

Supporting information for

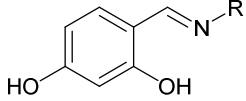
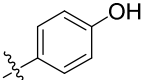
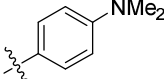
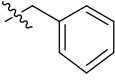
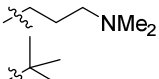

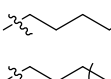

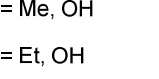
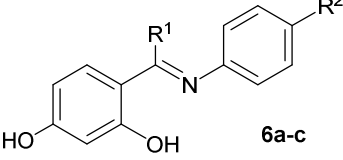
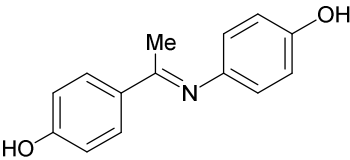
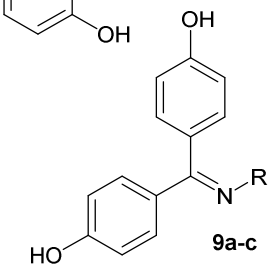
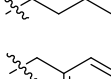
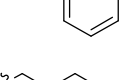
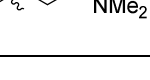
Triaryl-substituted Schiff Bases are High-Affinity Subtype-Selective Ligands for the Estrogen Receptor

Zong-Quan Liao, Chune Dong, Kathryn E. Carlson, Sathish Srinivasan, Jerome Nwkwuchu, Robert W. Chesnut, Abhishek Sharma, Kendall W. Nettles, John A. Katzenellenbogen,* and Hai-Bing Zhou*

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PART I. Table S1. Relative Binding Affinities (RBAs)^a of compounds **5-9** for the estrogen receptor α and β .

		Compd.	ER α	ER β	β/α	
	5a	R = 	0.004	0.181	45	
	5b	R = 	0.002	0.003	1.5	
	5c	R = 	0.002	0.003	1.5	
	5a-h	5d	R = 	0.005	0.004	0.8
	5e	R = 	0.002	<0.001	--	
	5f	R = 	0.005	0.008	1.6	
	5g	R = 	0.002	0.017	8.5	
	5h	R = 	0.007	0.013	1.9	
	6a	R ¹ , R ² = Me, OH	0.009	0.173	19	
	6b	R ¹ , R ² = Et, OH	0.013	0.040	3	
	6c	R ¹ , R ² = Me, Cl	0.016	0.029	2	
	7		0.018	0.048	2.5	
	8		<0.001	0.002	>2	
	9a	R = 	0.005	0.016	3.2	
	9b	R = 	0.024	0.186	7.8	
	9a-c	9c	R = 	0.015	0.292	20

^a See footnote for **Table 1**. Only single affinity measurements were made of these low affinity compounds.

PART II. Analytical techniques

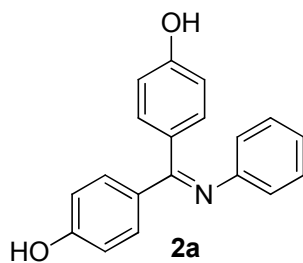
^1H NMR and ^{13}C NMR spectra were recorded on a Bruker AV400 spectrometer (400 MHz, ^1H NMR; 101 MHz, ^{13}C NMR) at room temperature. NMR spectra were calibrated to the solvent signals of CDCl_3 (δ 7.26 and 77.00), Acetone- d_6 (δ 2.05 and 29.84, 206.26), or DMSO- d_6 (δ 2.50 and 39.43). The chemical shifts are provided in ppm and the coupling constants in Hz. The following abbreviations for multiplicities are used: s, singlet; d, doublet; dd, double doublet; t, triplet; dt, double triplet; q, quadruplet; m, multiplet; br, broad. Chlorobenzene was dried over CaH_2 and distilled prior to use. Glassware was oven-dried, assembled while hot, and cooled under an inert atmosphere. Unless otherwise noted, all reactions were conducted in an inert atmosphere. Reaction progress was monitored using analytical thin-layer chromatography (TLC). Visualization was achieved by UV light (254 nm). Flash chromatography was performed with silica gel (0.040-0.063 mm) packing. High resolution mass spectra (HRMS) were measured on IonSpec 4.7 Tesla FTMS using MALDI/DHB. Melting points were obtained on X-4 melting point apparatus (Beijing TECH Instruments, Co.,Ltd.) and are uncorrected.

PART III. Summary of HPLC results

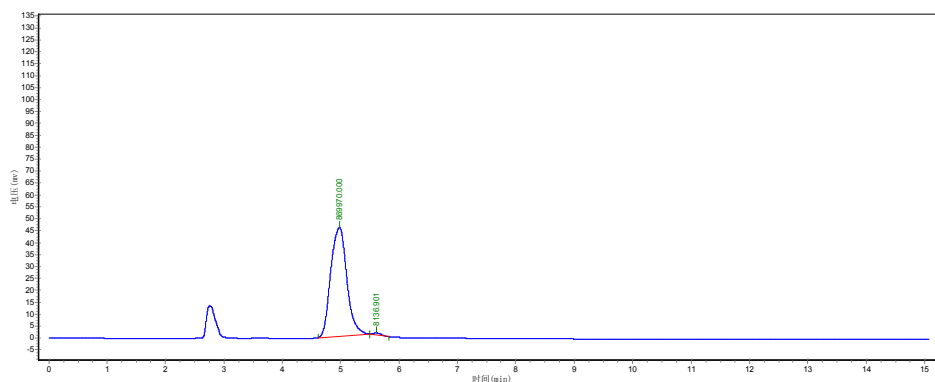
All the HPLC were conducted on SHIMADZU-10A and all the results were obtained under the condition of UV1000-254nm.

Cmpd	Normal Phase	Ret. Time	%Purity	Reverse Phase	Ret. Time	%Purity
2a	40:60 Hexane: EtOAc	4.980	99.0734	40:60 H ₂ O: CH ₃ CN	3.743	99.3673
2b	40:60 Hexane: EtOAc	4.773	100	40:60 H ₂ O: CH ₃ CN	4.590	100
2c	40:60 Hexane: EtOAc	4.630	99.5166	40:60 H ₂ O: CH ₃ CN	4.238	99.3923
2d	40:60 Hexane: EtOAc	4.820	95.4036	40:60 H ₂ O: CH ₃ CN	4.128	95.6785
2e	40:60 Hexane: EtOAc	4.933	97.9549	40:60 H ₂ O: CH ₃ CN	4.128	97.7321
2f	40:60 Hexane: EtOAc	4.892	99.3141	40:60 H ₂ O: CH ₃ CN	4.283	99.7822
2g	40:60 Hexane: EtOAc	4.945	98.9508	40:60 H ₂ O: CH ₃ CN	4.614	98.6860
2h	40:60 Hexane: EtOAc	4.898	98.0660	40:60 H ₂ O: CH ₃ CN	4.553	98.4772
2i	40:60 Hexane: EtOAc	4.760	98.9375	40:60 H ₂ O: CH ₃ CN	4.860	99.4761
2j	40:60 Hexane: EtOAc	5.018	98.6698	40:60 H ₂ O: CH ₃ CN	3.838	97.1999
2k	40:60 Hexane: EtOAc	4.628	98.1290	40:60 H ₂ O: CH ₃ CN	4.805	95.1603
2l	40:60 Hexane: EtOAc	6.660	97.5193	40:60 H ₂ O: CH ₃ CN	3.697	97.0678
2n	40:60 Hexane: EtOAc	8.950	96.0365	40:60 H ₂ O: CH ₃ CN	4.525	97.1370
4a	40:60 Hexane: EtOAc	4.842	100	40:60 H ₂ O: CH ₃ CN	3.665	100
4b	40:60 Hexane: EtOAc	4.873	100	40:60 H ₂ O: CH ₃ CN	4.368	99.5620
4c	40:60 Hexane: EtOAc	4.972	99.3654	40:60 H ₂ O: CH ₃ CN	4.262	99.3437
4d	40:60 Hexane: EtOAc	5.460	99.6515	40:60 H ₂ O: CH ₃ CN	4.368	99.2738
4e	40:60 Hexane: EtOAc	7.080	98.5416	40:60 H ₂ O: CH ₃ CN	4.332	98.8311
4f	40:60 Hexane: EtOAc	5.140	100	40:60 H ₂ O: CH ₃ CN	4.515	99.7220
4g	40:60 Hexane: EtOAc	5.132	97.0697	40:60 H ₂ O: CH ₃ CN	4.843	98.7303
4h	40:60 Hexane: EtOAc	4.992	96.2784	40:60 H ₂ O: CH ₃ CN	4.863	99.5213
4i	40:60 Hexane: EtOAc	5.310	97.8483	40:60 H ₂ O: CH ₃ CN	4.768	98.2337
4j	40:60 Hexane: EtOAc	4.462	99.5828	40:60 H ₂ O: CH ₃ CN	4.062	99.1691
4k	40:60 Hexane: EtOAc	3.748	97.1470	40:60 H ₂ O: CH ₃ CN	5.127	99.2799
4l	40:60 Hexane: EtOAc	4.717	97.4688	40:60 H ₂ O: CH ₃ CN	4.007	97.4333
4n	40:60 Hexane: EtOAc	9.630	97.8223	40:60 H ₂ O: CH ₃ CN	5.147	97.2463

PART IV. HPLC spectra of final compounds



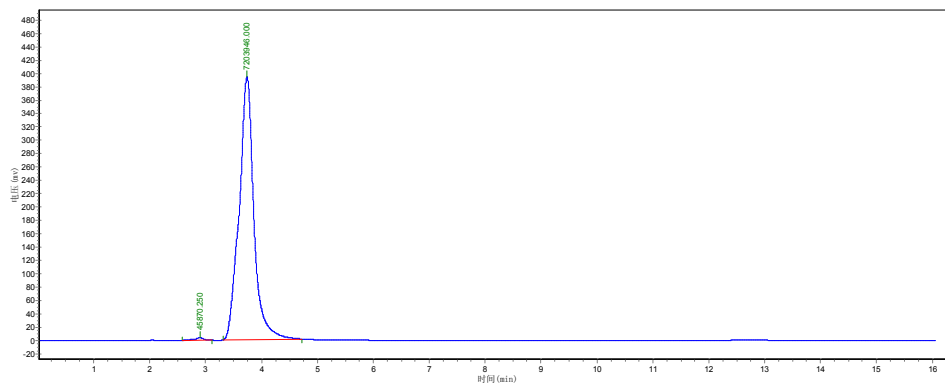
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.980	45565.527	869970.000	99.0734
2	5.610	831.822	8136.901	0.9266

