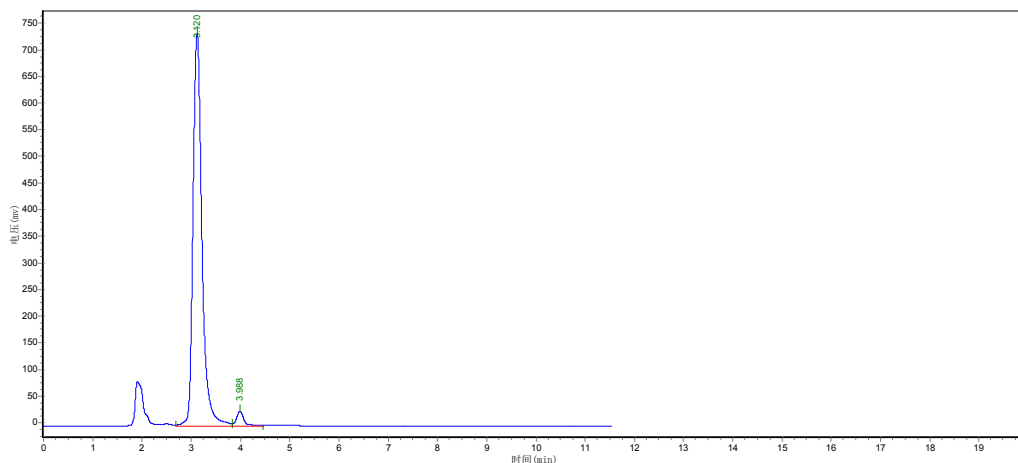
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	3.927	4029.172	65529.375	1.8516
	4.515	164671.750	3473528.500	98.1484
Totals		168700.922	3539057.875	100.0000

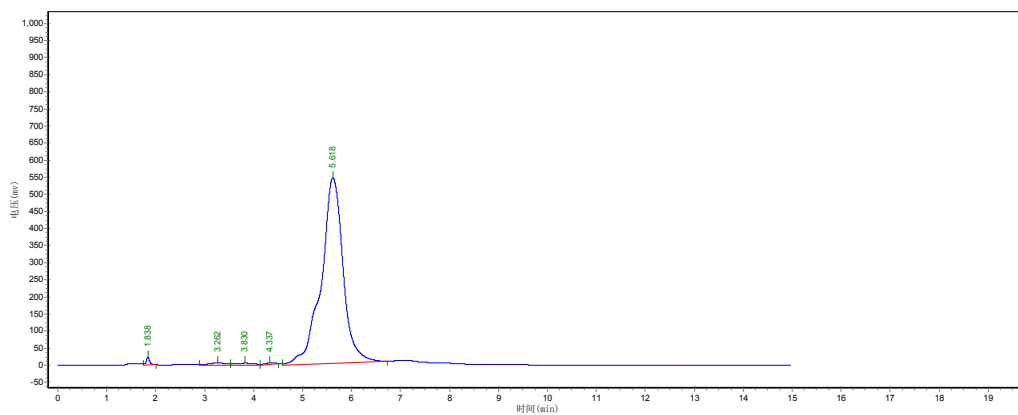


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

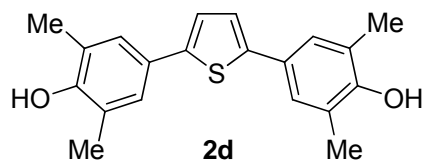


Name	Retention Time	Peak height	Area	Area Percent
	3.120	737009.563	9326274.000	96.8973
	3.988	27344.520	298628.000	3.1027
Totals		764354.082	9624902.000	100.0000

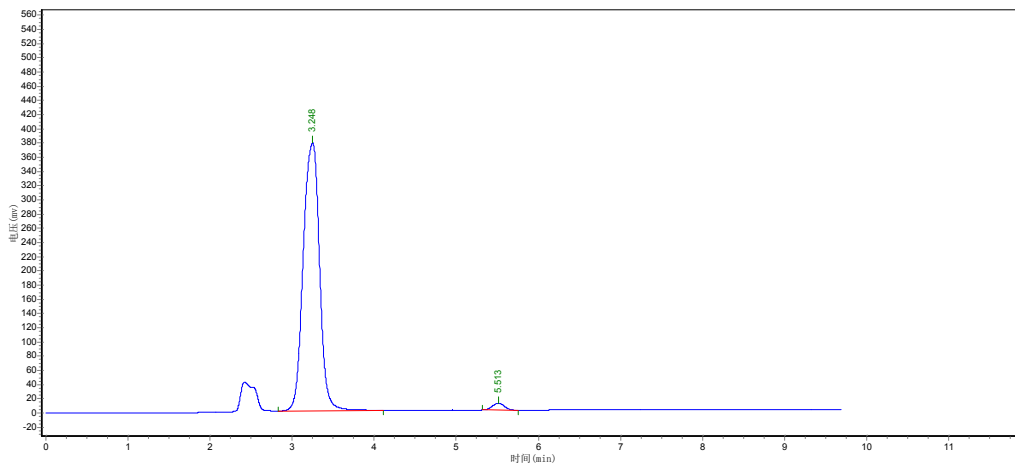
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	1.838	23930.510	120391.617	0.6881
	3.262	8299.011	202101.453	1.1550
	3.830	6317.469	190425.531	1.0883
	4.337	4104.927	65385.520	0.3737
	5.618	543700.625	16919074.000	96.6949
Totals		586352.542	17497378.121	100.0000

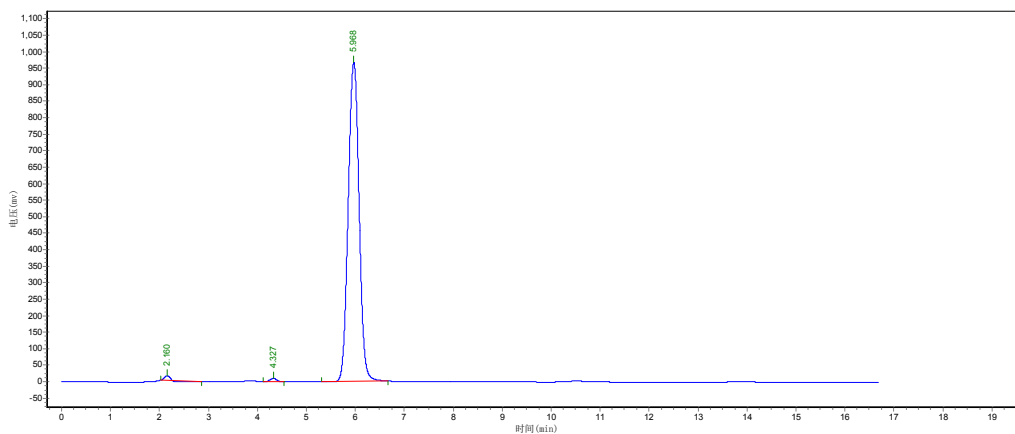


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

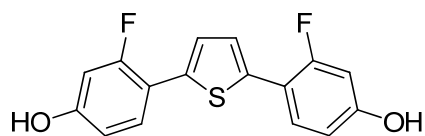


Name	Retention Time	Peak height	Area	Area Percent
	3.248	377613.344	5237528.000	98.1529
	5.513	9491.735	98560.797	1.8471
Totals		387105.079	5336088.797	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

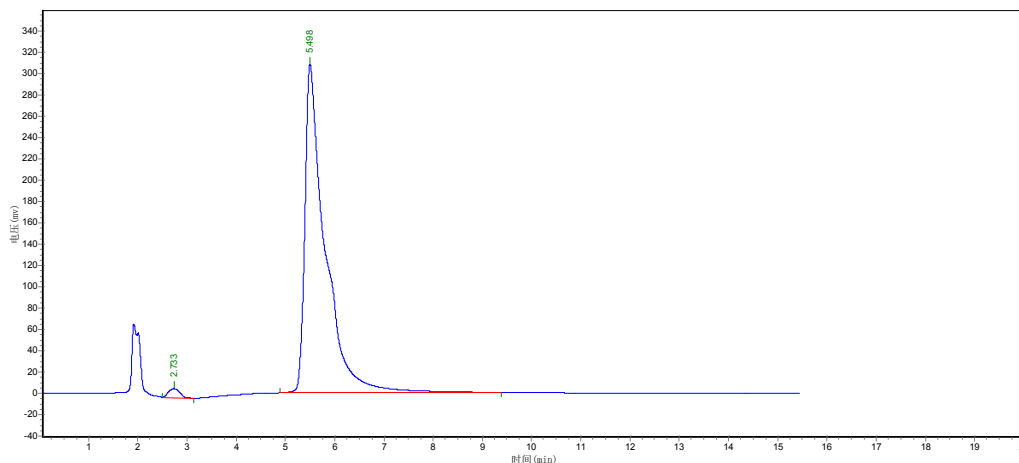


Name	Retention Time	Peak height	Area	Area Percent
	2.160	14440.305	56210.852	0.3730
	4.327	10442.141	107757.813	0.7150
	5.968	968068.750	14907494.000	98.9121
Totals		992951.196	15071462.665	100.0000



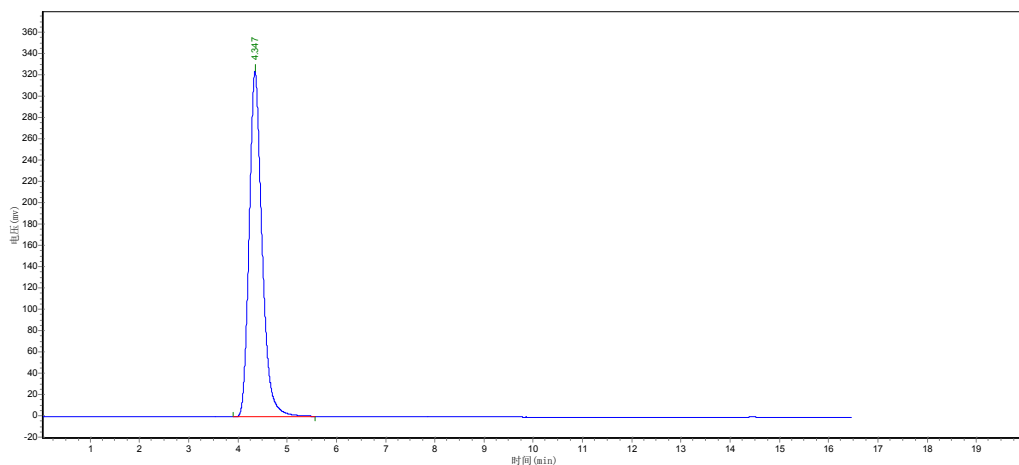
**2e**

Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)



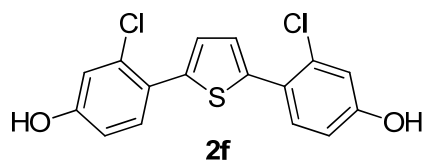
Name	Retention Time	Peak height	Area	Area Percent
	2.733	8464.650	132414.594	1.4876
	5.498	308393.063	8768765.000	98.5124
Totals		316857.713	8901179.594	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

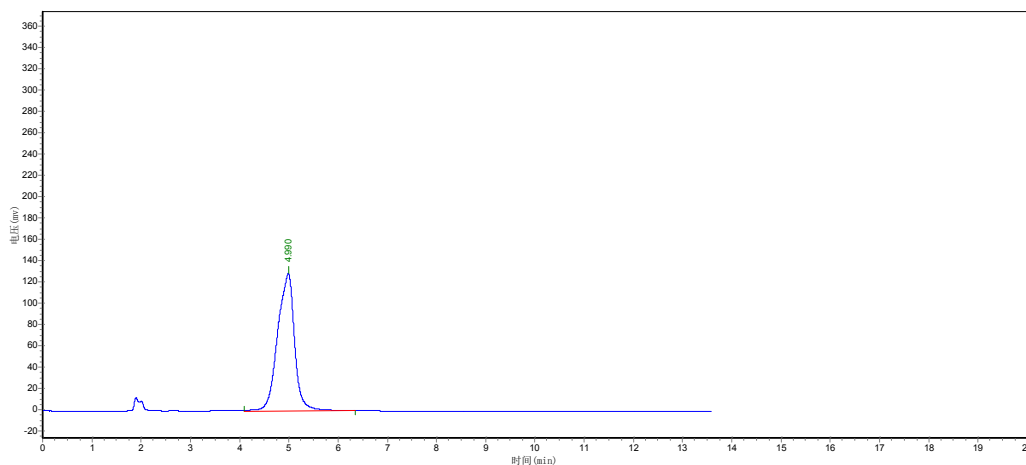


Name	Retention Time	Peak height	Area	Area Percent
	4.347	323917.563	5874576.000	100.0000
Totals		323917.563	5874576.000	100.0000



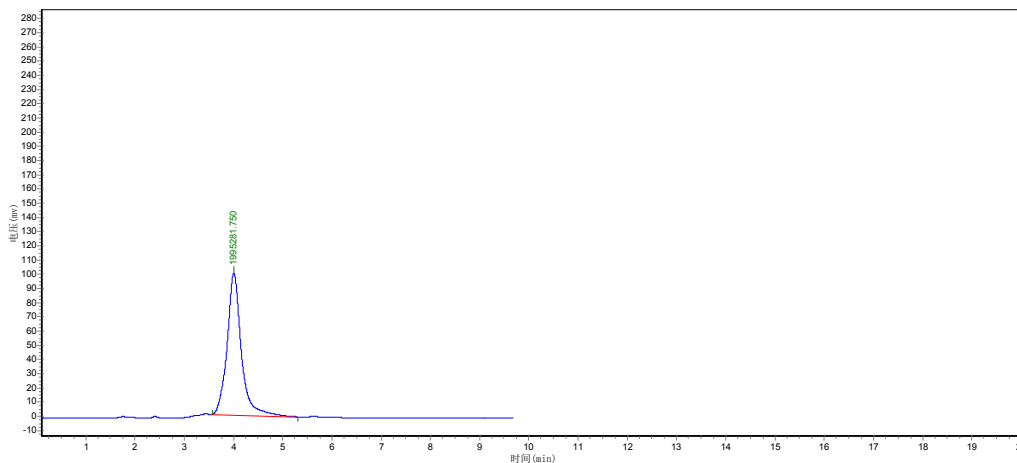


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

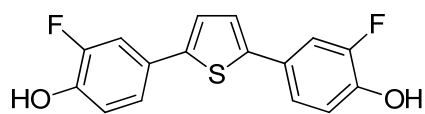


Name	Retention Time	Peak height	Area	Area Percent
Totals	4.990	128946.484	3090375.750	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

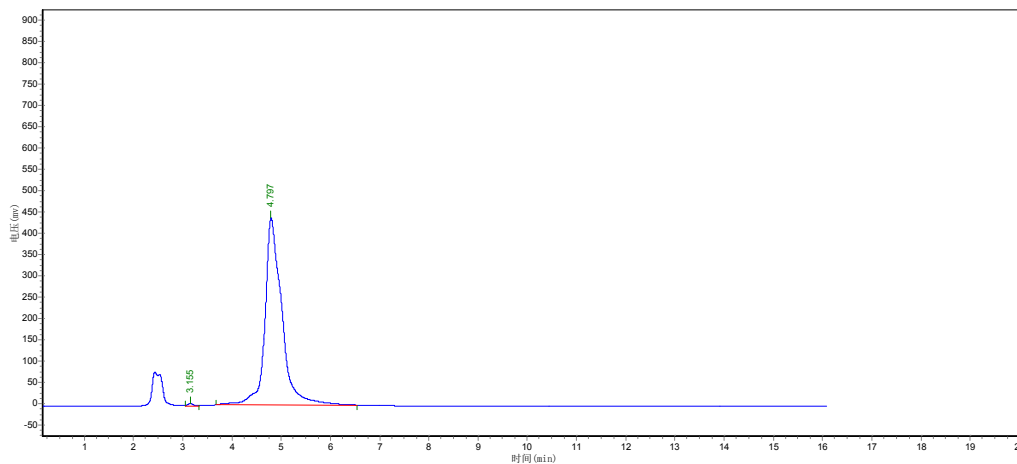


Name	Retention Time	Peak height	Area	Area Percent
Totals	4.007	99777.359	1995281.750	100.0000



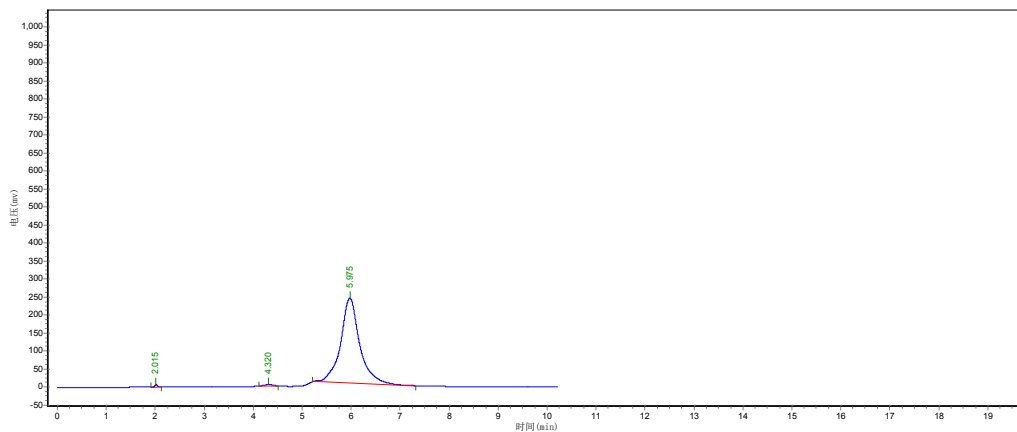
**2g**

Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

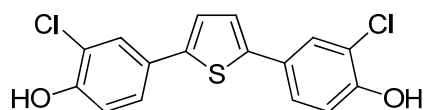


Name	Retention Time	Peak height	Area	Area Percent
	3.155	6850.424	69360.430	0.6598
	4.797	438312.781	10443035.000	99.3402
Totals		445163.205	10512395.430	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

