

Supporting Information for

**Chemoselective N-H Functionalization of Indole Derivatives via Reissert-type
Reaction Catalyzed by Chiral Phosphoric Acid**

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Table of Contents

Optimization of conditions	S2-S4
X-Ray of 4aa	S5-S6
Copies of NMR spectra and HPLC chromatographs	S7-S96

Optimization of conditions

Table S-1 Screening of chiral phosphoric acids.

2a (1 equiv) + 3a (1 equiv) $\xrightarrow[p\text{-xylene, 25 } ^\circ\text{C}]{(S)\text{-1 (10 mol\%)} \text{ Boc}_2\text{O (1 equiv)}}$ 4aa

(S)-1

1a: R = 1-naphthyl
 1g: R = 4-NO₂-C₆H₄
 1h: R = 9-(10-Br)-anthryl
 1c: R = 9-phenanthryl
 1d: R = 2,4,6-(*i*Pr)₃-C₆H₂
 1e: R = SiPh₃
 1f: R = 2,4,6-(Cy)₃-C₆H₂
 1i: R = PPh₂

(S)-1b

(S)-1j

entry ^a	(S)-1	yield (%) ^b	ee (%) ^c
1	1a	85	31
2	1b	87	46
3	1c	82	64
4	1d	89	64
5	1e	82	70
6	1f	89	76
7	1g	95	39
8	1h	85	44
9	1i	85	44
10	1j	57	11

^a Reaction condition: 10 mol% of (S)-1, 0.2 mmol of **2a**, 0.2 mmol of **3a**, 0.2 mmol of Boc₂O in 2 mL *p*-xylene, 25 °C, 3 d. ^b Isolated yield. ^c Determined by HPLC analysis.

Table S-2 Screening of solvents.

2a (1 equiv) + 3a (1 equiv) $\xrightarrow[\text{solvent, 25 } ^\circ\text{C}]{(S)\text{-1f (10 mol\%)} \text{ Boc}_2\text{O (1 equiv)}}$ 4aa

(S)-1f

entry ^a	solvent	yield (%) ^b	ee (%) ^c
1	<i>p</i> -xylene	89	76

2	toluene	81	75
3	<i>o</i> -xylene	82	76
4	<i>m</i> -xylene	93	76
5	THF	14	68
6	Et ₂ O	69	76
7	DCM	37	59
8	PhCl	73	79
9	PhF	80	77

^a Reaction condition: 10 mol% of (*S*)-**1f**, 0.2 mmol of **2a**, 0.2 mmol of **3a**, 0.2 mmol of Boc₂O in 2 mL solvent, 25 °C, 3 d. ^b Isolated yield. ^c Determined by HPLC analysis.

Table S-3 Screening of activation reagent.

entry ^a	activator	R	yield (%) ^b	ee (%) ^c
1	Boc ₂ O	Boc	93	83
2	(CH ₃ CO) ₂ O	CH ₃ CO	0	--
3	(CH ₃ OCO) ₂ O	CH ₃ OCO	0	--
4	TrocCl	Troc	77	2
5	PhOCOCl	PhOCO	82	-2

^a Reaction condition: 10 mol% of (*S*)-**1f**, 0.2 mmol of **2a**, 0.2 mmol of **3a**, 0.2 mmol of activator in 2 mL *m*-xylene, 25 °C, 3 d. ^b Isolated yield. ^c Determined by HPLC analysis.

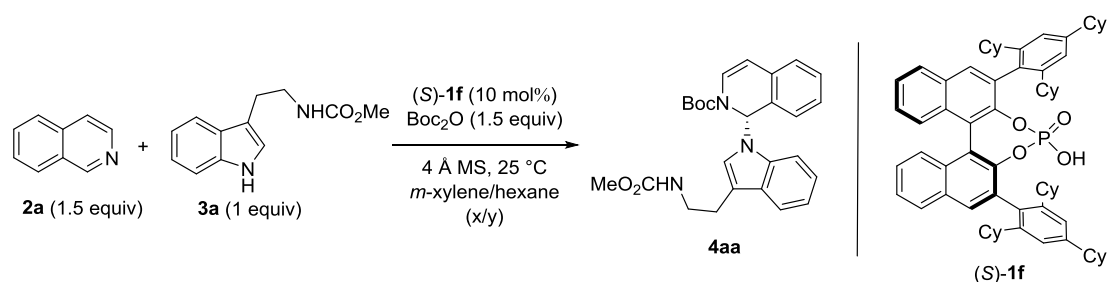
Table S-4 Screening of substrate ratio/additive/Ag salt.^a

entry	additive	x:y:z	yield (%) ^b	ee (%) ^c
-------	----------	-------	------------------------	---------------------

1	-	1:1:1	93	76
2	-	1:1:1.5	91	78
3	-	1:1:2	92	77
4	3 Å MS	1:1:2	91	79
5	4 Å MS	1:1:2	93	82
6	5 Å MS	1:1:2	92	80
7	-	1.5:1:1.5	93	80
8	4 Å MS	1.5:1:1.5	93	83
9 ^d	4 Å MS	1.5:1:1.5	92	74
10 ^e	4 Å MS	1.5:1:1.5	99	8
11 ^f	4 Å MS	1.5:1:1.5	97	8

^a Reaction condition: 10 mol% of (S)-**1f**, 0.2 mmol of **3** in 2 mL *m*-xylene, 25 °C, 3 d. ^b Isolated yield. ^c Determined by HPLC analysis. ^d 10 mol% of (S)-**1d** was used. ^e 10 mol% of (S)-**1d**-Ag was used, t = 12 h. ^f 10 mol% of (S)-**1d**-Ag was used, in dark, t = 12 h.

Table S-5 Screening of mixed solvents



entry ^a	x:y	time (h)	yield (%) ^b	ee (%) ^c
1	1:0	72 h	93	83
2	3:1	24 h	98	76
3	1:1	24 h	97	80
4	1:3	24 h	91	80
5	0:1	72 h	63	69

^a Reaction condition: 10 mol% of (S)-**1f**, 0.3 mmol of **2a**, 0.2 mmol of **3a**, 0.3 mmol of Boc₂O in 2 mL solvent, 25 °C. ^b Isolated yield. ^c Determined by HPLC analysis.

X-Ray structure of (*R*)-**4aa** (CCDC 1851528)

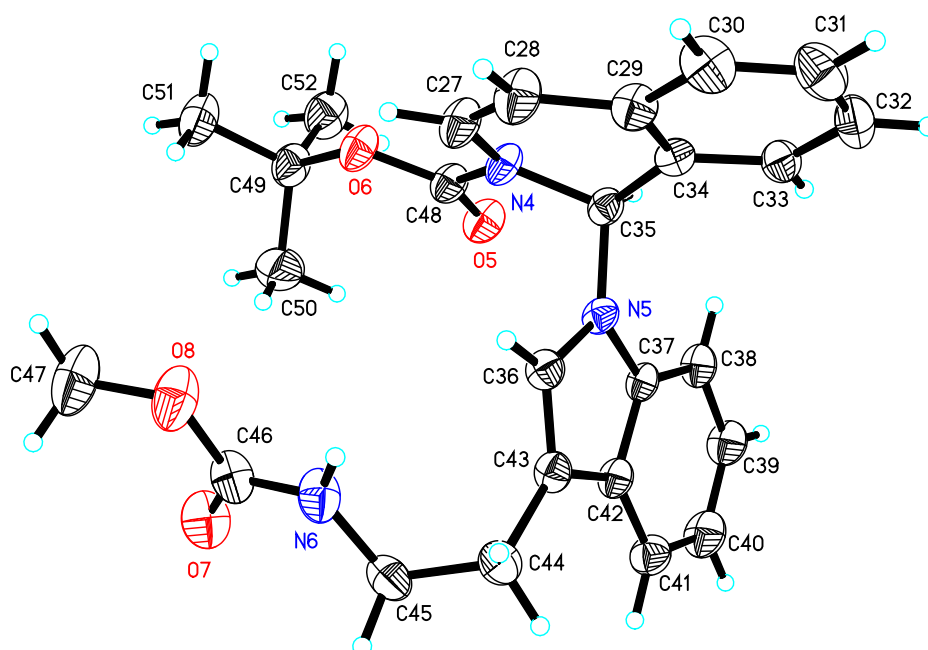


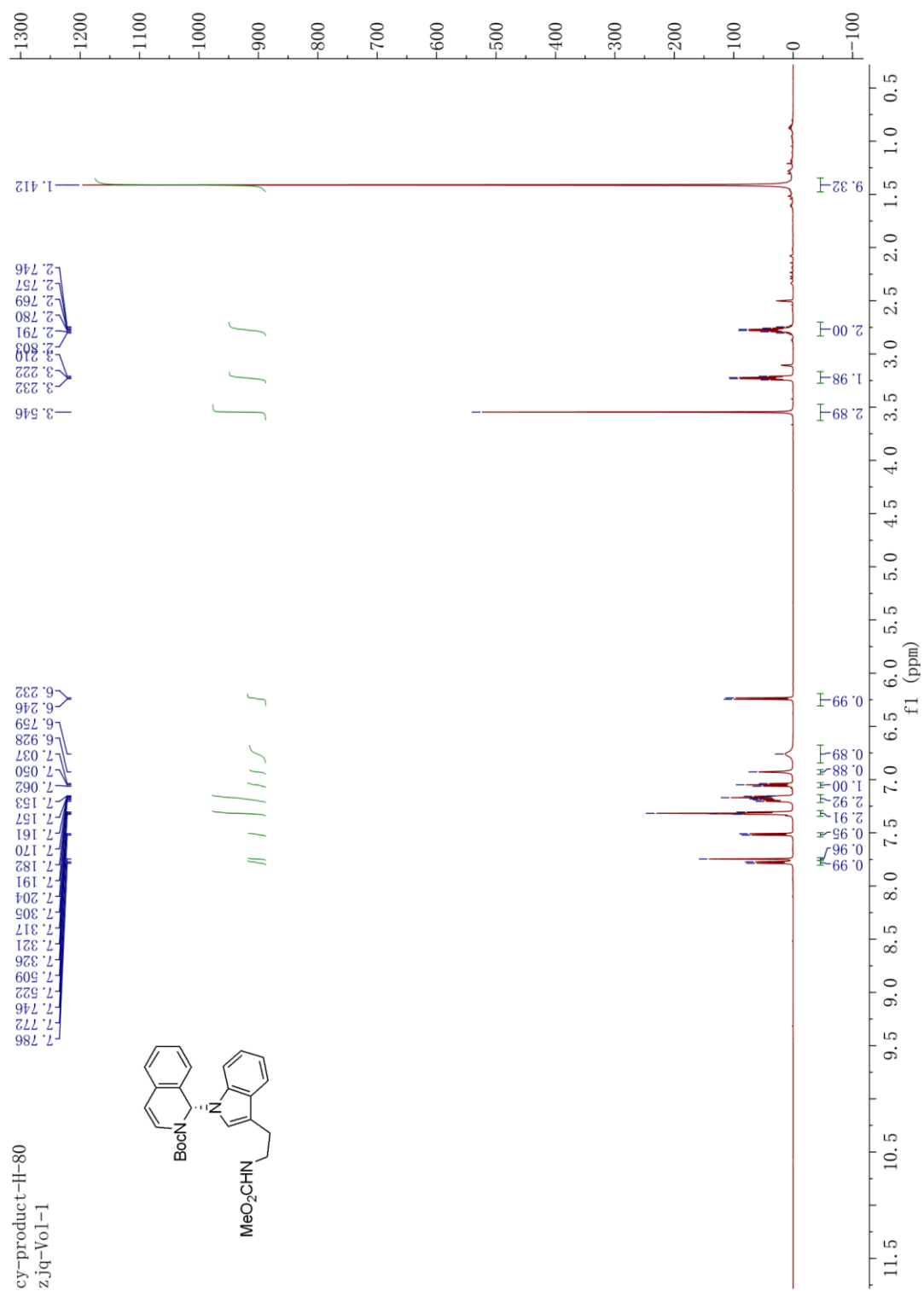
Table 1. Crystal data and structure refinement for cu_d8v18305_0m.

Identification code	cu_d8v18305_0m	
Empirical formula	C ₂₆ H ₂₉ N ₃ O ₄	
Formula weight	447.52	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 8.9053(2) Å	α = 90 °
	b = 29.8896(7) Å	β =
	c = 10.0393(2) Å	γ = 90 °
Volume	2442.69(9) Å ³	
Z	4	
Density (calculated)	1.217 Mg/m ³	
Absorption coefficient	0.670 mm ⁻¹	
F(000)	952	

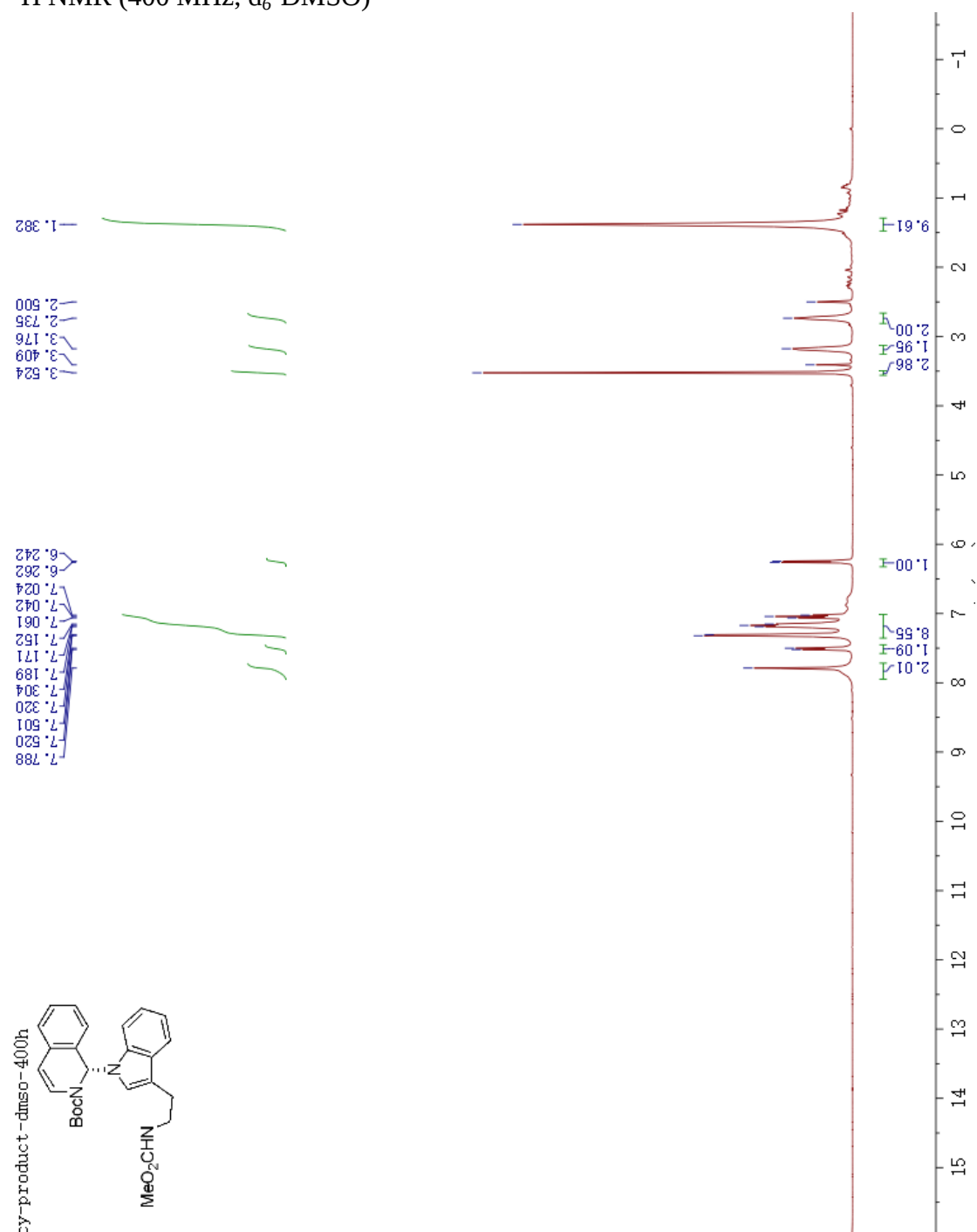
Crystal size	0.180 x 0.150 x 0.120 mm ³
Theta range for data collection	2.957 to 66.468 °
Index ranges	-10<=h<=10, -35<=k<=35, -11<=l<=11
Reflections collected	34541
Independent reflections	8568 [R(int) = 0.1106]
Completeness to theta = 67.679 °	97.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7533 and 0.4553
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8568 / 1 / 604
Goodness-of-fit on F ²	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0698, wR2 = 0.1763
R indices (all data)	R1 = 0.0865, wR2 = 0.1981
Absolute structure parameter	0.0(2)
Extinction coefficient	0.0131(14)
Largest diff. peak and hole	0.258 and -0.225 e.Å ⁻³

NMR Spectra and HPLC Chromatographs of **4aa**

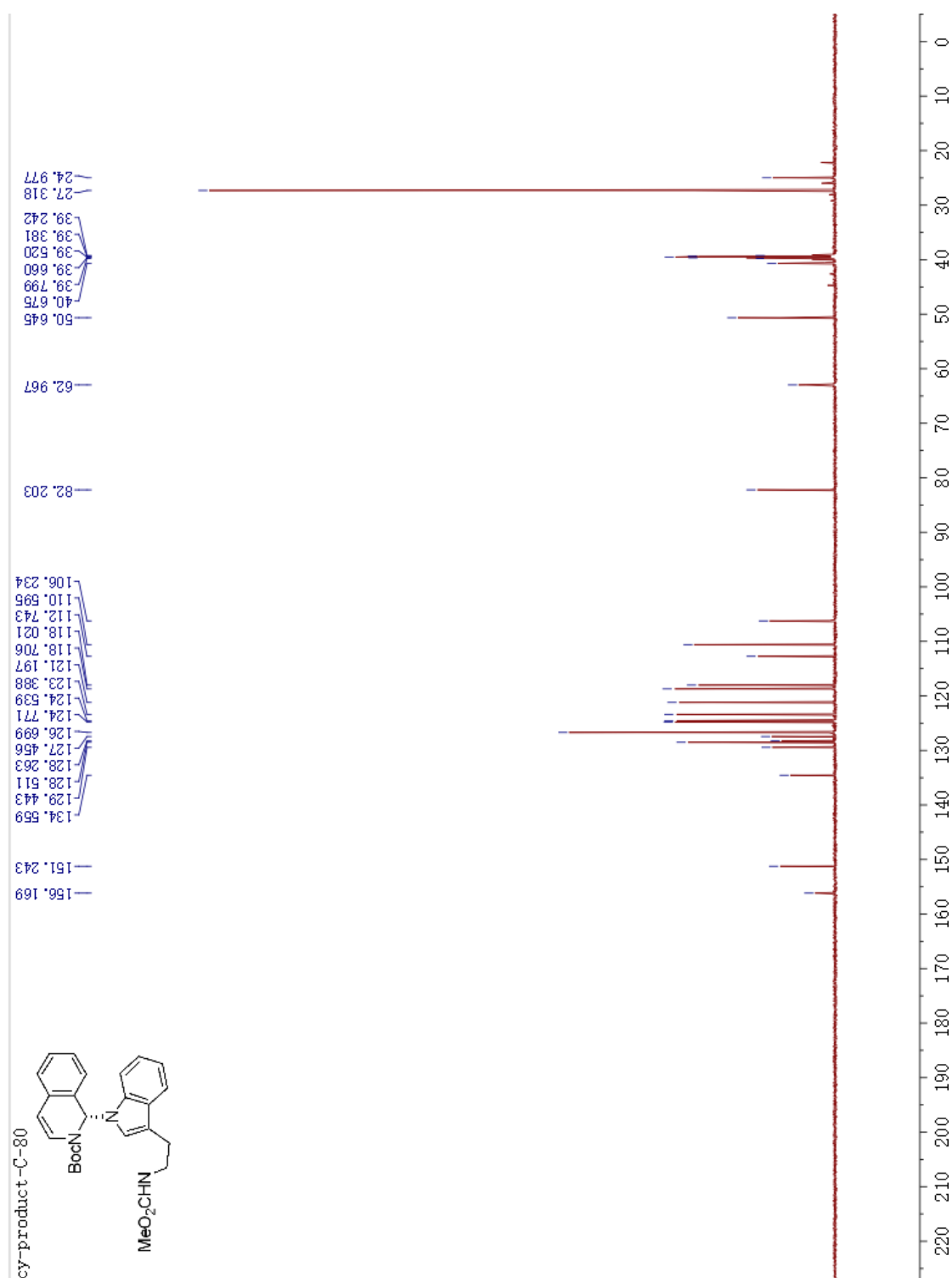
^1H NMR (600 MHz, $\text{d}_6\text{-DMSO}$, 80 $^\circ\text{C}$)



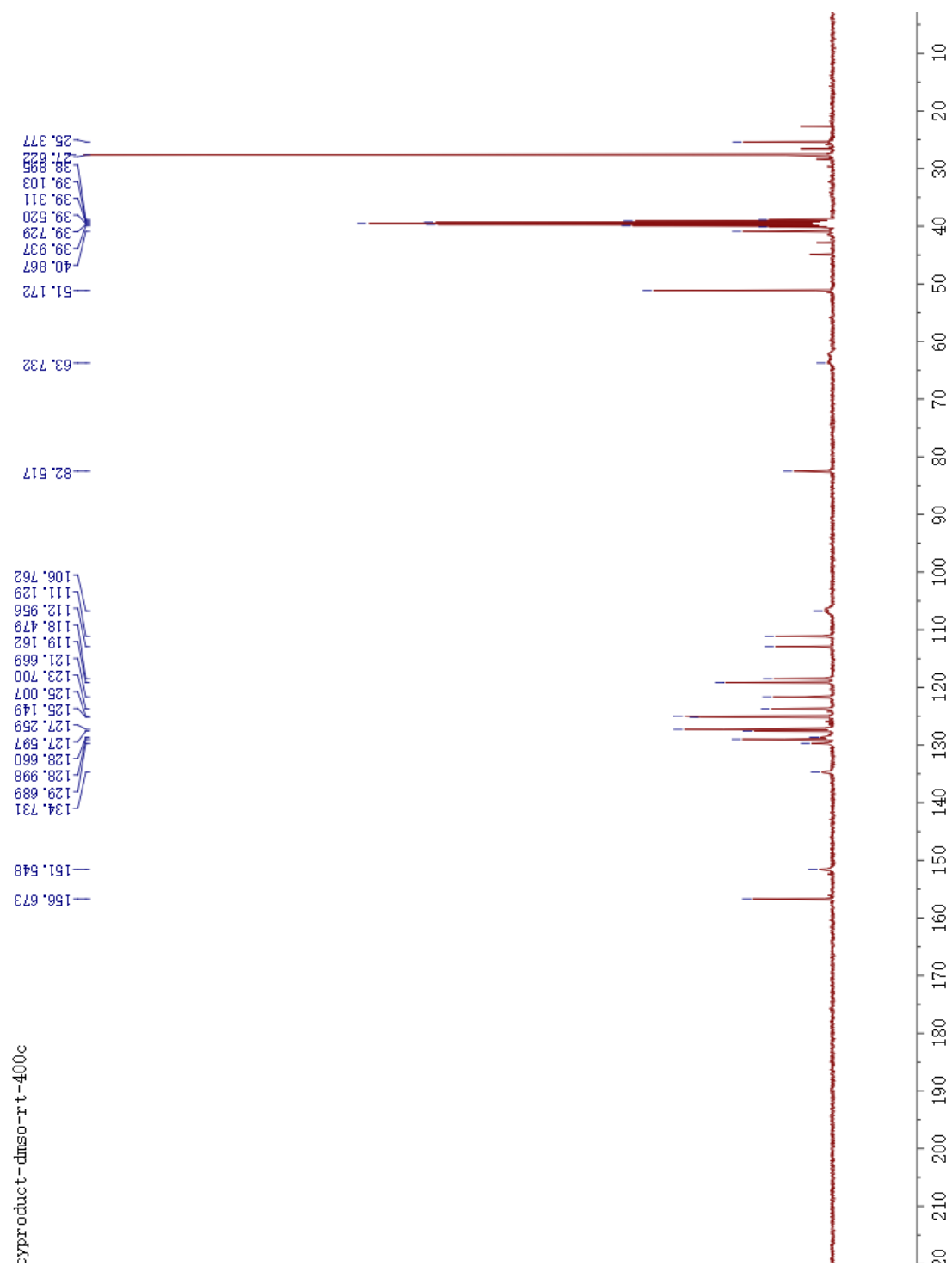
^1H NMR (400 MHz, $\text{d}_6\text{-DMSO}$)



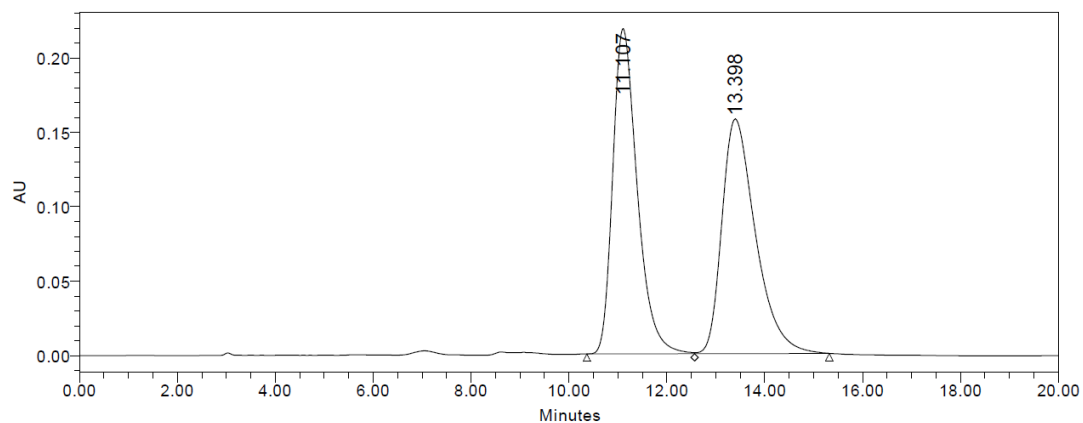
^{13}C NMR (151 MHz, $\text{d}_6\text{-DMSO}$, 80 $^\circ\text{C}$)



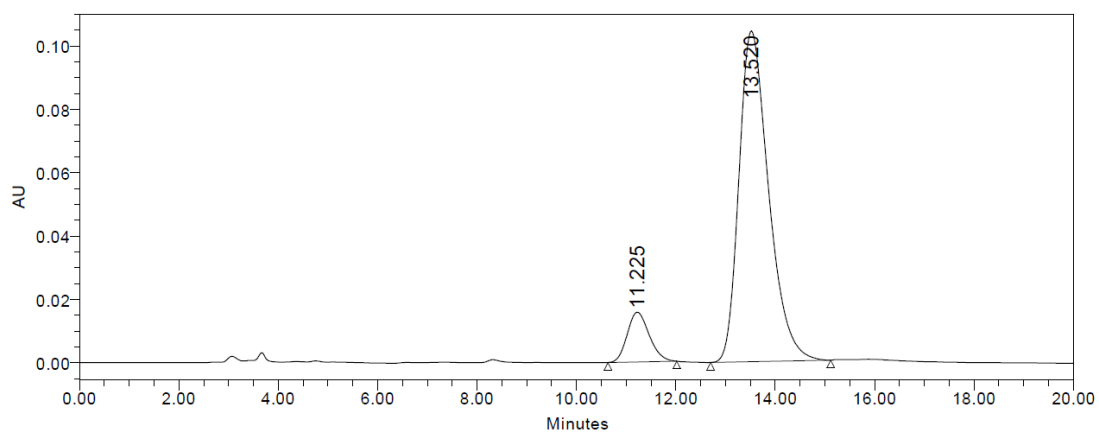
^{13}C NMR (100 MHz, $\text{d}_6\text{-DMSO}$)



xyproduct-dmsd-rt-400c

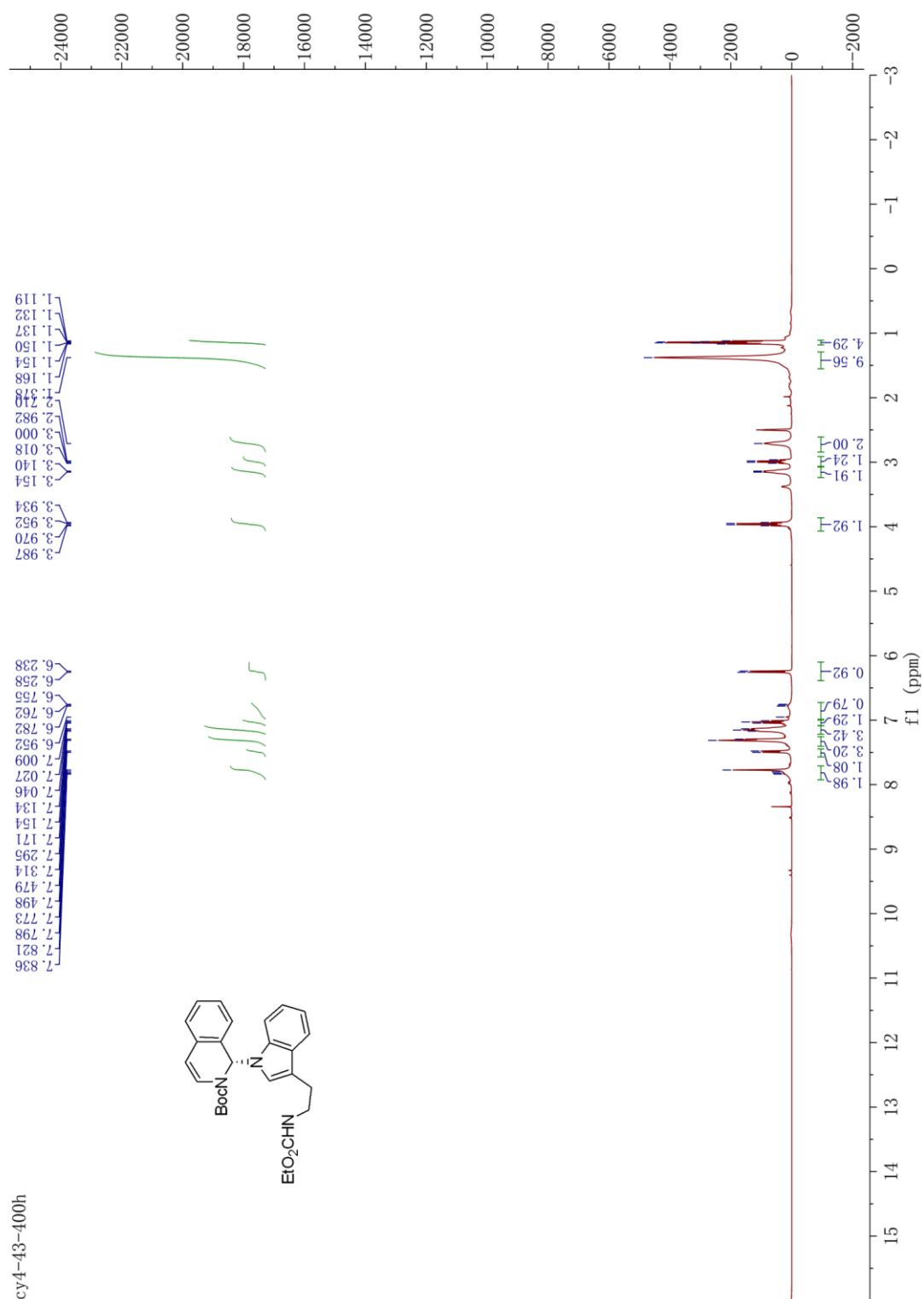


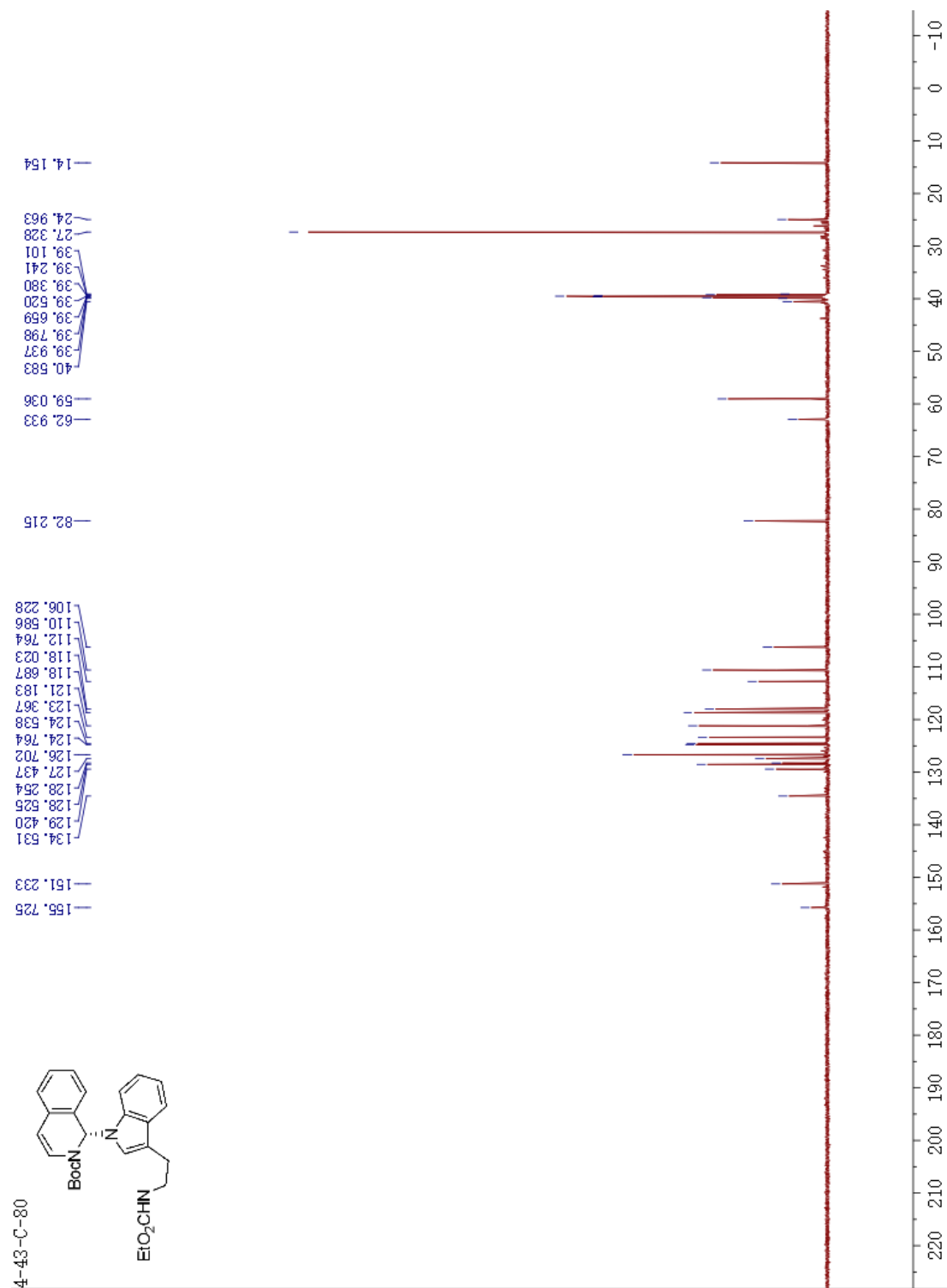
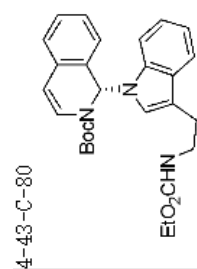
	RT	Area	% Area	Height
1	11.107	7596100	50.24	218559
2	13.398	7524812	49.76	157625

