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Supporting Information

Diastereo- and Enantioselective Construction of Chiral Cyclopenta[*b*]indole Framework via A Catalytic Asymmetric Tandem Cyclization of 2-Indolymethanols with 2-Naphthols

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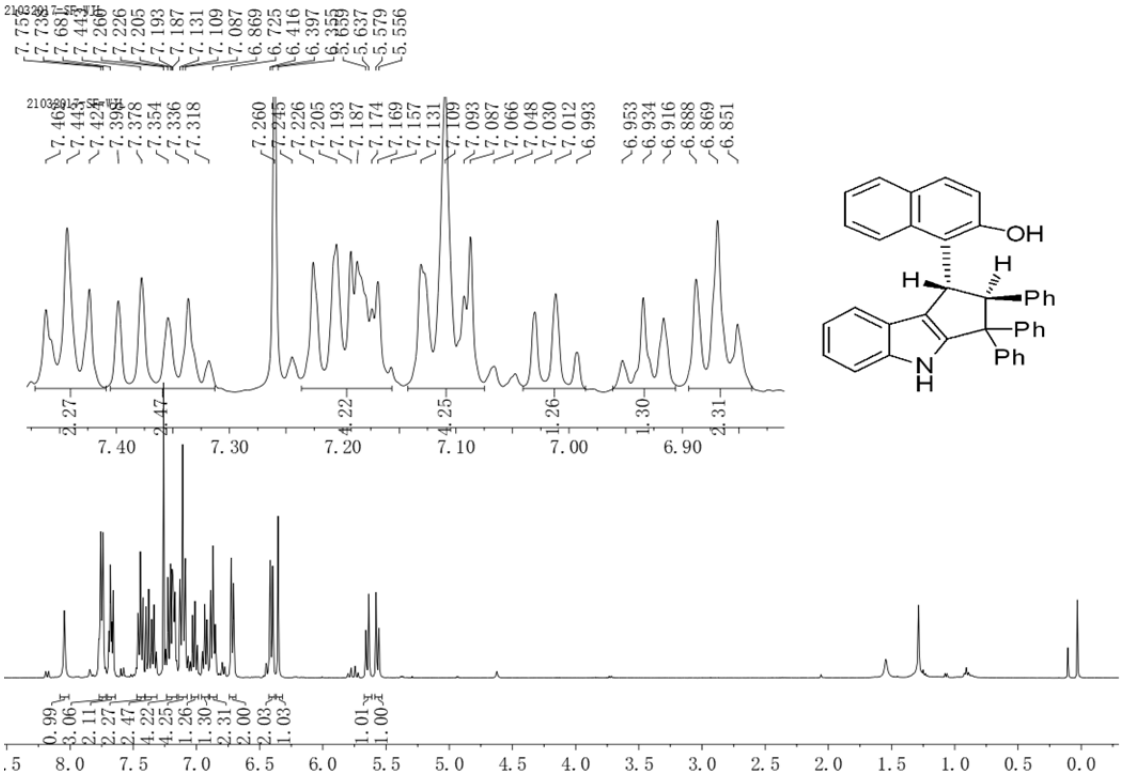
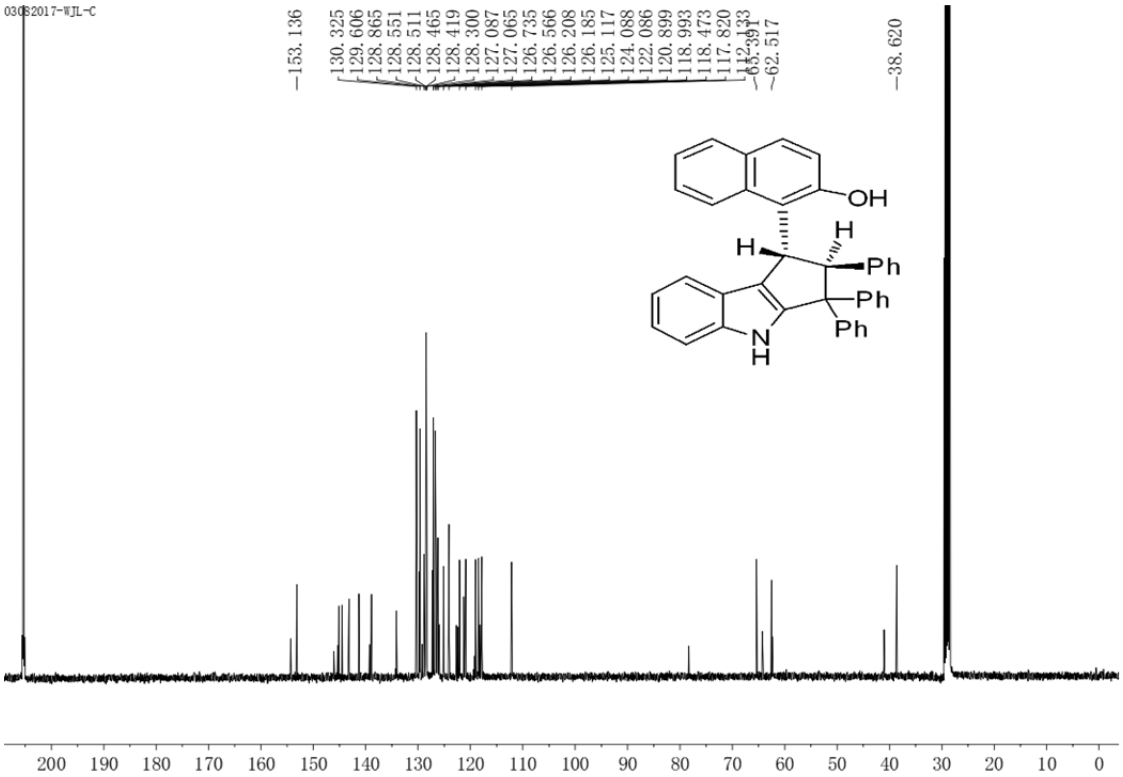
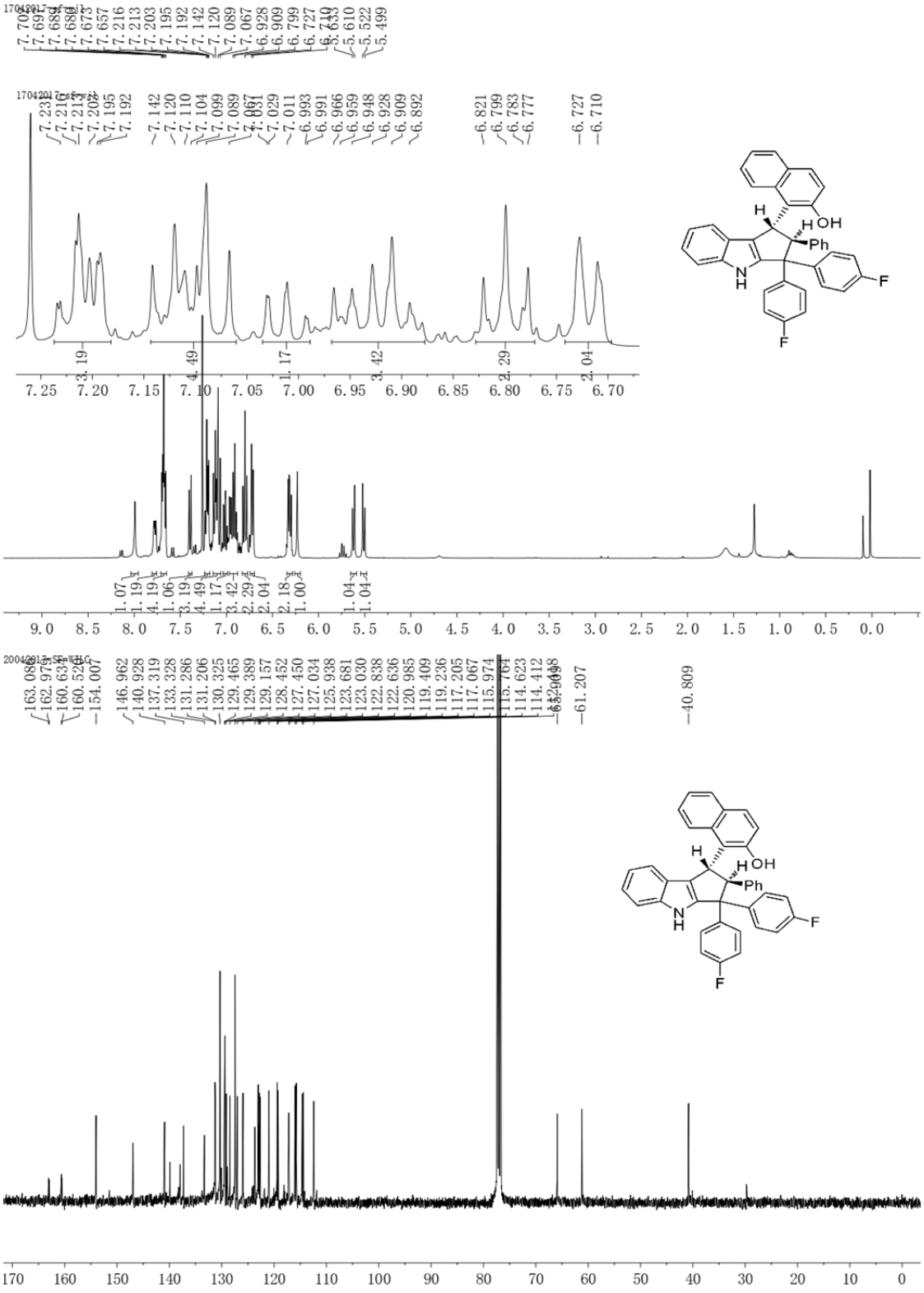




3ba (inseparable diastereomers of 87:13 dr)



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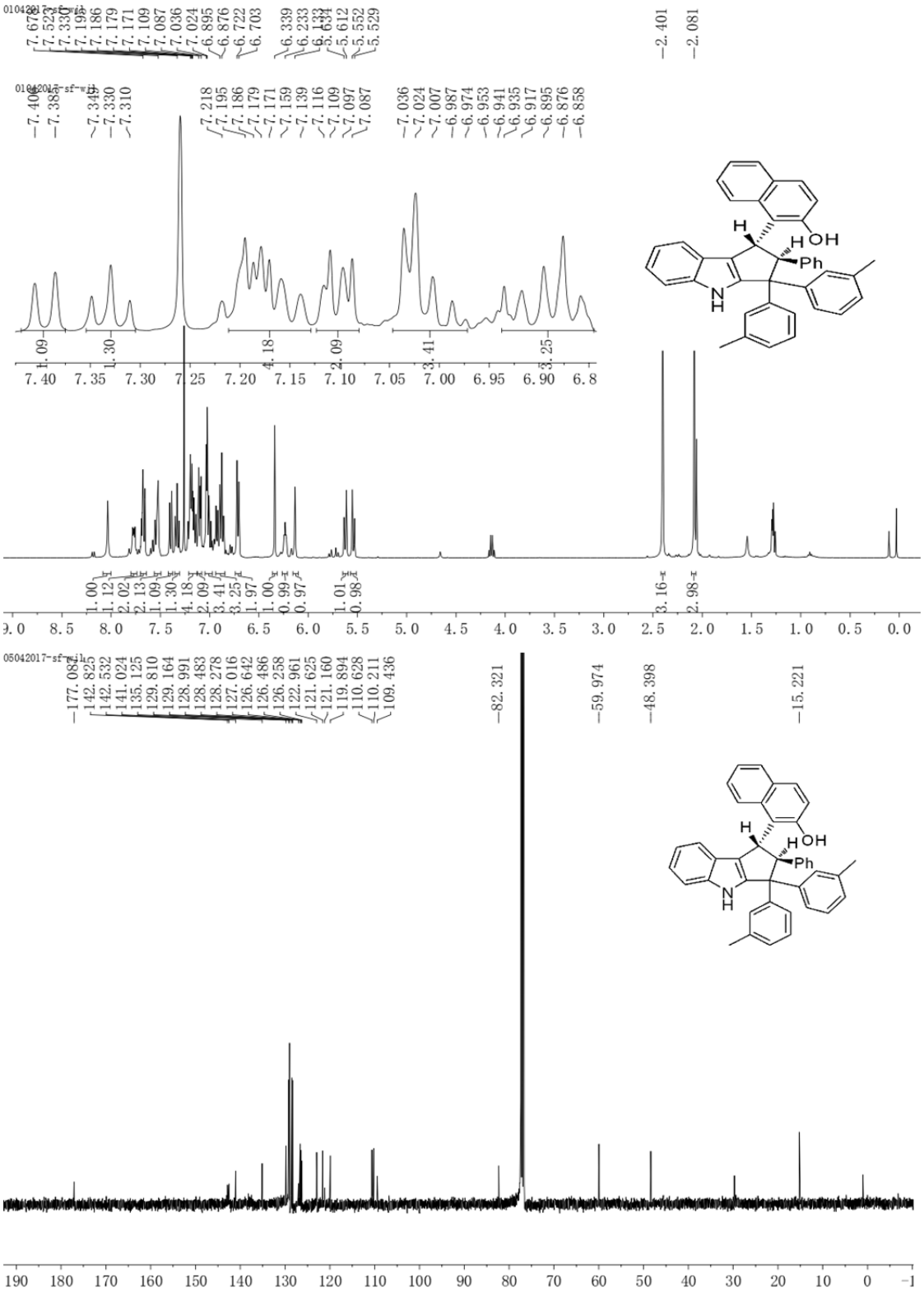

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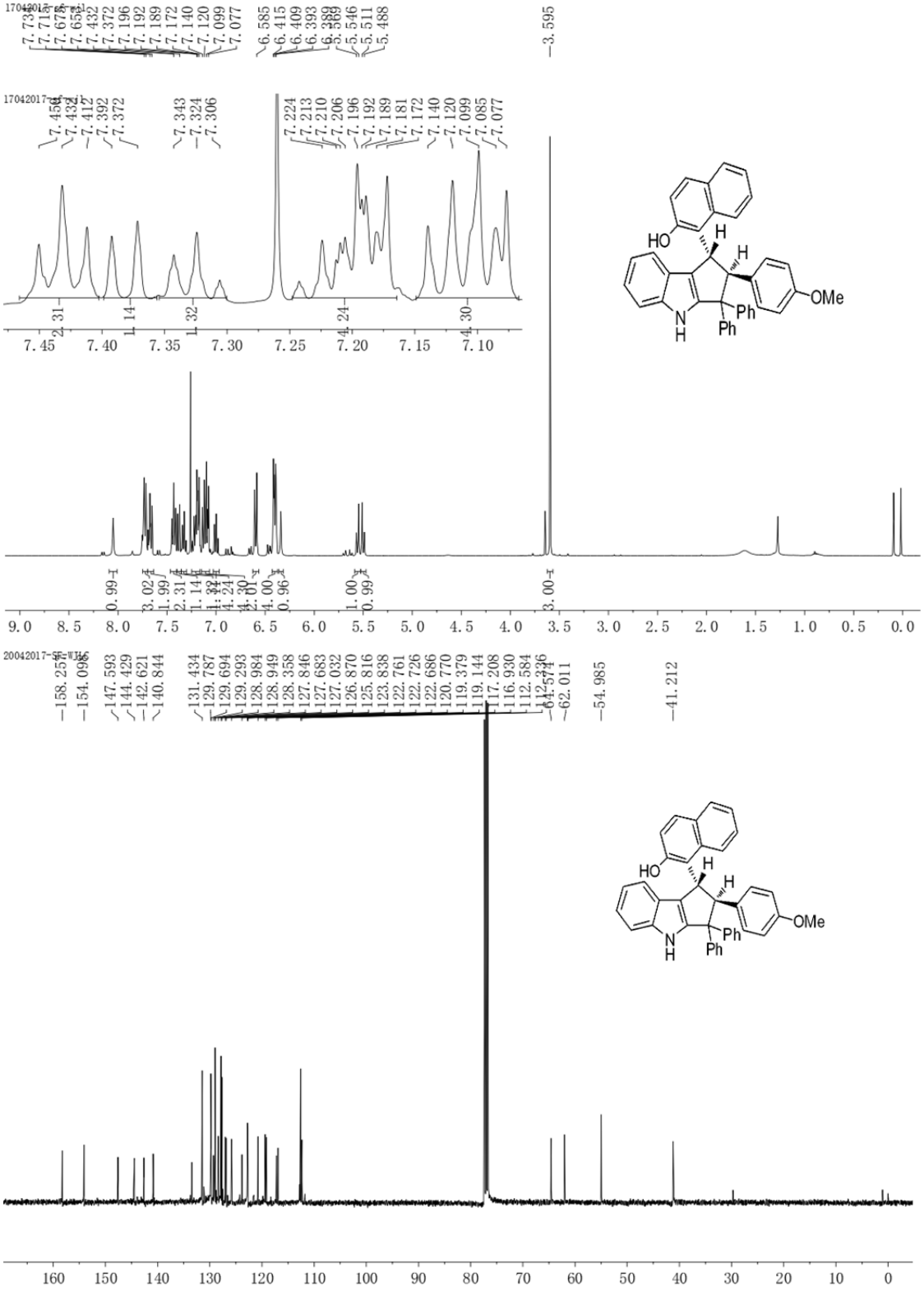

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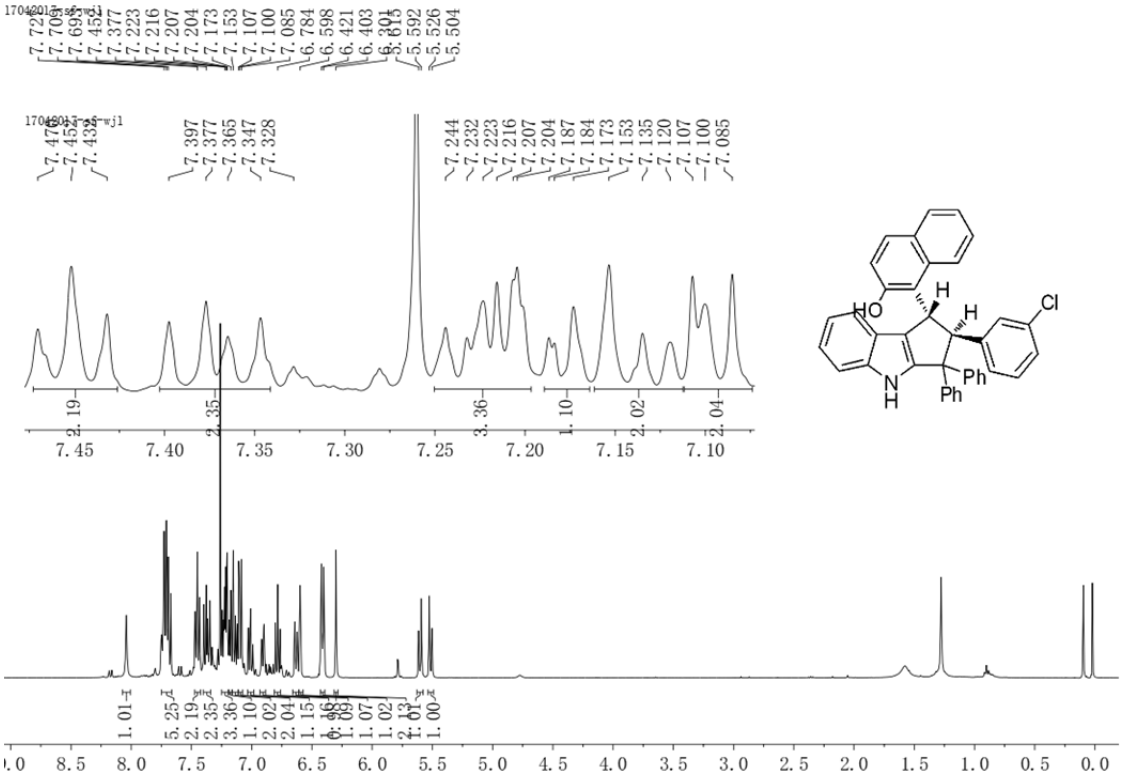