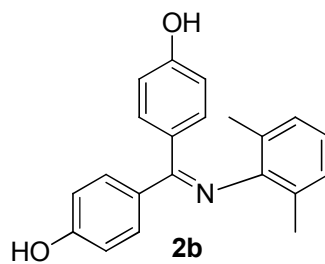
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Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

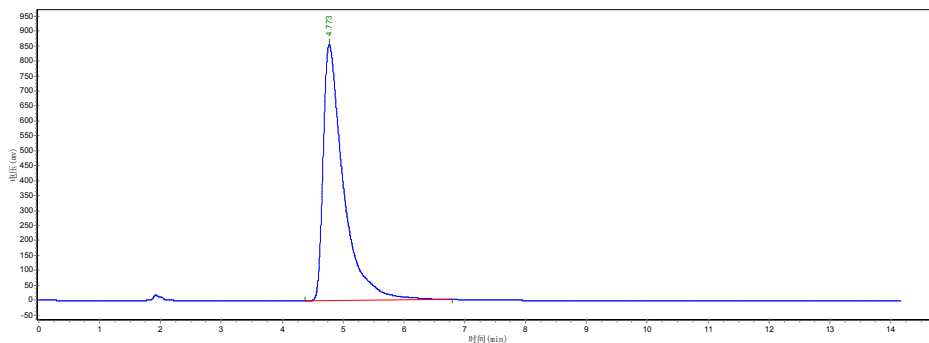


No.	Retention time	Peak height	Peak area	Percent
1	2.897	3703.155	45870.250	0.6327
2	3.743	393839.656	7203946.000	99.3673

total 100



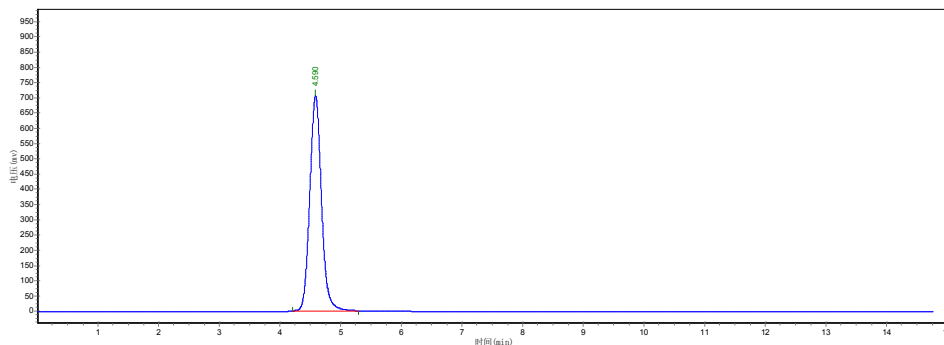
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.773	856766.000	19856186.000	100.0000

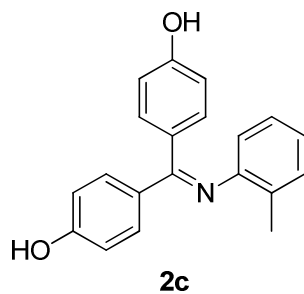
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Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

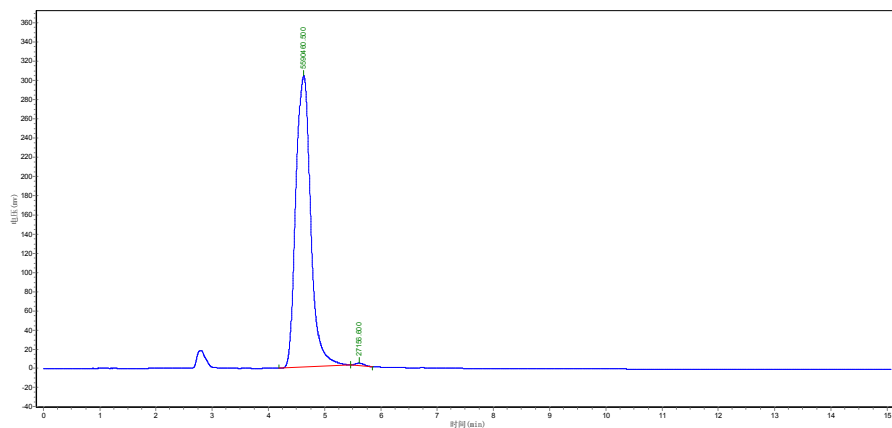


No.	Retention time	Peak height	Peak area	Percent
1	4.590	704877.938	9437654.000	100.0000

total 100



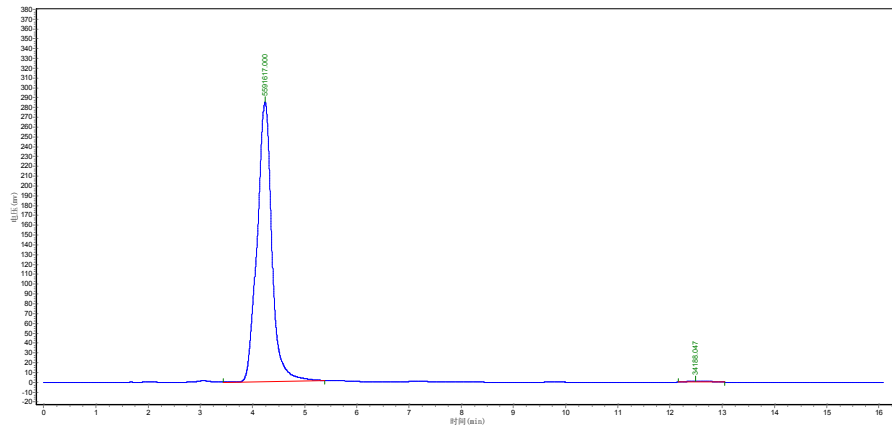
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.630	303418.531	5590460.500	99.5166
2	5.407	2611.669	27156.600	0.4834

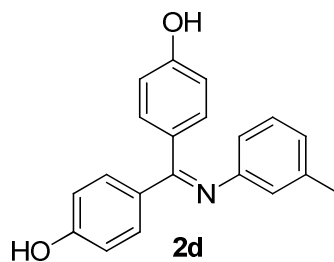
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Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

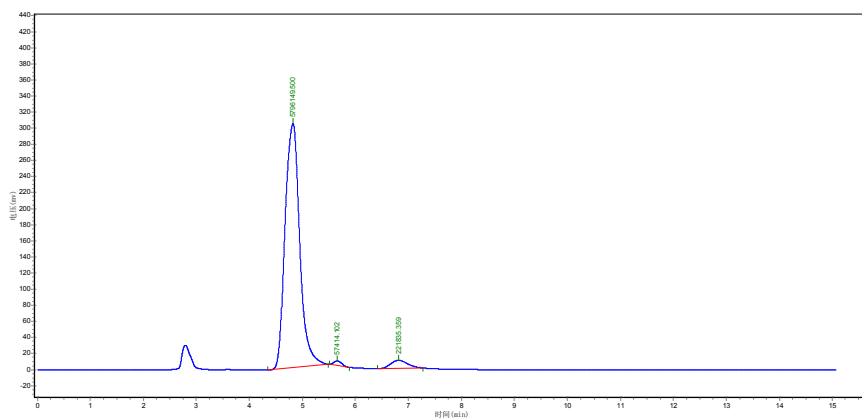


No.	Retention time	Peak height	Peak area	Percent
1	4.238	284735.750	5591617.000	99.3923
2	12.483	1164.254	34188.047	0.6077

total 100



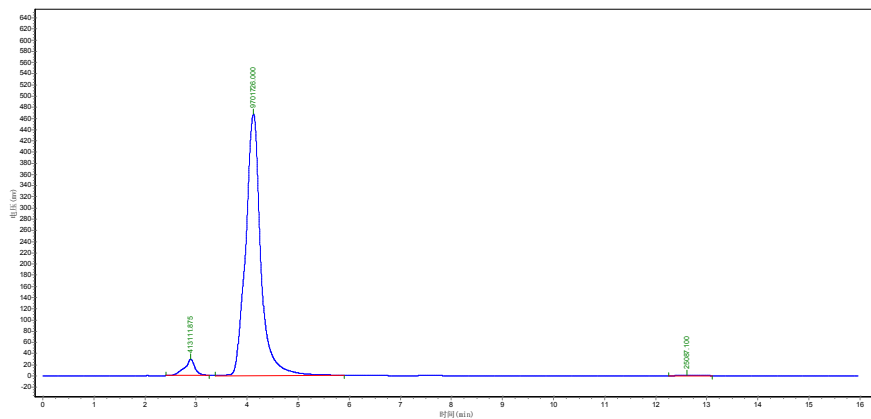
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.820	303074.375	5796149.500	95.4036
2	5.655	5487.177	57414.102	0.9450
3	6.822	9957.286	221835.359	3.6514

total 100

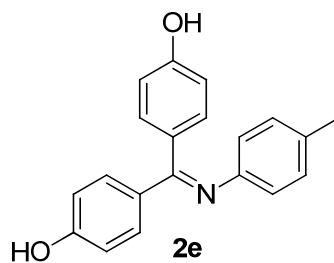
Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)



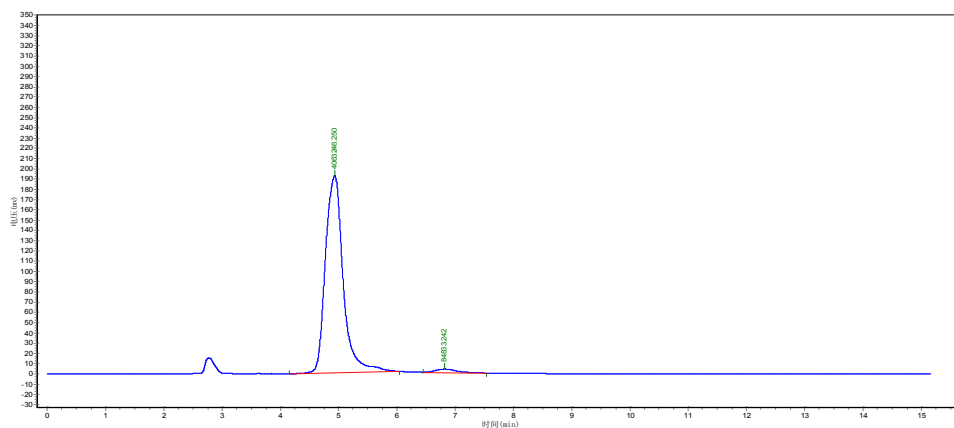
No.	Retention time	Peak height	Peak area	Percent
1	2.895	29605.164	413111.875	4.0741
2	4.128	467146.188	9701726.000	95.6785
3	12.612	940.070	25087.100	0.2474

total

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Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)