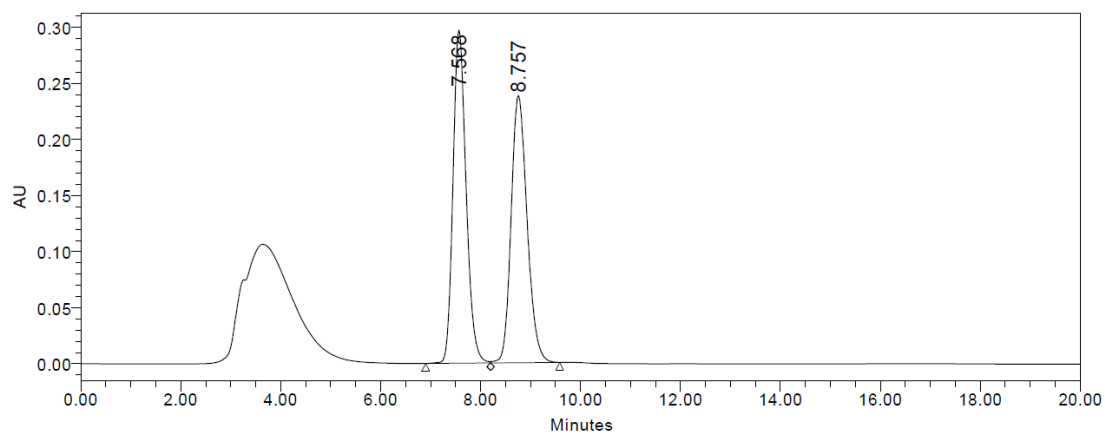


	RT	Area	% Area	Height
1	11.225	483707	10.05	15738
2	13.520	4331084	89.95	104467

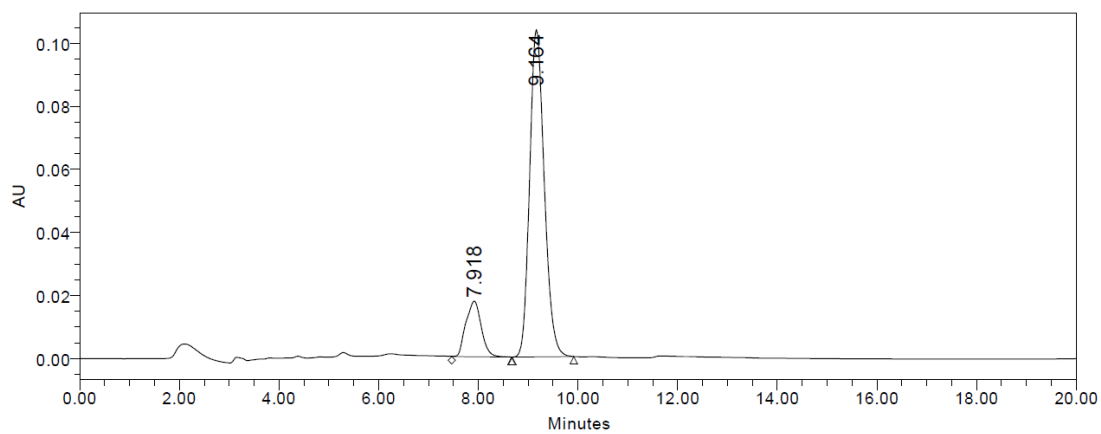
NMR Spectra and HPLC Chromatographs of **4ab**







	RT	Area	% Area	Height
1	7.568	5412703	50.65	297097
2	8.757	5274572	49.35	238262



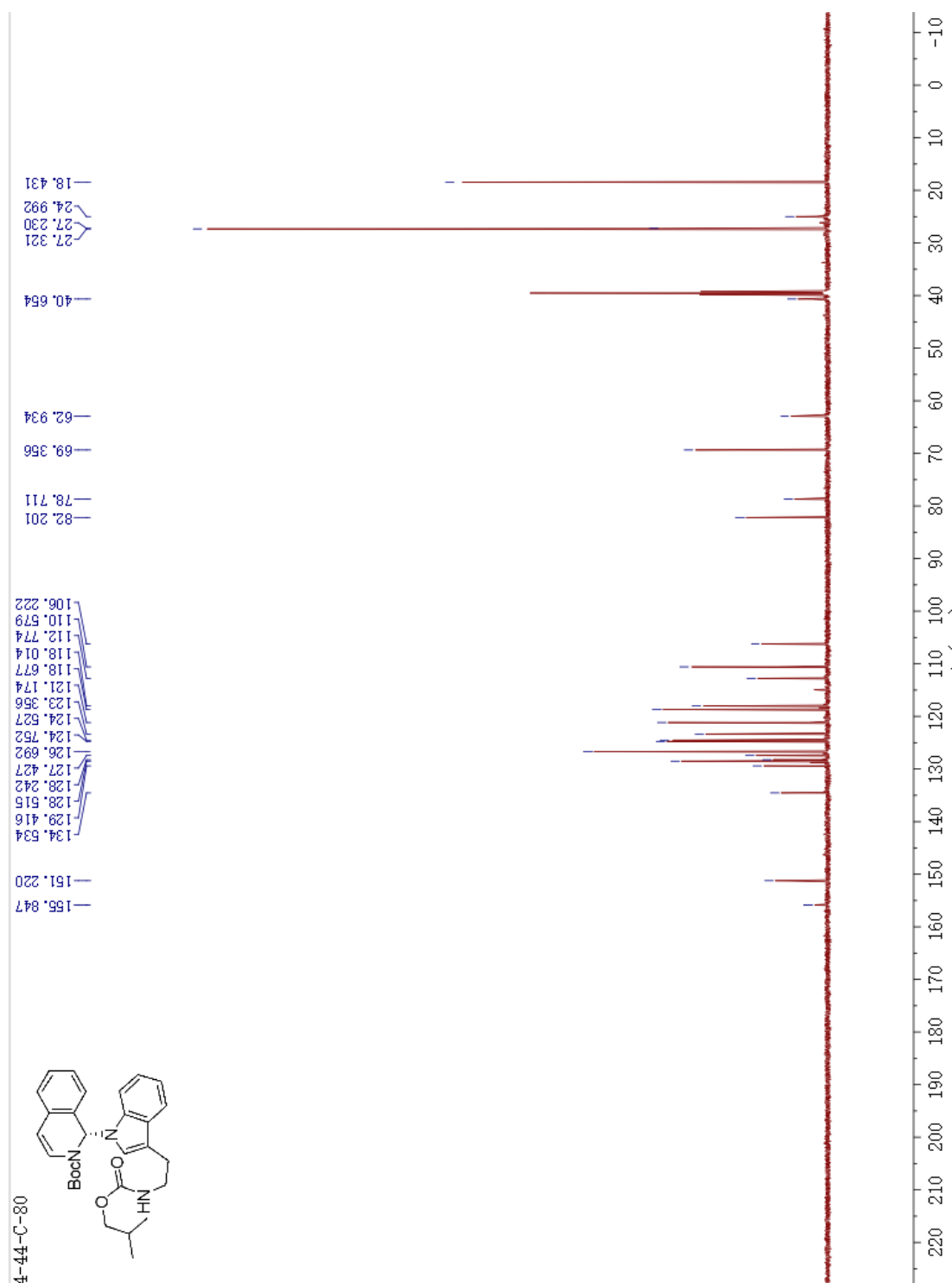
	RT	Area	% Area	Height
1	7.918	377210	15.11	17635
2	9.164	2118742	84.89	103706

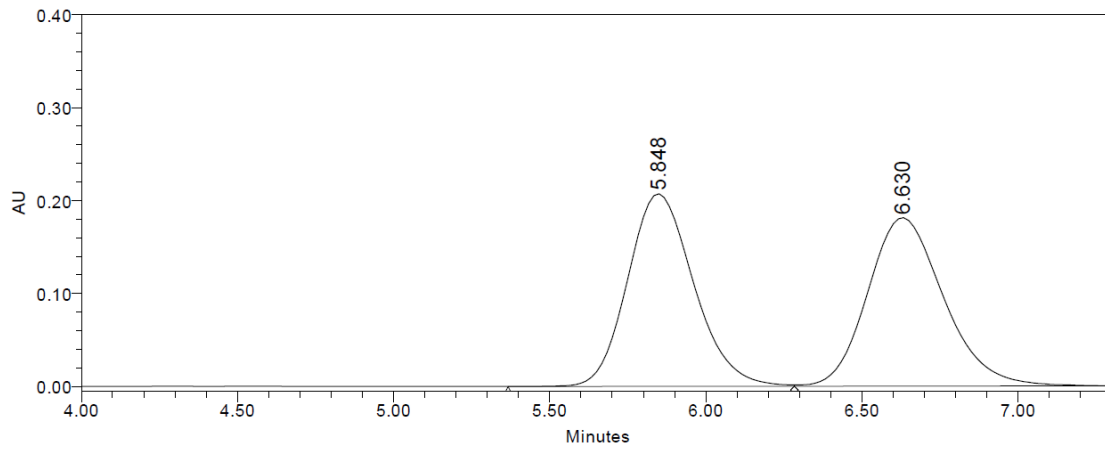
py-4-44-H-80

Chemical structure of compound 44 is shown below the spectrum:

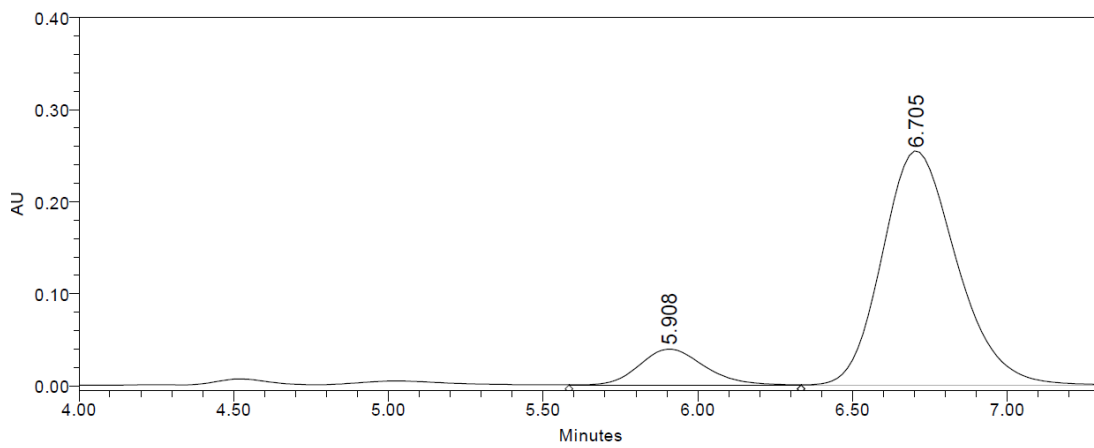
CC1CN(C(=O)O1)C2c3ccccc3n2[C@@H]4C=CC=C[C@H]4c5ccccc5

The structure is a complex molecule featuring a central carbon atom bonded to a phenyl ring, a pyridine ring, and a chiral auxiliary (Boc-protected amino acid derivative).



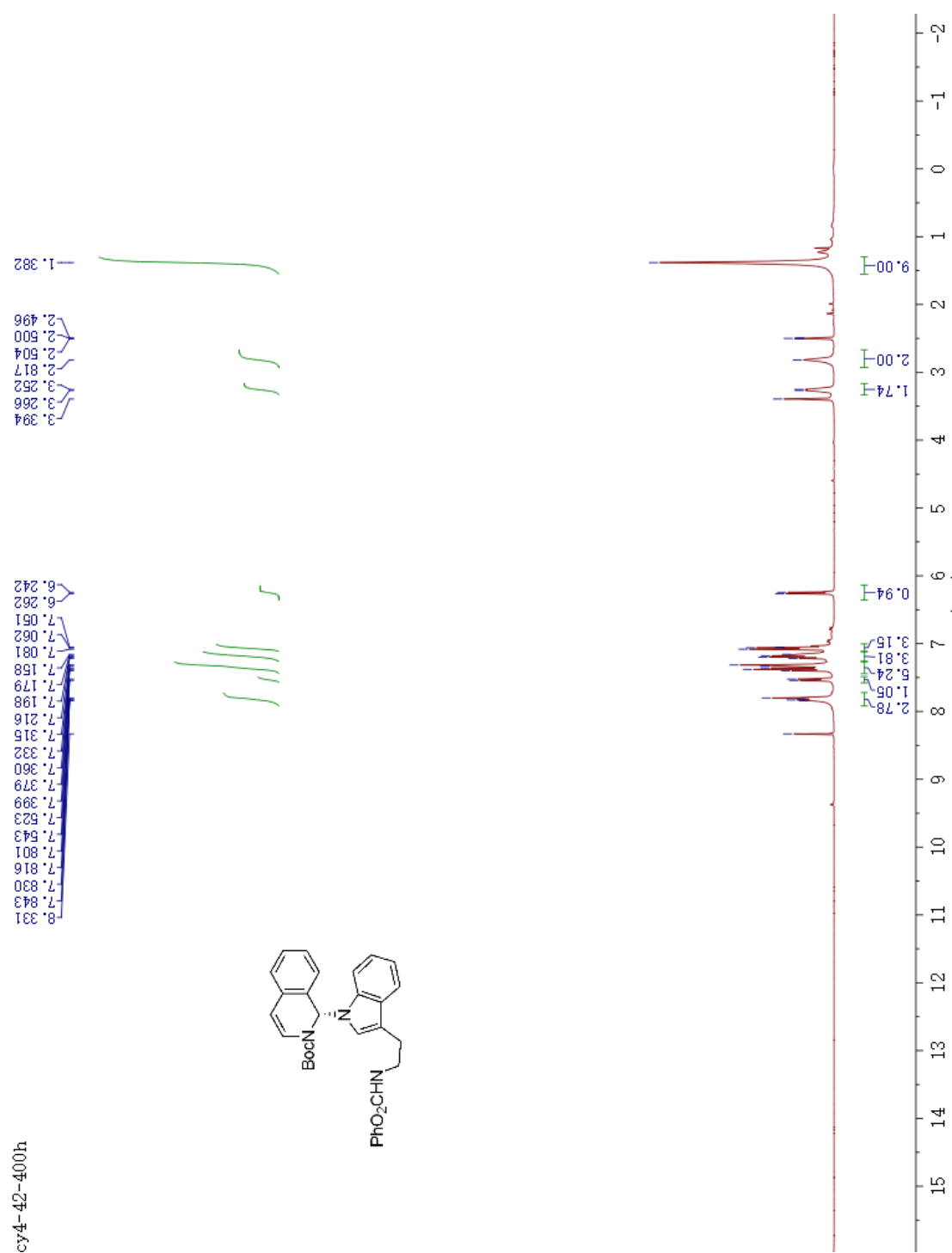


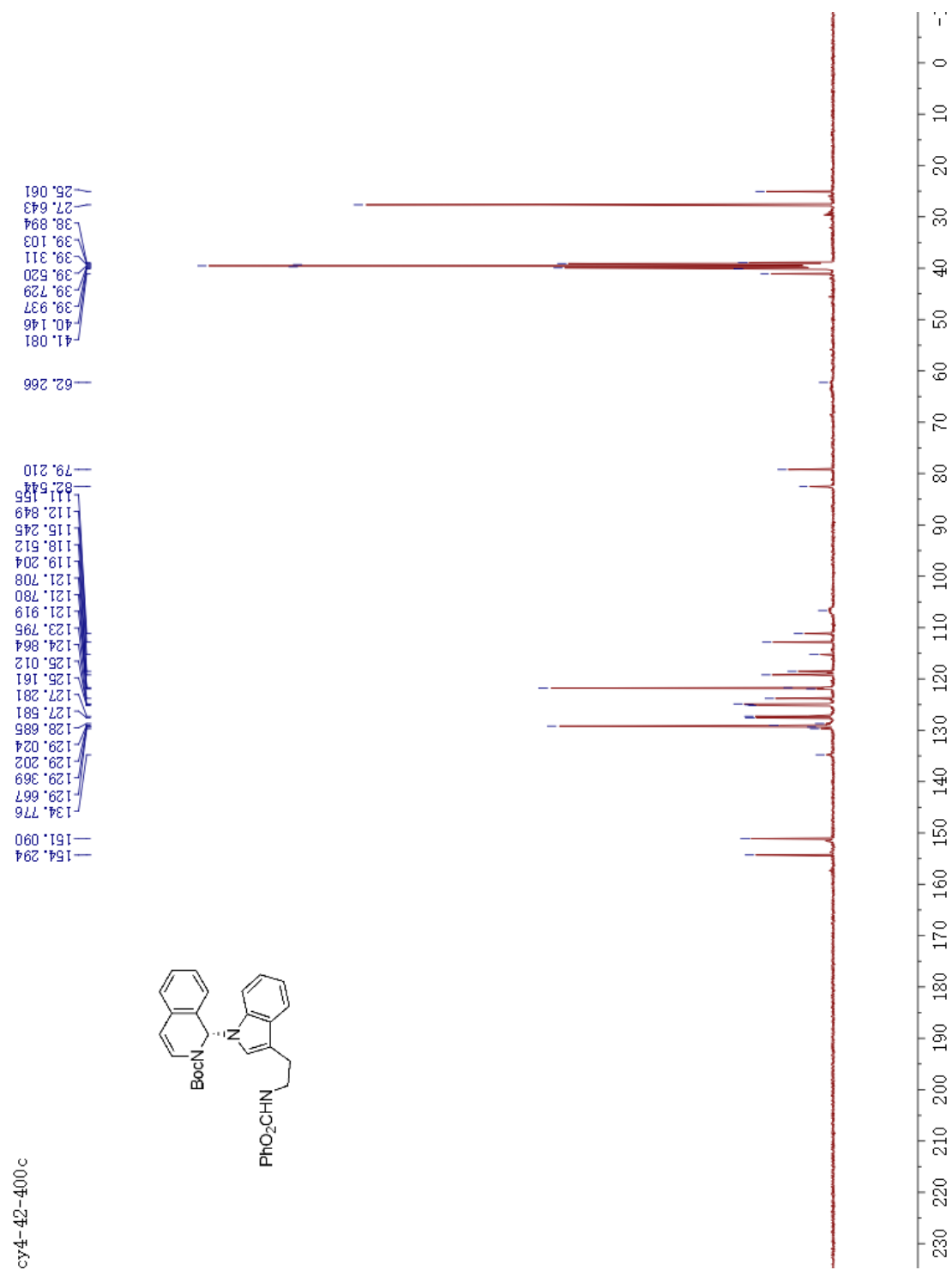
	RT	Area	% Area	Height
1	5.848	3047586	49.86	207129
2	6.630	3064764	50.14	181130

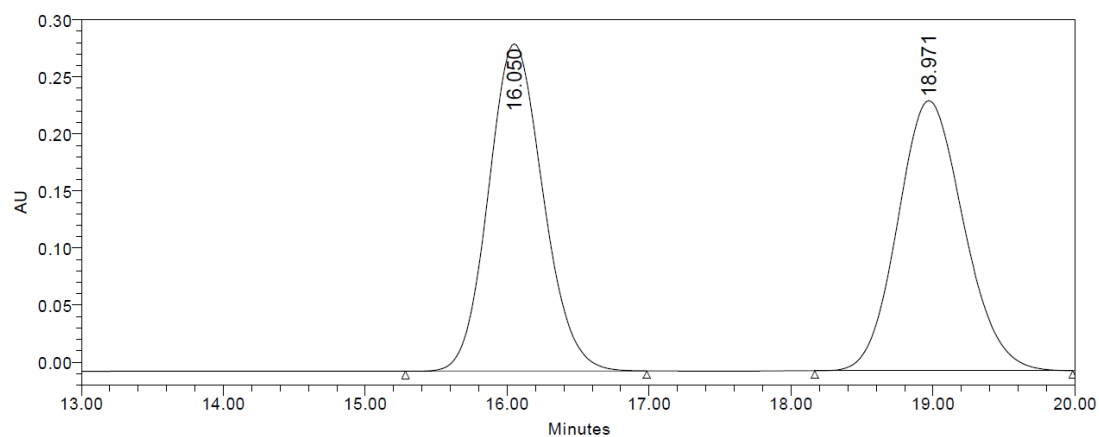


	RT	Area	% Area	Height
1	5.908	568794	11.81	39049
2	6.705	4248181	88.19	254157

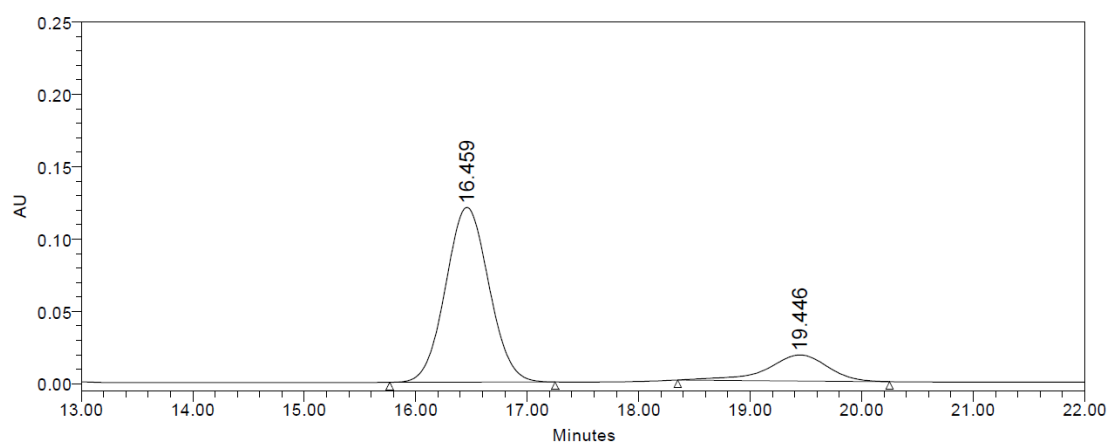
NMR Spectra and HPLC Chromatographs of **4ad**





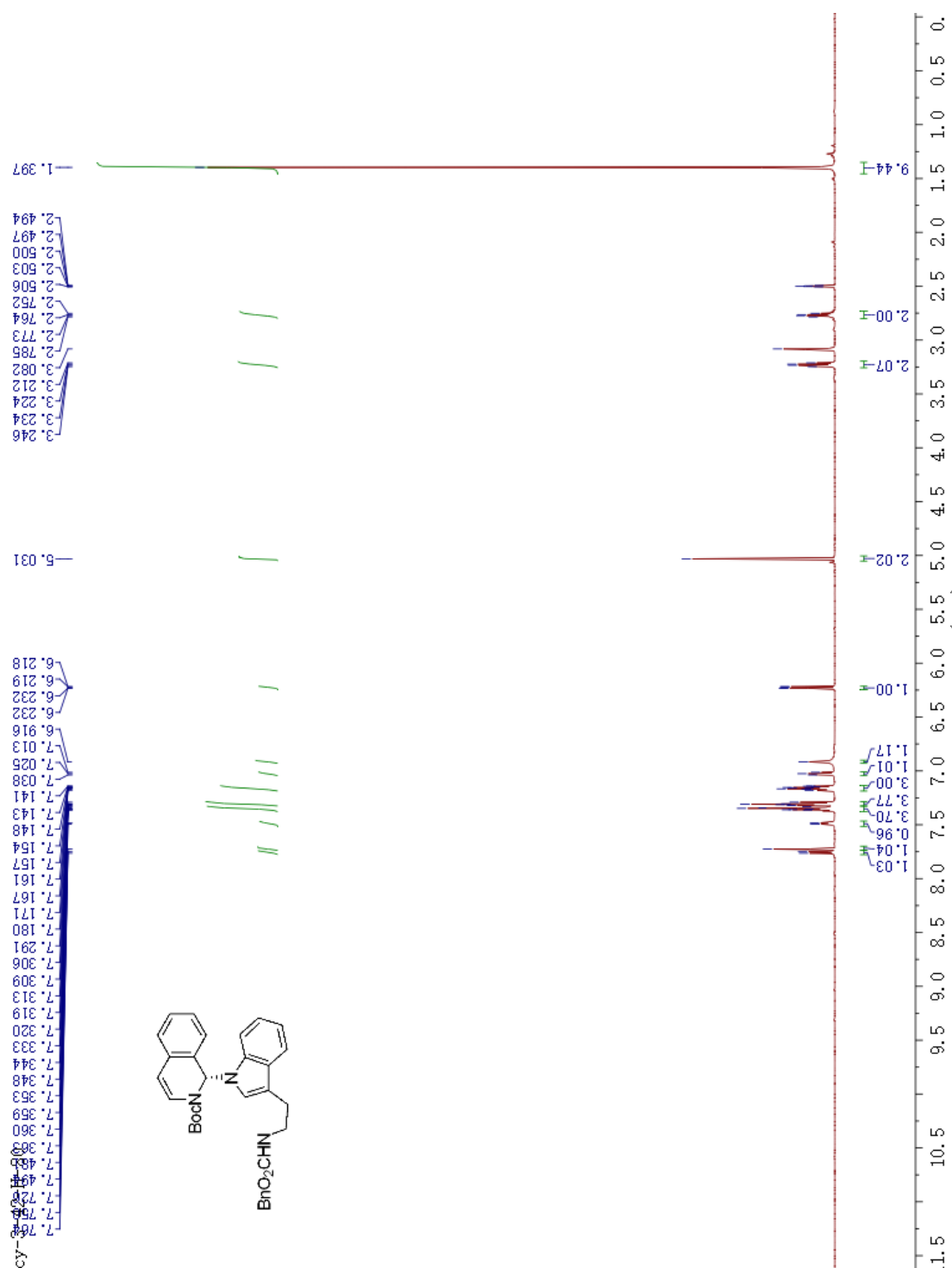


	RT	Area	% Area	Height
1	16.050	7648764	50.02	286611
2	18.971	7643888	49.98	236647

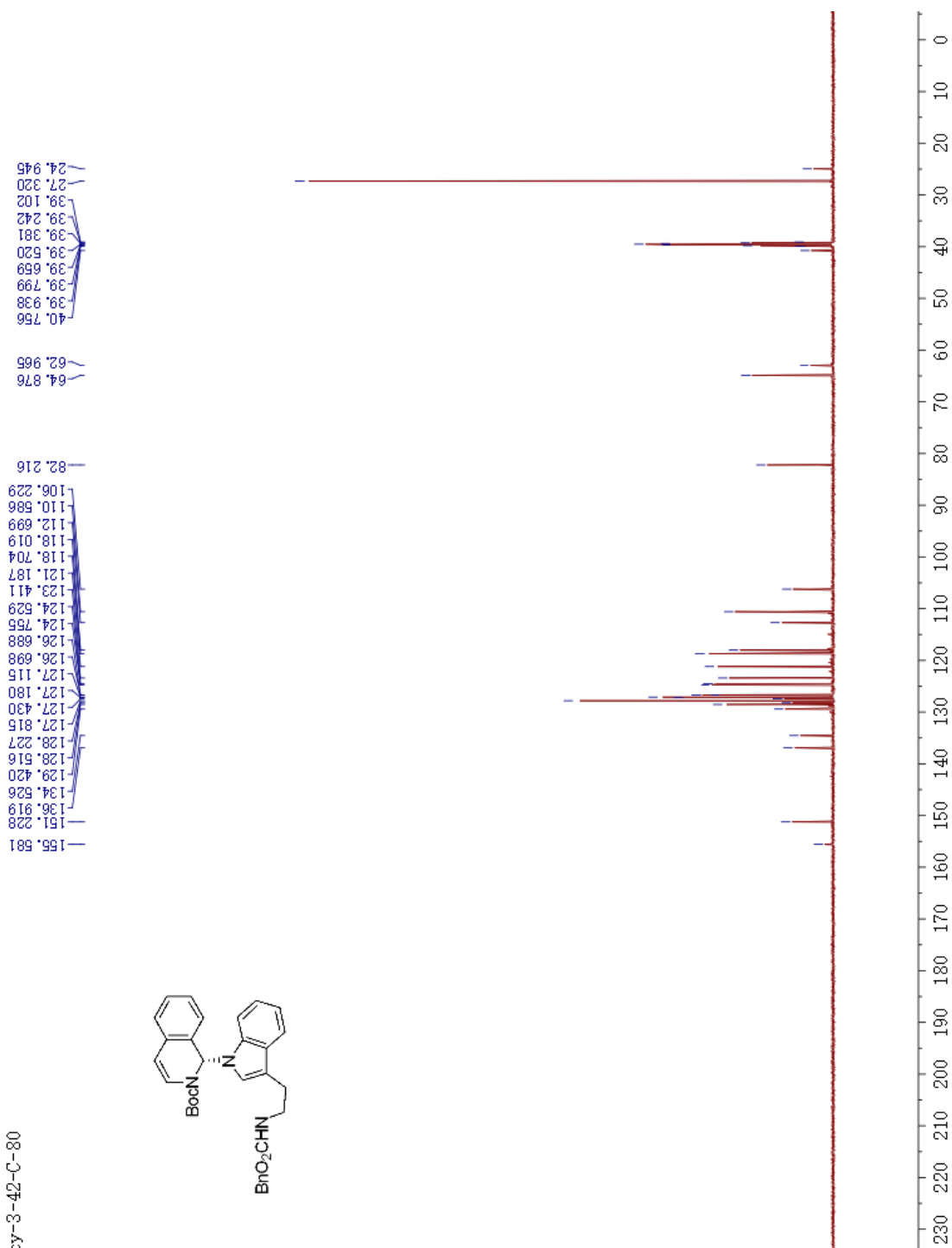
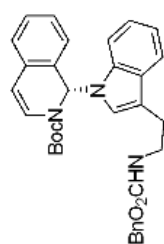


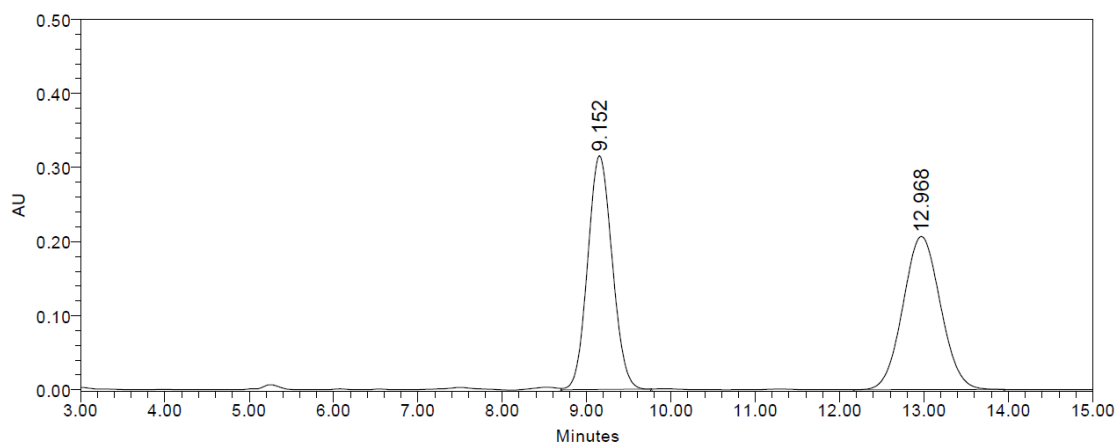
	RT	Area	% Area	Height
1	16.459	3265257	82.84	120872
2	19.446	676517	17.16	17979