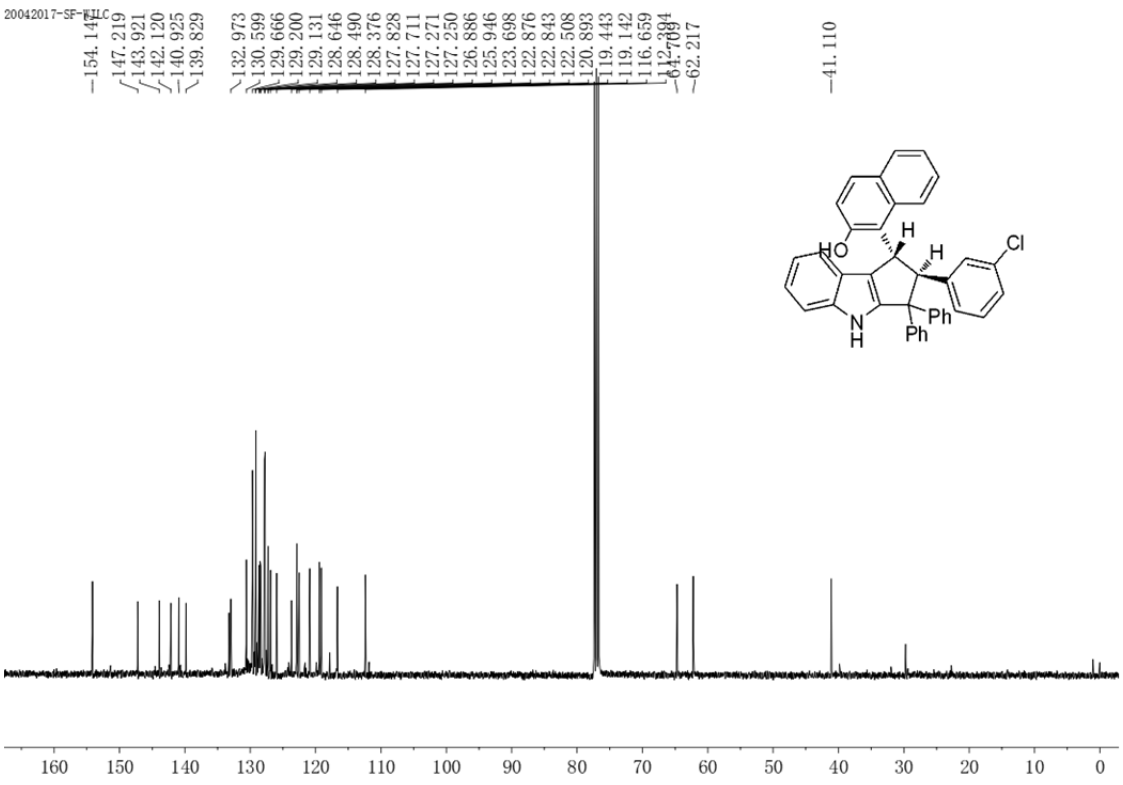

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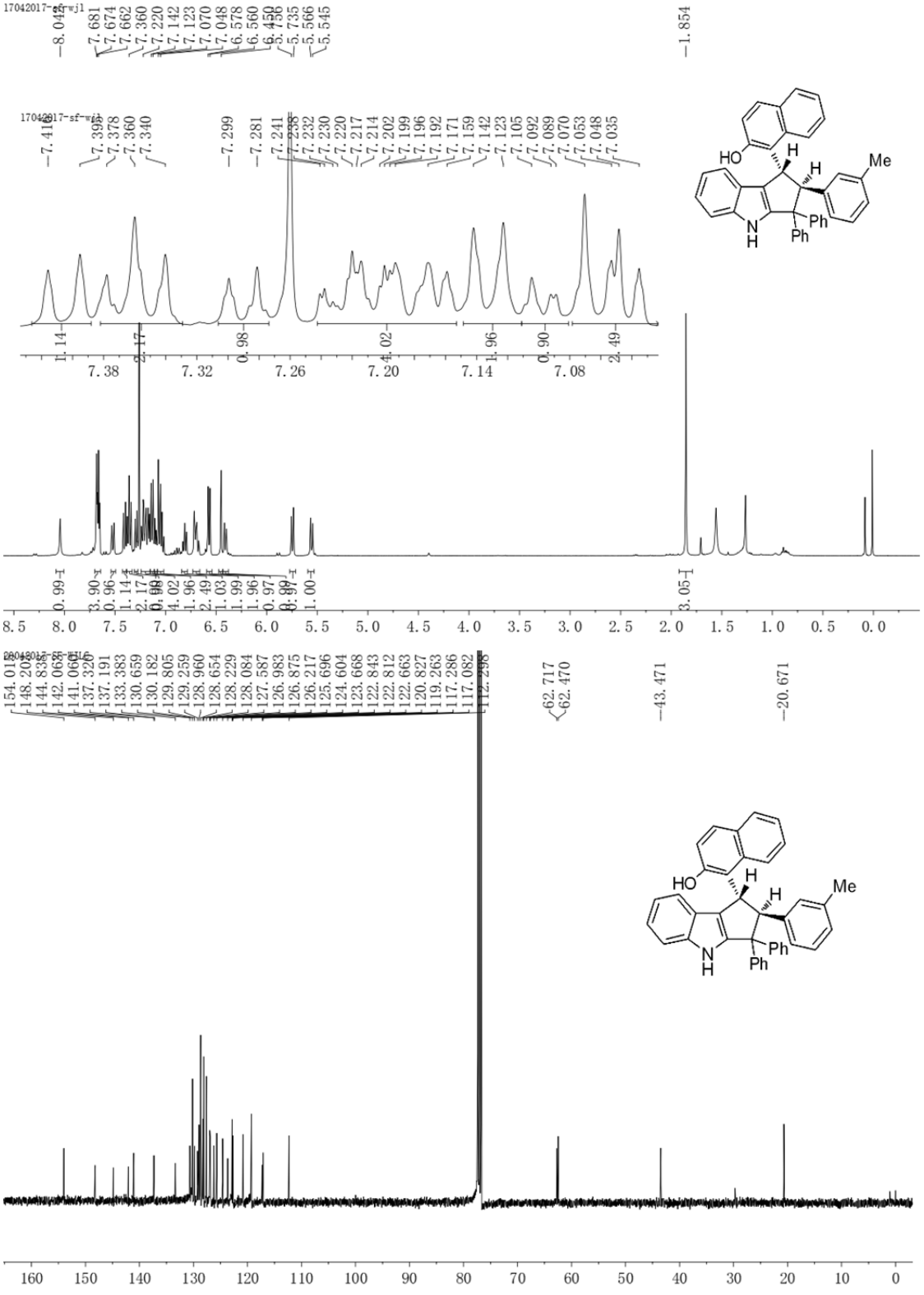

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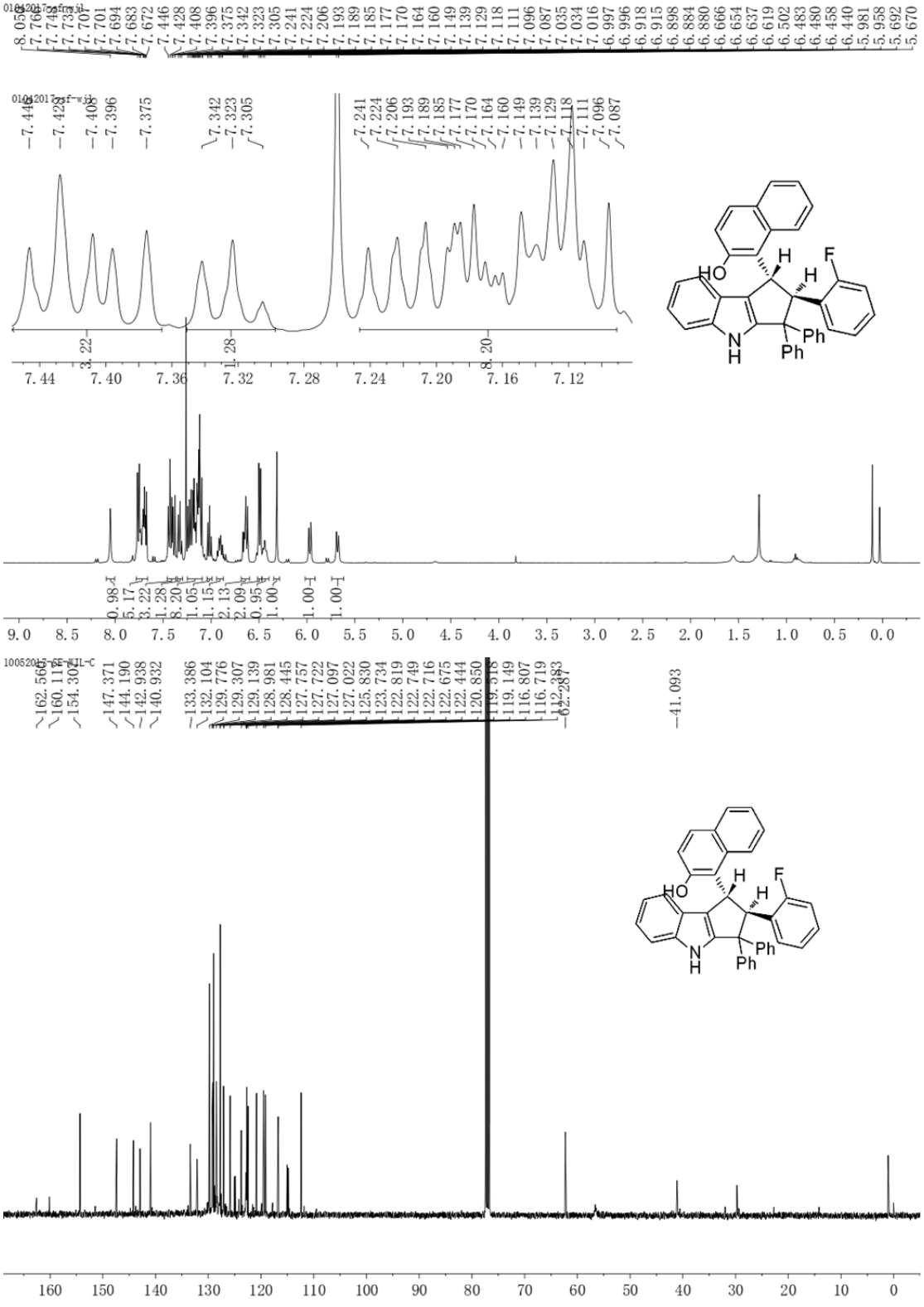

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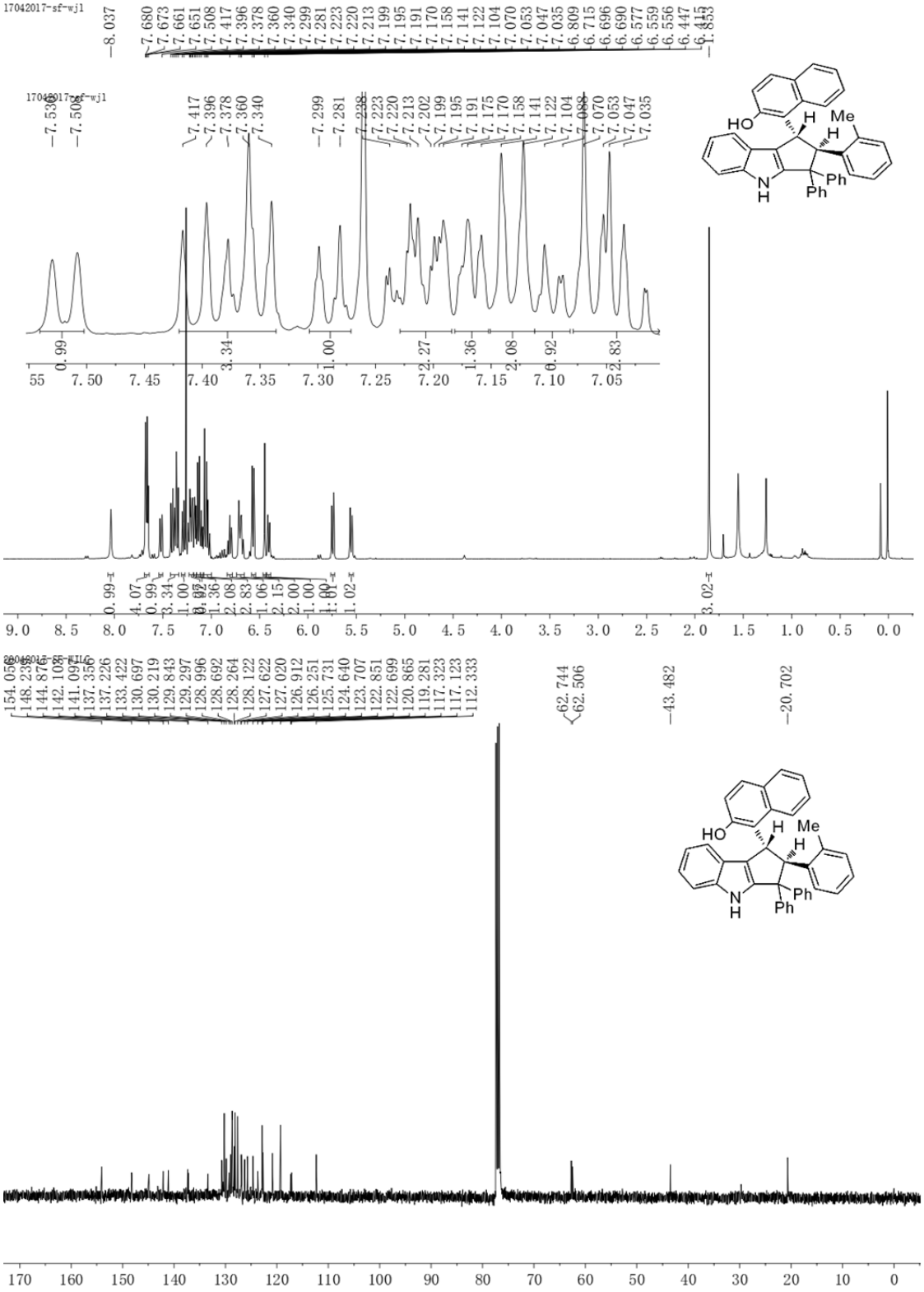

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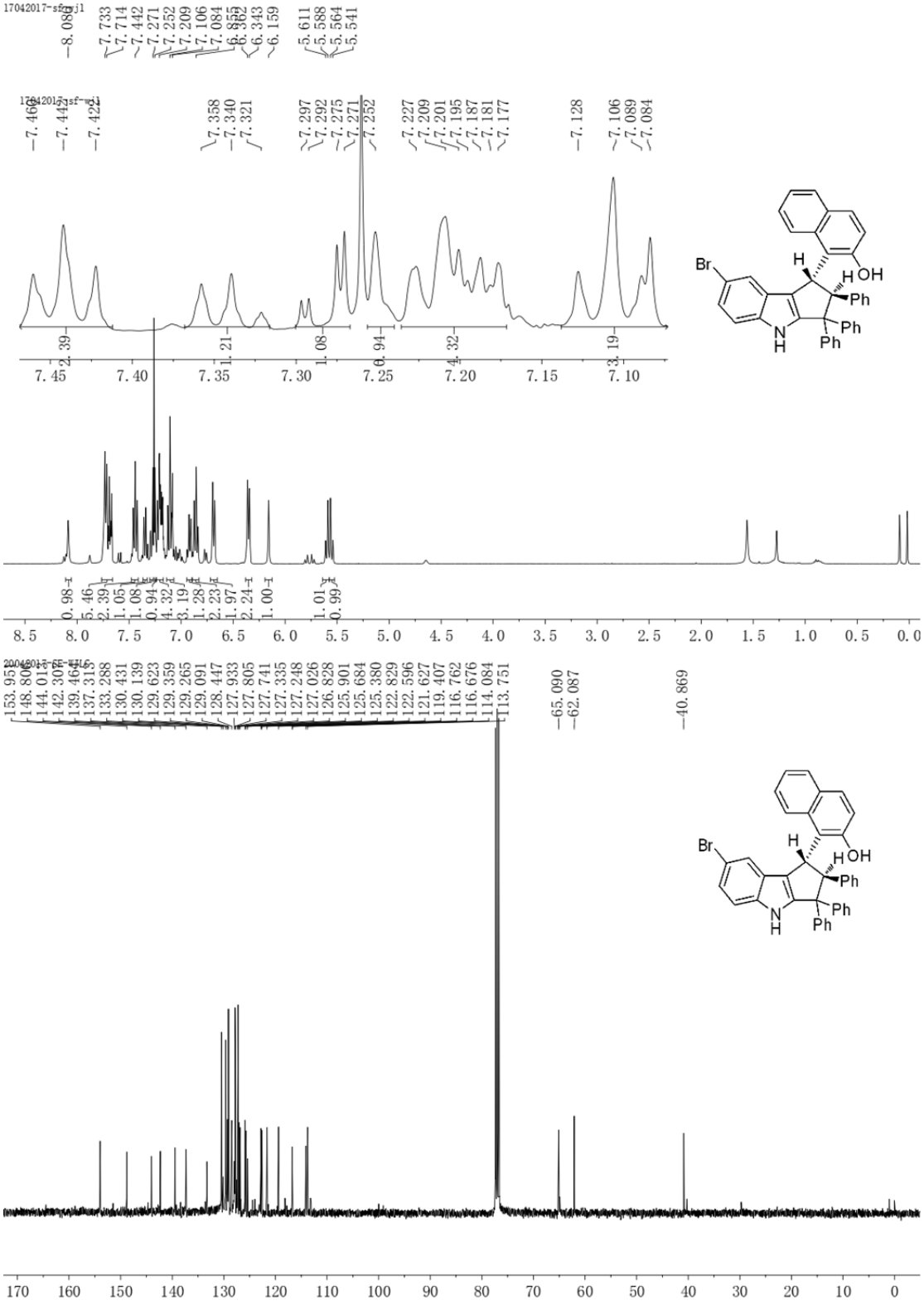

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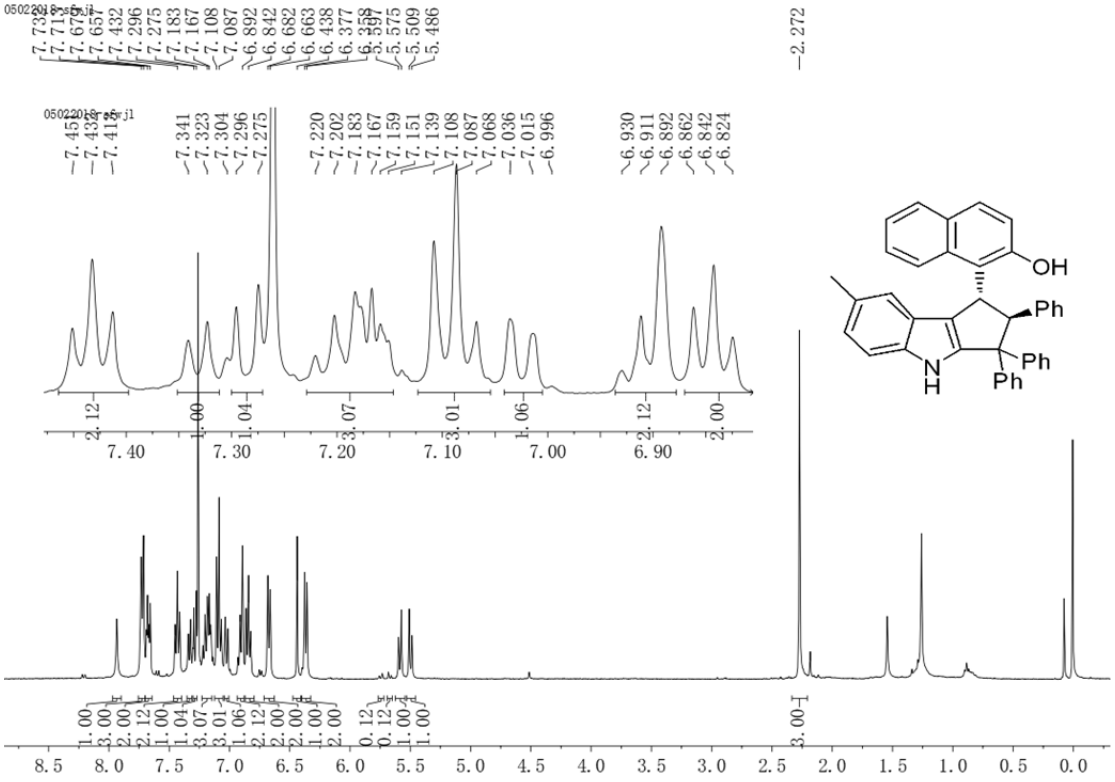