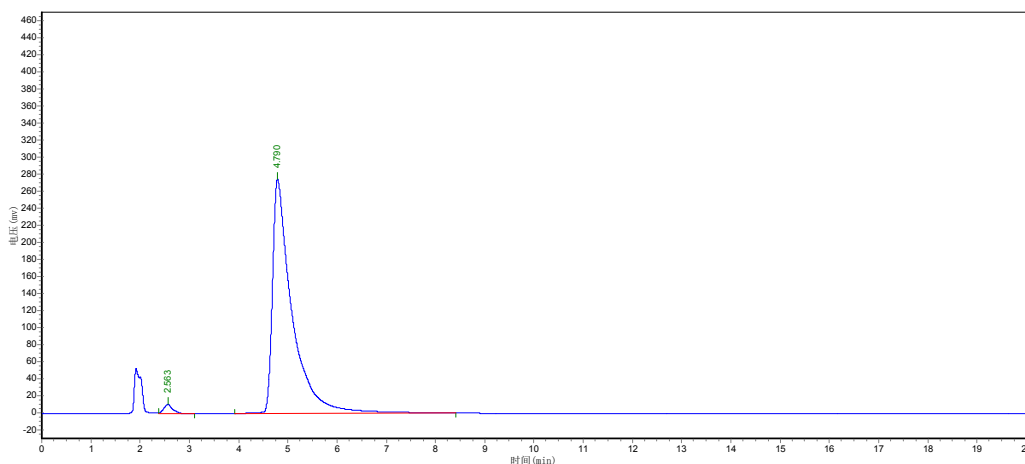


Name	Retention Time	Peak height	Area	Area Percent
	2.015	6950.916	33364.789	0.4458
	4.320	7420.315	198830.172	2.6566
	5.975	243385.359	7252122.500	96.8976
Totals		257756.590	7484317.461	100.0000



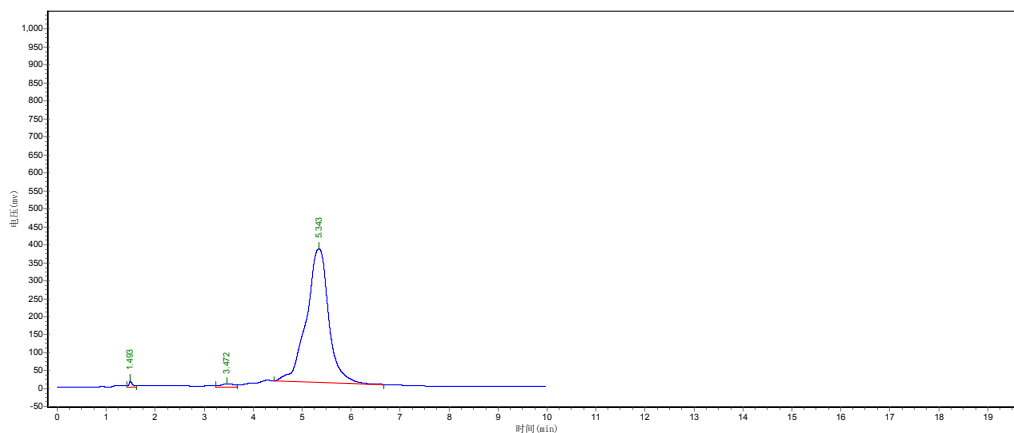
**2h**

Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

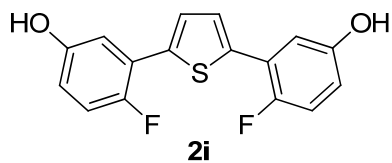


Name	Retention Time	Peak height	Area	Area Percent
	2.563	10979.554	140793.328	1.8166
	4.790	275276.063	7609512.000	98.1834
Totals		286255.617	7750305.328	100.0000

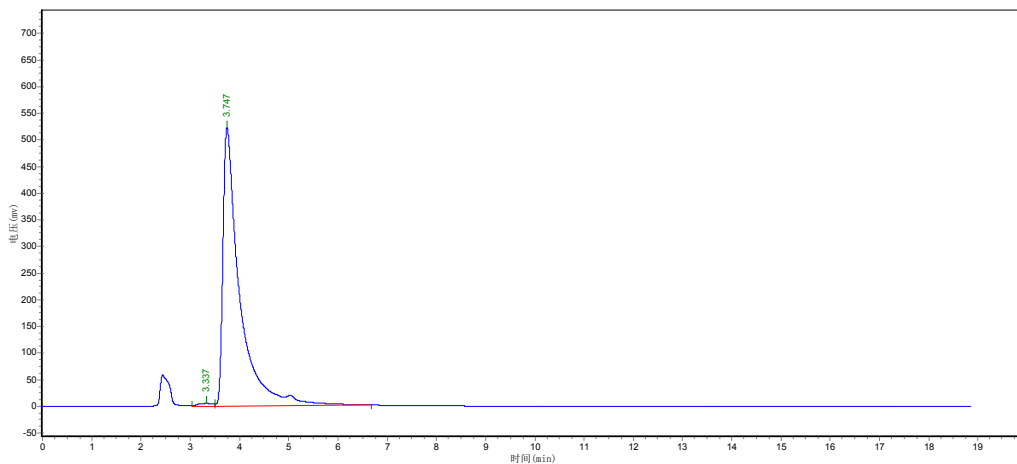
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	1.493	16517.520	88919.898	0.7582
	3.472	8838.831	173803.422	1.4821
	5.343	369749.219	11464286.000	97.7597
Totals		395105.570	11727009.320	100.0000

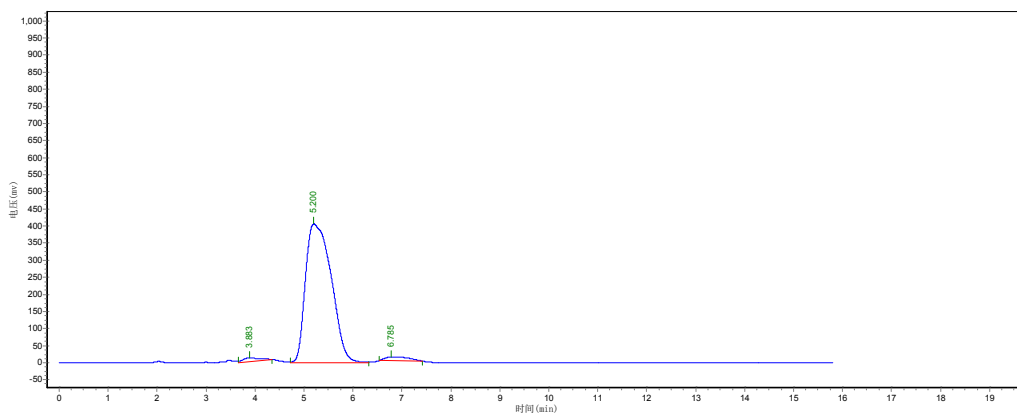


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

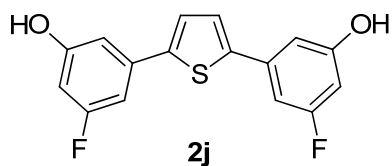


Name	Retention Time	Peak height	Area	Area Percent
	3.337	5998.810	124323.547	0.9929
	3.747	523721.500	12396871.000	99.0071
<b>Totals</b>		529720.310	12521194.547	100.0000

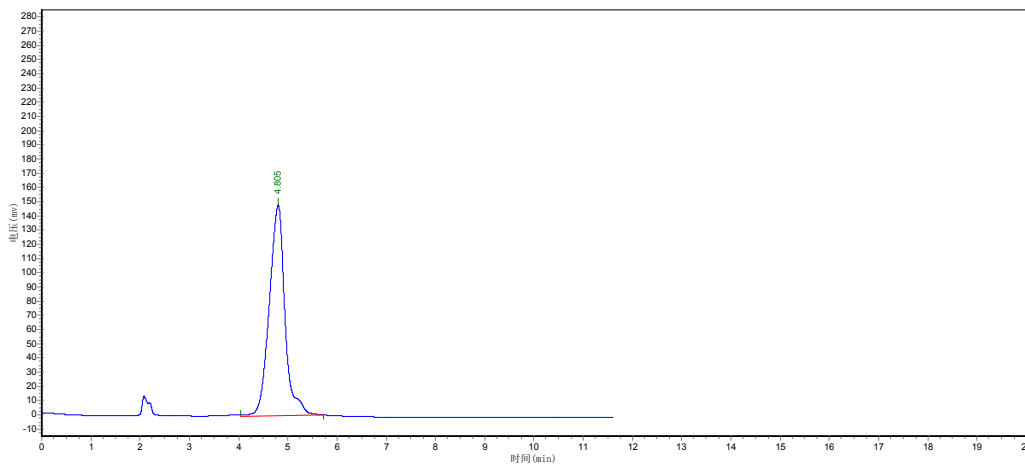
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	3.883	10809.248	260631.328	1.6754
	5.200	406582.250	14915171.000	95.8788
	6.785	10875.766	380475.875	2.4458
<b>Totals</b>		428267.264	15556278.203	100.0000

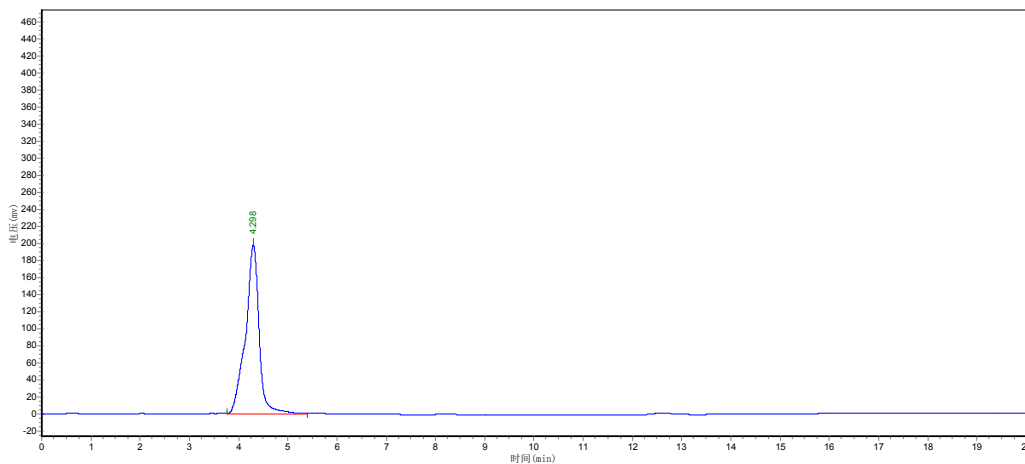


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

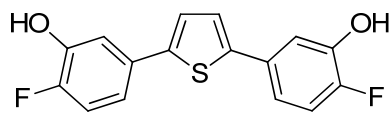


Name	Retention Time	Peak height	Area	Area Percent
	4.805	148272.266	3288432.500	100.0000
Totals		148272.266	3288432.500	100.0000

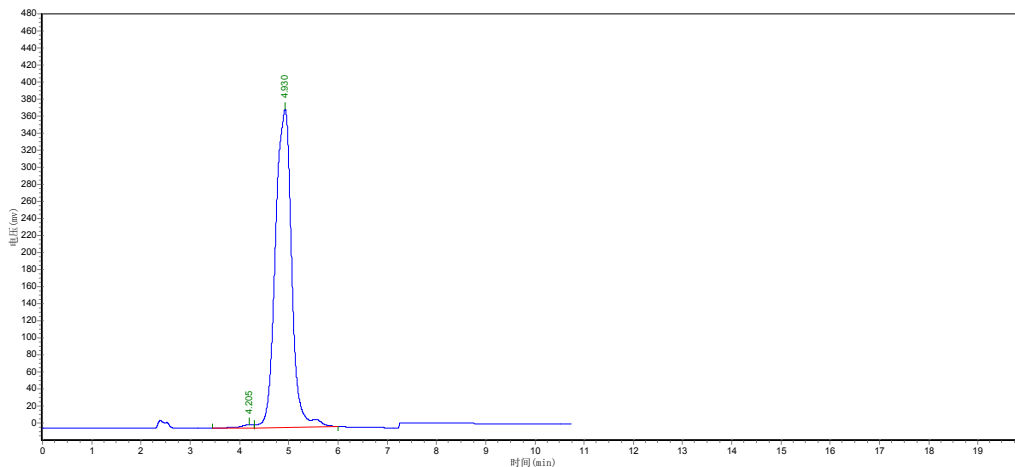
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	4.298	198462.484	3848356.250	100.0000
Totals		198462.484	3848356.250	100.0000

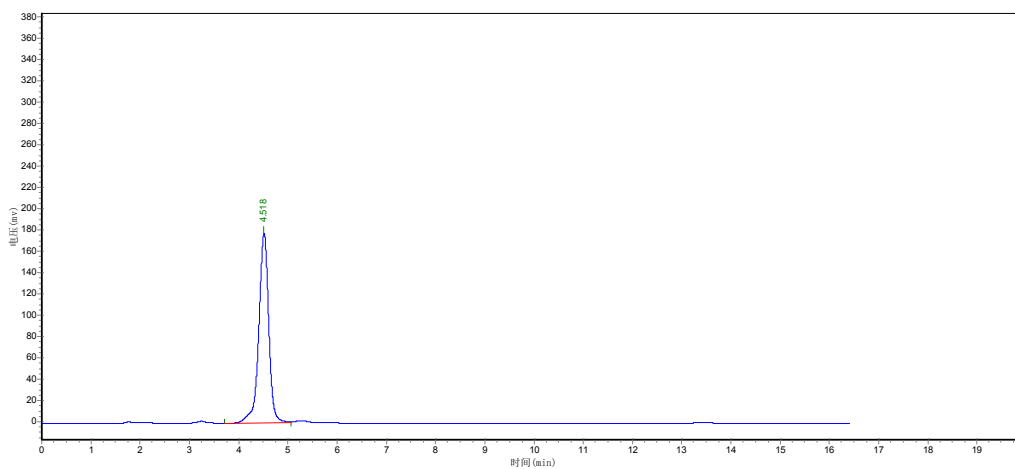


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

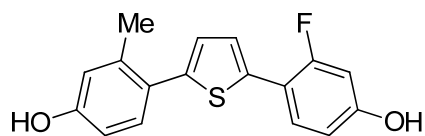


Name	Retention Time	Peak height	Area	Area Percent
	4.205	4309.459	87439.852	1.0116
	4.298	373332.000	8556315.000	98.9884
Totals		377641.459	8643754.852	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

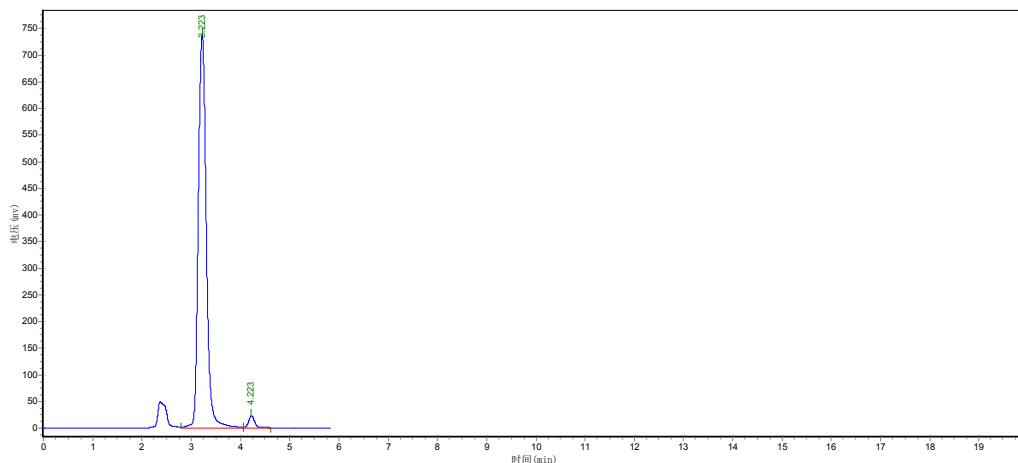


Name	Retention Time	Peak height	Area	Area Percent
	4.518	178184.375	2516533.750	100.0000
Totals		178184.375	2516533.750	100.0000



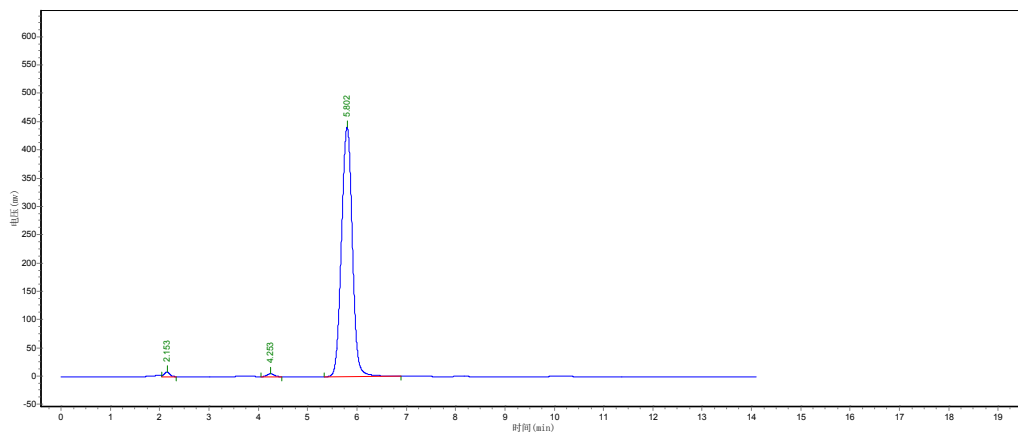
**2I**

Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

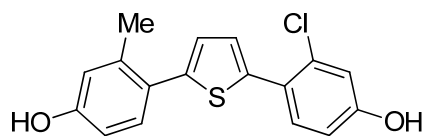


Name	Retention Time	Peak height	Area	Area Percent
	3.223	738001.750	8327328.000	97.7352
	4.223	22779.209	192968.703	2.2648
Totals		760780.959	8520296.703	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