NMR Spectra and HPLC Chromatographs of **4ae**

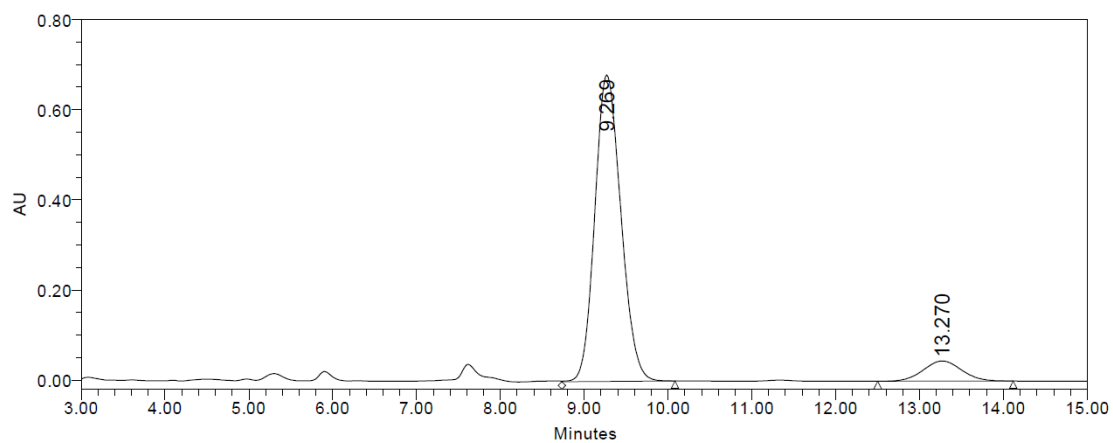


py-3-42-C-80



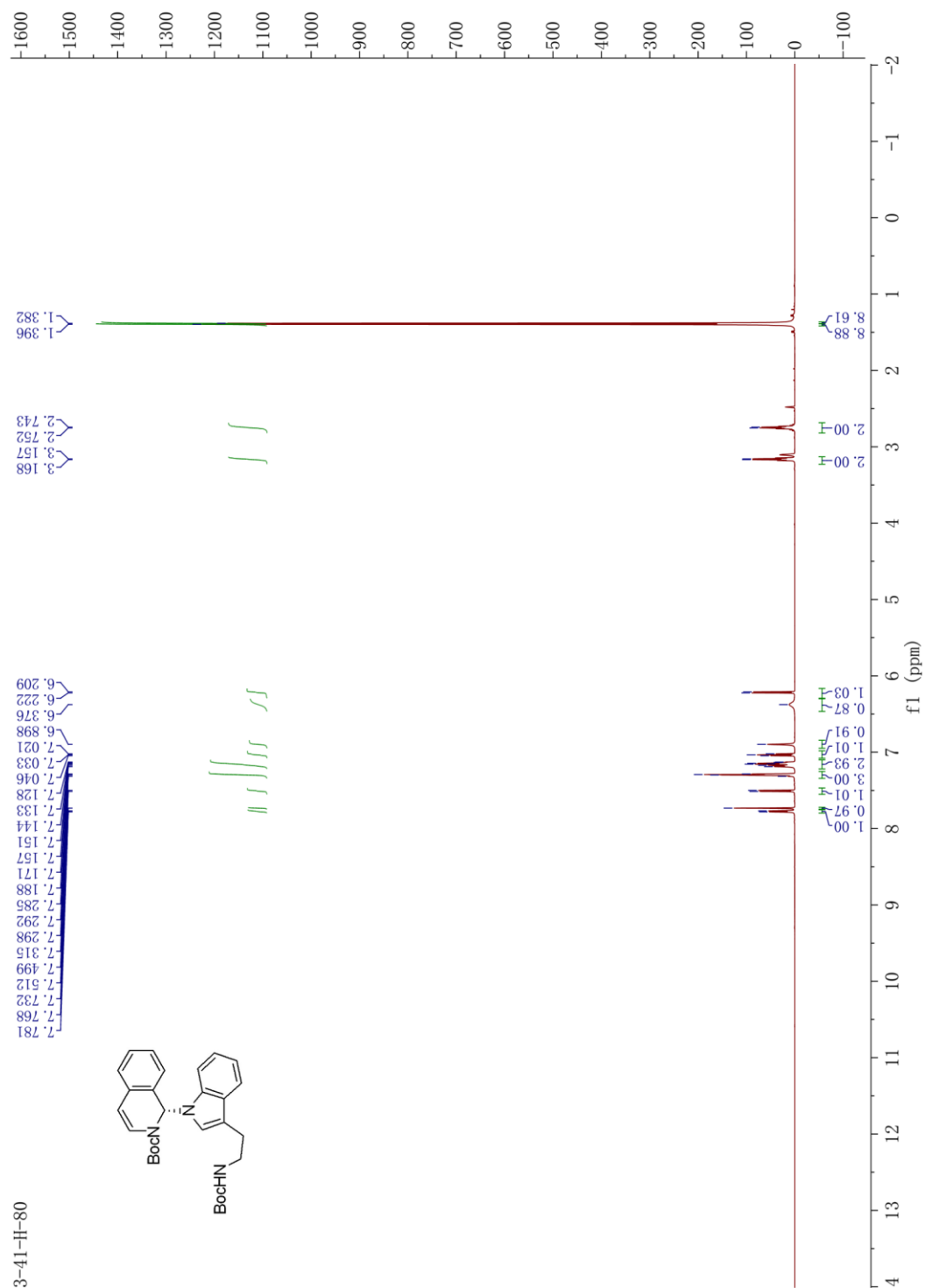


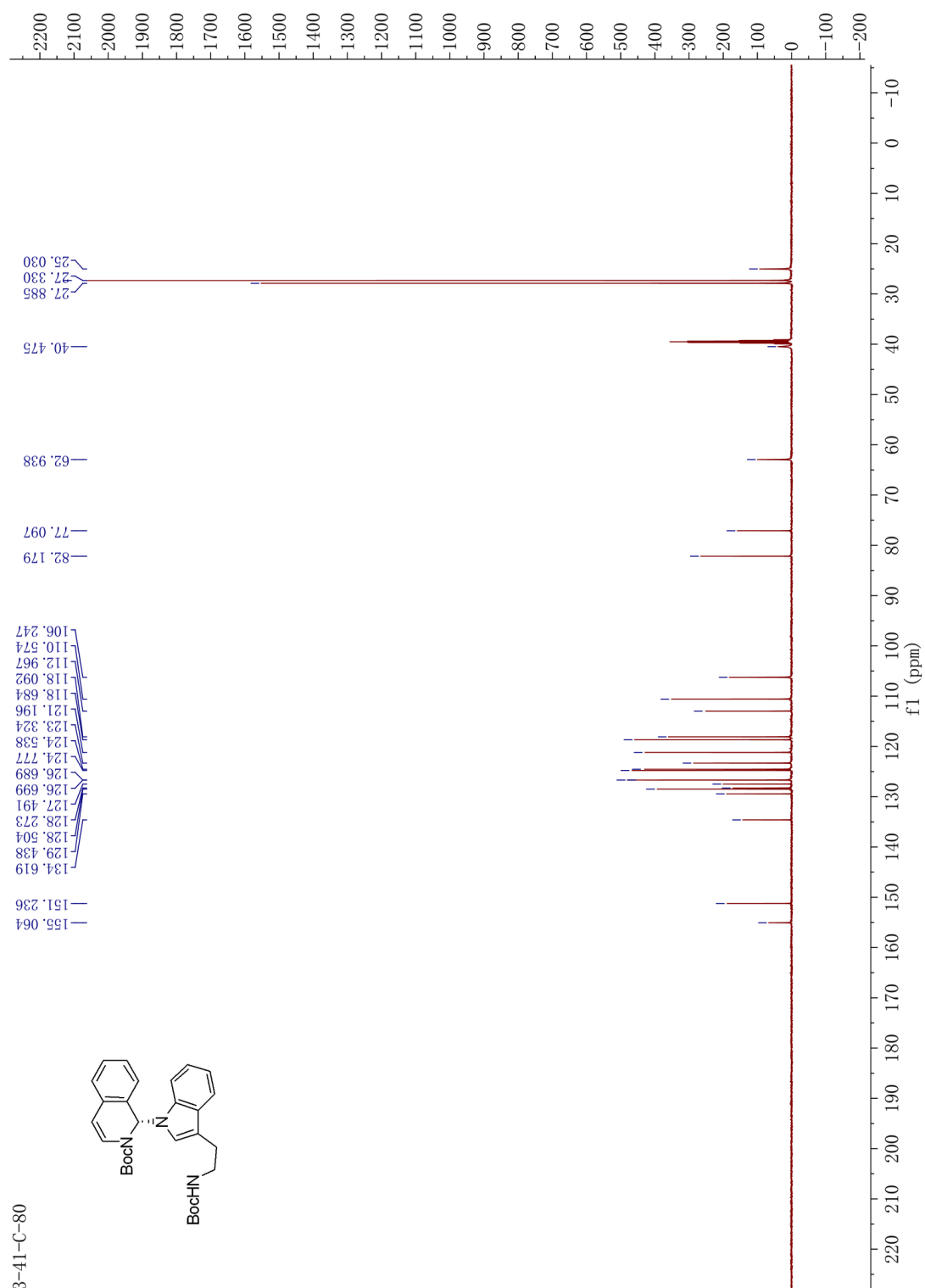
	RT	Area	% Area	Height
1	9.152	6362099	49.87	315530
2	12.968	6396460	50.13	206819

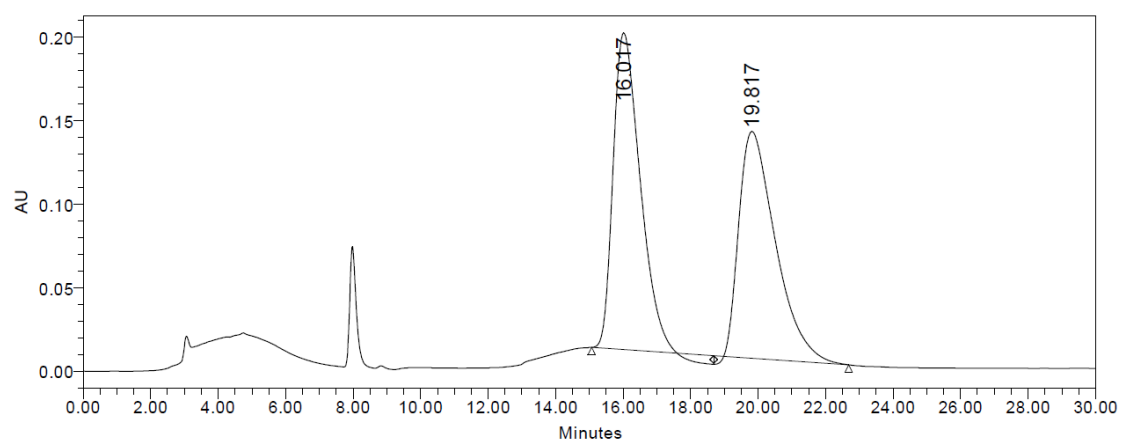


	RT	Area	% Area	Height
1	9.269	14675865	91.17	680033
2	13.270	1422006	8.83	44706

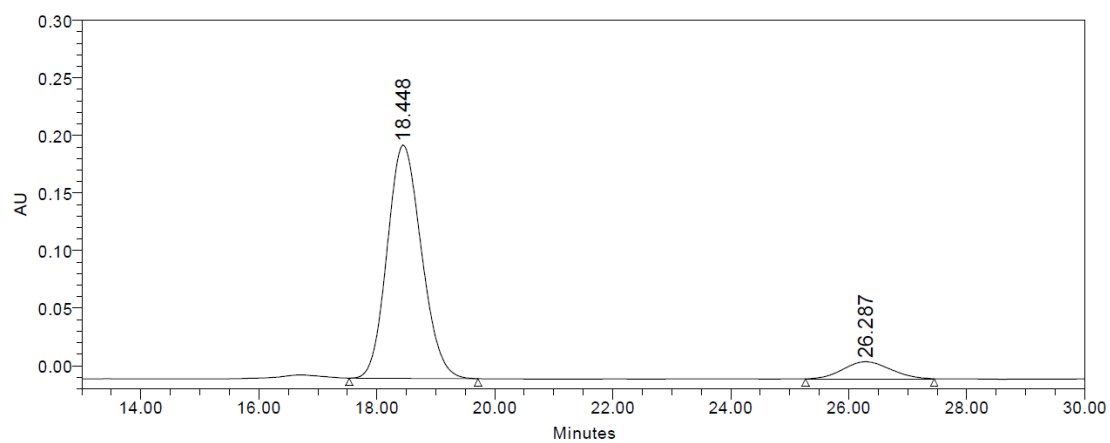
NMR Spectra and HPLC Chromatographs of **4af**



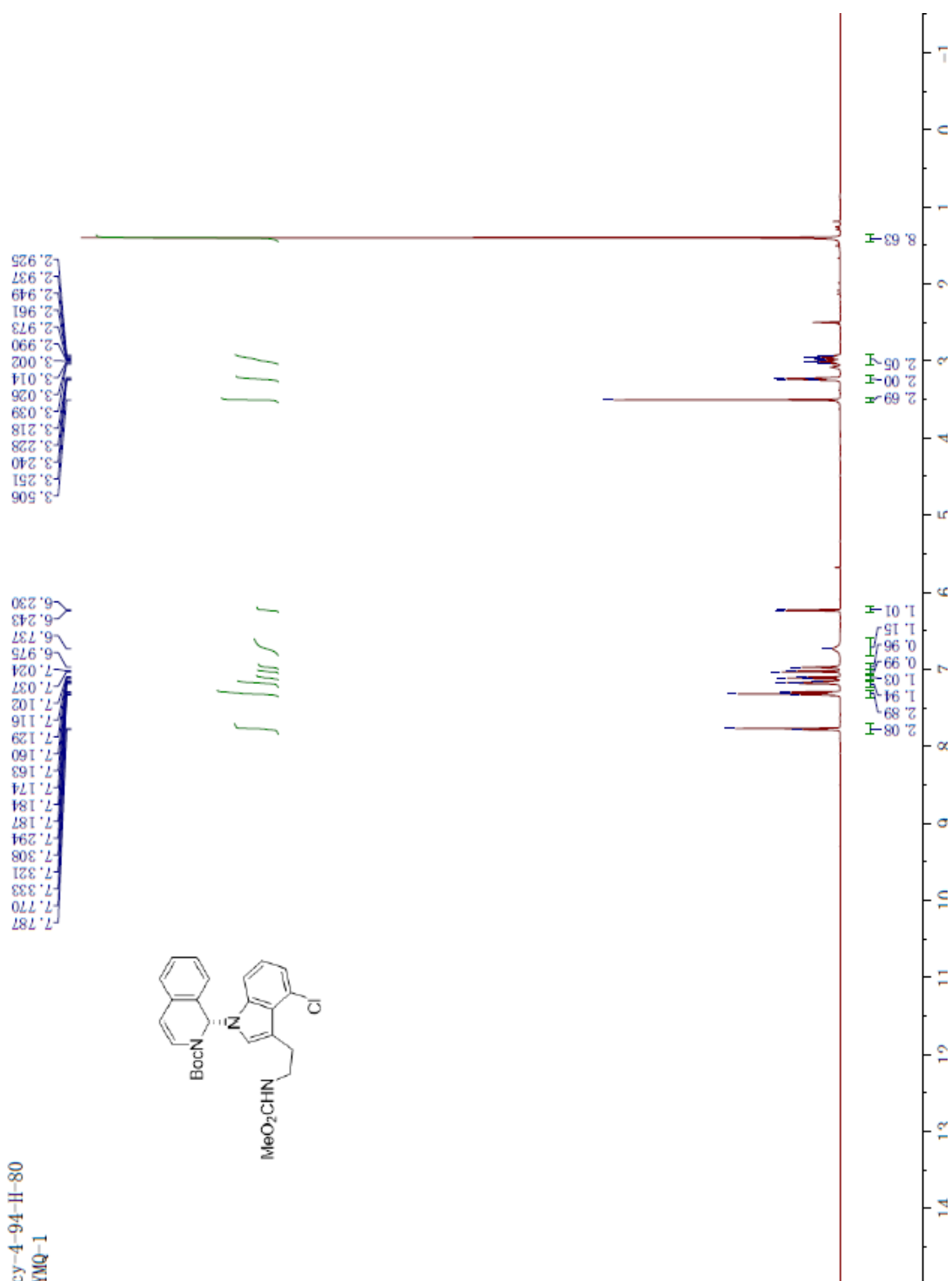


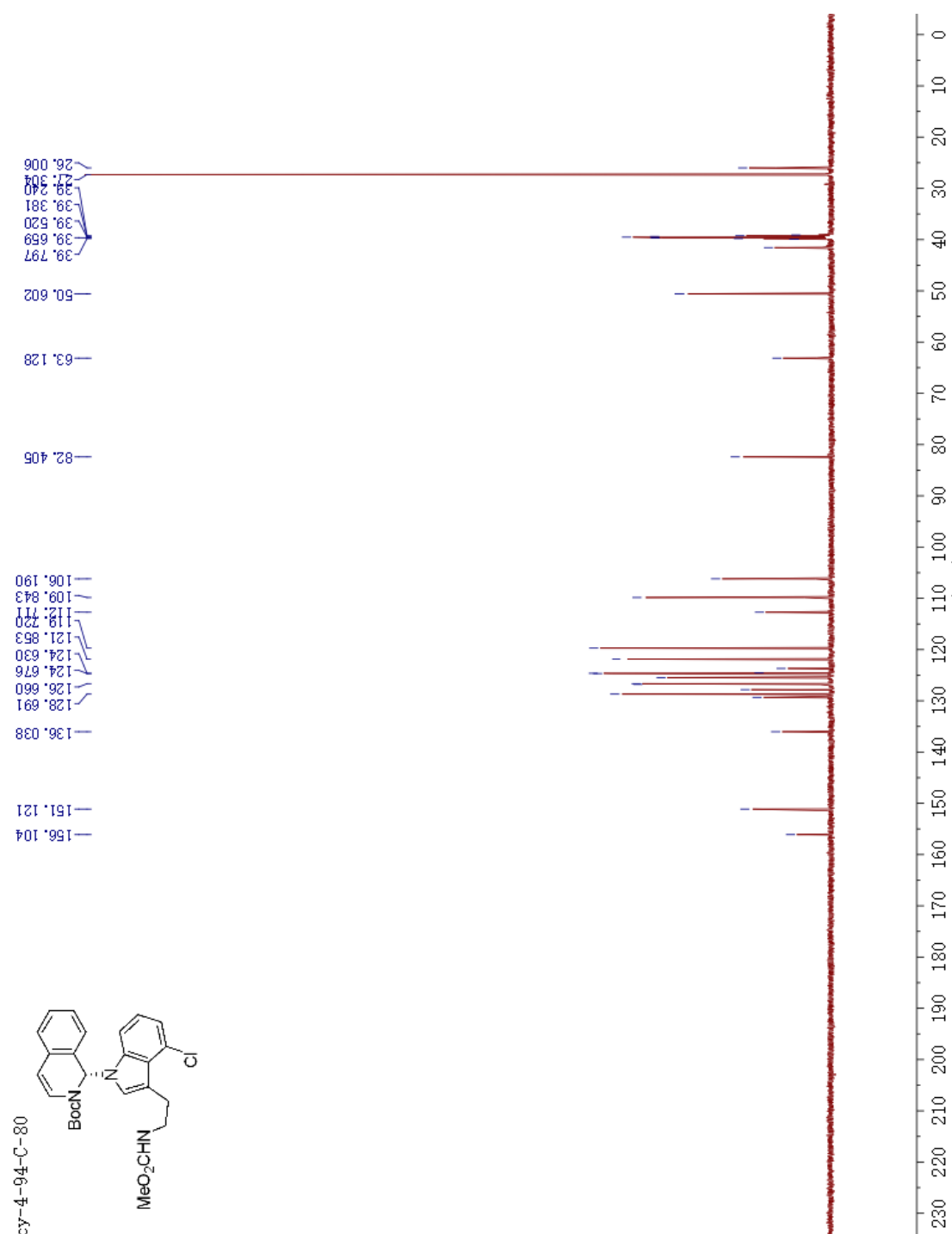


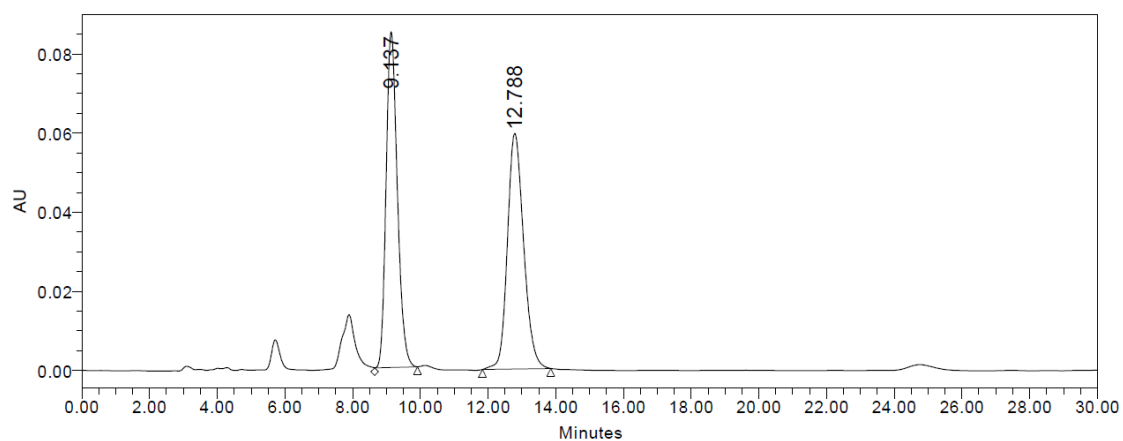
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1	16.017	10858167	51.29	189673
2	19.817	10314020	48.71	135789



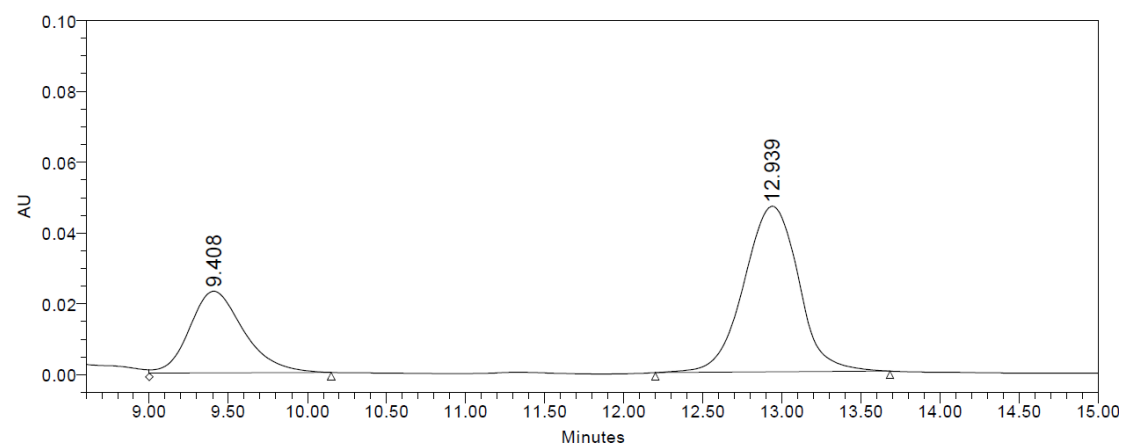
	RT	Area	% Area	Height
1	18.448	8175276	90.90	202504
2	26.287	818798	9.10	14744

cy-4-94-H-80
YMQ-1





	RT	Area	% Area	Height
1	9.137	1954013	49.64	84866
2	12.788	1982249	50.36	59526



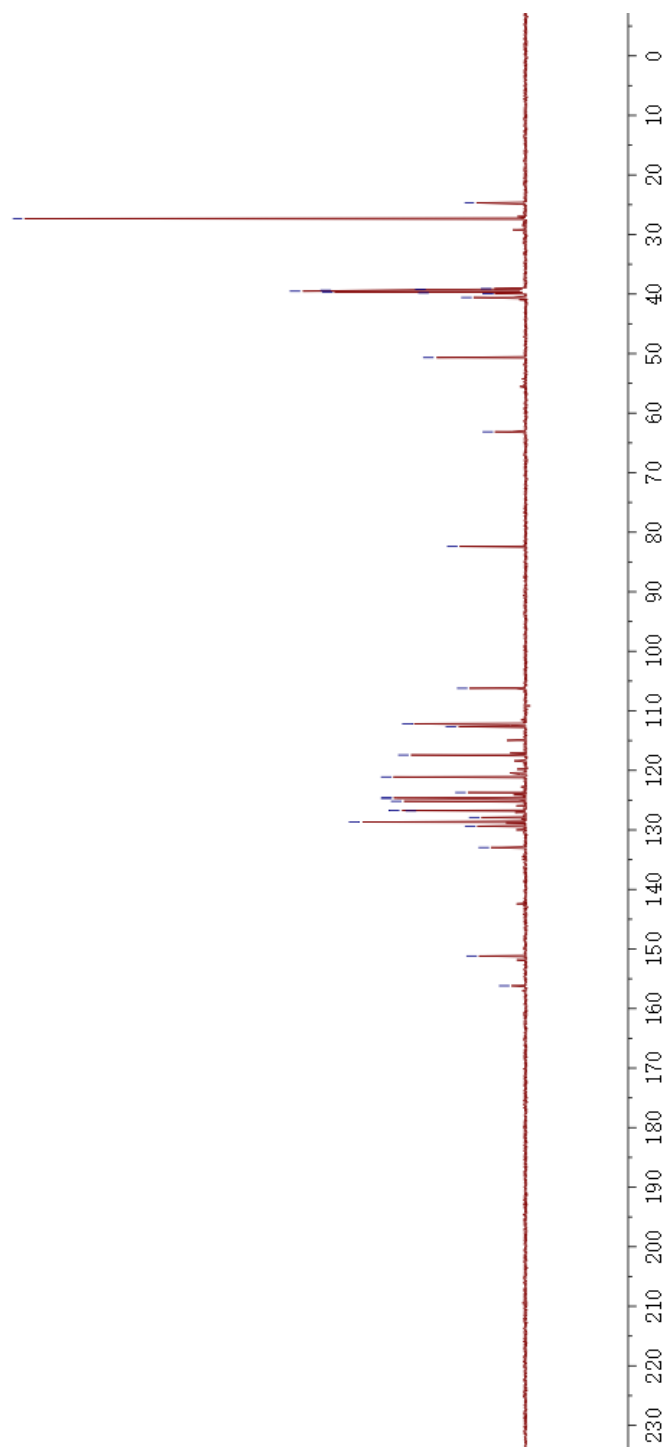
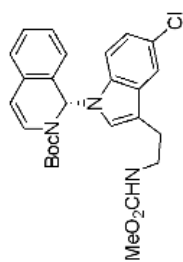
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1	9.408	547906	32.79	23053
2	12.939	1123221	67.21	46776

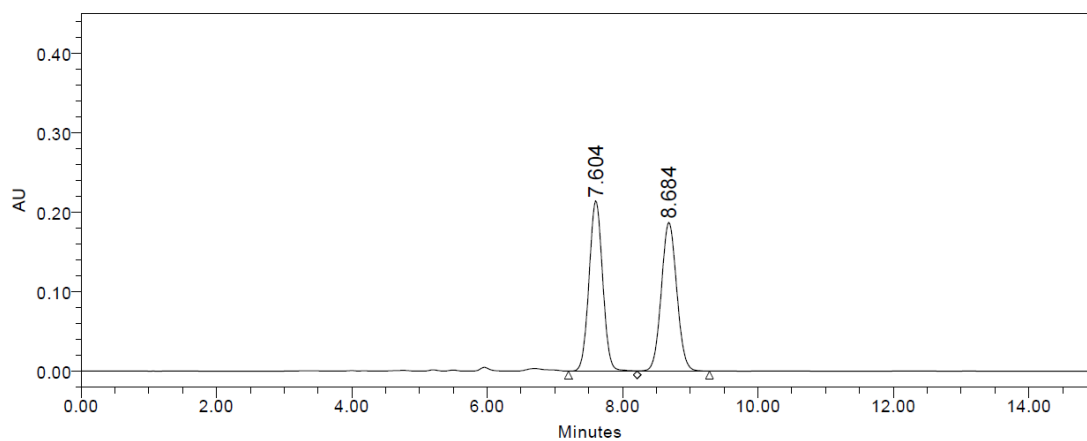
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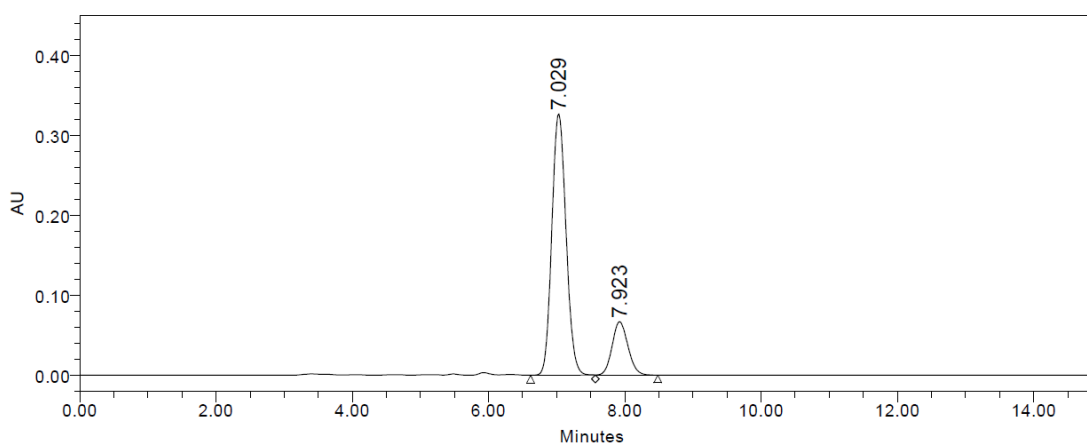
cy-5-6-C-80

156.175
151.173
132.957
129.372
128.684
127.905
126.799
126.747
125.182
124.668
124.621
123.718
121.102
117.417
112.640
112.164
106.215
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50.672
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39.799
39.660
39.520
39.381
39.242
27.328
24.681



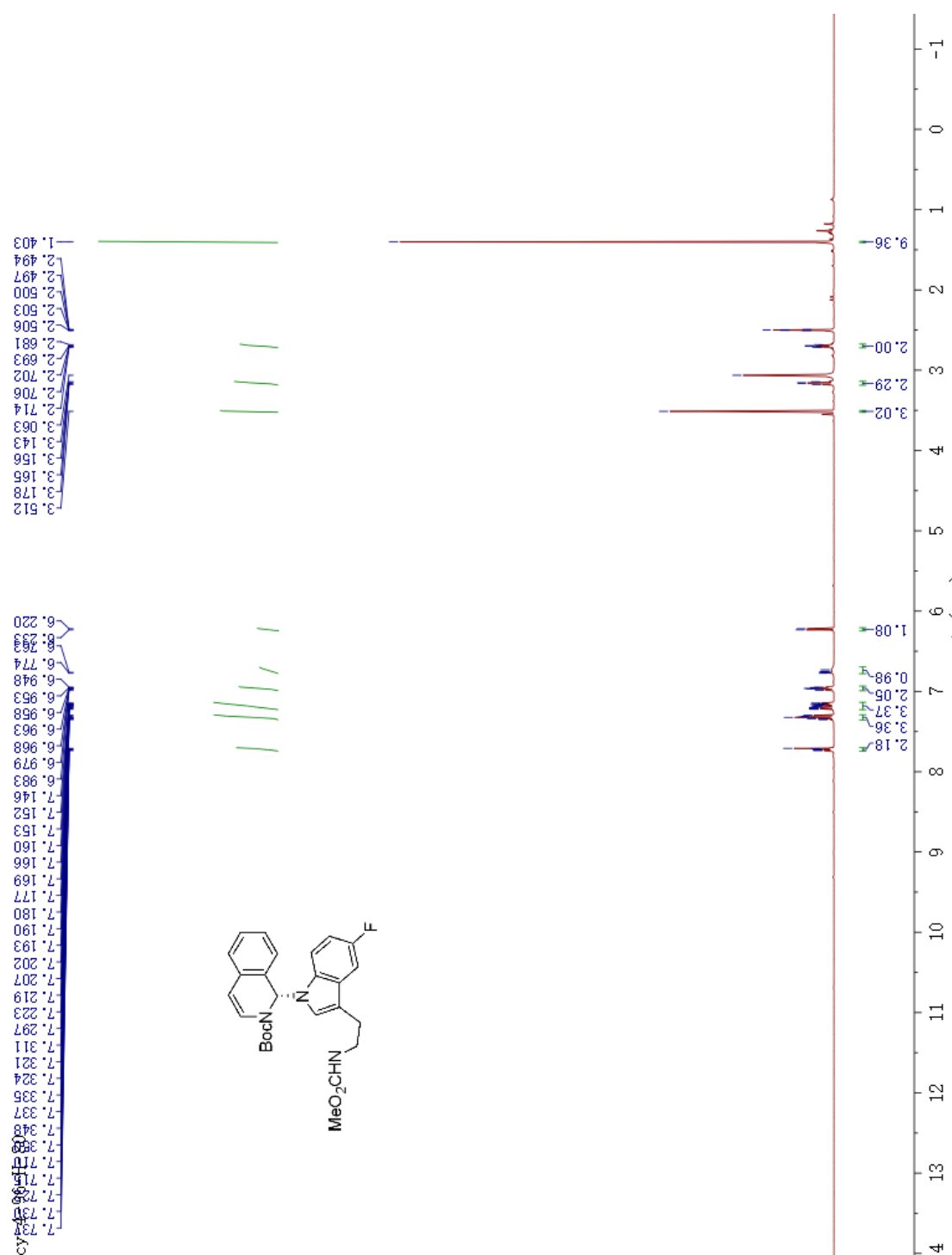


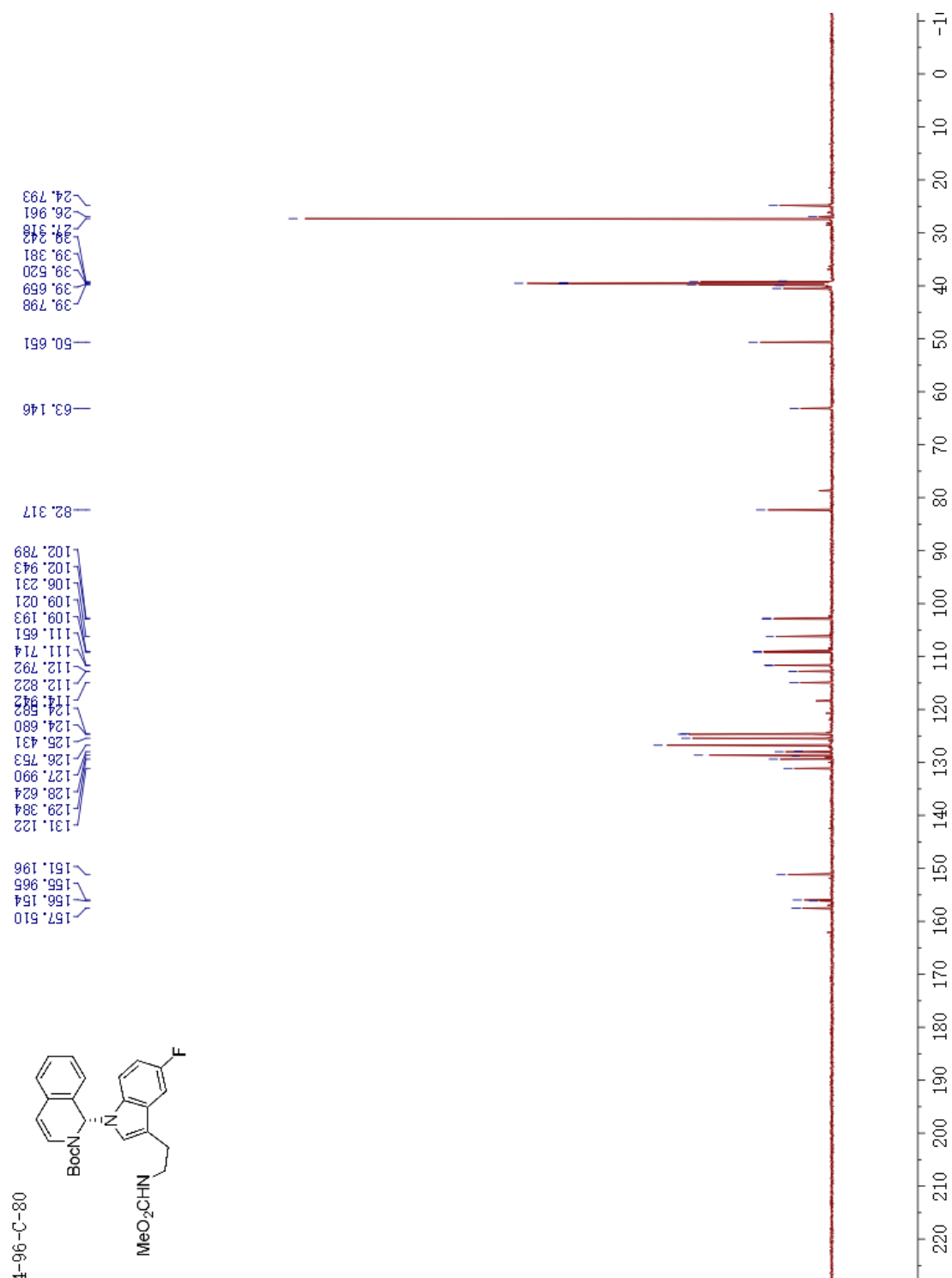
	RT	Area	% Area	Height
1	7.604	2991880	50.18	214480
2	8.684	2970797	49.82	187175



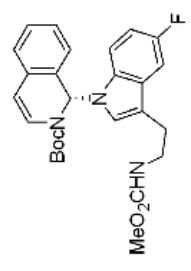
	RT	Area	% Area	Height
1	7.029	4746655	81.47	327286
2	7.923	1079519	18.53	67019

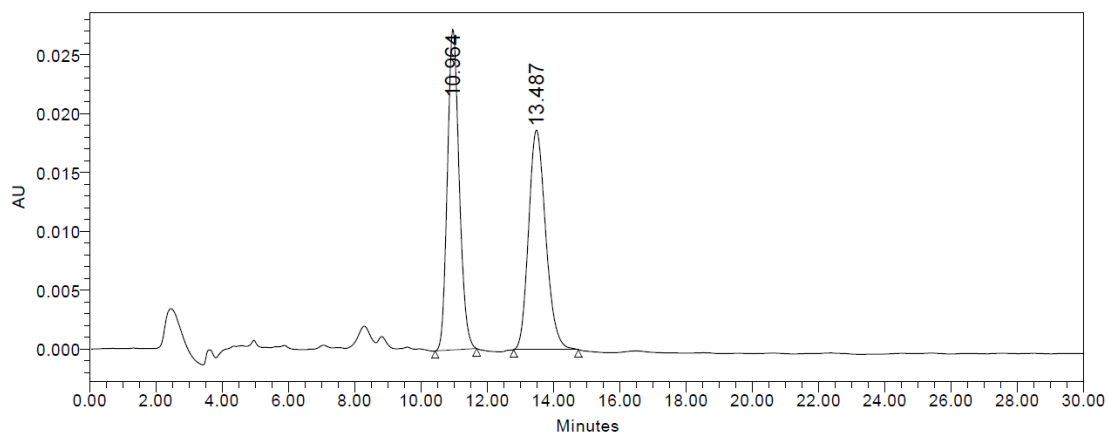
NMR Spectra and HPLC Chromatographs of **4ai**