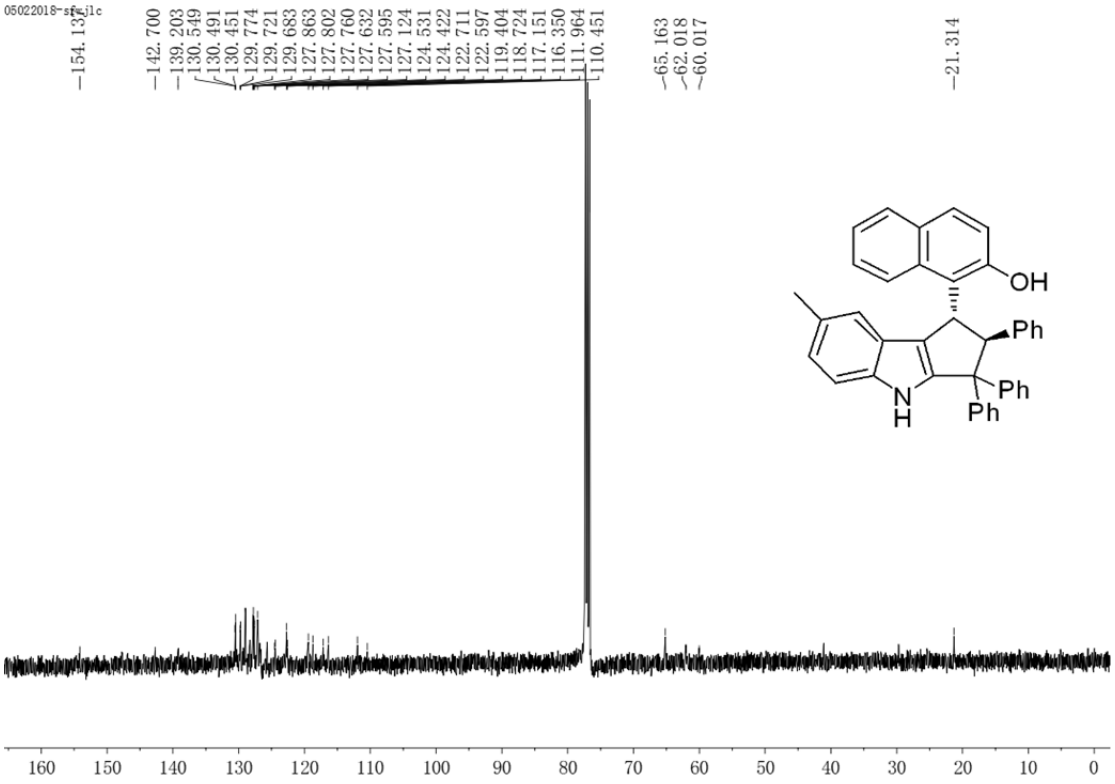

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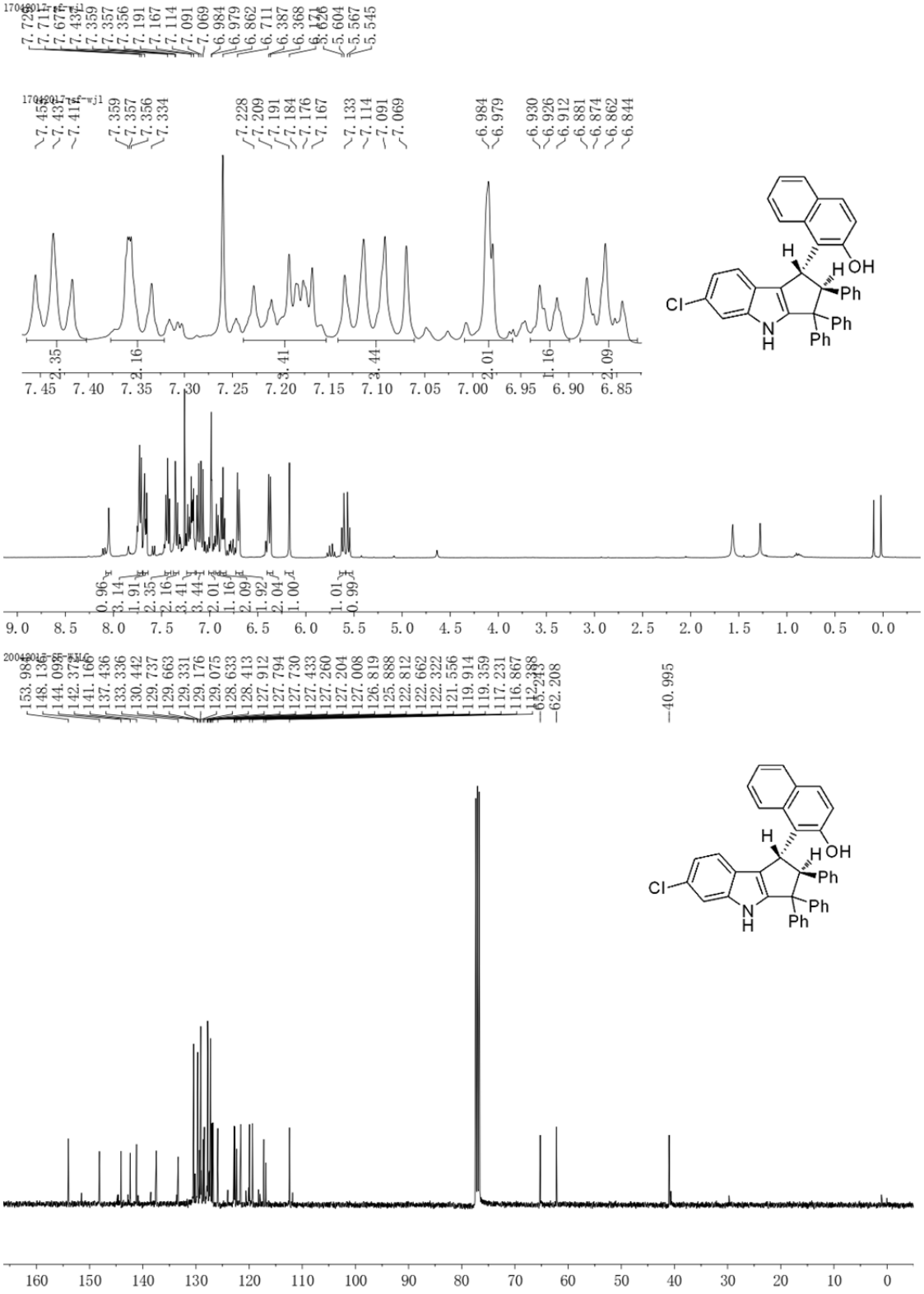

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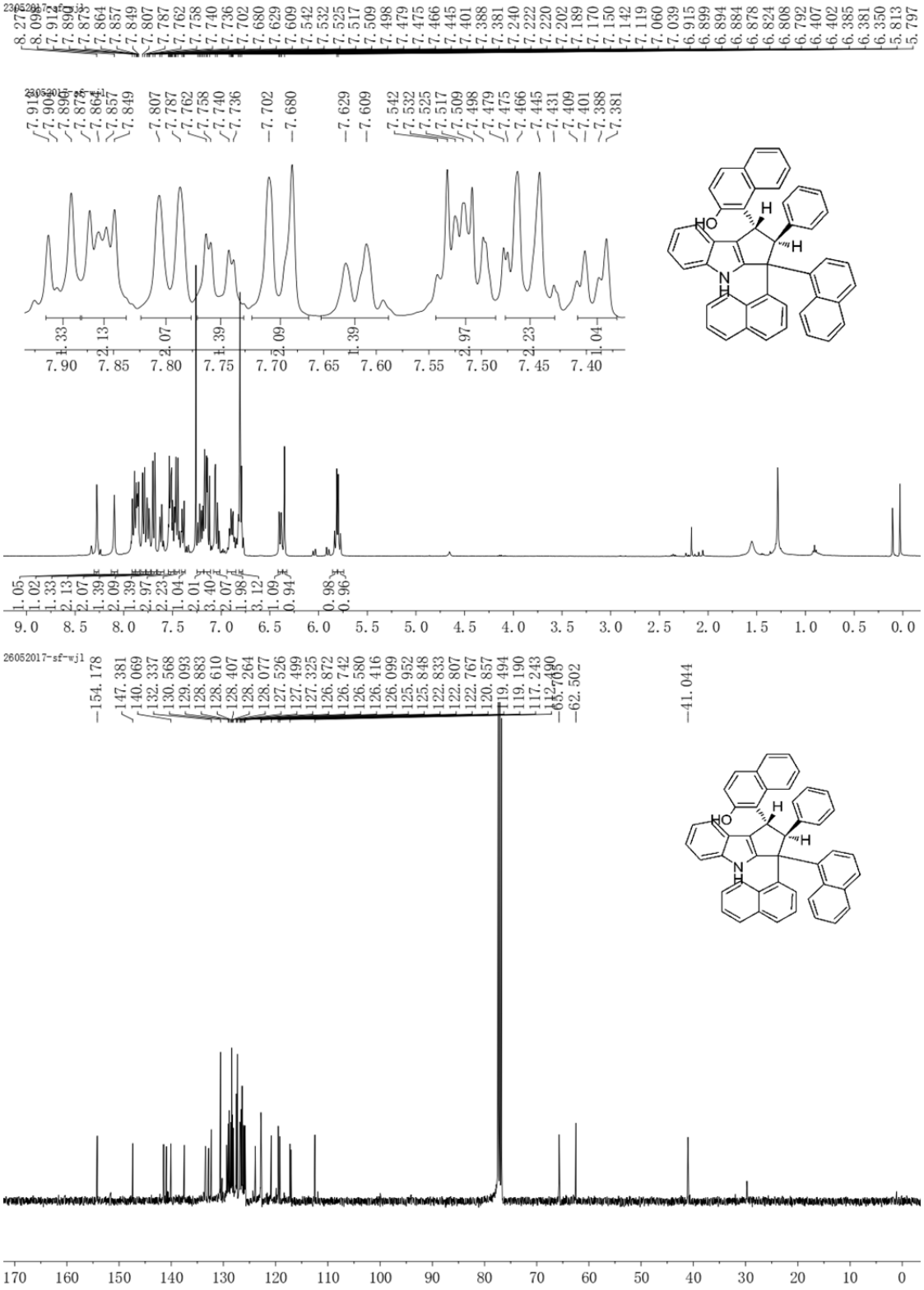
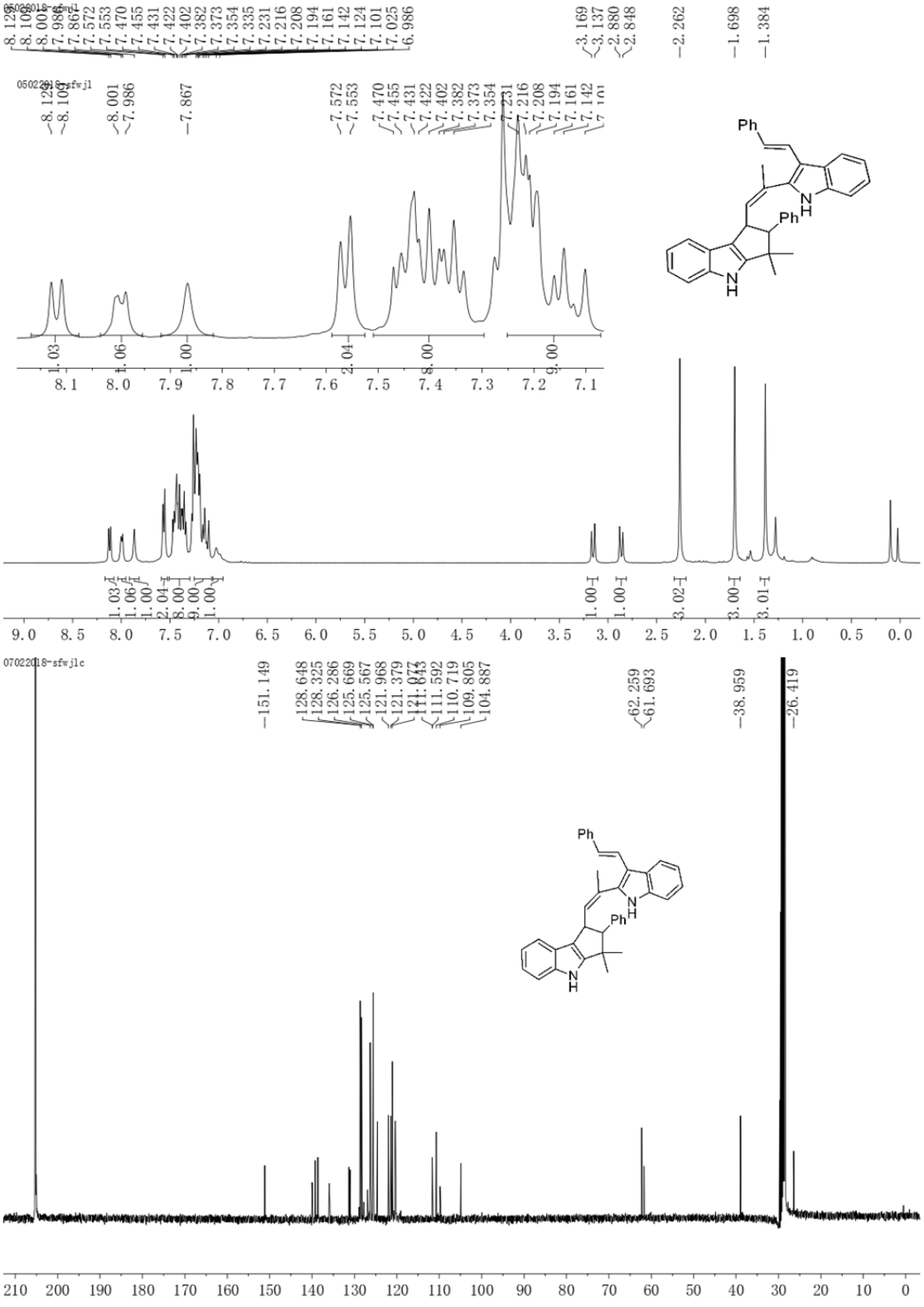


Compound 6



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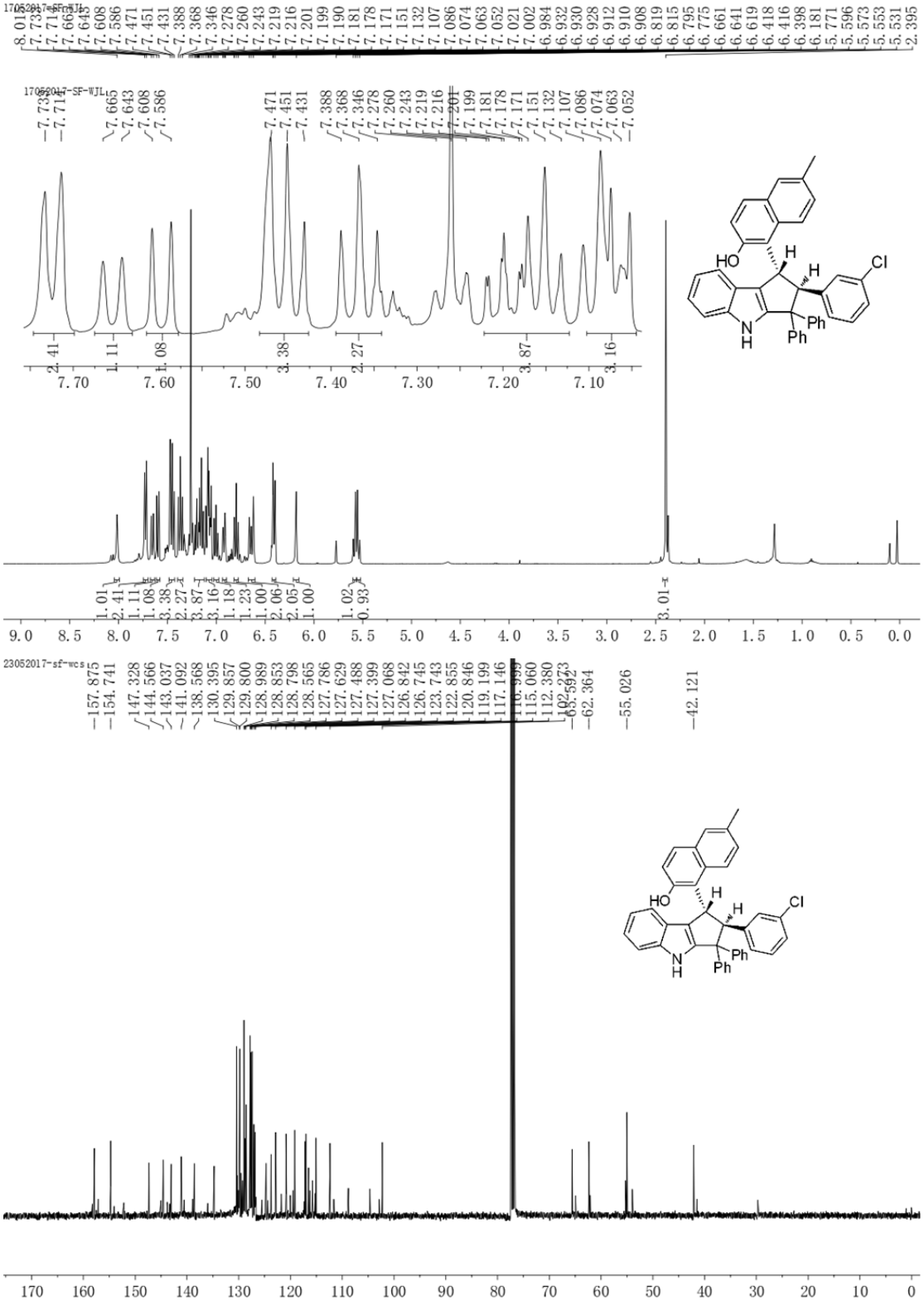

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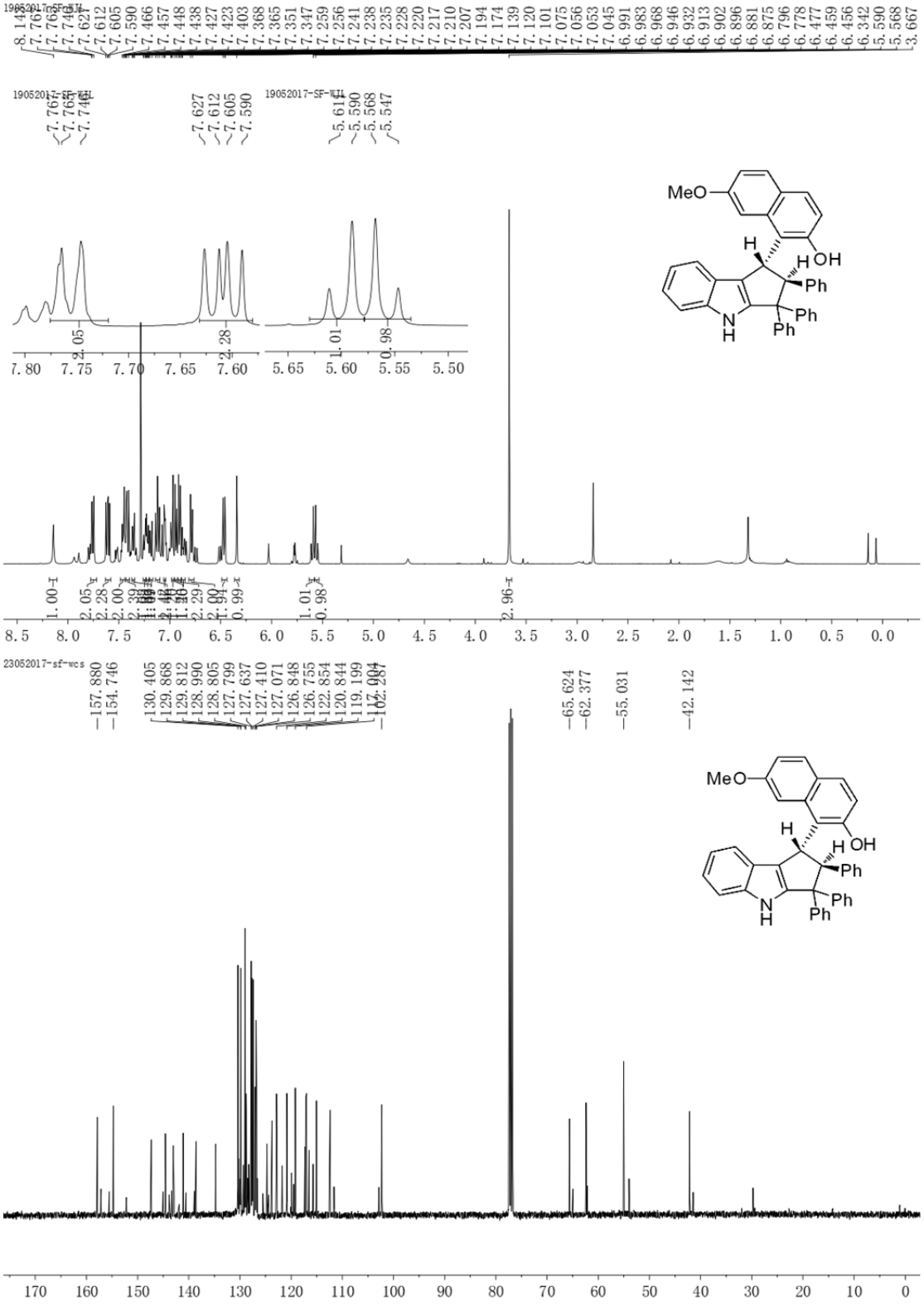