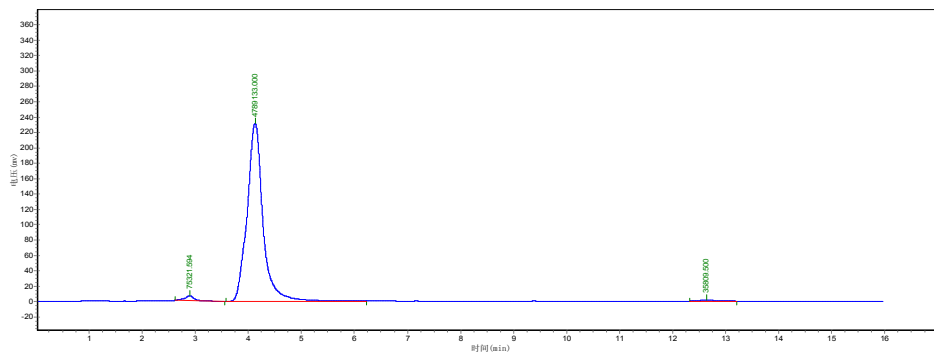


No.	Retention time	Peak height	Peak area	Percent
1	4.933	192296.313	4063246.250	97.9549
2	6.815	3464.734	84833.242	2.0451

total

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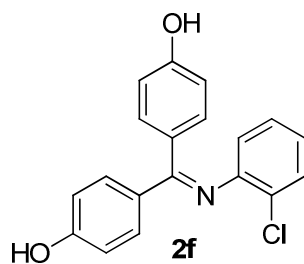
Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)



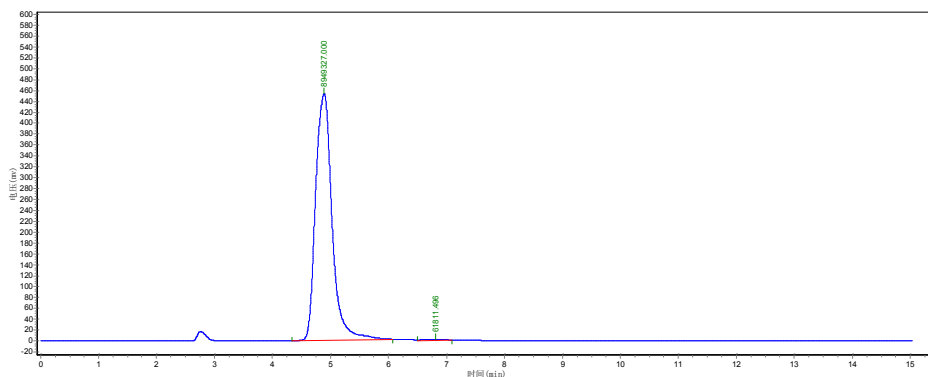
No.	Retention time	Peak height	Peak area	Percent
1	2.893	6382.281	75321.594	1.5371
2	4.128	231311.297	4789133.000	97.7321
3	12.640	1236.823	35809.500	0.7308

total

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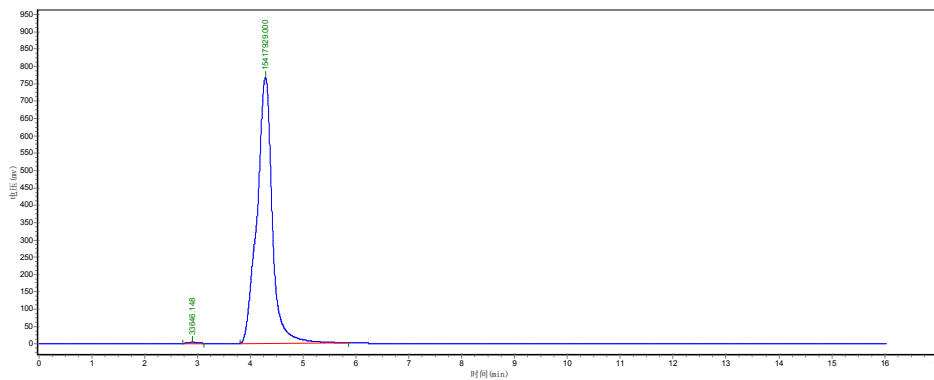
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.892	452863.688	8949327.000	99.3141
2	6.815	2329.834	61811.496	0.6859

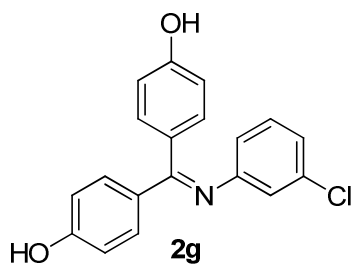
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Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

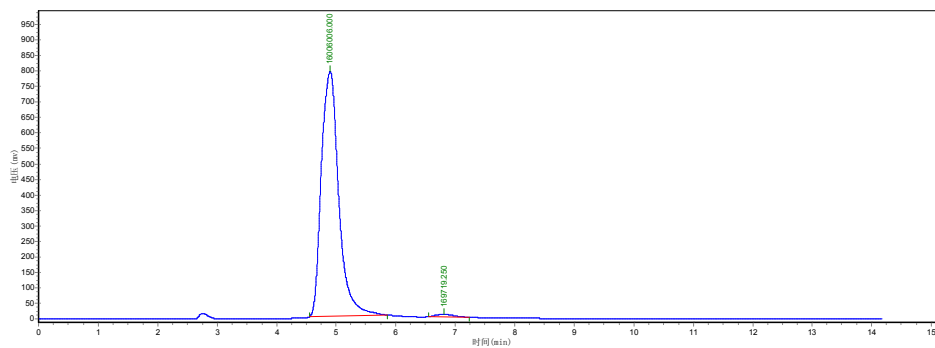


No.	Retention time	Peak height	Peak area	Percent
1	2.903	3217.693	33646.148	0.2178
2	4.283	766449.188	15417929.000	99.7822

total 100



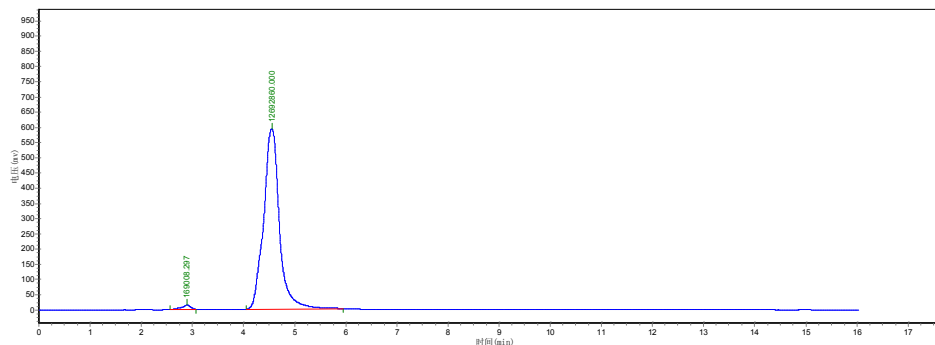
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.945	790553.813	16006006.000	98.9508
2	6.902	8259.269	169719.250	1.0492

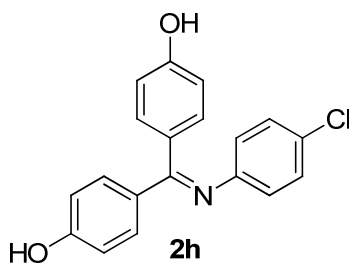
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Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

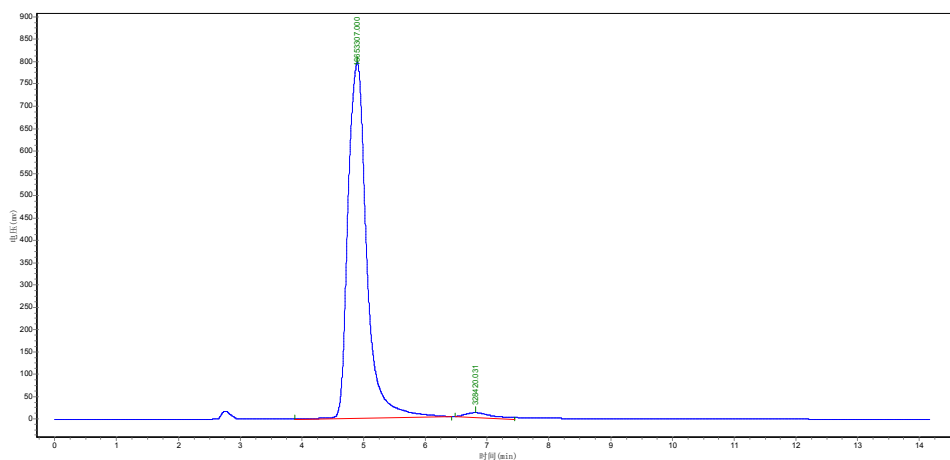


No.	Retention time	Peak height	Peak area	Percent
1	2.923	13925.279	169008.297	1.3140
2	4.614	592433.125	12692860.000	98.6860

total 100



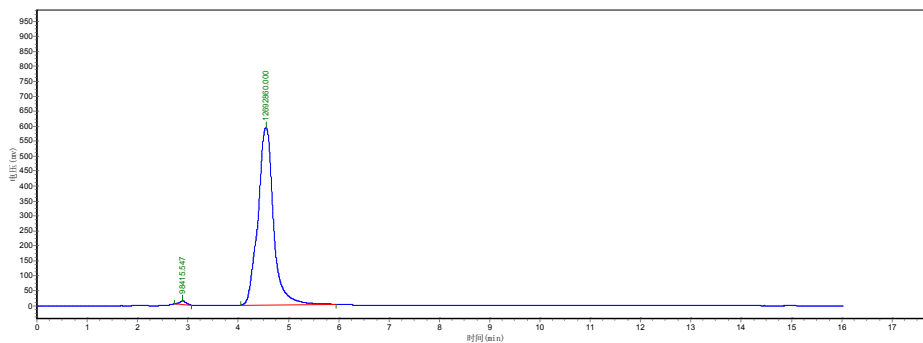
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.898	796373.438	16653307.000	98.0660
2	6.810	10742.045	328420.031	1.9340

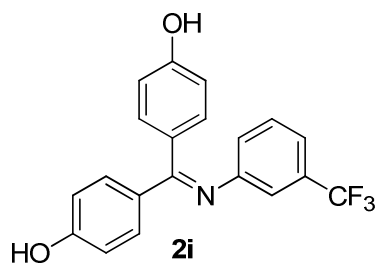
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Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

