

Design, Synthesis, and Biological Evaluation of X19: A Matrine pyrazole derivatives Therapeutic Candidate

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§ T. X. and S. D. contributed equally to this work.

X19

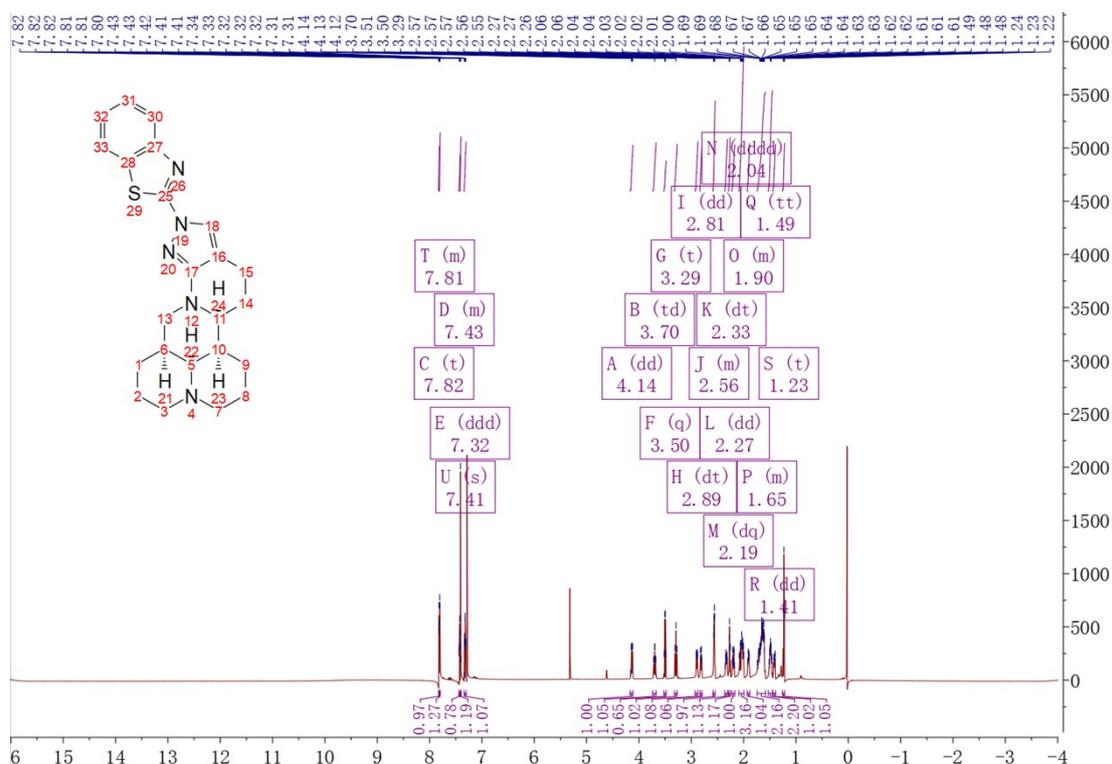


Fig s1. Comparison of partial ¹H NMR spectra of compounds X19

The ¹H NMR spectrum of compound X19 is presented in the Figure. The chemical shifts (δ) for the protons at positions 33 and 30 were observed at 7.81 and 7.82 ppm, respectively. Similarly, the signals corresponding to protons 31 and 32 appeared at δ 7.43 and 7.41 ppm, while the proton at position 18 resonated at δ 7.32 ppm.

Table of Molecular Docking Scores for All Compounds

compound	LibDockscore
X1	119.6636
X2	112.9162
X3	124.3719
X4	127.1987
X5	119.791
X6	115.203
X7	117.0185
X8	116.319
X9	114.6218
X10	118.834
X11	111.7392
X12	115.73
X13	113.123
X14	117.482

X15	115.698
X16	119.457
X17	128.492
X18	101.789
X19	143.6006
X20	124.159
X21	115.807
X22	113.129

The effect of X19 on the volume of xenograft tumors in nude mice

	Control	Sorafenib (40 mg/kg)	Matrine (40 mg/kg)	X19 (40 mg/kg)
1d	0.106 ± 0.012	0.099 ± 0.008	0.098 ± 0.01	0.1±0.012
4d	0.172 ± 0.015	0.136 ± 0.01	0.145 ± 0.013	0.133±0.015
7d	0.266 ± 0.021	0.182 ± 0.012	0.197 ± 0.016	0.175±0.017
10d	0.372 ± 0.026	0.236 ± 0.016	0.269 ± 0.018	0.236±0.02
13d	0.515 ± 0.033	0.301 ± 0.017	0.37 ± 0.024	0.314±0.025
16d	0.698 ± 0.04	0.408 ± 0.025	0.492 ± 0.03	0.381±0.033
19d	0.917 ± 0.048	0.488 ± 0.024	0.625 ± 0.034	0.483±0.034
22d	1.184 ± 0.056	0.573 ± 0.025	0.738 ± 0.034	0.576±0.035
25d	1.444 ± 0.065	0.66 ± 0.029	0.837 ± 0.041	0.645±0.041
28d	1.718 ± 0.079	0.748 ± 0.031	0.93 ± 0.043	0.719±0.043

Effect of X19 on the body weight of nude mice with axillary xenograft tumors

	Control	Sorafenib (40 mg/kg)	Matrine (40 mg/kg)	X19 (40 mg/kg)
1d	18.4 ± 0.4	18.6 ± 0.4	18.5 ± 0.4	18.5±0.4
4d	18.8 ± 0.5	19 ± 0.4	18.8 ± 0.4	18.8±0.3

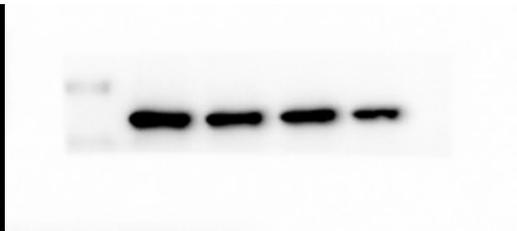
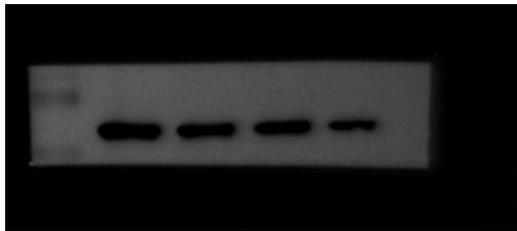
7d	19.2 ± 0.5	19.2 ± 0.4	19.3 ± 0.4	19.2±0.3
10d	19.6 ± 0.5	19.5 ± 0.5	19.6 ± 0.4	19.5±0.3
13d	20.1 ± 0.5	19.8 ± 0.5	20 ± 0.5	19.8±0.3
16d	20.5 ± 0.5	20 ± 0.4	20.4 ± 0.4	20.1±0.3
19d	21 ± 0.5	20.3 ± 0.4	20.8 ± 0.4	20.4±0.3
22d	21.5 ± 0.6	20.6 ± 0.4	21.2 ± 0.4	20.8±0.3
25d	22 ± 0.6	21 ± 0.5	21.6 ± 0.5	21.1±0.3
28d	22.5 ± 0.5	21.4 ± 0.5	22 ± 0.5	21.5±0.4

Effect of X19 on the weight of transplanted tumors in nude mice

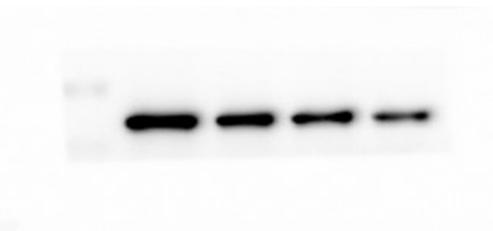
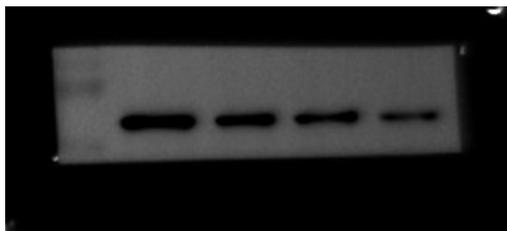
	Control	Sorafenib (40 mg/kg)	Matrine (40 mg/kg)	X19 (40 mg/kg)
1	2.07	0.93	1.11	0.98
2	2.11	0.84	1.25	0.96
3	2.23	0.77	1.17	0.91
4	2.15	0.85	1.21	0.86
5	1.86	0.98	1.29	0.88
6	1.92	1.02	1.12	0.92
X	2.06	0.90	1.19	0.92
S	0.14	0.09	0.07	0.05
P		0.000	0.000	0.000
TGI		56.32%	42.06%	55.35%

The original western blot result plots

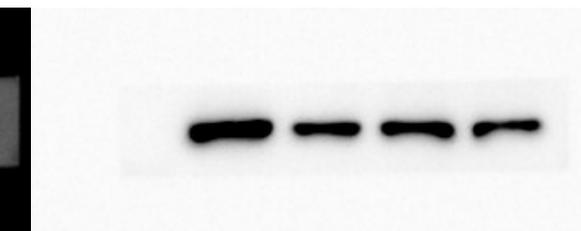
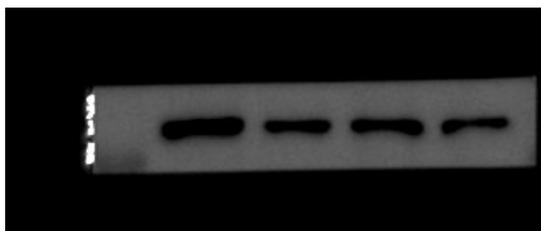
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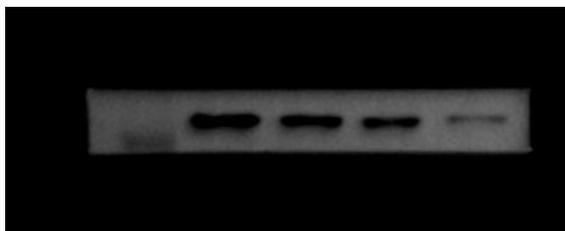
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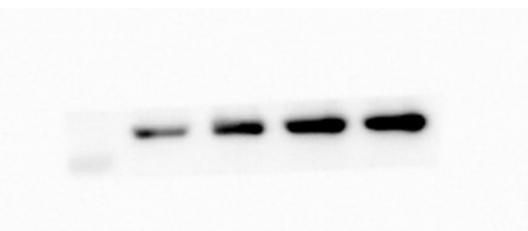
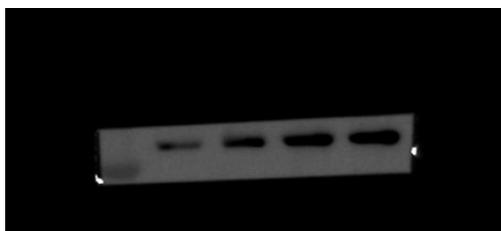
STAT



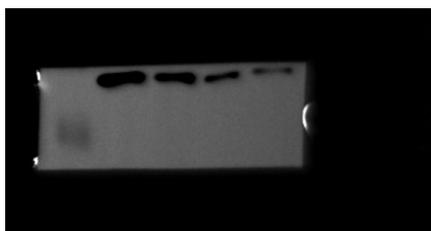
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Bax



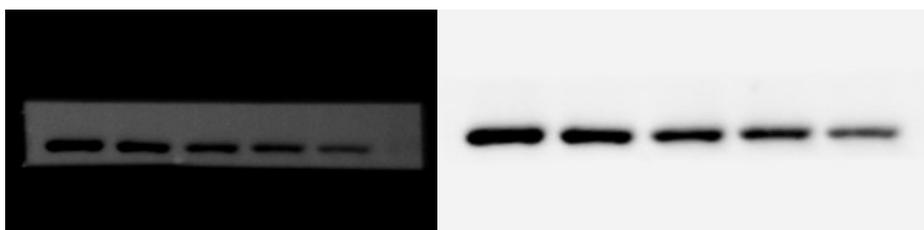
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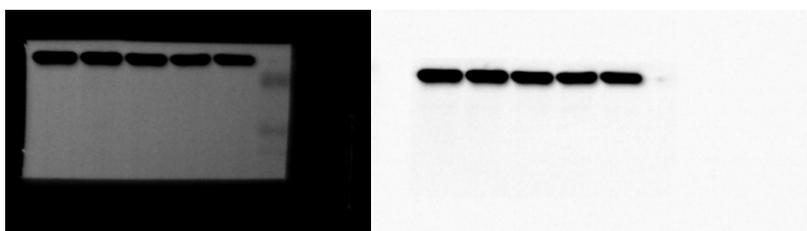
GAPDH



p-STAT

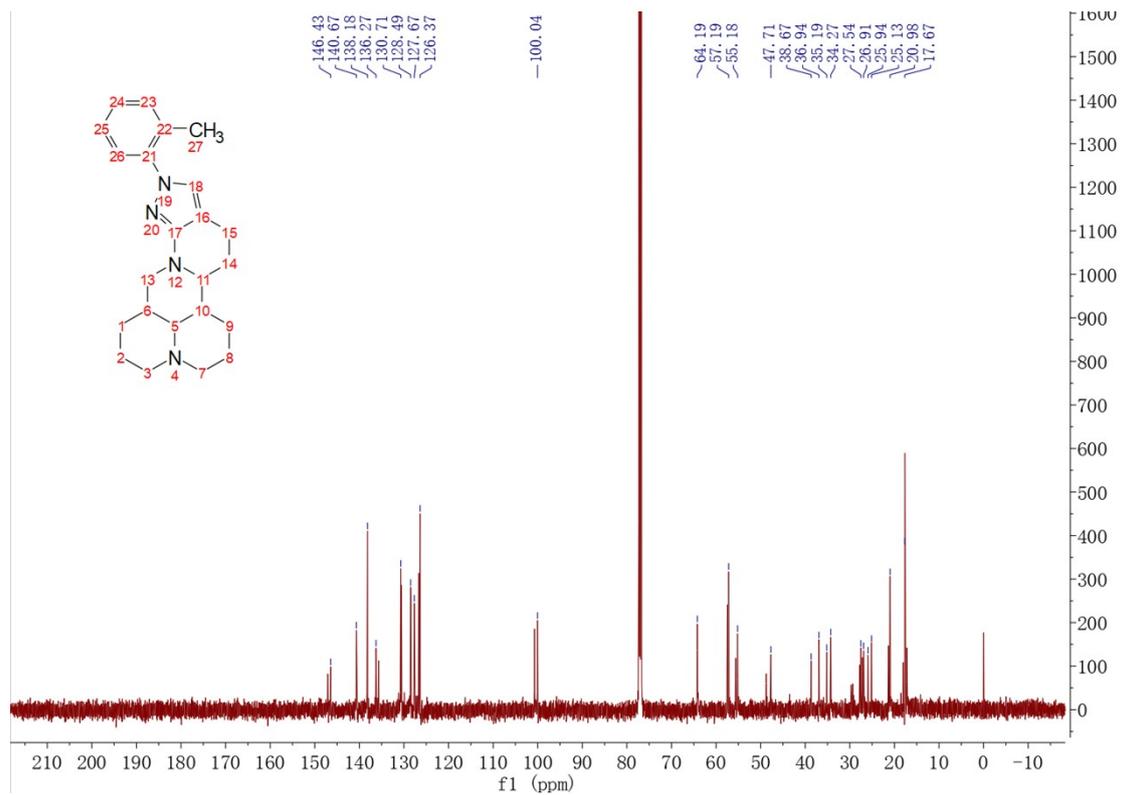
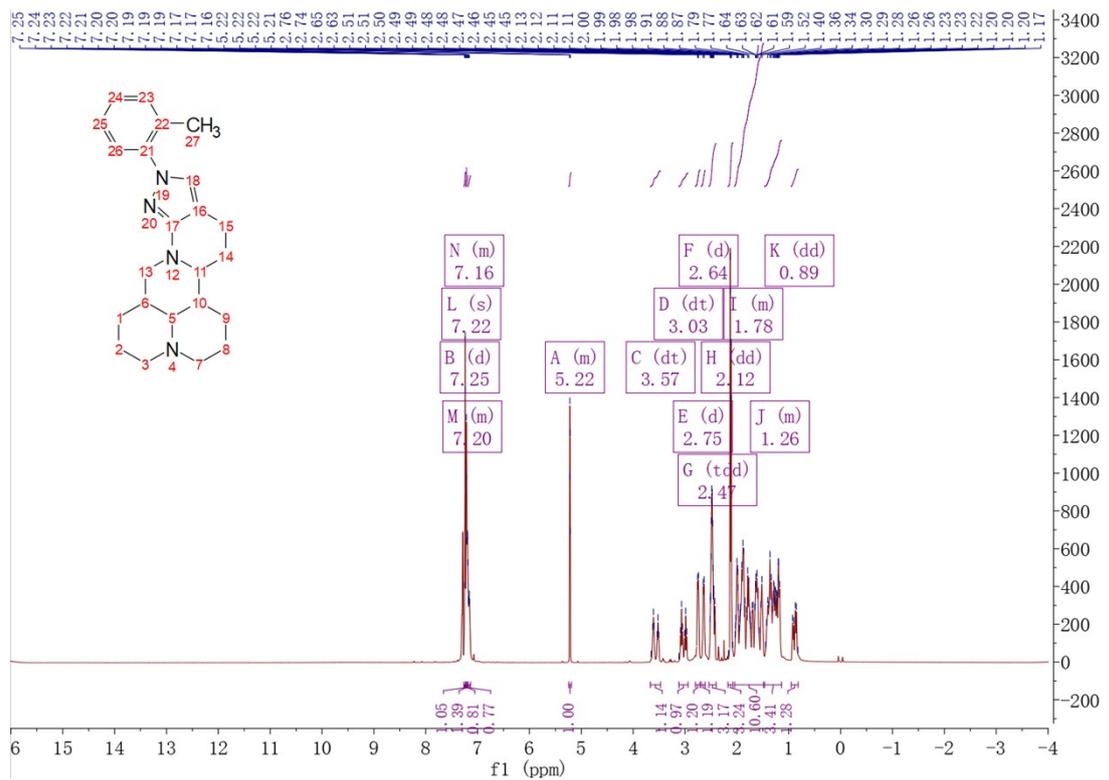


GAPDH



¹H-NMR, ¹³C-NMR, HRMS spectra and HPLC chromatogram of target compounds

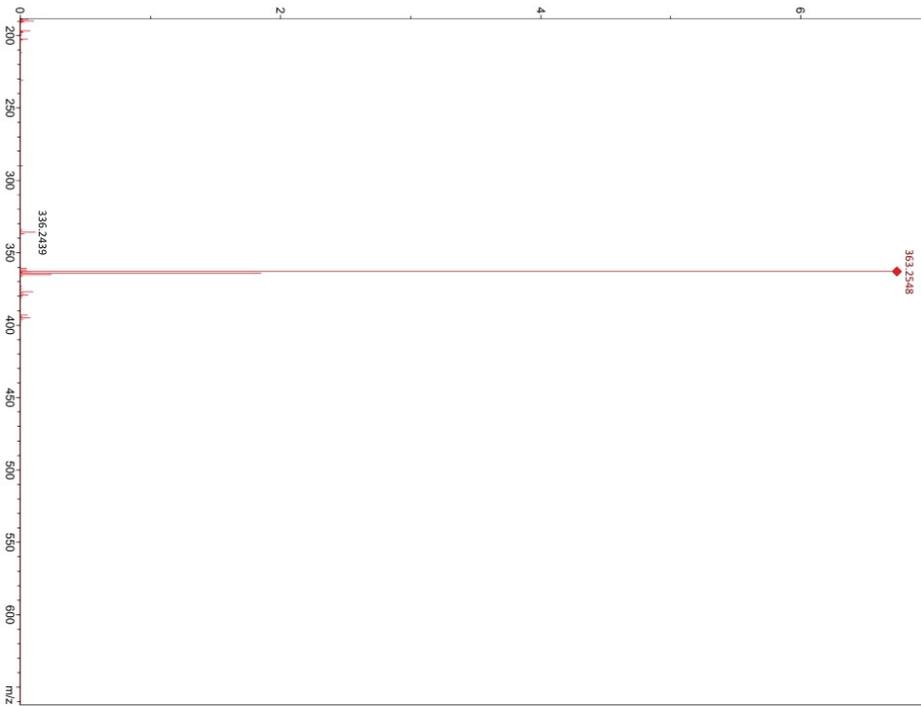
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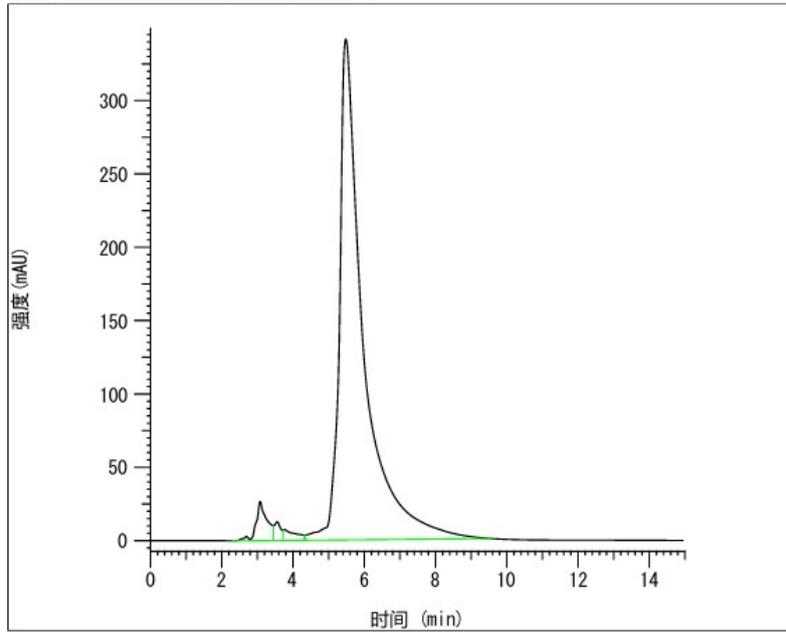
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Intens:
x10⁶

X32_REF_01_4980d - MS_5.omin #117

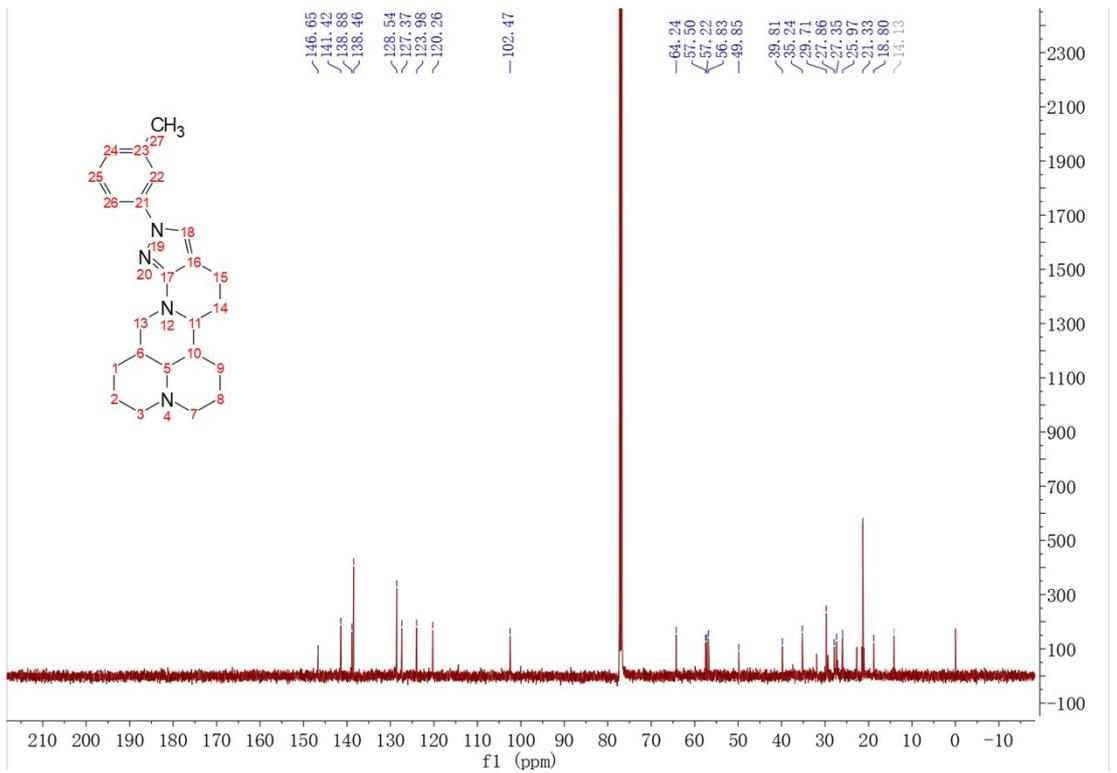
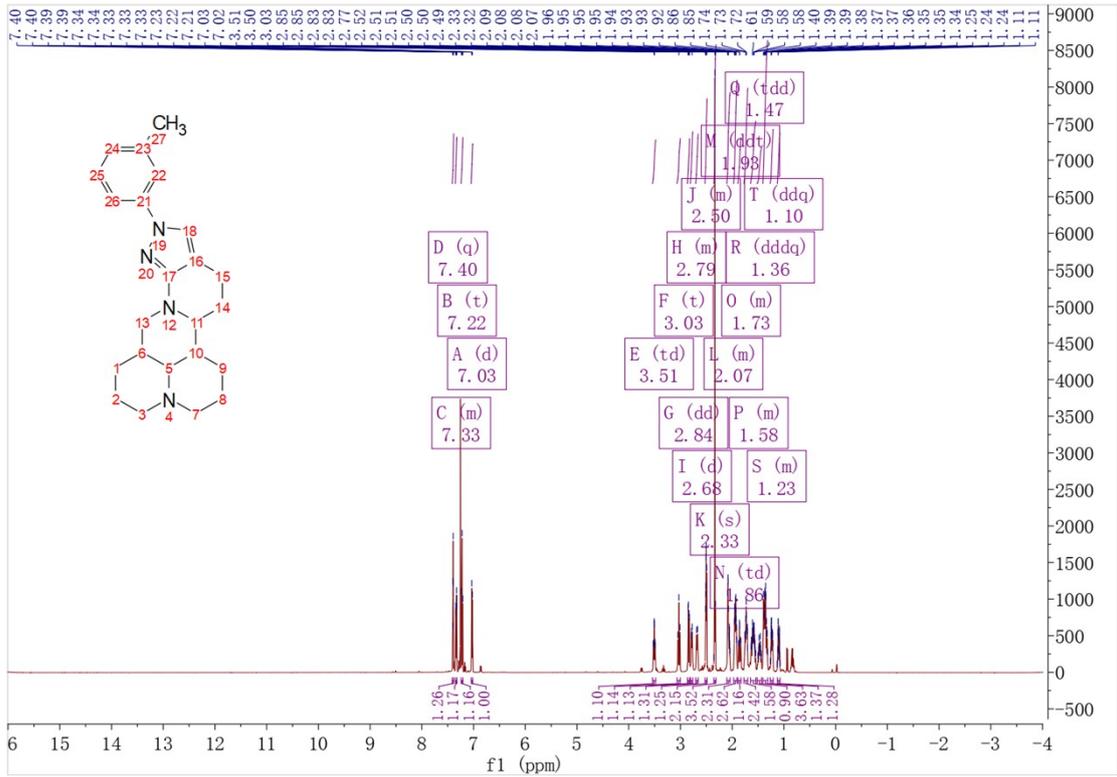


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5410 UV Detector Ch1 样品ID: 6 UNK006 (254nm) 次数: 1