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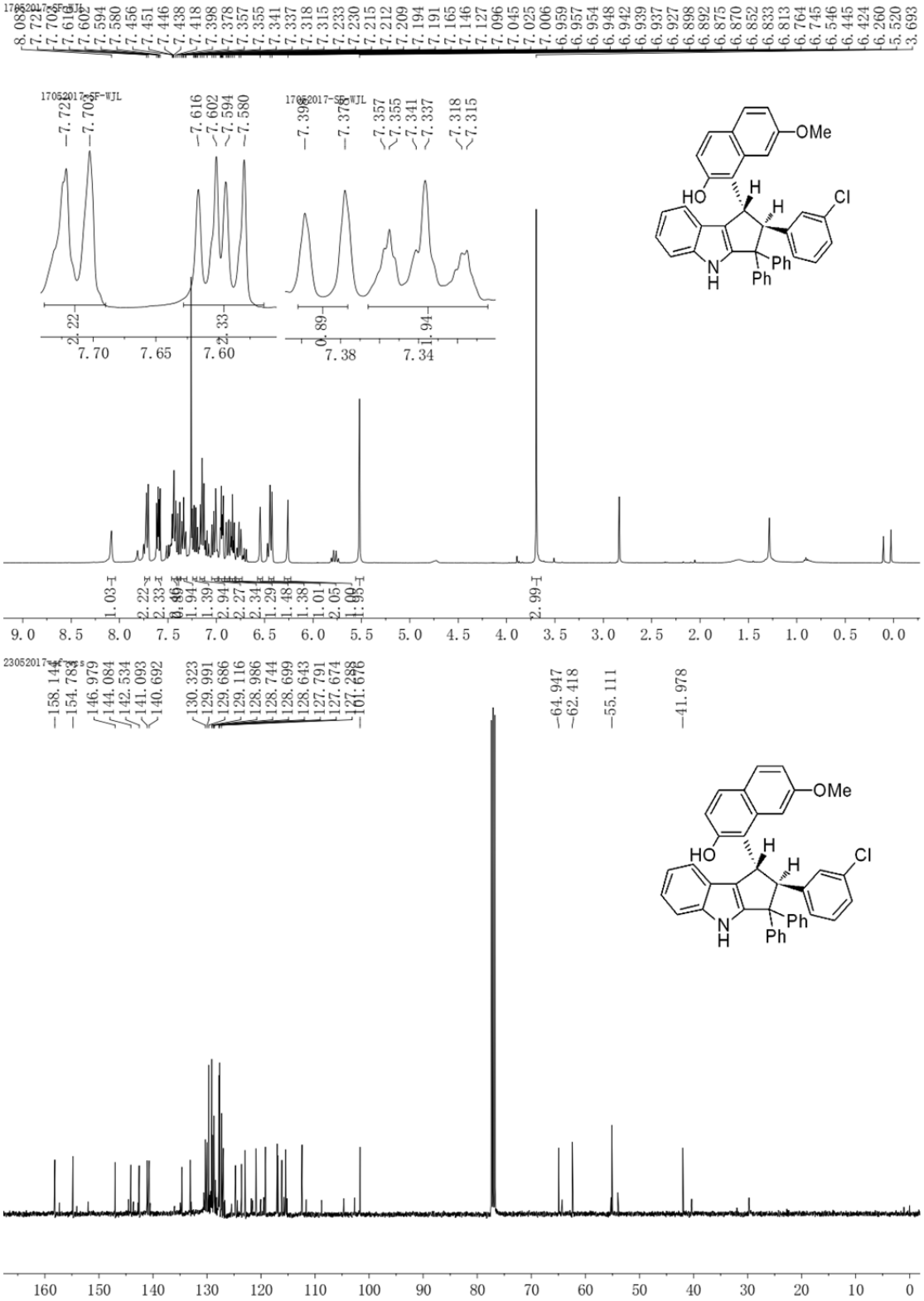
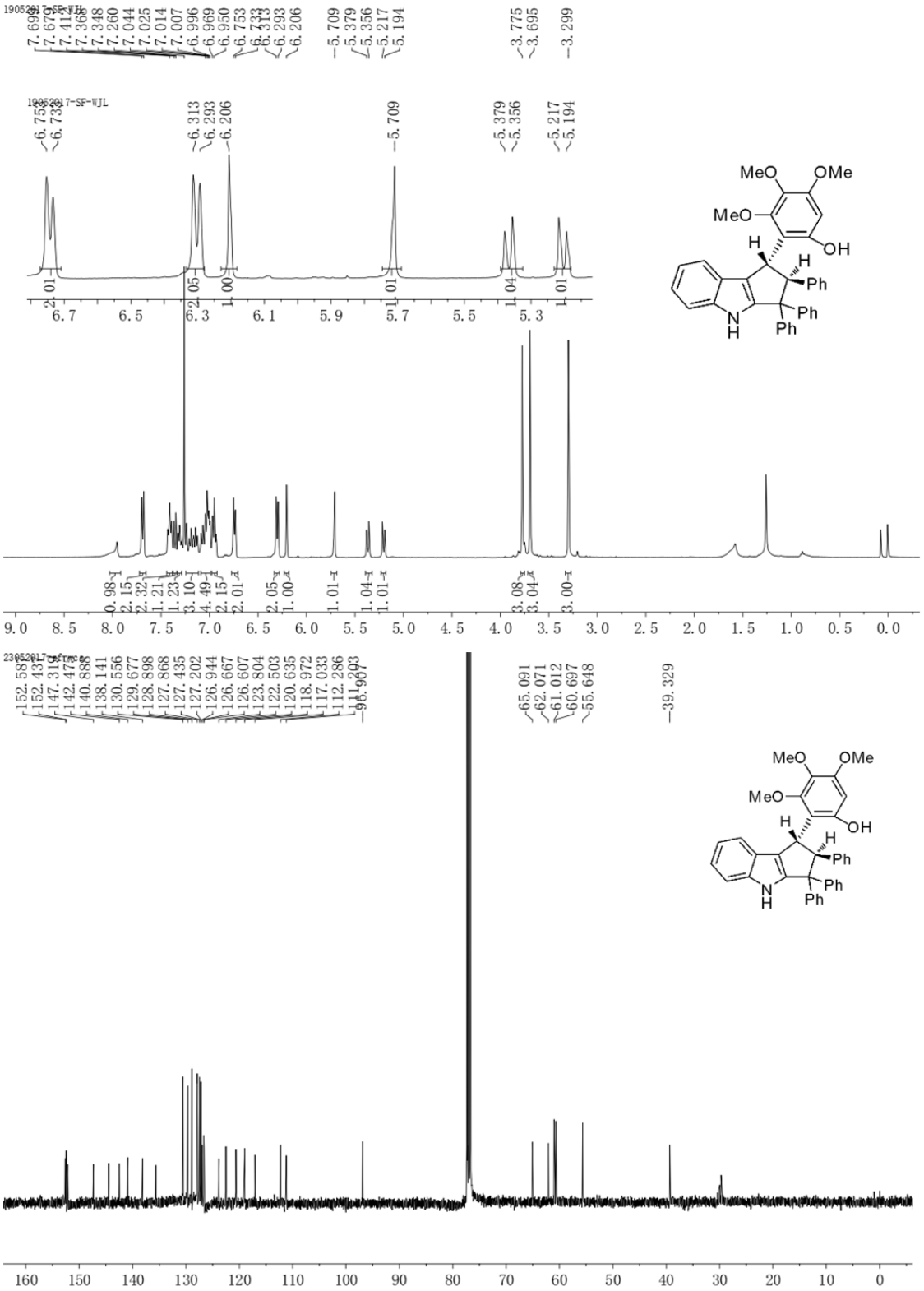
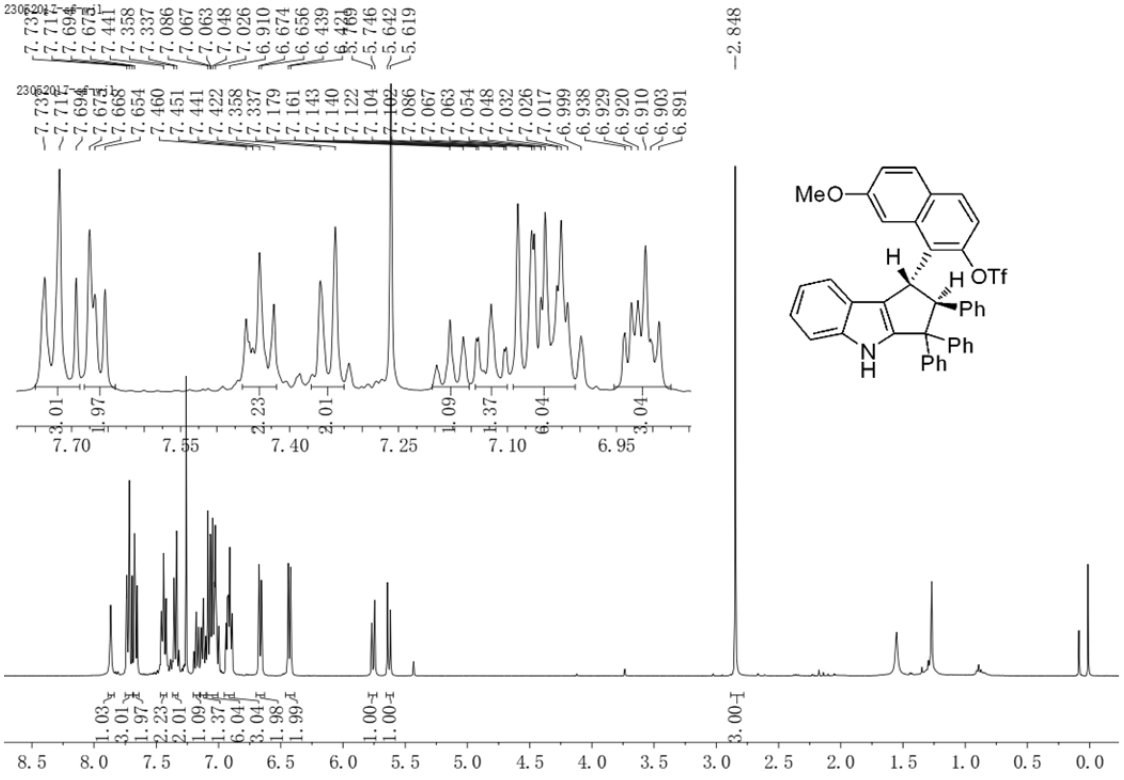
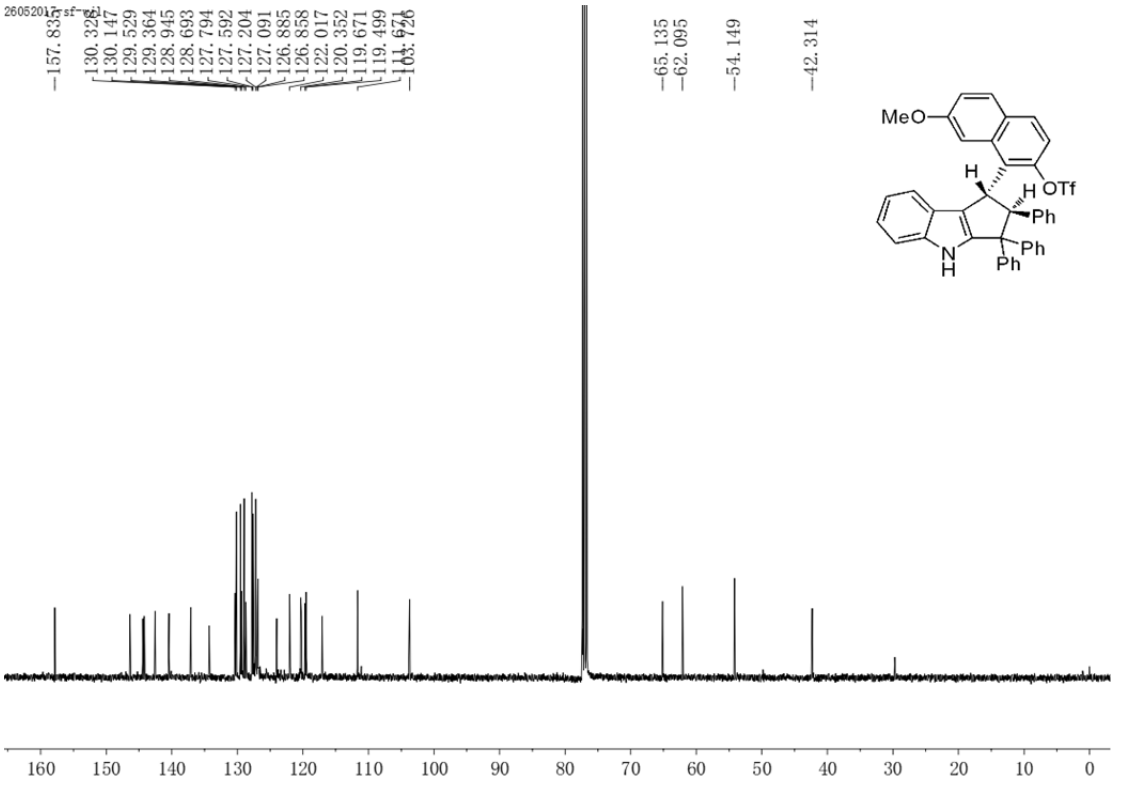


3ad



Compound 7

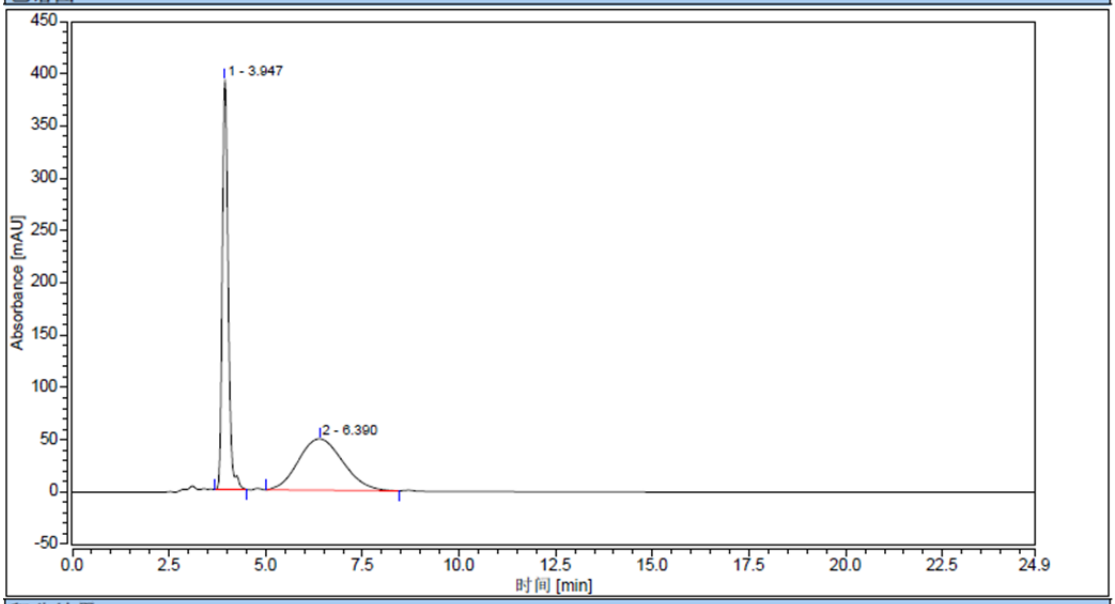




2. HPLC spectra of products 3 and 6-7

3aa

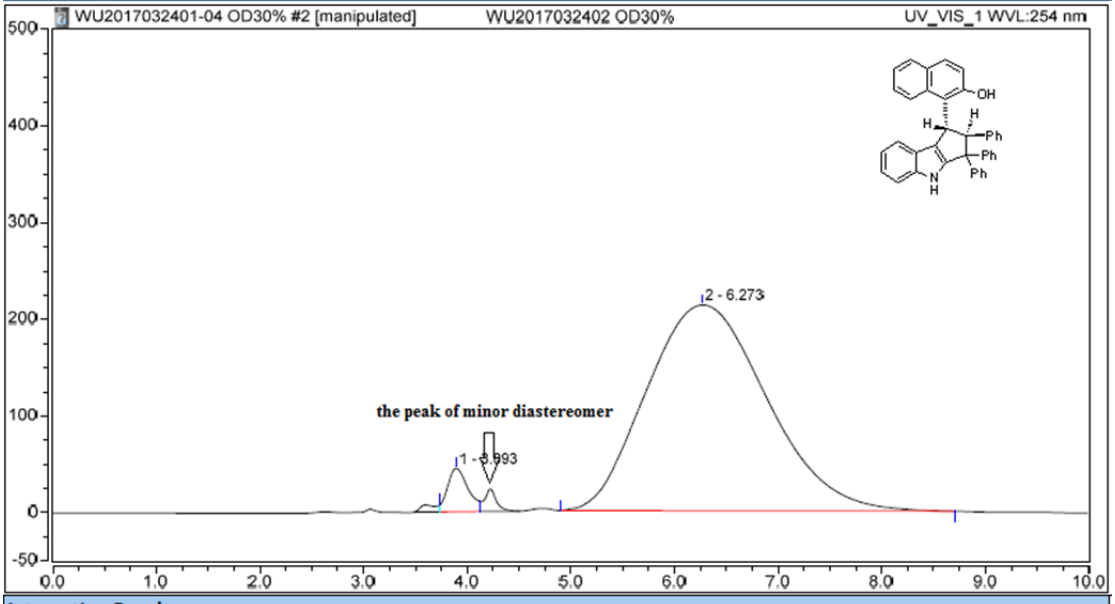
色谱图



积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		3.947	68.218	391.867	50.99	88.87	n.a.
2		6.390	65.581	49.099	49.01	11.13	n.a.
总和:			133.799	440.966	100.00	100.00	

Chromatogram

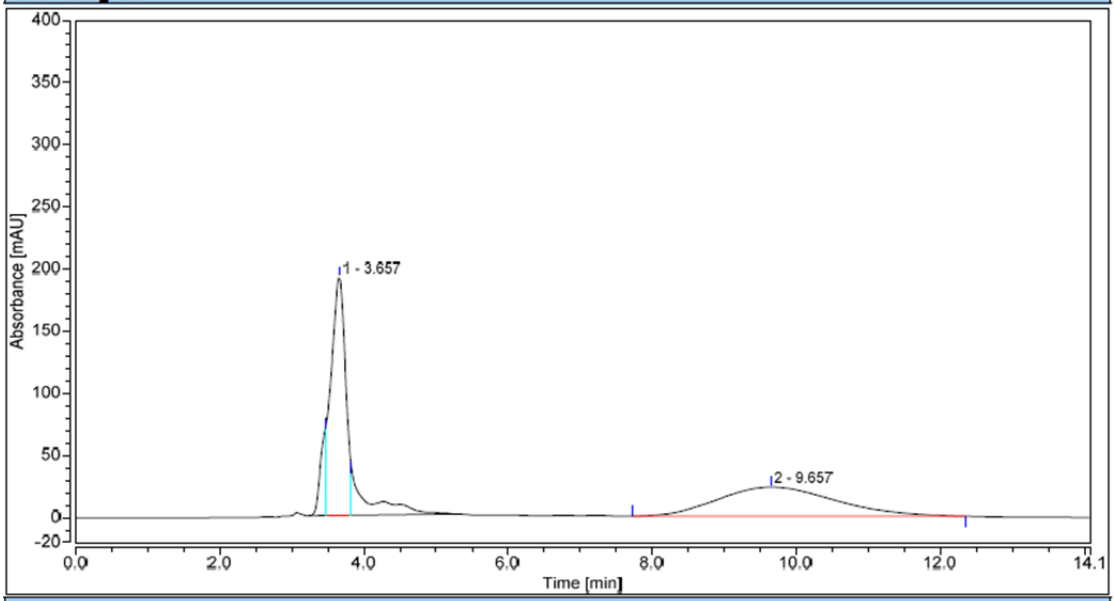


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		3.893	10.138	44.971	3.42	17.44	n.a.
2		6.273	285.959	212.897	96.58	82.56	n.a.
Total:			296.097	257.869	100.00	100.00	