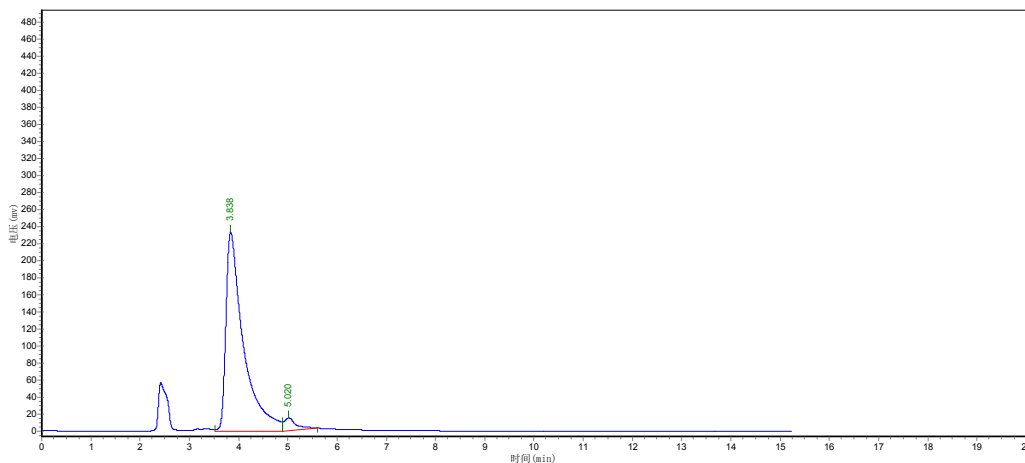


Name	Retention Time	Peak height	Area	Area Percent
	2.153	8825.018	68943.492	1.0147
	4.253	5085.852	48515.098	0.7140
	5.802	440713.219	6677234.000	98.2713
Totals		454624.089	6794692.590	100.0000



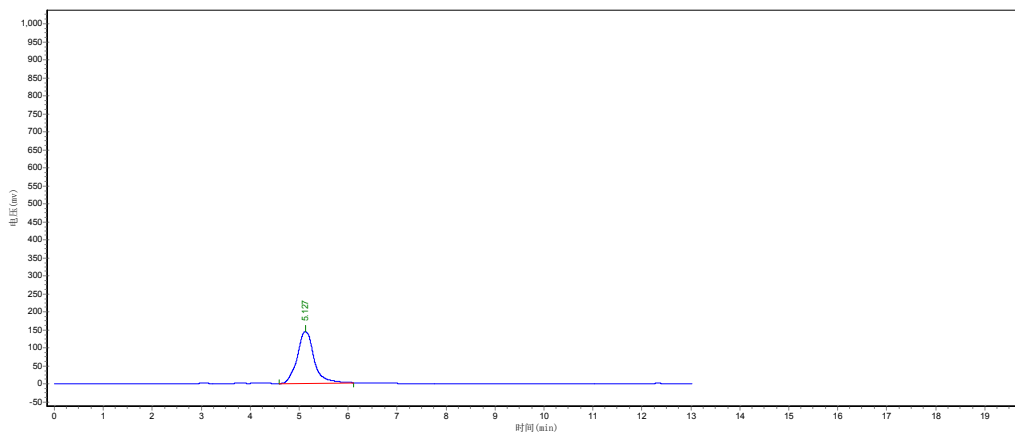
**2m**

Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)



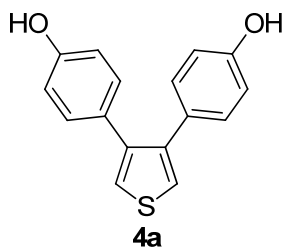
Name	Retention Time	Peak height	Area	Area Percent
	3.838	233712.094	5787899.000	95.6289
	5.020	15164.579	264558.656	4.3711
Totals		248876.673	6052457.656	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

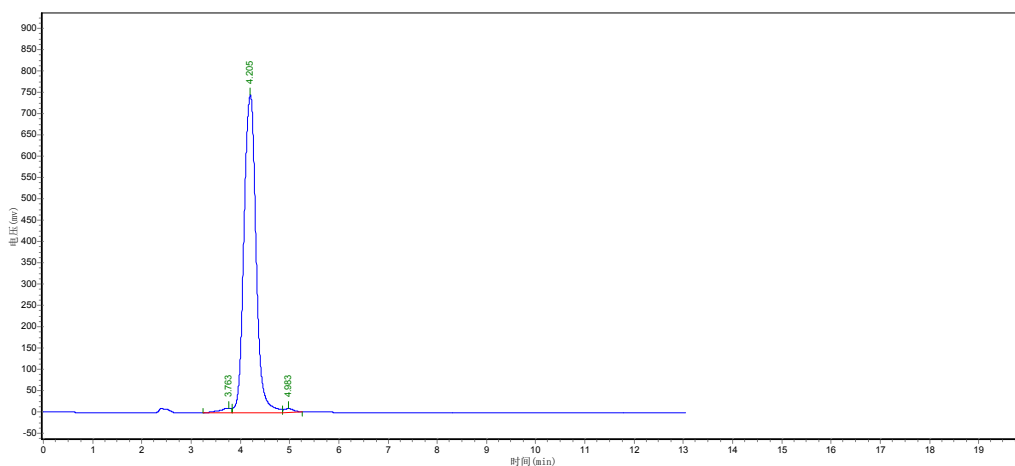


Name	Retention Time	Peak height	Area	Area Percent
	5.127	143277.453	3413929.000	100.0000
Totals		143277.453	3413929.000	100.0000



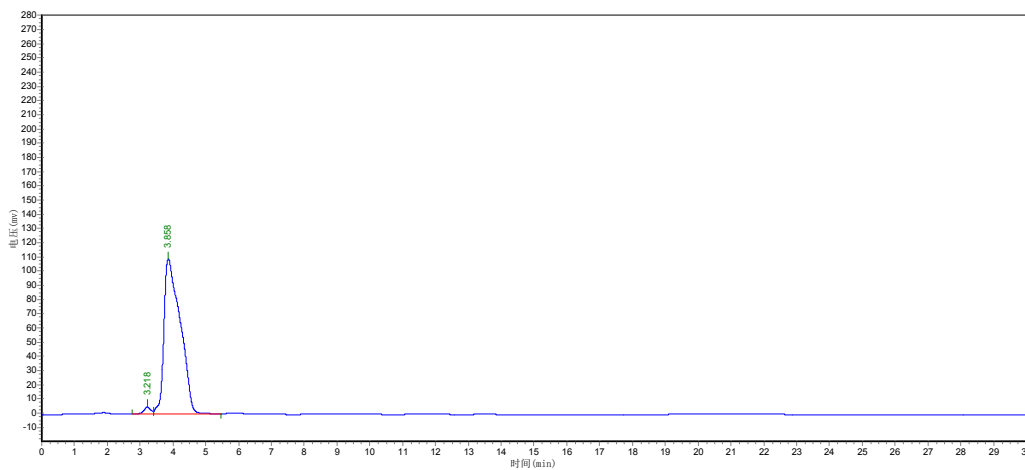


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

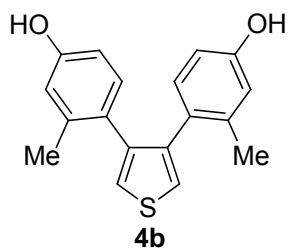


Name	Retention Time	Peak height	Area	Area Percent
	3.435	687079.875	10677790.000	95.6272
	4.055	43494.699	488263.563	4.3727
<b>Totals</b>		<b>730574.574</b>	<b>11166053.563</b>	<b>100.0000</b>

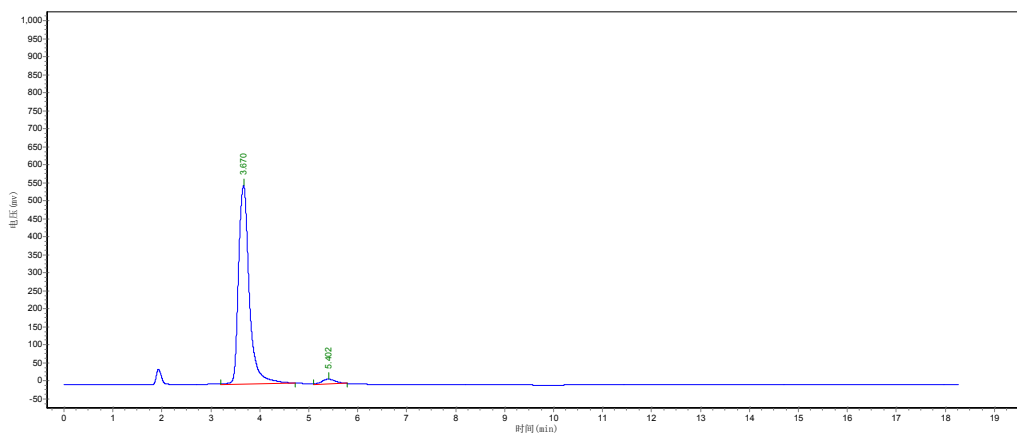
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	3.218	5168.713	75431.430	1.9488
	3.858	109204.406	3795189.000	98.0512
<b>Totals</b>		<b>114373.119</b>	<b>3870620.430</b>	<b>100.0000</b>

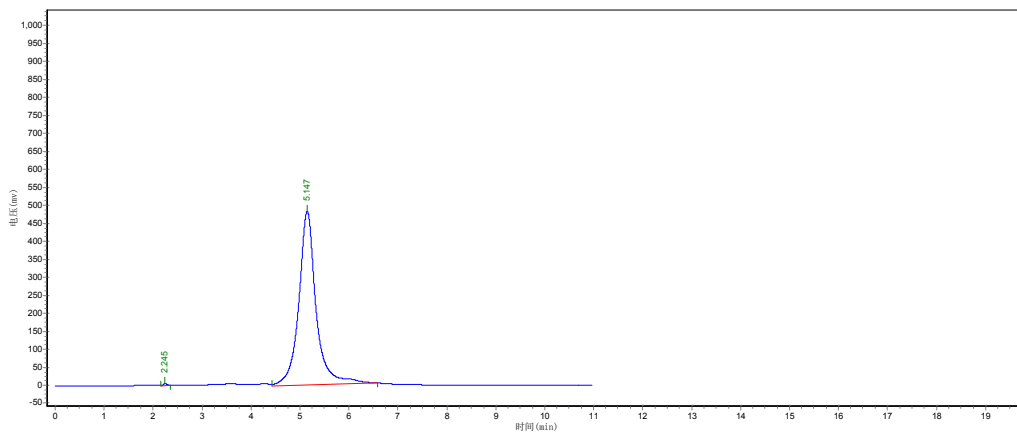


Normal Phase(Method 40:60 EtOAc:Hex, Flow rate 1.0 mL/min)

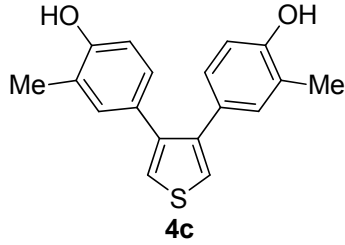


Name	Retention Time	Peak height	Area	Area Percent
	3.670	552535.813	8447569.000	96.6890
	5.402	14168.037	289280.406	3.3110
<b>Totals</b>		<b>566703.850</b>	<b>8736849.406</b>	<b>100.0000</b>

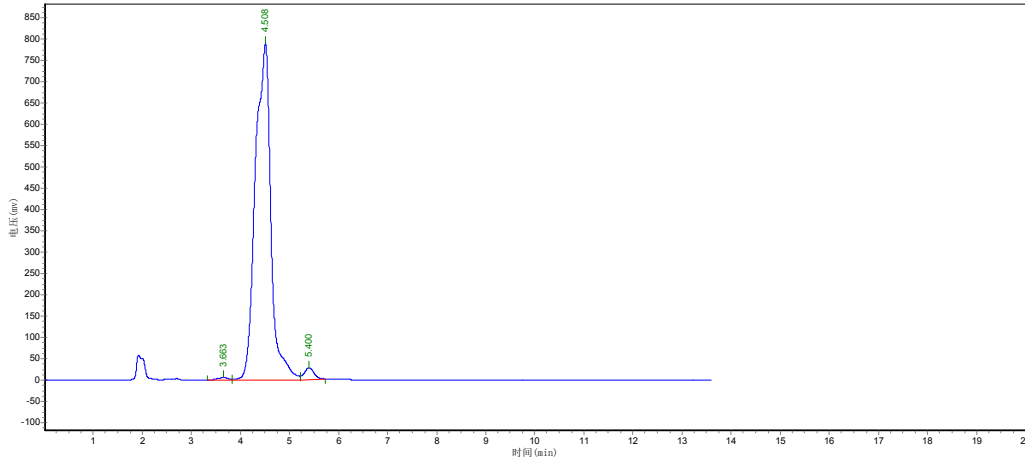
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	2.245	6308.801	31386.576	0.2655
	5.147	481230.594	11790560.000	99.7345
<b>Totals</b>		<b>487539.395</b>	<b>11821946.576</b>	<b>100.0000</b>

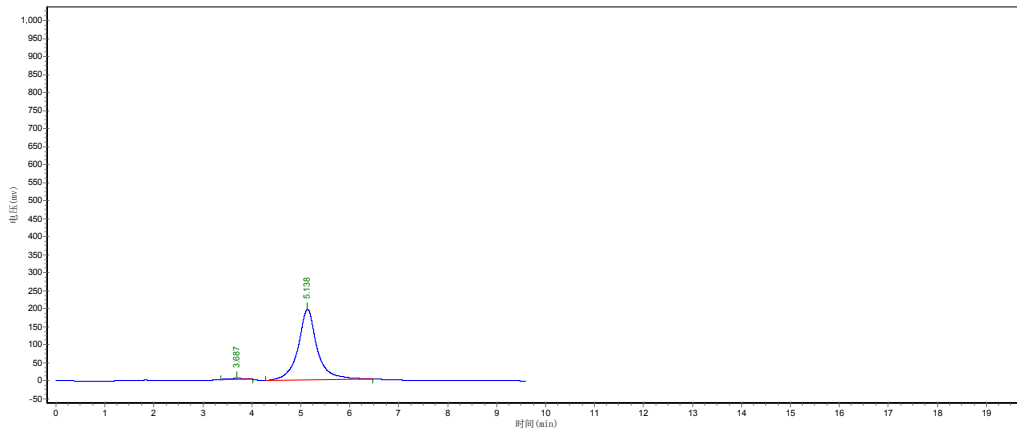


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

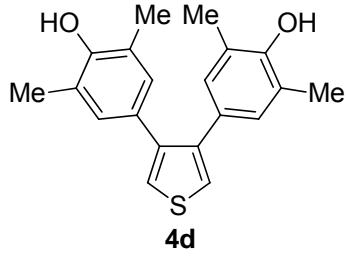


Name	Retention Time	Peak height	Area	Area Percent
	3.663	5594.049	86859.820	0.4855
	4.508	789576.875	17412258.000	97.3305
	5.400	27655.203	390712.188	2.1840
<b>Totals</b>		<b>822826.127</b>	<b>17889830.008</b>	<b>100.0000</b>

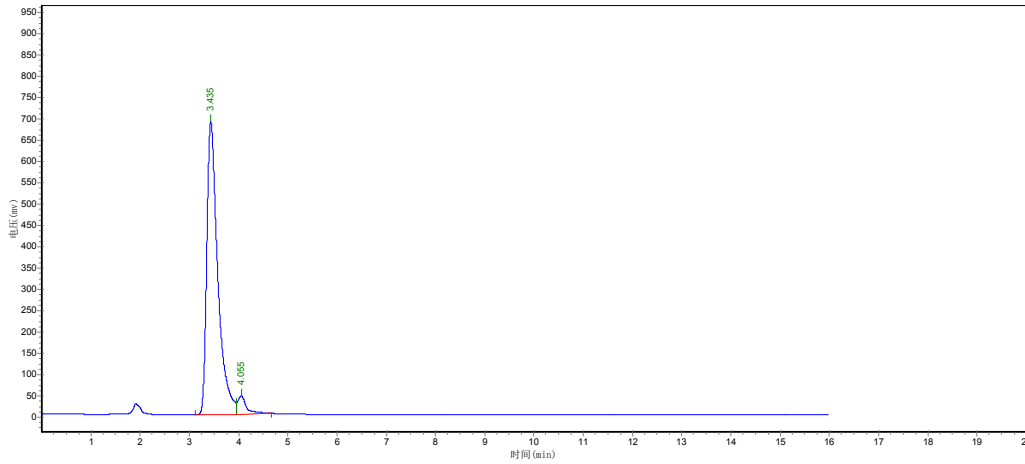
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	3.687	1656.342	32066.596	0.5687
	5.138	197740.422	5606437.500	99.4313
<b>Totals</b>		<b>199396.764</b>	<b>5638504.096</b>	<b>100.0000</b>