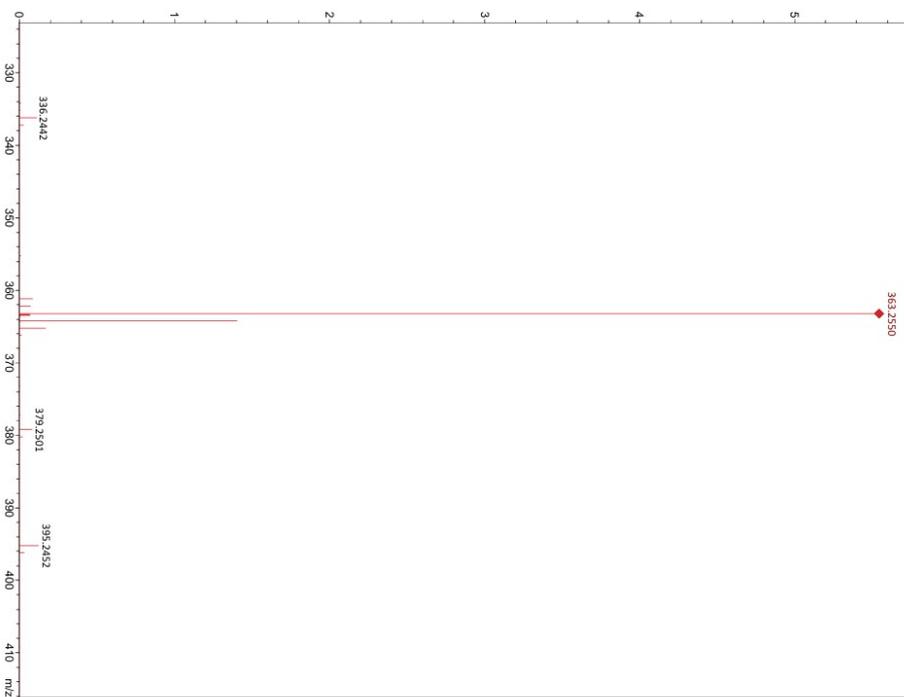
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1	峰1	3.077	5653 66	3.388	2675 3	7.126	---	---	---	---	543	27	0.31	---	---	---	---	---
2	峰2	3.777	1852 94	1.110	7251	1.931	---	---	---	---	---	7	---	---	---	---	---	---
3	峰3	5.483	1593 7829	95.50	3414 46	90.94 3	---	---	---	---	555	342	0.55	---	---	---	---	---
			1668 8490	100.0	3754 50	100.0 00												



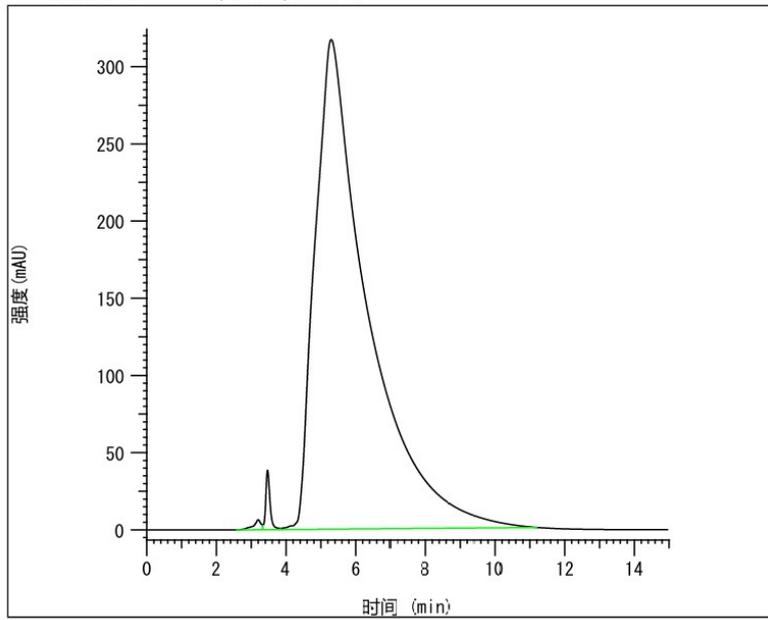
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X10
g

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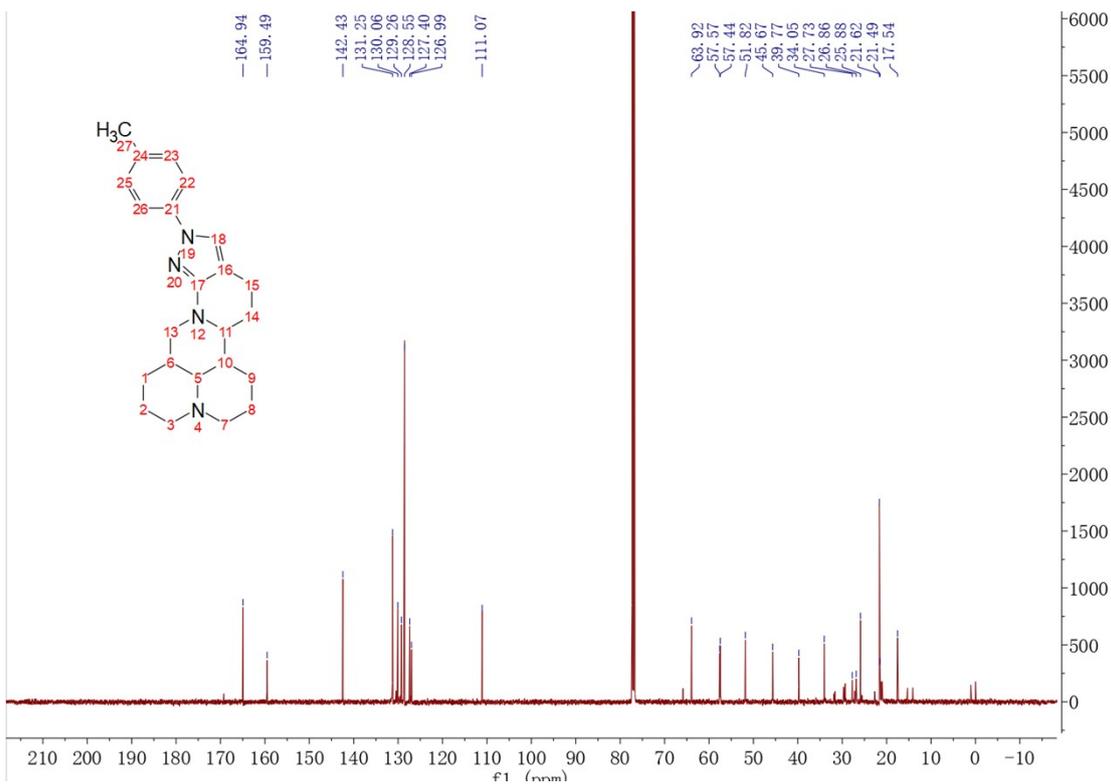
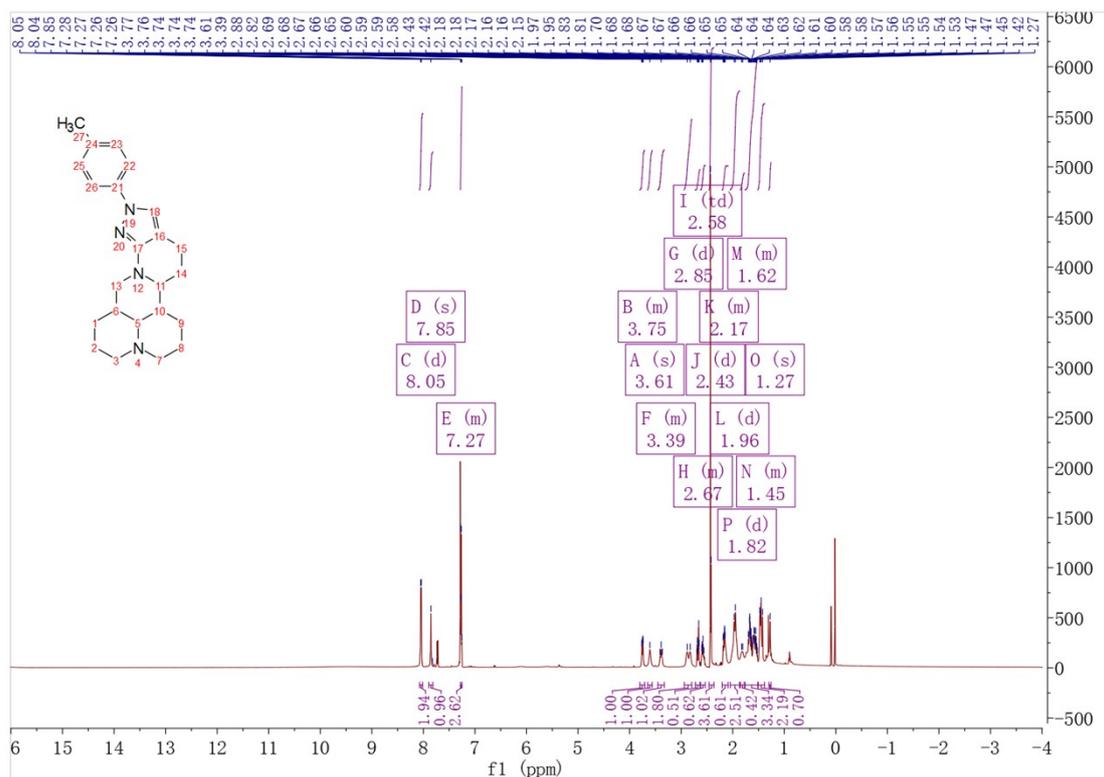


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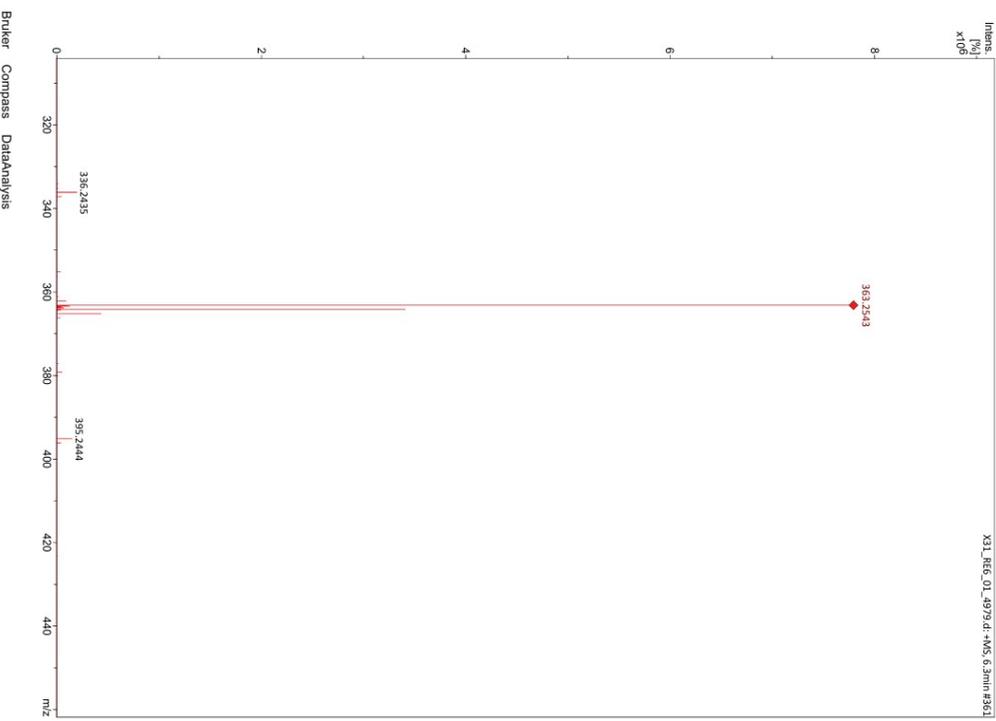
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1	峰1	3.197	9729 1	0.289	6444	1.779	---	---	---	---	1350	7	0.20	---	---	---	---	---
2	峰2	3.467	3289 69	0.977	3866 2	10.67 6	---	---	---	---	4592	39	0.12	---	---	---	---	---
3	峰3	5.293	3326 1063	98.73 4	3170 32	87.54 5	---	---	---	---	73	318	1.46	---	---	---	---	---
			3368 7323	100.0 00	3621 37	100.0 00												

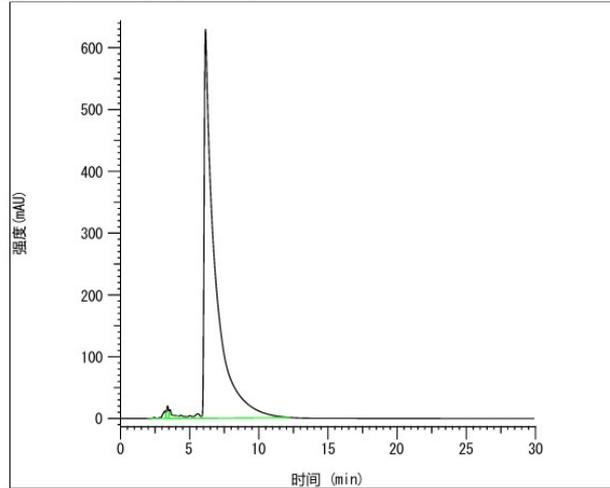


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Intens. [%]
x10⁶ X31_REF_01_4979.d:MS 6.min#361



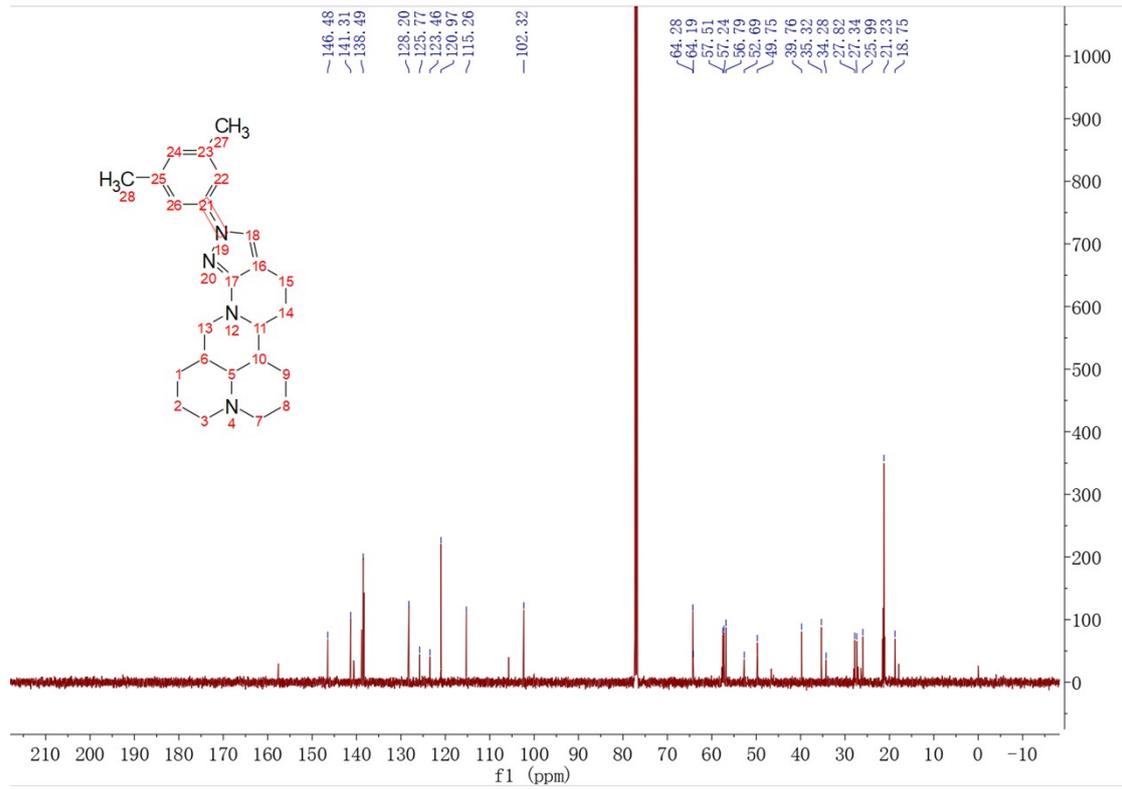
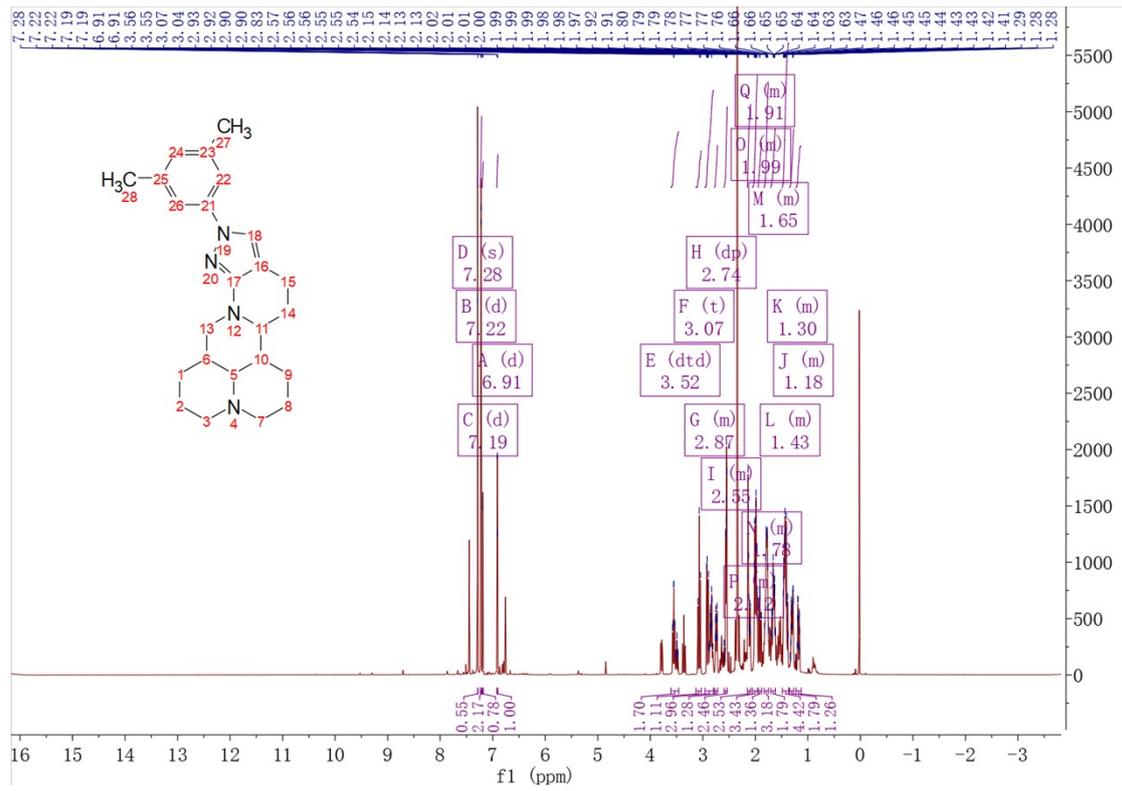
5410 UV Detector Ch1 样品ID: 4 UNK004 (254nm) 次数: 1



5410 UV Detector Ch1 样品ID: 4 UNK004 (254nm) 次数: 1

No.	成分名	RT	面积	面积%	高度	高度%	浓度	单位	浓度2	单位2	N	强度	半峰宽	相对RT	校正RT	纯度(平均)	纯度(3点)	纯度(2点)
1	峰1	2.250	4584	0.013	684	0.098	---	---	---	---	---	0	---	---	---	---	---	---
2	峰2	2.440	19417	0.056	2010	0.287	---	---	---	---	2494	2	0.12	---	---	---	---	---
3	峰3	3.207	186437	0.539	12133	1.735	---	---	---	---	---	12	---	---	---	---	---	---
4	峰4	3.403	200022	0.578	20643	2.953	---	---	---	---	---	21	---	---	---	---	---	---
5	峰5	3.580	263182	0.760	14449	2.067	---	---	---	---	---	14	---	---	---	---	---	---
6	峰6	3.873	6510	0.019	573	0.082	---	---	---	---	---	5	---	---	---	---	---	---
7	峰7	4.333	96294	0.278	4677	0.669	---	---	---	---	---	5	---	---	---	---	---	---
8	峰8	4.677	34792	0.101	2968	0.424	---	---	---	---	---	3	---	---	---	---	---	---
9	峰9	5.020	87803	0.254	4170	0.596	---	---	---	---	---	4	---	---	---	---	---	---
10	峰10	5.597	180717	0.522	7300	1.044	---	---	---	---	1002	8	0.42	---	---	---	---	---
11	峰11	6.143	33535743	96.88	629534	90.045	---	---	---	---	615	630	0.58	---	---	---	---	---
			34615501	100.000	699139	100.000												

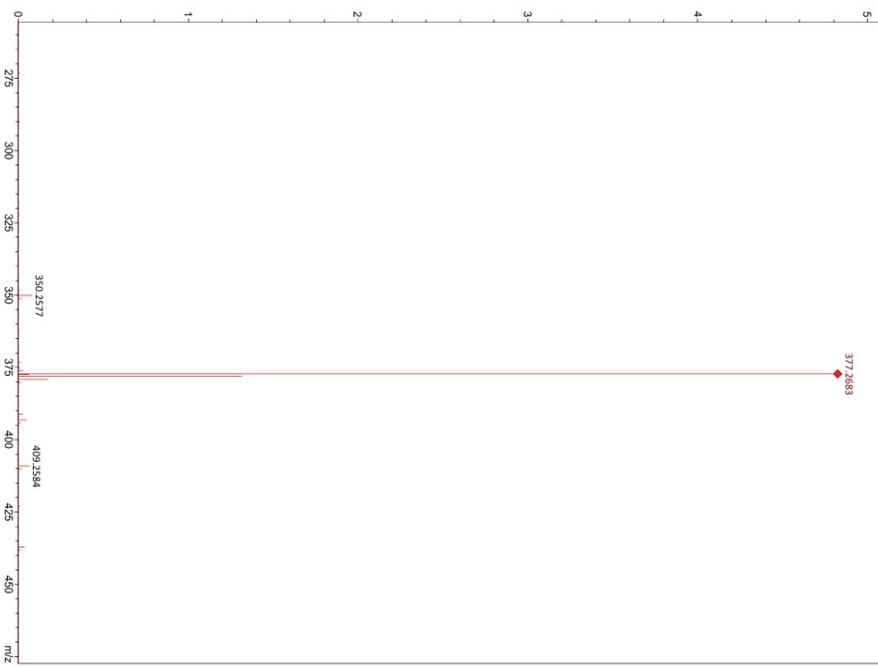
X4



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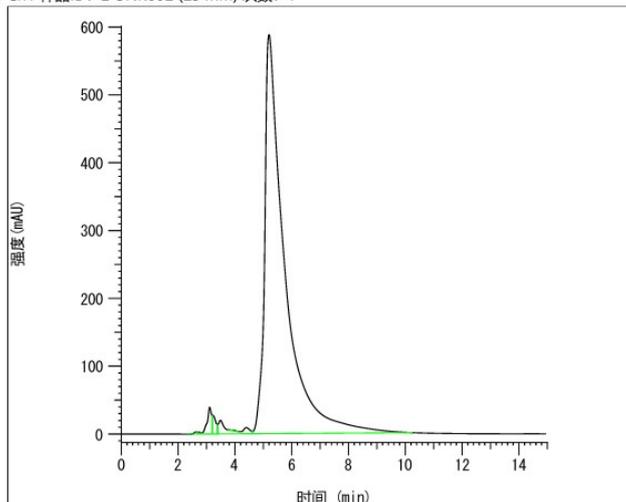
Intensity
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Bruker Compass DataAnalysis

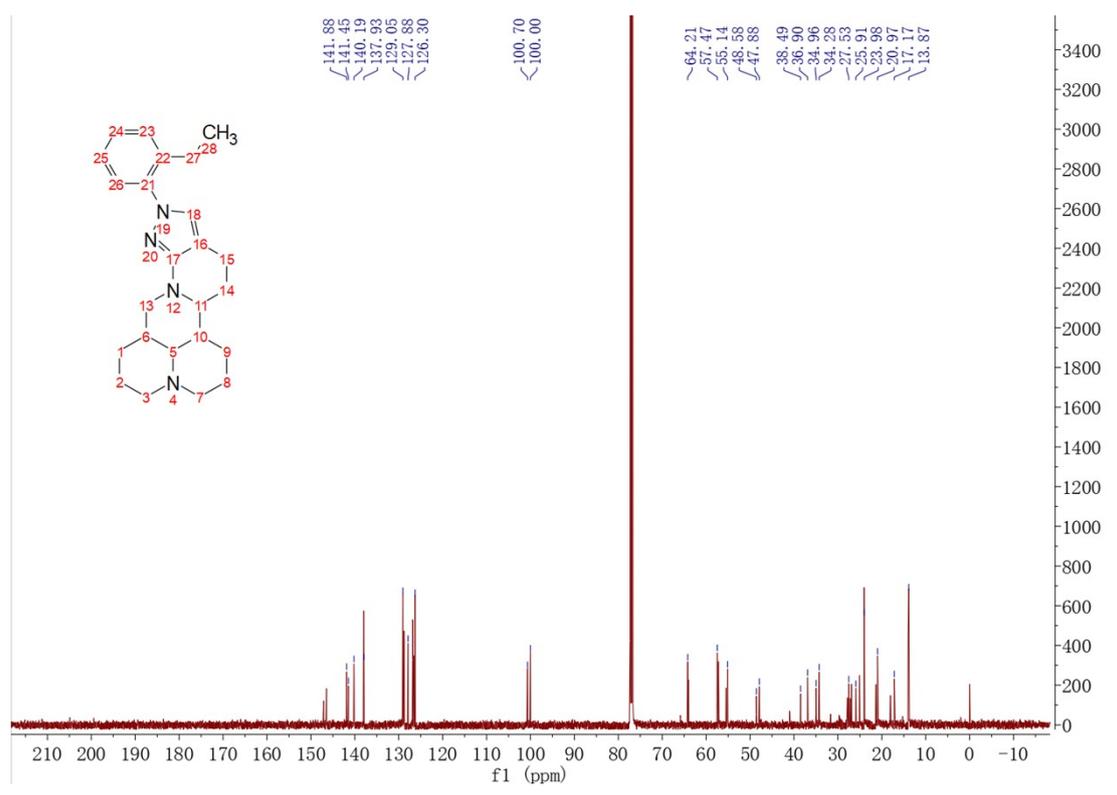
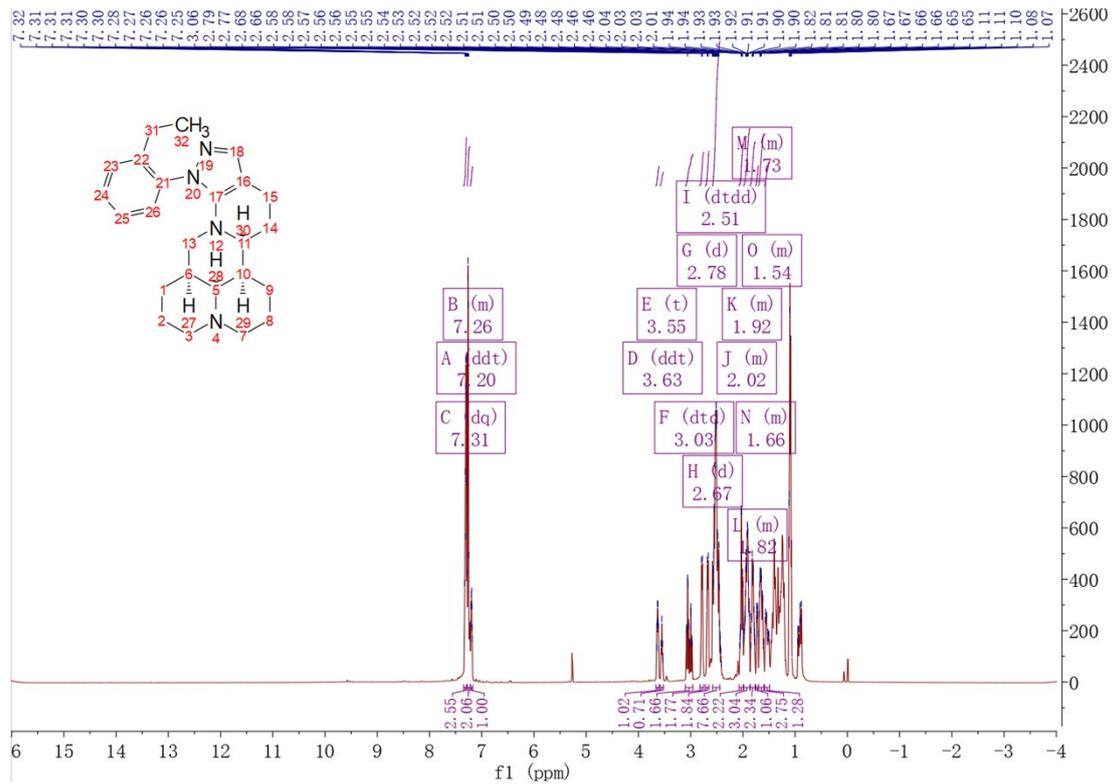
5410 UV Detector Ch1 样品ID: 2 UNK002 (254nm) 次数: 1