3ba

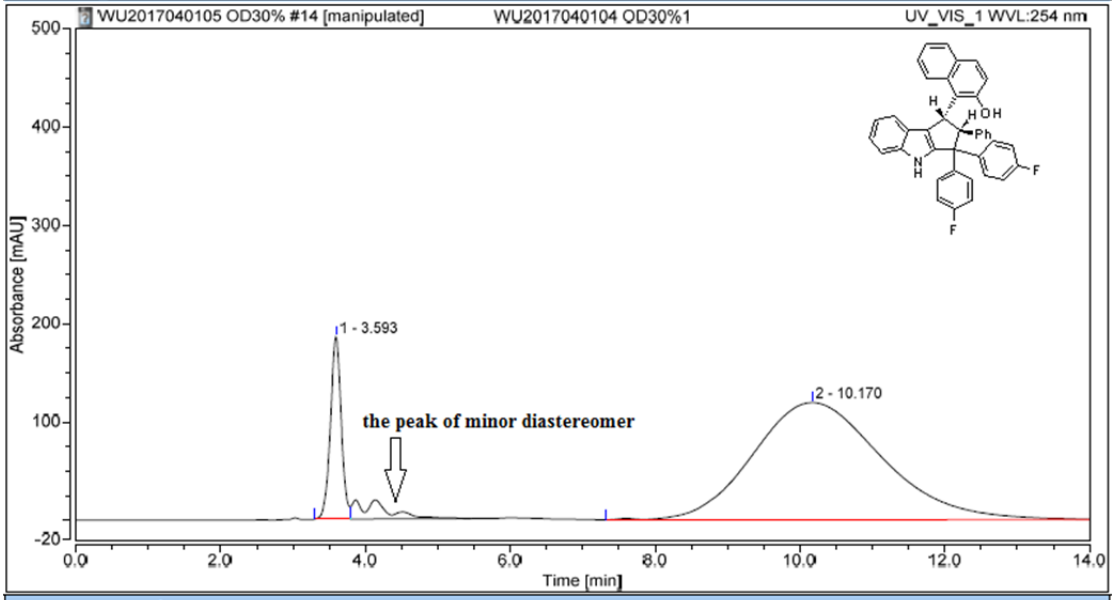
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		3.657	44.471	191.486	50.17	89.12	n.a.
2		9.657	44.175	23.383	49.83	10.88	n.a.
Total:			**88.646**	**214.869**	**100.00**	**100.00**	

Chromatogram

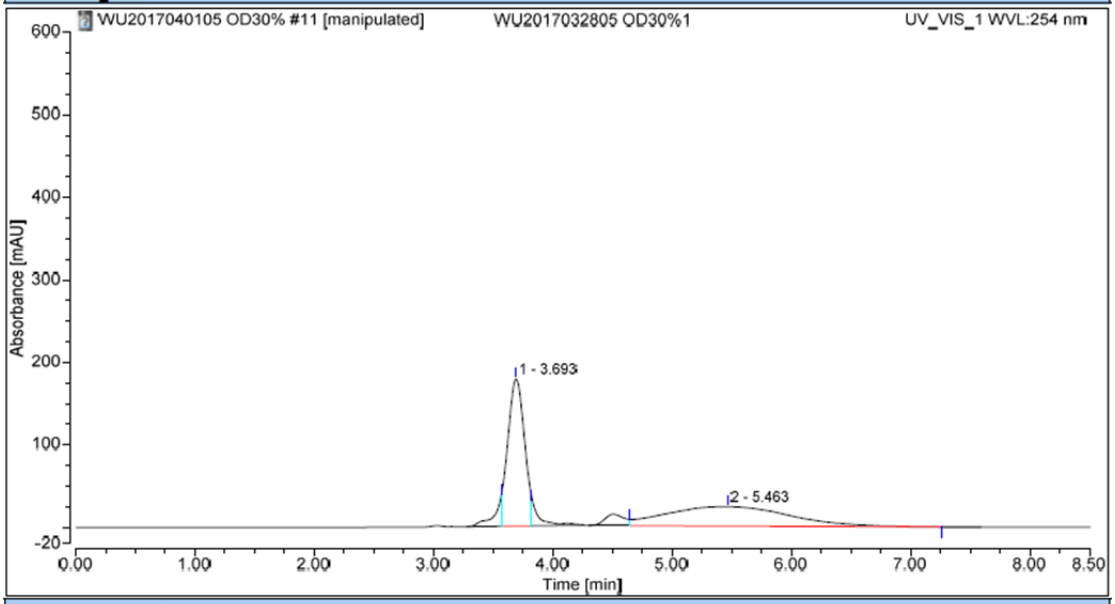


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		3.593	32.116	185.423	11.52	60.88	n.a.
2		10.170	246.576	119.169	88.48	39.12	n.a.
Total:			**278.691**	**304.592**	**100.00**	**100.00**	

3ca

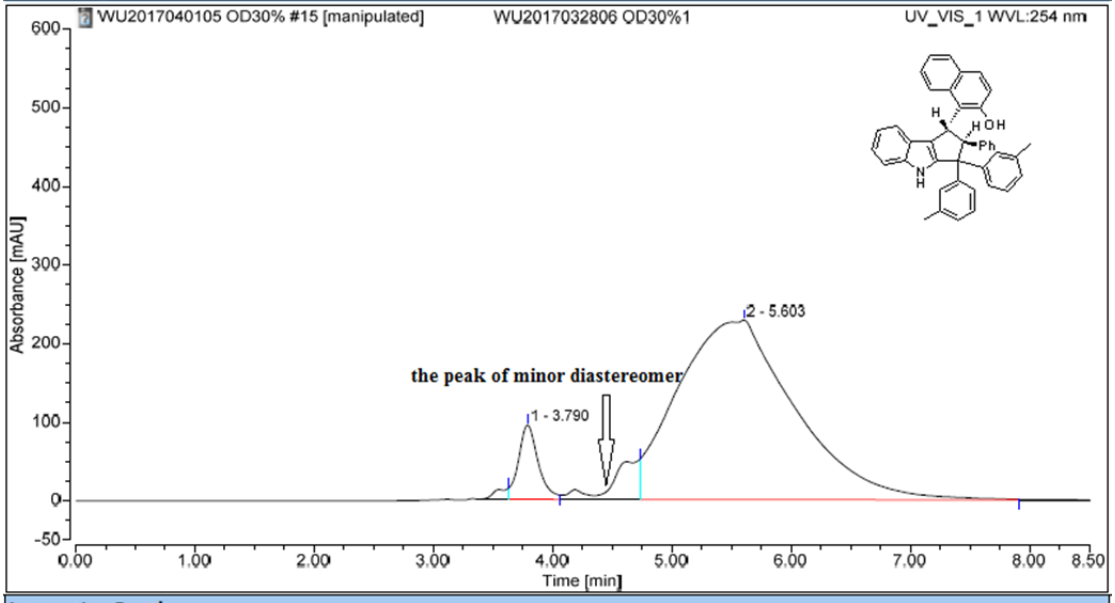
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		3.693	28.207	178.532	49.87	88.25	n.a.
2		5.463	28.352	23.769	50.13	11.75	n.a.
Total:			**56.558**	**202.301**	**100.00**	**100.00**	

Chromatogram

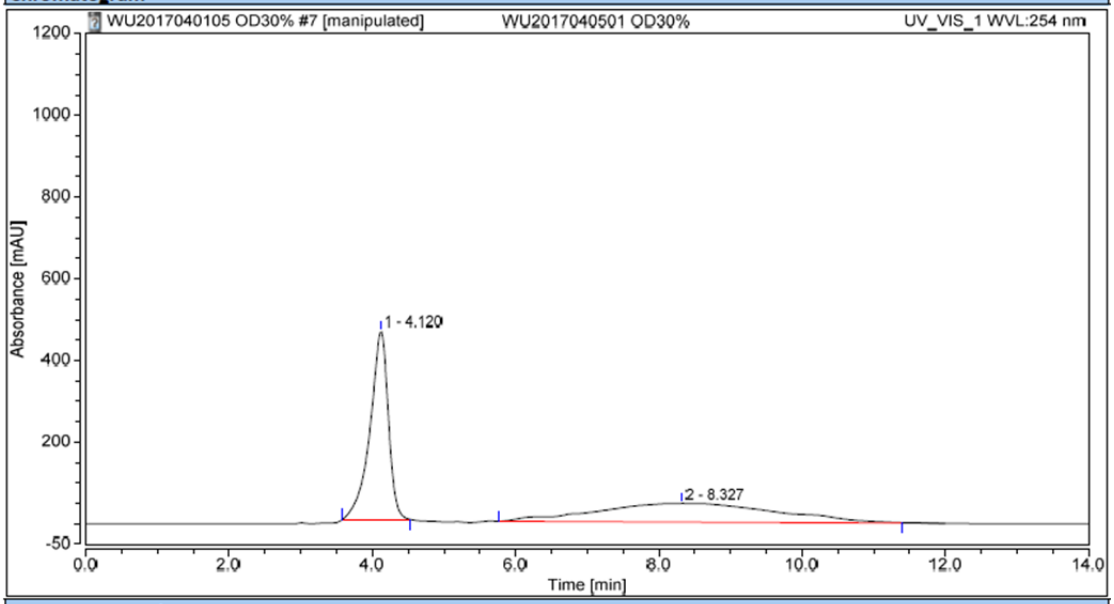


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		3.790	18.052	94.493	6.50	29.28	n.a.
2		5.603	259.873	228.187	93.50	70.72	n.a.
Total:			**277.925**	**322.680**	**100.00**	**100.00**	

3da

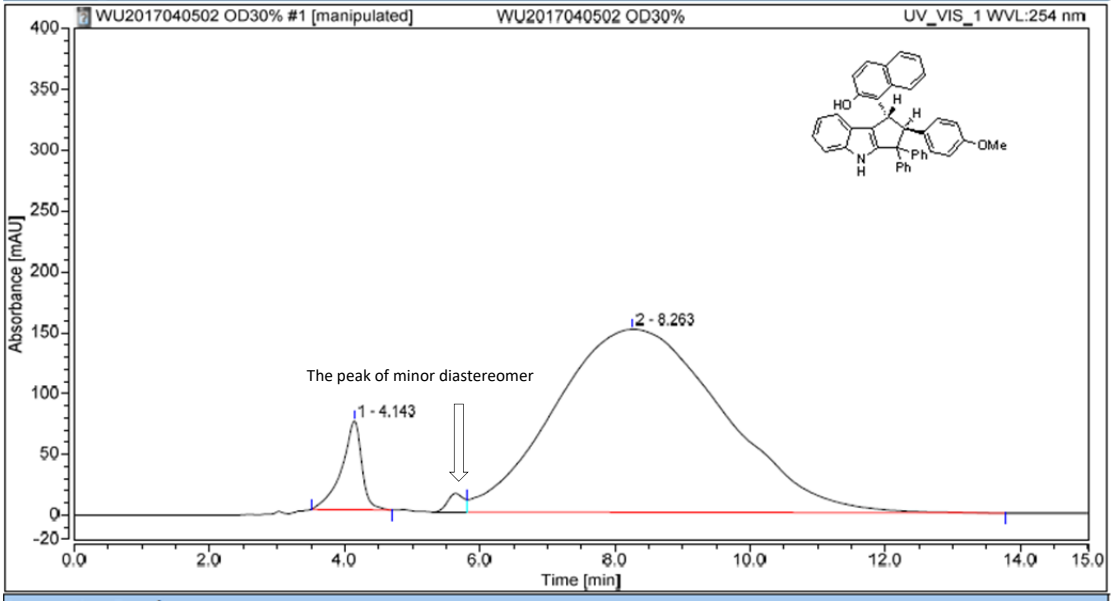
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.120	136.207	460.219	50.34	90.94	n.a.
2		8.327	134.350	45.834	49.66	9.06	n.a.
Total:			**270.558**	**506.054**	**100.00**	**100.00**	

Chromatogram

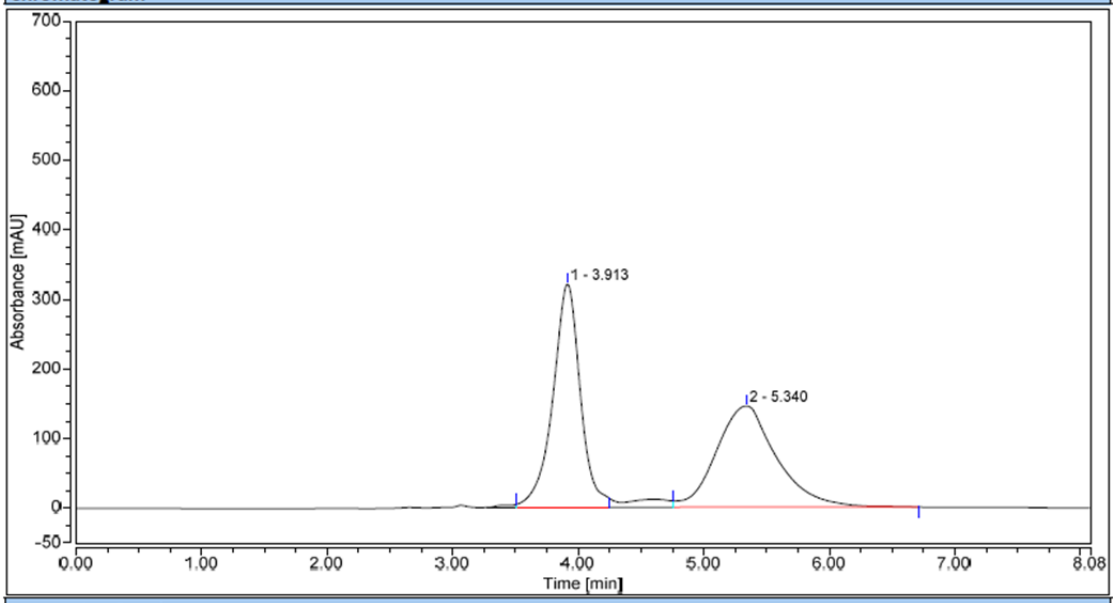


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.143	25.143	72.973	5.46	32.65	n.a.
2		8.263	435.422	150.548	94.54	67.35	n.a.
Total:			**460.565**	**223.521**	**100.00**	**100.00**	

3ea

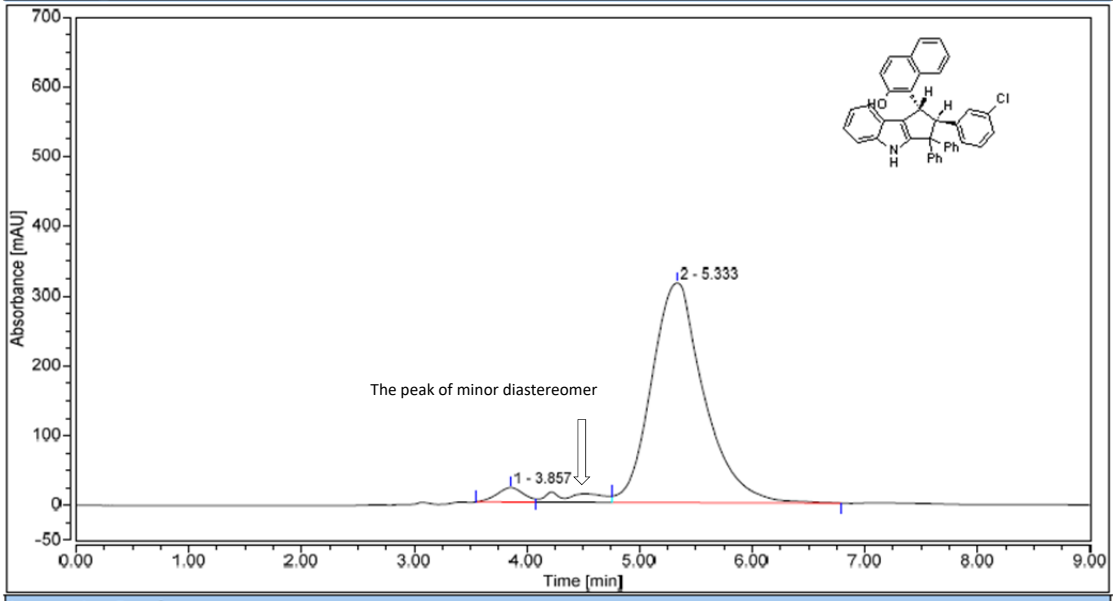
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		3.913	81.308	320.820	50.13	68.84	n.a.
2		5.340	80.877	145.220	49.87	31.16	n.a.
Total:			**162.186**	**466.040**	**100.00**	**100.00**	

Chromatogram

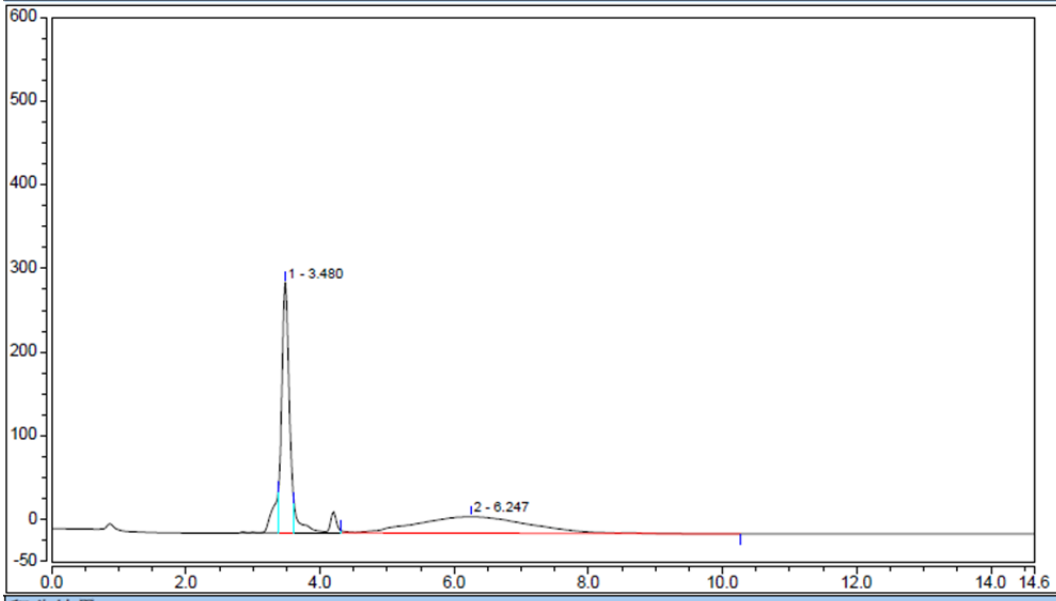


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		3.857	5.587	20.655	3.19	6.16	n.a.
2		5.333	169.818	314.606	96.81	93.84	n.a.
Total:			**175.405**	**335.261**	**100.00**	**100.00**	

3fa

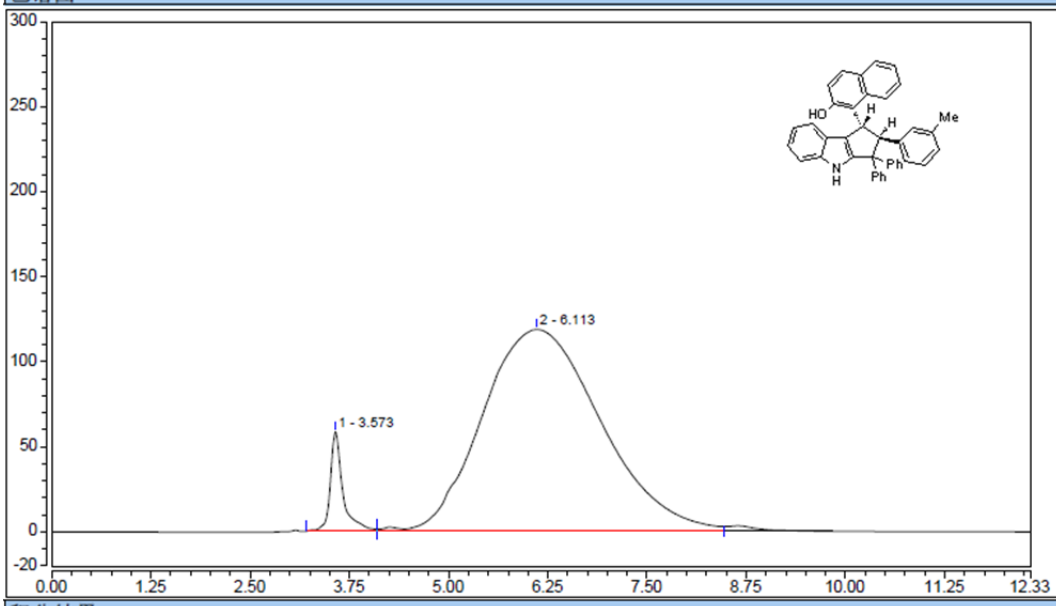
色谱图



积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		3.480	37.741	298.996	49.47	93.80	n.a.
2		6.247	38.552	19.753	50.53	6.20	n.a.
总和:			**76.294**	**318.749**	**100.00**	**100.00**	