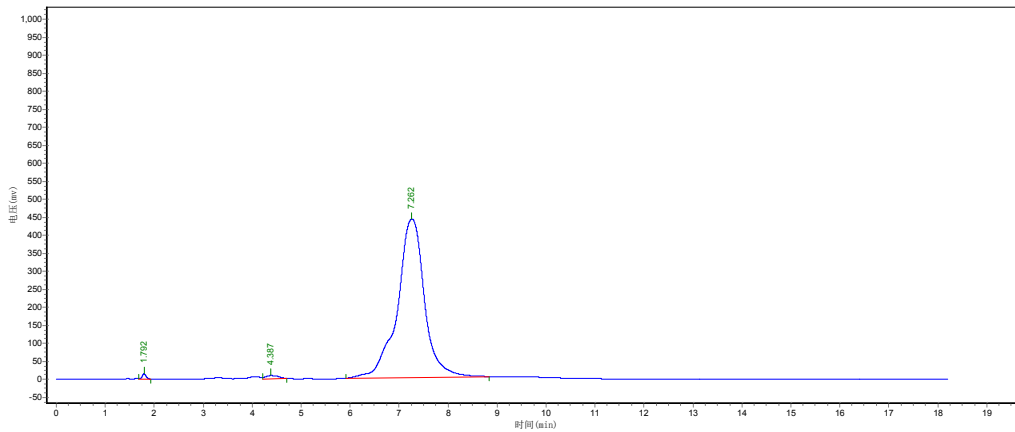


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

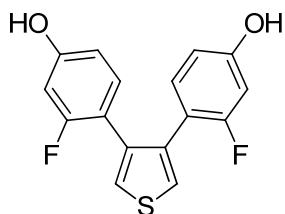


Name	Retention Time	Peak height	Area	Area Percent
	3.435	687079.875	10677790.000	95.0513
	4.055	44192.273	555927.438	4.9487
<b>Totals</b>		<b>731272.948</b>	<b>11233717.438</b>	<b>100.0000</b>

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

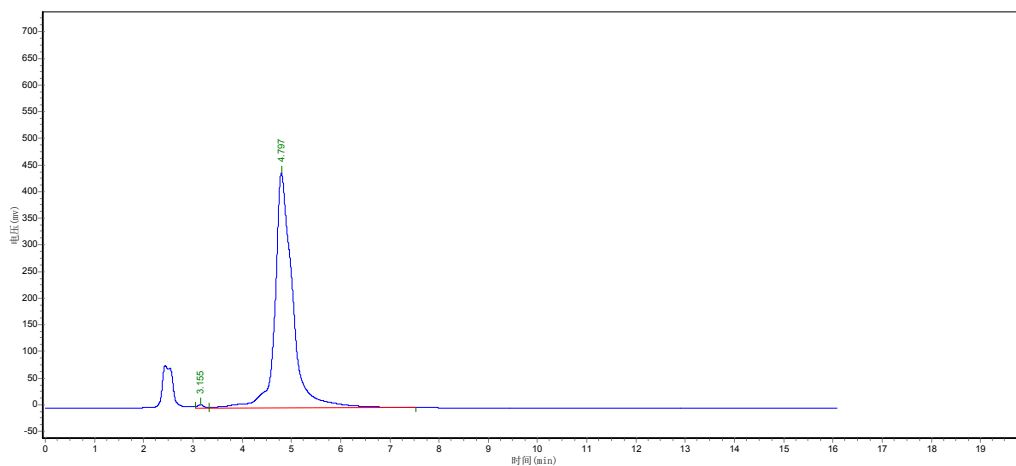


Name	Retention Time	Peak height	Area	Area Percent
	1.792	15864.683	97023.703	0.5452
	4.387	10386.066	233831.047	1.3139
	7.262	443163.031	17466204.000	98.1410
<b>Totals</b>		<b>469413.780</b>	<b>17797058.750</b>	<b>100.0000</b>



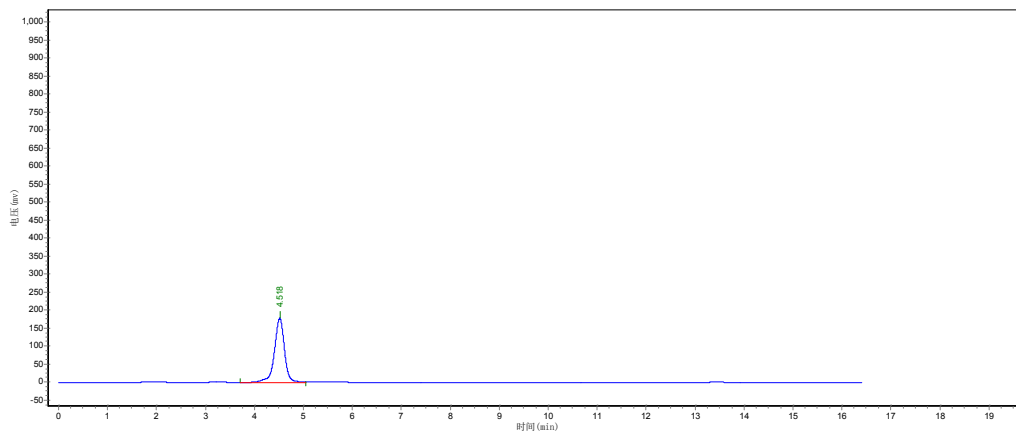
**4e**

Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

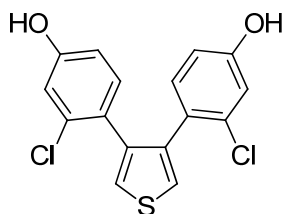


Name	Retention Time	Peak height	Area	Area Percent
	3.155	6850.424	69360.430	0.6213
	4.797	441618.781	11093890.000	99.3787
Totals		448469.205	11163250.430	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

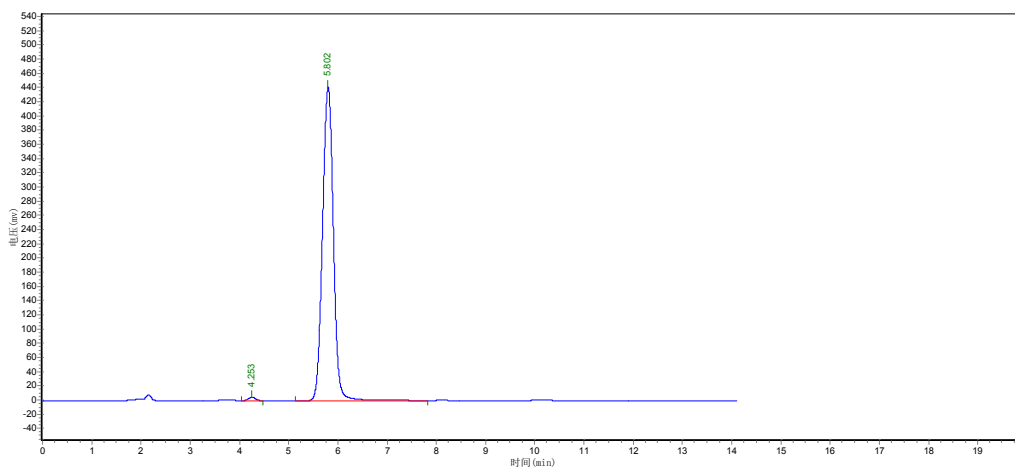


Name	Retention Time	Peak height	Area	Area Percent
	4.518	178184.375	2516533.750	100.0000
Totals		178184.375	2516533.750	100.0000



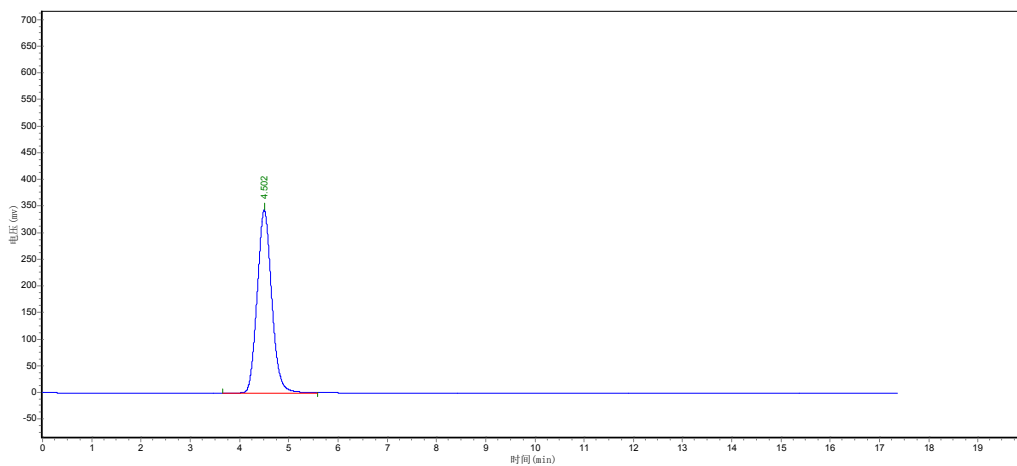
**4f**

Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

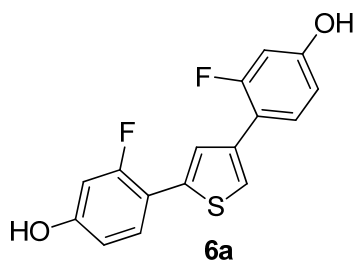


Name	Retention Time	Peak height	Area	Area Percent
	4.253	5085.852	48515.098	0.7075
Totals	5.802	441520.719	6808895.500	99.2925
		446606.570	6857410.598	100.0000

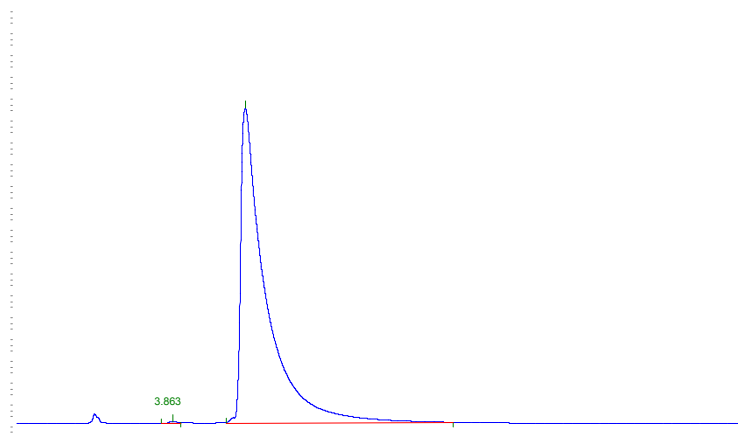
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	4.502	343937.344	7073932.000	100.0000
Totals		343937.344	7073932.000	100.0000

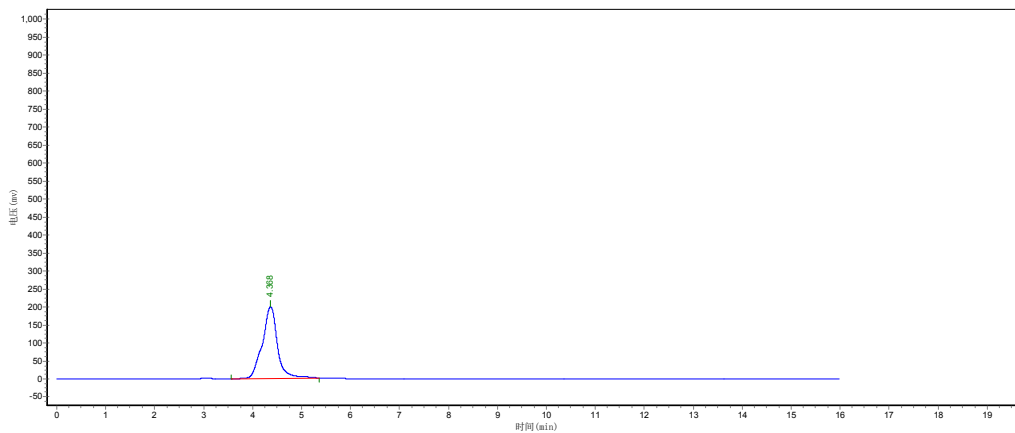


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

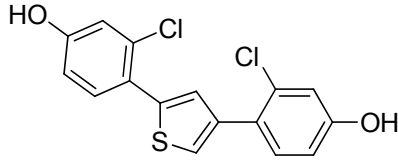


Name	Retention Time	Peak height	Area	Area Percent
	3.863	5641.618	84202.594	0.2688
	5.653	721665.063	31244736.000	99.7312
Totals		727306.681	31328938.594	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

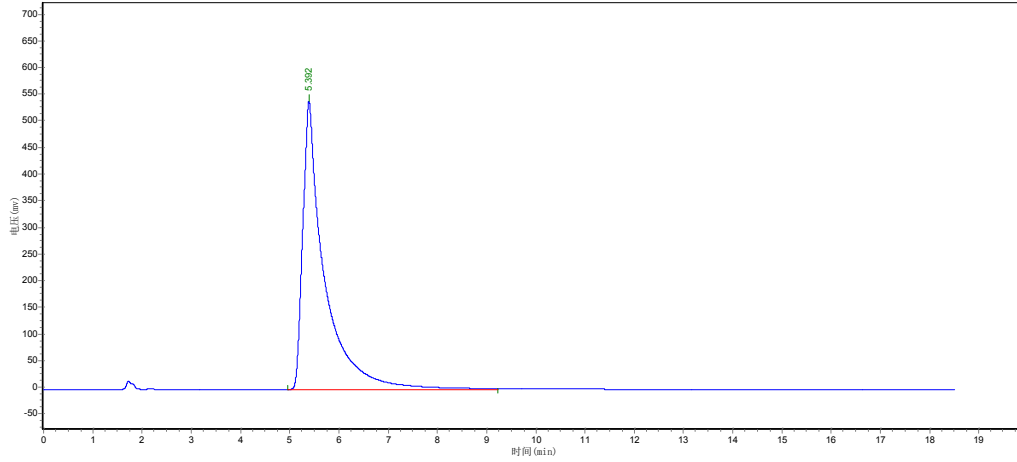


Name	Retention Time	Peak height	Area	Area Percent
	4.368	197315.859	4060958.750	100.0000
Totals		197315.859	4060958.750	100.0000



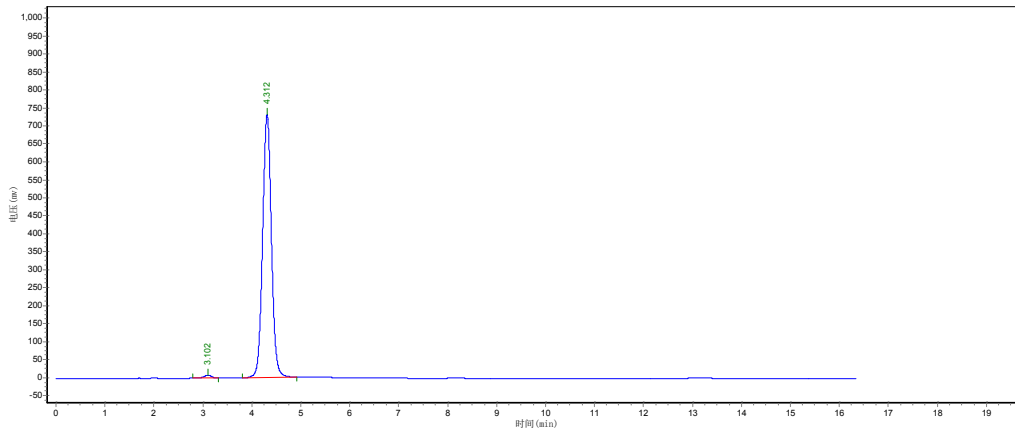
**6b**

Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)



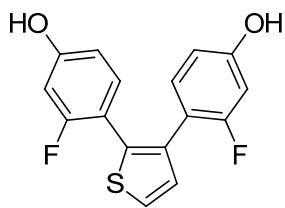
Name	Retention Time	Peak height	Area	Area Percent
Totals	5.392	541999.125	16820268.000	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



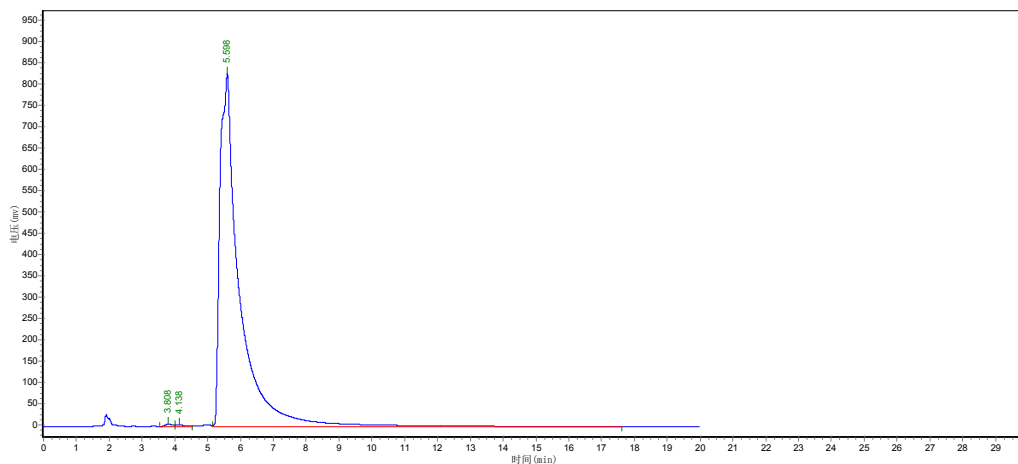
Name	Retention Time	Peak height	Area	Area Percent
	3.102	8499.513	89030.250	0.9482
	4.312	731945.188	9300281.000	99.0518
Totals		740444.701	9389311.25	100.0000