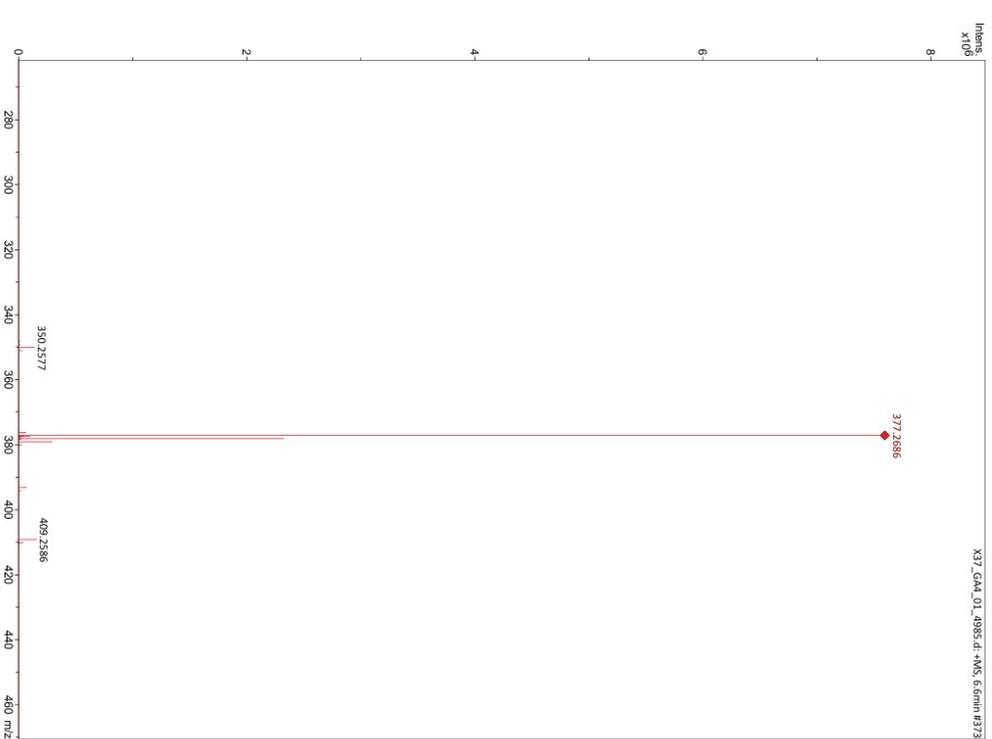
5410 UV Detector Ch1 样品ID: 2 UNK002 (254nm) 次数: 1

No.	成分名	RT	面积	面 积%	高度	高 度%	浓度	单位	浓度2	单位2	N	强度	半峰 宽	相对 RT	校正 RT	纯度 (平均)	纯度 (3点)	纯度 (2点)
1	峰1	2.633	24509	0.082	3265	0.472	---	---	---	---	---	3	---	---	---	---	---	---
2	峰2	2.733	17727	0.059	2967	0.429	---	---	---	---	---	3	---	---	---	---	---	---
3	峰3	3.113	435944	1.454	39414	5.695	---	---	---	---	---	39	---	---	---	---	---	---
4	峰4	3.230	223066	0.744	27290	3.943	---	---	---	---	---	27	---	---	---	---	---	---
5	峰5	3.490	386846	1.290	20204	2.919	---	---	---	---	---	20	---	---	---	---	---	---
6	峰6	3.797	2527	0.008	390	0.056	---	---	---	---	---	6	---	---	---	---	---	---
7	峰7	3.953	8222	0.027	1075	0.155	---	---	---	---	---	6	---	---	---	---	---	---
8	峰8	4.397	163185	0.544	9199	1.329	---	---	---	---	1458	10	0.27	---	---	---	---	---
9	峰9	5.203	2872429	95.792	588305	85.002	---	---	---	---	407	589	0.61	---	---	---	---	---
			29984455	100.000	692107	100.000												

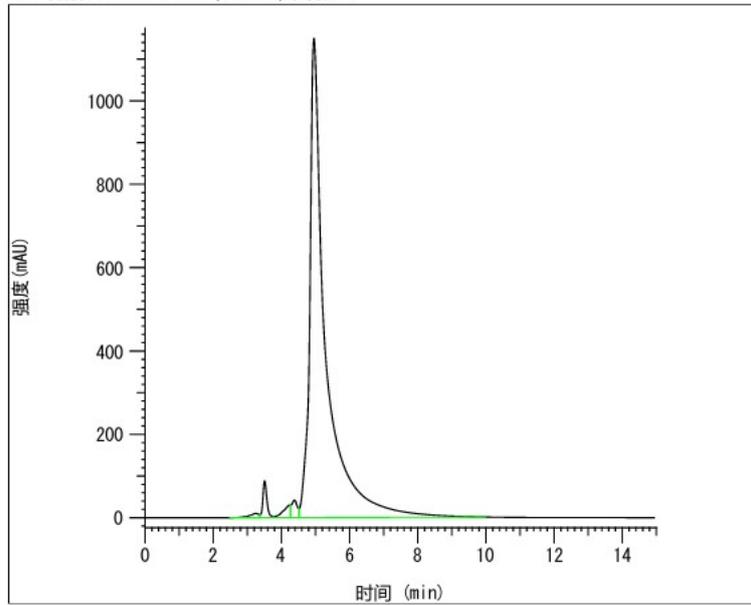
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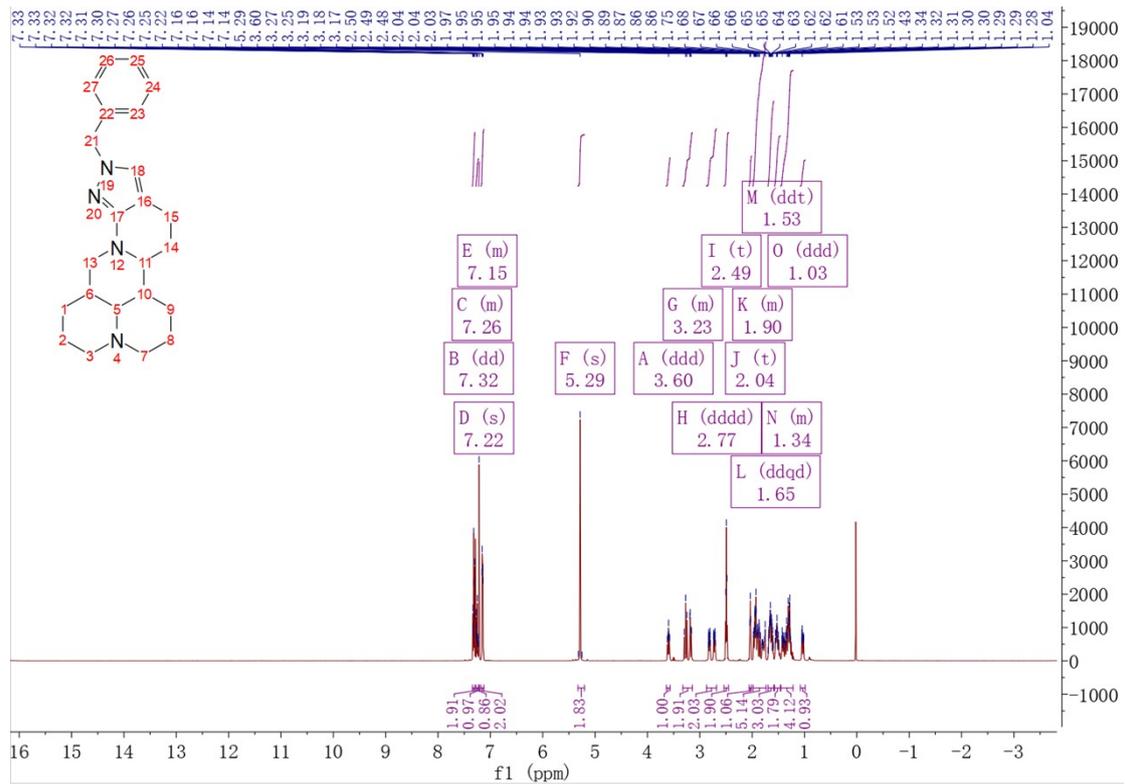


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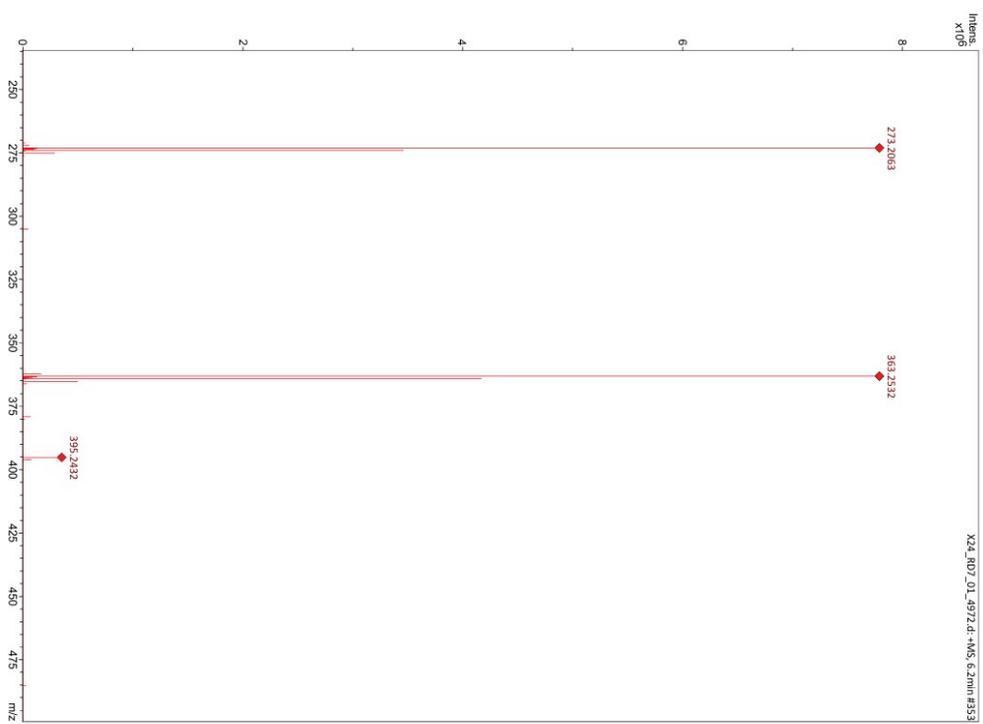


5410 UV Detector Ch1 样品ID: 2 UNK002 (254nm) 次数: 1

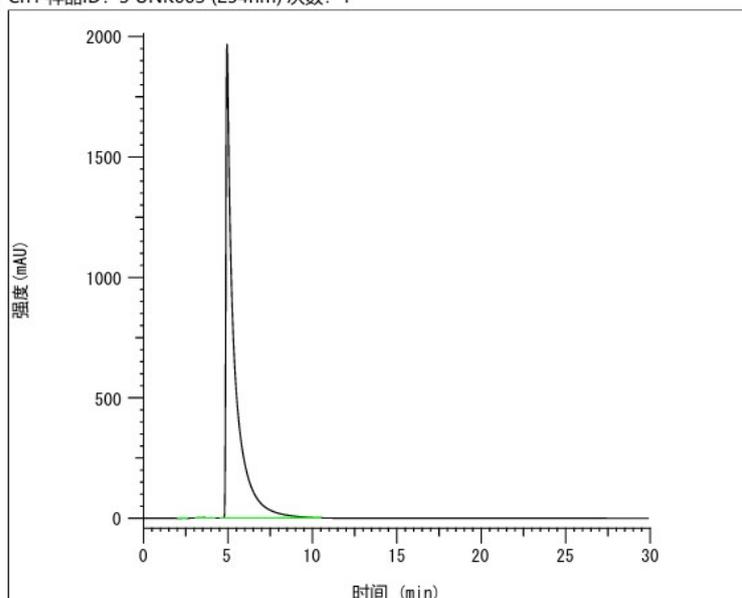
No.	成分名	RT	面积	面积%	高度	高度%	浓度	单位	浓度2	单位2	N	强度	半峰宽	相对RT	校正RT	纯度(平均)	纯度(3点)	纯度(2点)
1	峰1	3.253	194751	0.498	10113	0.766	---	---	---	---	---	10	---	---	---	---	---	---
2	峰2	3.507	732087	1.872	88462	6.700	---	---	---	---	4716	89	0.12	---	---	---	---	---
3	峰3	4.240	430895	1.102	29665	2.247	---	---	---	---	---	30	---	---	---	---	---	---
4	峰4	4.383	490105	1.254	41838	3.169	---	---	---	---	---	42	---	---	---	---	---	---
5	峰5	4.953	37249248	95.27	1150154	87.118	---	---	---	---	1223	1151	0.33	---	---	---	---	---
			39097086	100.000	1320231	100.000												



Window Display Report

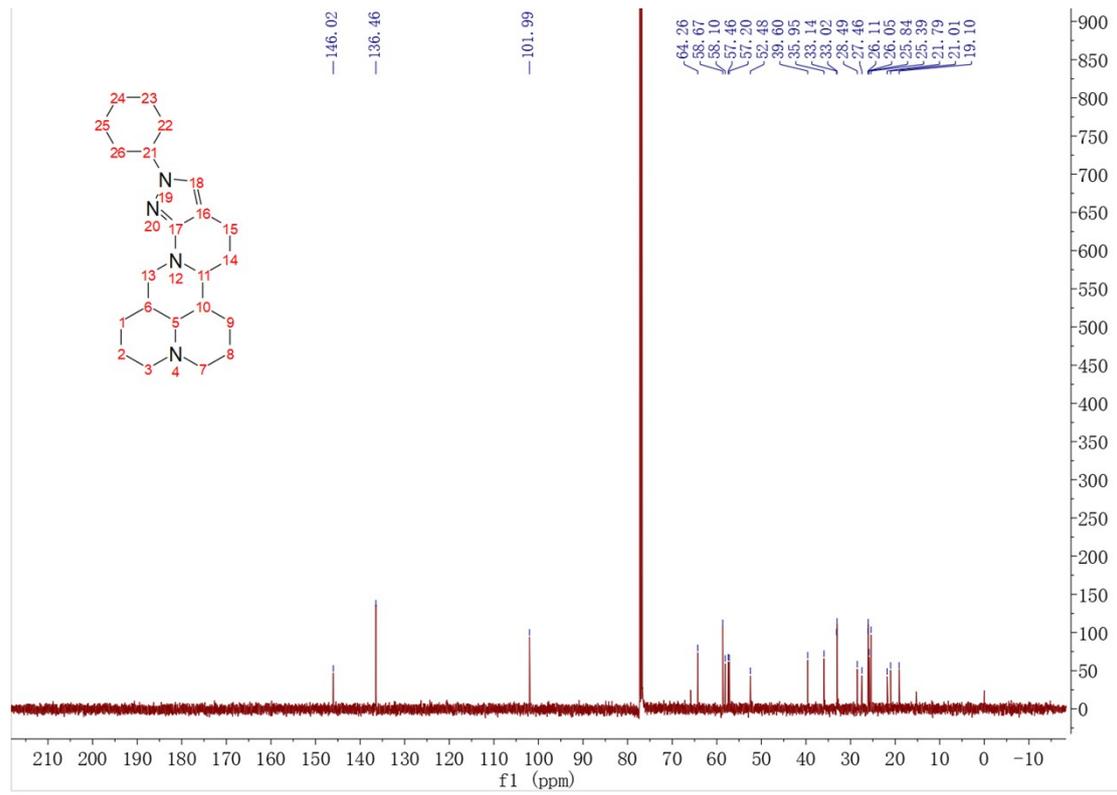
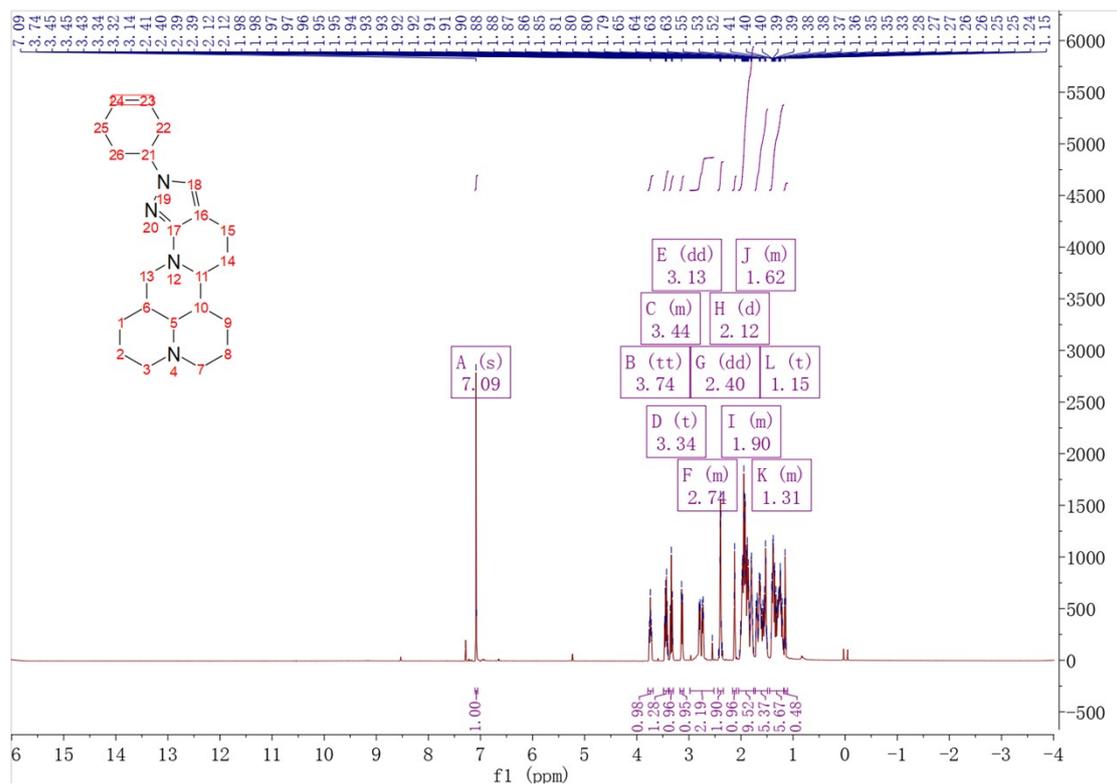


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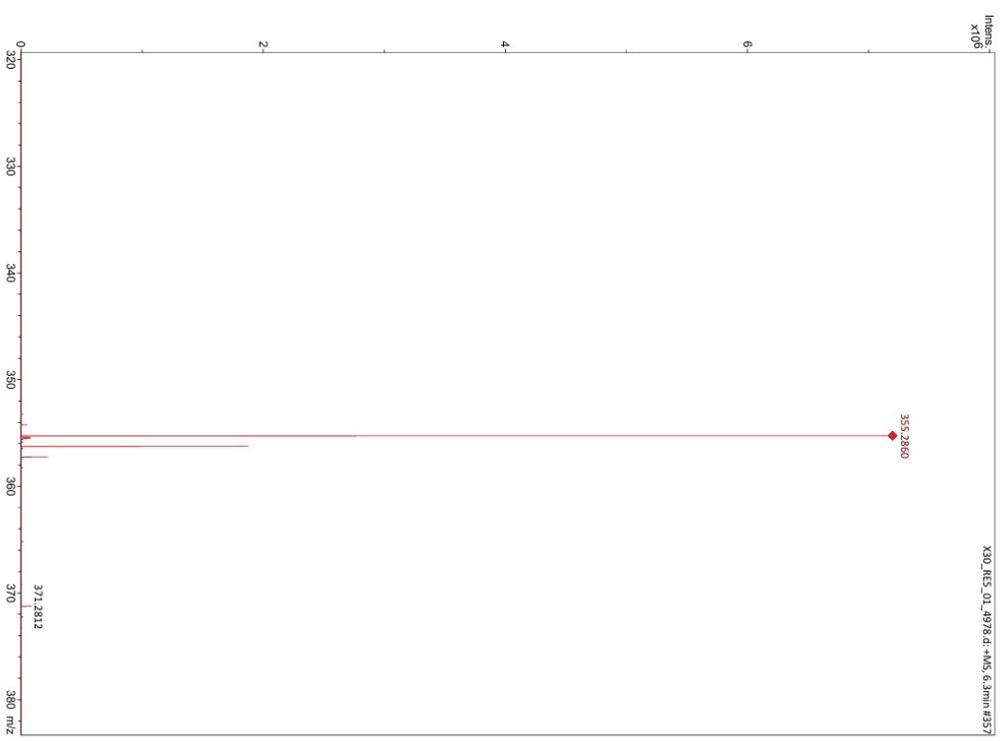


5410 UV Detector Ch1 样品ID: 3 UNK003 (254nm) 次数: 1

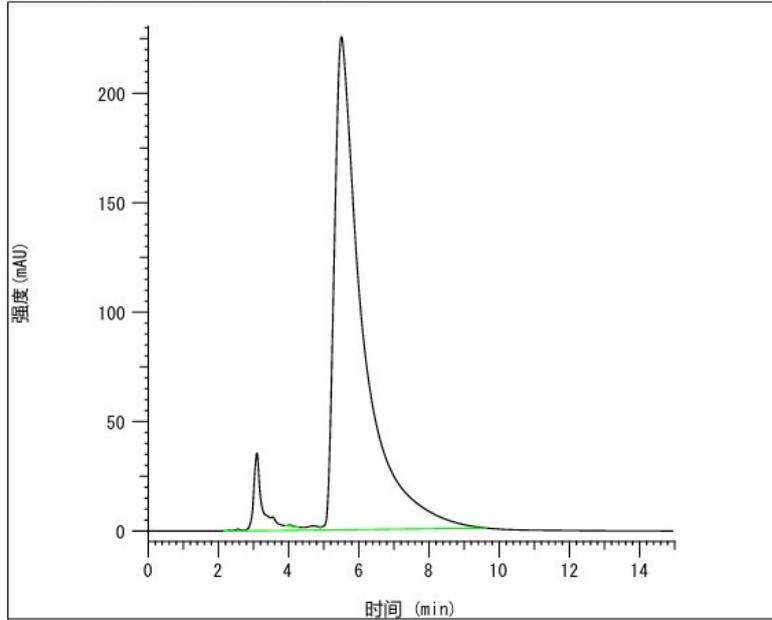
No.	成分名	RT	面积	面 积%	高度	高 度%	浓度	单位	浓度2	单位2	N	强度	半峰 宽	相对 RT	校正 RT	纯度 (平均)	纯度 (3点)	纯度 (2点)
1	峰1	2.127	2077	0.003	352	0.018	---	---	---	---	2869	0	0.09	---	---	---	---	---
2	峰2	2.390	1013	0.016	1112	0.056	---	---	---	---	2273	1	0.12	---	---	---	---	---
3	峰3	3.187	4508	0.007	731	0.037	---	---	---	---	---	2	---	---	---	---	---	---
4	峰4	3.363	1421	0.022	1356	0.069	---	---	---	---	---	2	---	---	---	---	---	---
5	峰5	3.570	1925	0.030	2162	0.109	---	---	---	---	3871	3	0.14	---	---	---	---	---
6	峰6	4.043	3637	0.006	435	0.022	---	---	---	---	5044	1	0.13	---	---	---	---	---
7	峰7	4.947	6432	99.91	1969	99.68	---	---	---	---	1252	1971	0.33	---	---	---	---	---
			6437	100.0	1976	100.0												
			8481	100.0	1976	100.0												



Window Display Report



5410 UV Detector Ch1 样品ID: 3 UNK003 (254nm) 次数: 1



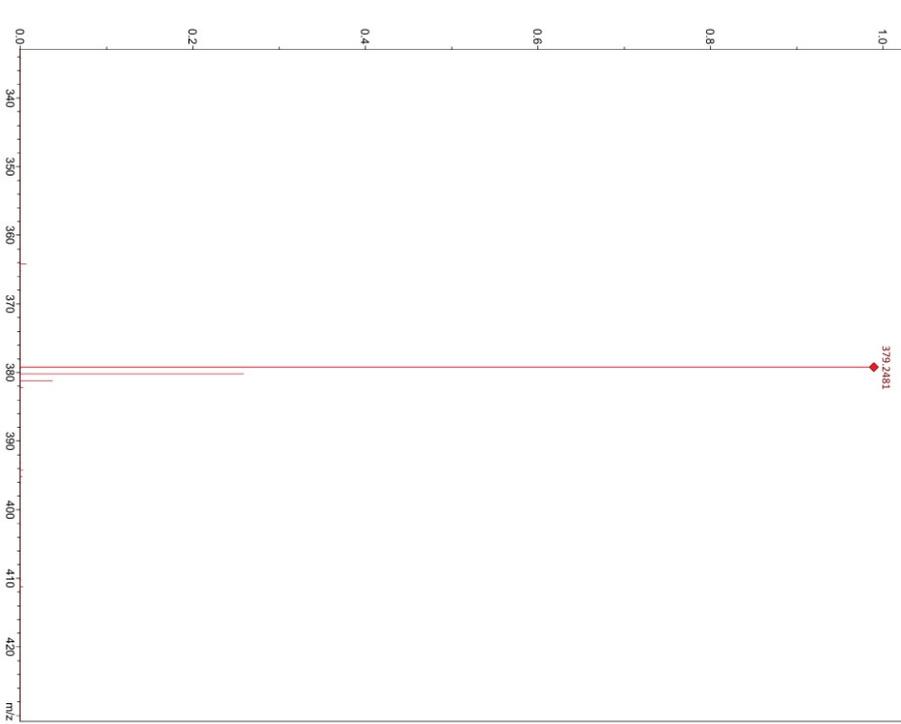
5410 UV Detector Ch1 样品ID: 3 UNK003 (254nm) 次数: 1

No.	成分名	RT	面积	面积%	高度	高度%	浓度	单位	浓度2	单位2	N	强度	半峰宽	相对RT	校正RT	纯度(平均)	纯度(3点)	纯度(2点)
1	峰1	2.317	2170	0.016	323	0.123	---	---	---	---	---	0	---	---	---	---	---	---
2	峰2	3.097	6539 29	4.923	3556 9	13.49 1	---	---	---	---	1673	36	0.18	---	---	---	---	---
3	峰3	4.033	5516	0.042	542	0.205	---	---	---	---	3710	3	0.16	---	---	---	---	---
4	峰4	4.700	5658 0	0.426	1917	0.727	---	---	---	---	---	2	---	---	---	---	---	---
5	峰5	5.503	1256 4890	94.59	2253 04	85.45 4	---	---	---	---	335	226	0.71	---	---	---	---	---
			1328 3084	100.0	2636 53	100.0 00												