色谱图

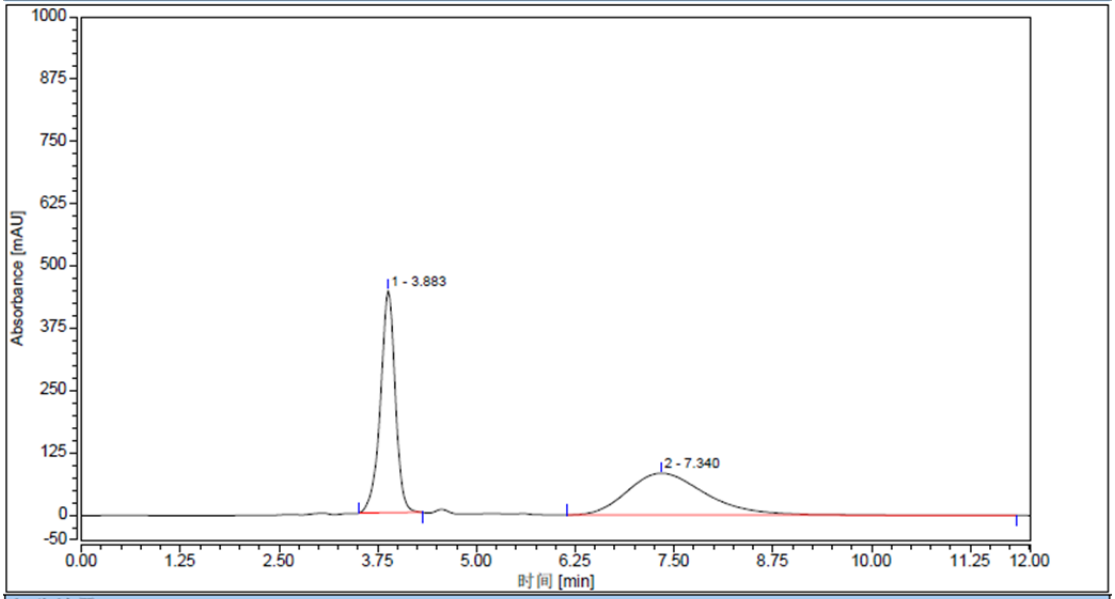


积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		3.573	10.820	58.375	5.01	32.98	n.a.
2		6.113	204.997	118.652	94.99	67.02	n.a.
总和:			**215.817**	**177.027**	**100.00**	**100.00**	

3ga

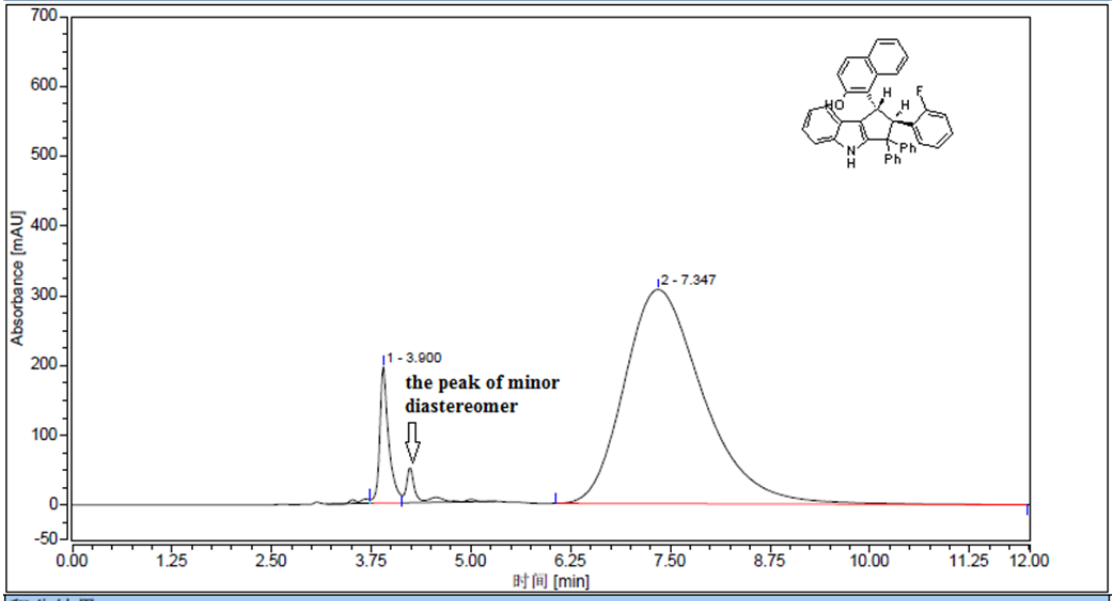
色谱图



积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		3.883	97.231	445.648	49.99	84.13	n.a.
2		7.340	97.264	84.065	50.01	15.87	n.a.
总和:			194.495	529.713	100.00	100.00	

色谱图

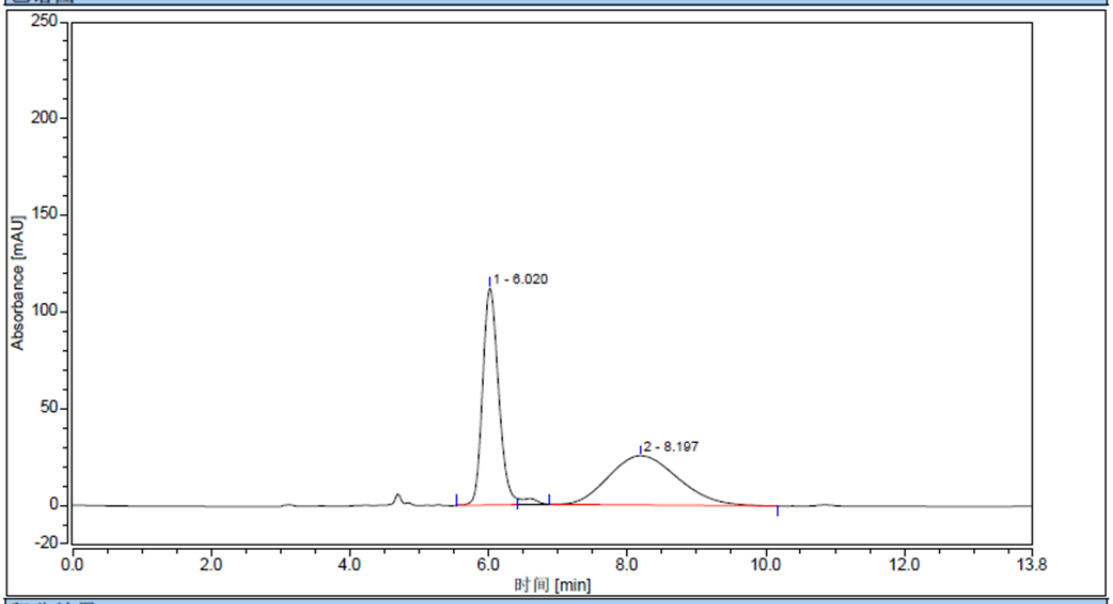


积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		3.900	25.262	195.440	6.71	38.93	n.a.
2		7.347	351.250	306.610	93.29	61.07	n.a.
总和:			376.511	502.050	100.00	100.00	

3ha

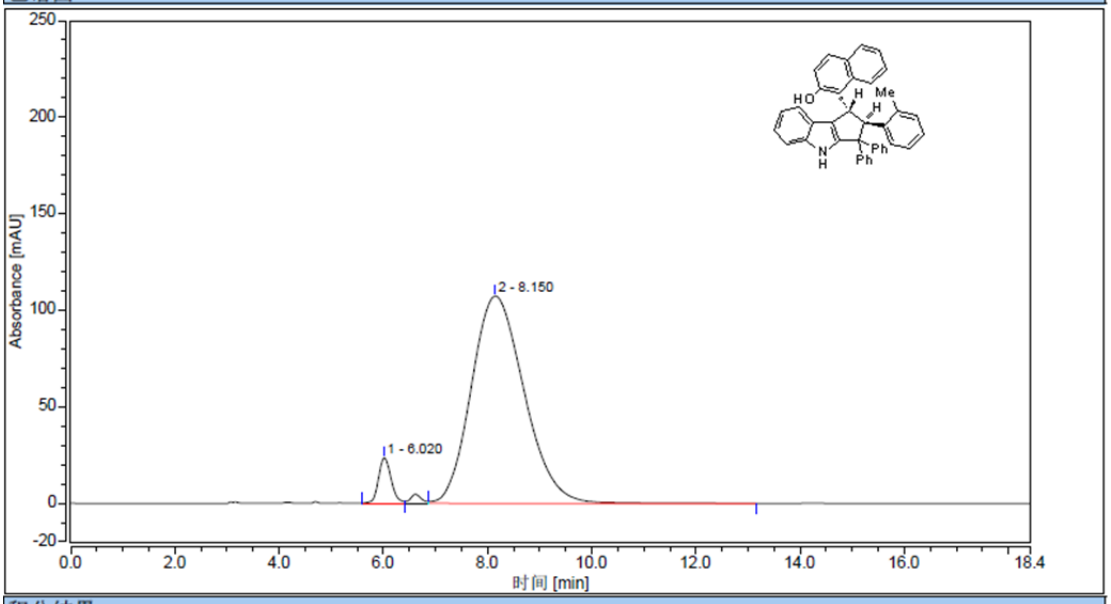
色谱图



积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		6.020	29.784	112.265	50.37	81.55	n.a.
2		8.197	29.346	25.407	49.63	18.45	n.a.
总和:			**59.130**	**137.672**	**100.00**	**100.00**	

色谱图

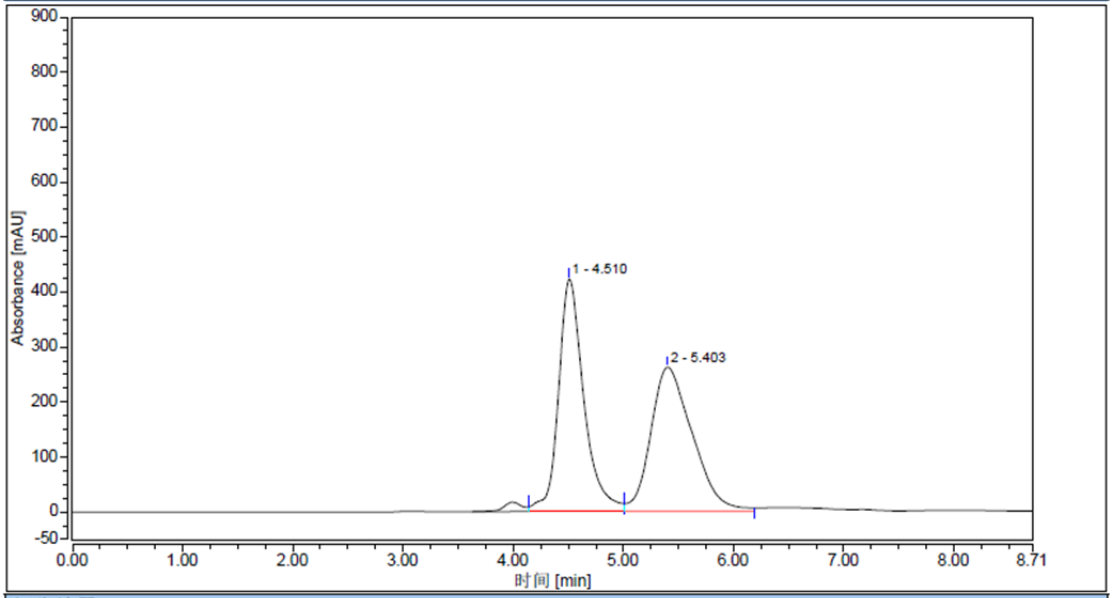


积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		6.020	6.620	23.554	4.99	17.99	n.a.
2		8.150	126.102	107.363	95.01	82.01	n.a.
总和:			**132.721**	**130.917**	**100.00**	**100.00**	

3ia

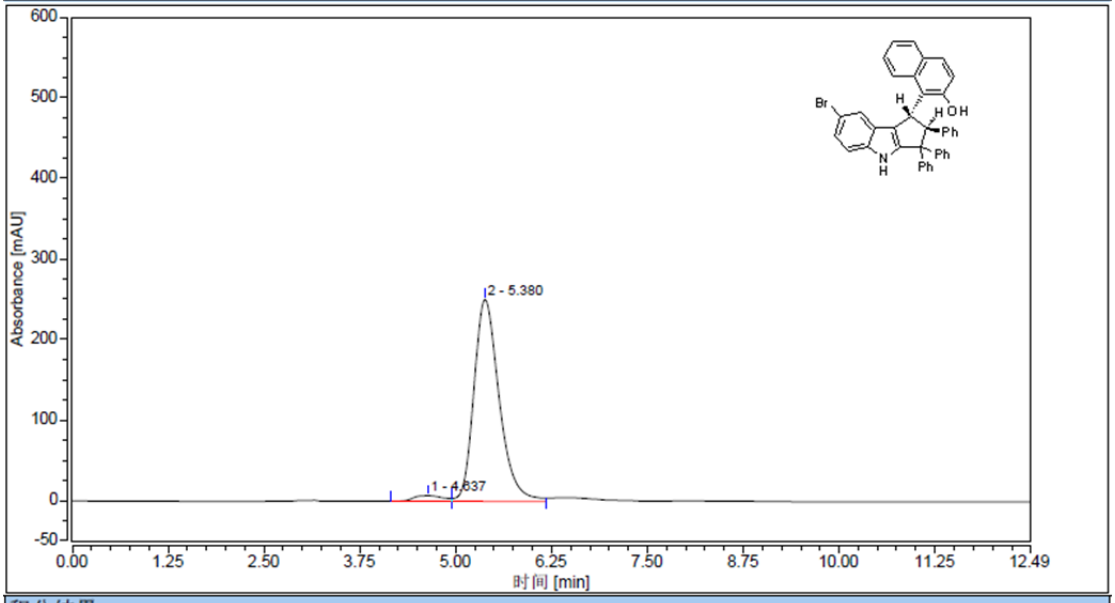
色谱图



积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		4.510	112.464	423.139	49.57	61.76	n.a.
2		5.403	114.395	262.043	50.43	38.24	n.a.
总和:			226.859	685.182	100.00	100.00	

色谱图

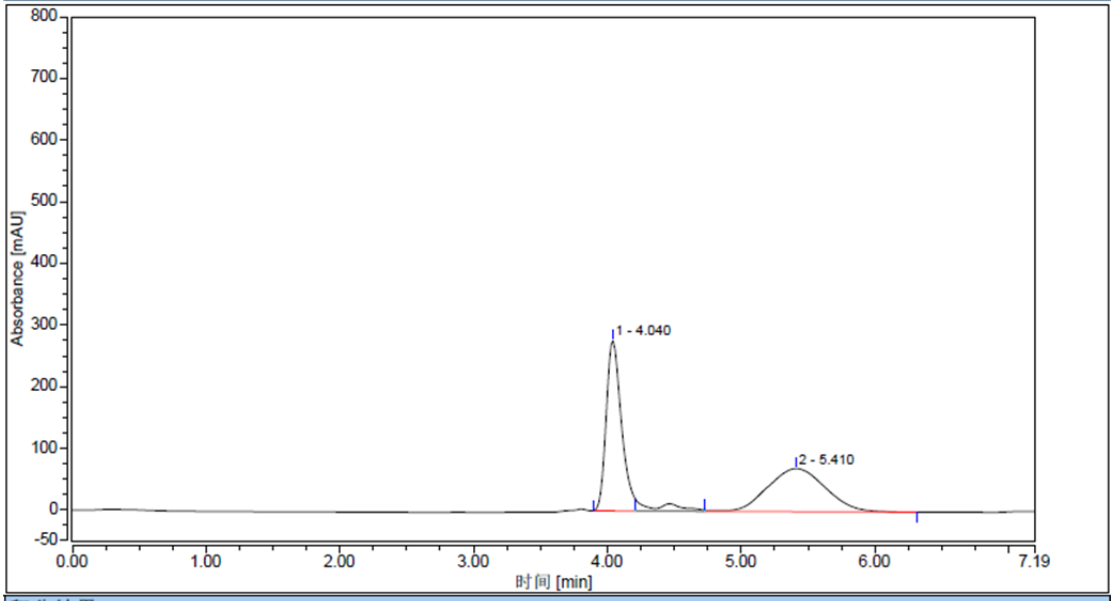


积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		4.637	3.066	6.937	3.10	2.69	n.a.
2		5.380	95.675	250.757	96.90	97.31	n.a.
总和:			98.741	257.693	100.00	100.00	

3ja

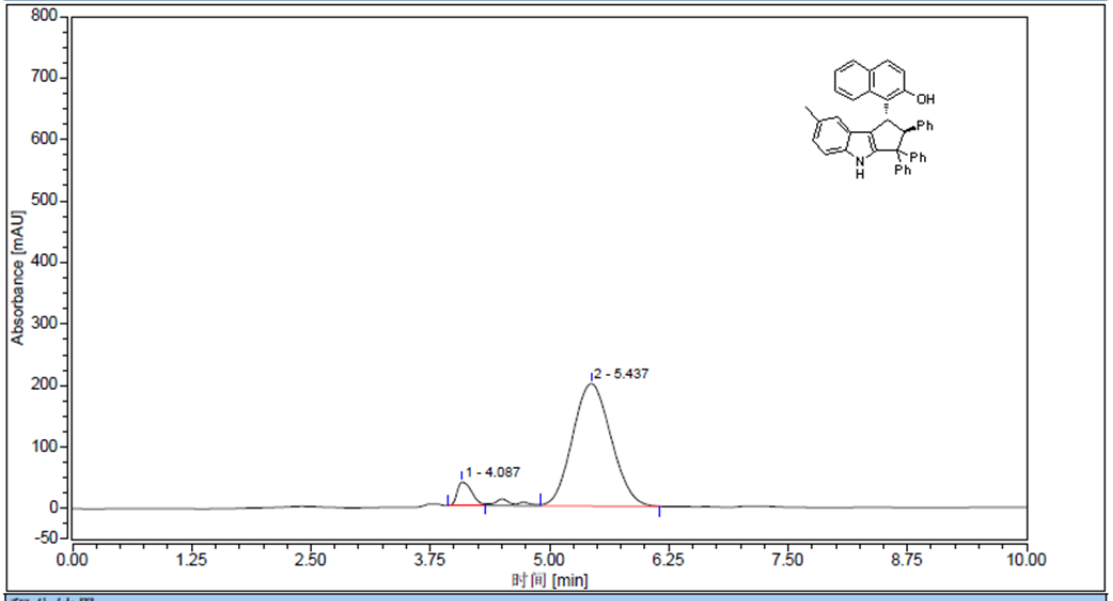
色谱图



积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		4.040	35.794	276.610	50.83	79.89	n.a.
2		5.410	34.629	69.626	49.17	20.11	n.a.
总和:			**70.422**	**346.236**	**100.00**	**100.00**	

色谱图

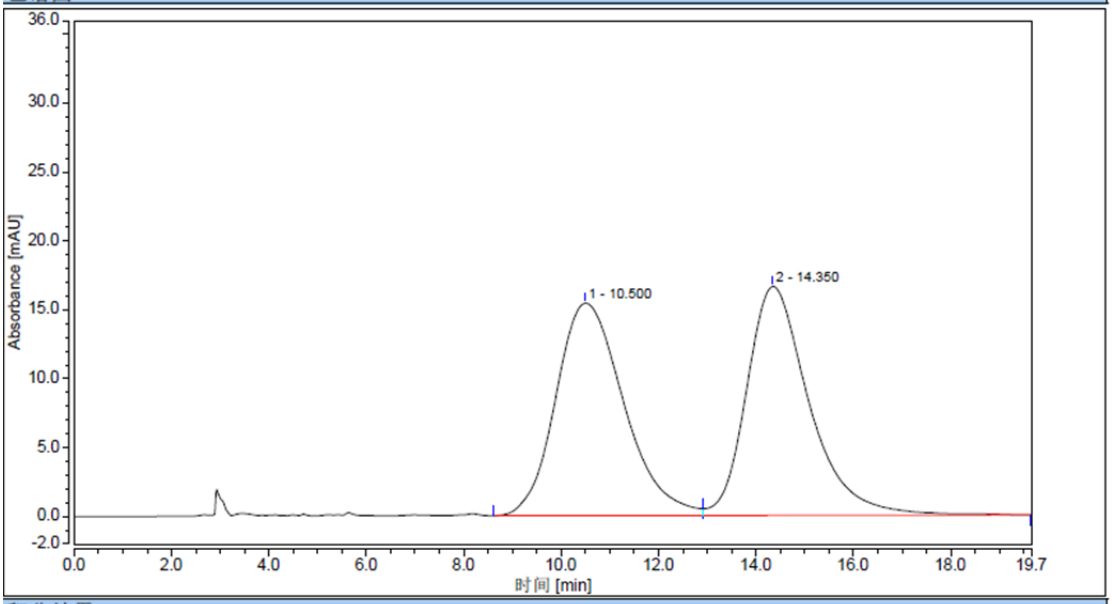


积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		4.087	6.812	38.431	6.80	16.17	n.a.
2		5.437	93.412	199.268	93.20	83.83	n.a.
总和:			**100.224**	**237.699**	**100.00**	**100.00**	