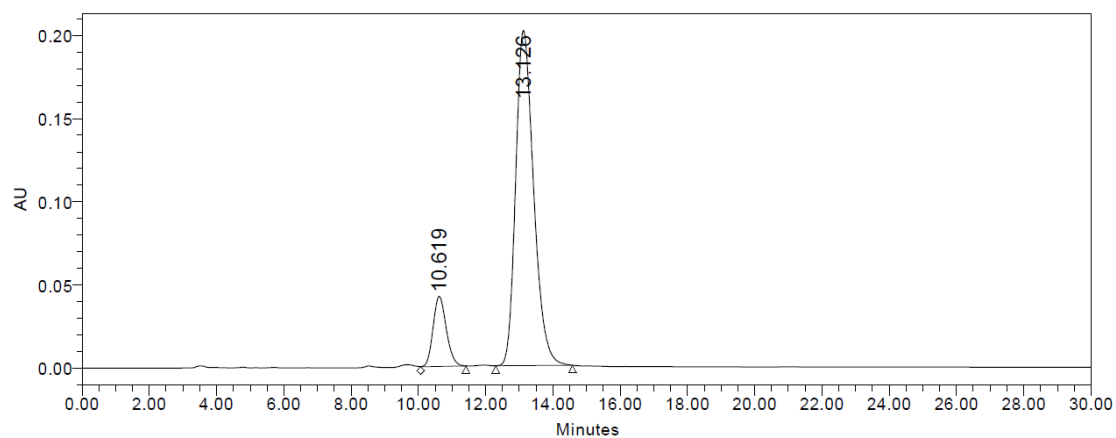


cy4-96-400f
Std Fluorine





	RT	Area	% Area	Height
1	10.964	674092	50.17	27226
2	13.487	669502	49.83	18668

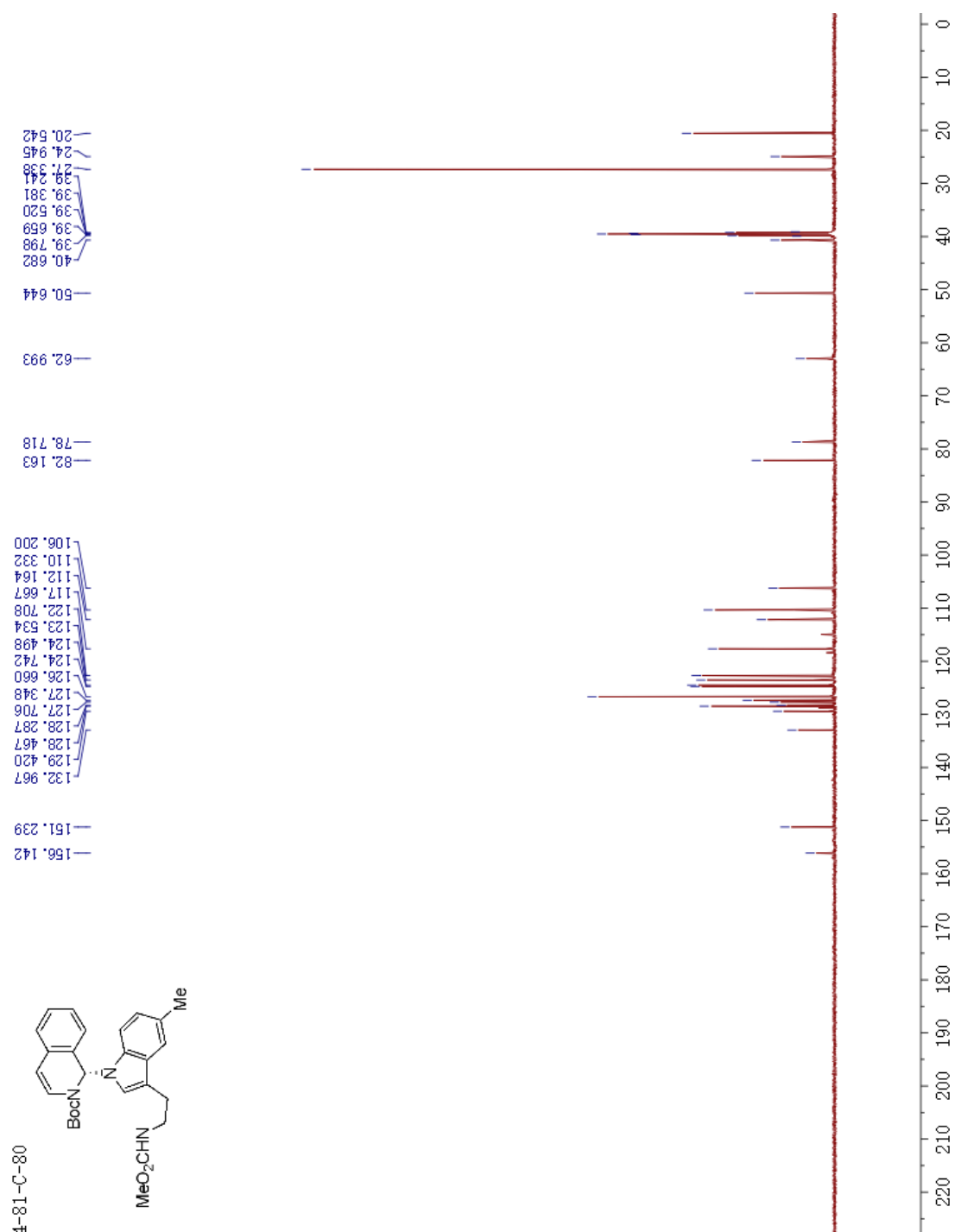


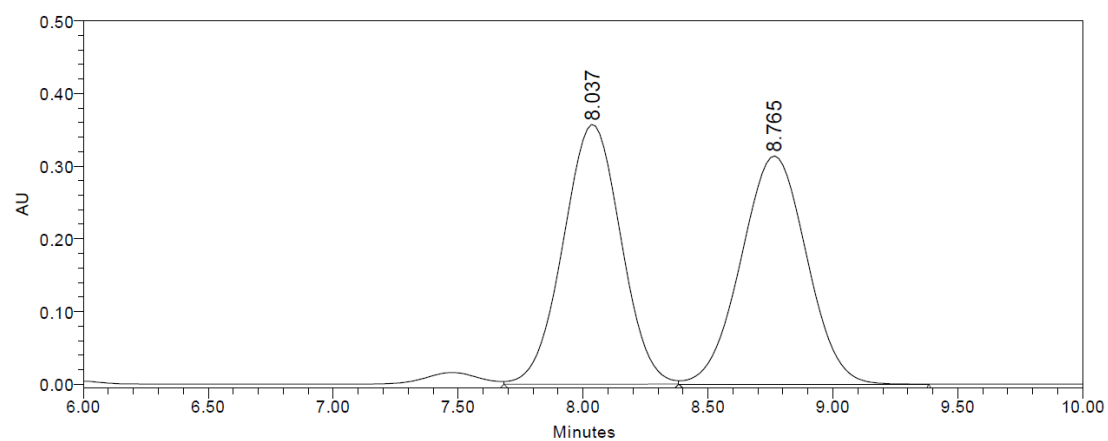
	RT	Area	% Area	Height
1	10.619	1153302	13.37	42225
2	13.126	7473245	86.63	201540

NMR Spectra and HPLC Chromatographs of **4aj**

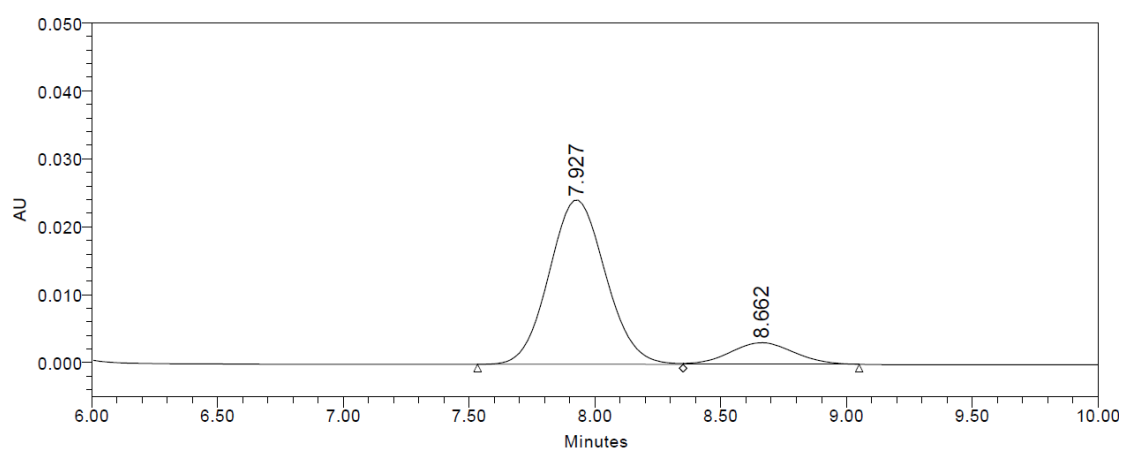


cy4-81



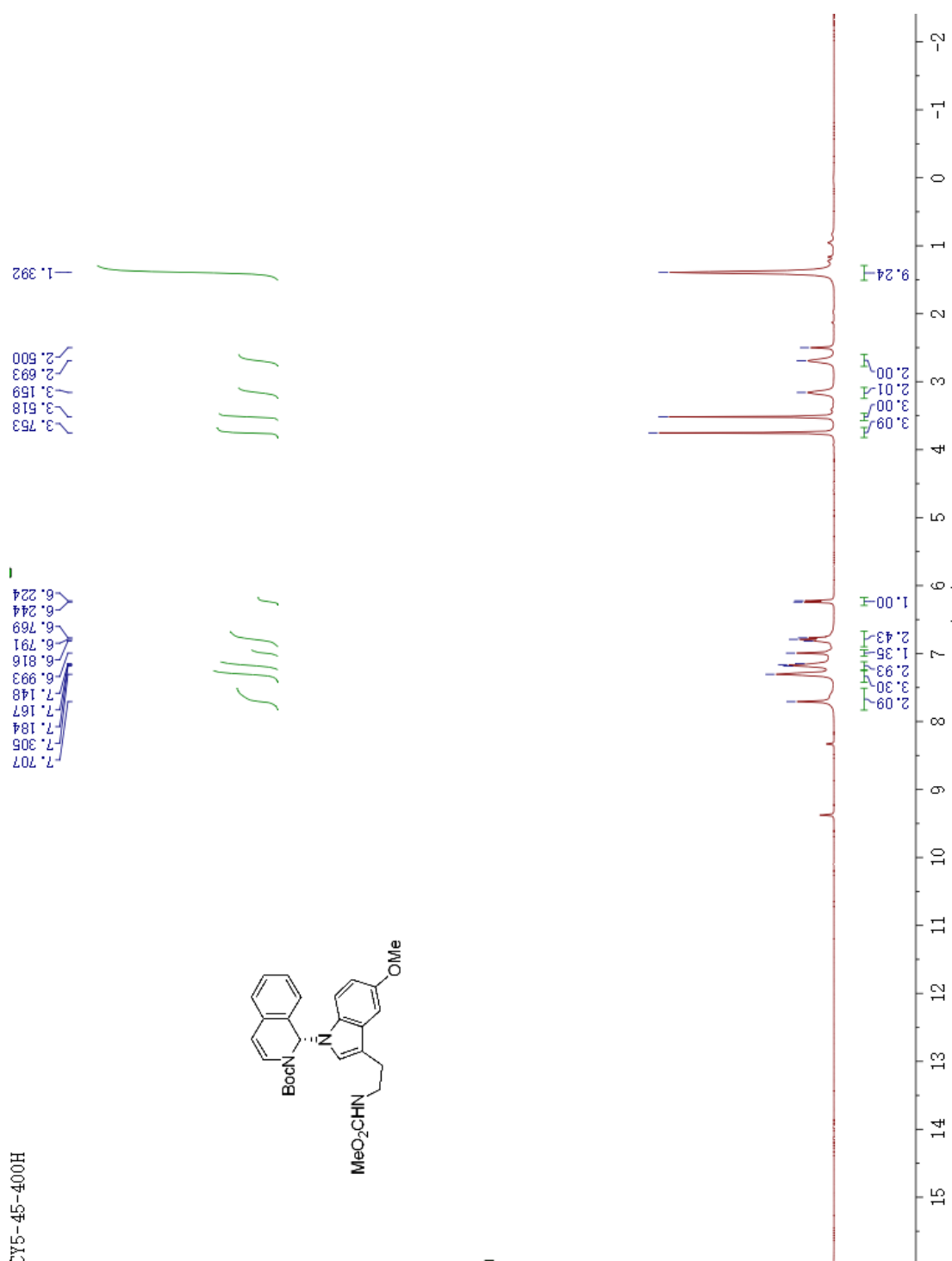


	RT	Area	% Area	Height
1	8.037	5737106	50.04	357476
2	8.765	5728152	49.96	313869

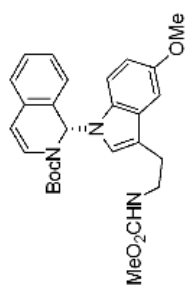


	RT	Area	% Area	Height
1	7.927	377744	87.05	24213
2	8.662	56219	12.95	3184

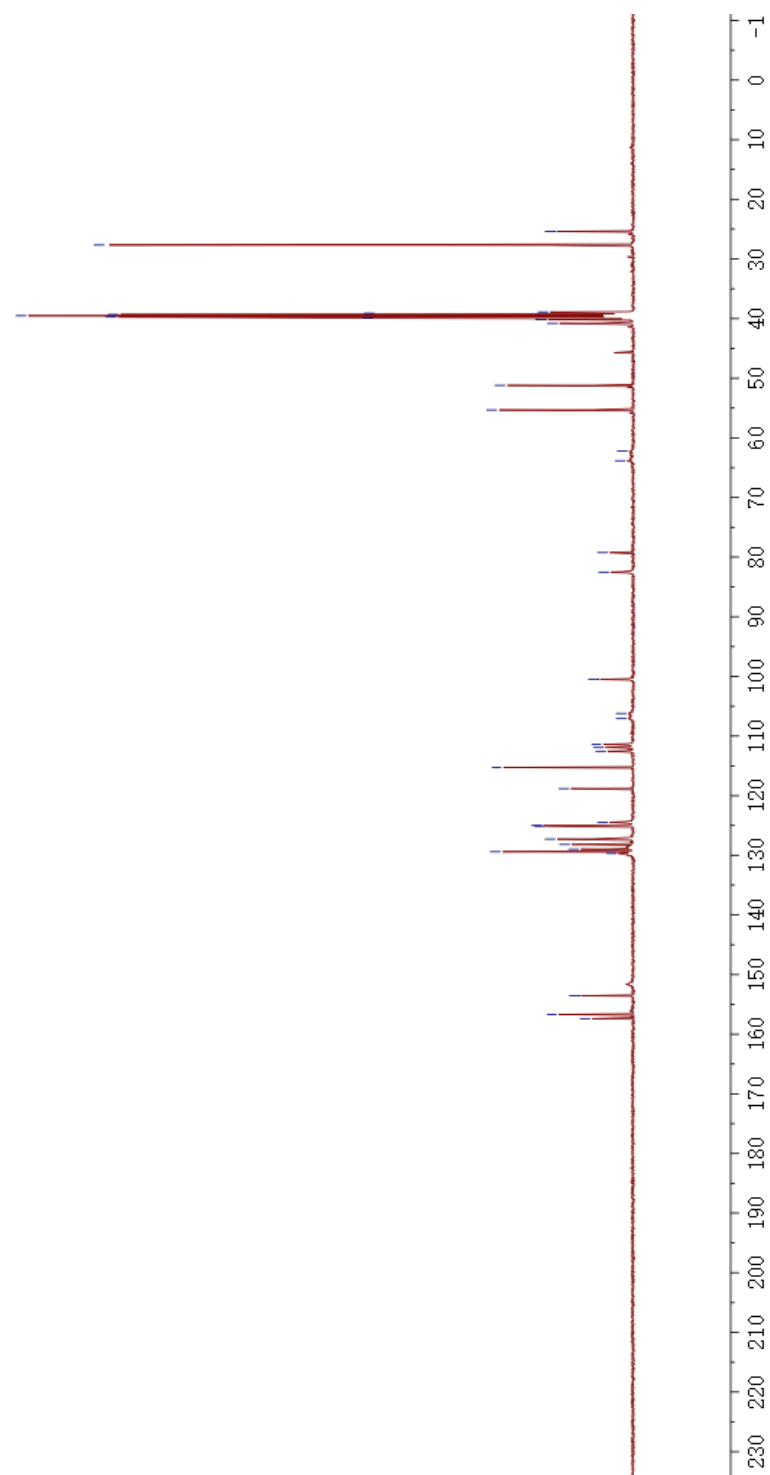
NMR Spectra and HPLC Chromatographs of **4ak**

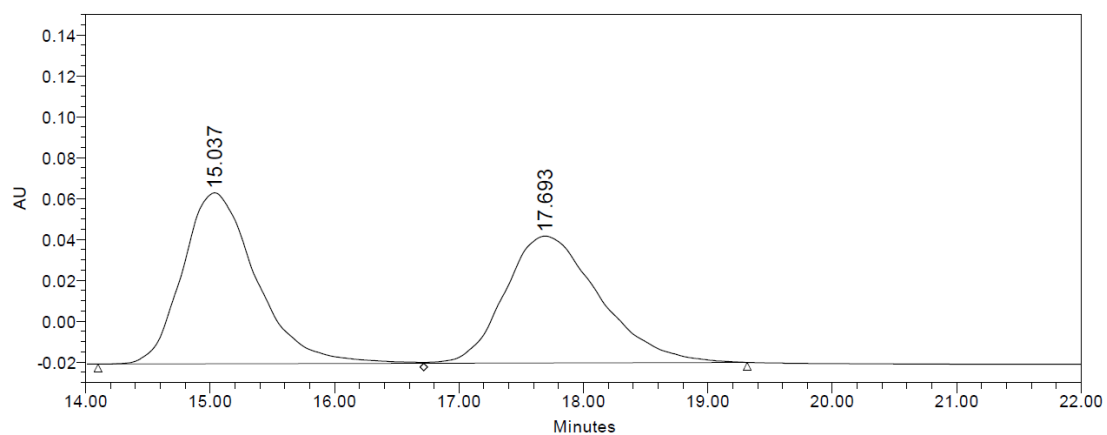


7Y5-45-400H

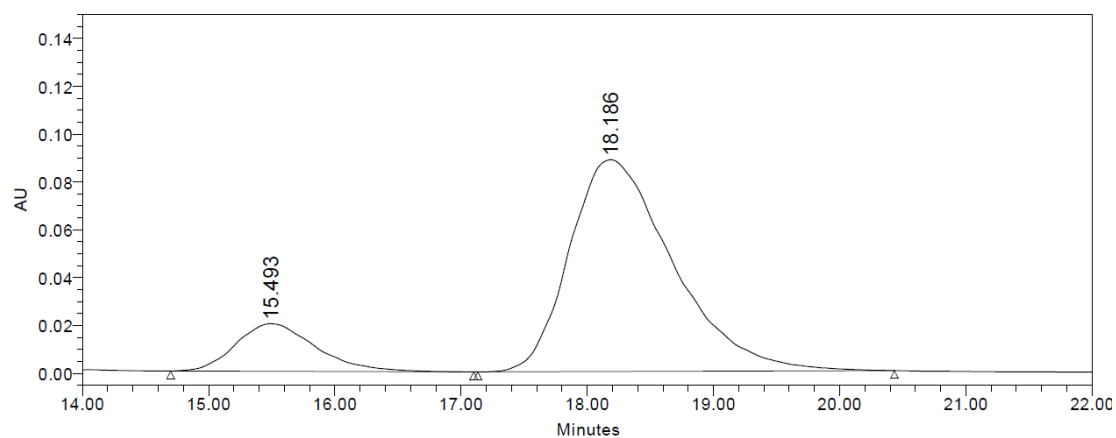


157.392
156.893
153.550
129.673
129.401
128.985
128.182
127.285
125.122
125.000
124.451
118.818
115.267
112.552
111.915
111.402
107.071
106.222
100.503
82.518
79.232
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62.233
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51.205
40.146
39.937
39.728
39.520
39.311
27.888
25.383



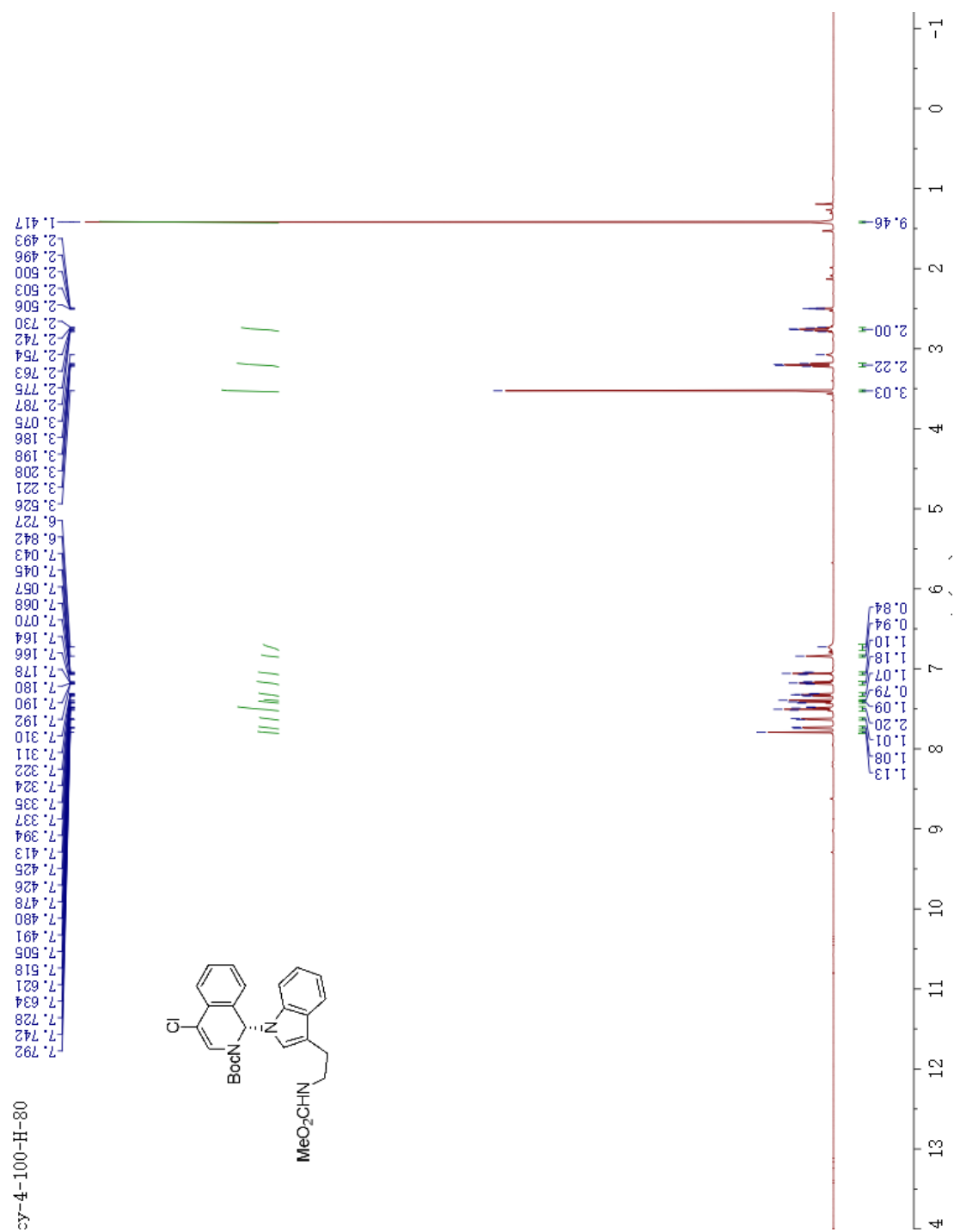


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1	15.037	3441649	51.29	83633
2	17.693	3269130	48.71	62070

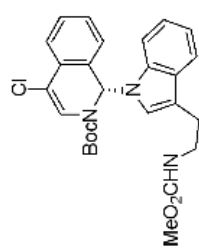


	RT	Area	% Area	Height
1	15.493	874163	14.78	19874
2	18.186	5041311	85.22	88586

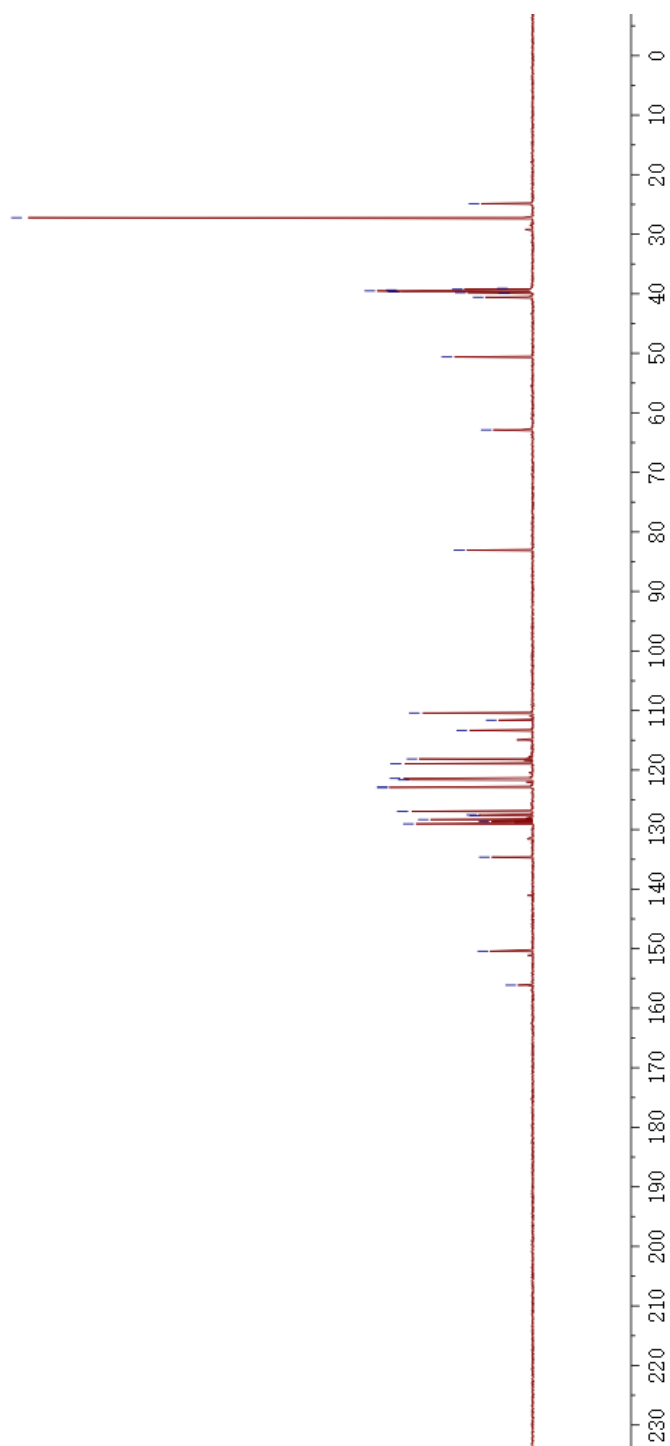
NMR Spectra and HPLC Chromatographs of **4ba**

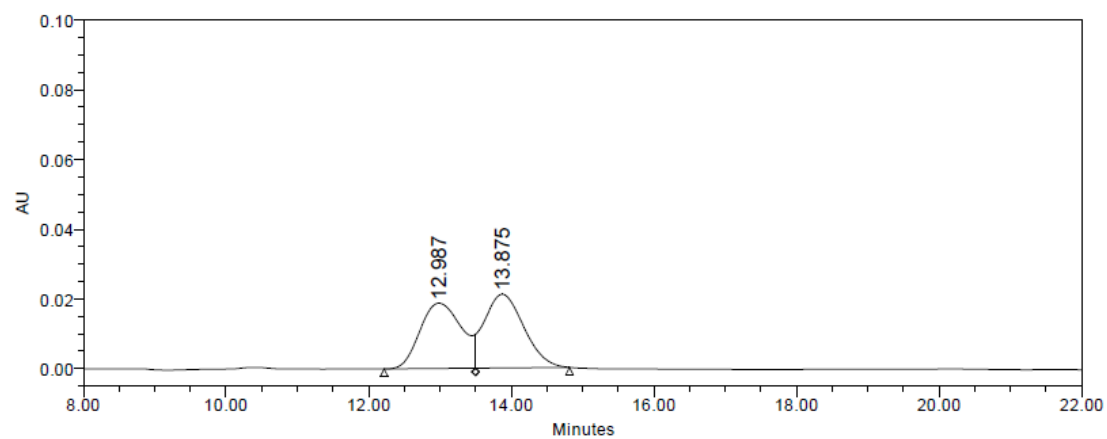


cy-4-100-C-80

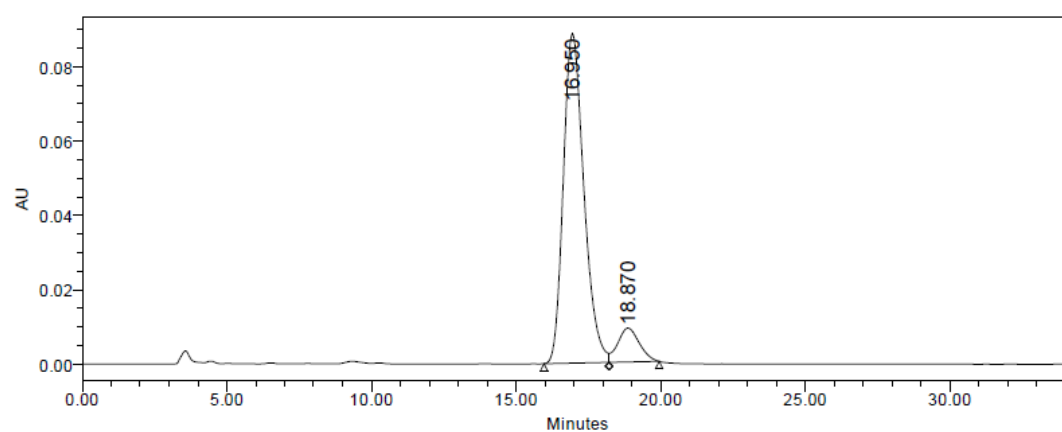


156.131
150.418
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127.647
127.537
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121.403
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24.861



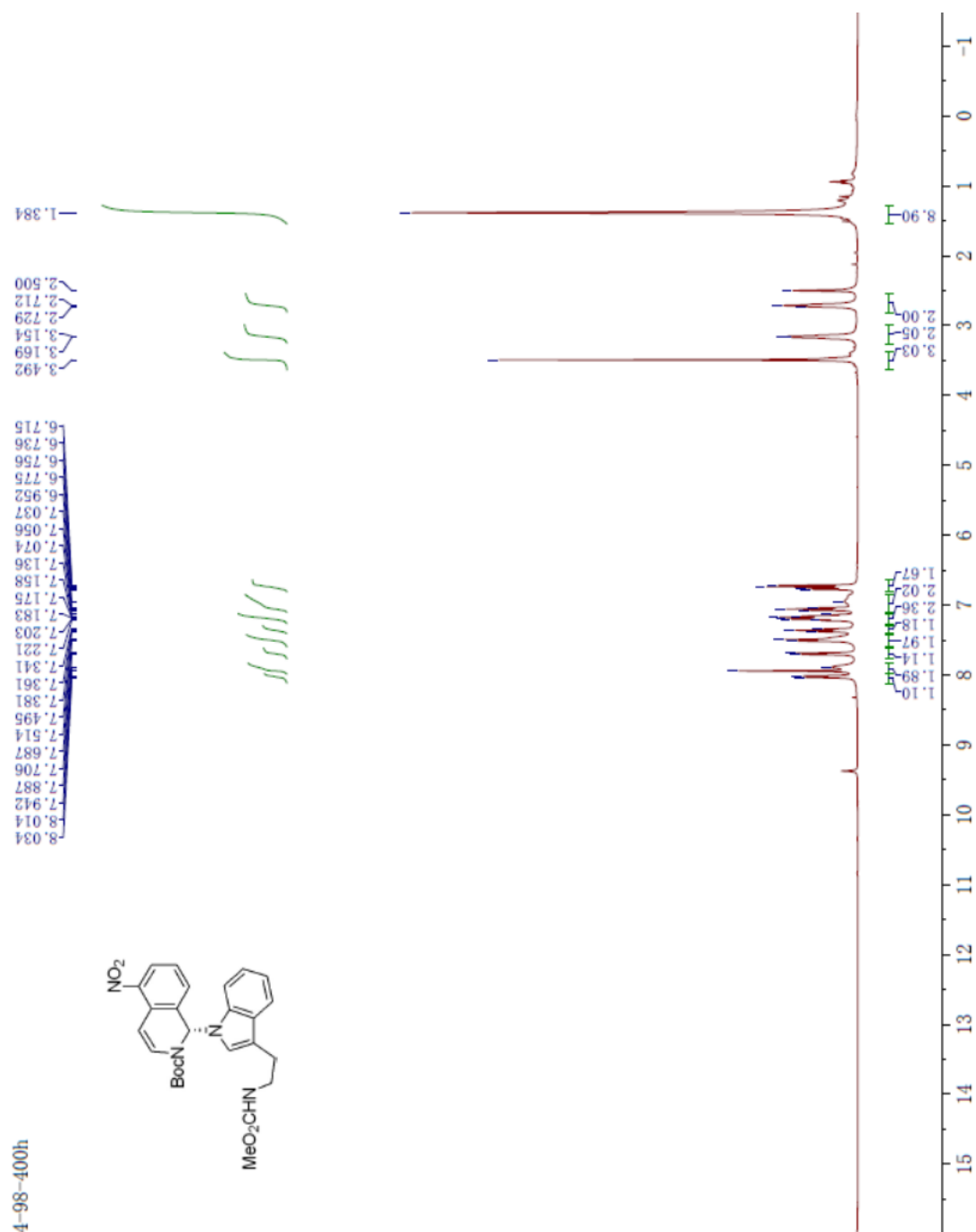


	RT	Area	% Area	Height
1	12.987	764861	48.55	18747
2	13.875	810402	51.45	21157

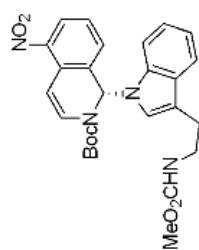


	RT	Area	% Area	Height
1	16.950	4377673	90.22	88590
2	18.870	474366	9.78	9131

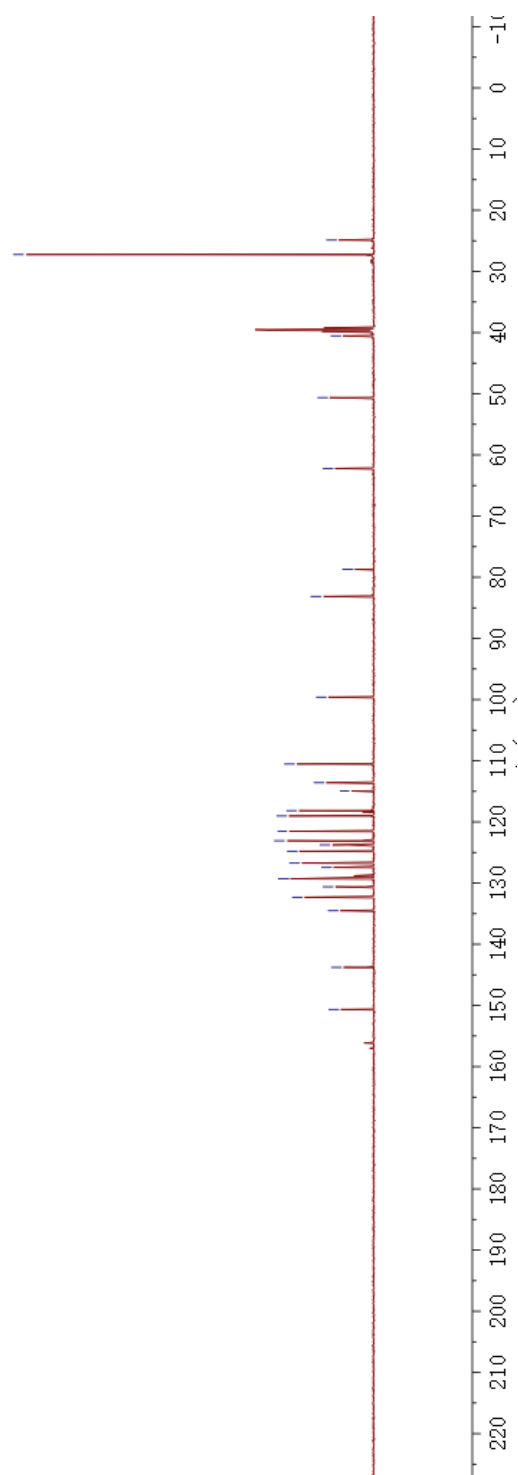
NMR Spectra and HPLC Chromatographs of **4ca**