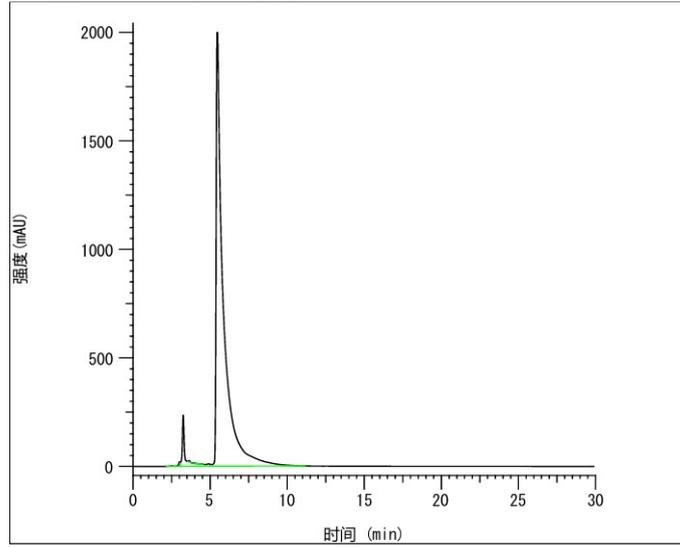
X8

Window Display Report

Intens $\times 10^6$ XZ3_006_01_4971.d-MMS, 5.5min#333

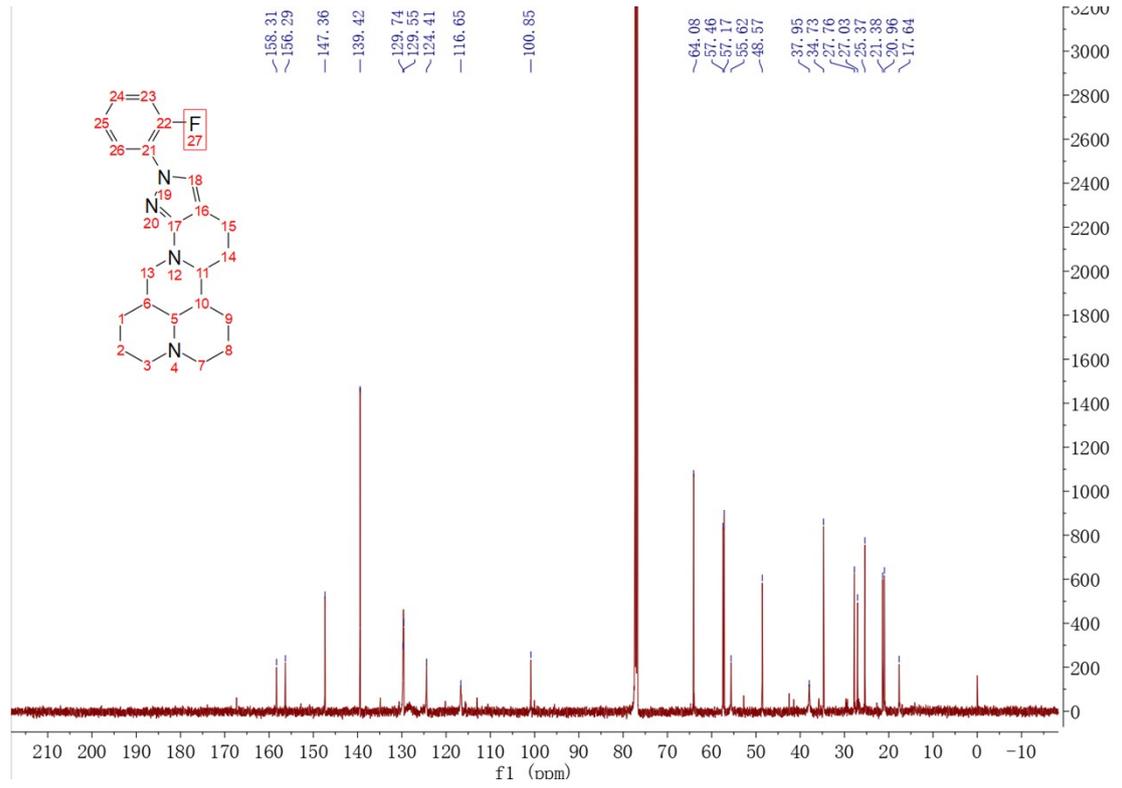
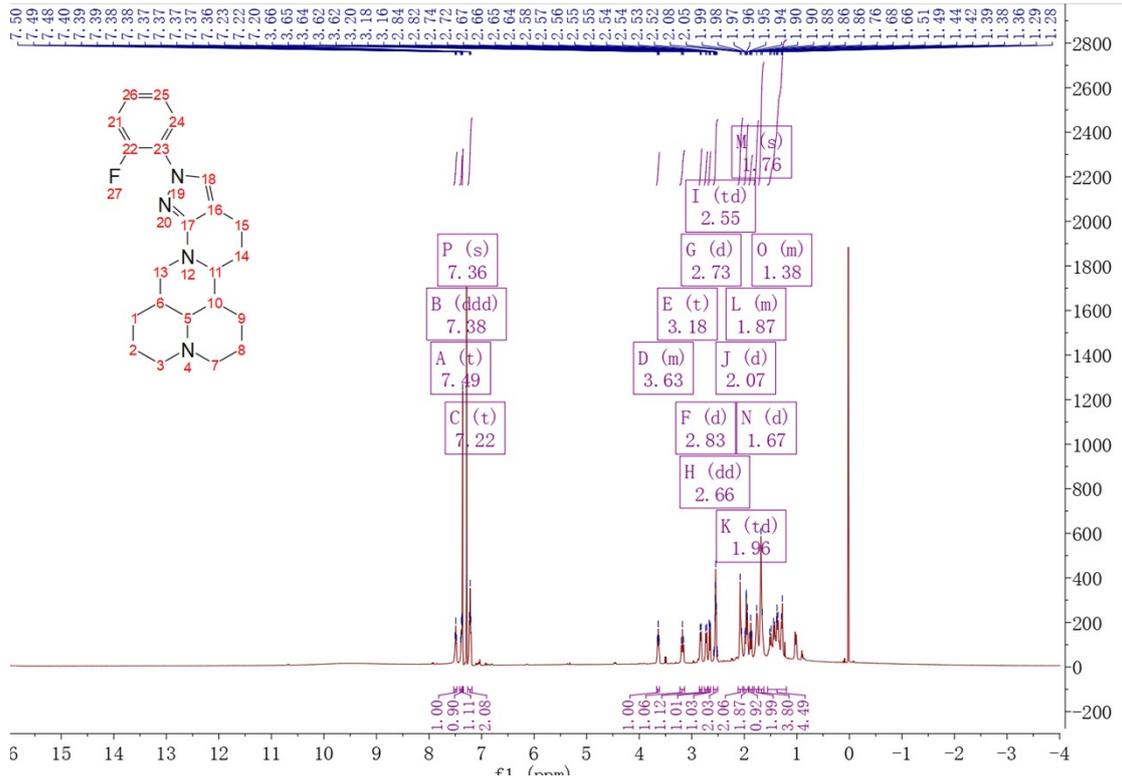


5410 UV Detector Ch1 样品ID: 3 UNK003 (254nm) 次数: 1



5410 UV Detector Ch1 样品ID: 3 UNK003 (254nm) 次数: 1

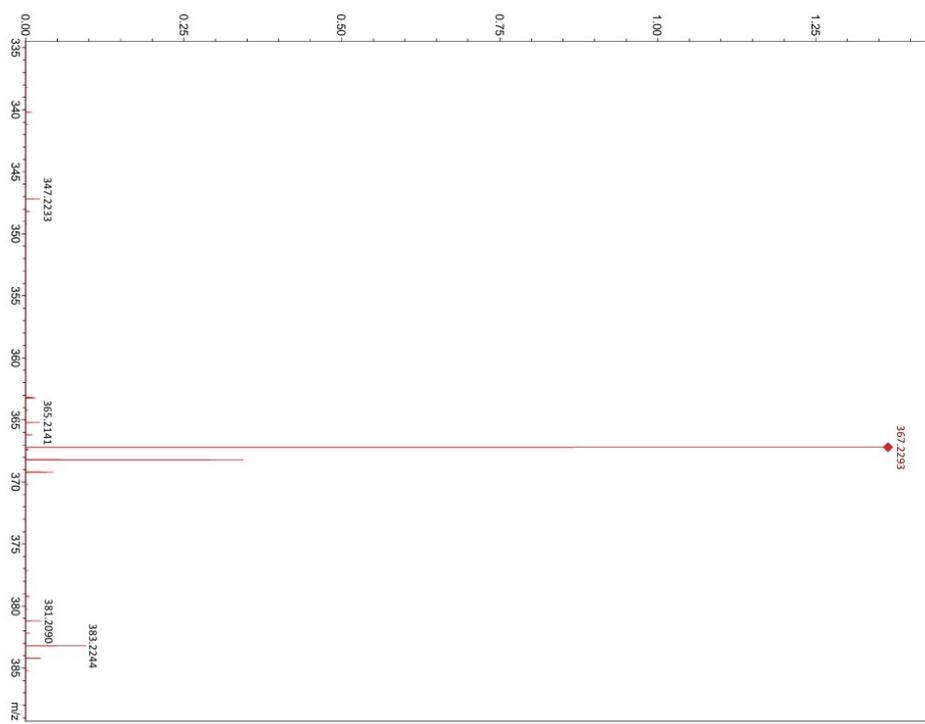
No.	成分名	RT	面积	面积%	高度	高度%	浓度	单位	浓度2	单位2	N	强度	半峰宽	相对RT	校正RT	纯度(平均)	纯度(3点)	纯度(2点)
1	峰1	2.320	4886	0.007	717	0.032	---	---	---	---	---	1	---	---	---	---	---	---
2	峰2	2.513	21952	0.032	2264	0.100	---	---	---	---	1906	2	0.14	---	---	---	---	---
3	峰3	3.253	2976834	4.382	238023	10.566	---	---	---	---	4406	238	0.12	---	---	---	---	---
4	峰4	3.633	56724	0.084	6574	0.292	---	---	---	---	3315	27	0.15	---	---	---	---	---
5	峰5	3.947	22303	0.033	3063	0.136	---	---	---	---	6058	17	0.12	---	---	---	---	---
6	峰6	4.160	7146	0.011	856	0.038	---	---	---	---	---	13	---	---	---	---	---	---
7	峰7	4.410	14082	0.021	1838	0.082	---	---	---	---	---	12	---	---	---	---	---	---
8	峰8	5.487	64822543	95.430	1999425	88.754	---	---	---	---	1416	2000	0.34	---	---	---	---	---
			67926470	100.000	2252759	100.000												



Window Display Report

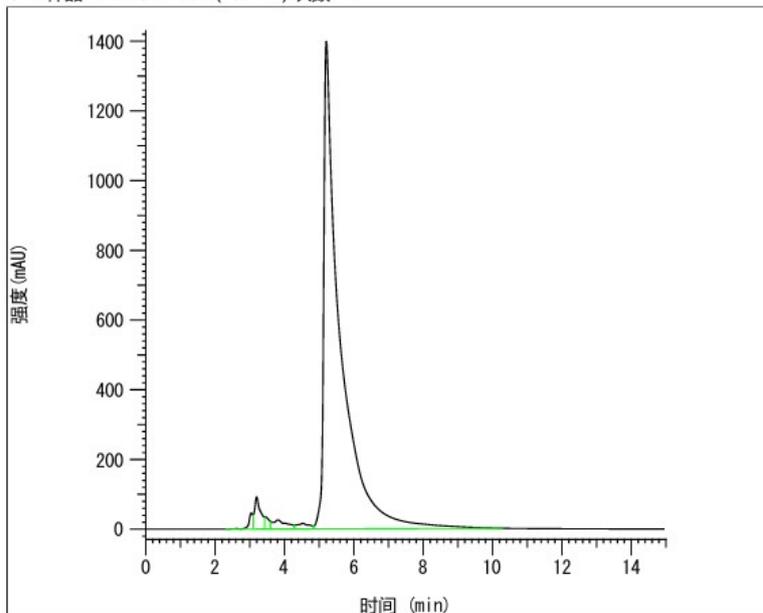
Invent:
K106

X33_N68_01_4981.d -MS, 5.8mm #329



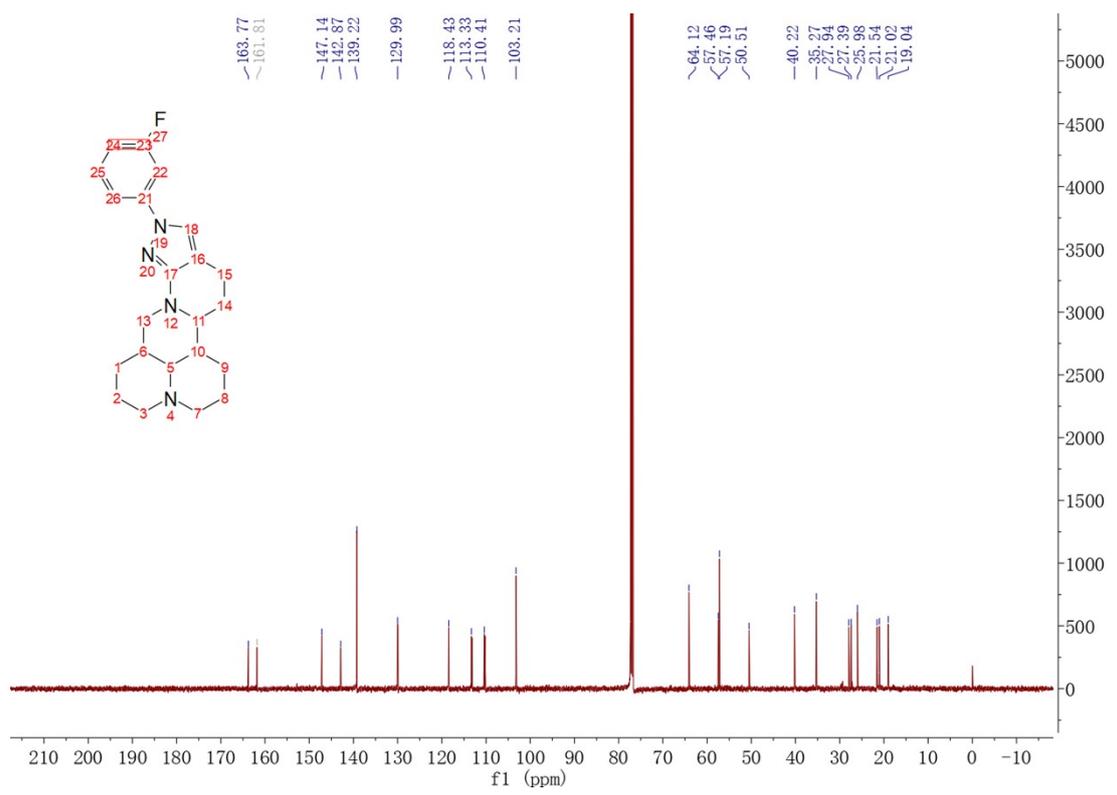
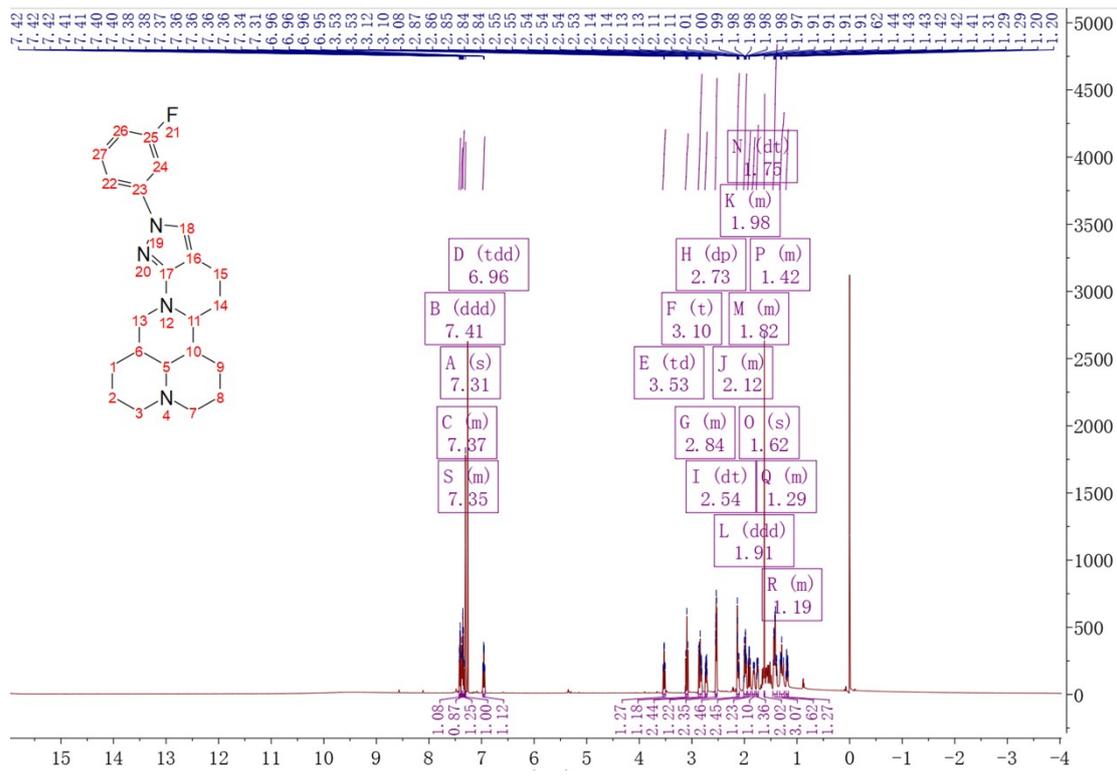
Bruker Compass DataAnalysis

5410 UV Detector Ch1 样品ID: 4 UNK004 (254nm) 次数: 1

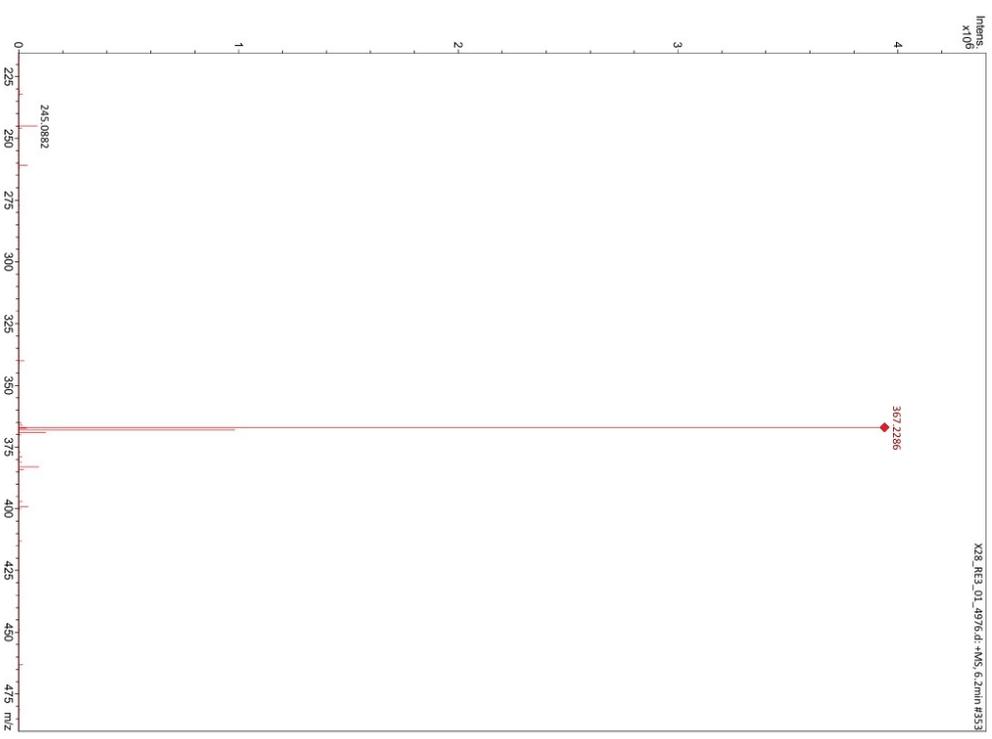


5410 UV Detector Ch1 样品ID: 4 UNK004 (254nm) 次数: 1

No.	成分名	RT	面积	面积%	高度	高度%	浓度	单位	浓度2	单位2	N	强度	半峰宽	相对RT	校正RT	纯度(平均)	纯度(3点)	纯度(2点)
1	峰1	2.480	6025	0.013	915	0.060	---	---	---	---	---	1	---	---	---	---	---	---
2	峰2	2.623	13011	0.027	1538	0.101	---	---	---	---	1794	2	0.15	---	---	---	---	---
3	峰3	3.197	1145013	2.394	92255	6.043	---	---	---	---	1301	93	0.21	---	---	---	---	---
4	峰4	4.007	738326	1.544	16471	1.079	---	---	---	---	---	17	---	---	---	---	---	---
5	峰5	4.530	403871	0.844	16082	1.053	---	---	---	---	---	17	---	---	---	---	---	---
6	峰6	5.207	45521056	95.1700	1399377	91.664	---	---	---	---	1190	1400	0.36	---	---	---	---	---
			47827302	100.000	1526639	100.000												

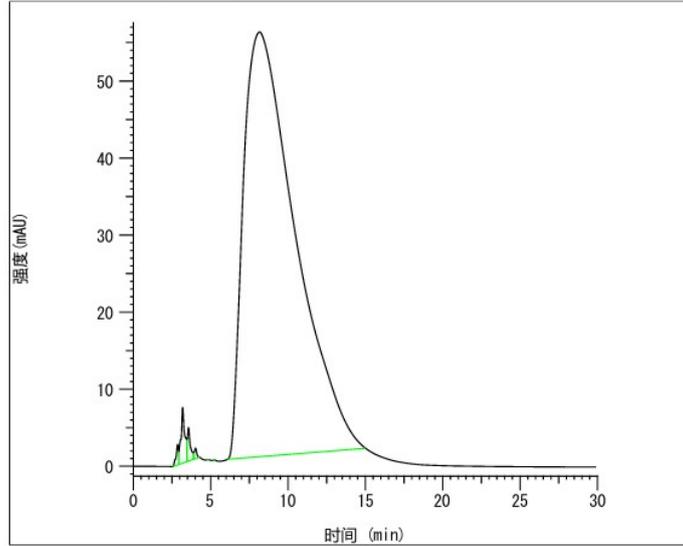


Window Display Report



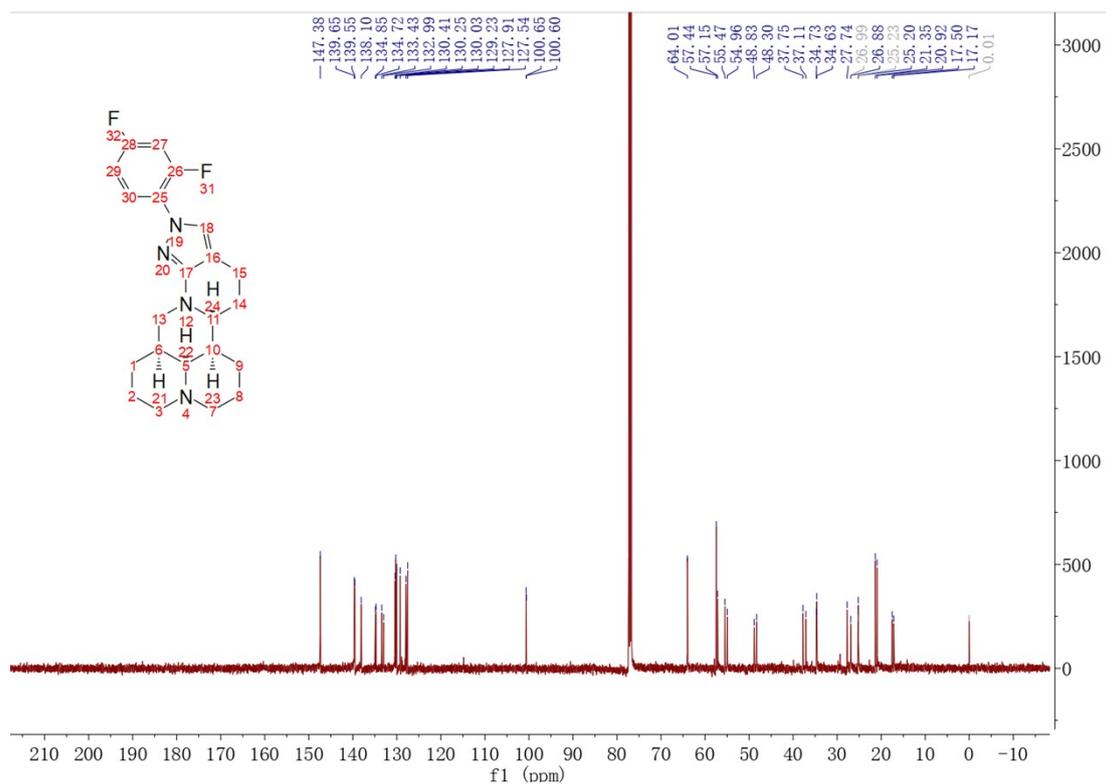
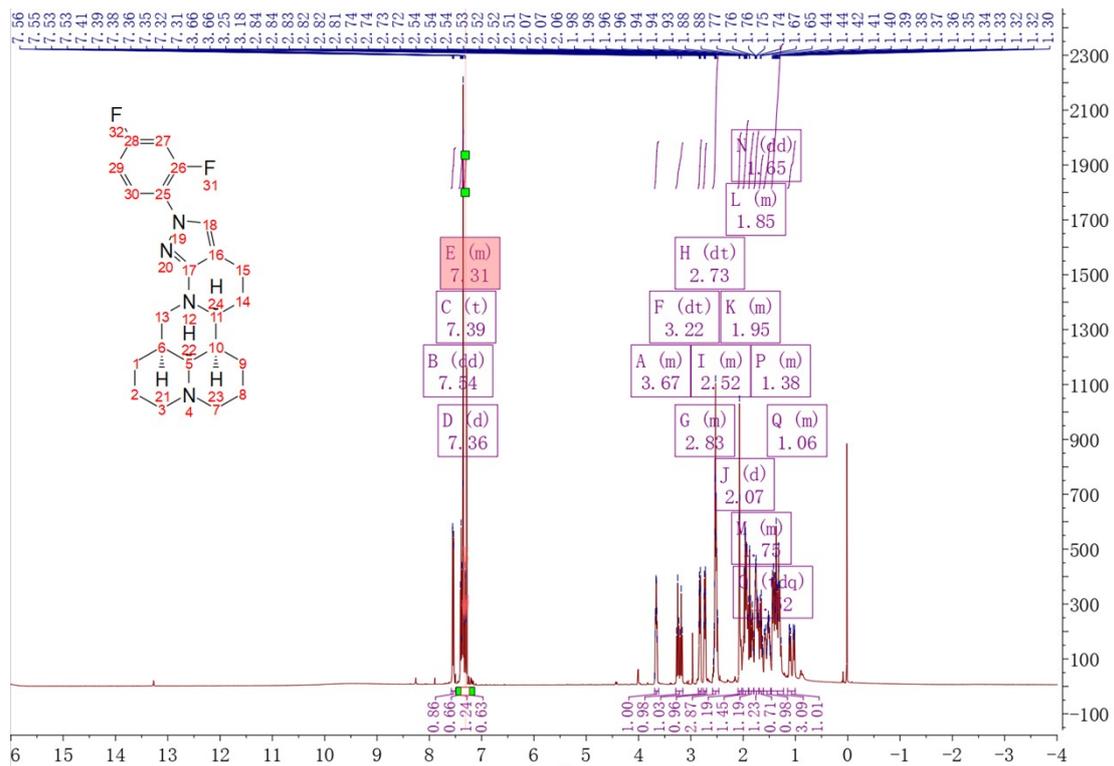
Bruker Compass DataAnalysis