3ka

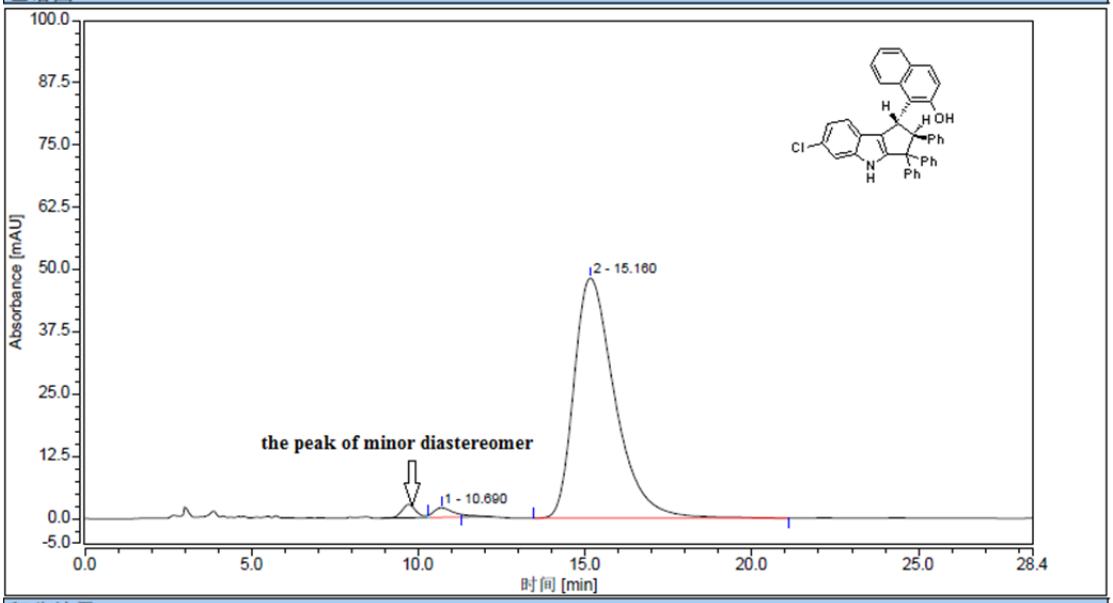
色谱图



积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		10.500	24.917	15.419	50.26	48.14	n.a.
2		14.350	24.664	16.611	49.74	51.86	n.a.
总和:			**49.581**	**32.029**	**100.00**	**100.00**	

色谱图

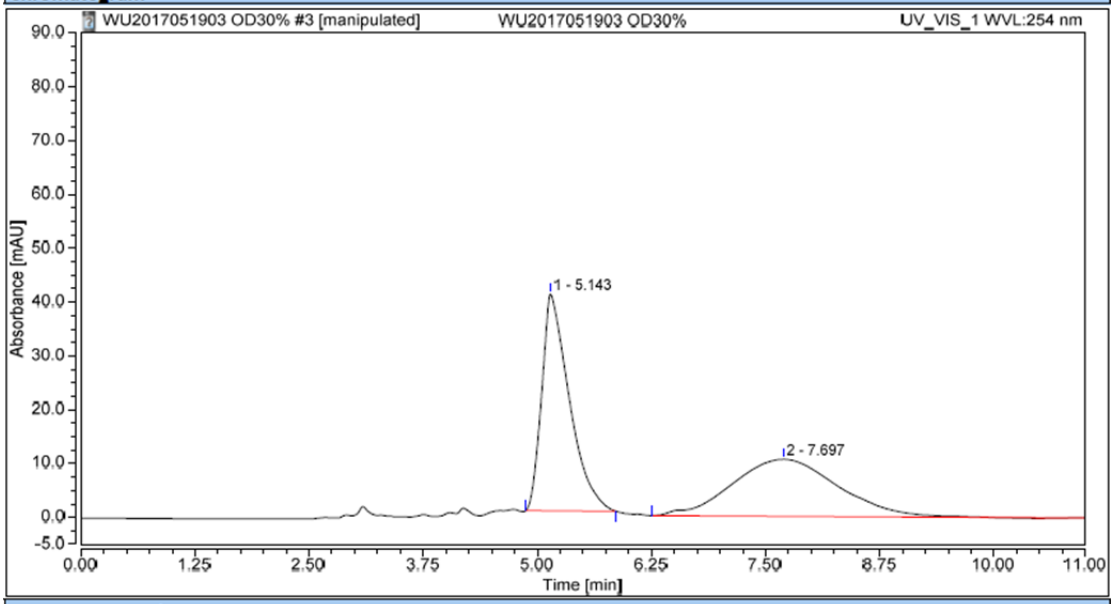


积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		10.690	1.256	1.928	1.80	3.85	n.a.
2		15.160	68.648	48.183	98.20	96.15	n.a.
总和:			**69.904**	**50.111**	**100.00**	**100.00**	

3la

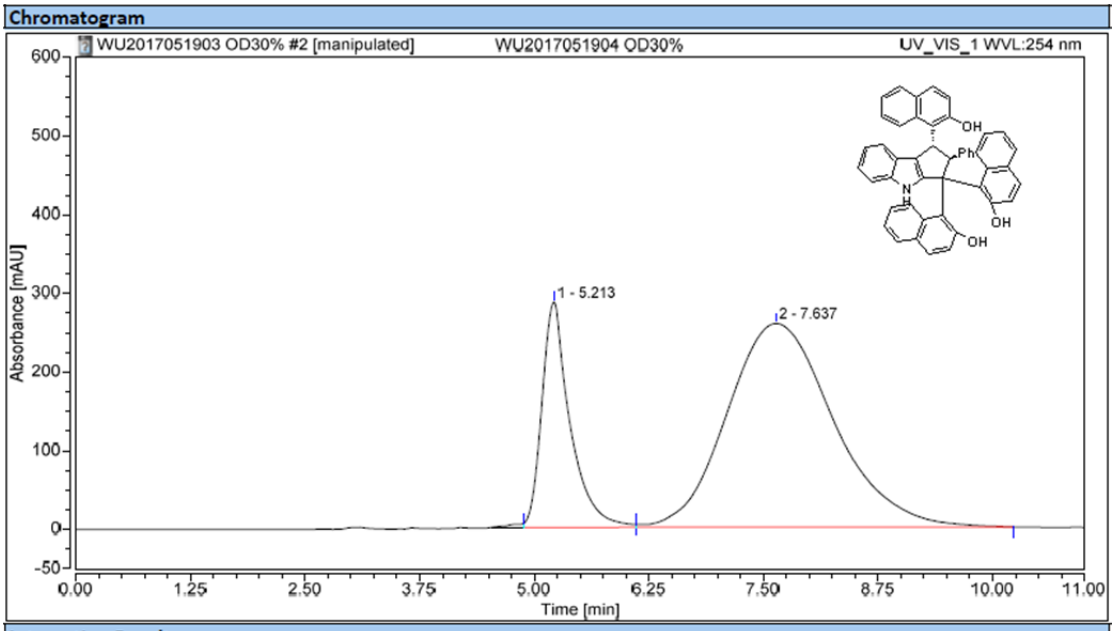
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.143	14.093	40.288	50.05	79.19	n.a.
2		7.697	14.062	10.589	49.95	20.81	n.a.
Total:			**28.155**	**50.878**	**100.00**	**100.00**	

Chromatogram

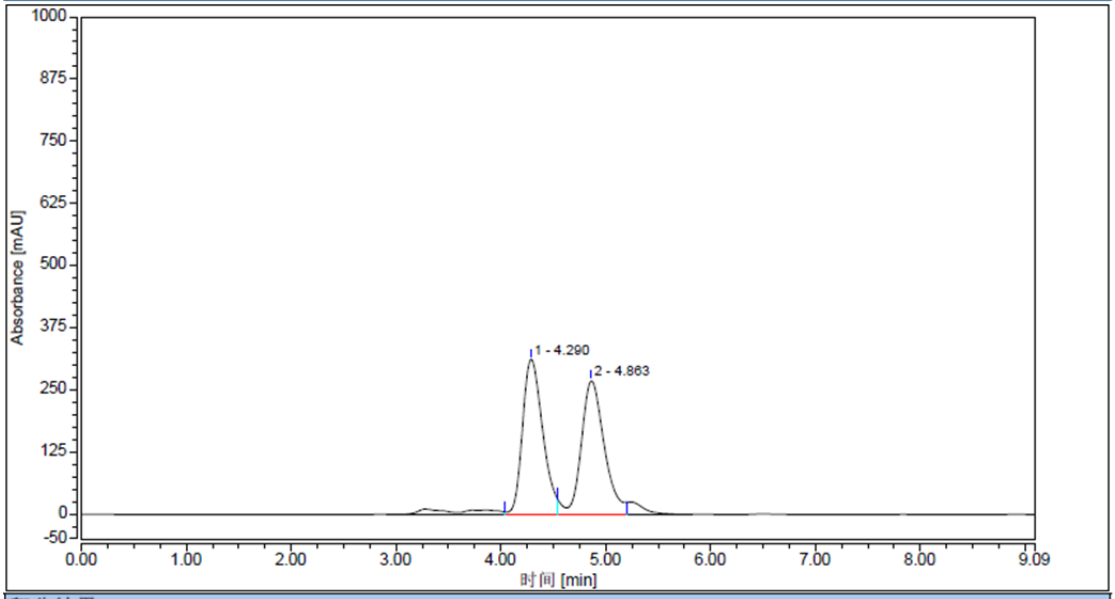


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.213	101.811	286.275	22.64	52.51	n.a.
2		7.637	347.803	258.886	77.36	47.49	n.a.
Total:			**449.614**	**545.162**	**100.00**	**100.00**	

Compound 6

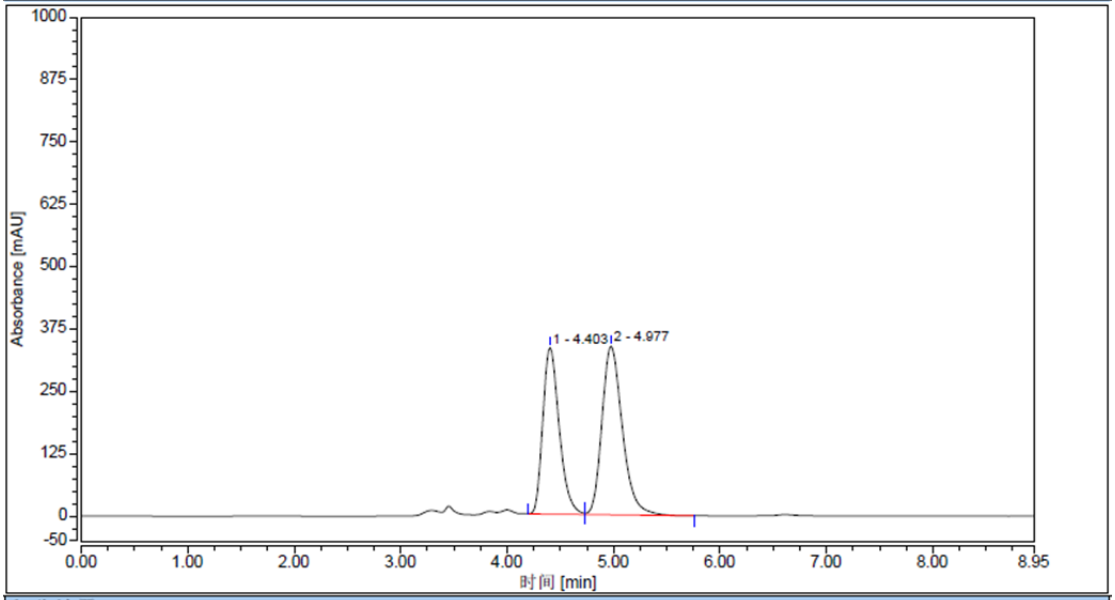
色谱图



积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		4.290	69.195	311.577	50.23	53.71	n.a.
2		4.863	68.561	268.503	49.77	46.29	n.a.
总和:			**137.756**	**580.080**	**100.00**	**100.00**	

色谱图

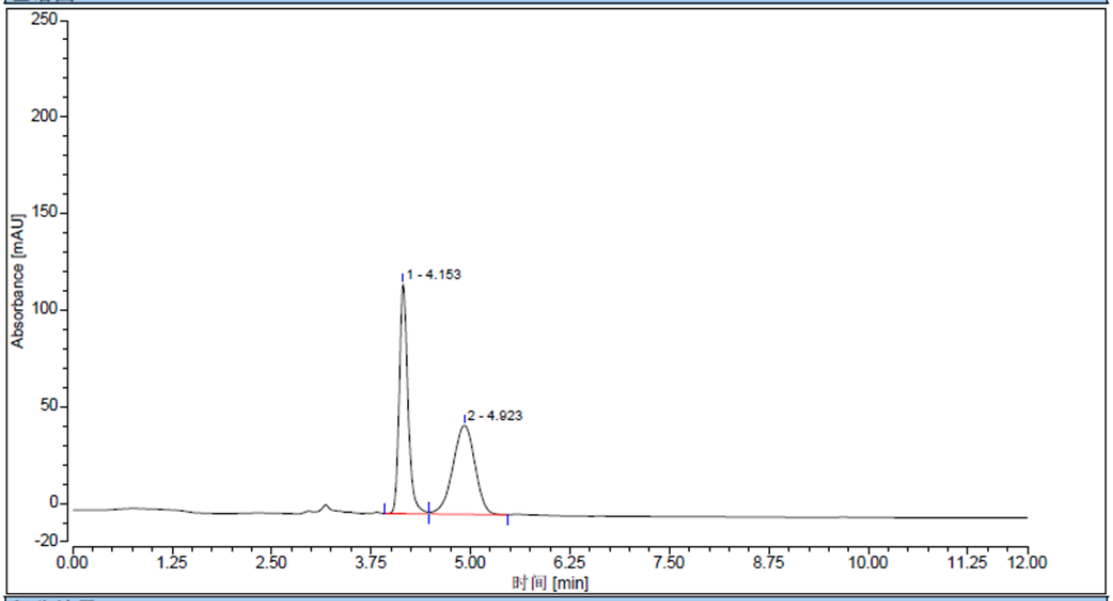


积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		4.403	59.451	333.479	44.16	49.67	n.a.
2		4.977	75.175	337.899	55.84	50.33	n.a.
总和:			**134.626**	**671.378**	**100.00**	**100.00**	

3eb

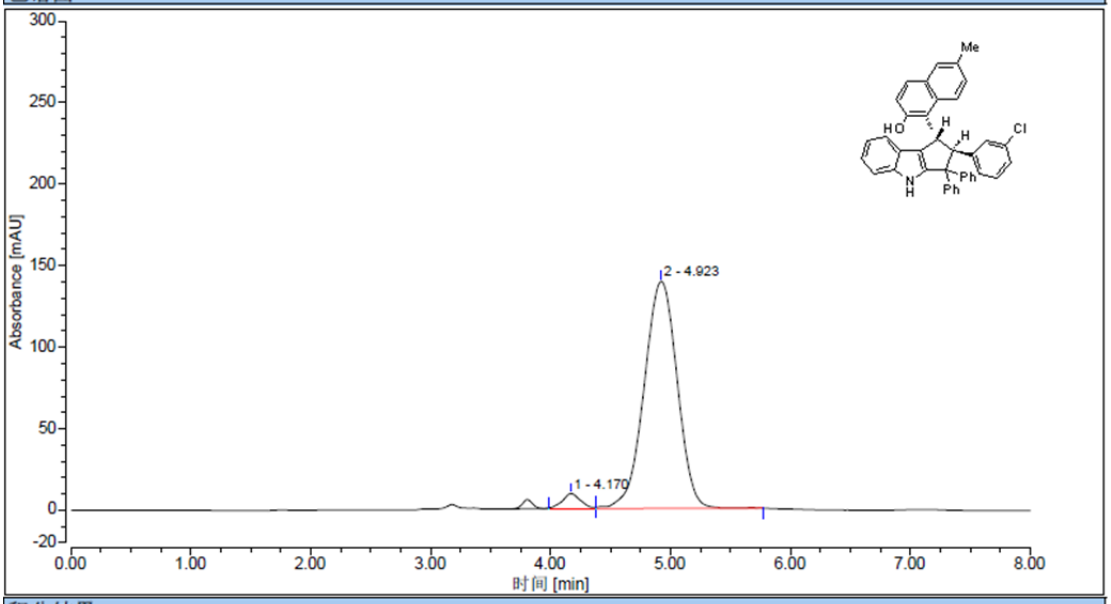
色谱图



积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		4.153	14.958	118.943	50.25	72.04	n.a.
2		4.923	14.809	46.163	49.75	27.96	n.a.
总和:			**29.767**	**165.107**	**100.00**	**100.00**	

色谱图

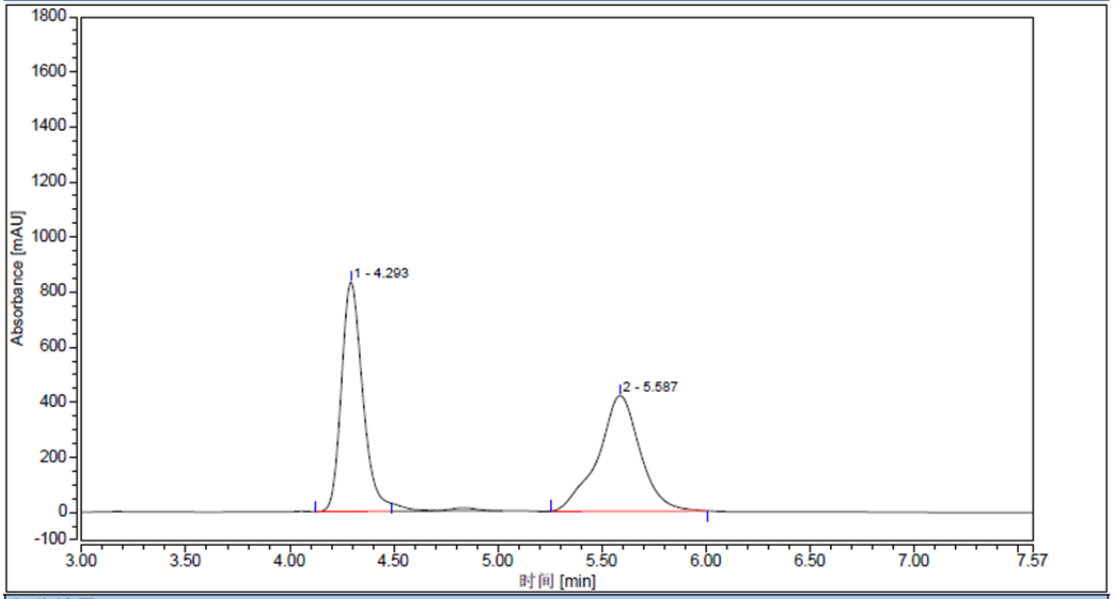


积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		4.170	1.633	9.302	3.54	6.26	n.a.
2		4.923	44.521	139.316	96.46	93.74	n.a.
总和:			**46.154**	**148.618**	**100.00**	**100.00**	