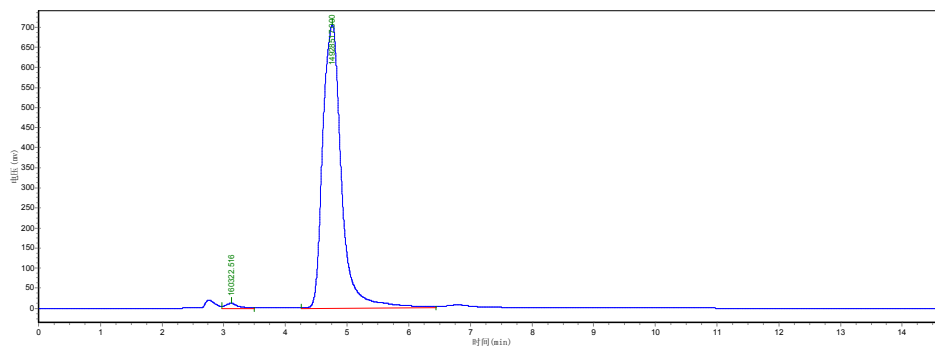


No.	Retention time	Peak height	Peak area	Percent
1	2.895	14950.634	198718.000	1.5228
2	4.553	593562.750	12851158.000	98.4772

total 100



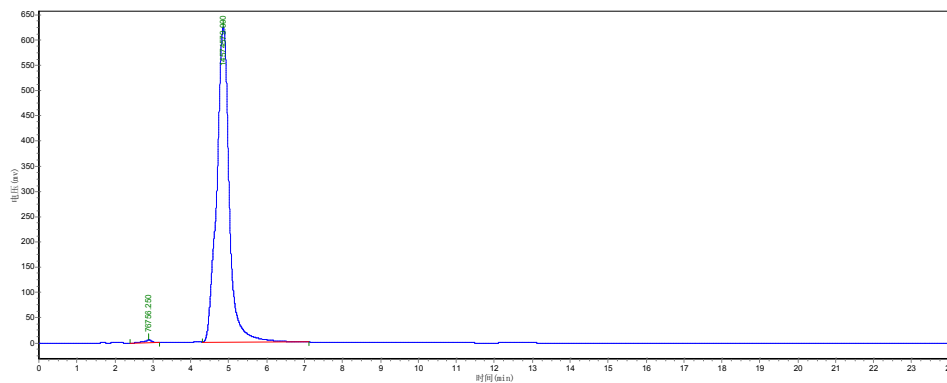
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	3.120	11588.420	160322.516	1.0625
2	4.760	706350.875	14928517.000	98.9375

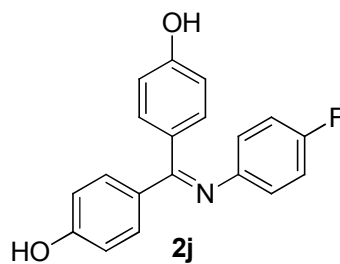
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Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

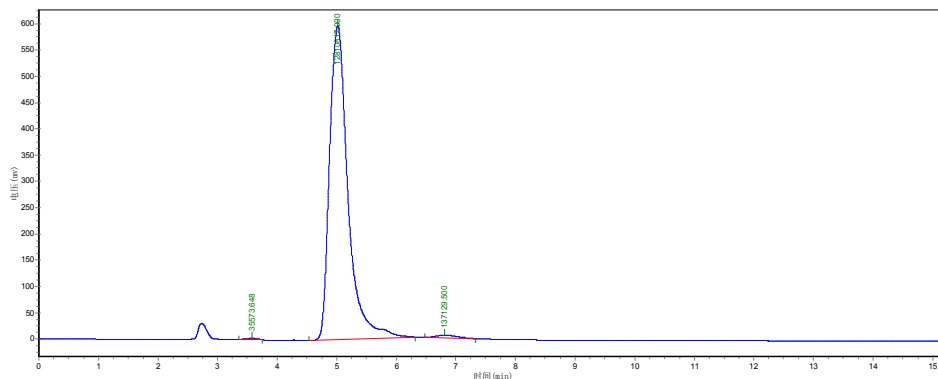


No.	Retention time	Peak height	Peak area	Percent
1	2.893	5679.271	76756.250	0.5239
2	4.860	625021.063	14574579.000	99.4761

total 100



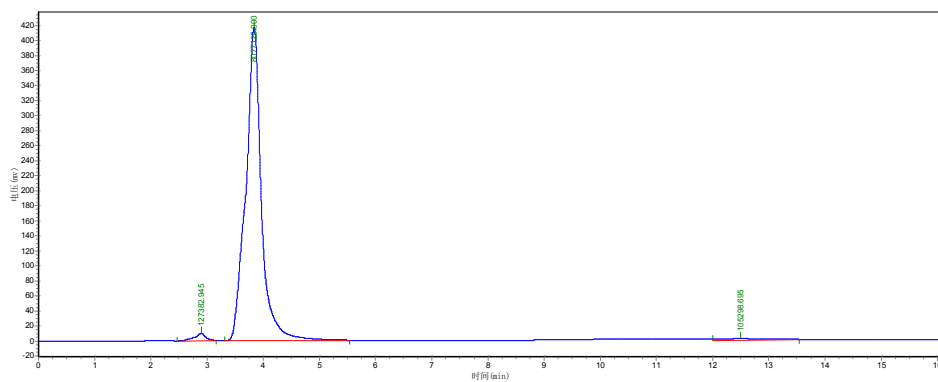
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	3.578	2537.218	35573.648	0.2740
2	5.018	597045.750	12810817.000	98.6698
3	6.813	5749.064	137129.500	1.0562

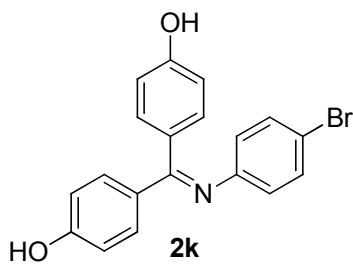
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Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

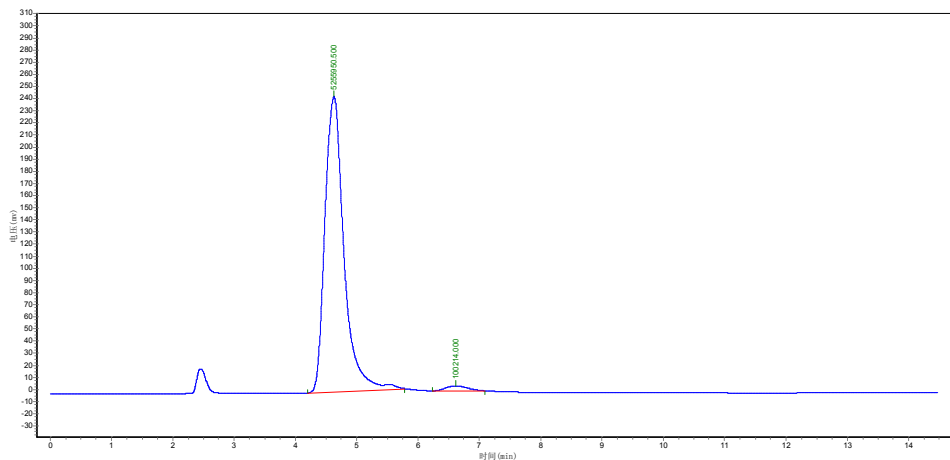


No.	Retention time	Peak height	Peak area	Percent
1	2.895	9543.234	127382.945	1.5329
2	3.838	416943.406	8077125.000	97.1999
3	12.500	1980.607	105298.695	1.2672

total 100



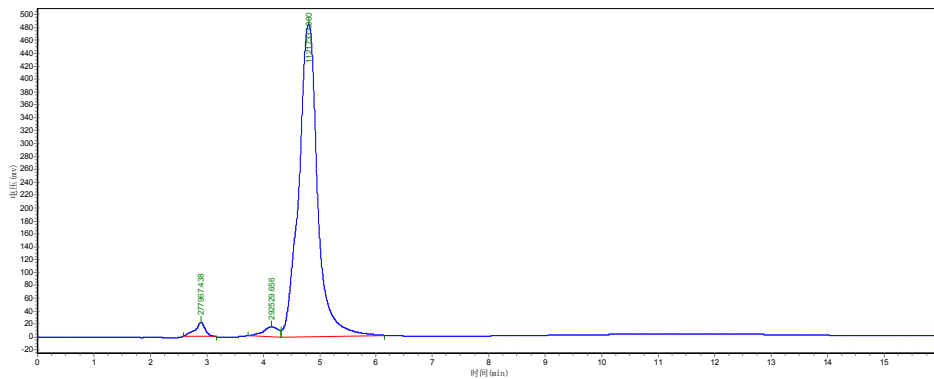
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.628	243823.969	5255950.500	98.1290
2	6.612	4162.609	100214.000	1.8710

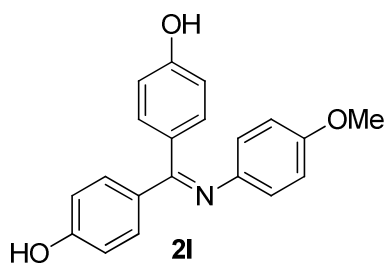
total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