5410 UV Detector Ch1 样品ID: 4 UNK004 (254nm) 次数: 1

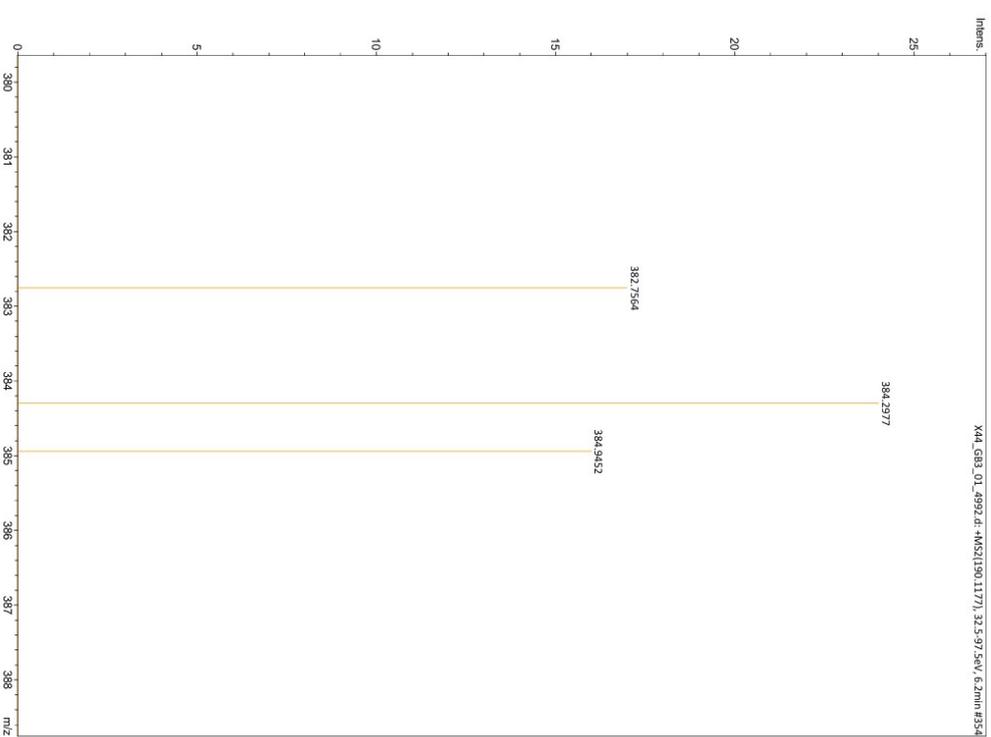


5410 UV Detector Ch1 样品ID: 4 UNK004 (254nm) 次数: 1

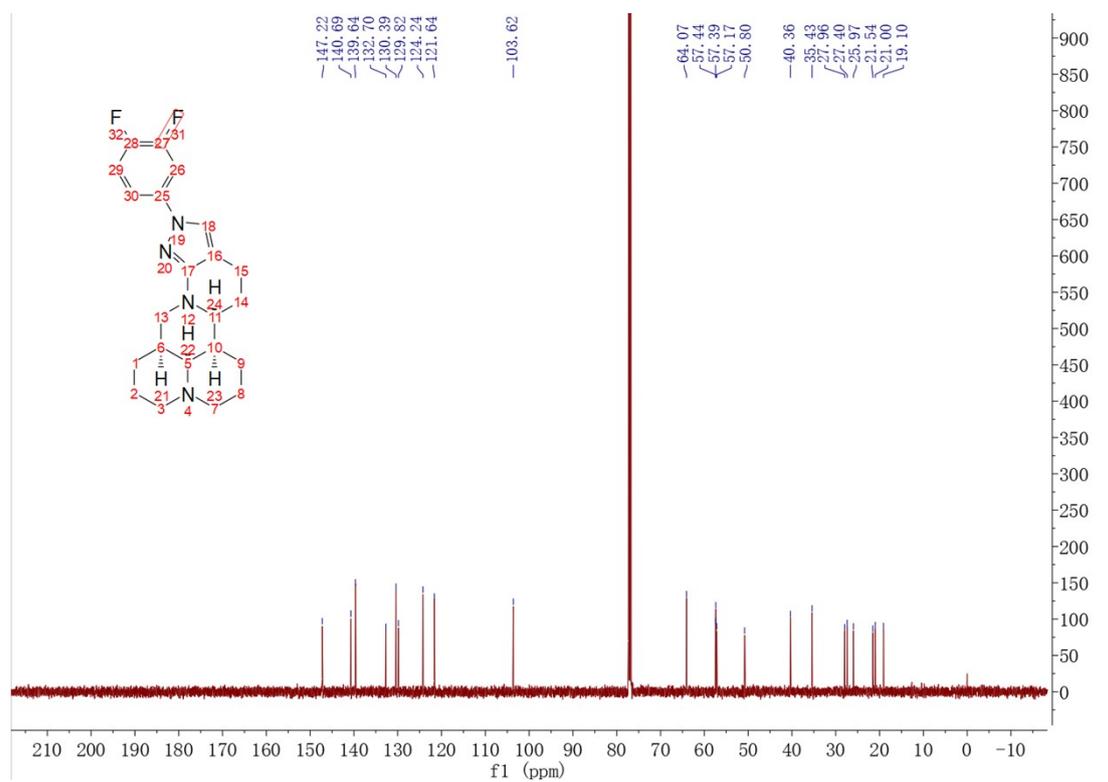
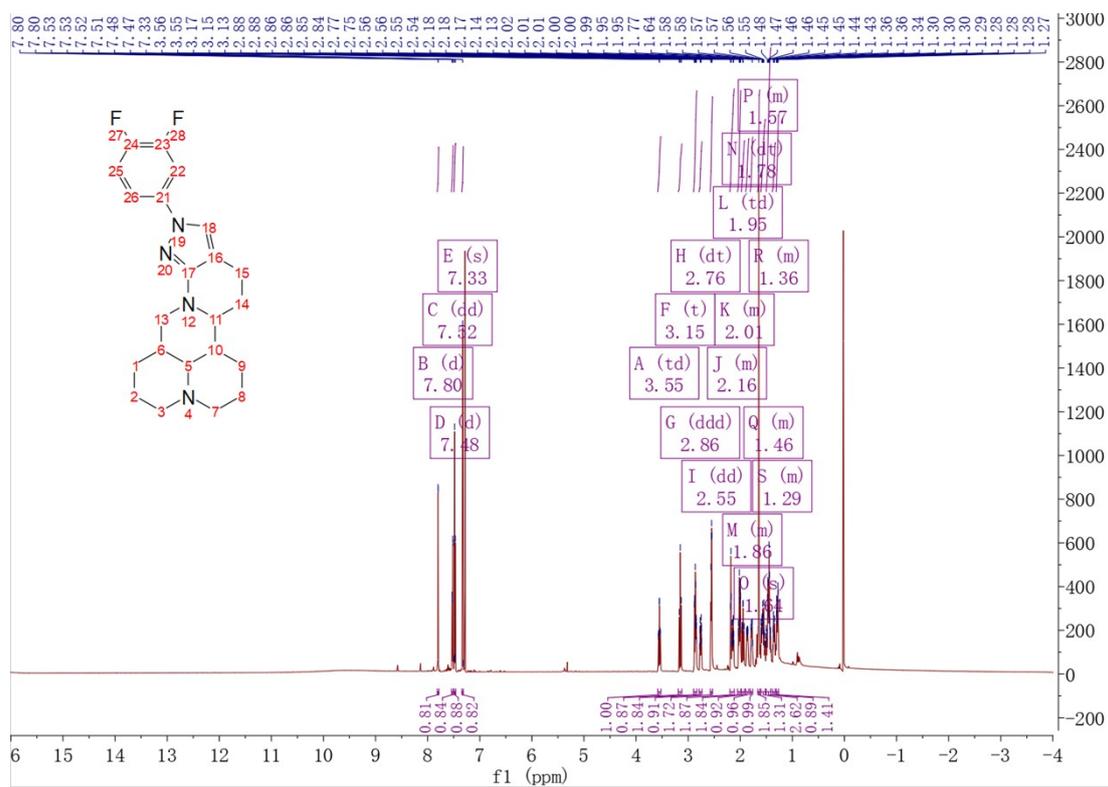
No.	成分名	RT	面积	面积%	高度	高度%	浓度	单位	浓度2	单位2	N	强度	半峰宽	相对RT	校正RT	纯度(平均)	纯度(3点)	纯度(2点)
1	峰1	2.867	29000	0.223	2670	3.765	---	---	---	---	---	3	---	---	---	---	---	---
2	峰2	3.187	122764	0.943	7268	10.251	---	---	---	---	1297	8	0.21	---	---	---	---	---
3	峰3	3.567	57875	0.444	4383	6.182	---	---	---	---	---	5	---	---	---	---	---	---
4	峰4	4.020	15319	0.118	1353	1.908	---	---	---	---	---	2	---	---	---	---	---	---
5	峰5	4.813	254	0.002	39	0.055	---	---	---	---	10592	1	0.11	---	---	---	---	---
6	峰6	5.237	173	0.001	35	0.049	---	---	---	---	18756	1	0.09	---	---	---	---	---
7	峰7	8.163	12796334	98.26	55149	77.790	---	---	---	---	28	56	3.62	---	---	---	---	---
			13021718	100.000	70895	100.000												



Window Display Report



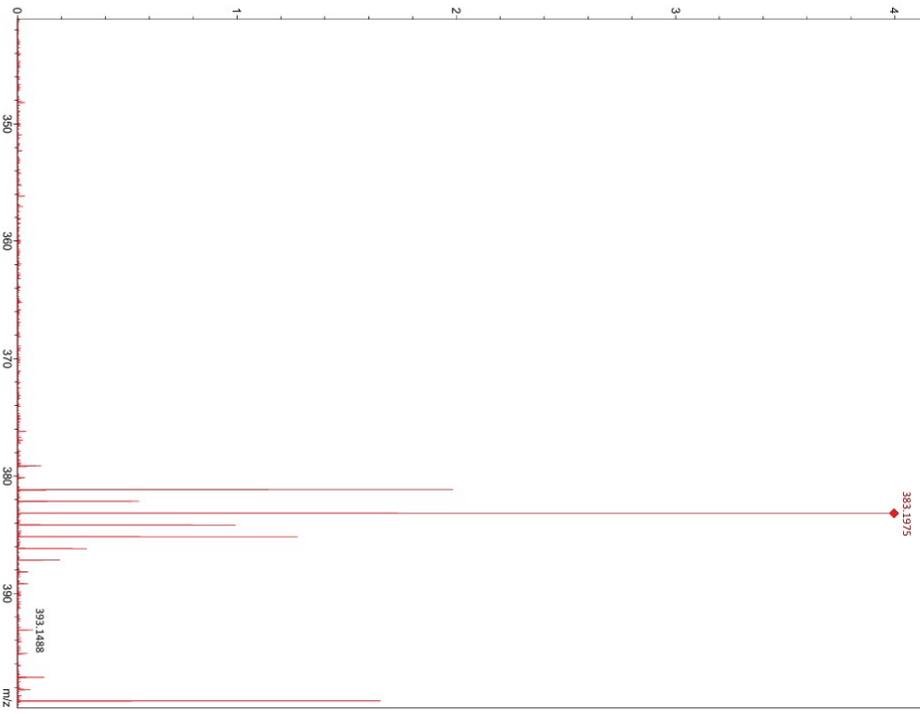
X12



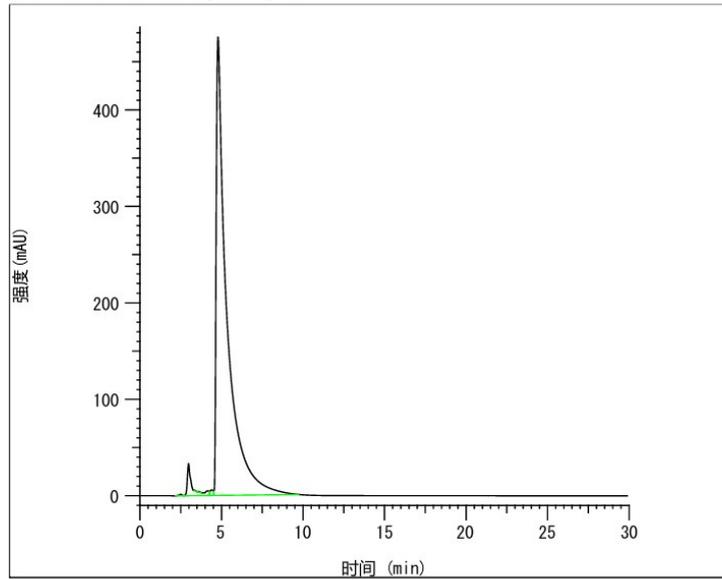
Window Display Report

Interna
X104

XZ2_R05_01_1970.d+.MS.7.0min.F938

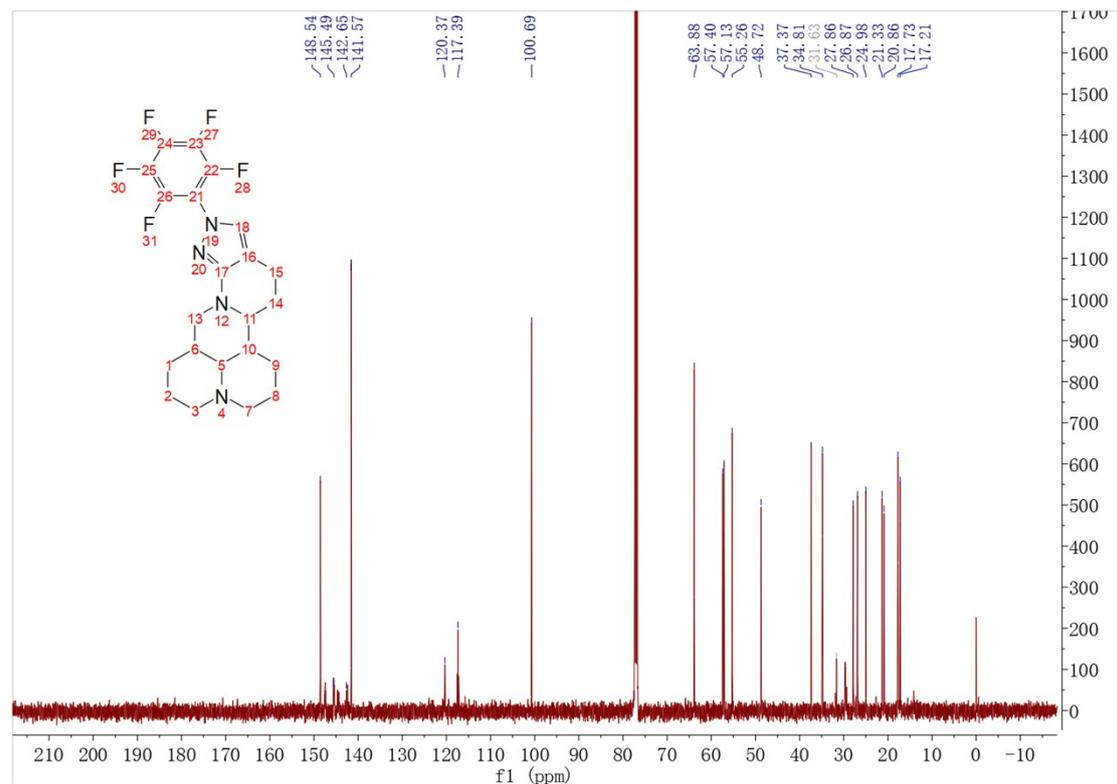
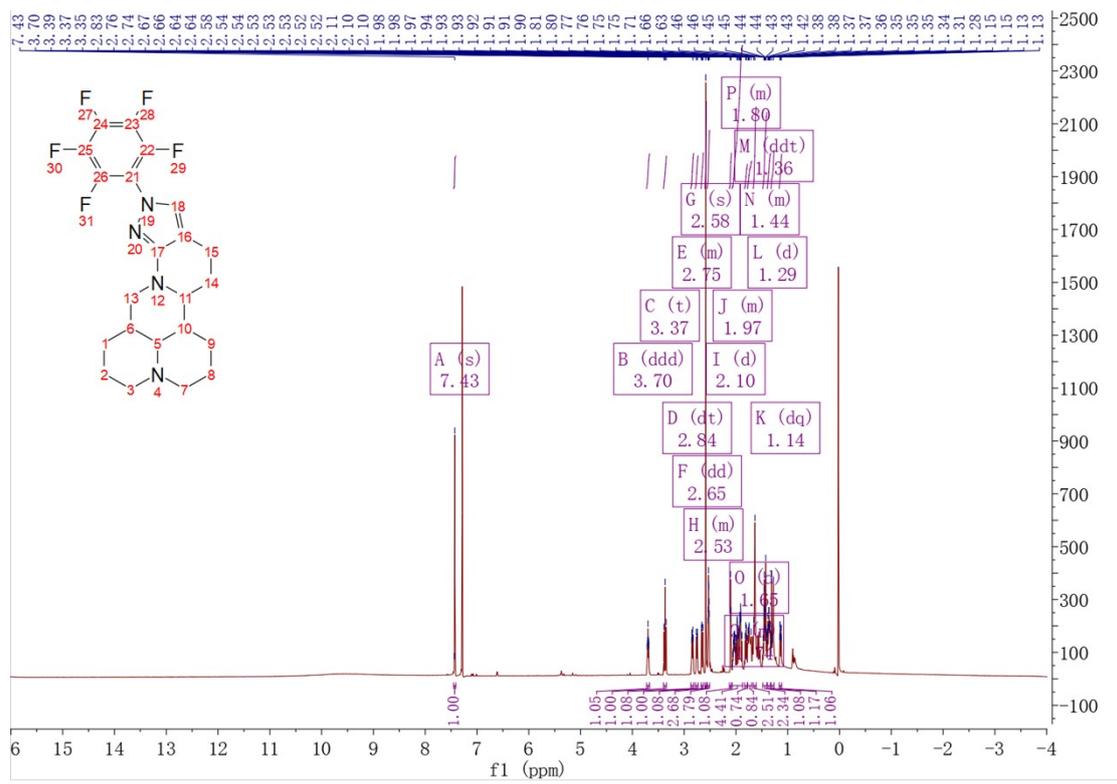


5410 UV Detector Ch1 样品ID: 5 UNK005 (254nm) 次数: 1

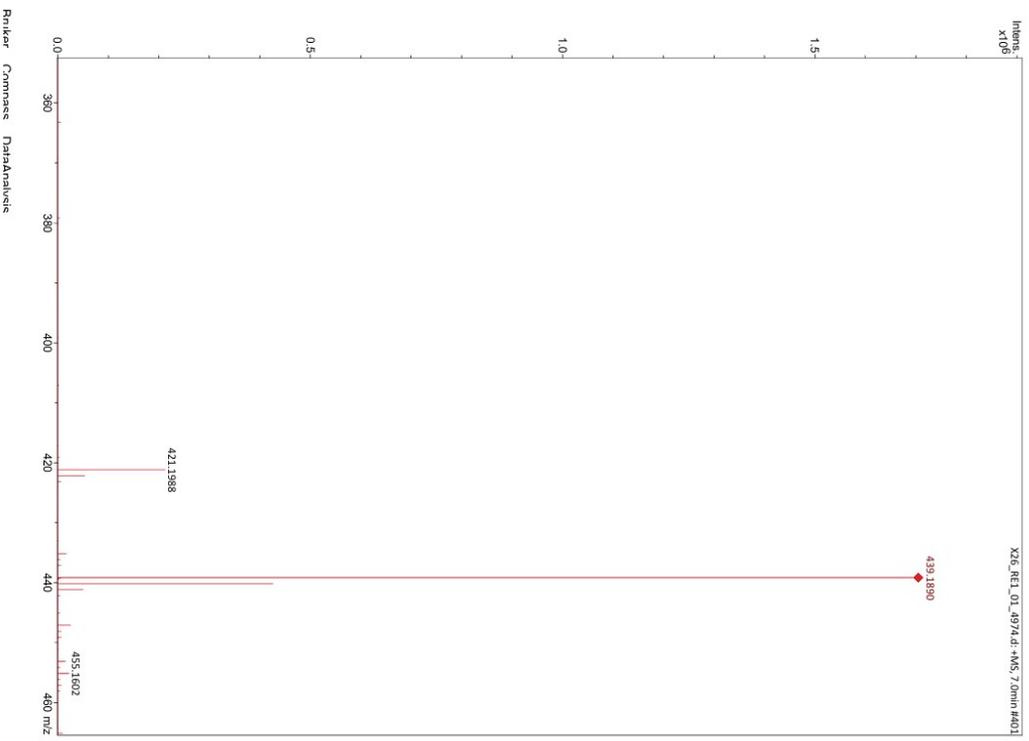


5410 UV Detector Ch1 样品ID: 5 UNK005 (254nm) 次数: 1

No.	成分名	RT	面积	面积%	高度	高度%	浓度	单位	浓度2	单位2	N	强度	半峰宽	相对RT	校正RT	纯度(平均)	纯度(3点)	纯度(2点)
1	峰1	2.347	4494	0.020	678	0.129	---	---	---	---	---	1	---	---	---	---	---	---
2	峰2	2.500	15968	0.072	1770	0.338	---	---	---	---	2088	2	0.13	---	---	---	---	---
3	峰3	2.980	613324	2.755	33492	6.399	---	---	---	---	1087	33	0.21	---	---	---	---	---
4	峰4	3.357	4524	0.020	587	0.112	---	---	---	---	---	6	---	---	---	---	---	---
5	峰5	3.580	7036	0.032	747	0.143	---	---	---	---	4394	5	0.13	---	---	---	---	---
6	峰6	4.173	77700	0.349	4732	0.904	---	---	---	---	---	5	---	---	---	---	---	---
7	峰7	4.400	80281	0.361	5838	1.115	---	---	---	---	---	6	---	---	---	---	---	---
8	峰8	4.790	21459969	96.391	475571	90.860	---	---	---	---	469	476	0.52	---	---	---	---	---
			22263296	100.000	523414	100.000												

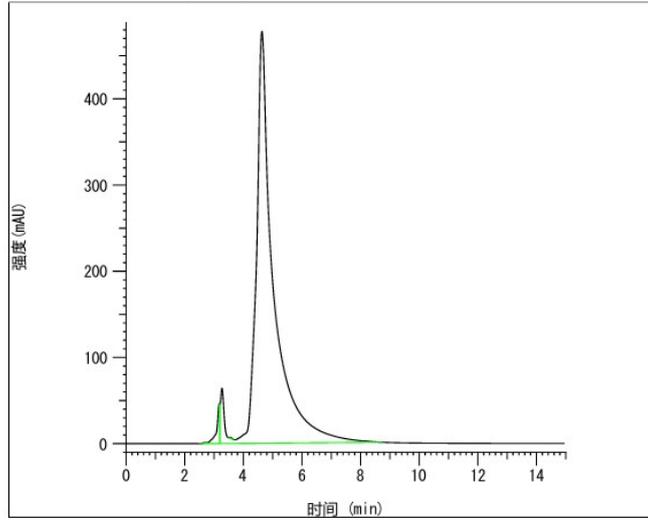


Window Display Report



峰值检测详细结果

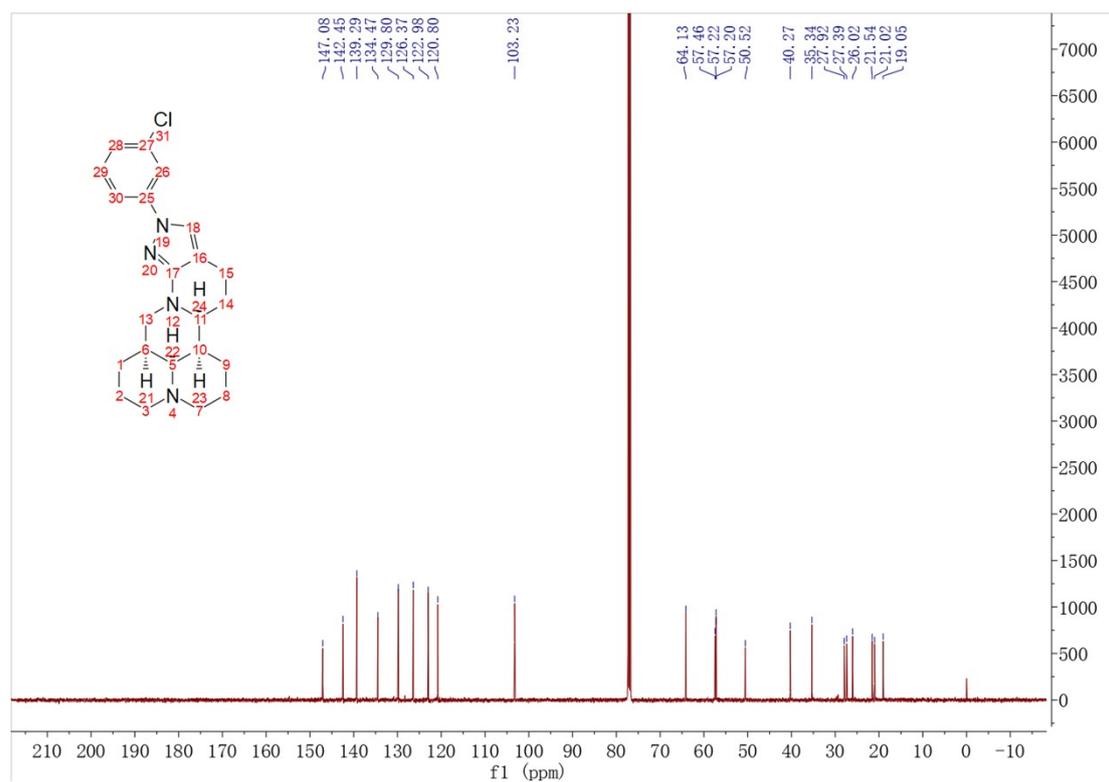
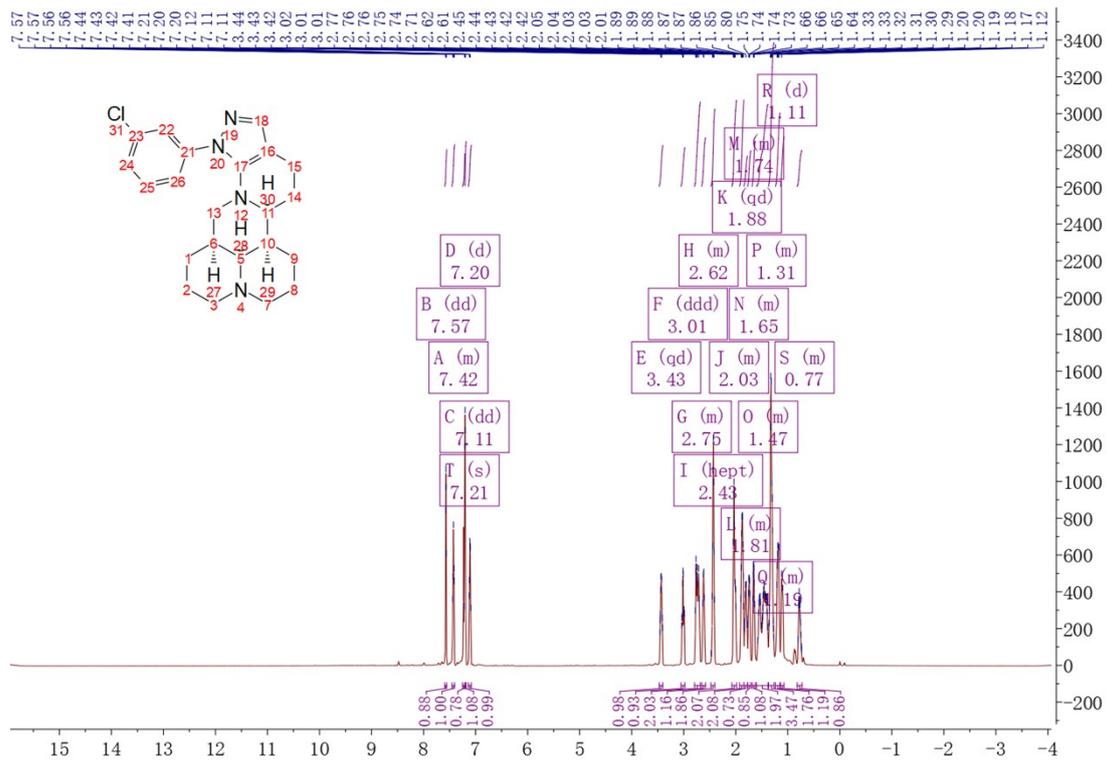
5410 UV Detector Ch1 样品ID: 1 UNK001 (254nm) 次数: 1



5410 UV Detector Ch1 样品ID: 1 UNK001 (254nm) 次数: 1

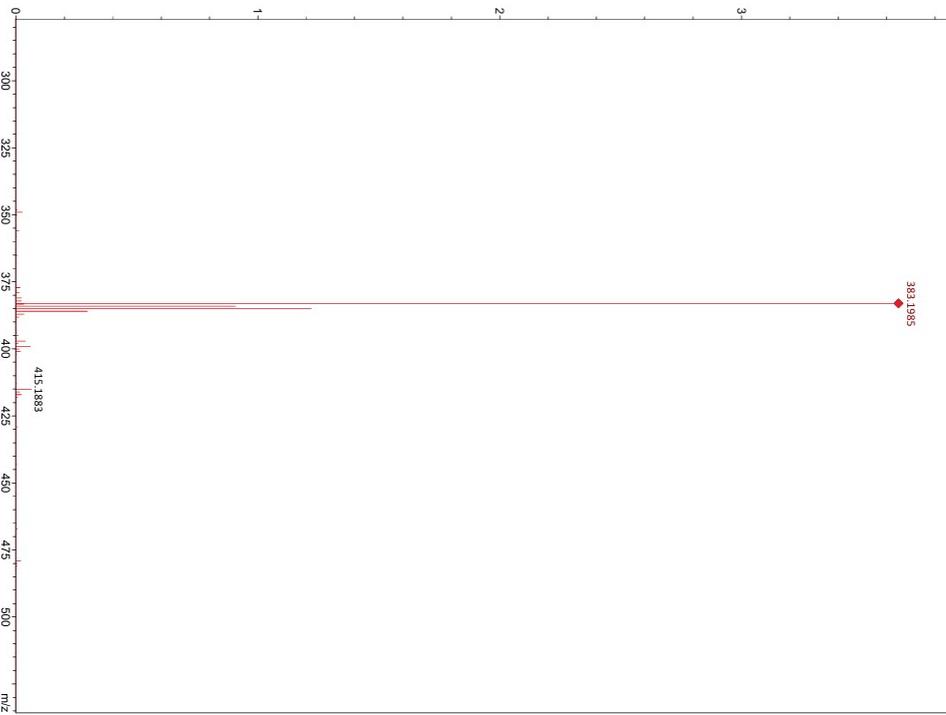
No.	成分名	RT	面积	面积%	高度	高度%	浓度	单位	浓度2	单位2	N	强度	半峰宽	相对RT	校正RT	纯度(平均)	纯度(3点)	纯度(2点)
1	峰1	2.667	7874	0.039	1127	0.191	---	---	---	---	---	1	---	---	---	---	---	---