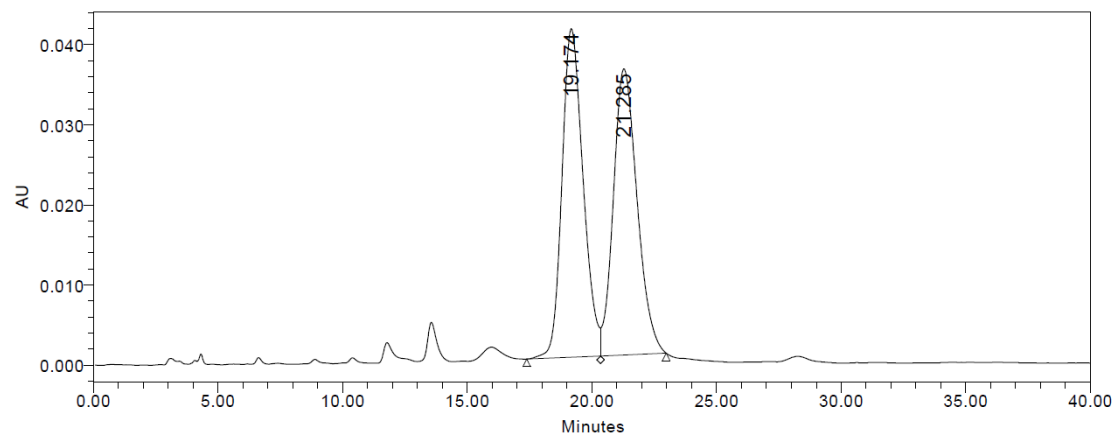


4-98-C-80

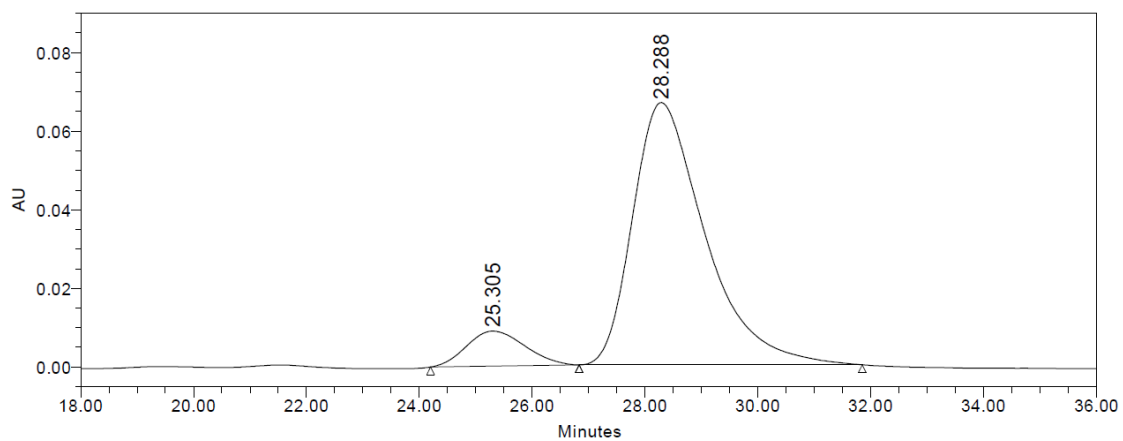


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124.780
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99.592
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78.710
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50.628
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	RT	Area	% Area	Height
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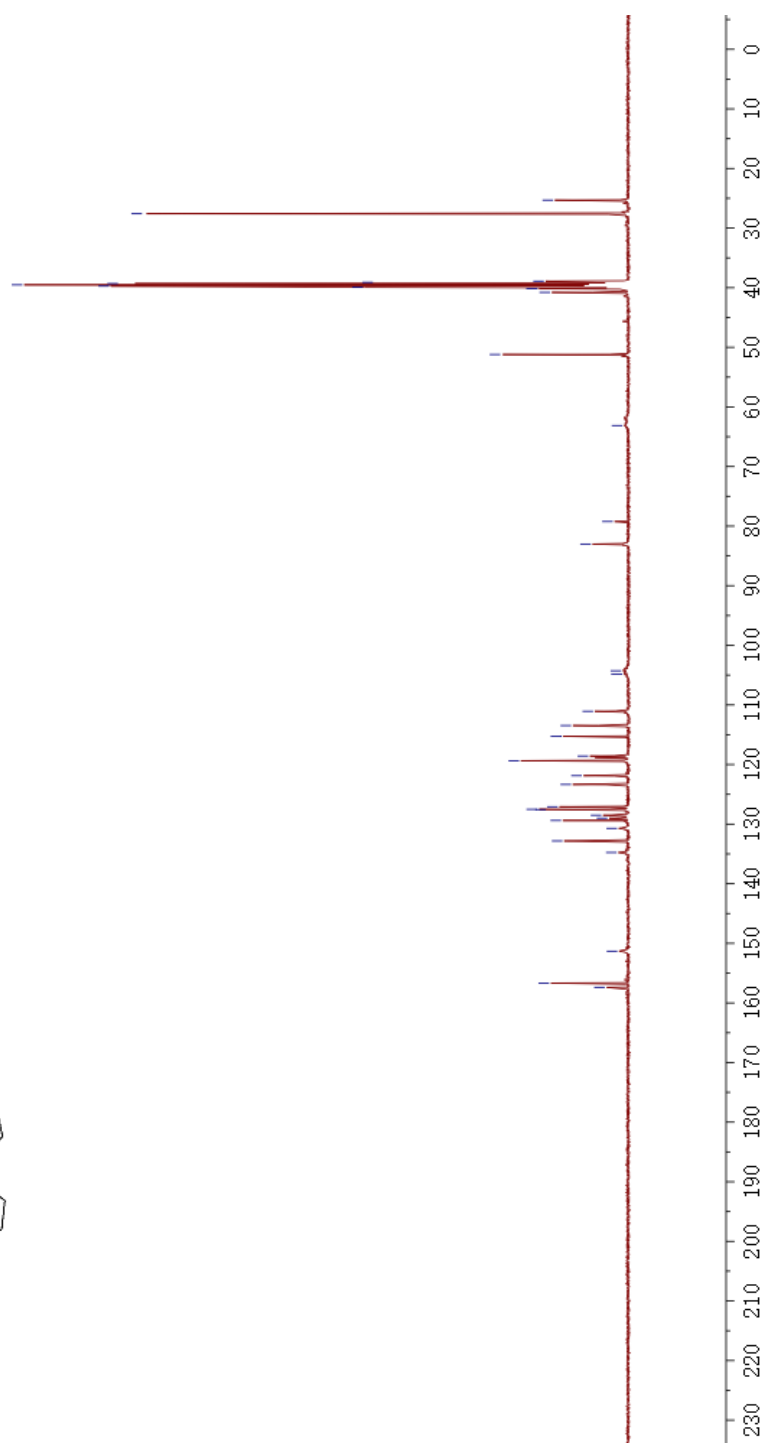
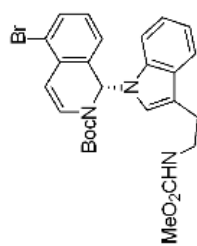
	RT	Area	% Area	Height
1	25.305	638719	9.69	8908
2	28.288	5949850	90.31	66739

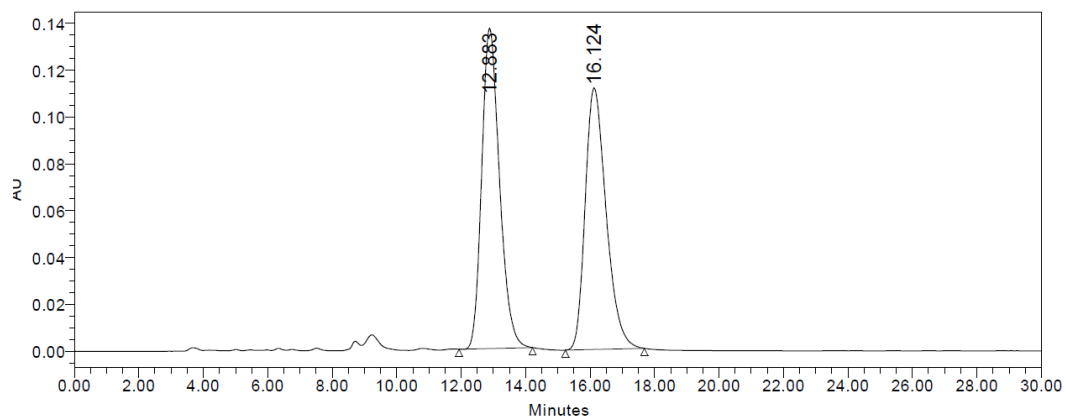
NMR Spectra and HPLC Chromatographs of **4da**



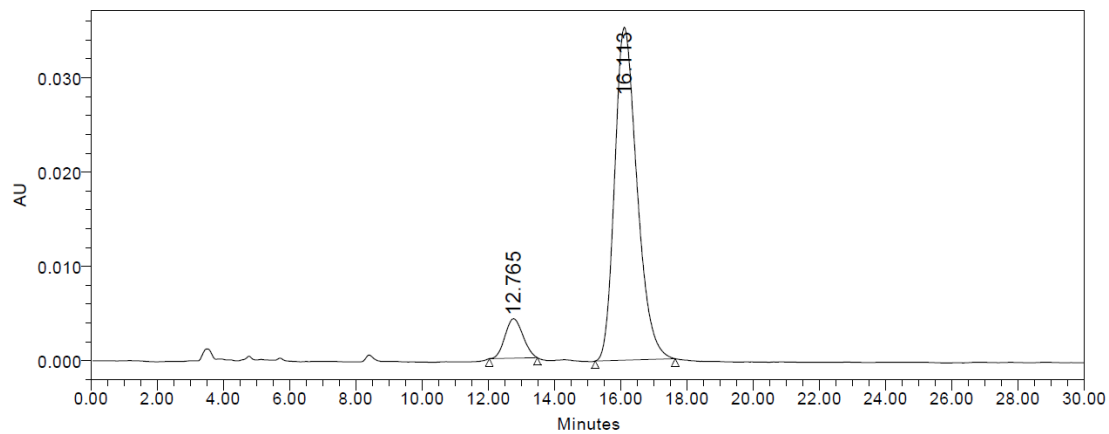
5-11 -400c

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127.080
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27.590
25.305



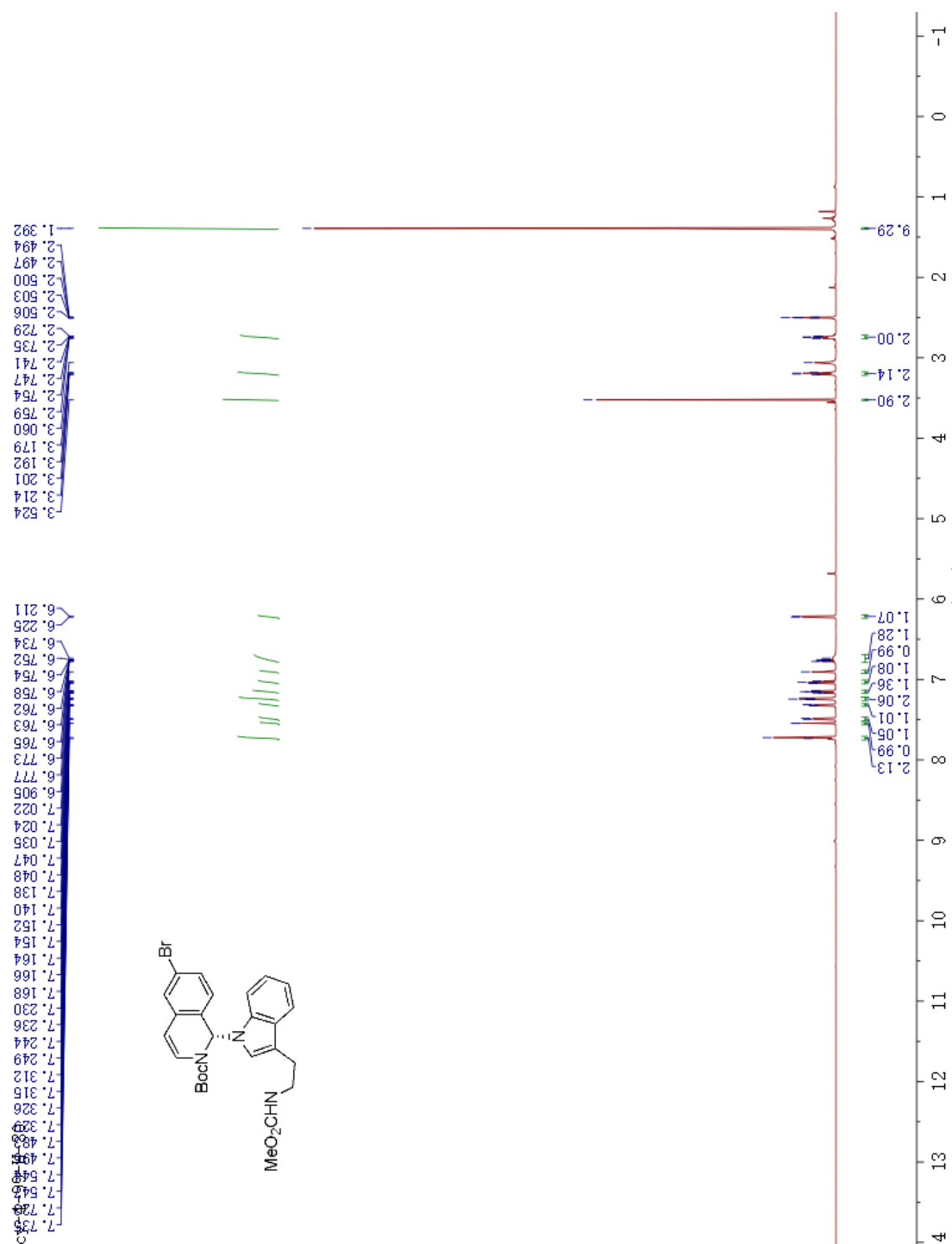


	RT	Area	% Area	Height
1	12.883	5245550	50.94	136702
2	16.124	5051598	49.06	111647

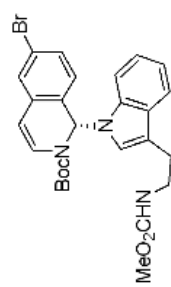


	RT	Area	% Area	Height
1	12.765	156800	8.64	4170
2	16.113	1657335	91.36	35263

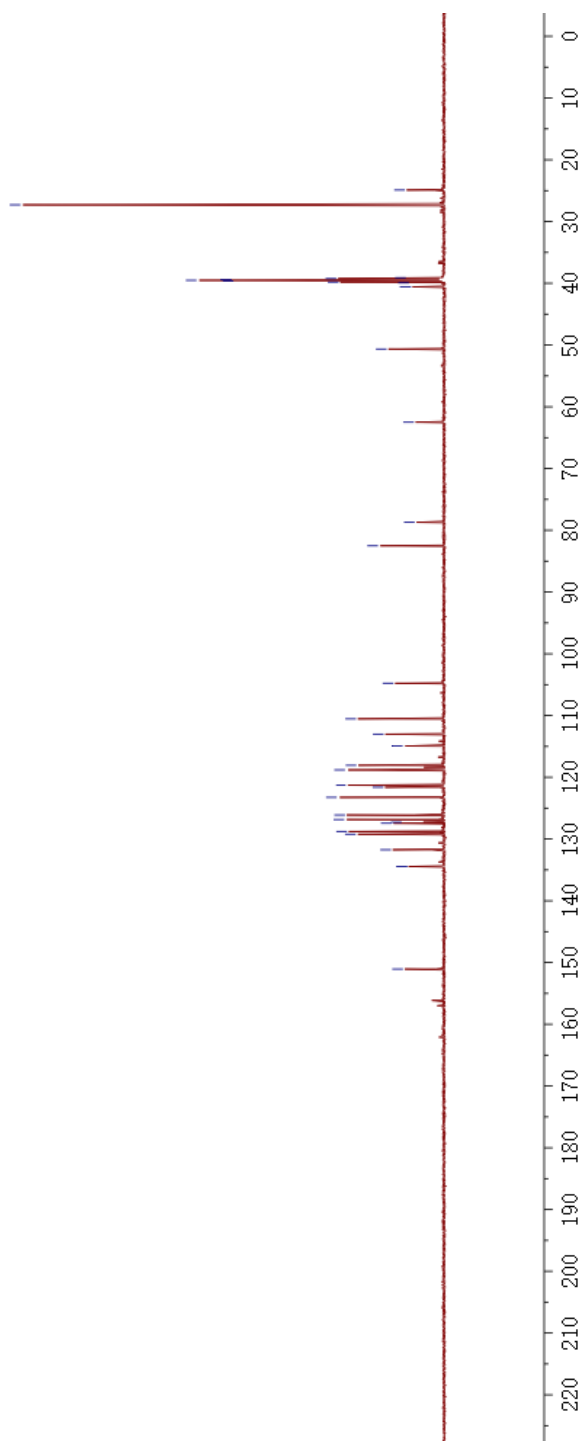
NMR Spectra and HPLC Chromatographs of **4ea**

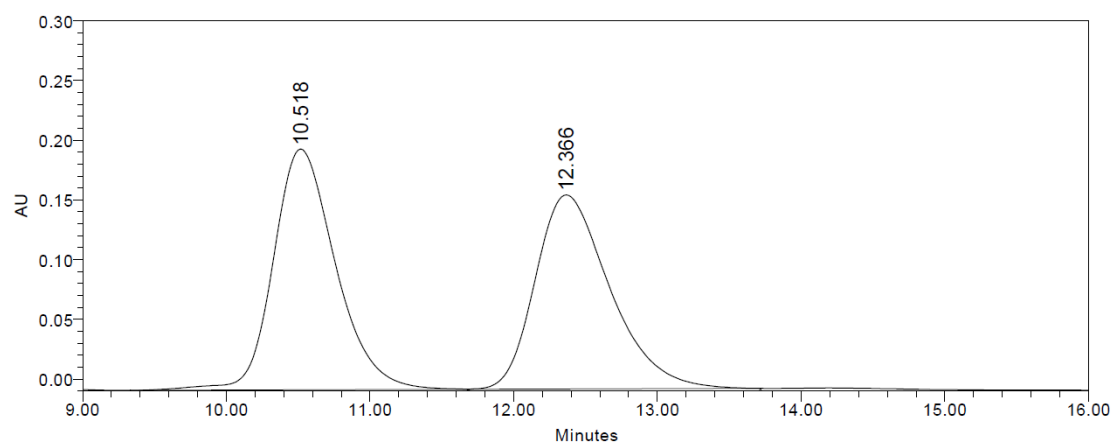


4-99-C-80

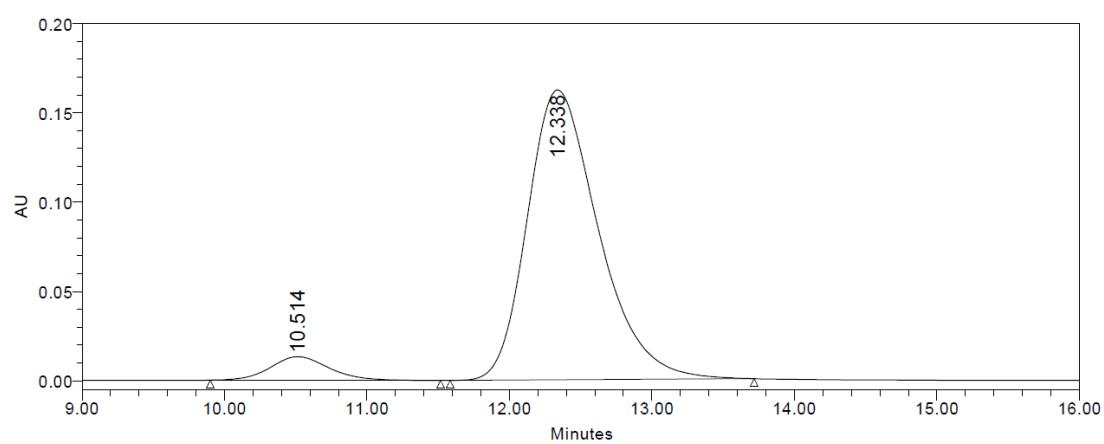


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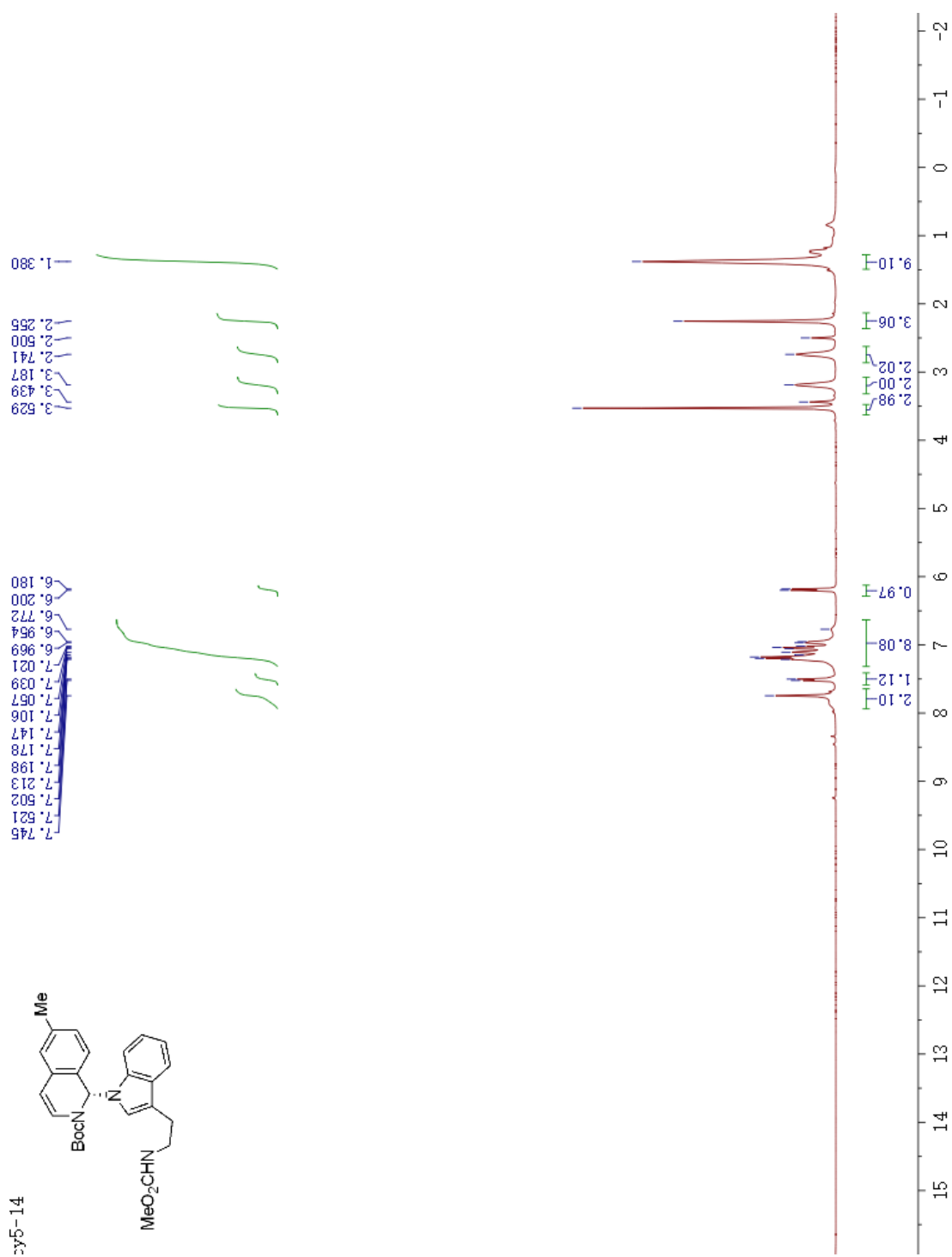


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1	10.518	6084908	50.90	201713
2	12.366	5870692	49.10	162556

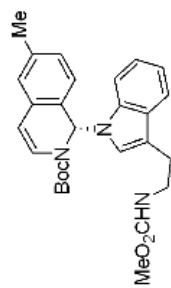


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1	10.514	379083	6.31	13212
2	12.338	5624635	93.69	162255

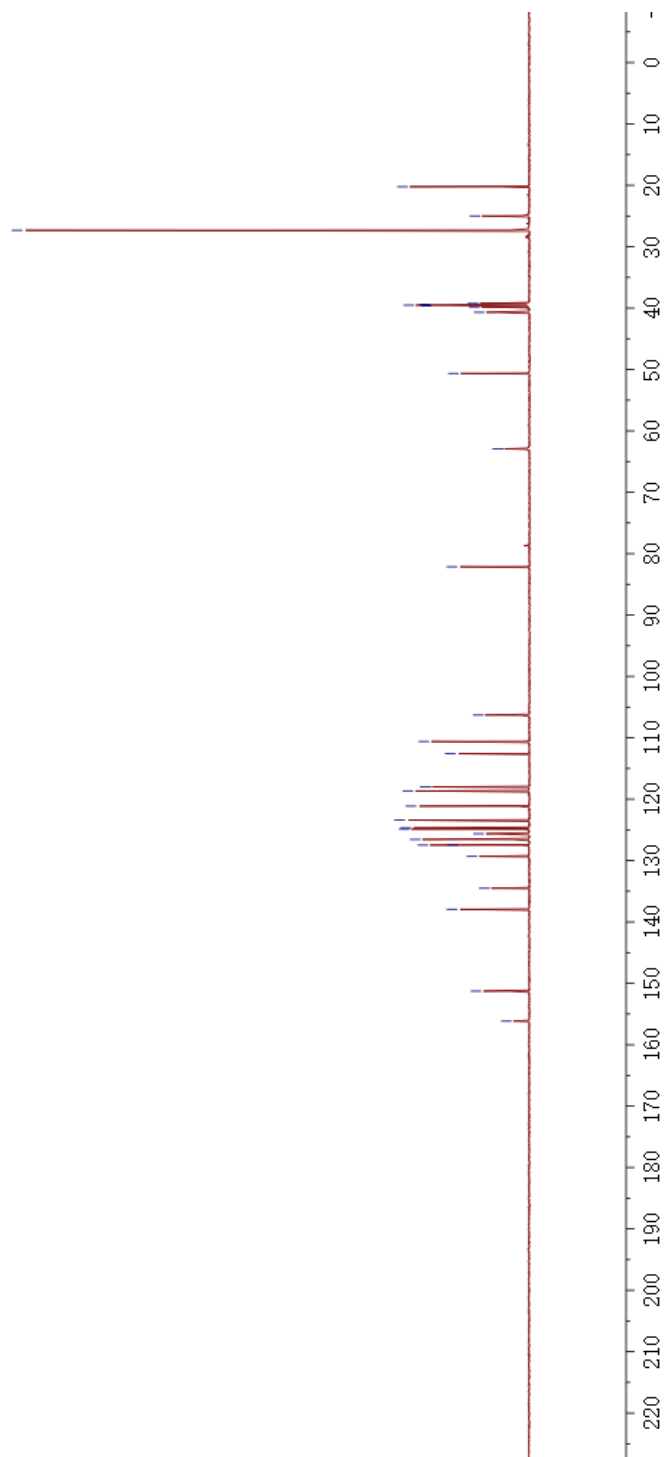
NMR Spectra and HPLC Chromatographs of **4fa**

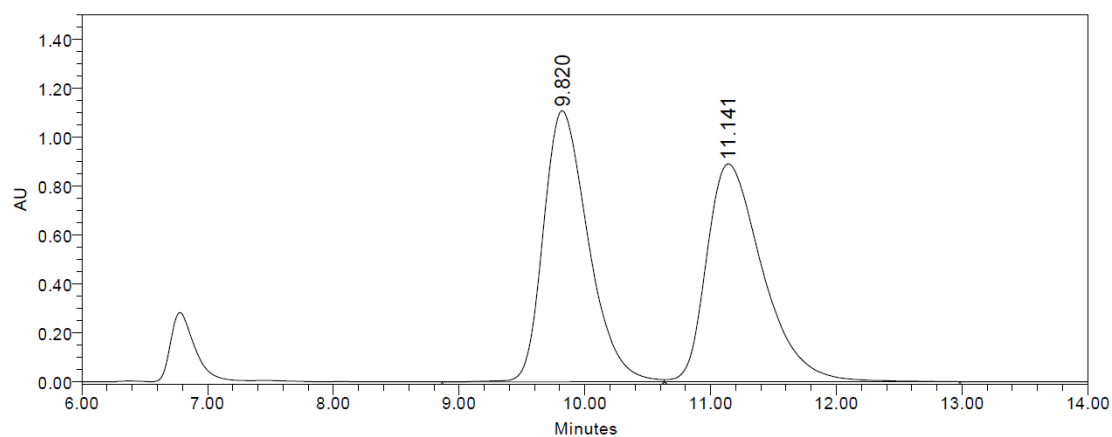


5-14-C-80

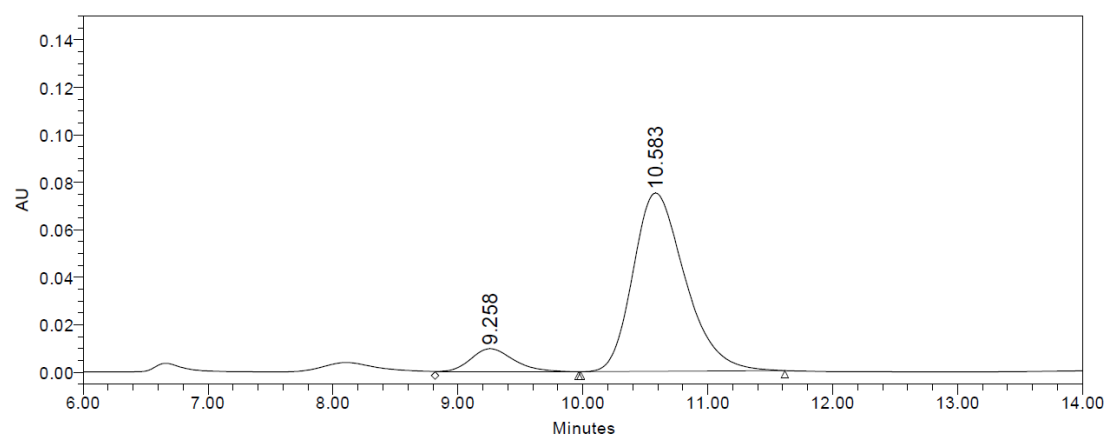


156.165
151.269
137.935
134.516
129.323
127.483
127.460
126.557
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124.880
124.889
123.420
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24.984
20.222



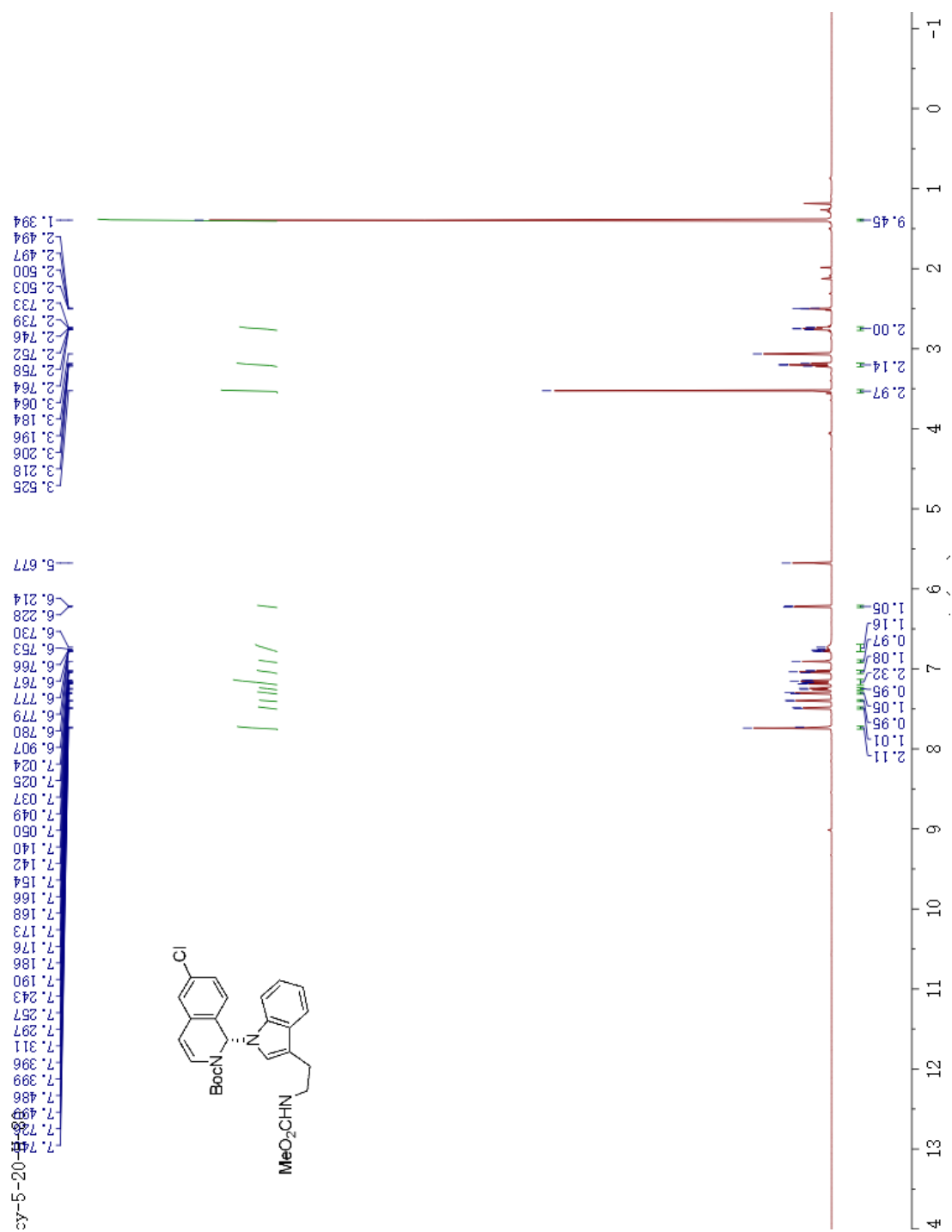


	RT	Area	% Area	Height
1	9.820	27383216	49.90	1108668
2	11.141	27487723	50.10	891571