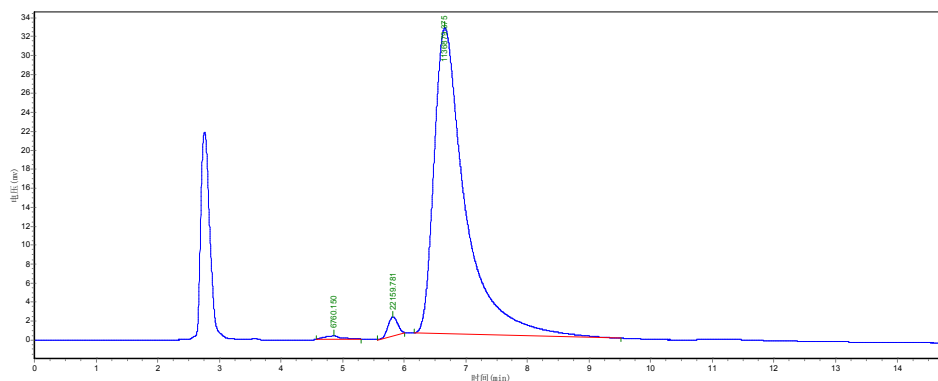


No.	Retention time	Peak height	Peak area	Percent
1	2.895	22001.090	277967.438	2.3581
2	4.150	15585.571	292529.656	2.4816
3	4.805	484846.188	11217337.000	95.1603

total 100



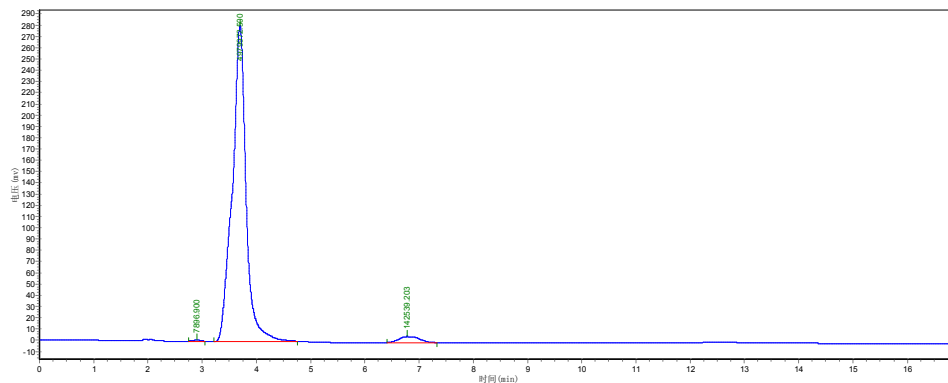
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.857	342.995	6760.150	0.5799
2	5.818	2001.558	22159.781	1.9008
3	6.660	32248.516	1136879.375	97.5193

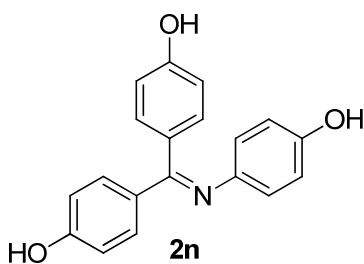
total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

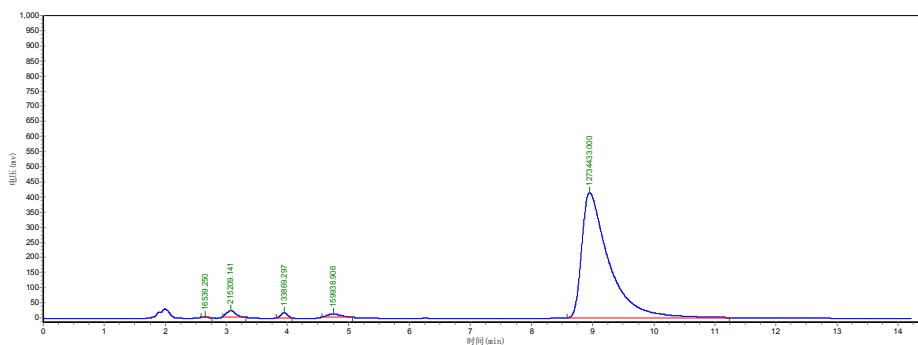


No.	Retention time	Peak height	Peak area	Percent
1	2.902	923.000	7896.900	0.1539
2	3.697	280619.688	4979972.500	97.0678
3	6.777	5369.090	142539.203	2.7783

total 100



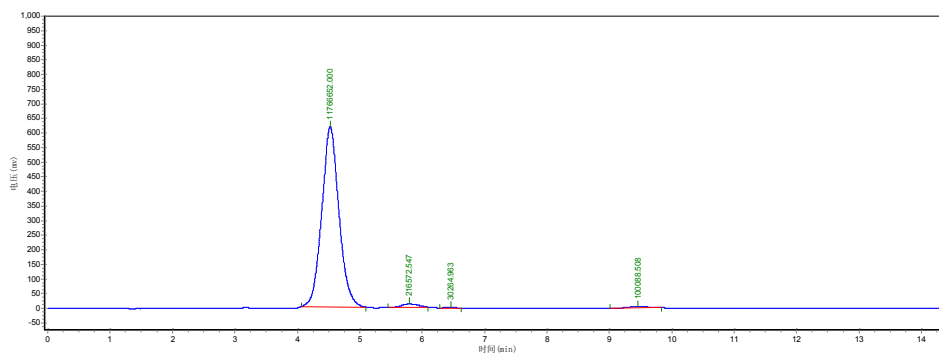
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	2.650	2686.515	16539.250	0.1247
2	3.075	20911.350	215209.141	1.6230
3	3.947	17989.904	133869.297	1.0096
4	4.752	10440.277	159938.906	1.2062
5	8.950	414700.594	12734433.000	96.0365

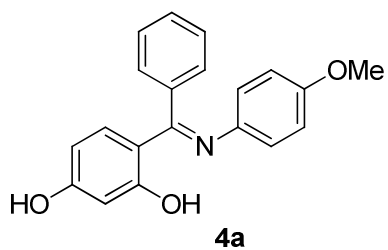
total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

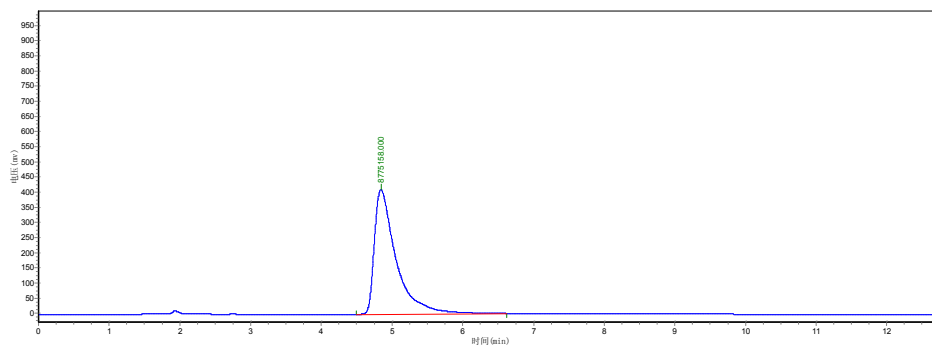


No.	Retention time	Peak height	Peak area	Percent
1	4.525	616574.813	11766652.000	97.1360
2	5.797	11557.197	216572.547	1.7878
3	6.455	1721.950	30264.963	0.2498
4	9.457	4640.454	100088.508	0.8263

total 100



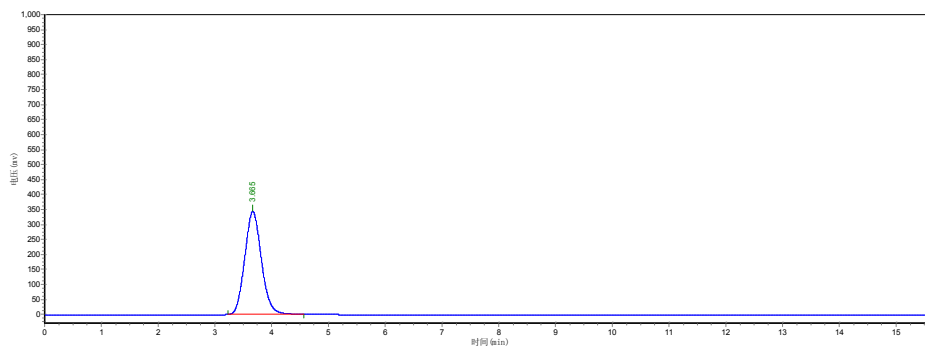
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.842	411060.375	8775158.000	100.0000

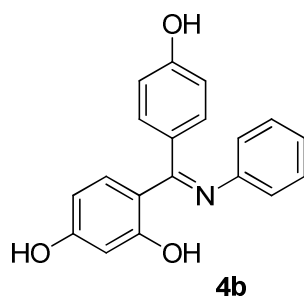
total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

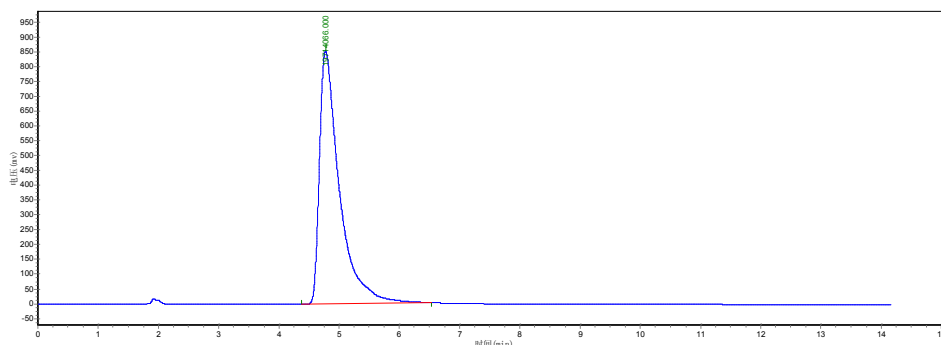


No.	Retention time	Peak height	Peak area	Percent
1	3.665	343985.469	7007134.500	100.0000

total 100



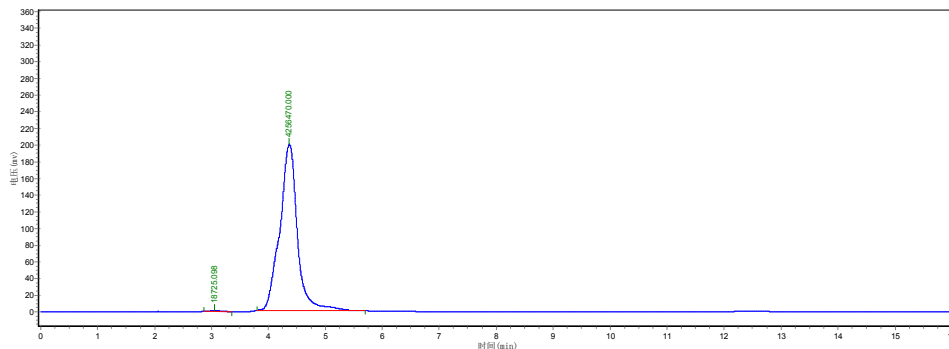
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.873	856403.875	19714066.000	100.0000

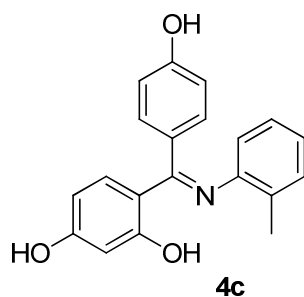
total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