2	峰2	3.180	325881	1.610	46146	7.816	---	---	---	---	---	46	---	---	---	---	---	---
3	峰3	3.270	662486	3.273	64237	10.880	---	---	---	---	---	64	---	---	---	---	---	---
4	峰4	3.547	6341	0.031	1030	0.174	---	---	---	---	---	7	---	---	---	---	---	---
5	峰5	4.633	19236596	95.047	477852	80.939	---	---	---	---	646	478	0.43	---	---	---	---	---
			20239178	100.000	590391	100.000												

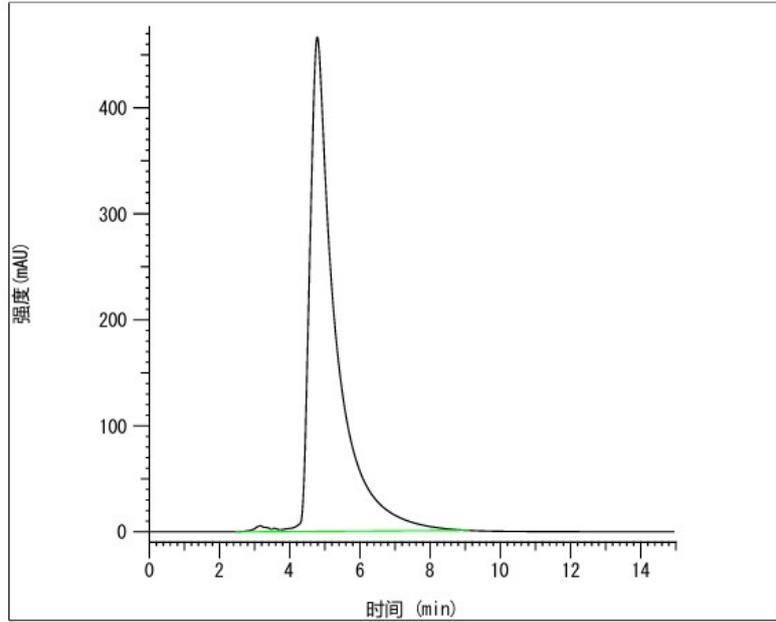


Window Display Report

Inventis X100 X38_GA5_01_4986.d - MS, 6.3min #361

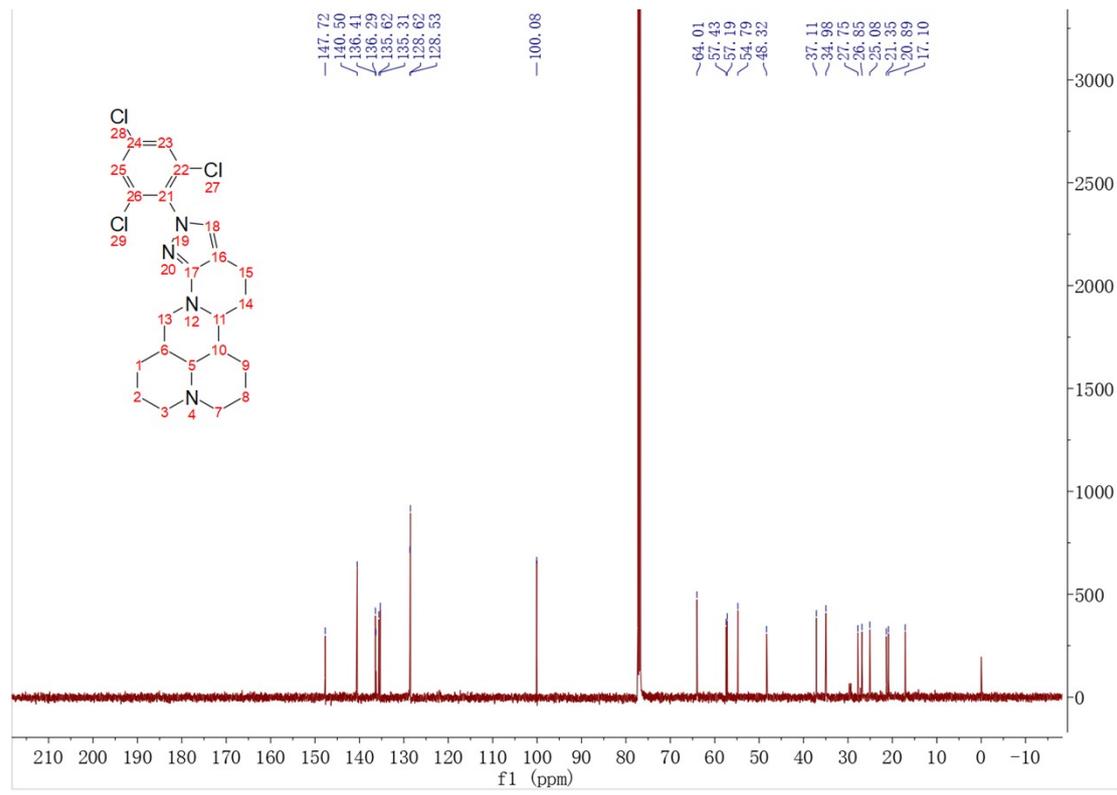
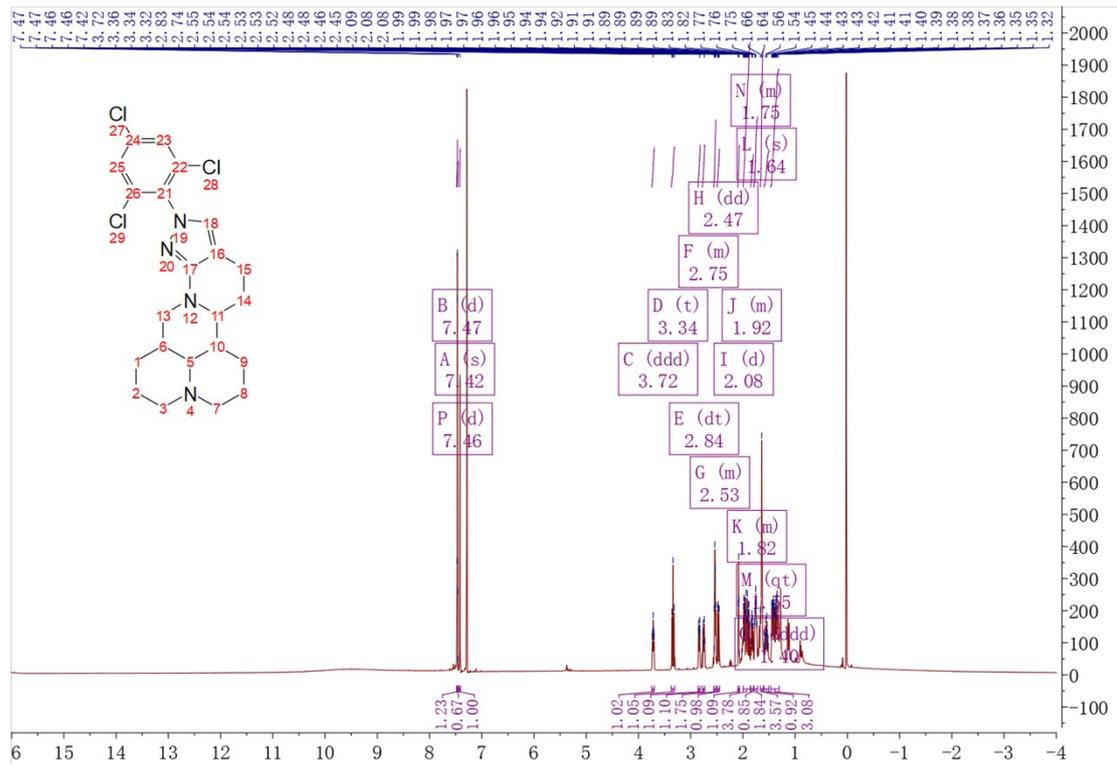


5410 UV Detector Ch1 样品ID: 4 UNK004 (254nm) 次数: 1

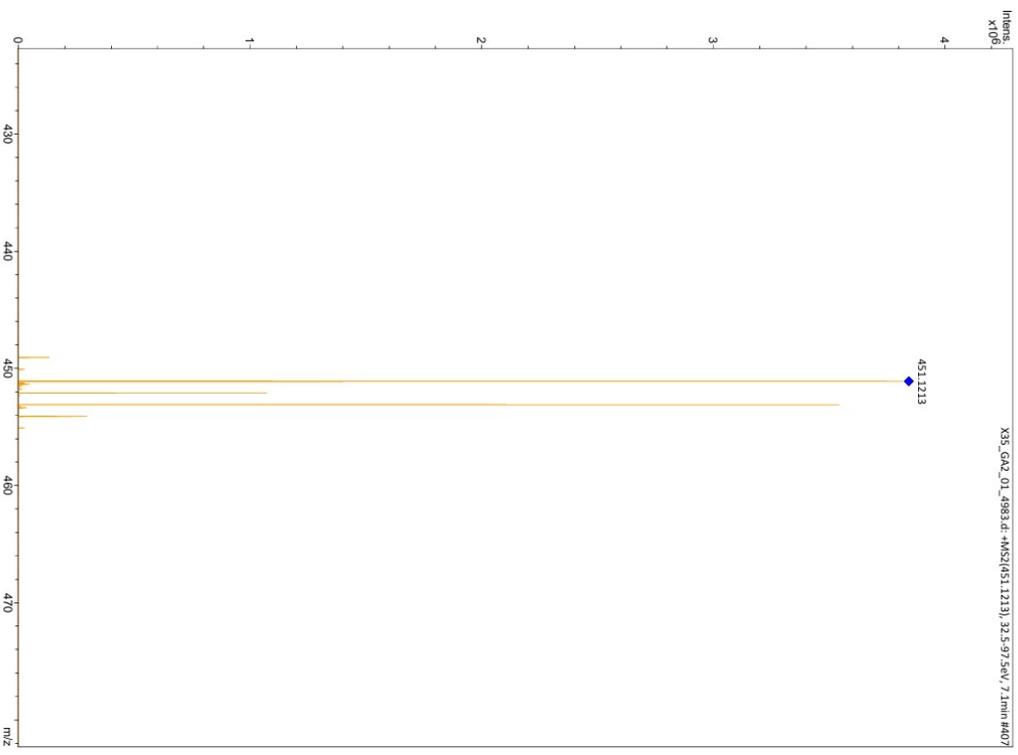


5410 UV Detector Ch1 样品ID: 4 UNK004 (254nm) 次数: 1

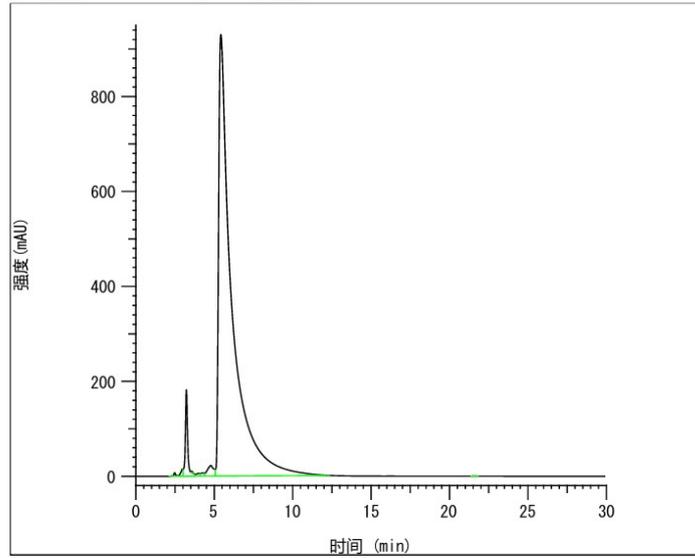
No.	成分名	RT	面积	面积%	高度	高度%	浓度	单位	浓度2	单位2	N	强度	半峰宽	相对RT	校正RT	纯度(平均)	纯度(3点)	纯度(2点)
1	峰1	3.163	144917	0.609	5587	1.176	---	---	---	---	276	6	0.45	---	---	---	---	---
2	峰2	3.563	36760	0.154	3112	0.655	---	---	---	---	---	3	---	---	---	---	---	---
3	峰3	4.787	23613339	99.237	466367	98.169	---	---	---	---	310	467	0.64	---	---	---	---	---
			23795017	100.000	475066	100.000												



Window Display Report

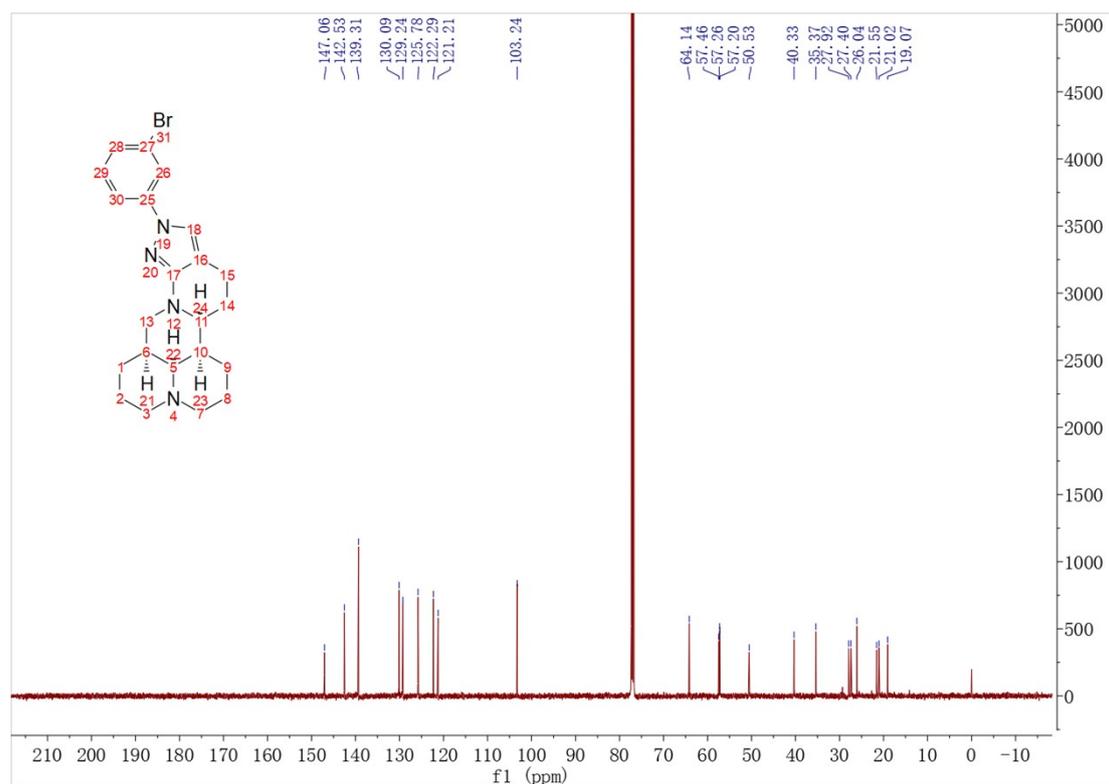
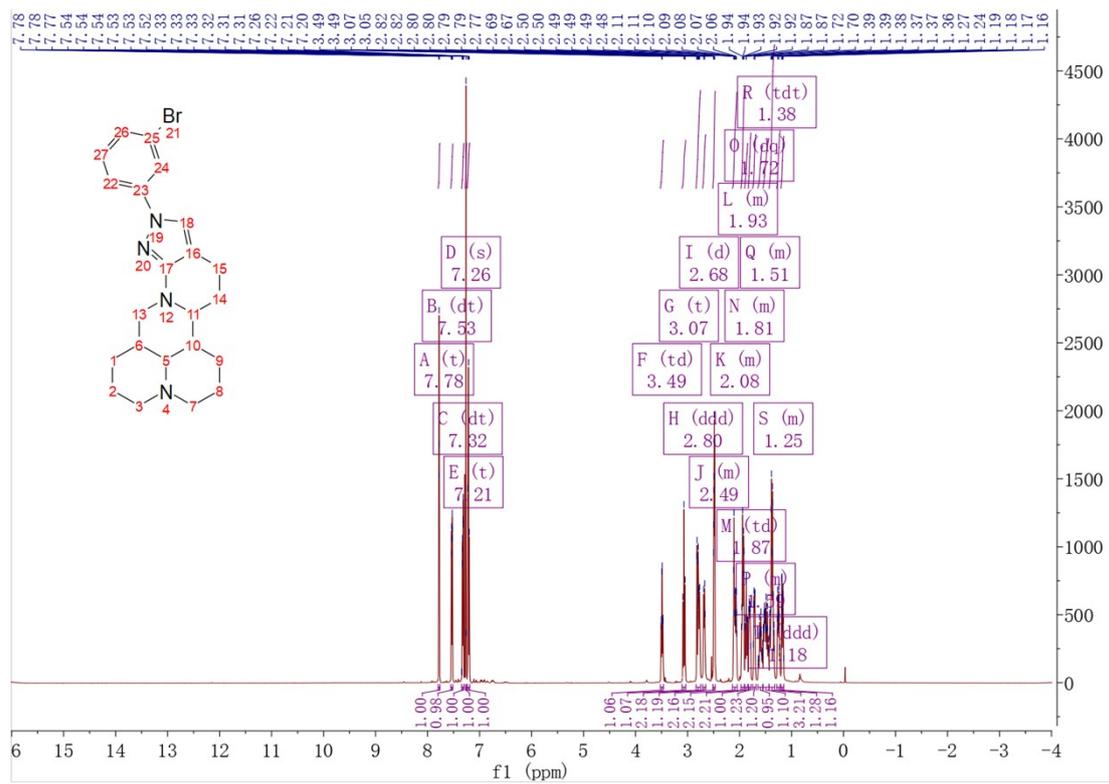


5410 UV Detector Ch1 样品ID: 2 UNK002 (254nm) 次数: 1

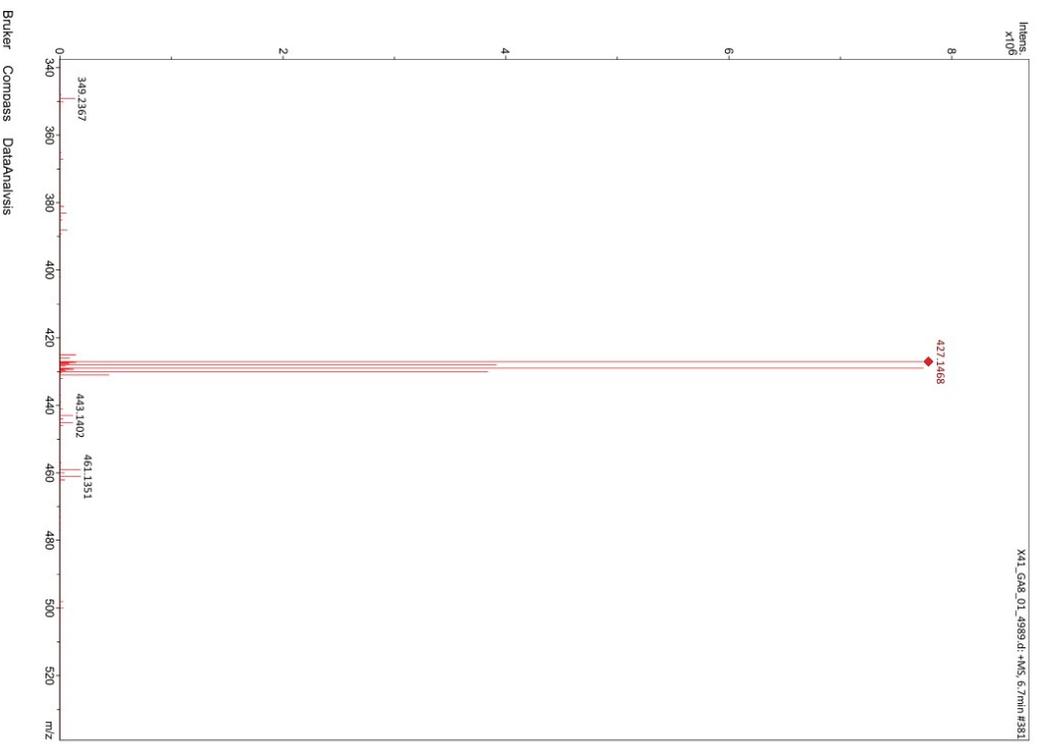


5410 UV Detector Ch1 样品ID: 2 UNK002 (254nm) 次数: 1

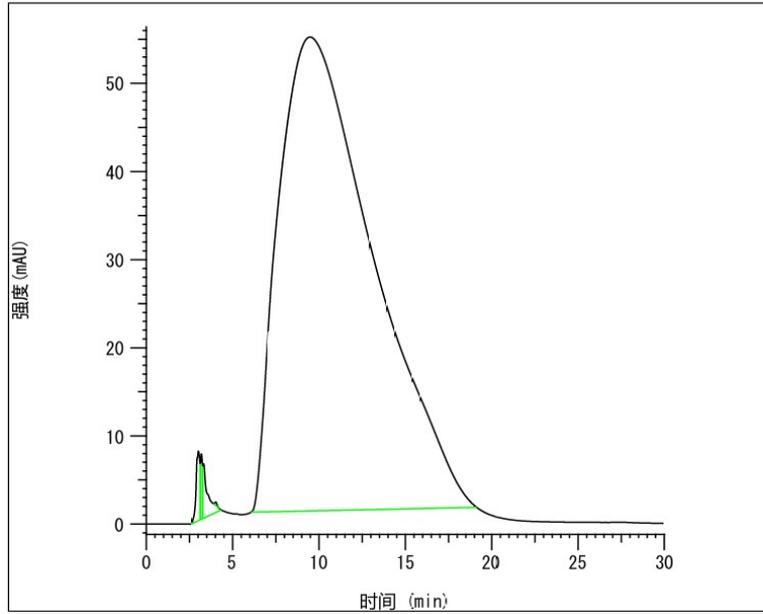
No.	成分名	RT	面积	面积%	高度	高度%	浓度	单位	浓度2	单位2	N	强度	半峰宽	相对RT	校正RT	纯度(平均)	纯度(3点)	纯度(2点)
1	峰1	2.337	8775	0.016	1380	0.121	---	---	---	---	---	1	---	---	---	---	---	---
2	峰2	2.473	59646	0.106	7843	0.689	---	---	---	---	3342	8	0.10	---	---	---	---	---
3	峰3	3.220	1885072	3.336	182377	16.029	---	---	---	---	3182	182	0.13	---	---	---	---	---
4	峰4	3.570	19543	0.035	3139	0.276	---	---	---	---	7070	11	0.10	---	---	---	---	---
5	峰5	4.023	117389	0.208	5889	0.518	---	---	---	---	---	6	---	---	---	---	---	---
6	峰6	4.263	105031	0.186	6840	0.601	---	---	---	---	---	7	---	---	---	---	---	---
7	峰7	5.423	54314565	96.113	930229	81.759	---	---	---	---	368	931	0.67	---	---	---	---	---
8	峰8	21.613	1198	0.000	67	0.007	---	---	---	---	24252	0	0.33	---	---	---	---	---
			56511218	100.000	1137763	100.000												



Window Display Report

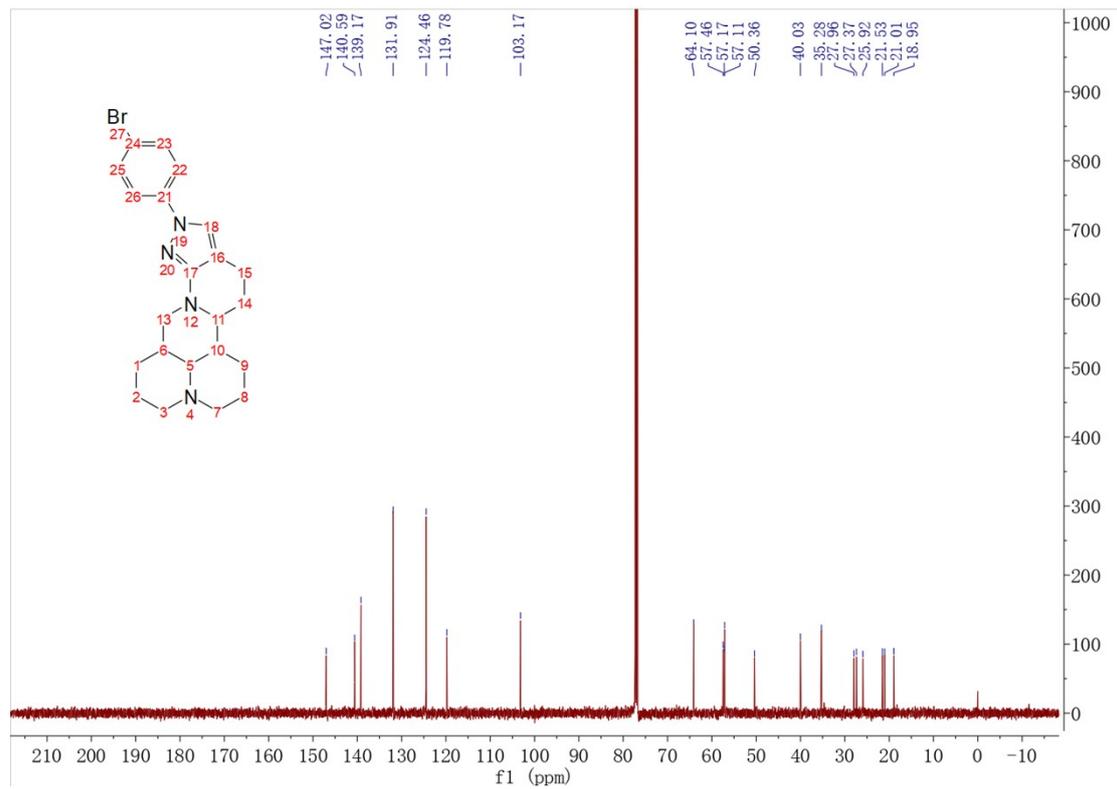
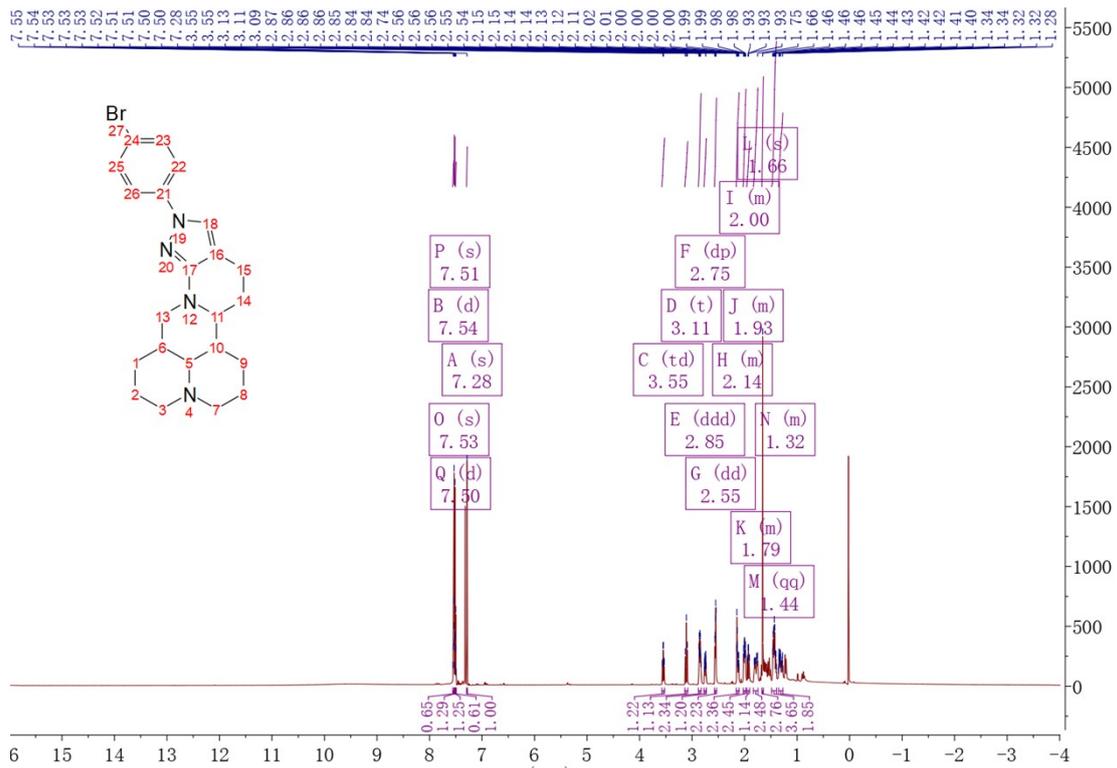