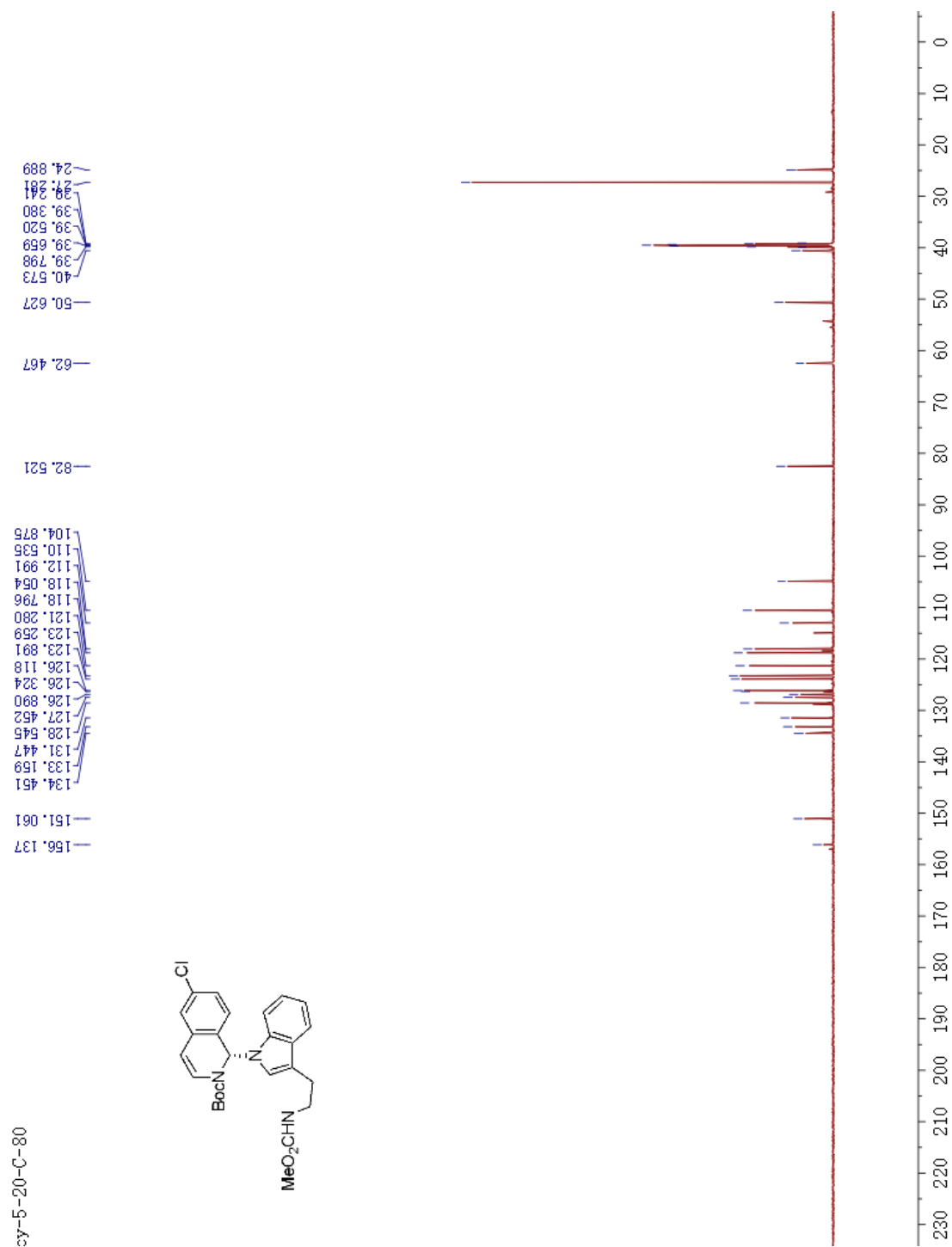
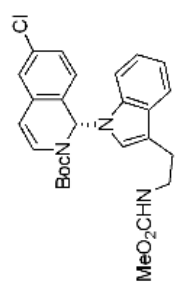


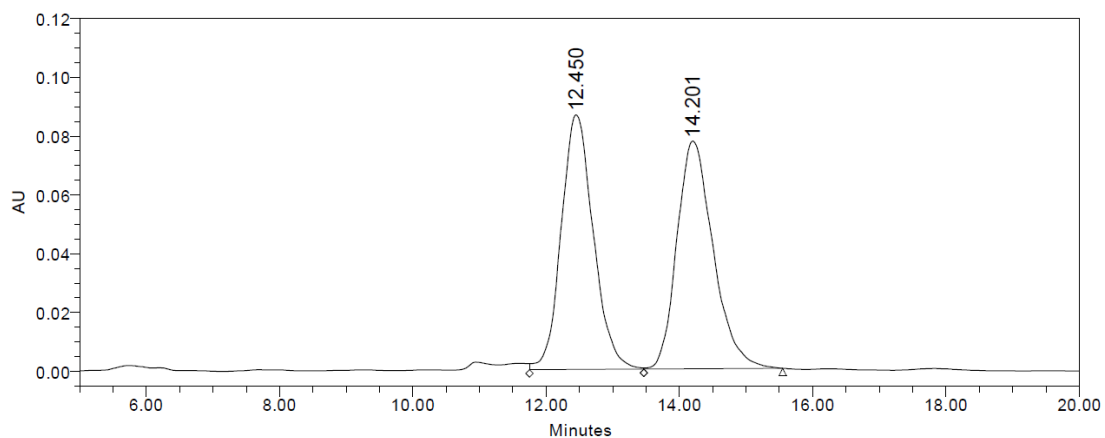
	RT	Area	% Area	Height
1	9.258	231373	9.61	9682
2	10.583	2177203	90.39	75142

NMR Spectra and HPLC Chromatographs of **4ga**

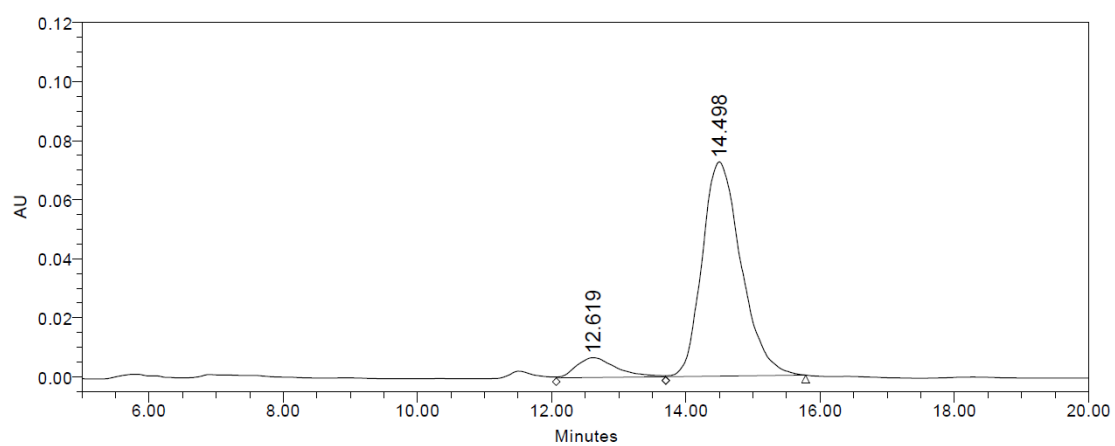


cy-5-20-C-80



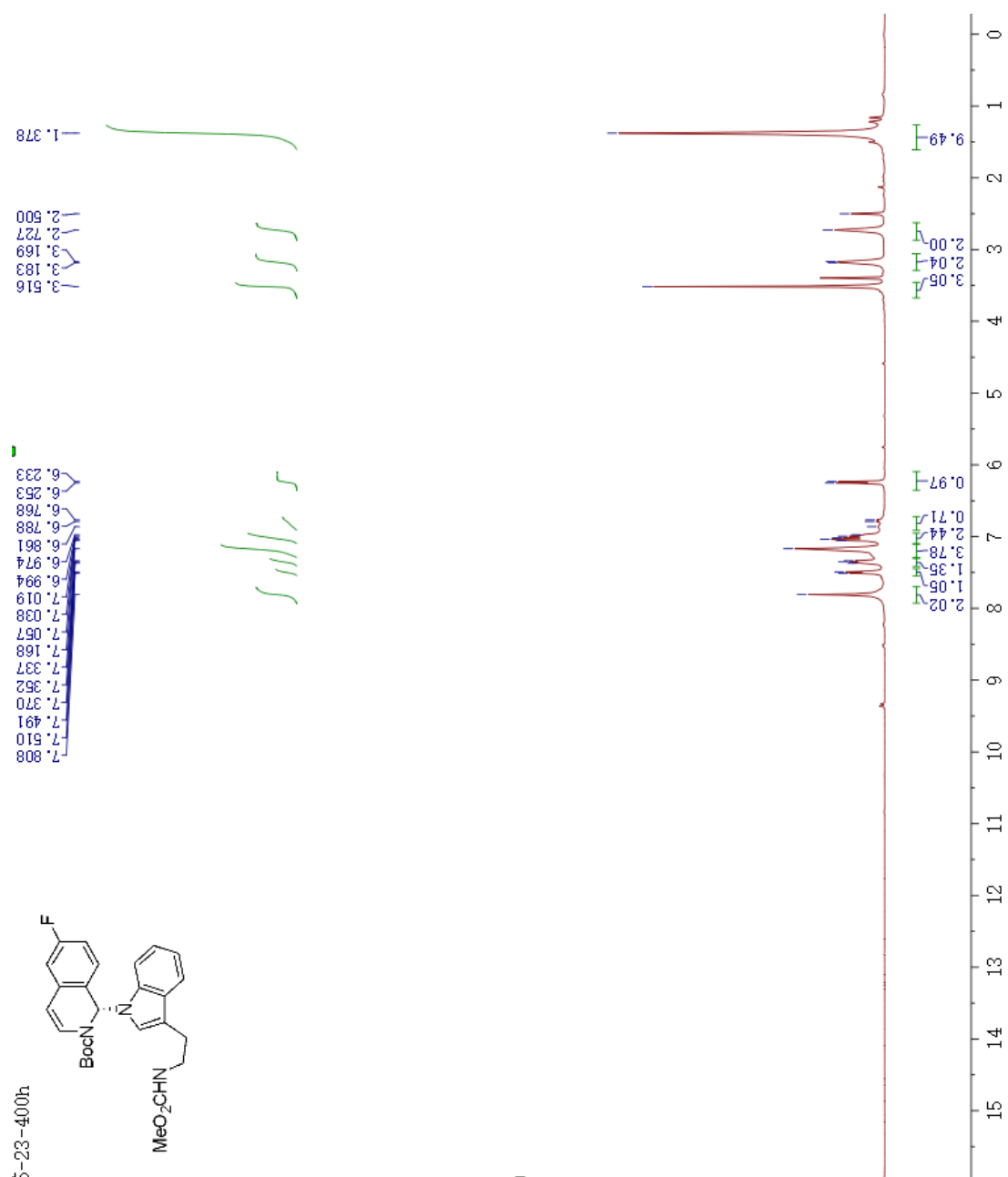


	RT	Area	% Area	Height
1	12.450	2902103	49.76	86537
2	14.201	2929747	50.24	77374

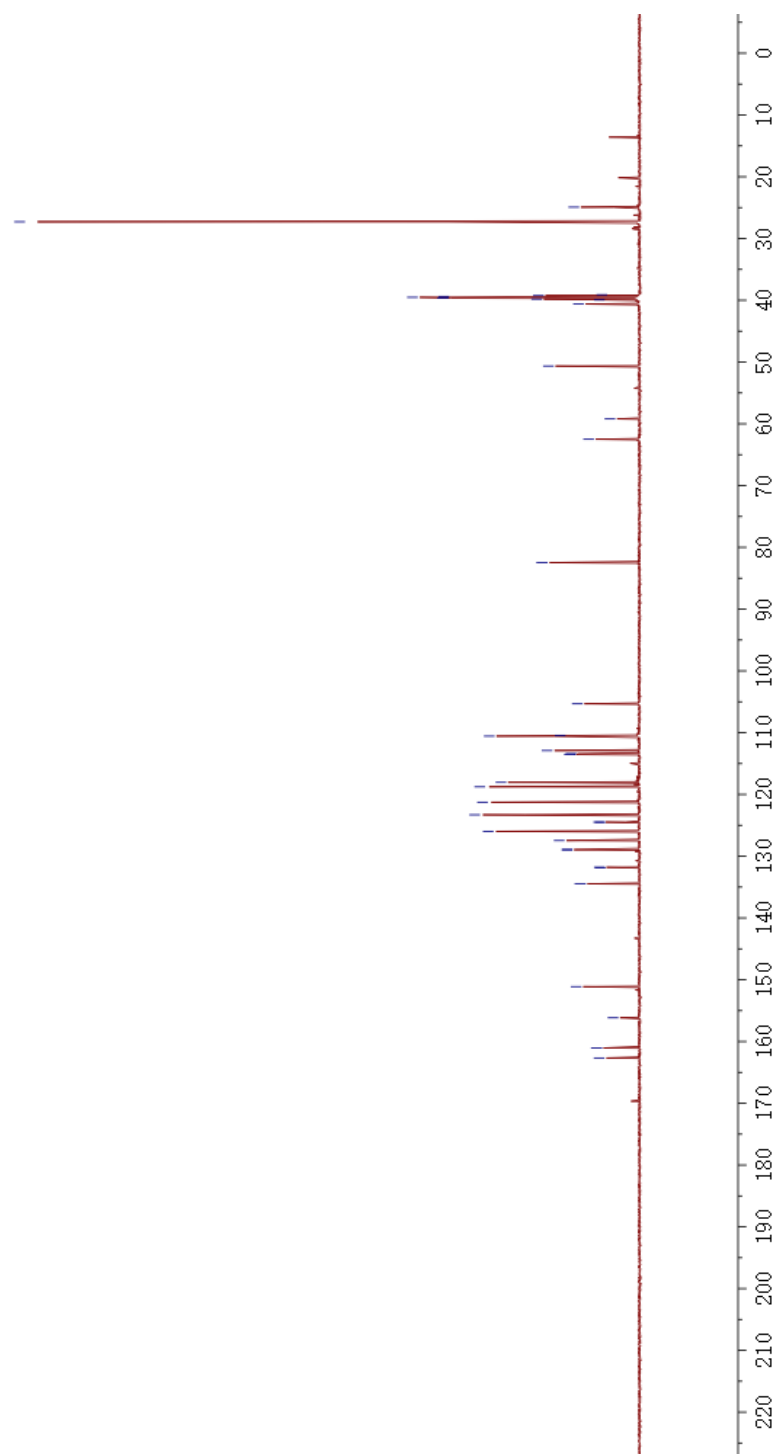
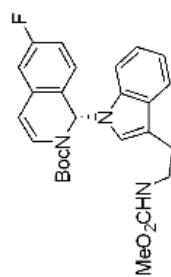


	RT	Area	% Area	Height
1	12.619	276191	8.63	6705
2	14.498	2925054	91.37	72528

NMR Spectra and HPLC Chromatographs of **4ha**

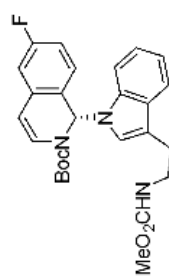


5-23-C-80

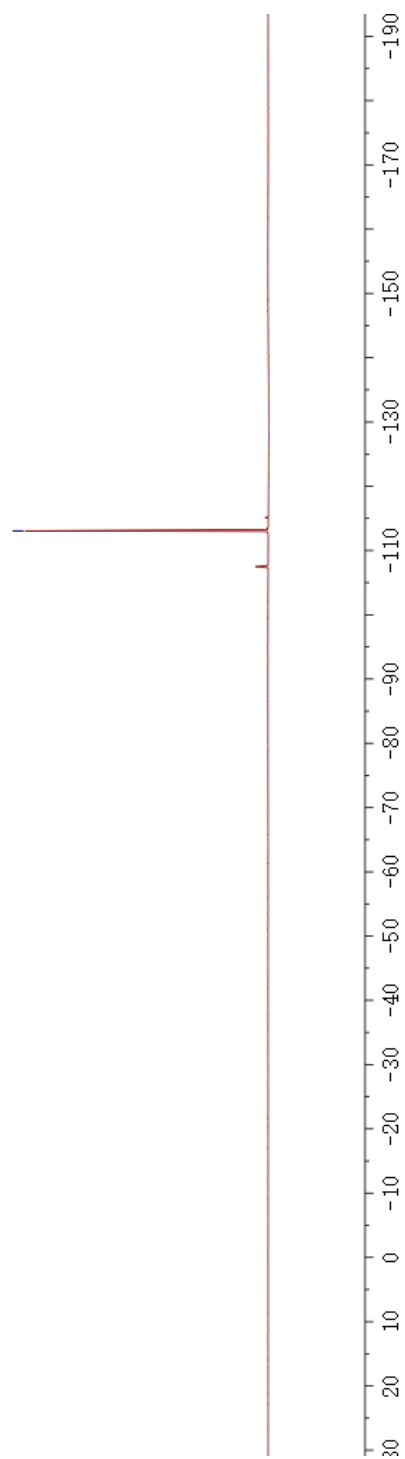


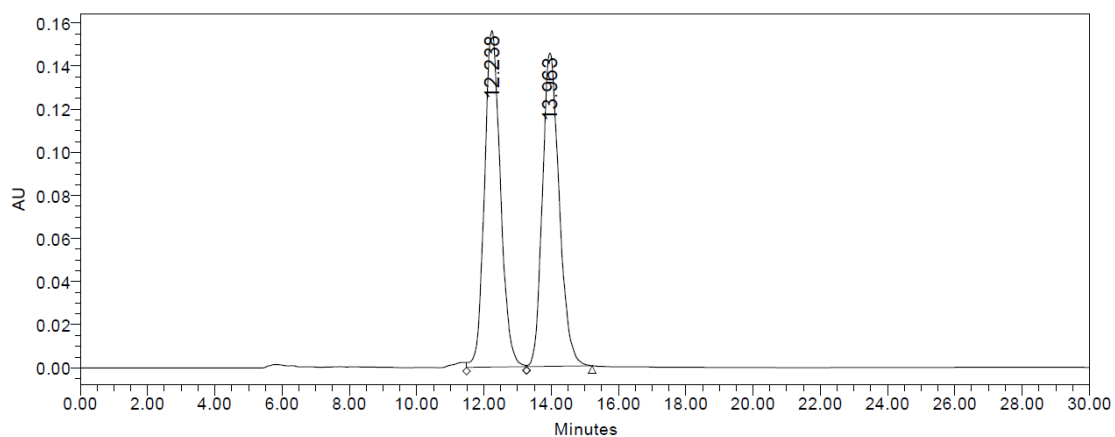
5-23 -600F-80

STANDARD PROTON PARAMETERS

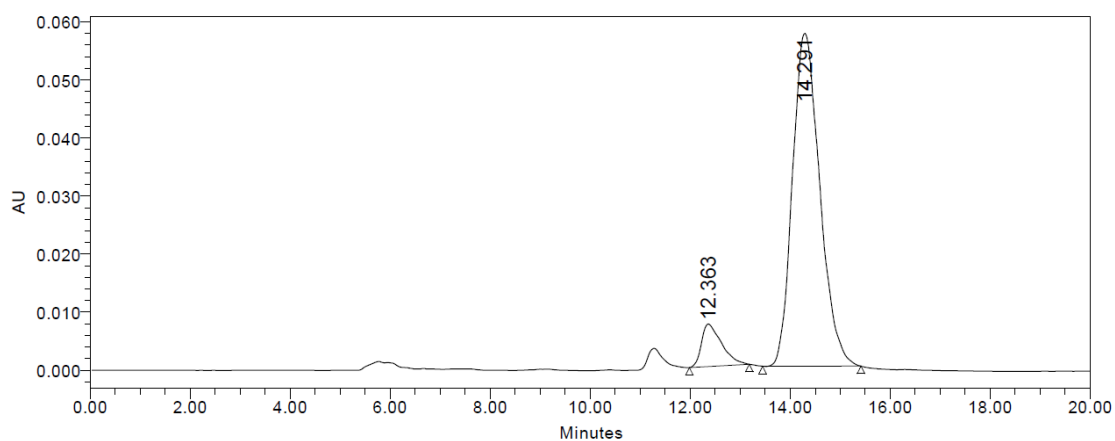


113.062
113.062



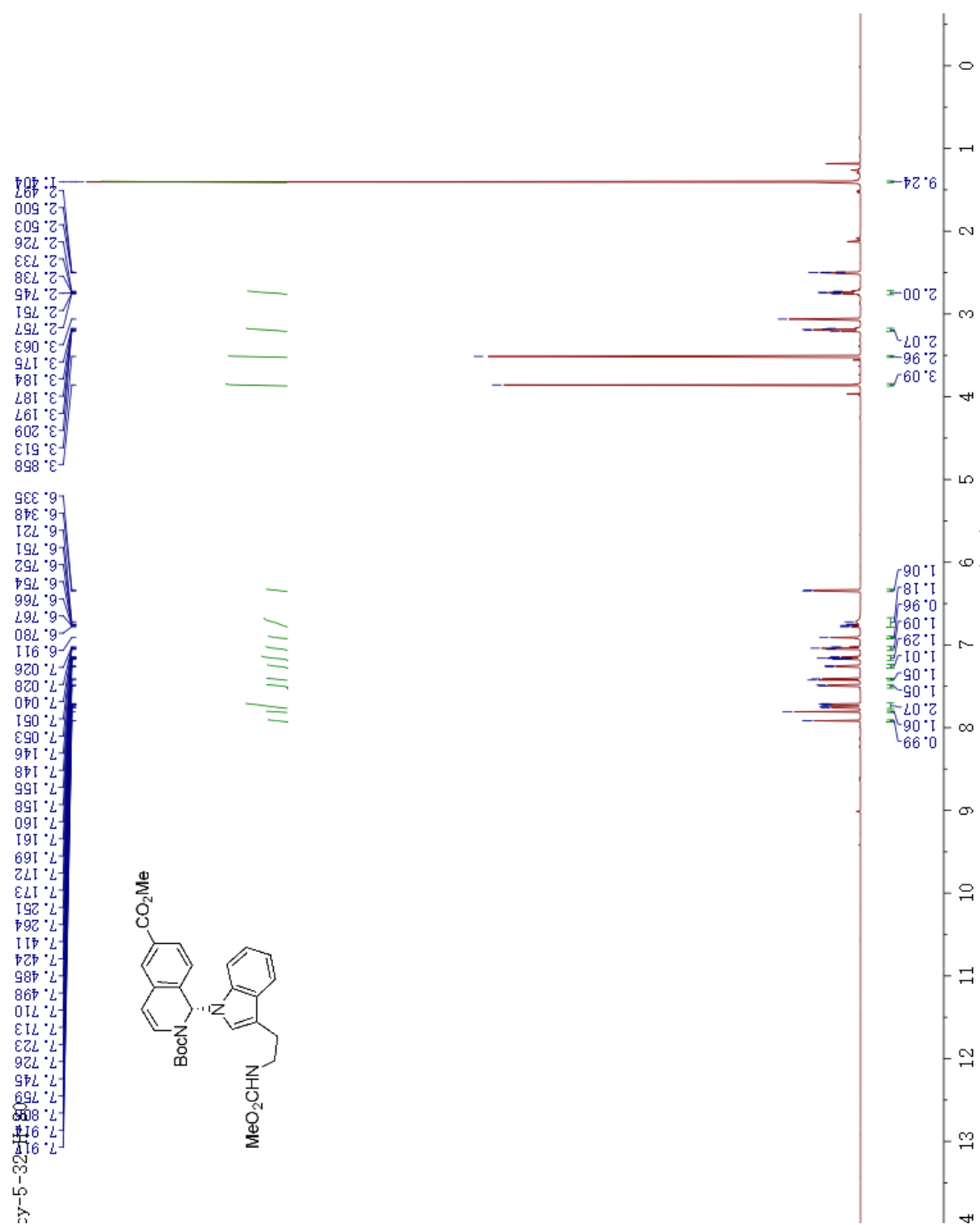


	RT	Area	% Area	Height
1	12.238	5154810	50.44	156009
2	13.963	5064423	49.56	145390

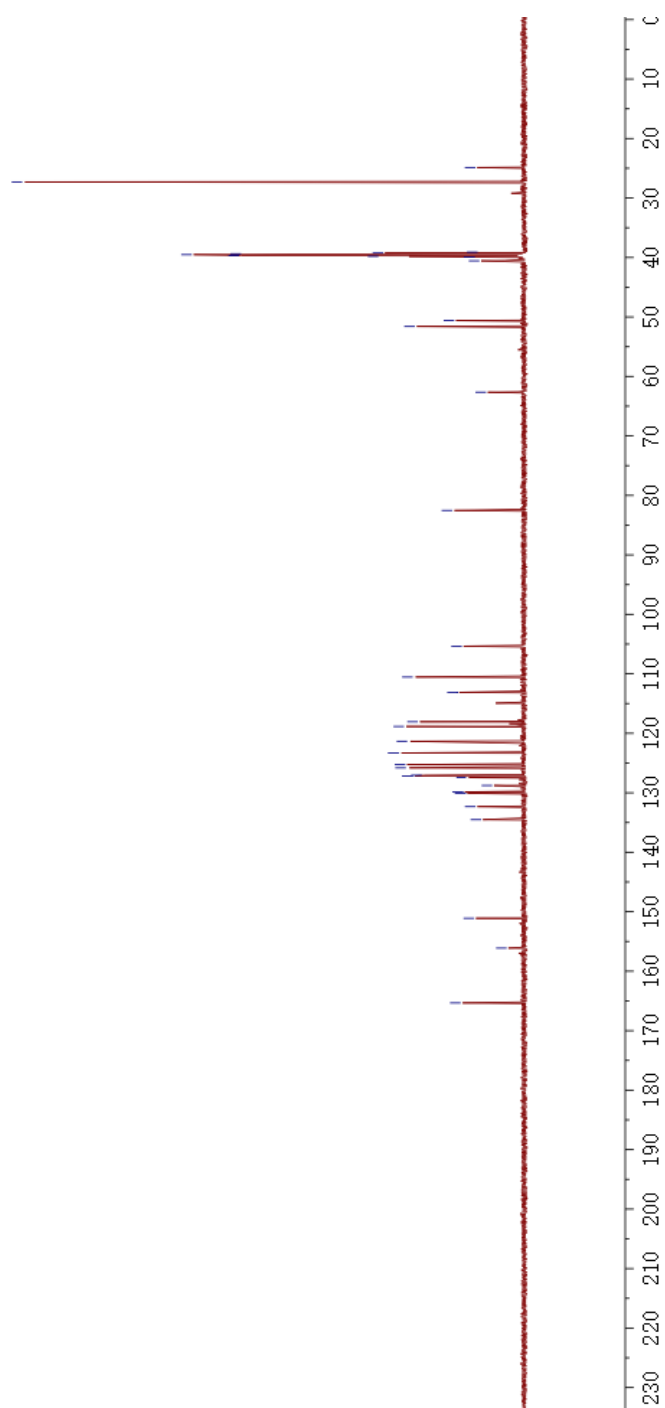
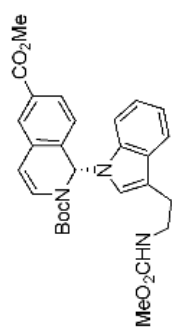
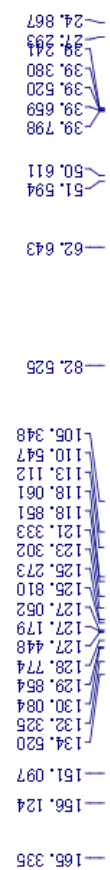


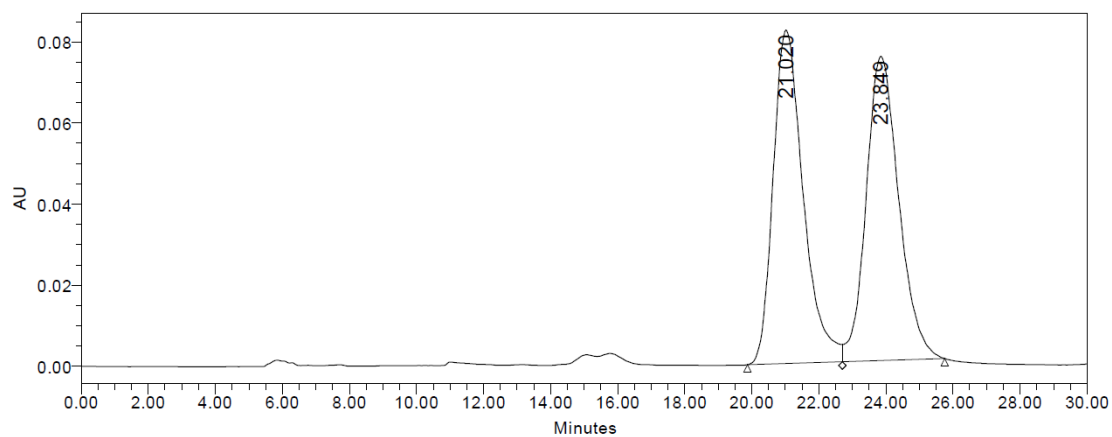
	RT	Area	% Area	Height
1	12.363	204107	8.57	7312
2	14.291	2178859	91.43	57259

NMR Spectra and HPLC Chromatographs of **4ia**

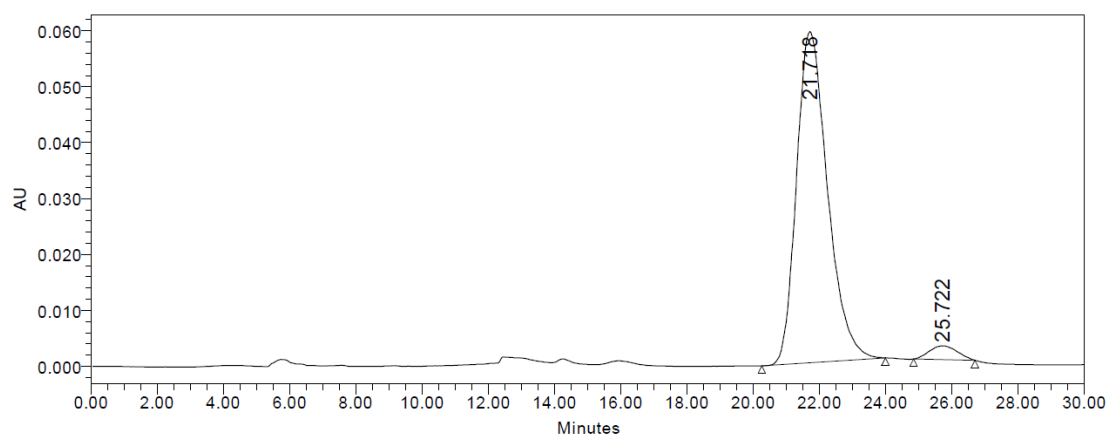


cy-5-32-C-80



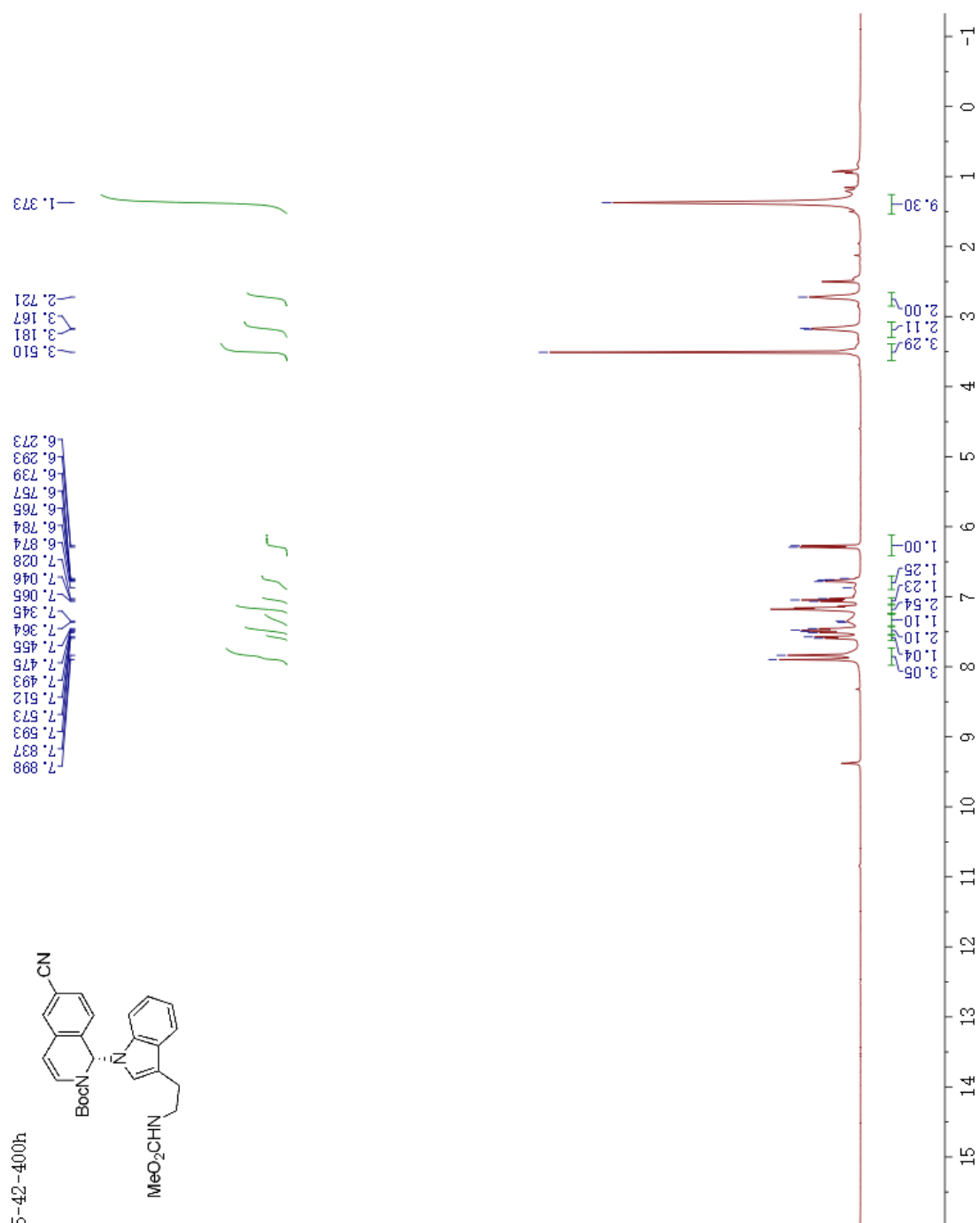


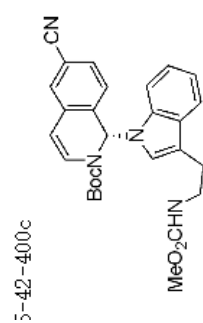
	RT	Area	% Area	Height
1	21.020	5114539	50.22	82180
2	23.849	5070176	49.78	75007