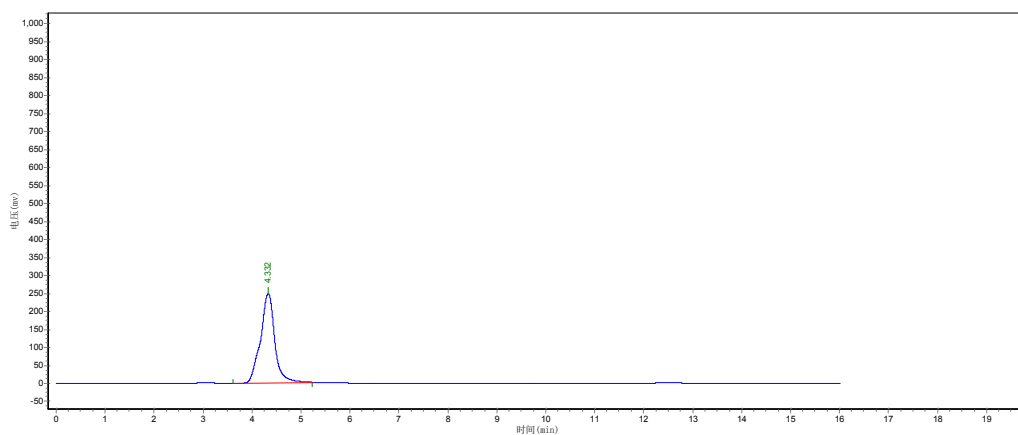
**8a**

Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

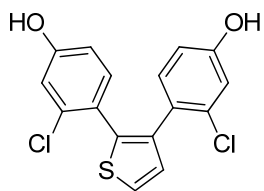


Name	Retention Time	Peak height	Area	Area Percent
	3.808	6262.274	93087.719	0.2710
	4.138	3517.807	68057.898	0.1982
	5.598	827602.313	34184120.000	99.5308
Totals		837382.394	34345265.617	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

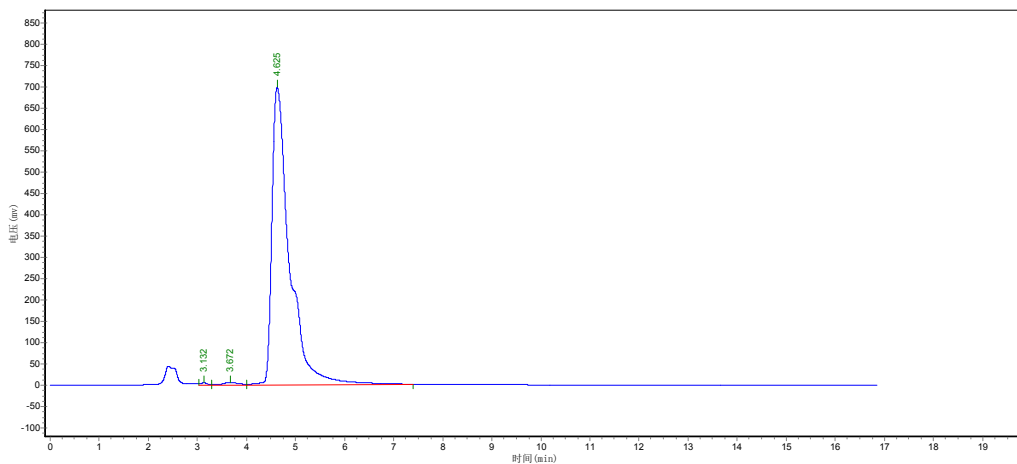


Name	Retention Time	Peak height	Area	Area Percent
	4.332	249522.125	5203304.500	100.0000
Totals		249522.125	5203304.500	100.0000



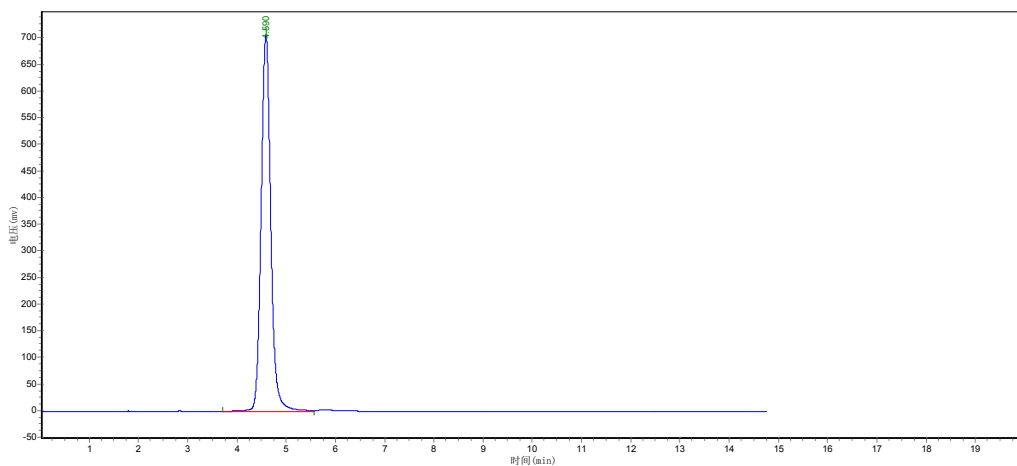
**8b**

Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

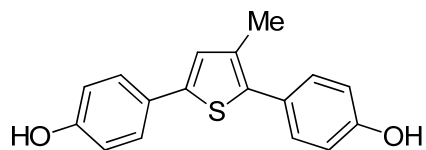


Name	Retention Time	Peak height	Area	Area Percent
	3.132	6010.696	60064.996	0.3418
	3.672	6408.811	172141.234	0.9796
	4.625	698588.000	17340244.000	98.6786
Totals		711007.507	17572450.230	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

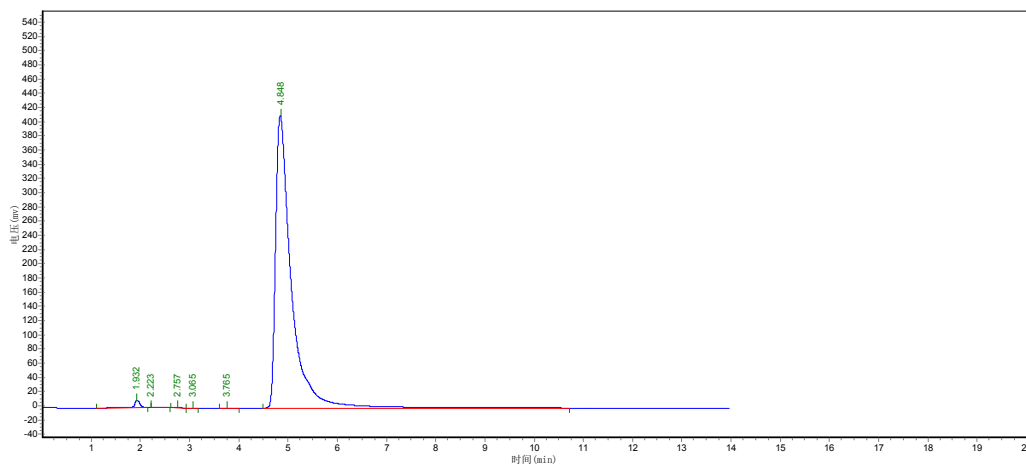


Name	Retention Time	Peak height	Area	Area Percent
	4.590	707387.438	9649499.000	100.0000
Totals		707387.438	9649499.000	100.0000



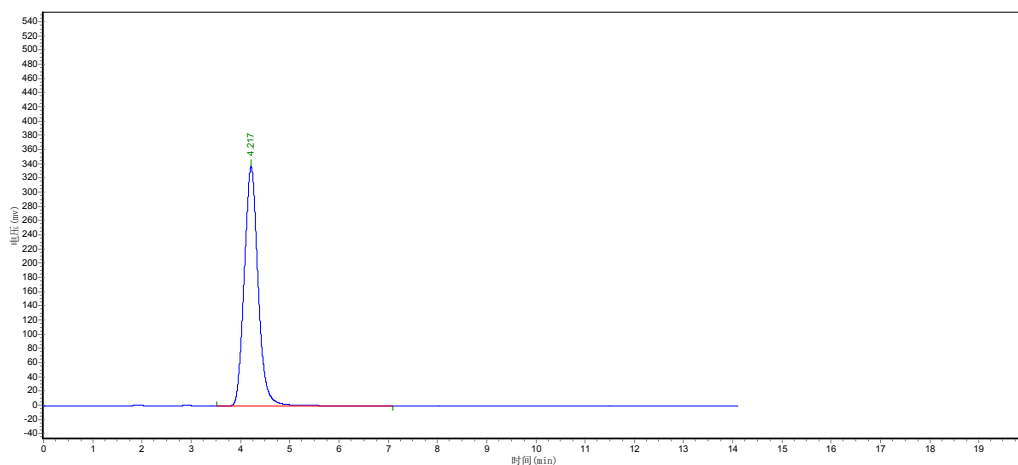
**10a**

Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

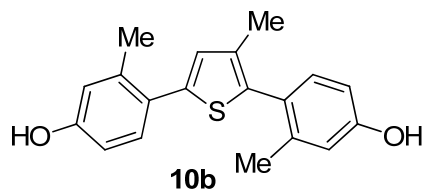


Name	Retention Time	Peak height	Area	Area Percent
Totals	4.848	411299.719	9102504.000	100.0000
Totals		411299.719	9102504.000	100.0000

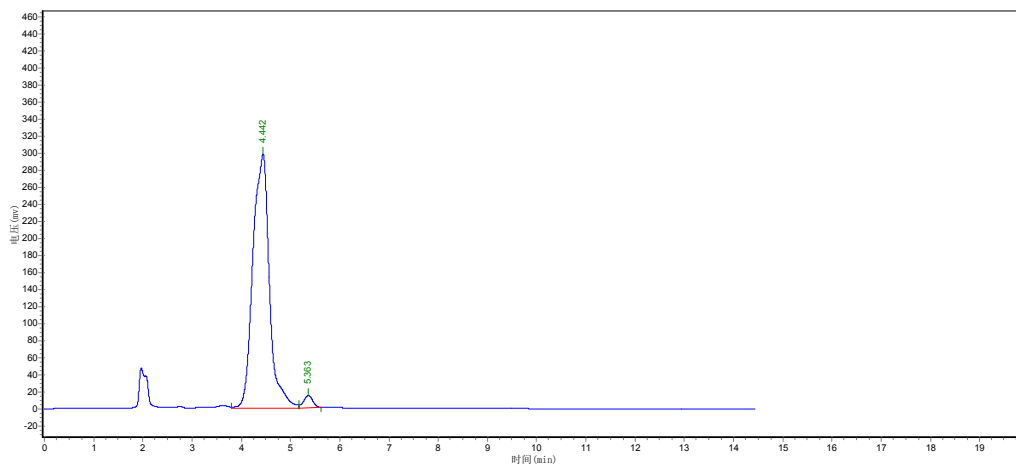
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
Totals	4.217	336551.594	6596959.000	100.0000
Totals		336551.594	6596959.000	100.0000

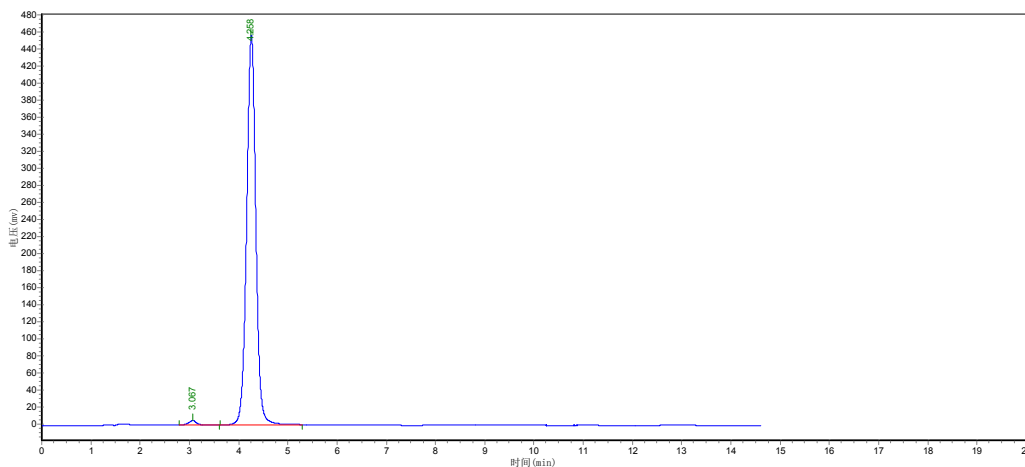


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

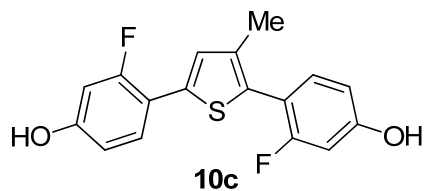


Name	Retention Time	Peak height	Area	Area Percent
	4.442	297818.031	6931385.500	97.4312
	5.363	14160.913	182745.031	2.5688
Totals		311978.944	7114130.531	100.0000

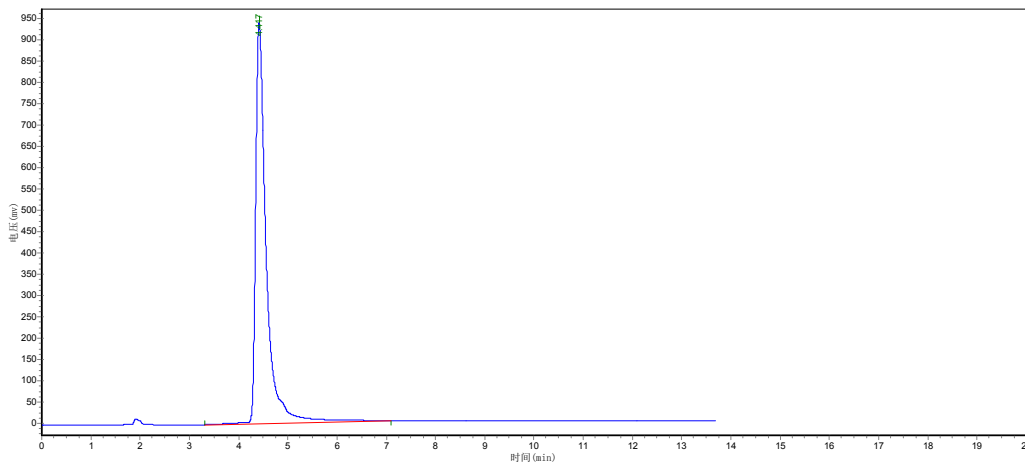
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	3.067	5459.500	62780.805	1.0422
	4.258	457213.844	5960887.000	98.9578
Totals		462673.344	6023667.803	100.0000

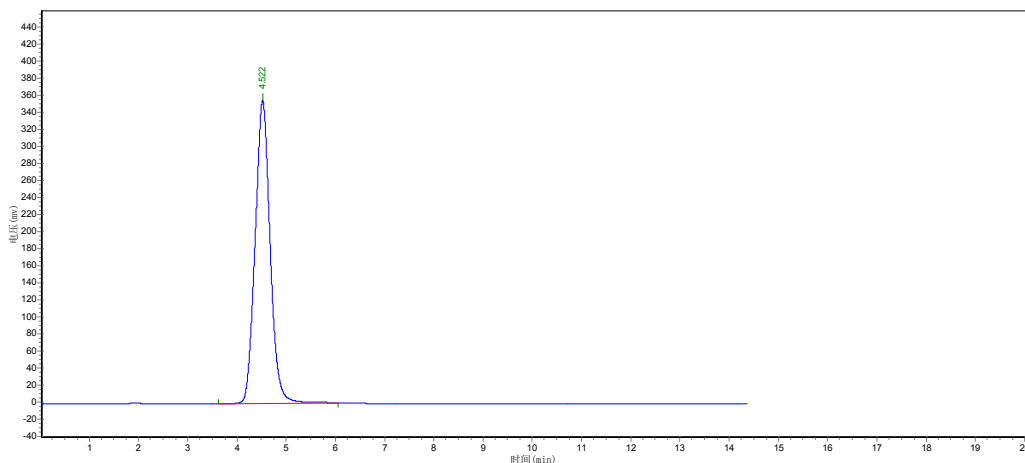


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

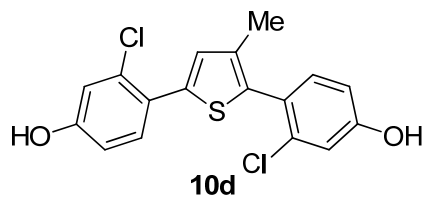


Name	Retention Time	Peak height	Area	Area Percent
	4.417	940445.000	14073680.000	100.0000
Totals		940445.000	14073680.000	100.0000

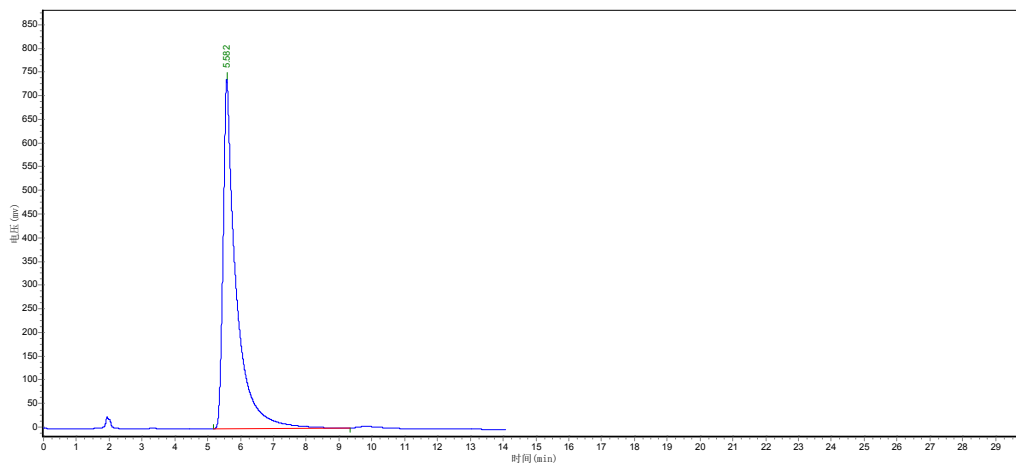
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	4.522	355866.875	7531634.000	100.0000
Totals		355866.875	7531634.000	100.0000