5410 UV Detector Ch1 样品ID: 2 UNK002 (254nm) 次数: 1



5410 UV Detector Ch1 样品ID: 2 UNK002 (254nm) 次数: 1

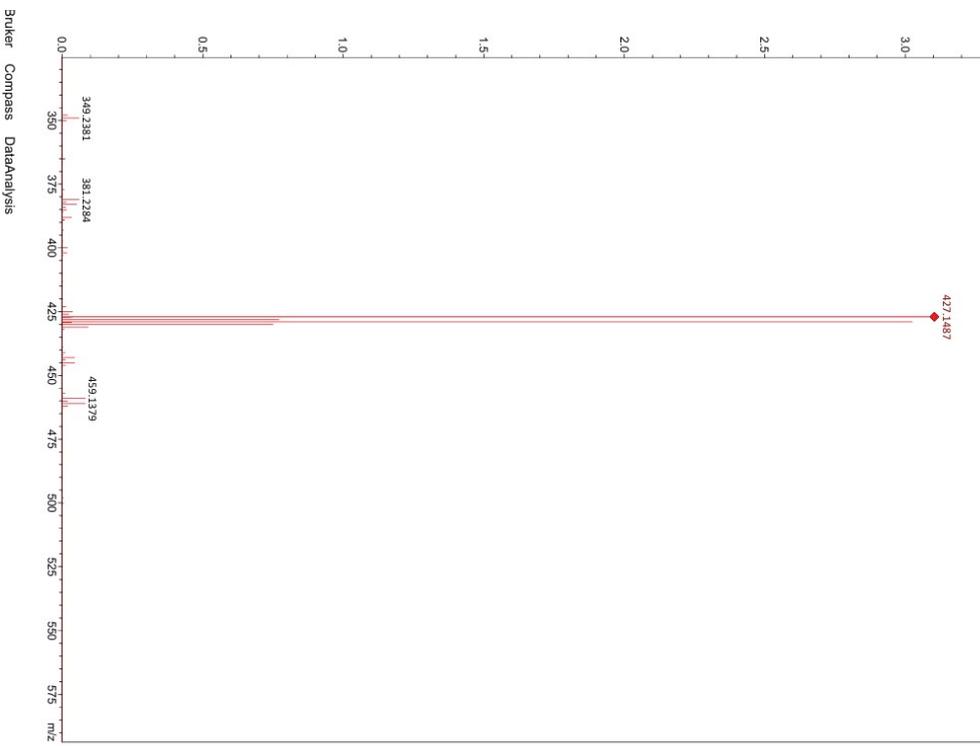
No.	成分名	RT	面积	面积%	高度	高度%	浓度	单位	浓度2	单位2	N	强度	半峰宽	相对RT	校正RT	纯度(平均)	纯度(3点)	纯度(2点)
1	峰1	3.013	1173	0.565	7896	10.43	---	---	---	---	---	8	---	---	---	---	---	---
2	峰2	3.190	5952	0.287	7439	9.831	---	---	---	---	---	8	---	---	---	---	---	---
3	峰3	3.317	1225	0.591	6171	8.154	---	---	---	---	---	7	---	---	---	---	---	---
4	峰4	4.017	3142	0.015	384	0.507	---	---	---	---	4682	2	0.14	---	---	---	---	---
5	峰5	9.480	2045	98.54	5378	71.07	---	---	---	---	13	55	6.13	---	---	---	---	---
			2075	100.0	7567	100.0												
			4307	00	4	00												



Window Display Report

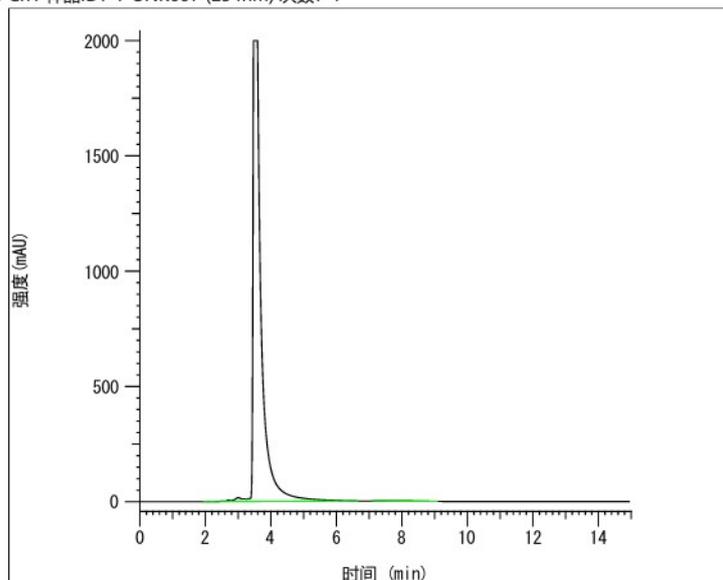
Interna
X100

X39_0605_01_4987.d -MS 6.6min#377



Brucker Compass DataAnalysis

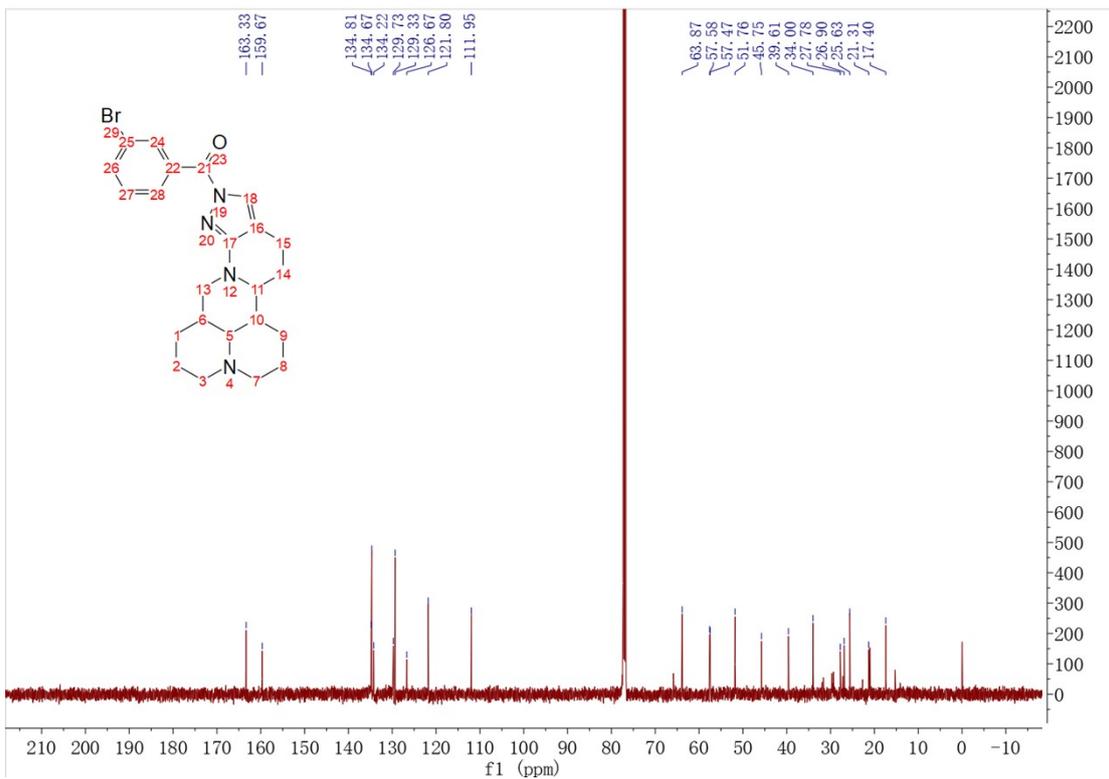
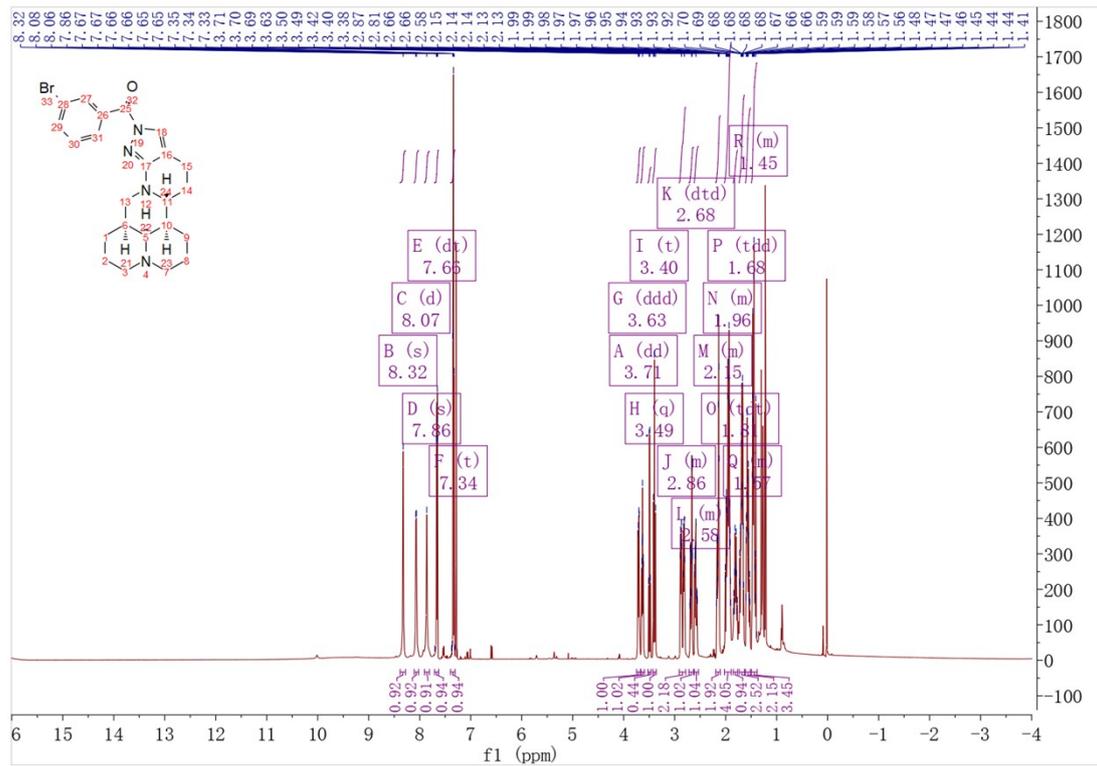
5410 UV Detector Ch1 样品ID: 7 UNK007 (254nm) 次数: 1



5410 UV Detector Ch1 样品ID: 7 UNK007 (254nm) 次数: 1

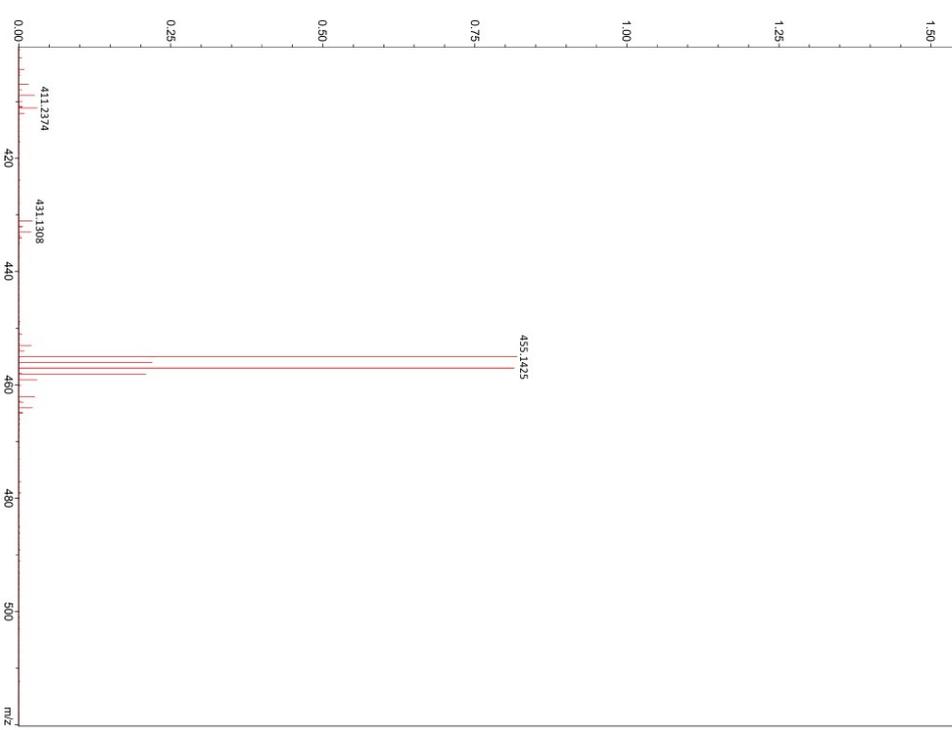
No.	成分名	RT	面积	面 积%	高度	高 度%	浓度	单位	浓度2	单位2	N	强度	半峰 宽	相对 RT	校正 RT	纯度 (平均) (3点)	纯度 (2点)
1	峰1	2.083	5013	0.014	493	0.024	---	---	---	---	---	1	---	---	---	---	---
2	峰2	2.493	23248	0.065	2779	0.137	---	---	---	---	---	3	---	---	---	---	---
3	峰3	2.703	54833	0.153	7047	0.348	---	---	---	---	---	8	---	---	---	---	---
4	峰4	3.000	324586	0.905	17108	0.844	---	---	---	---	---	18	---	---	---	---	---
5	峰5	3.593	35355945	98.57	1998837	98.576	---	---	---	---	1438	2000	0.22	---	---	---	---
6	峰6	7.757	102312	0.285	1444	0.071	---	---	---	---	274	4	1.10	---	---	---	---
			35865936	100.0	202700	100.000											

X18

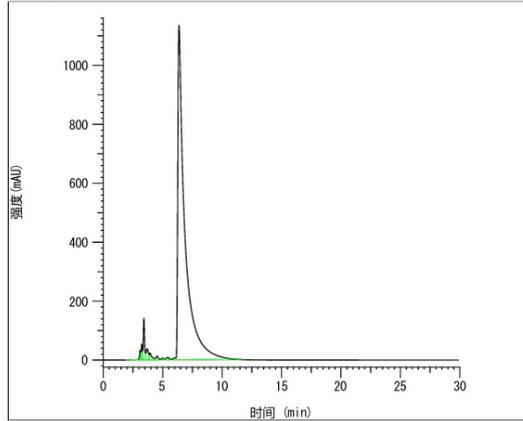


Window Display Report

Intens. x10⁵ XZ5_F08_01_4973.d - MS, 10.7min.669



5410 UV Detector Ch1 样品ID: 2 UNK002 (254nm) 次数: 1

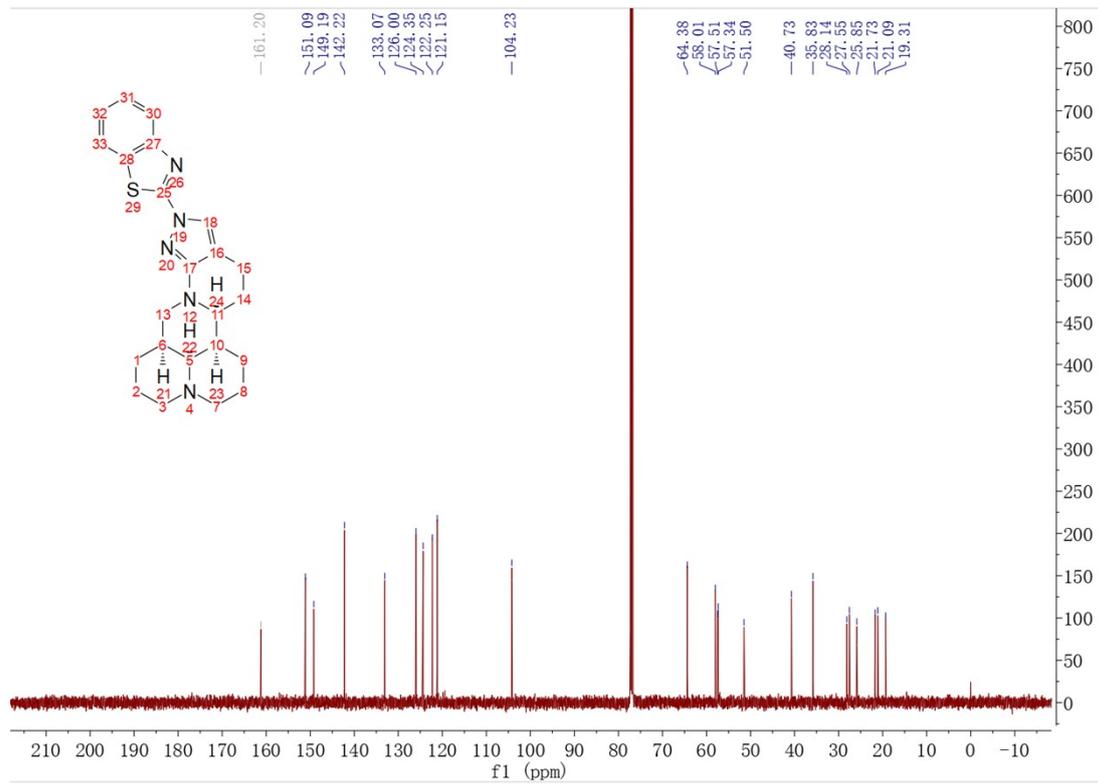


5410 UV Detector Ch1 样品ID: 2 UNK002 (254nm) 次数: 1

No	成分名	RT	面积	面积%	高度	高度%	浓度	单位	浓度2	单位2	N	强度	半峰宽	相对RT	校正RT	纯度(平均)	纯度(3点)	纯度(2点)
1	峰1	2.073	3298	0.007	531	0.040	---	---	---	---	---	0	---	---	---	---	---	---
2	峰2	2.303	15739	0.032	1335	0.102	---	---	---	---	2319	1	0.11	---	---	---	---	---
3	峰3	3.107	243734	0.497	34153	2.604	---	---	---	---	---	34	---	---	---	---	---	---
4	峰4	3.243	386055	0.788	54890	4.186	---	---	---	---	---	55	---	---	---	---	---	---
5	峰5	3.693	505459	1.032	38199	2.913	---	---	---	---	---	38	---	---	---	---	---	---
6	峰6	3.940	340064	0.694	24134	1.840	---	---	---	---	---	24	---	---	---	---	---	---
7	峰7	4.993	90790	0.185	6096	0.465	---	---	---	---	---	6	---	---	---	---	---	---
8	峰8	5.447	176383	0.360	8870	0.676	---	---	---	---	1577	9	0.32	---	---	---	---	---
9	峰9	6.027	122399	0.250	6860	0.523	---	---	---	---	---	7	---	---	---	---	---	---
10	峰10	6.367	47118008	96.15	1136336	86.65	---	---	---	---	1039	1137	0.46	---	---	---	---	---

		4900	100.0	1311	100.0													
		1929	00	403	00													

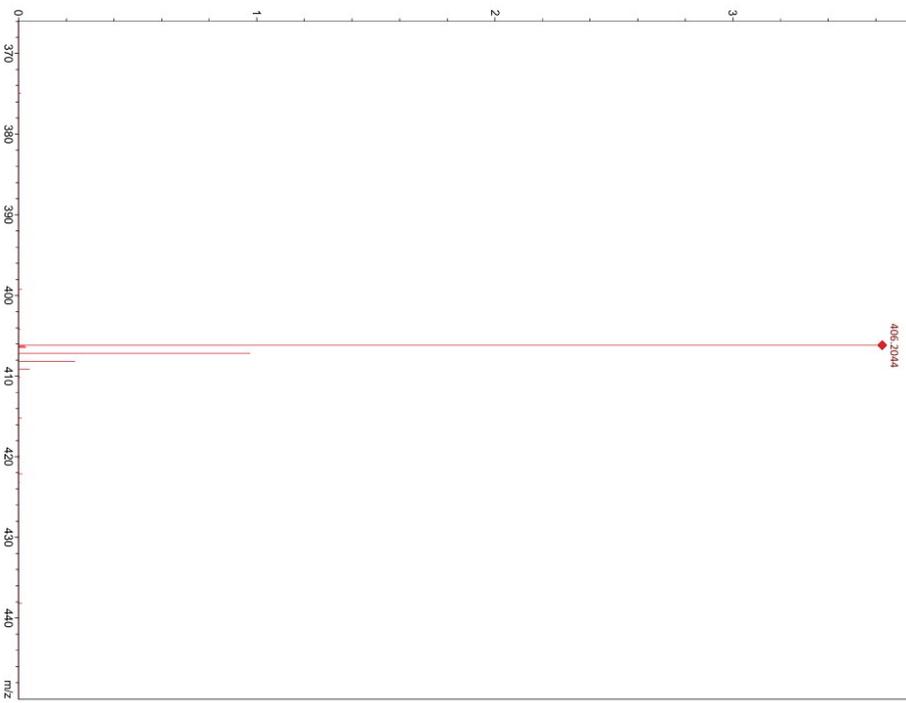
5410 UV Detector Ch1 样品ID: 3 UNK003 (254nm) 次数: 1



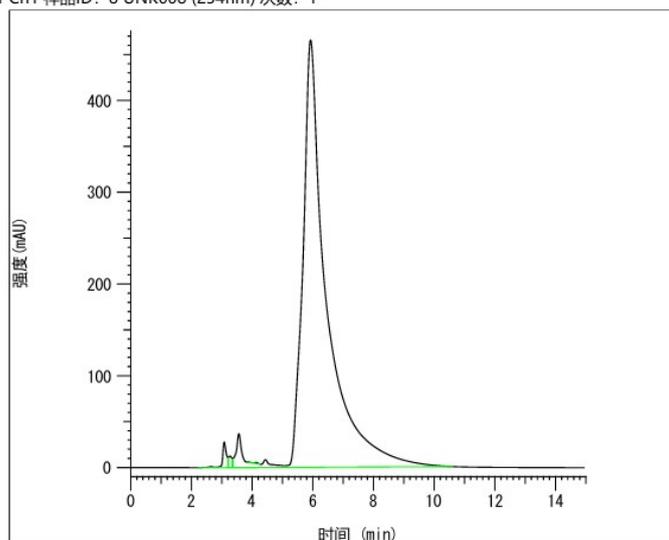
Window Display Report

Intens
X10⁶

X36_GAS_01_19984.D -MS, 7.1min.FIG5



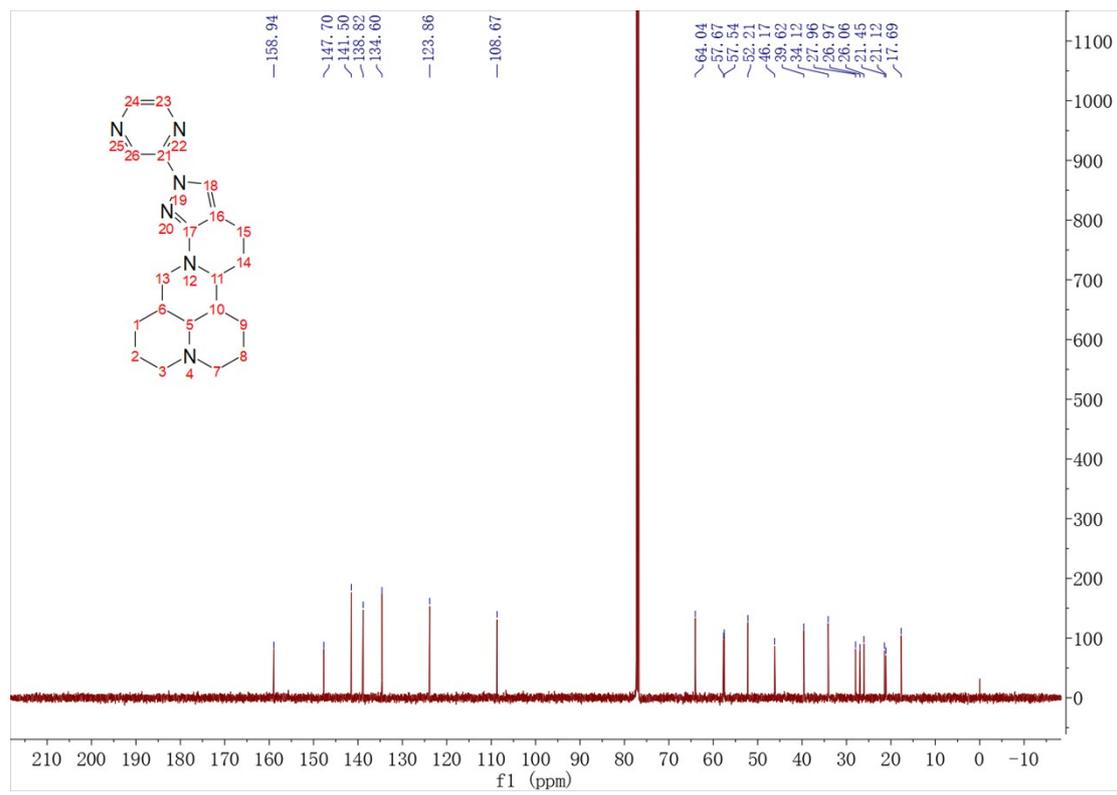
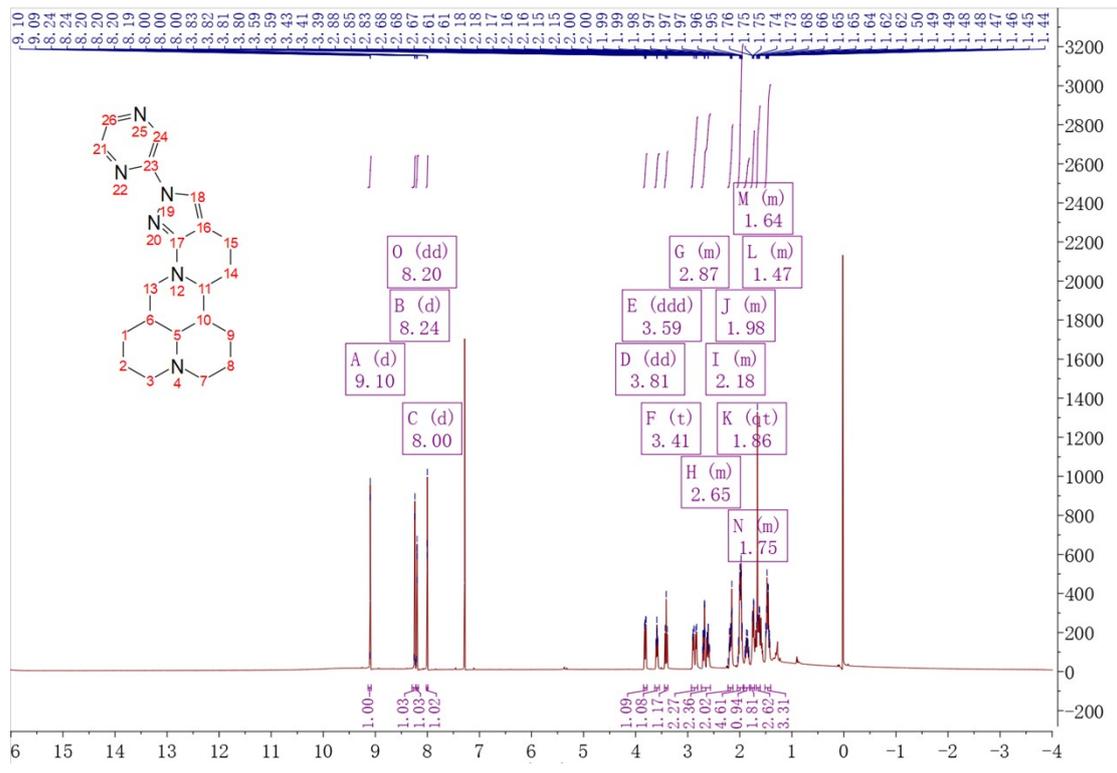
5410 UV Detector Ch1 样品ID: 8 UNK008 (254nm) 次数: 1