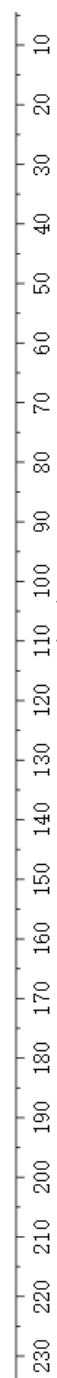
	RT	Area	% Area	Height
1	21.718	3846627	96.42	59144
2	25.722	142669	3.58	2445

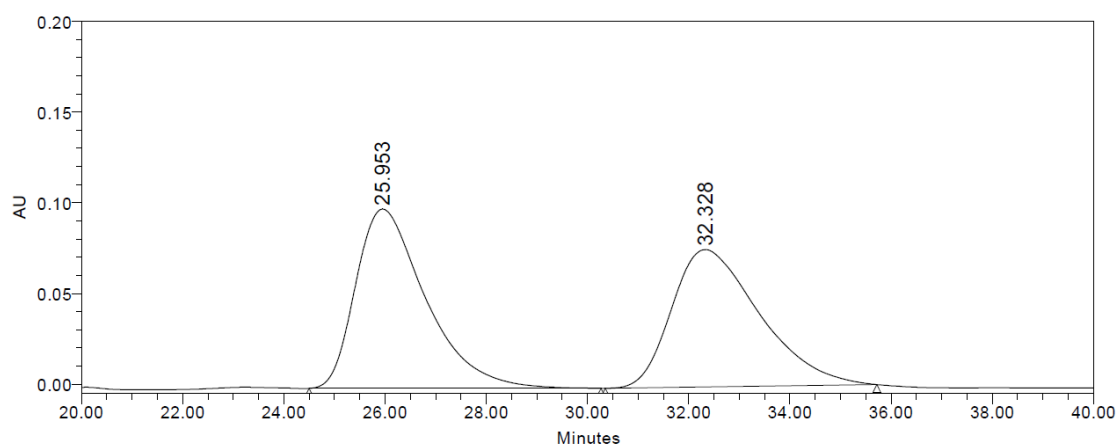
NMR Spectra and HPLC Chromatographs of **4ja**



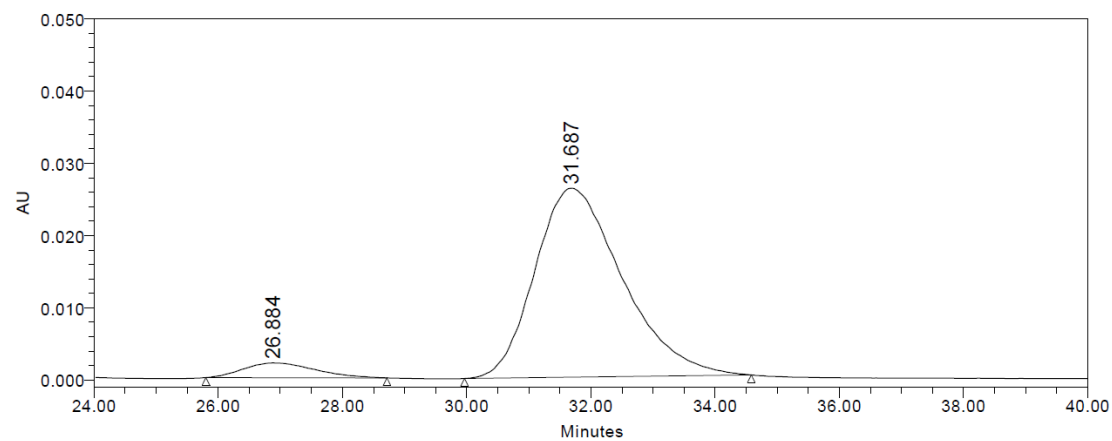


157.394
156.682
151.388
129.404
128.668
128.432
127.626
127.211
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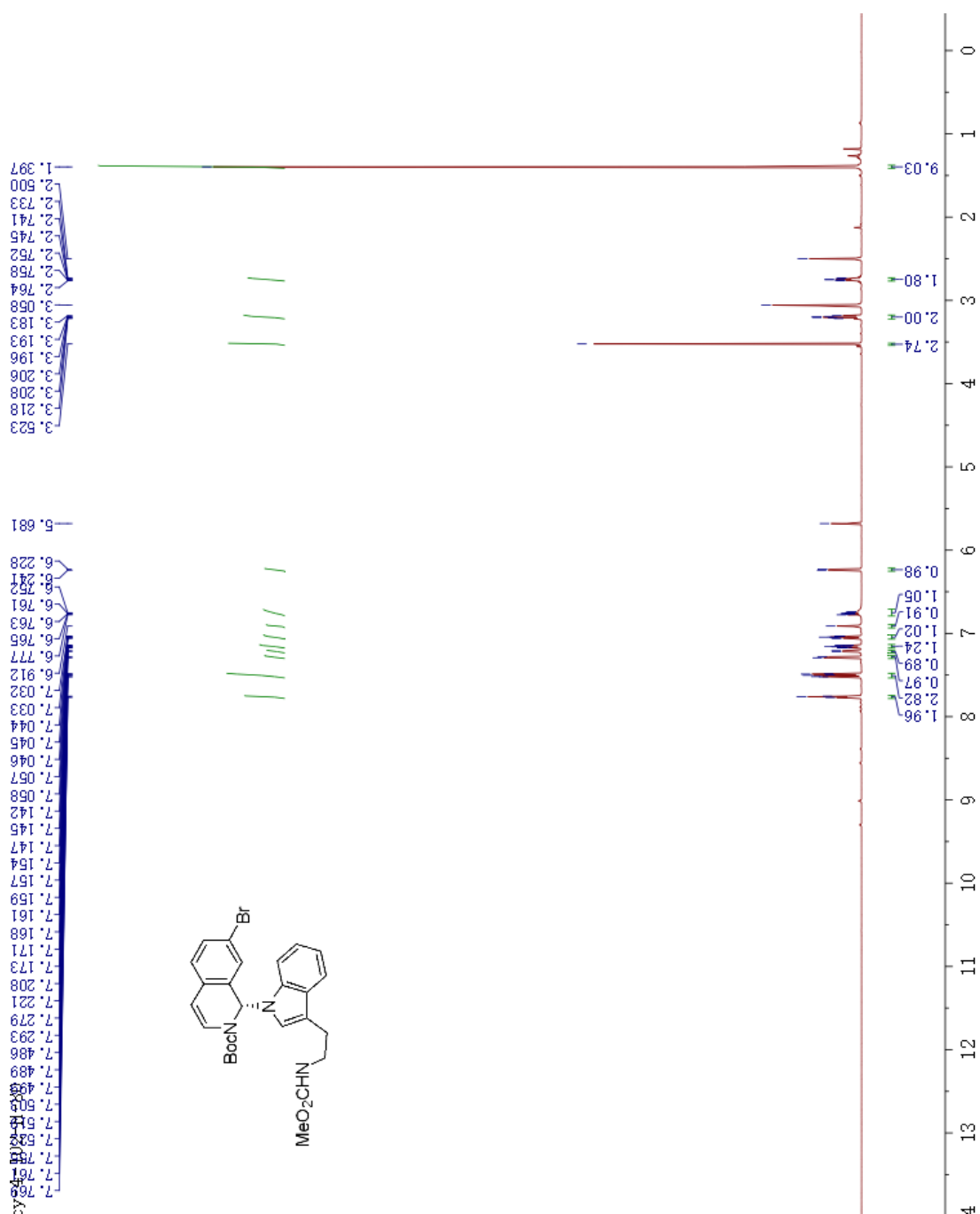


	RT	Area	% Area	Height
1	25.953	9489431	51.06	98814
2	32.328	9096559	48.94	75686



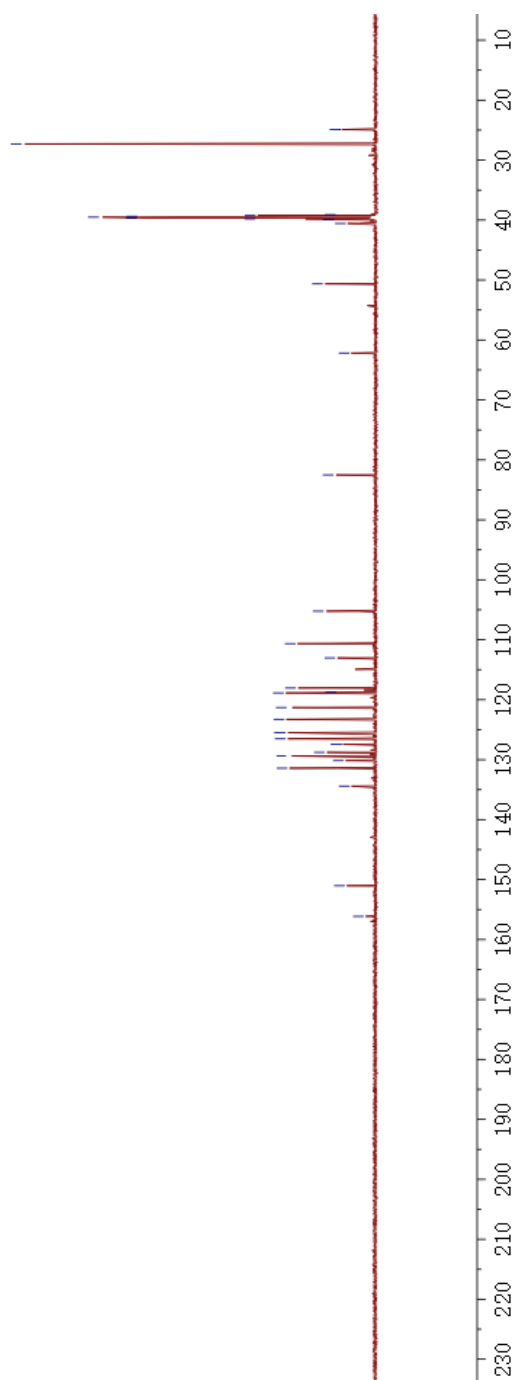
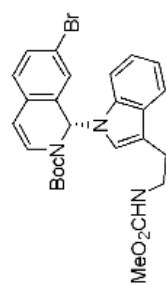
	RT	Area	% Area	Height
1	26.884	164141	6.02	2051
2	31.687	2561314	93.98	26166

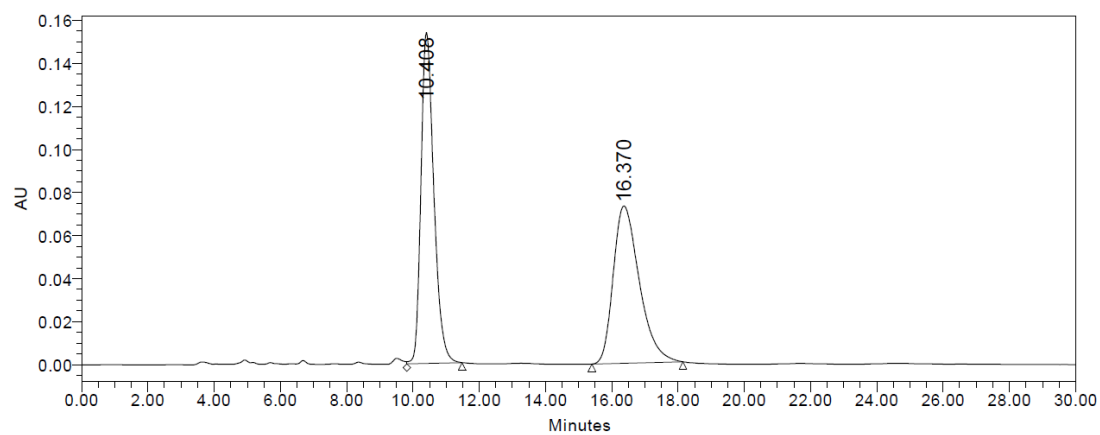
NMR Spectra and HPLC Chromatographs of **4ka**



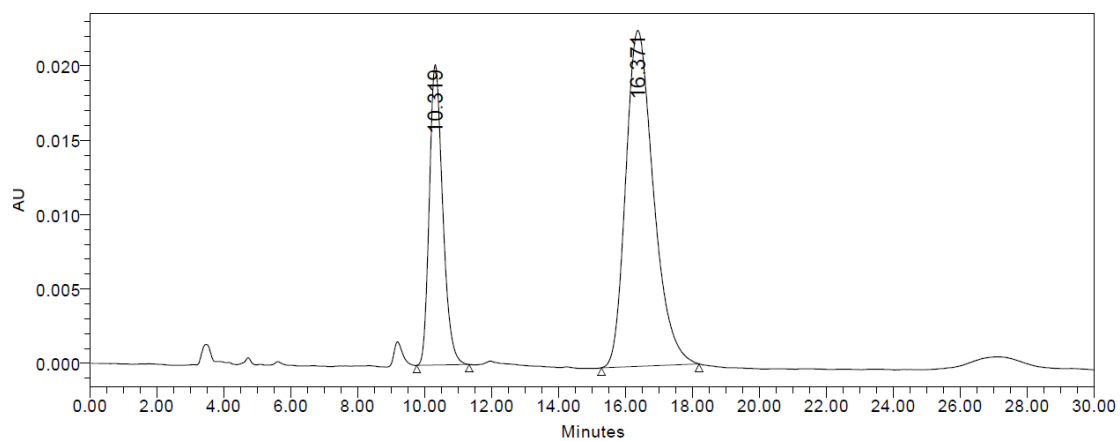
cy-4-102-C-80

156.141
151.028
134.407
131.431
130.167
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24.896



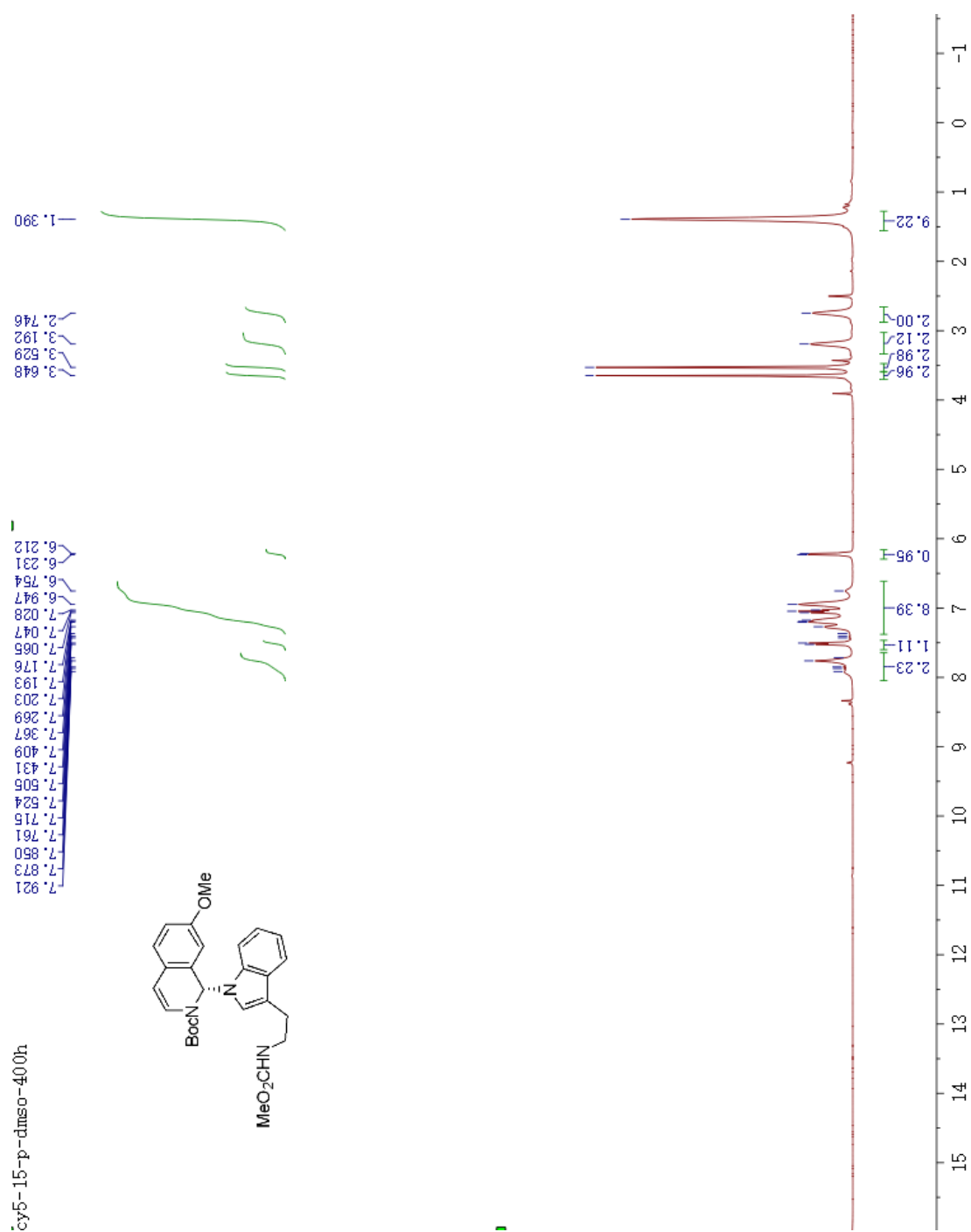


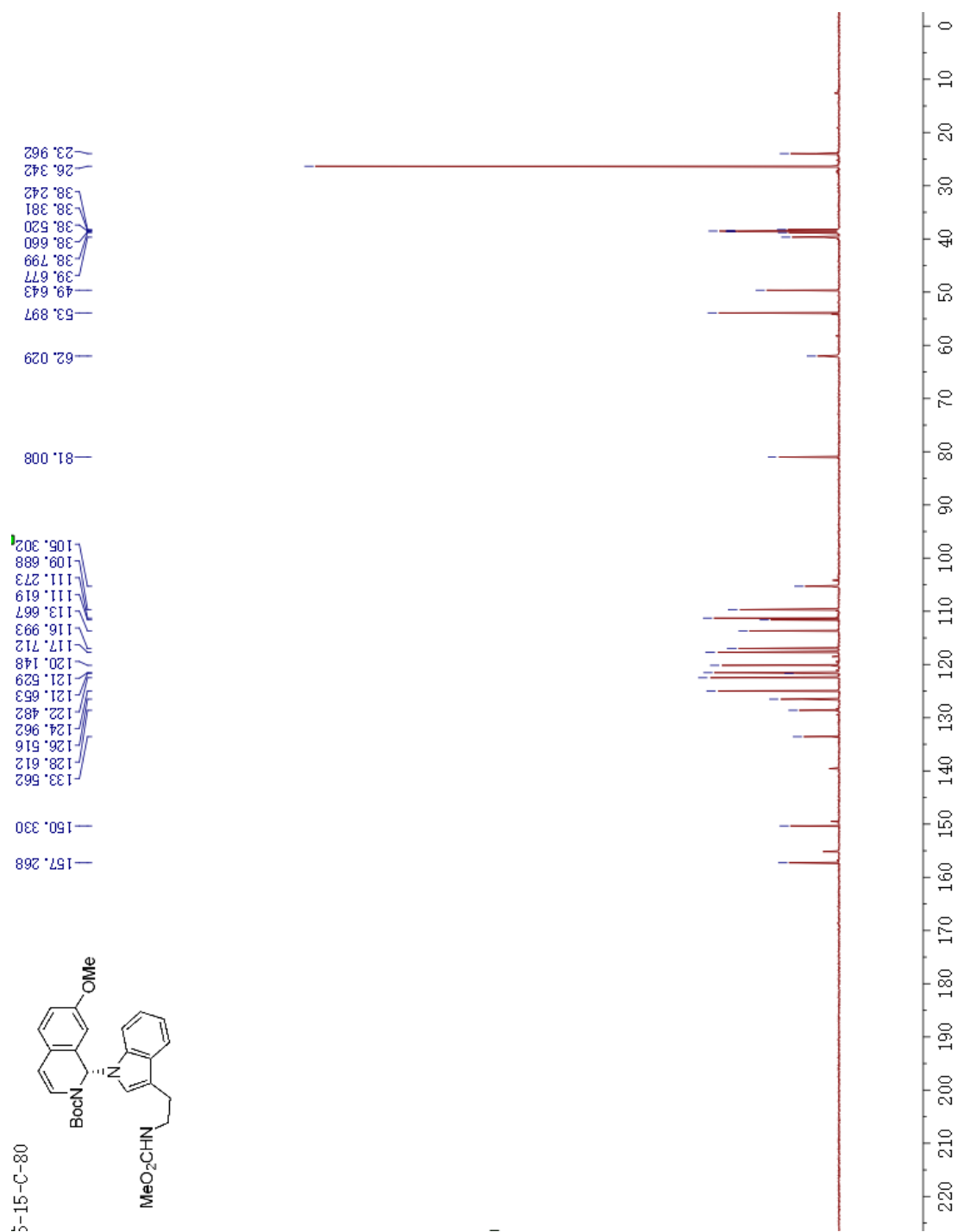
	RT	Area	% Area	Height
1	10.408	4149118	50.95	153761
2	16.370	3994288	49.05	73035

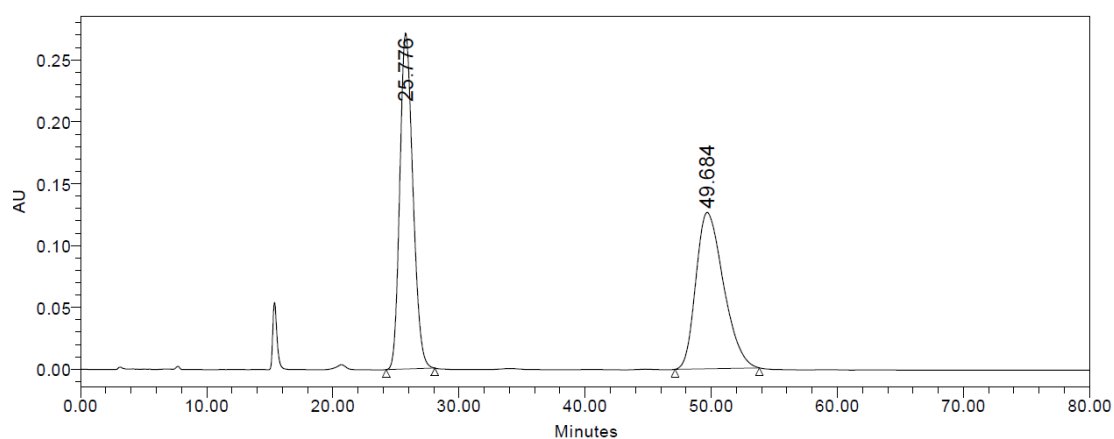


	RT	Area	% Area	Height
1	10.319	560832	30.12	20207
2	16.371	1301246	69.88	22581

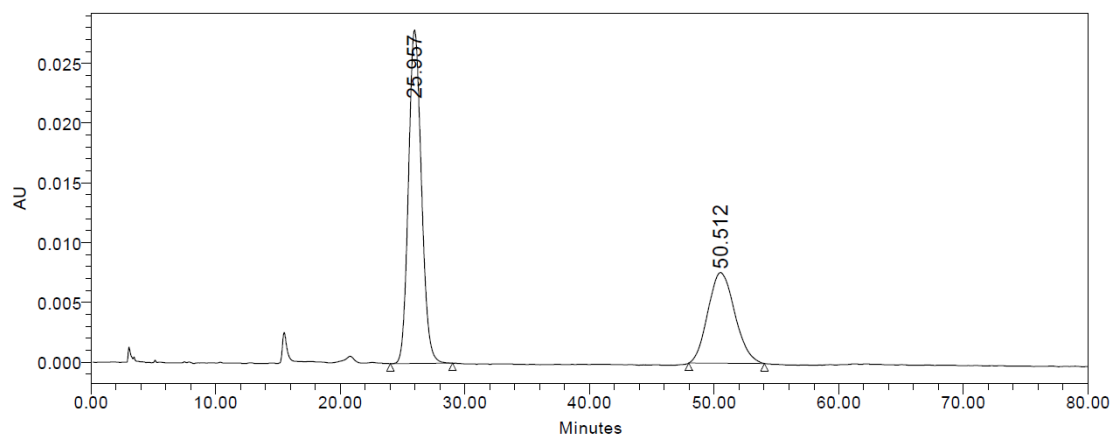
NMR Spectra and HPLC Chromatographs of **4la**





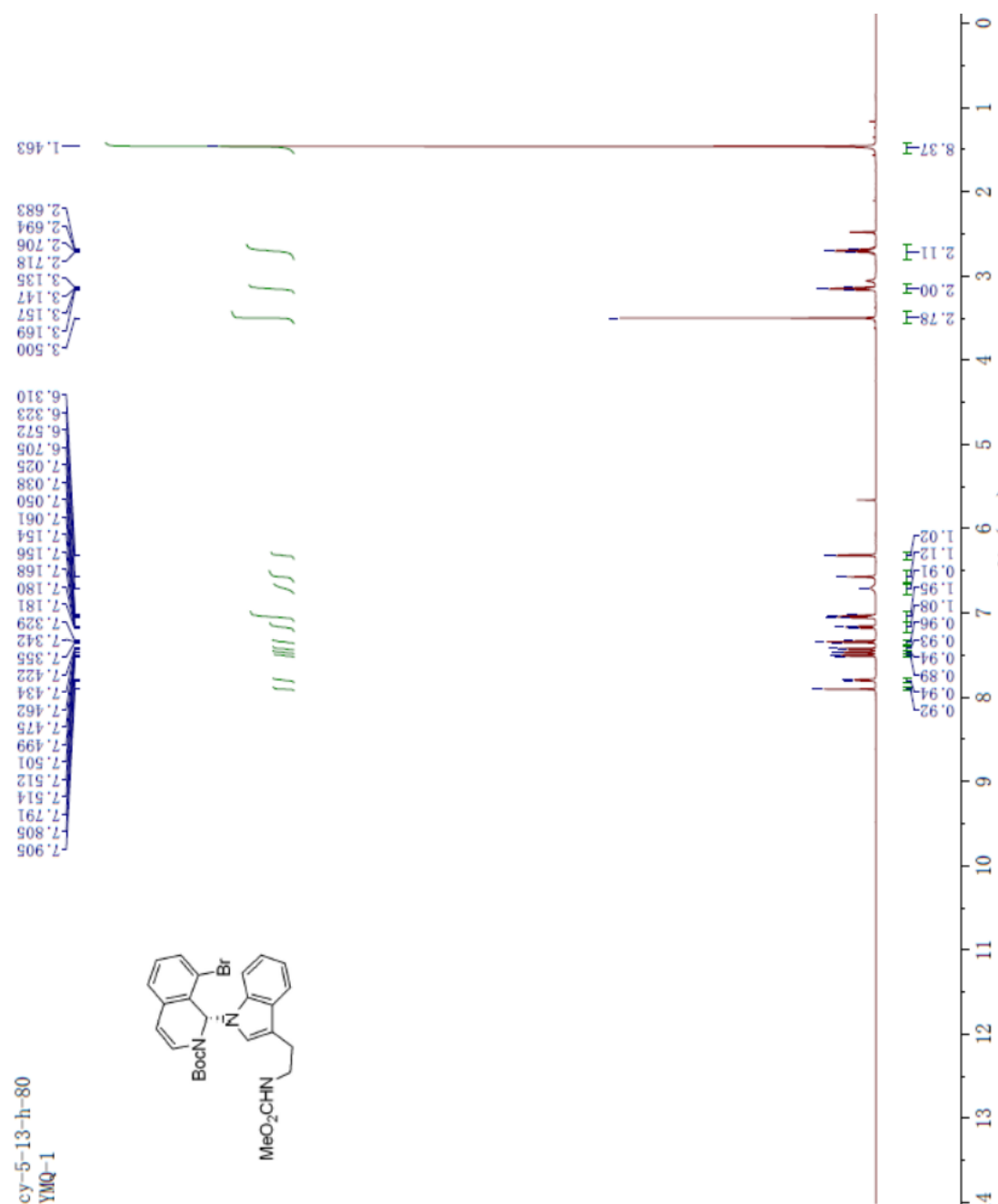


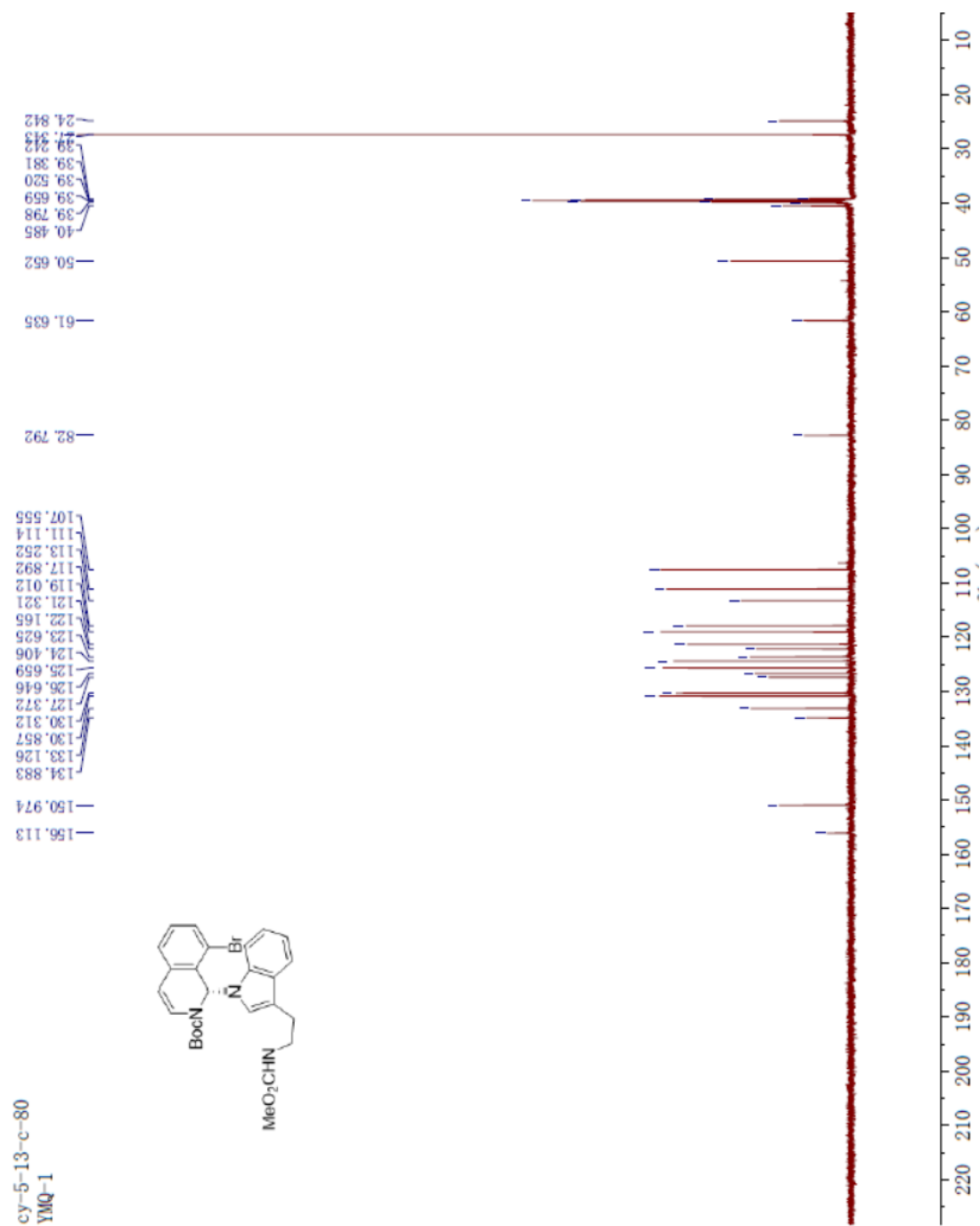
	RT	Area	% Area	Height
1	25.776	19544787	50.41	271316
2	49.684	19225346	49.59	126305

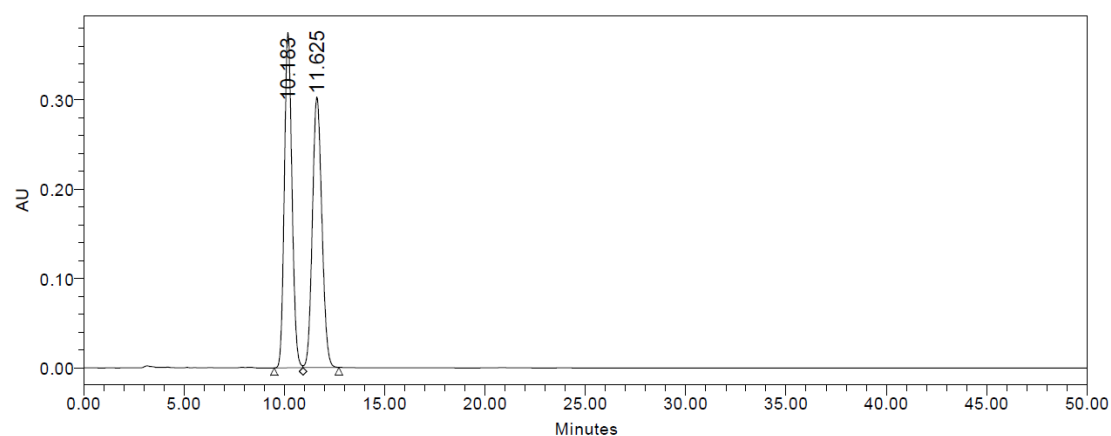


	RT	Area	% Area	Height
1	25.957	2018817	63.91	27893
2	50.512	1140019	36.09	7585

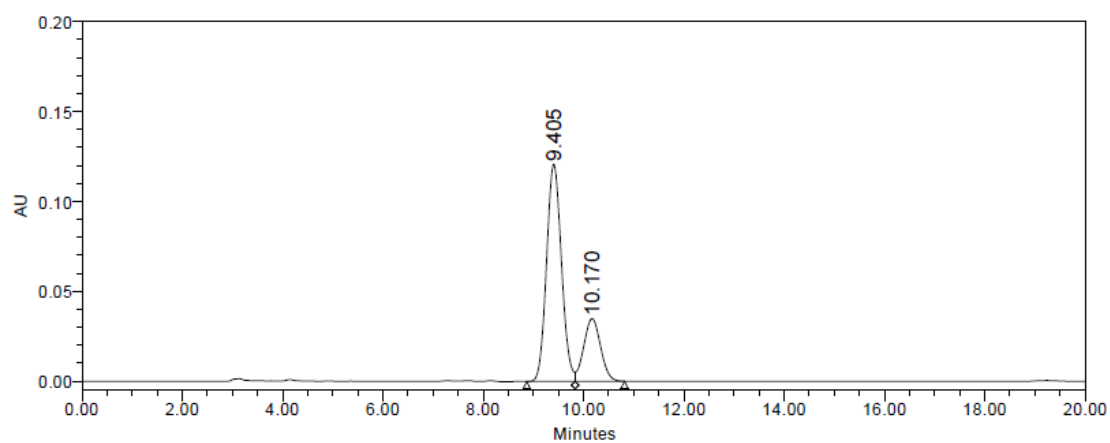
NMR Spectra and HPLC Chromatographs of **4ma**