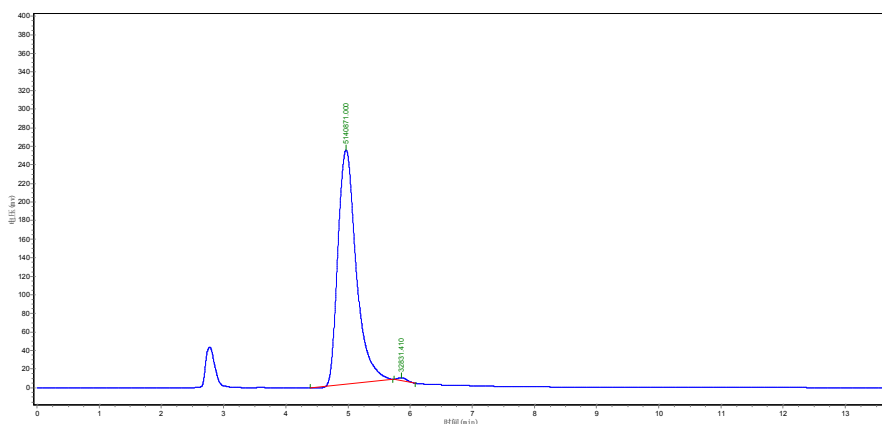


No.	Retention time	Peak height	Peak area	Percent
1	3.058	1608.083	18725.098	0.4380
2	4.368	198907.078	4256470.000	99.5620

total 100



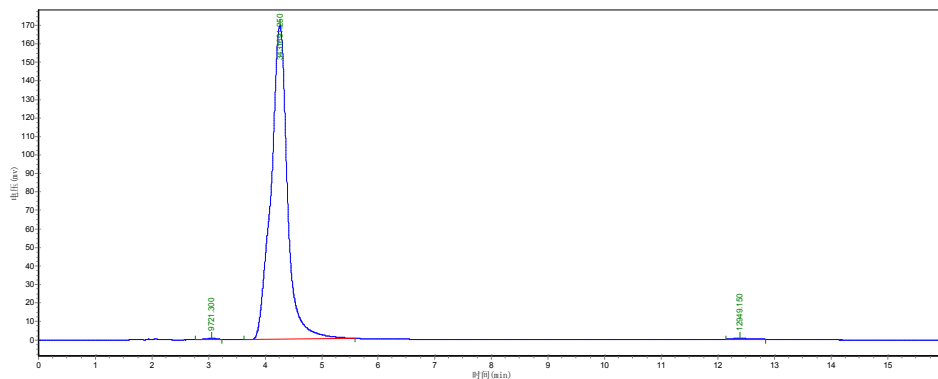
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.972	252006.688	5140871.000	99.3654
2	5.858	3324.104	32831.410	0.6346

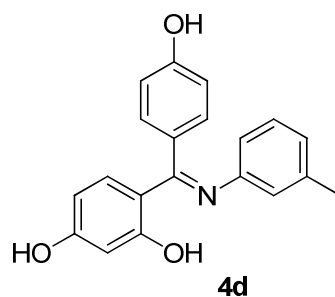
total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

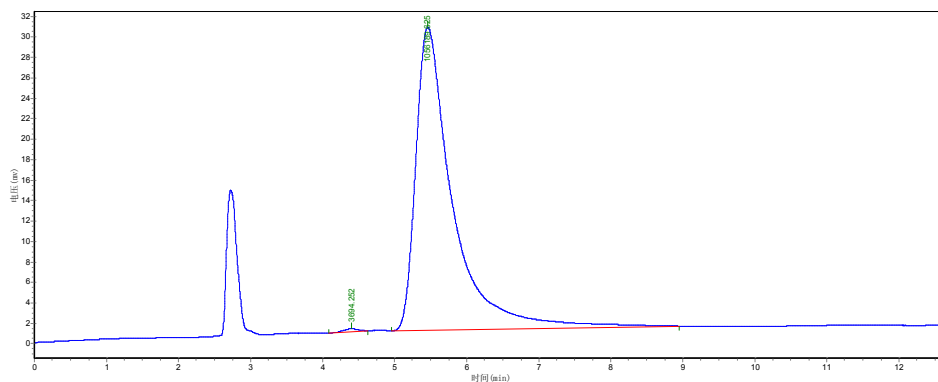


No.	Retention time	Peak height	Peak area	Percent
1	3.158	787.440	9721.300	0.2814
2	4.262	169487.391	3431691.250	99.3437
3	12.385	552.400	12949.150	0.3749

total 100



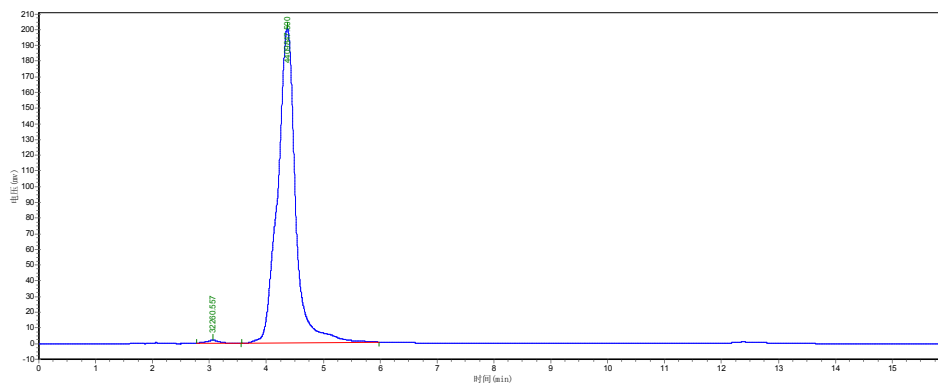
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.402	270.967	3694.252	0.3486
2	5.460	29625.785	1056189.625	99.6515

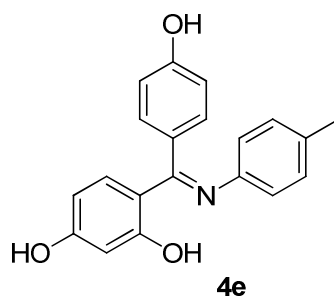
total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

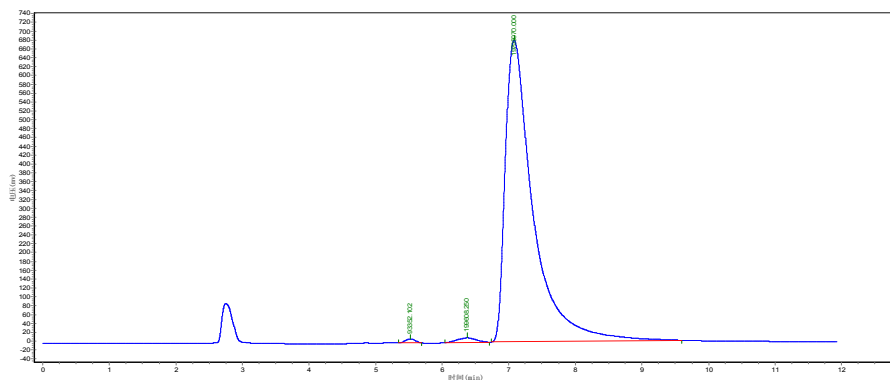


No.	Retention time	Peak height	Peak area	Percent
1	3.058	1997.052	32260.557	0.7262
2	4.368	200327.063	4409847.500	99.2738

total 100



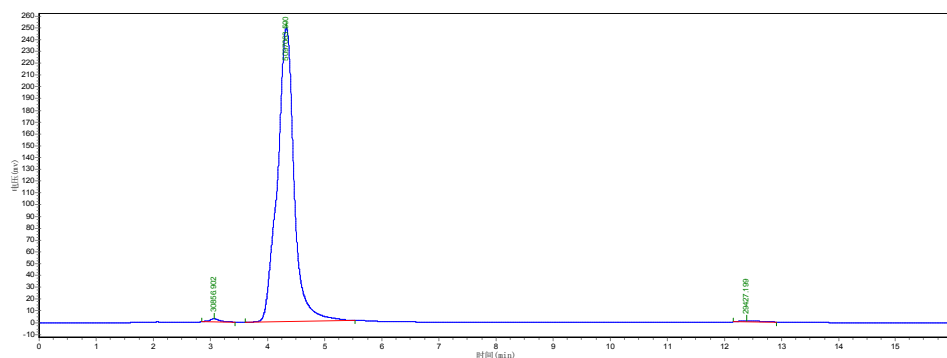
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	5.520	8812.868	93352.102	0.4647
2	6.375	10372.841	199608.250	0.9937
3	7.080	681073.938	19795070.000	98.5416

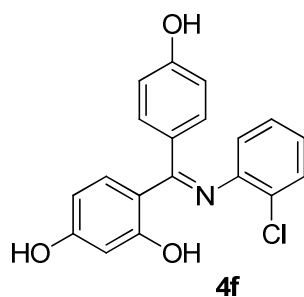
total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

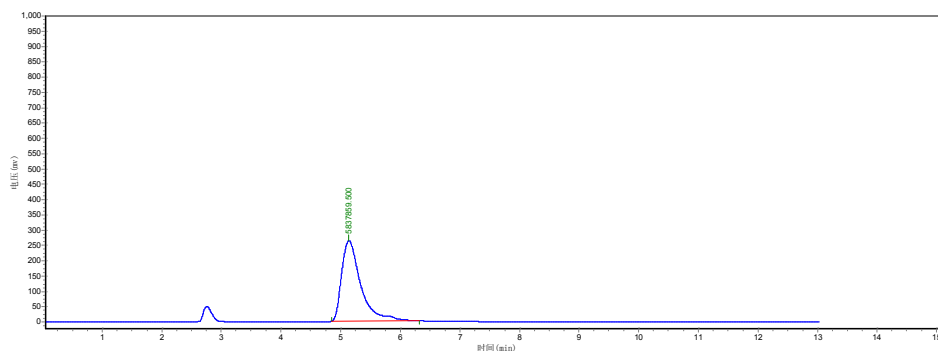


No.	Retention time	Peak height	Peak area	Percent
1	3.065	2476.125	30856.902	0.5983
2	4.332	248876.813	5097063.500	98.8311
3	12.400	1099.558	29427.199	0.5706

total 100



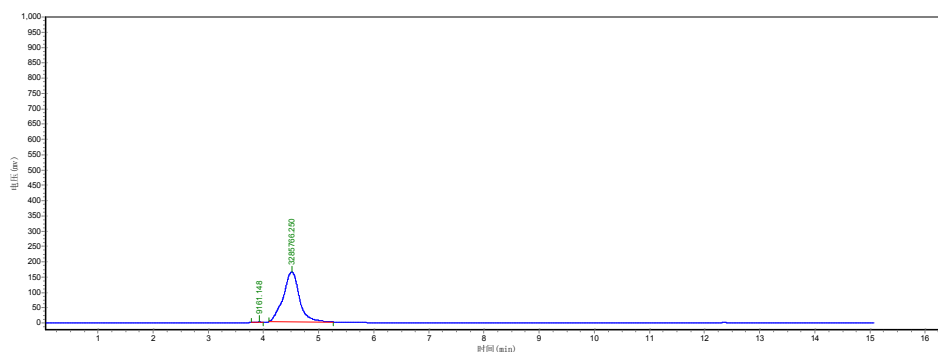
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	5.140	264948.375	6034239.500	100.0000