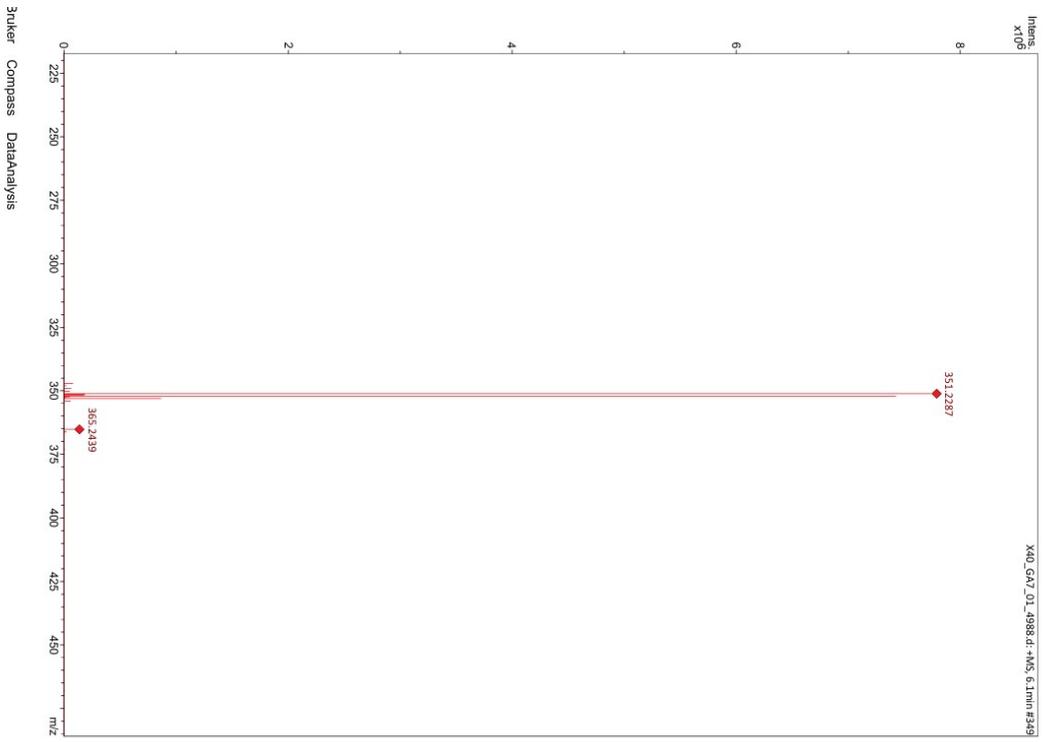
5410 UV Detector Ch1 样品ID: 8 UNK008 (254nm) 次数: 1

No.	成分名	RT	面积	面积%	高度	高度%	浓度	单位	浓度2	单位2	N	强度	半峰宽	相对RT	校正RT	纯度(平均)	纯度(3点)	纯度(2点)
1	峰1	2.647	16230	0.062	1320	0.238	---	---	---	---	1820	1	0.15	---	---	---	---	---
2	峰2	3.080	228105	0.872	27921	5.038	---	---	---	---	3377	28	0.12	---	---	---	---	---
3	峰3	3.273	102547	0.392	12545	2.263	---	---	---	---	---	12	---	---	---	---	---	---
4	峰4	3.563	617505	2.361	36936	6.664	---	---	---	---	2512	37	0.17	---	---	---	---	---
5	峰5	3.867	4217	0.016	369	0.067	---	---	---	---	---	6	---	---	---	---	---	---
6	峰6	4.127	8940	0.034	1167	0.211	---	---	---	---	---	5	---	---	---	---	---	---
7	峰7	4.437	170815	0.653	8443	1.523	---	---	---	---	3034	9	0.19	---	---	---	---	---
8	峰8	5.927	25008560	95.61	465520	83.996	---	---	---	---	515	466	0.61	---	---	---	---	---
			26156918	100.0	554200	100.0												

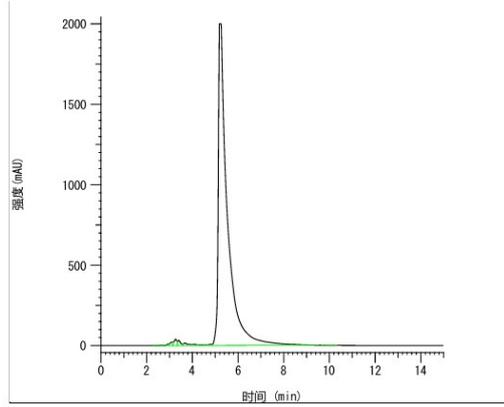
X20



Window Display Report



5410 UV Detector Ch1 样品ID: 2 UNK002 (254nm) 次数: 1

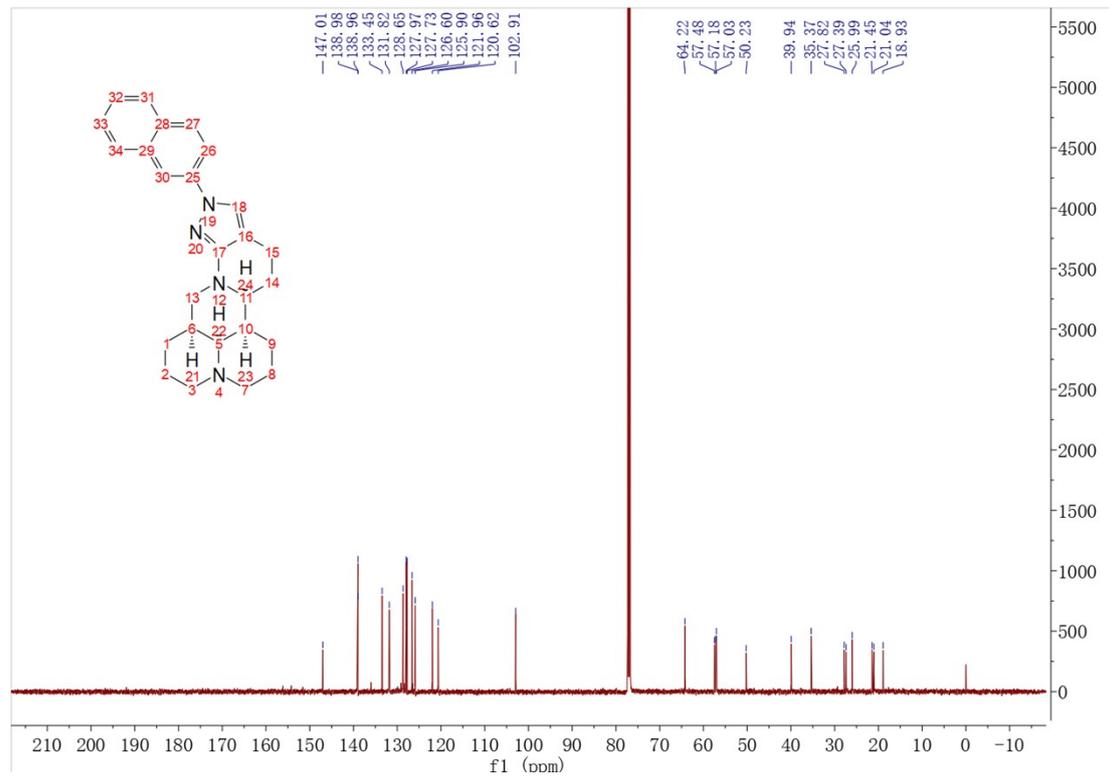
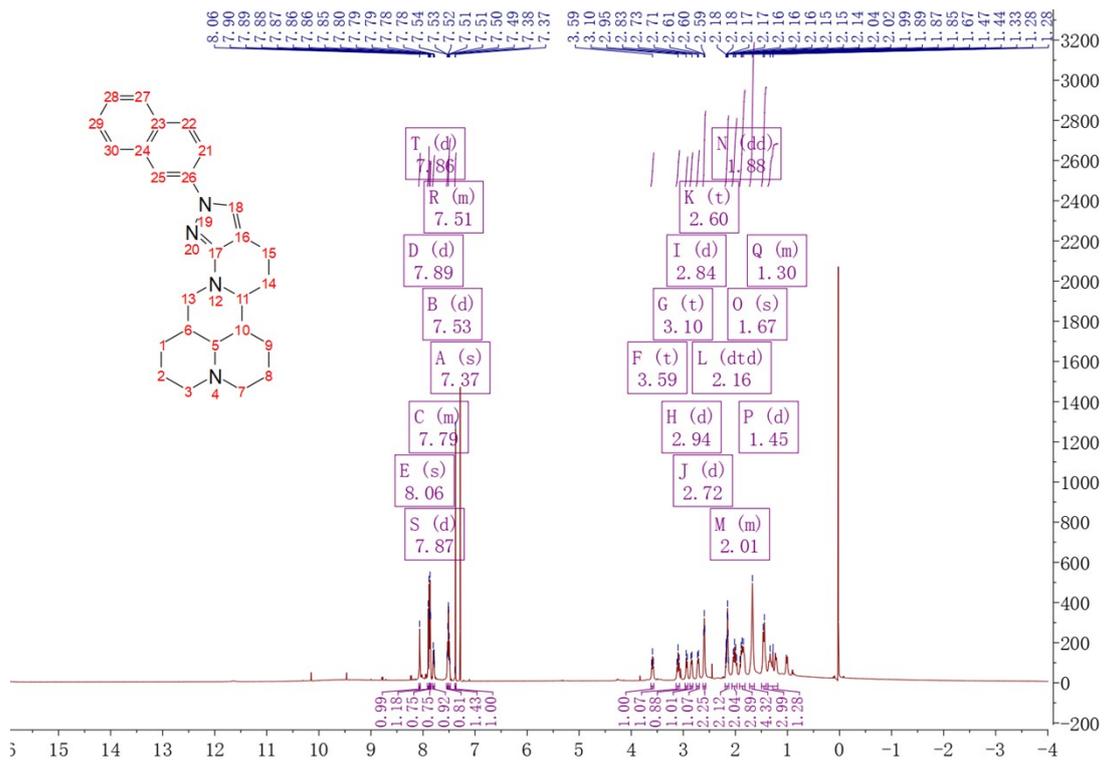


5410 UV Detector Ch1 样品ID: 2 UNK002 (254nm) 次数: 1

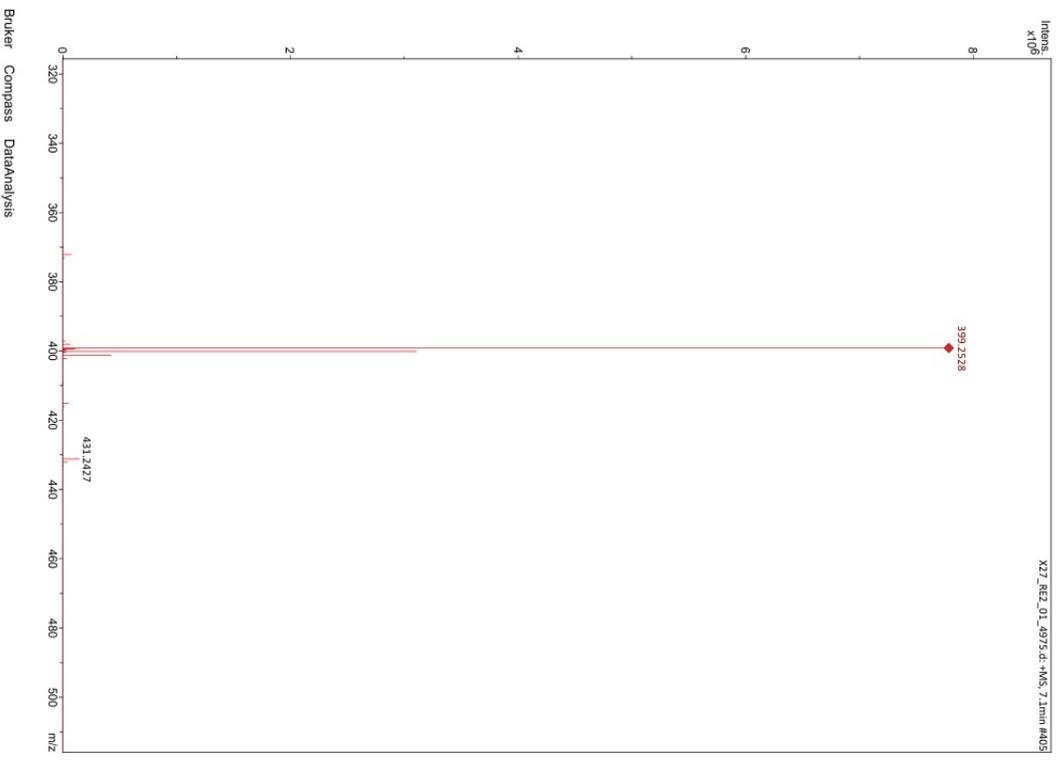
No.	成分名	RT	面积	面积%	高度	高度%	浓度	单位	浓度2	单位2	N	强度	半峰宽	相对RT	校正RT	纯度(平均)	纯度(3点)	纯度(2点)
1	峰1	2.640	26891	0.047	1948	0.091	---	---	---	---	914	2	0.21	---	---	---	---	---
2	峰2	2.943	63289	0.112	10739	0.500	---	---	---	---	---	11	---	---	---	---	---	---
3	峰3	3.103	184721	0.326	22265	1.037	---	---	---	---	---	22	---	---	---	---	---	---
4	峰4	3.263	352088	0.620	39921	1.860	---	---	---	---	---	40	---	---	---	---	---	---
5	峰5	3.403	290278	0.512	32291	1.505	---	---	---	---	---	33	---	---	---	---	---	---
6	峰6	3.673	231541	0.408	16653	0.776	---	---	---	---	---	17	---	---	---	---	---	---
7	峰7	4.083	91206	0.161	7099	0.331	---	---	---	---	---	8	---	---	---	---	---	---
8	峰8	4.273	69613	0.123	4798	0.224	---	---	---	---	---	5	---	---	---	---	---	---

9	峰9	4.607	36713	0.065	4392	0.205	---	---	---	---	---	5	---	---	---	---	---	---
10	峰10	4.797	68911	0.121	6727	0.313	---	---	---	---	---	7	---	---	---	---	---	---
11	峰11	5.260	55322485	97.491	1999106	93.145	---	---	---	---	1422	2000	0.33	---	---	---	---	---
12	峰12	9.743	832256746058	0.014100.0	2822146219	0.013100.0	---	---	---	---	---	3	---	---	---	---	---	---

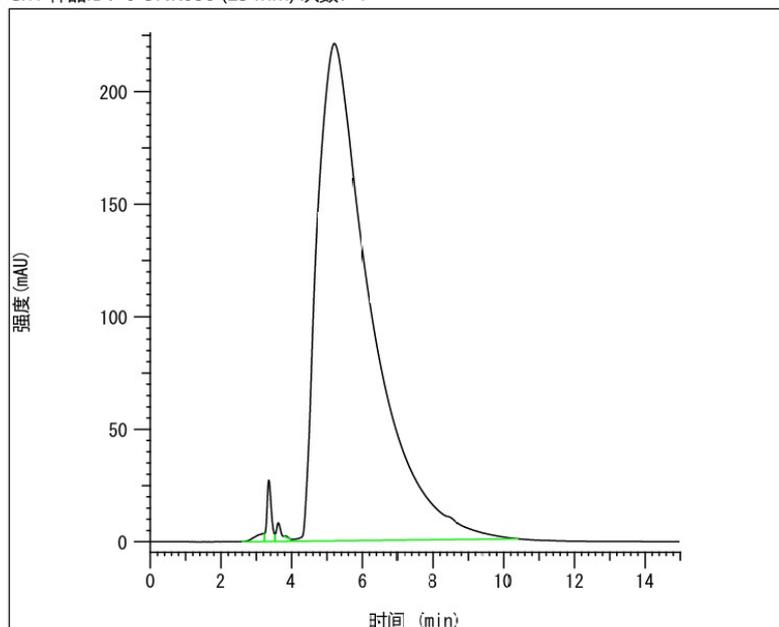
X21



Window Display Report



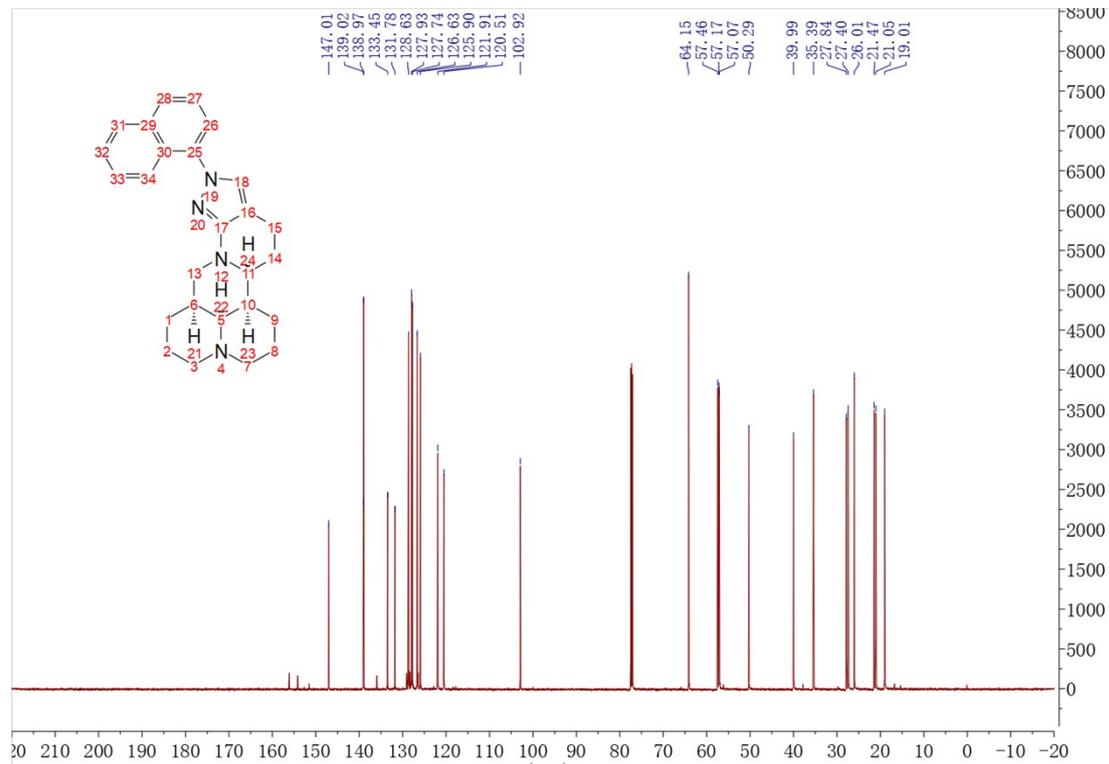
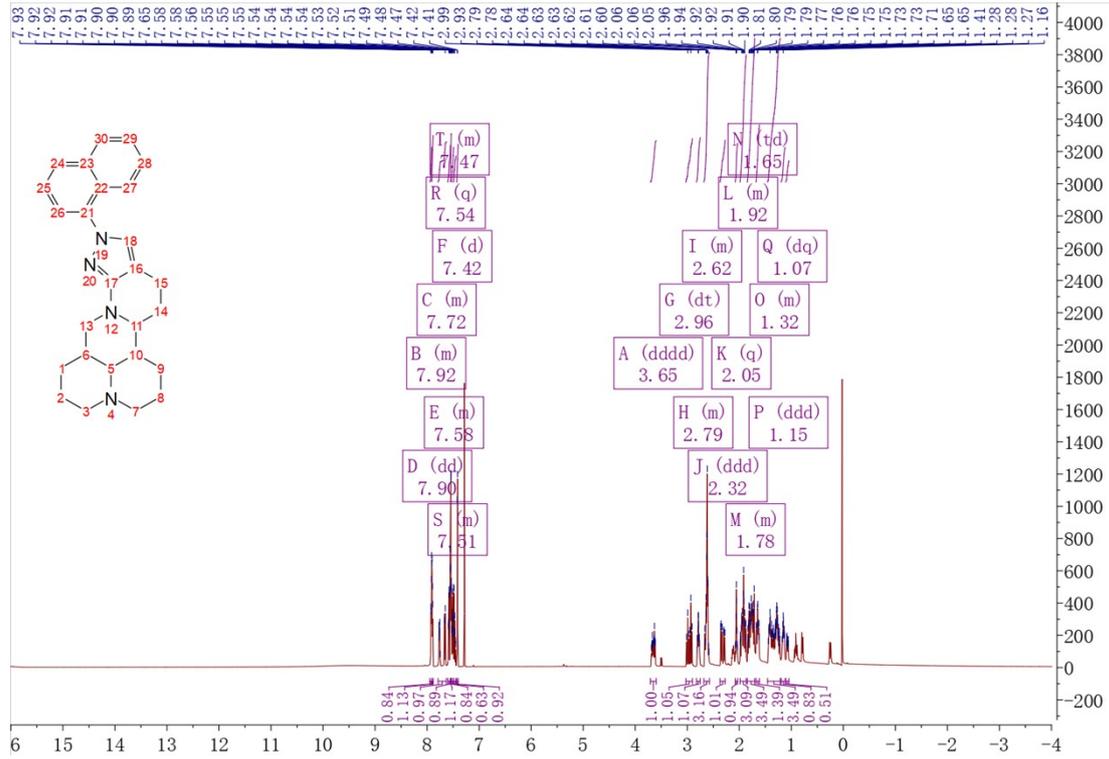
5410 UV Detector Ch1 样品ID: 6 UNK006 (254nm) 次数: 1



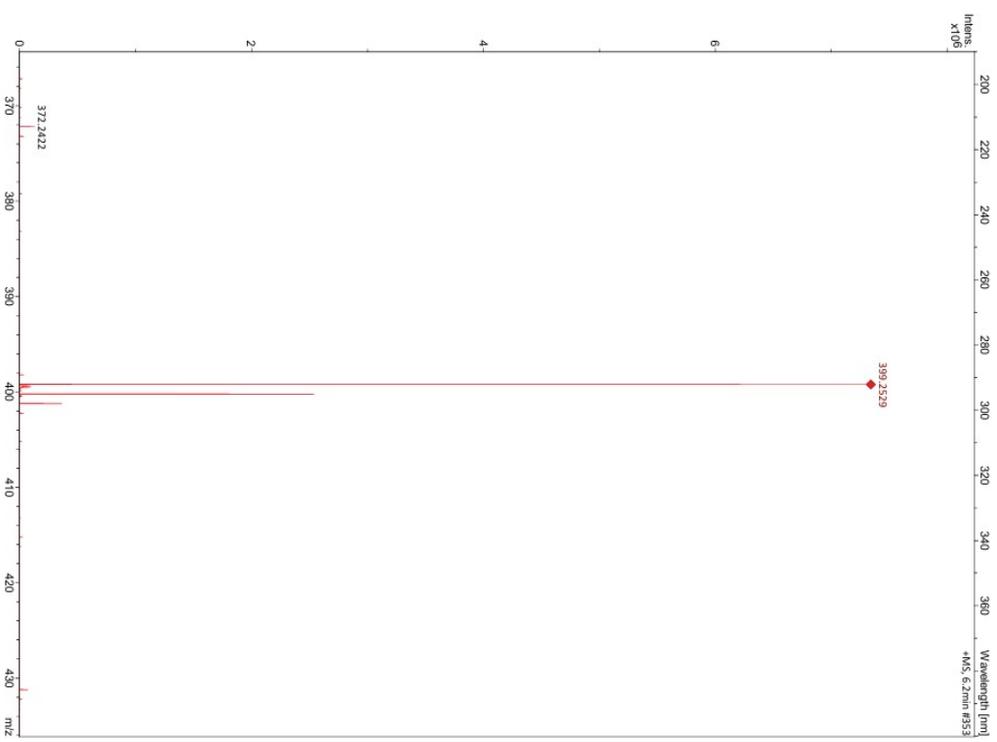
5410 UV Detector Ch1 样品ID: 6 UNK006 (254nm) 次数: 1

No.	成分名	RT	面积	面积%	高度	高度%	浓度	单位	浓度2	单位2	N	强度	半峰宽	相对RT	校正RT	纯度(平均)	纯度(3点)	纯度(2点)
1	峰1	3.187	63617	0.271	3562	1.367	---	---	---	---	---	4	---	---	---	---	---	---
2	峰2	3.353	233546	0.995	27259	10.463	---	---	---	---	3877	27	0.13	---	---	---	---	---
3	峰3	3.620	95618	0.407	8267	3.173	---	---	---	---	3598	8	0.14	---	---	---	---	---
4	峰4	3.830	3393	0.014	477	0.183	---	---	---	---	---	3	---	---	---	---	---	---
5	峰5	5.207	23081833	98.313	220961	84.814	---	---	---	---	64	221	1.53	---	---	---	---	---
			23478008	100.000	260525	100.000												

X22

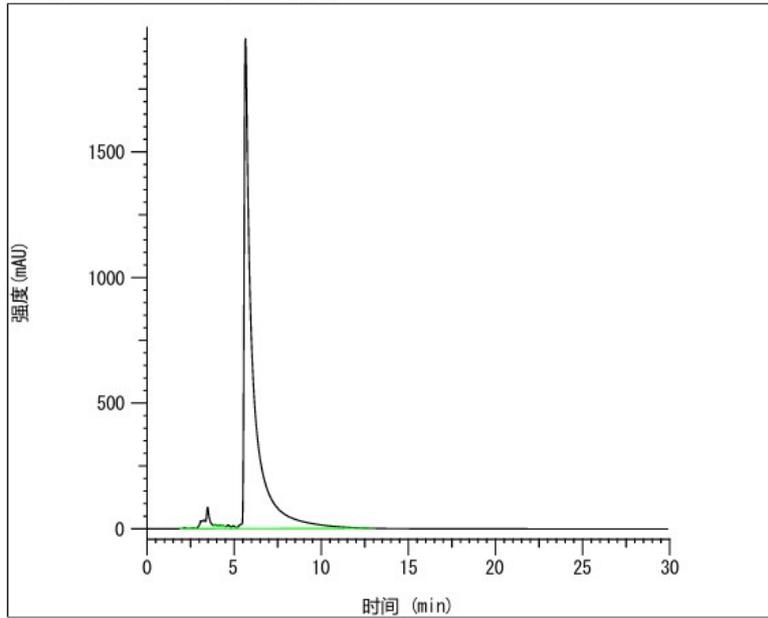


Window Display Report



峰值检测详细结果

5410 UV Detector Ch1 样品ID: 1 UNK001 (254nm) 次数: 1



5410 UV Detector Ch1 样品ID: 1 UNK001 (254nm) 次数: 1

No.	成分名	RT	面积	面 积%	高度	高 度%	浓度	单位	浓度2	单位2	N	强度	半峰 宽	相对 RT	校正 RT	纯度 (平均)	纯度 (3点)	纯度 (2点)
1	峰1	2.083	1032 4	0.015	2104	0.106	---	---	---	---	---	2	---	---	---	---	---	---
2	峰2	2.163	2341 488	3.415	4535	0.228	---	---	---	---	---	4	---	---	---	---	---	---

3	峰3	4.377	7809 8	0.114	2365	0.119	---	---	---	---	---	12	---	---	---	---	---	---
4	峰4	4.660	2034 71	0.297	1499 2	0.754	---	---	---	---	---	15	---	---	---	---	---	---
5	峰5	4.957	1532 40	0.224	1153 6	0.580	---	---	---	---	---	12	---	---	---	---	---	---
6	峰6	5.653	6577 4968	95.93 5	1953 505	98.21 3	---	---	---	---	1643	1954	0.33	---	---	---	---	---
			6856 1589	100.0 00	1989 036	100.0 00												

5410 UV Detector Ch1 样品ID: 2 UNK002 (254nm) 次数: 1