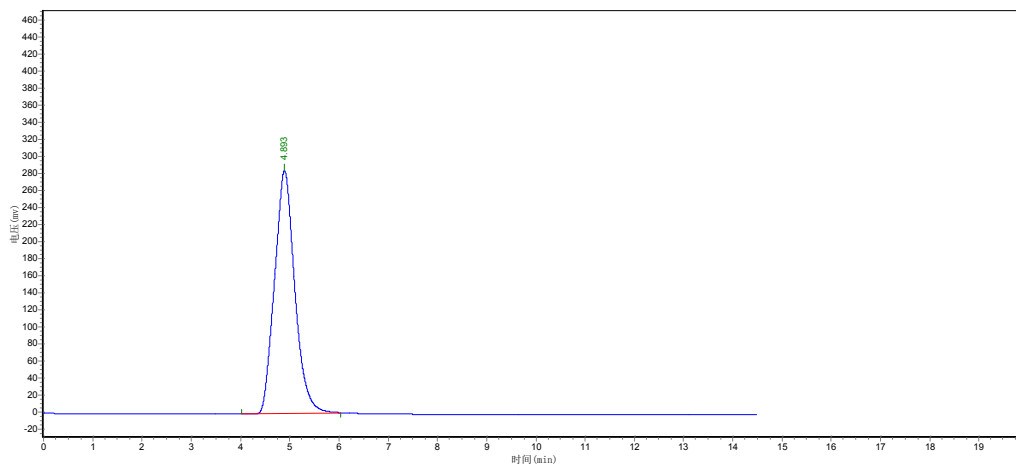


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

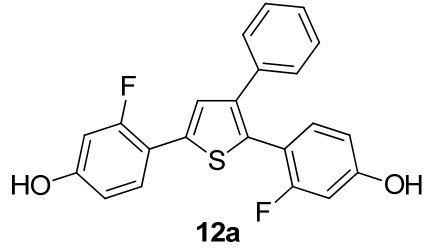


Name	Retention Time	Peak height	Area	Area Percent
Totals	5.582	738943.813	20204630.000	100.0000

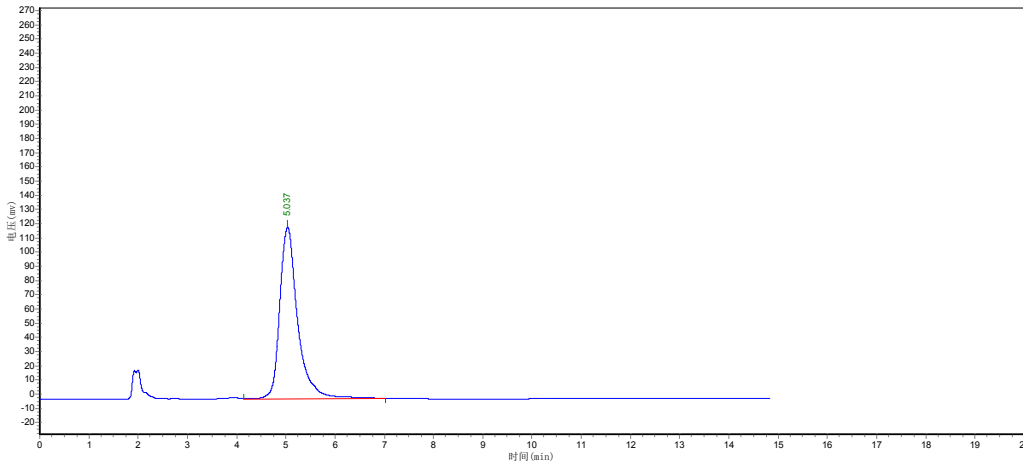
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
Totals	4.893	285099.375	8110905.000	100.0000

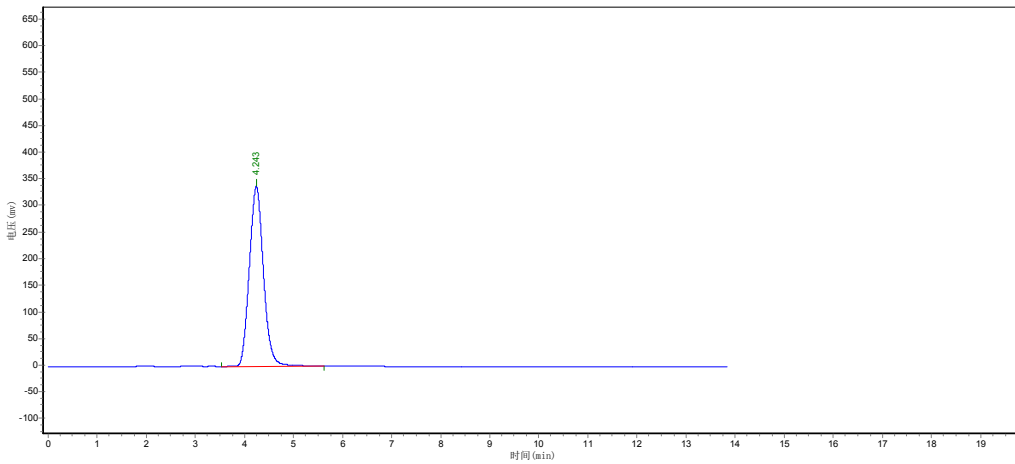


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

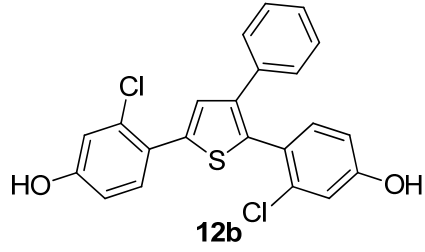


Name	Retention Time	Peak height	Area	Area Percent
	5.037	120751.820	3056137.750	100.0000
Totals		120751.820	3056137.750	100.0000

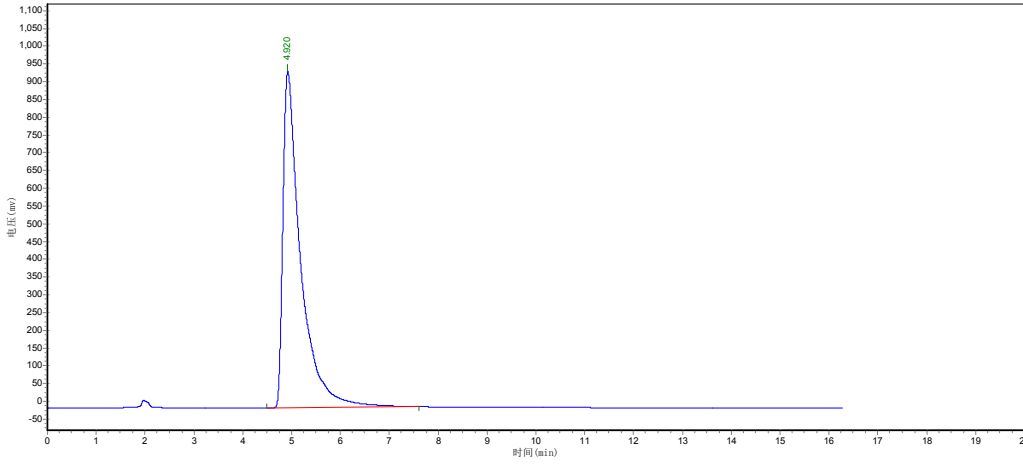
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	4.243	337712.156	6748891.000	100.0000
Totals		337712.156	6748891.000	100.0000

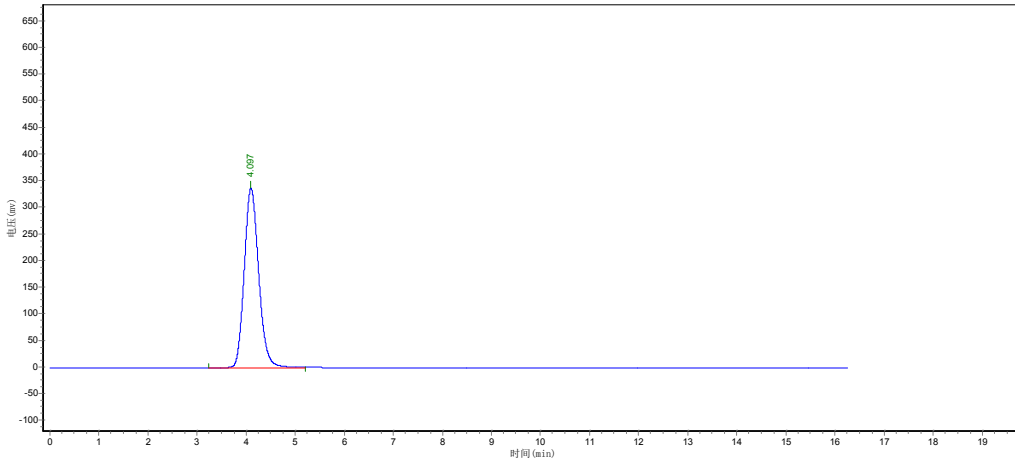


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)



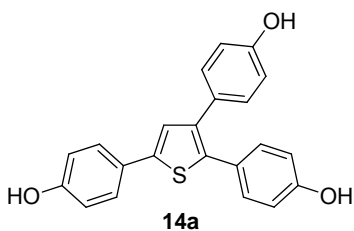
Name	Retention Time	Peak height	Area	Area Percent
	4.920	947742.063	23809662.000	100.0000
Totals		947742.063	23809662.000	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

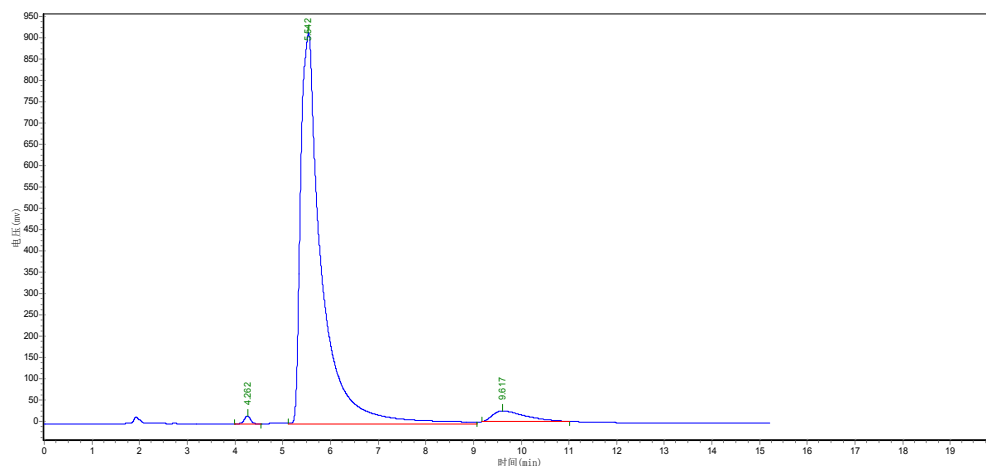


Name	Retention Time	Peak height	Area	Area Percent
	4.097	338044.969	6958047.000	100.0000
Totals		338044.969	6958047.000	100.0000



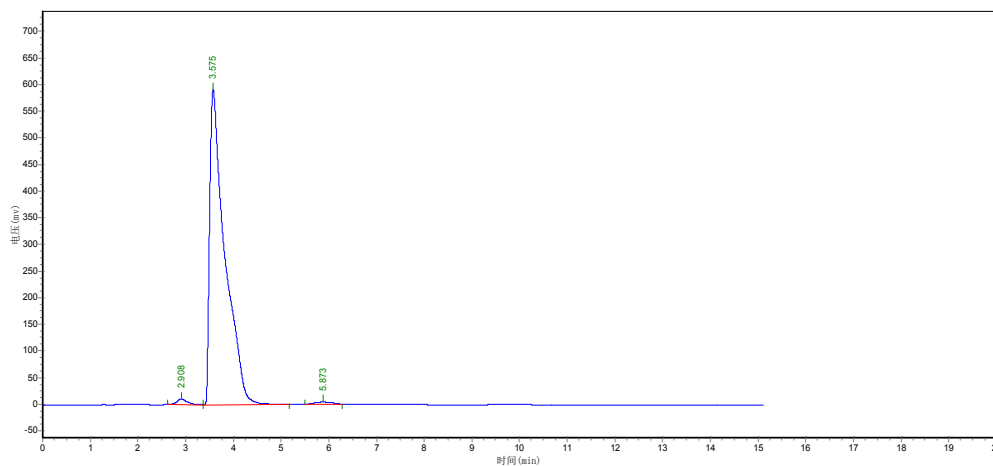


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

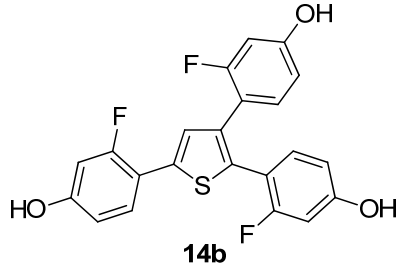


Name	Retention Time	Peak height	Area	Area Percent
	4.262	17894.713	162425.766	0.5575
	5.542	917130.375	27760694.000	95.2782
	9.617	25158.000	1213343.625	4.1643
Totals		960183.088	29136463.391	100.0000

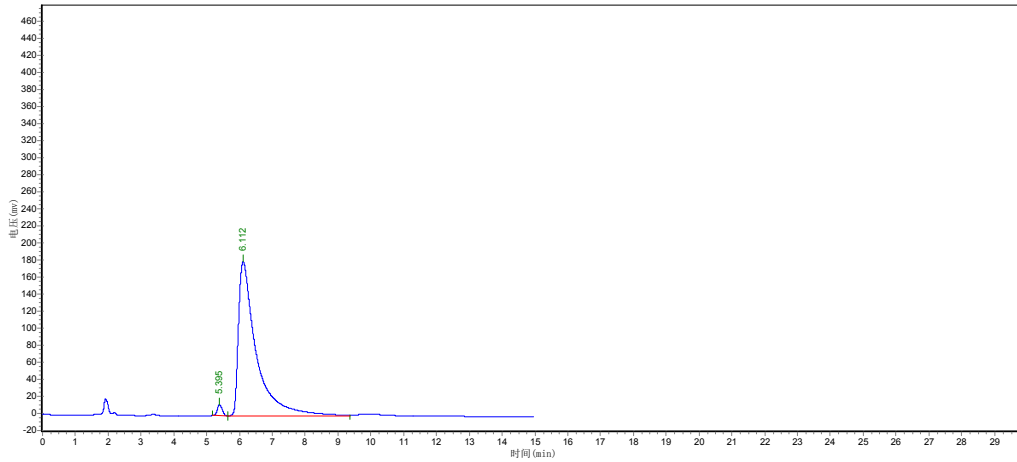
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	2.908	10464.652	160894.031	1.2025
	3.575	591265.563	13116912.000	98.0363
	5.873	3927.362	101843.500	0.7612
Totals		605657.576	13379649.531	100.0000

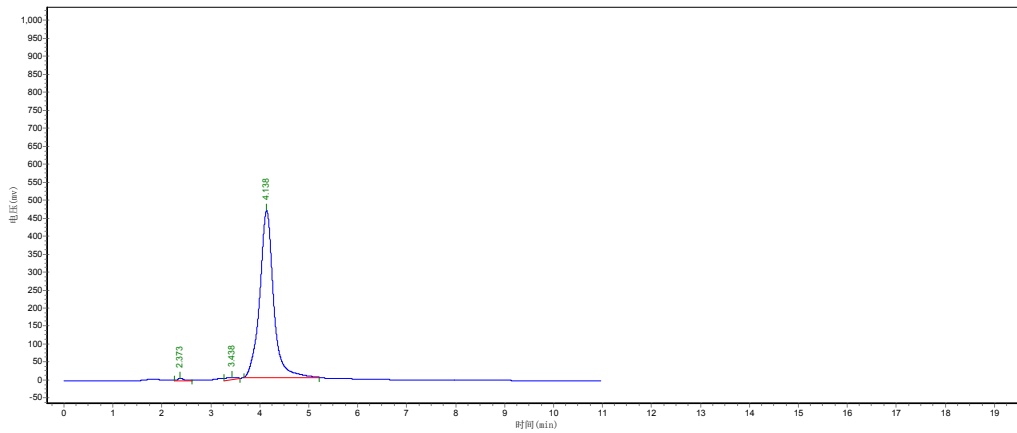


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

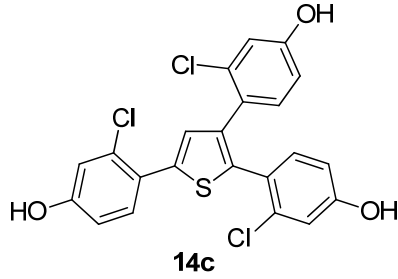


Name	Retention Time	Peak height	Area	Area Percent
	5.395	13006.758	139737.094	1.9780
	6.112	181363.469	6924822.500	98.0220
Totals		194370.227	7064559.594	100.0000

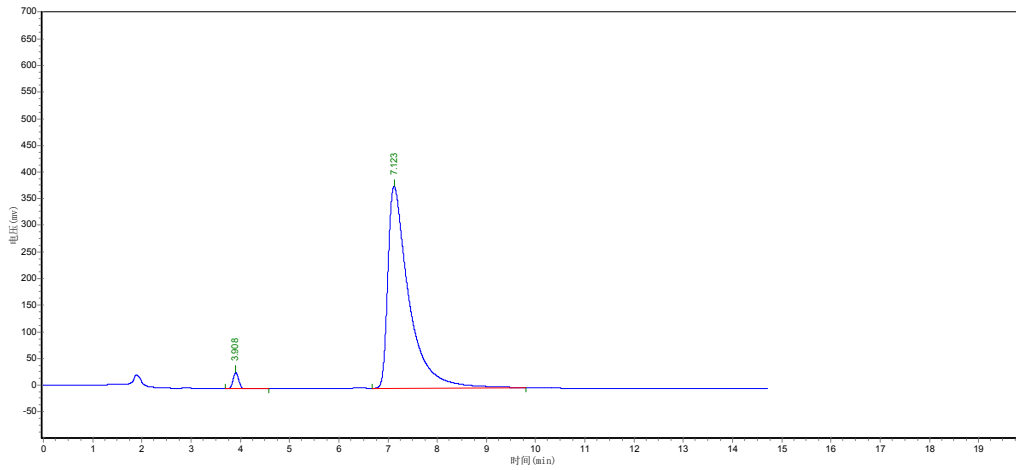
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	2.373	5894.809	38718.953	0.3921
	3.438	8794.950	154052.578	1.5599
	4.138	470355.875	9683217.000	98.0481
Totals		485045.634	9875988.531	100.0000