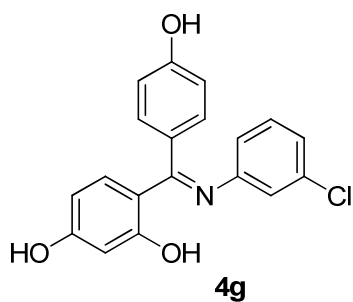
total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

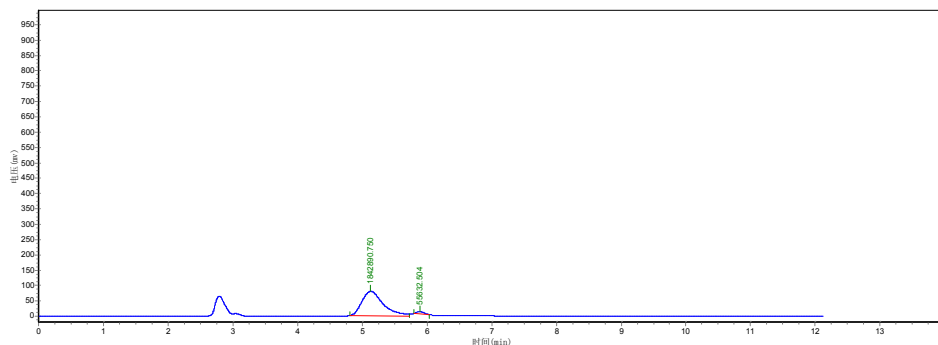


No.	Retention time	Peak height	Peak area	Percent
1	3.927	1157.953	9161.148	0.2780
2	4.515	161597.359	3285766.250	99.7220

total 100



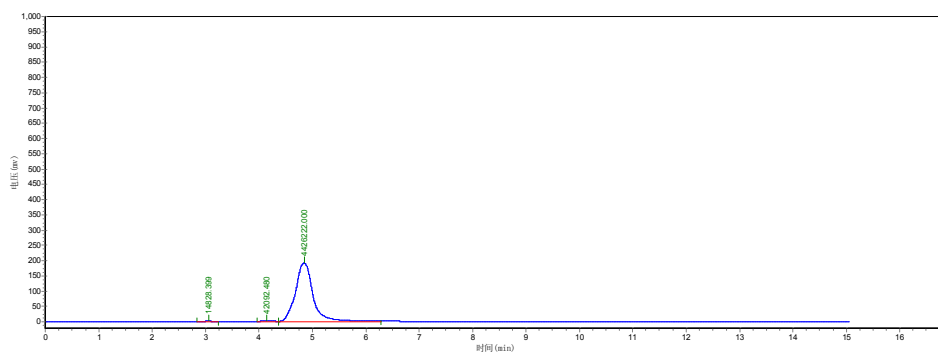
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	5.132	79443.859	1842890.750	97.0697
2	5.890	6801.754	55632.504	2.9303

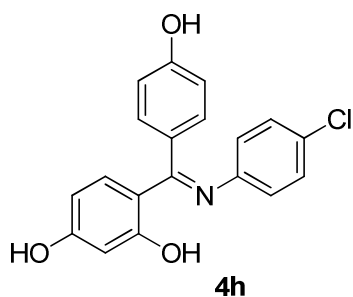
total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

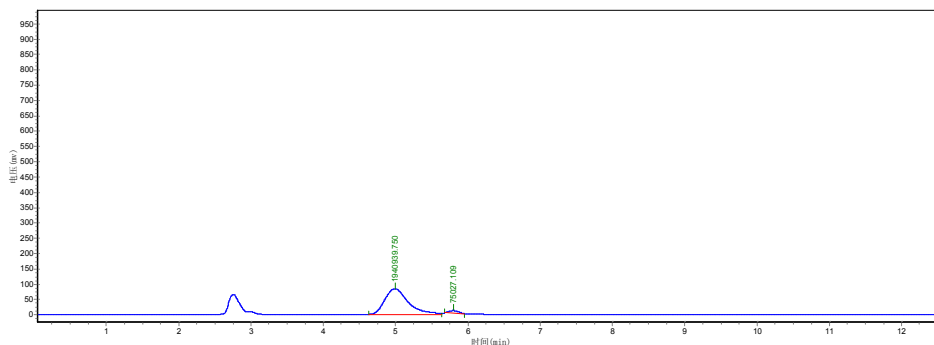


No.	Retention time	Peak height	Peak area	Percent
1	3.053	1324.133	14828.399	0.3308
2	4.148	2837.359	42092.480	0.9389
3	4.843	191665.156	4426222.000	98.7303

total 100



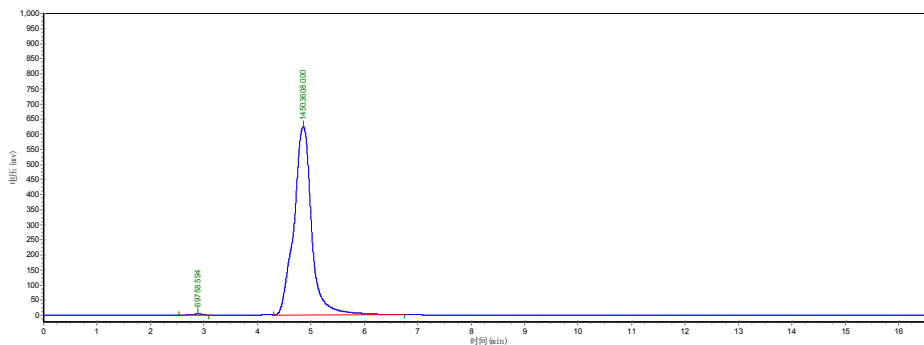
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.992	84615.273	1940939.750	96.2784
2	5.795	8269.368	75027.109	3.7216

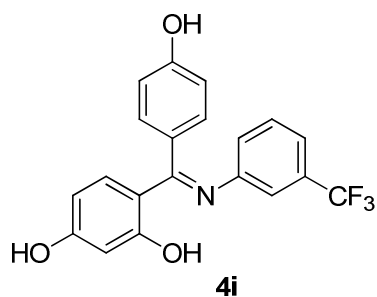
total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

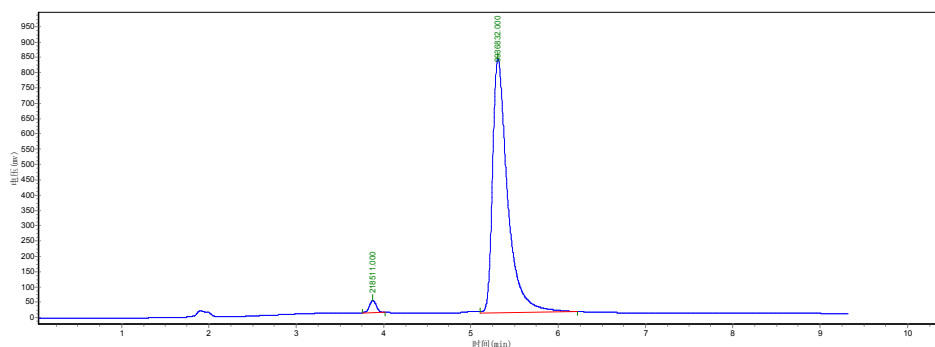


No.	Retention time	Peak height	Peak area	Percent
1	2.893	5449.716	69758.594	0.4787
2	4.863	624828.188	14503608.000	99.5213

total 100



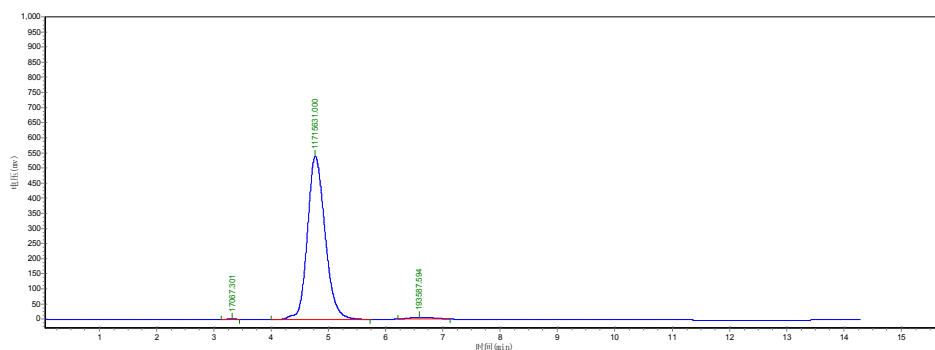
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	3.877	39731.176	218511.000	2.1517
2	5.310	829883.063	9936832.000	97.8483

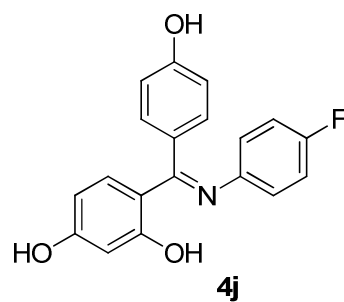
total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