3ac

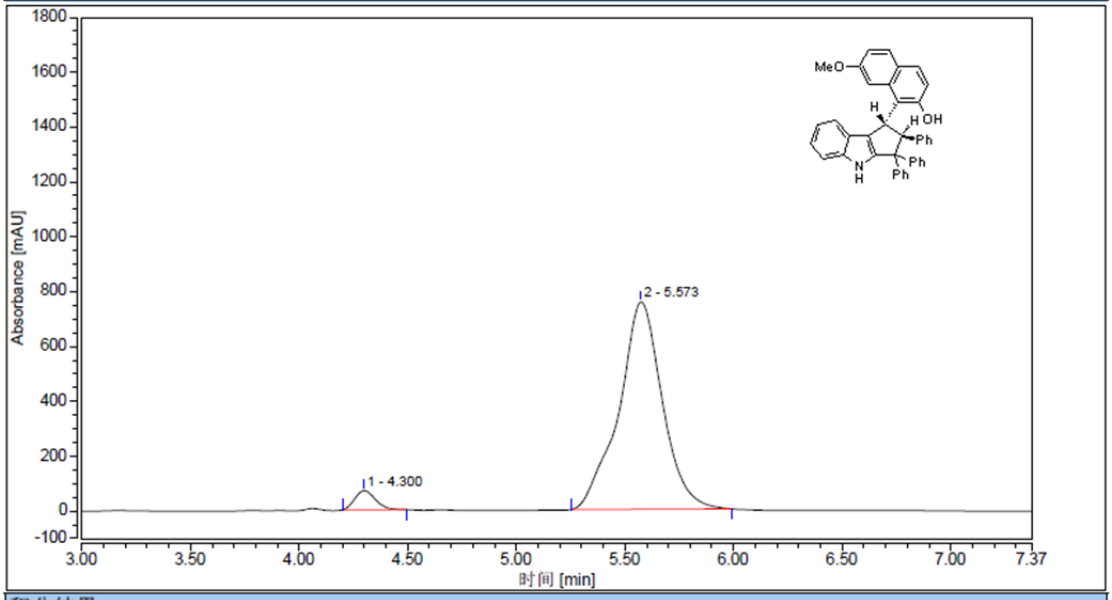
色谱图



积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		4.293	98.617	834.189	50.01	66.53	n.a.
2		5.587	98.569	419.722	49.99	33.47	n.a.
总和:			**197.186**	**1253.911**	**100.00**	**100.00**	

色谱图

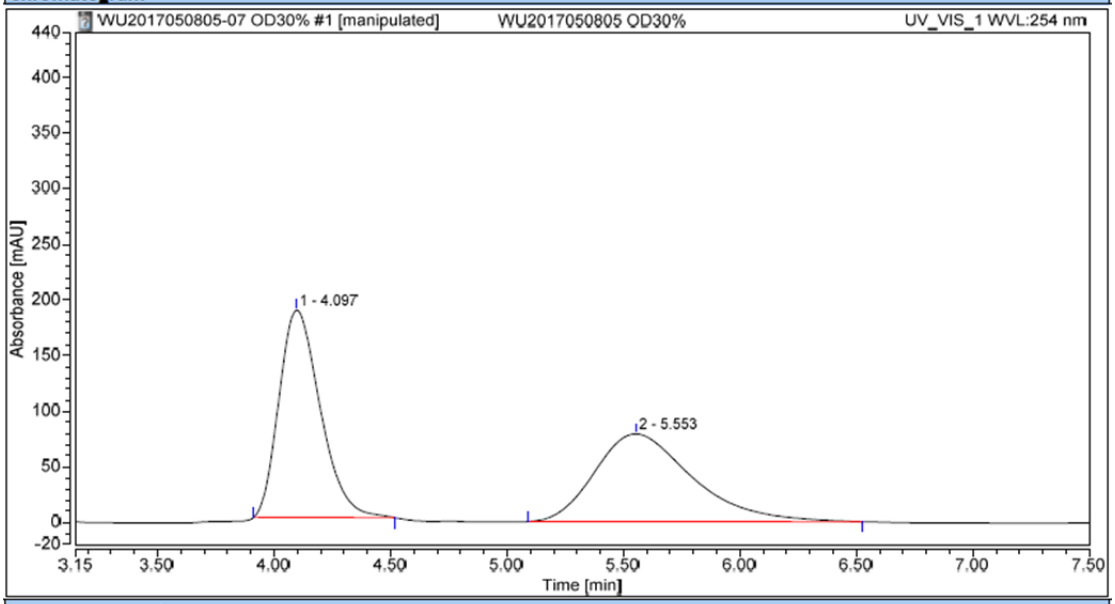


积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		4.300	7.654	69.598	4.17	8.43	n.a.
2		5.573	176.058	756.045	95.83	91.57	n.a.
总和:			**183.711**	**825.643**	**100.00**	**100.00**	

3ec

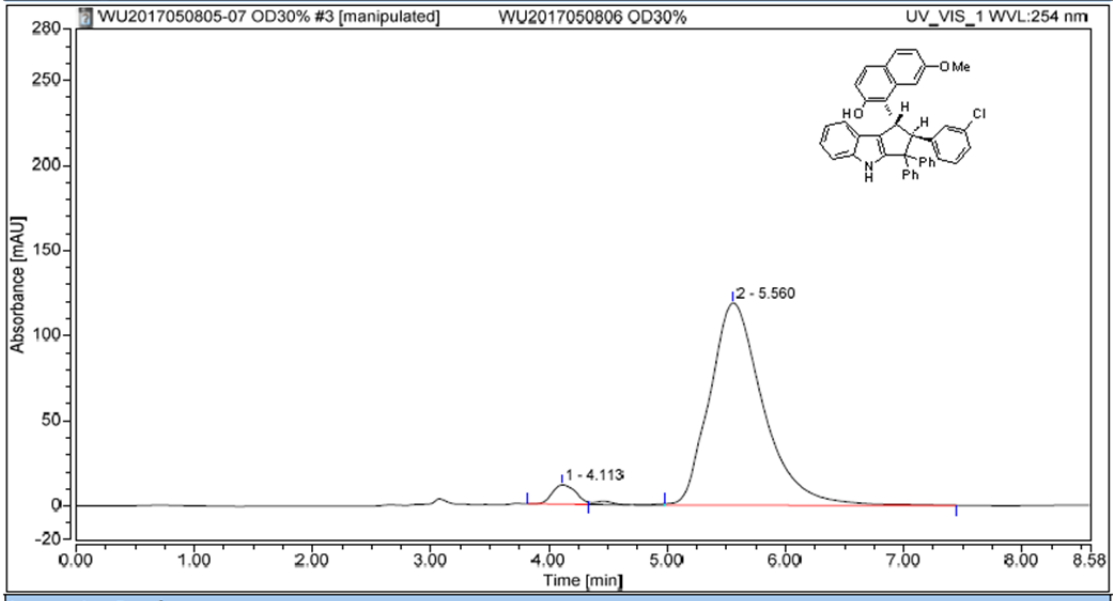
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.097	38.218	186.429	50.01	70.27	n.a.
2		5.553	38.205	78.888	49.99	29.73	n.a.
Total:			**76.423**	**265.317**	**100.00**	**100.00**	

Chromatogram

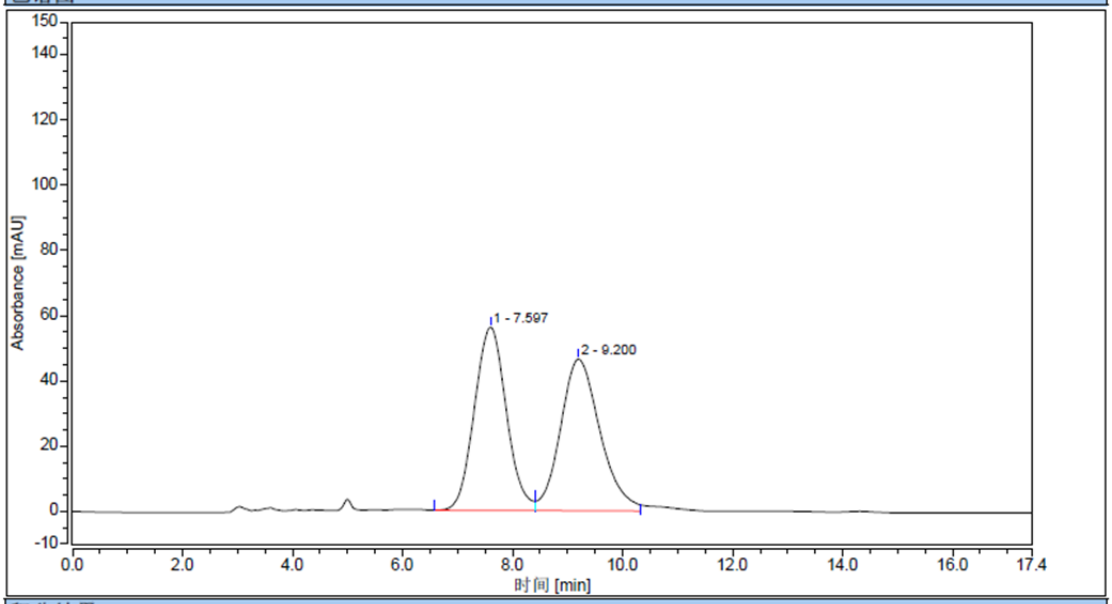


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.113	2.612	11.316	4.03	8.70	n.a.
2		5.560	62.194	118.807	95.97	91.30	n.a.
Total:			**64.807**	**130.123**	**100.00**	**100.00**	

3ad

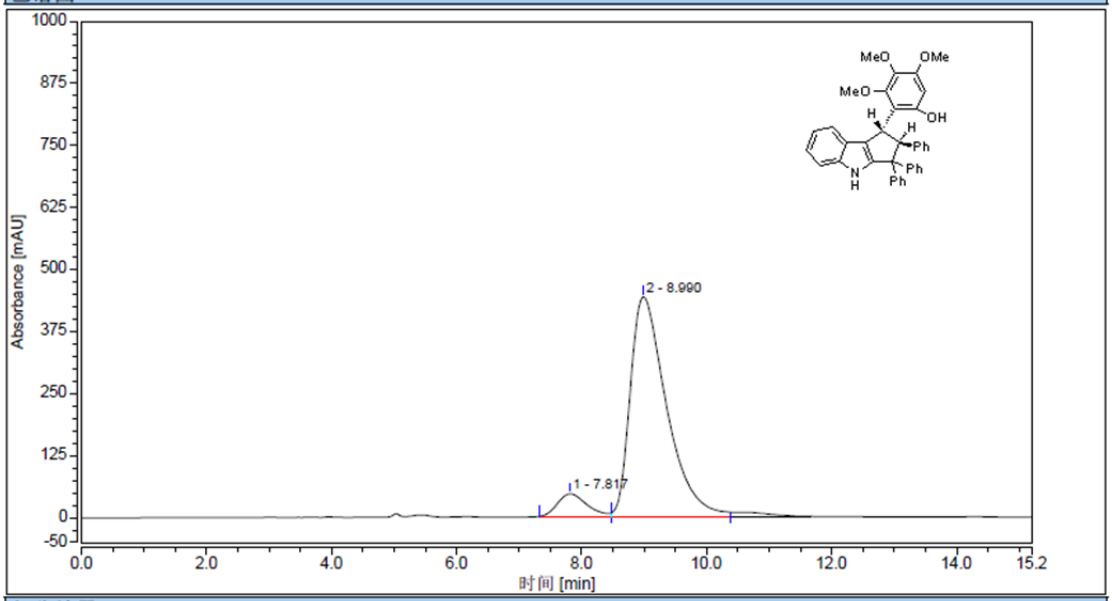
色谱图



积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		7.597	37.730	56.103	49.39	54.71	n.a.
2		9.200	38.667	46.451	50.61	45.29	n.a.
总和:			**76.397**	**102.553**	**100.00**	**100.00**	

色谱图

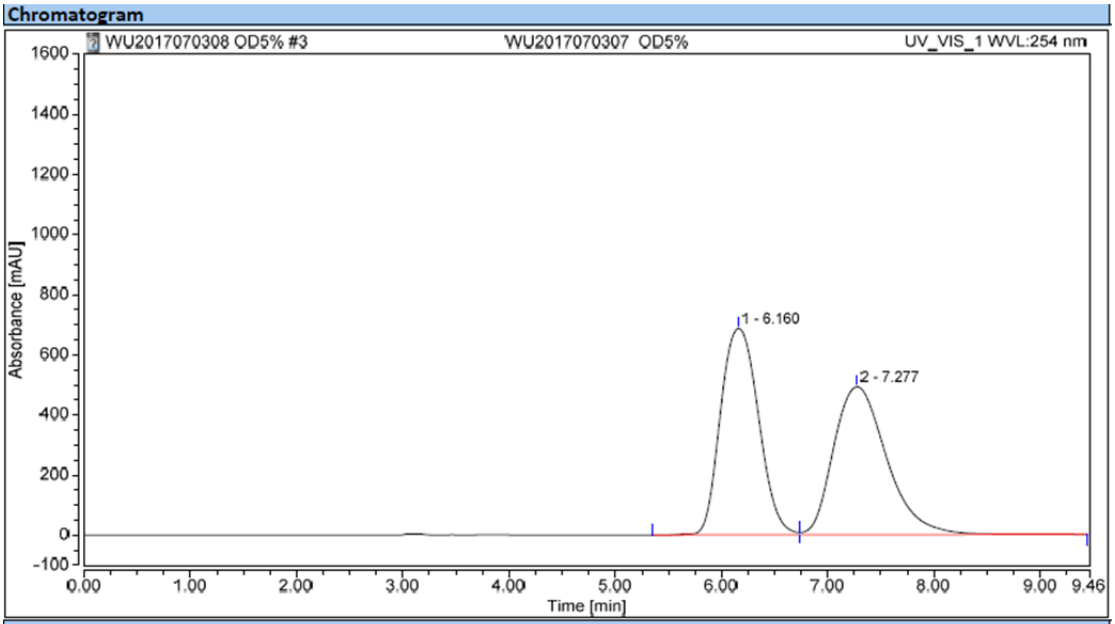


积分结果

序号	峰名称	保留时间 min	峰面积 mAU*min	峰高 mAU	相对峰面积 %	相对峰高 %	样品量 n.a.
1		7.817	24.788	45.365	7.72	9.30	n.a.
2		8.990	296.277	442.370	92.28	90.70	n.a.
总和:			**321.065**	**487.735**	**100.00**	**100.00**	

Compound 7

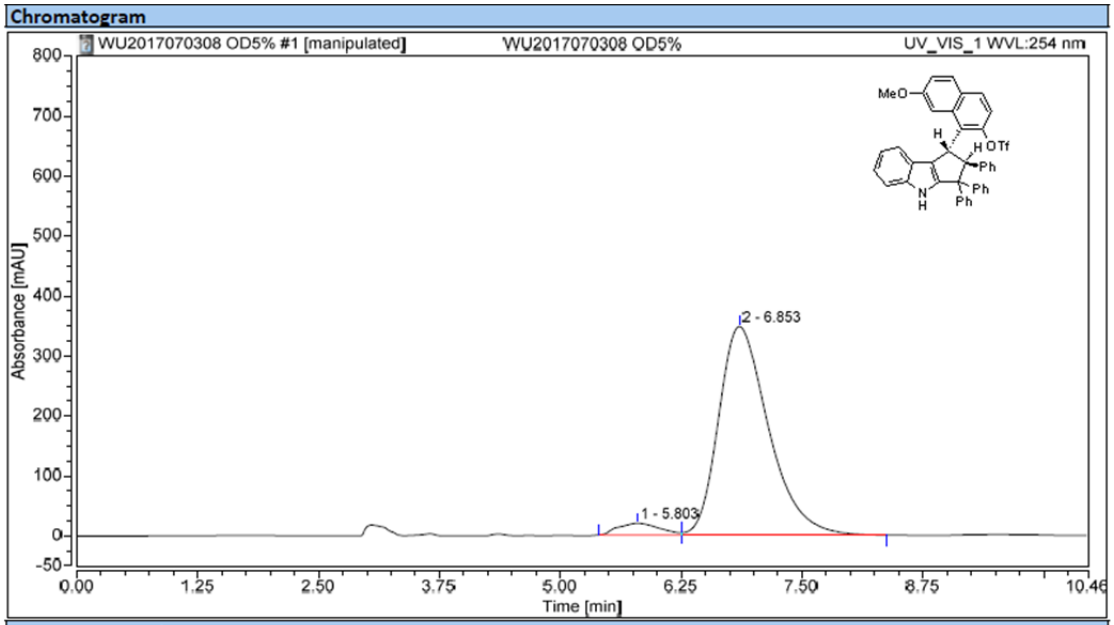
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.160	284.974	686.880	49.91	58.24	n.a.
2		7.277	286.012	492.501	50.09	41.76	n.a.
Total:			**570.986**	**1179.382**	**100.00**	**100.00**	

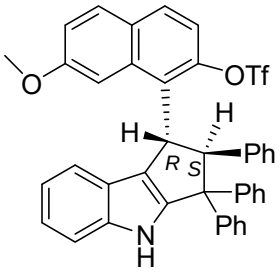
Chromatogram



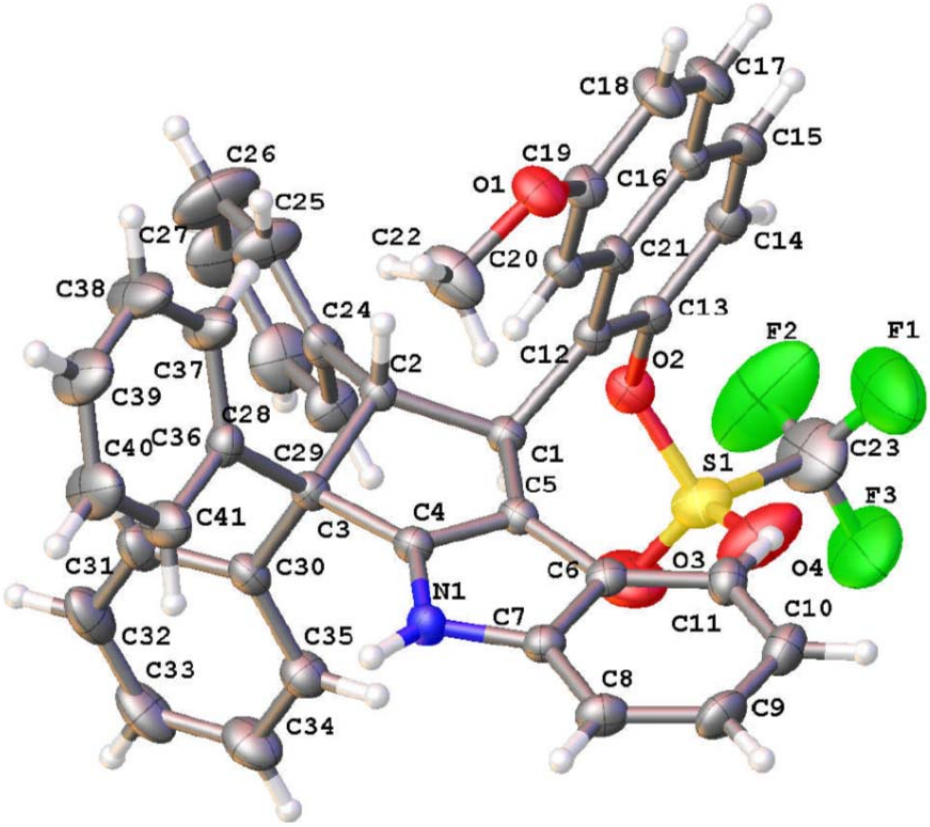
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.803	9.750	19.449	4.47	5.30	n.a.
2		6.853	208.458	347.784	95.53	94.70	n.a.
Total:			**218.208**	**367.232**	**100.00**	**100.00**	

3. X-ray single crystal data for compound 7



(1*R*,2*S*)-7



The thermal ellipsoid was drawn at the 30% probability level.

Empirical formula	C41 H30 F3 N O4 S	
Formula weight	689.72	
Temperature	296.15 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12$	
Unit cell dimensions	a = 12.0584(9) Å	α= 90°.
	b = 33.163(2) Å	β= 90°.
	c = 9.3861(7) Å	γ = 90°.
Volume	3753.4(5) $Å^3$	

Z	4
Density (calculated)	1.221 Mg/m^3
Absorption coefficient	0.141 mm^{-1}
F(000)	1432
Theta range for data collection	2.818 to 26.997°.
Index ranges	-13<=h<=15, -42<=k<=42, -9<=l<=11
Reflections collected	22036
Independent reflections	8151 [R(int) = 0.0302]
Completeness to theta = 25.242°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7458 and 0.6762
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8151 / 0 / 452
Goodness-of-fit on F^2	0.975
Final R indices [I>2sigma(I)]	R1 = 0.0533, wR2 = 0.1389
R indices (all data)	R1 = 0.0738, wR2 = 0.1530
Absolute structure parameter	0.12(3)
Extinction coefficient	n/a
Largest diff. peak and hole	0.232 and -0.259 $e.Å^{-3}$