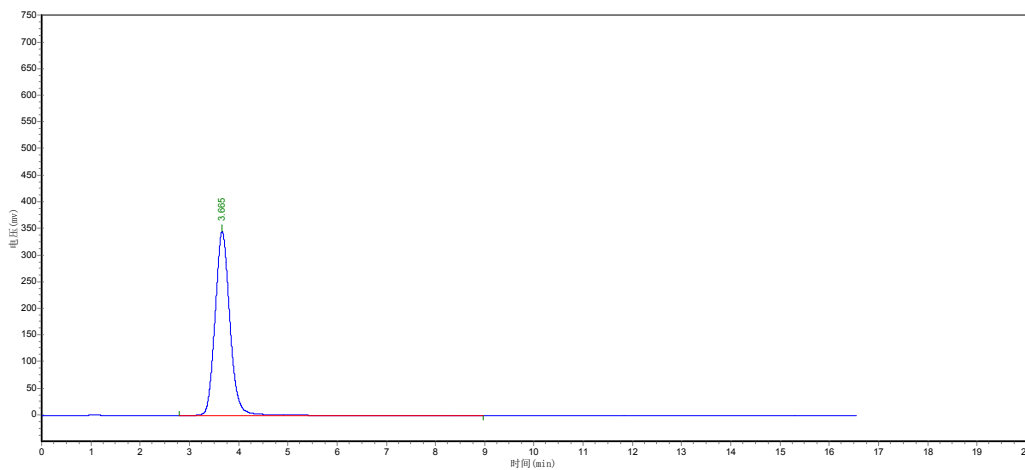


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

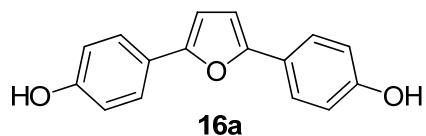


Name	Retention Time	Peak height	Area	Area Percent
	3.908	30094.238	240843.203	2.0811
	7.123	380223.938	11331844.000	97.9189
Totals		410318.176	11572687.203	100.0000

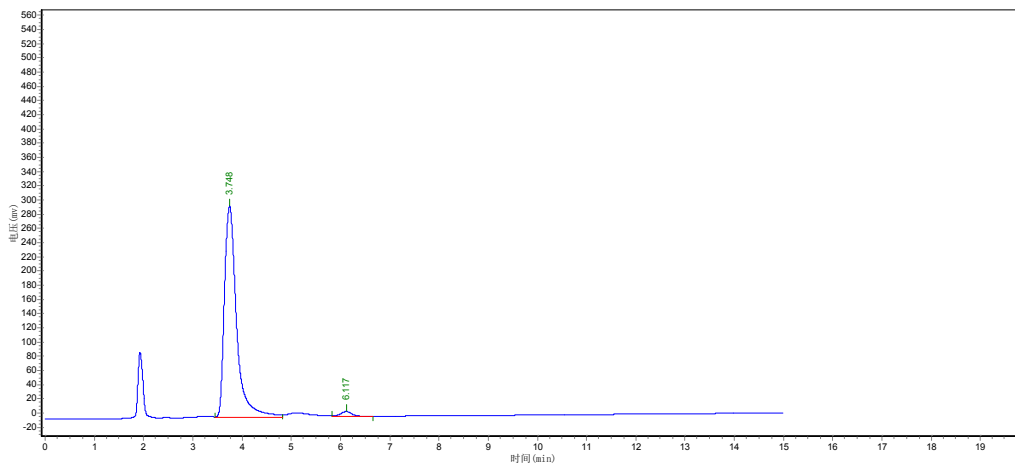
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	3.665	345578.375	7230601.000	100.0000
Totals		345578.375	7230601.000	100.0000

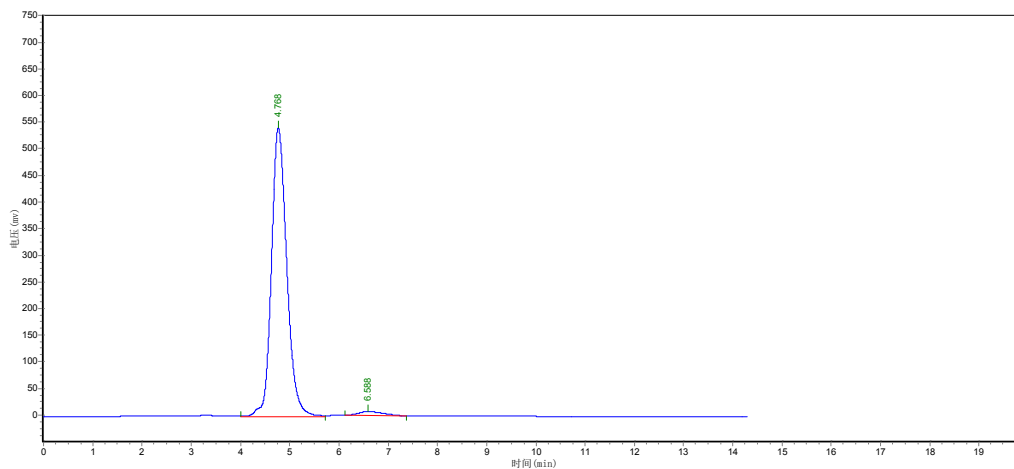


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

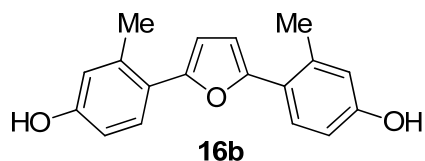


Name	Retention Time	Peak height	Area	Area Percent
	3.748	297348.281	5132034.500	97.8027
	6.117	6976.034	115298.758	2.1973
<b>Totals</b>		<b>304324.315</b>	<b>524733.258</b>	<b>100.0000</b>

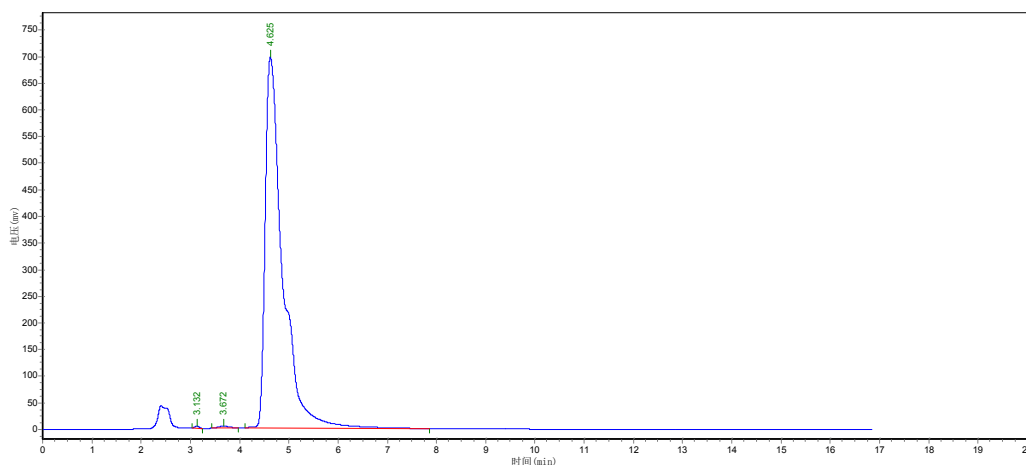
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	4.768	541923.813	11715631.000	97.7940
	6.588	7381.860	264276.813	2.2060
<b>Totals</b>		<b>549305.472</b>	<b>11979907.813</b>	<b>100.0000</b>

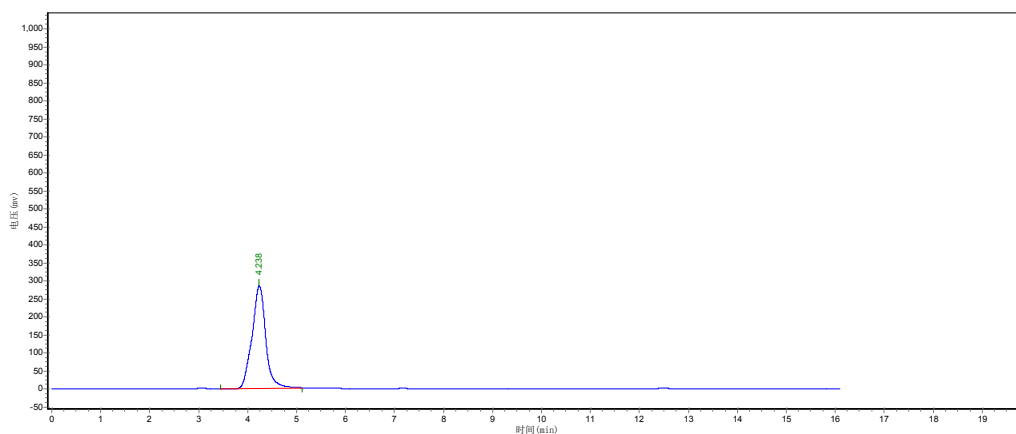


Normal Phase(Method 30:70 EtOAc:Hex, Flow rate 1.0 mL/min)

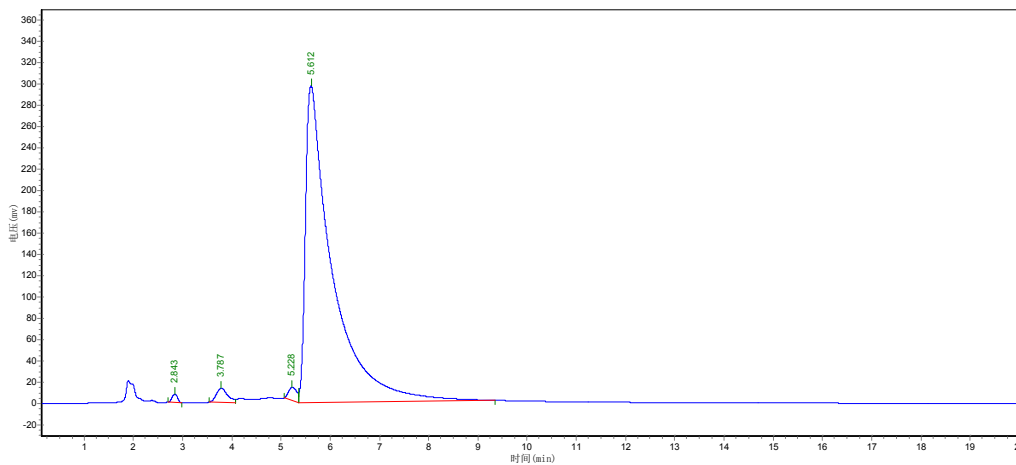
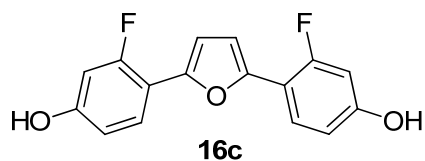


Name	Retention Time	Peak height	Area	Area Percent
	3.132	3222.698	19565.998	0.1140
	3.672	3856.399	62318.195	0.3631
Totals	4.625	696100.625	17079162.000	99.5229
		703179.723	17161046.193	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

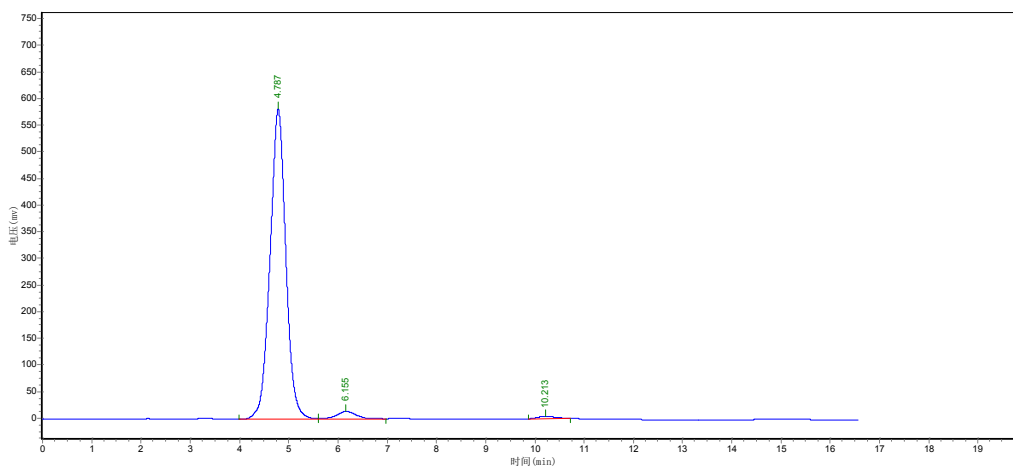


Name	Retention Time	Peak height	Area	Area Percent
Totals	4.238	284593.156	5572610.000	100.0000
		284593.156	5572610.000	100.0000

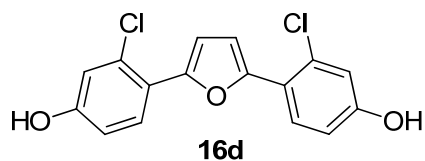


Name	Retention Time	Peak height	Area	Area Percent
	2.843	7724.186	59816.547	0.5134
	3.787	13382.565	216484.500	1.8580
	5.228	12258.151	151472.906	1.3000
	5.612	297576.531	11223725.000	96.3286
<b>Totals</b>		<b>330941.434</b>	<b>11651498.953</b>	<b>100.0000</b>

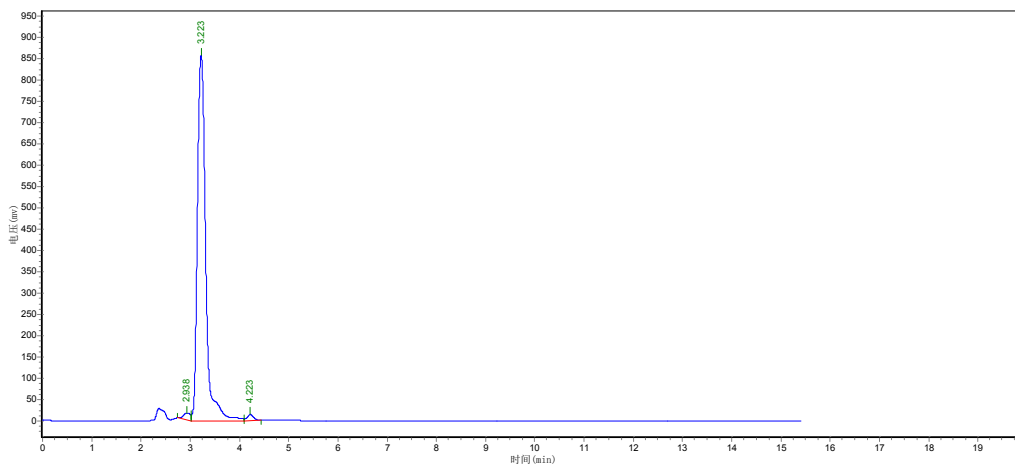
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	4.787	582933.125	13024212.000	95.6711
	6.155	14909.532	477646.406	3.5086
	10.213	4411.816	111668.750	0.8203
<b>Totals</b>		<b>602254.474</b>	<b>13613527.156</b>	<b>100.0000</b>

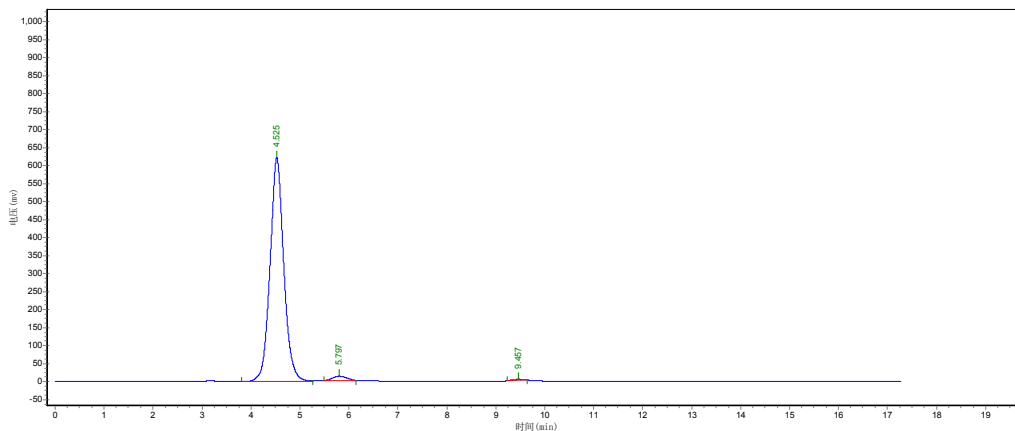


Normal Phase(Method 40:60 EtOAc:Hex, Flow rate 1.0 mL/min)

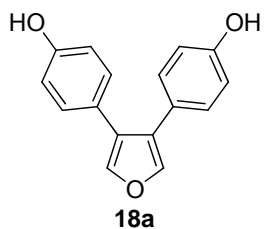


Name	Retention Time	Peak height	Area	Area Percent
	2.938	16467.893	157055.625	1.5177
	3.223	857877.438	10060491.000	97.2168
	4.223	14598.757	130963.344	1.2655
<b>Totals</b>		<b>888944.088</b>	<b>10348509.969</b>	<b>100.0000</b>