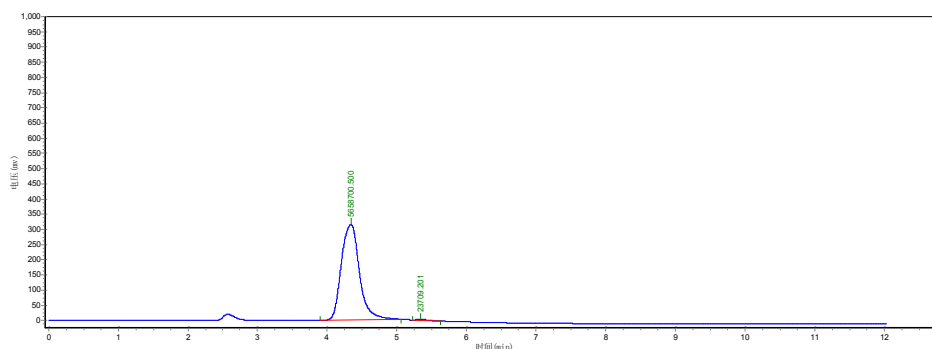


No.	Retention time	Peak height	Peak area	Percent
1	3.312	1500.217	17067.301	0.1431
2	4.768	541923.813	11715631.000	98.2337
3	6.588	6366.037	193587.594	1.6232

total 100



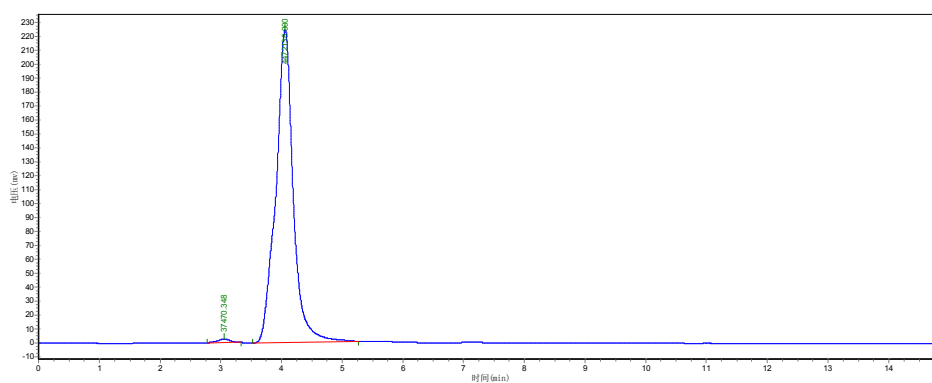
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.462	313899.969	5658700.500	99.5828
2	5.348	2015.966	23709.201	0.4172

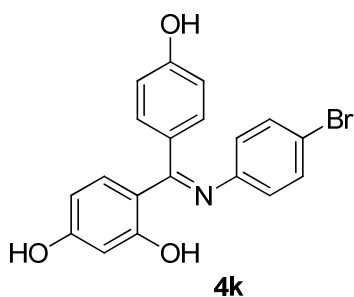
total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

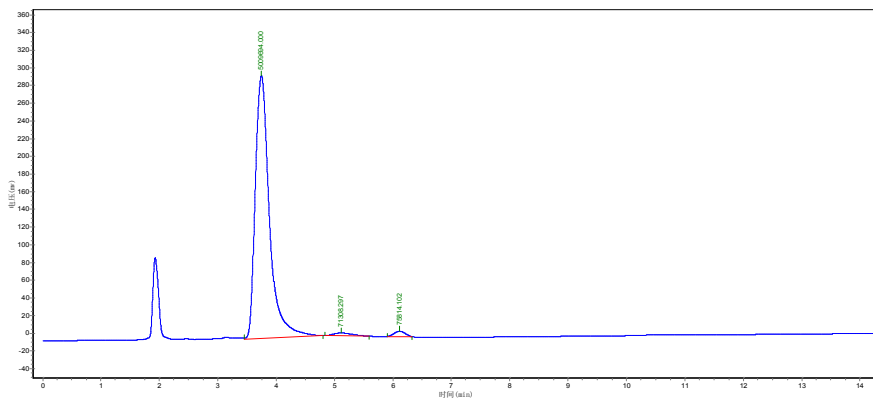


No.	Retention time	Peak height	Peak area	Percent
1	3.055	2660.687	37470.348	0.8309
2	4.062	224164.500	4472138.000	99.1691

total 100



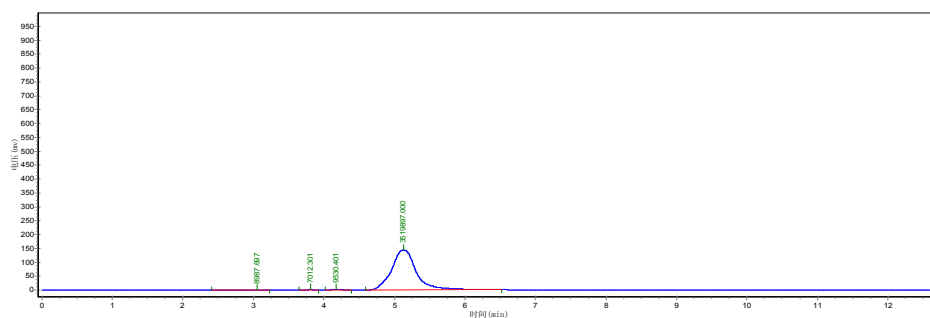
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	3.748	296705.031	5009694.000	97.1470
2	5.108	3173.552	71308.297	1.3828
3	6.117	5808.320	75814.102	1.4702

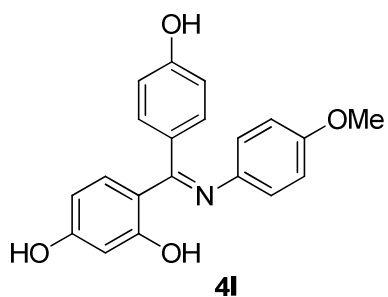
total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

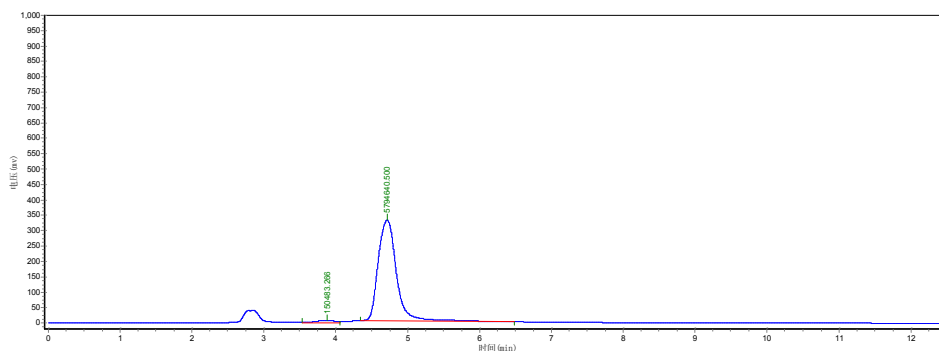


No.	Retention time	Peak height	Peak area	Percent
1	3.057	948.539	8987.697	0.2535
2	3.815	708.000	7012.301	0.1978
3	4.177	725.735	9530.401	0.2688
4	5.127	143966.922	3519897.000	99.2799

total 100



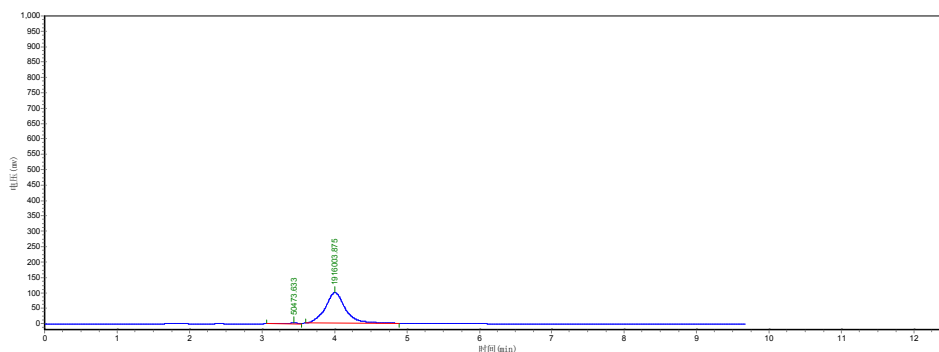
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	3.880	7601.659	150483.266	2.5312
2	4.717	326855.313	5794640.500	97.4688

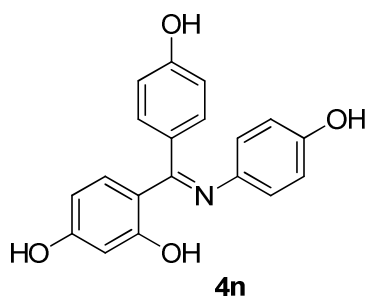
total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)

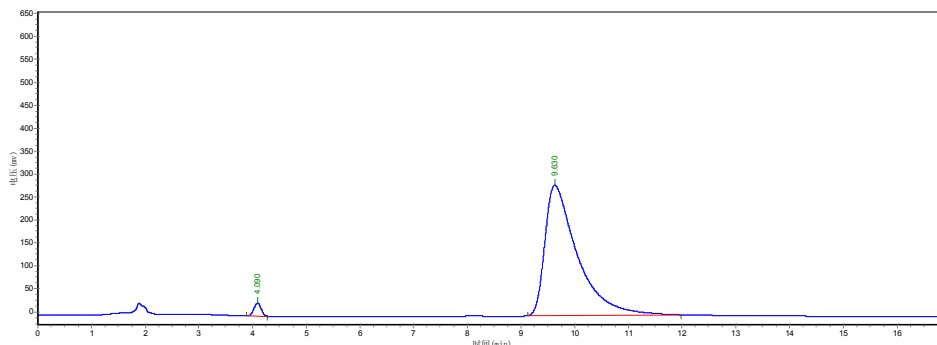


No.	Retention time	Peak height	Peak area	Percent
1	3.437	2761.152	50473.633	2.5667
2	4.007	98980.539	1916003.875	97.4333

total 100



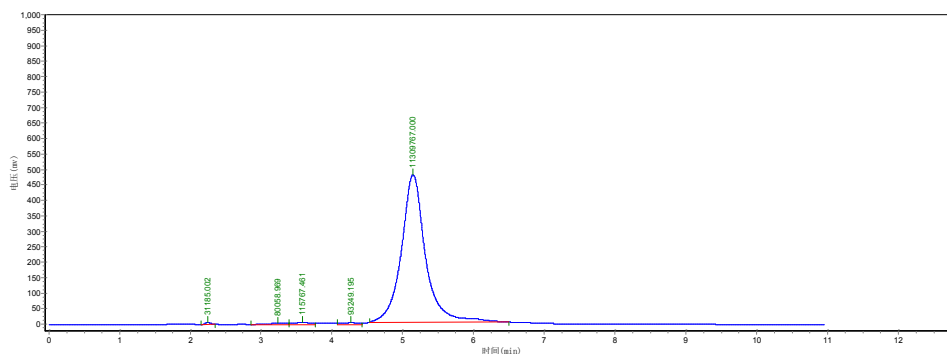
Normal Phase (Method 40:60 Hexane: EtOAc, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	4.090	27935.652	265599.375	2.1777
2	9.630	284386.000	11930706.000	97.8223

total 100

Reverse Phase (Method 40:60 H₂O:CH₃CN, Flow rate 0.7mL/min)



No.	Retention time	Peak height	Peak area	Percent
1	2.245	6293.490	31185.002	0.2681
2	3.238	4626.422	80058.969	0.6884
3	3.582	6729.552	115767.461	0.9954
4	4.272	5669.687	93249.195	0.8018
5	5.147	476242.719	11309767.000	97.2463

total 100