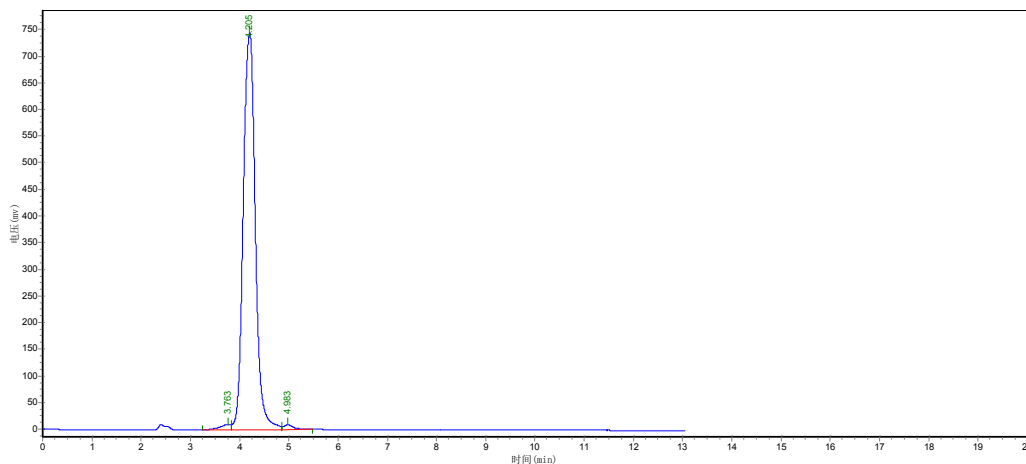
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	4.525	618868.375	11914657.000	96.9878
	5.797	12383.794	274586.000	2.2352
	9.457	4538.437	95459.102	0.7771
<b>Totals</b>		<b>635790.606</b>	<b>12284702.102</b>	<b>100.0000</b>

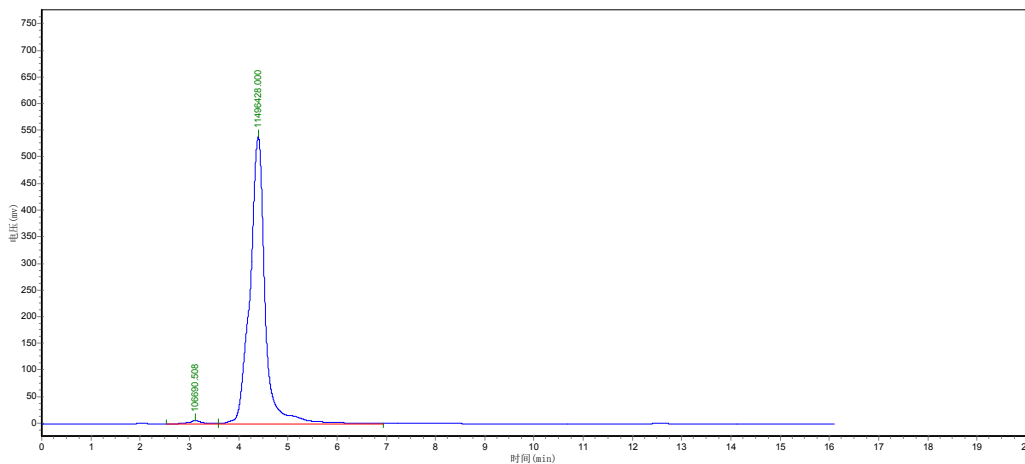


Normal Phase(Method 40:60 EtOAc:Hex, Flow rate 1.0 mL/min)



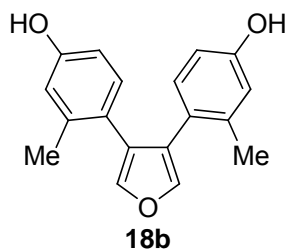
Name	Retention Time	Peak height	Area	Area Percent
	3.763	10376.232	165334.156	1.2683
	4.205	746491.250	12732914.000	97.6740
	4.983	9282.698	137889.266	1.0577
<b>Totals</b>		<b>766150.181</b>	<b>13036137.422</b>	<b>100.0000</b>

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

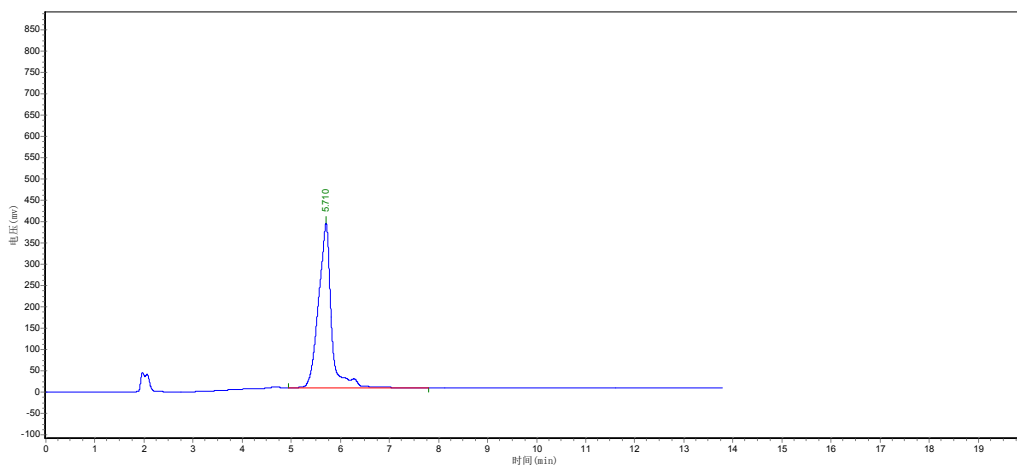


Name	Retention Time	Peak height	Area	Area Percent
	3.120	6059.301	106690.508	0.9195
	4.398	538291.938	11496428.000	99.0805
<b>Totals</b>		<b>544351.239</b>	<b>11603118.508</b>	<b>100.0000</b>



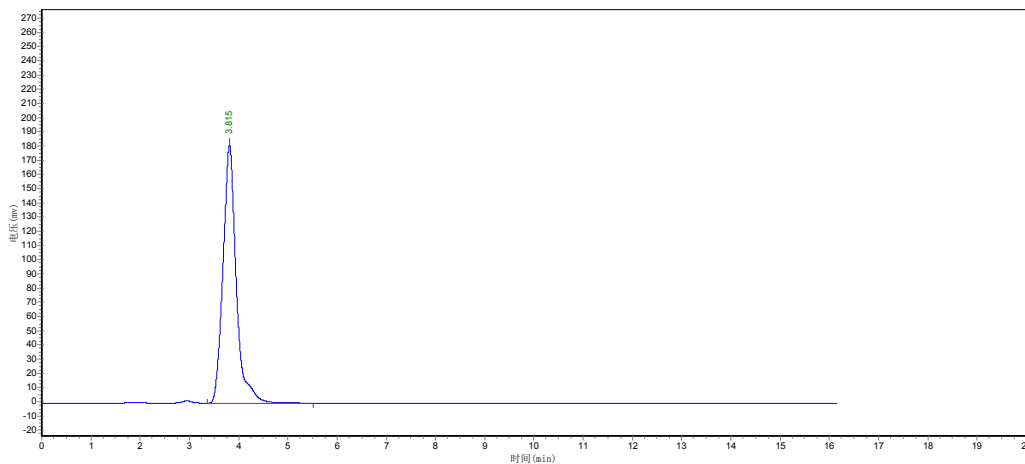


Normal Phase(Method 40:60 EtOAc:Hex, Flow rate 1.0 mL/min)

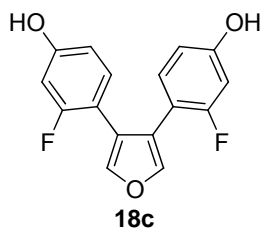


Name	Retention Time	Peak height	Area	Area Percent
Totals	5.710	385433.750	6997826.500	100.0000
Totals		385433.750	6997826.500	100.0000

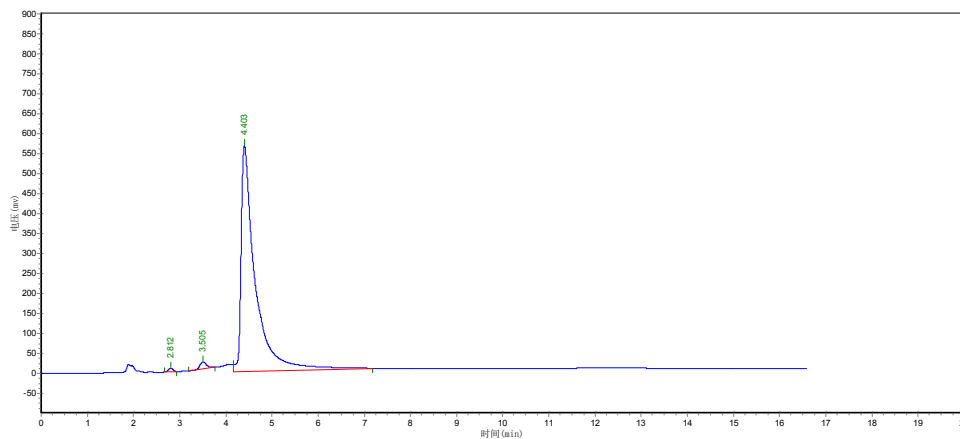
Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
Totals	3.815	181914.578	3387507.500	100.0000
Totals		181914.578	3387507.500	100.0000

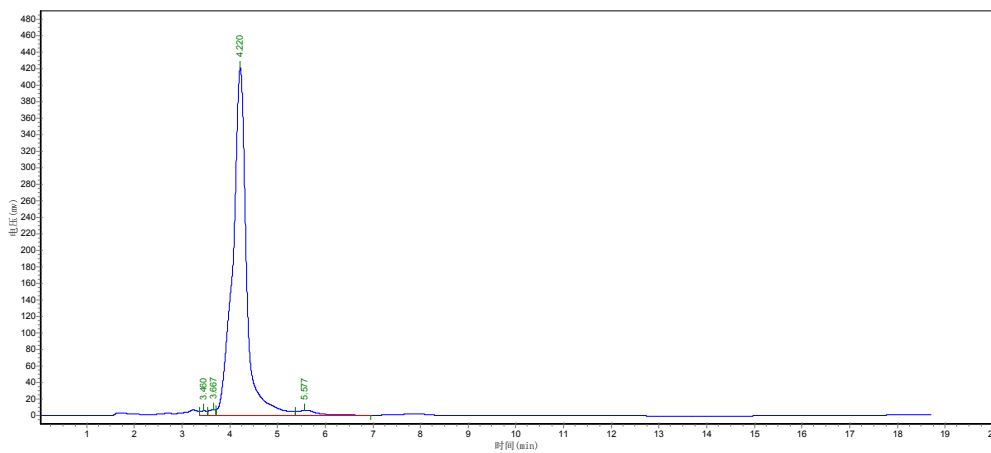


Normal Phase(Method 40:60 EtOAc:Hex, Flow rate 1.0 mL/min)

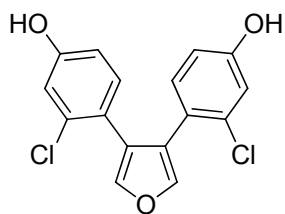


Name	Retention Time	Peak height	Area	Area Percent
	2.812	8764.337	60599.152	0.4982
	3.505	17162.057	164122.375	1.3494
Totals	4.403	564933.250	11937716.000	98.1523
		590859.644	12162437.527	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)

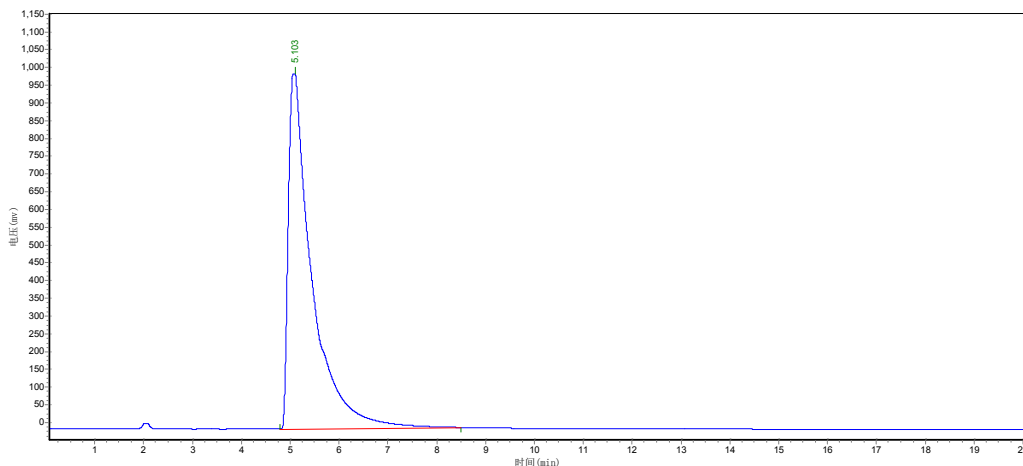


Name	Retention Time	Peak height	Area	Area Percent
	3.460	5615.458	57823.184	0.6586
	3.667	7453.568	70353.234	0.8013
	4.220	421406.906	8443249.000	96.1641
	5.577	5857.371	208618.359	2.3761
Totals		440333.303	8780043.777	100.0000



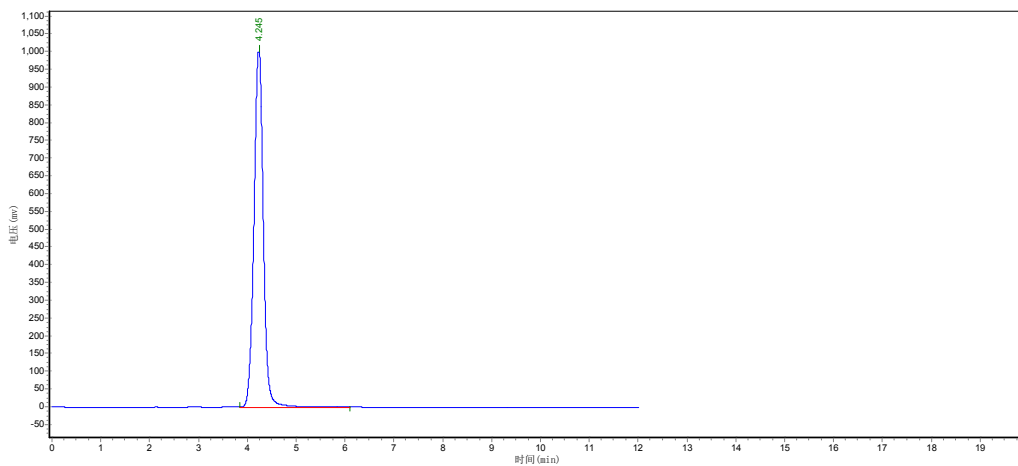
**18d**

Normal Phase(Method 40:60 EtOAc:Hex, Flow rate 1.0 mL/min)



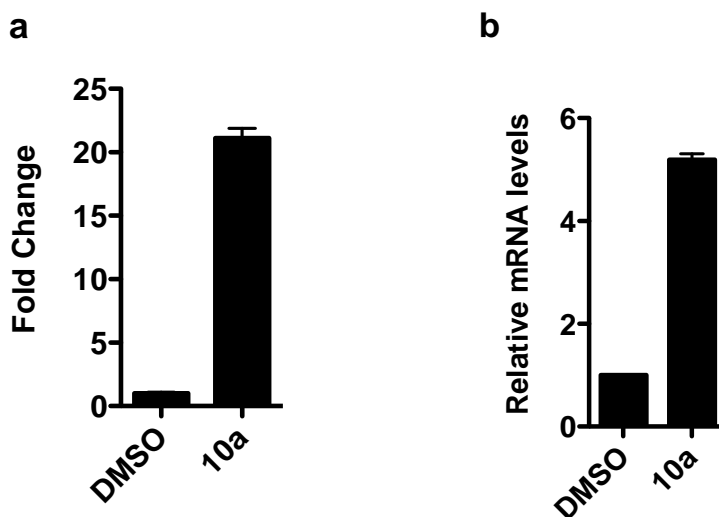
Name	Retention Time	Peak height	Area	Area Percent
	5.103	999067.500	33385538.000	100.0000
Totals		999067.500	33385538.000	100.0000

Reverse Phase(Method 70:30 CH<sub>3</sub>CN:H<sub>2</sub>O, Flow rate 0.7 mL/min)



Name	Retention Time	Peak height	Area	Area Percent
	4.245	1001028.750	13450566.000	100.0000
Totals		1001028.750	13450566.000	100.0000

### PART III. BIOLOGICAL ASSAYS FOR COMPOUND 10a



- a) Mammalian-two hybrid assay: HEK293T cells were transfected with VP16- ER $\alpha$  (bait), GAL4 SRC2 (prey) and 5X GAL4 UAS luciferase as the reporter. The next day, cells were plated at a density of 20,000 cells/well, incubated in 384-well plates overnight at 37 °C and 5% CO<sub>2</sub>, and treated with compounds dissolved in DMSO using a robotic pin-tool dispenser. Luciferase activity was measured after 24 hours using BriteLite reagent (Perkin-Elmer Inc., Shelton, CT) according to manufacturer's protocol.
- b) RT-QPCR for GREB1: Ishikawa cells were plated at a density of 20,000 cells/well in phenol red-free growth media, incubated in 384-well plates overnight at 37 °C and 5% CO<sub>2</sub>, and treated with compounds dissolved in DMSO using a robotic pin-tool dispenser. mRNA was extracted, converted to cDNA, and RT-QPCR for GREB1 was performed and normalized using GAPDH as a housekeeping gene.