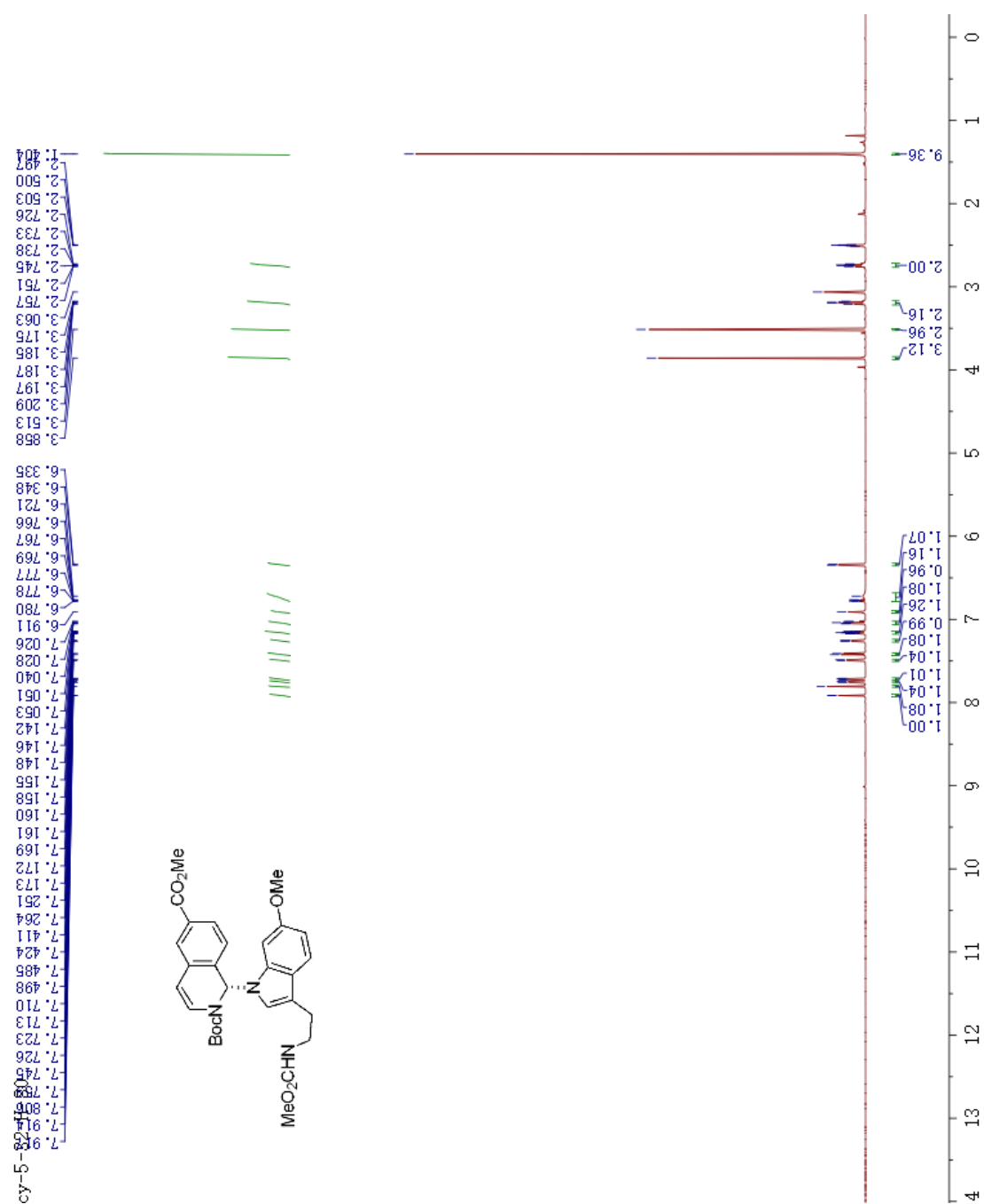


	RT	Area	% Area	Height
1	10.183	9897558	49.88	375092
2	11.625	9945297	50.12	302817



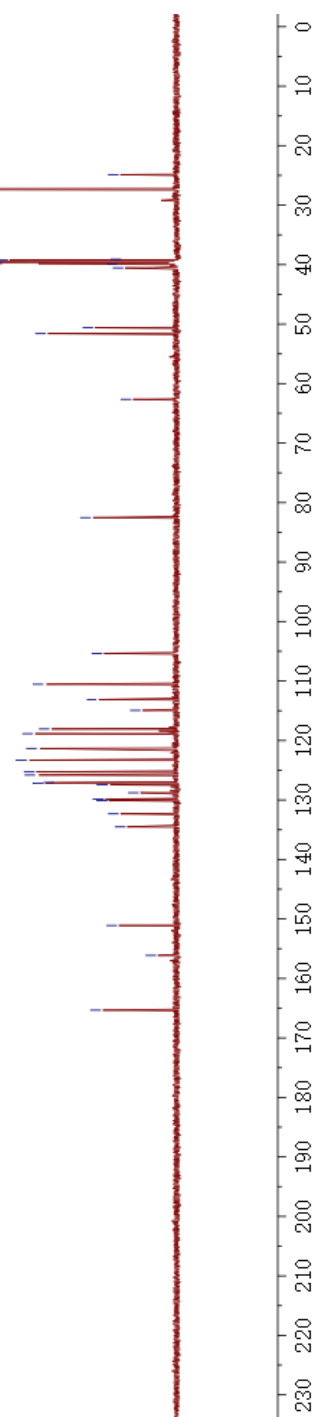
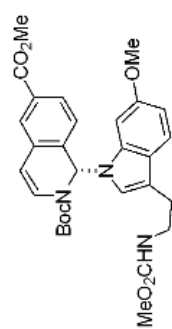
	RT	Area	% Area	Height
1	9.405	2494511	75.38	120908
2	10.170	814920	24.62	34944

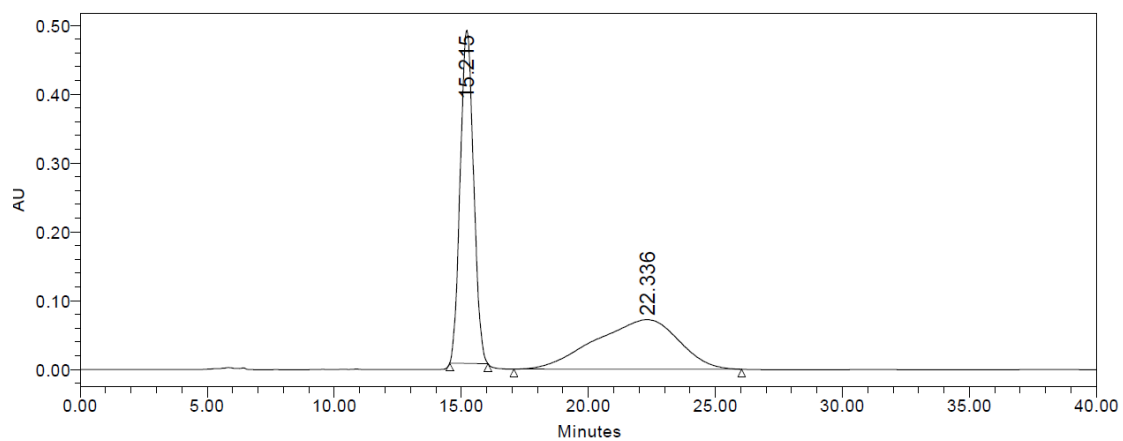
NMR Spectra and HPLC Chromatographs of **4il**



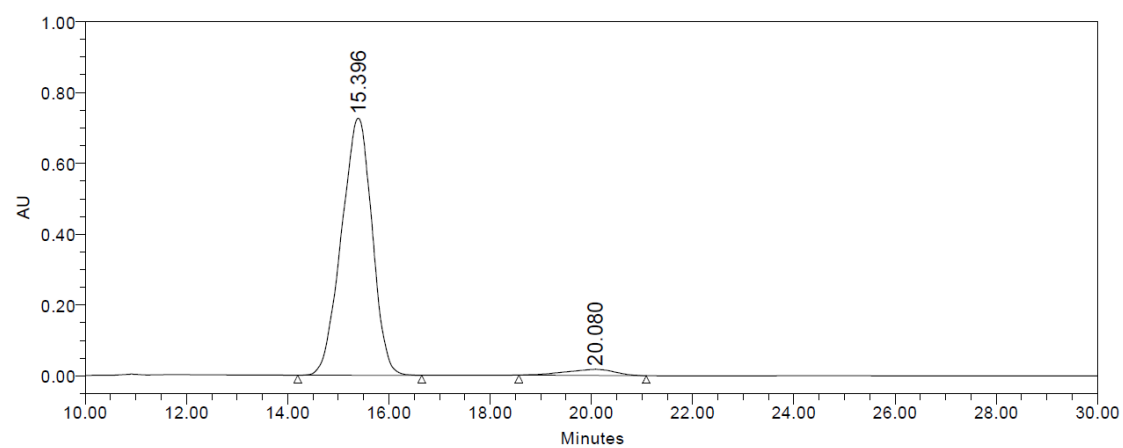
3γ-5-32-C-80

165.335
156.124
151.097
134.520
132.325
130.084
129.854
128.774
127.448
127.179
127.062
126.810
125.273
123.302
121.333
118.861
118.061
114.936
113.112
110.547
105.348
82.525
62.643
51.594
50.611
39.798
39.659
39.520
39.380
27.243
24.867



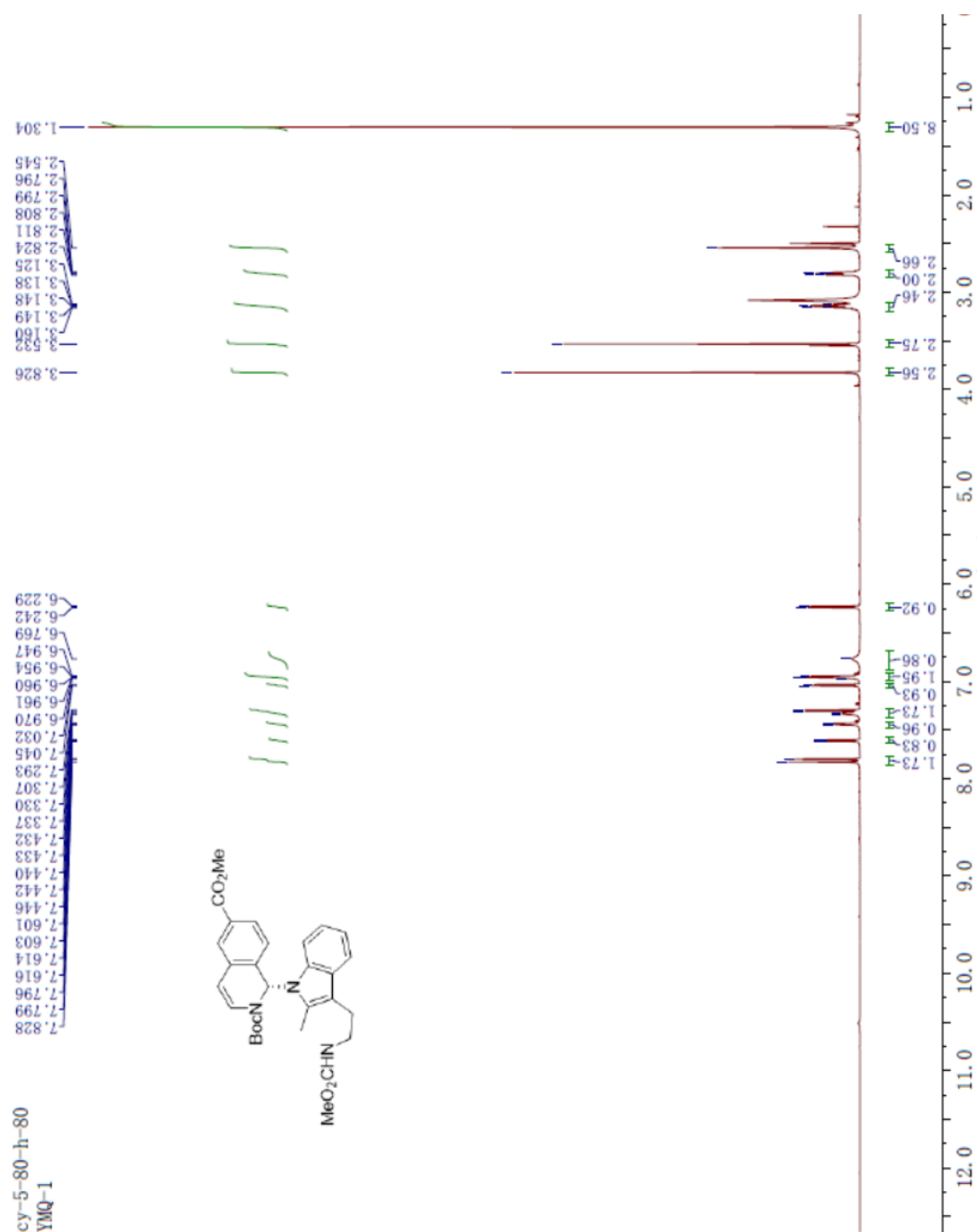


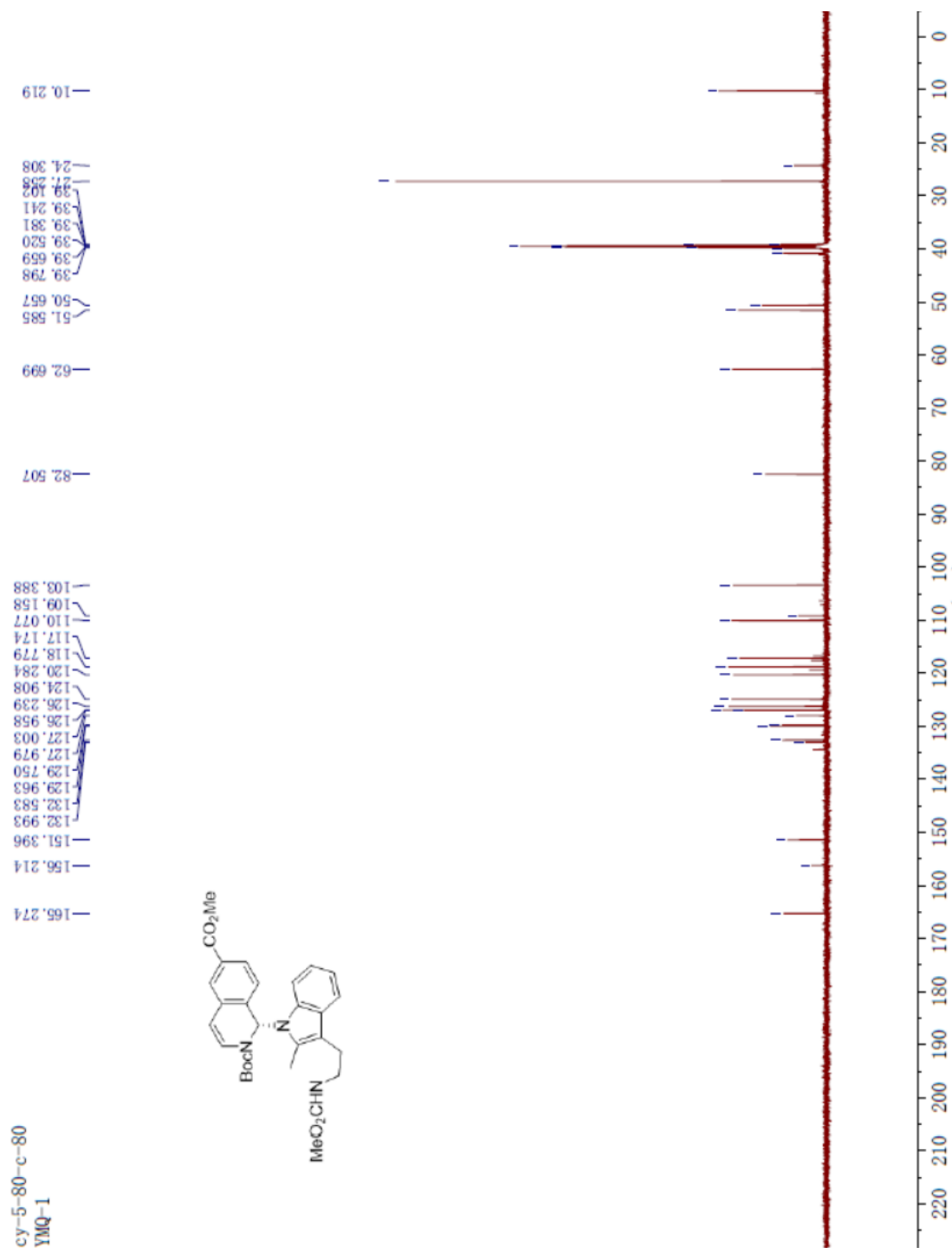
	RT	Area	% Area	Height
1	15.215	17704928	51.95	483866
2	22.336	16373938	48.05	72077

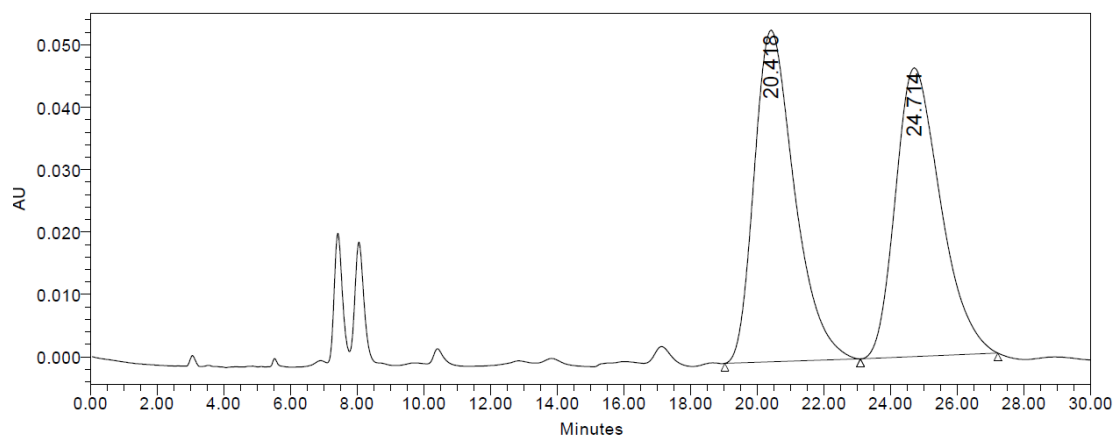


	RT	Area	% Area	Height
1	15.396	30466409	96.42	725573
2	20.080	1131958	3.58	16956

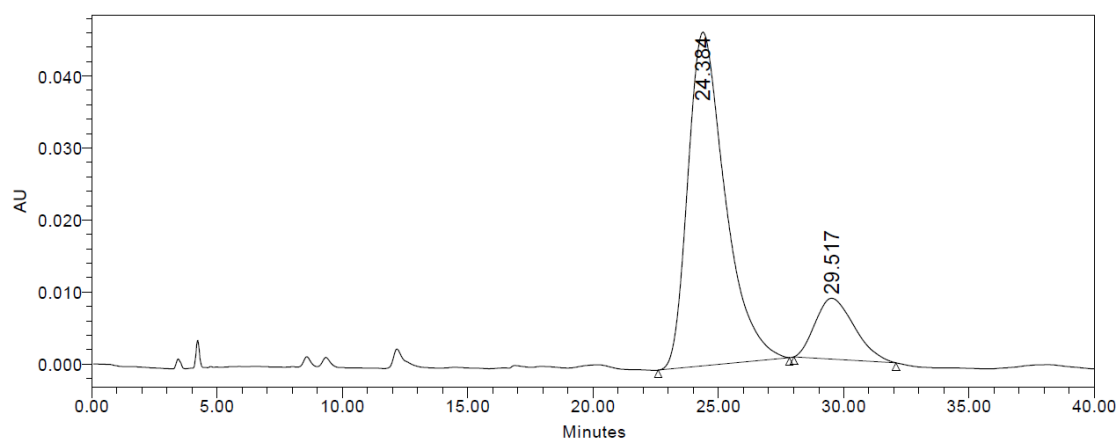
NMR Spectra and HPLC Chromatographs of **4im**





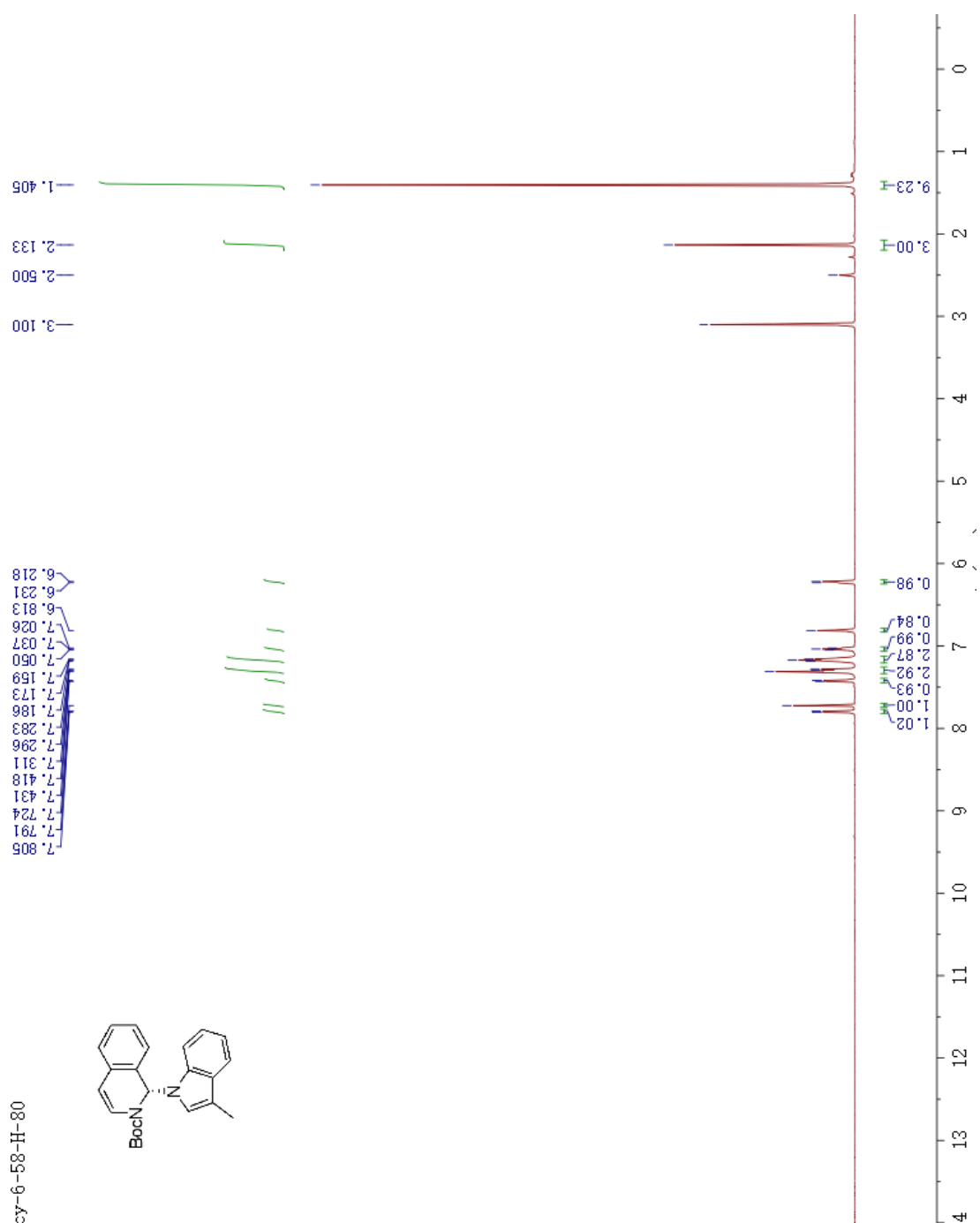


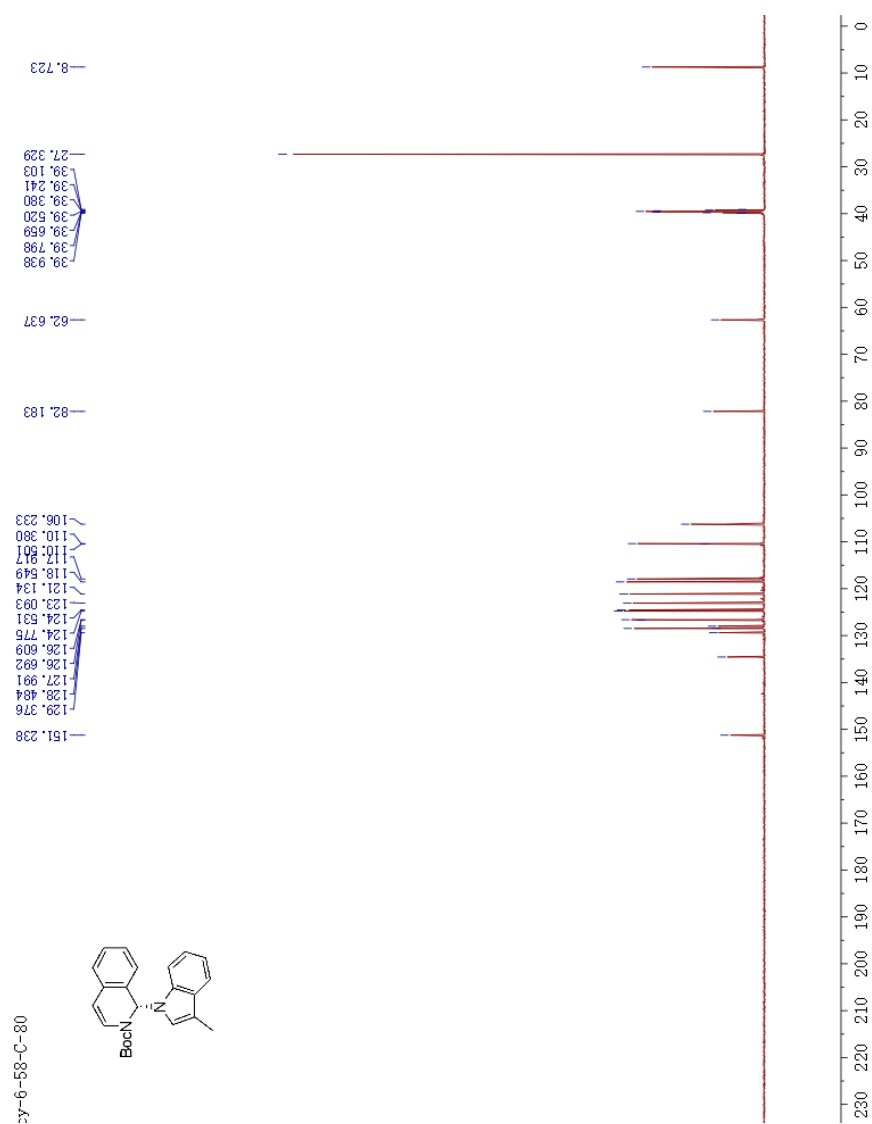
	RT	Area	% Area	Height
1	20.418	4468712	50.71	53110
2	24.714	4344028	49.29	46232

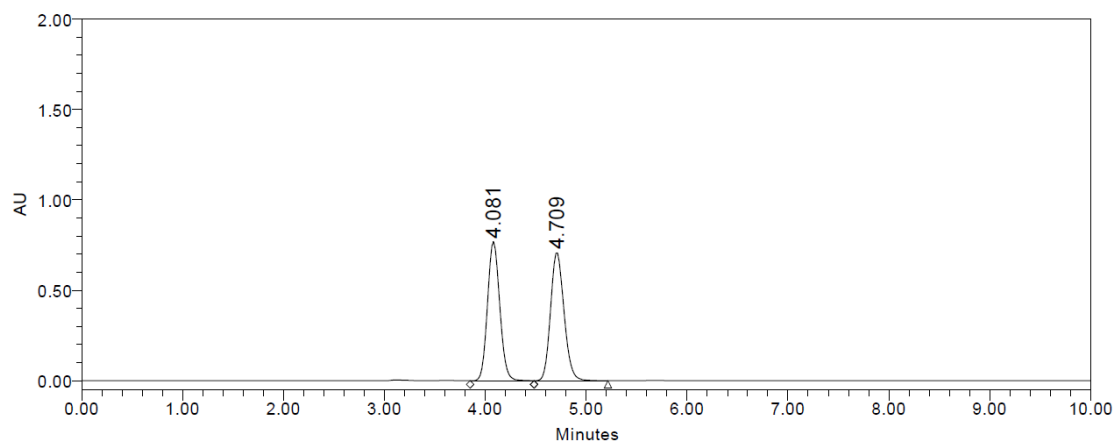


	RT	Area	% Area	Height
1	24.384	4785245	83.94	46326
2	29.517	915704	16.06	8437

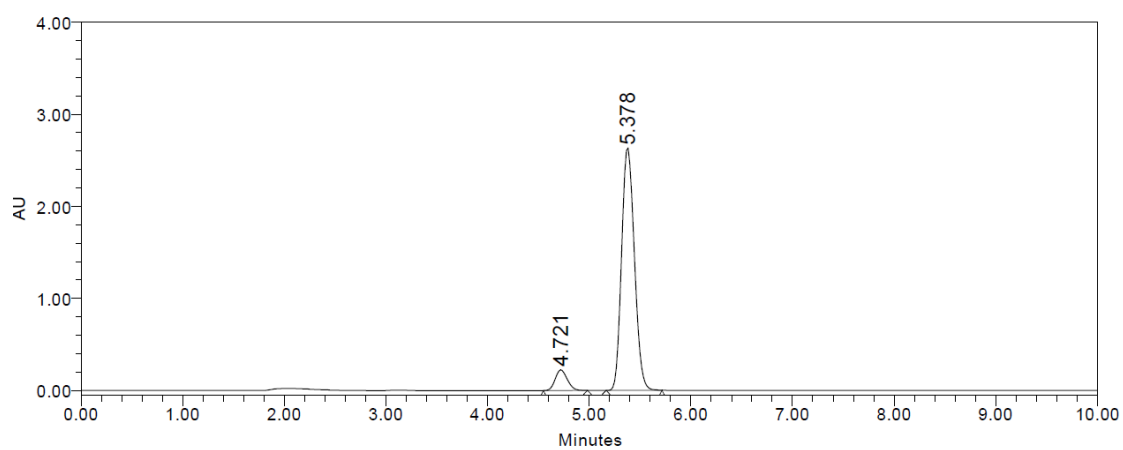
NMR Spectra and HPLC Chromatographs of **4an**





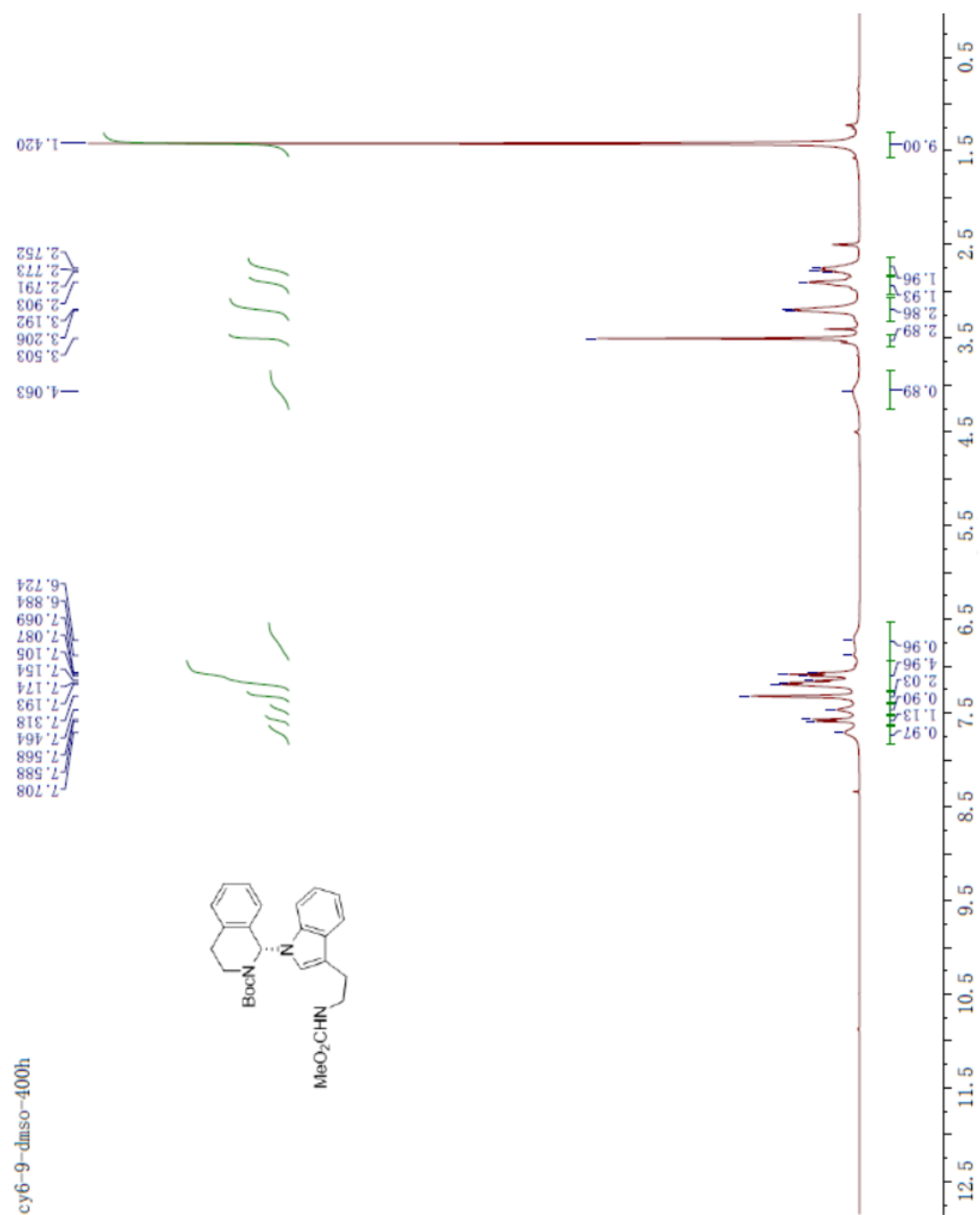


	RT	Area	% Area	Height
1	4.081	6467868	49.54	768568
2	4.709	6587071	50.46	708996

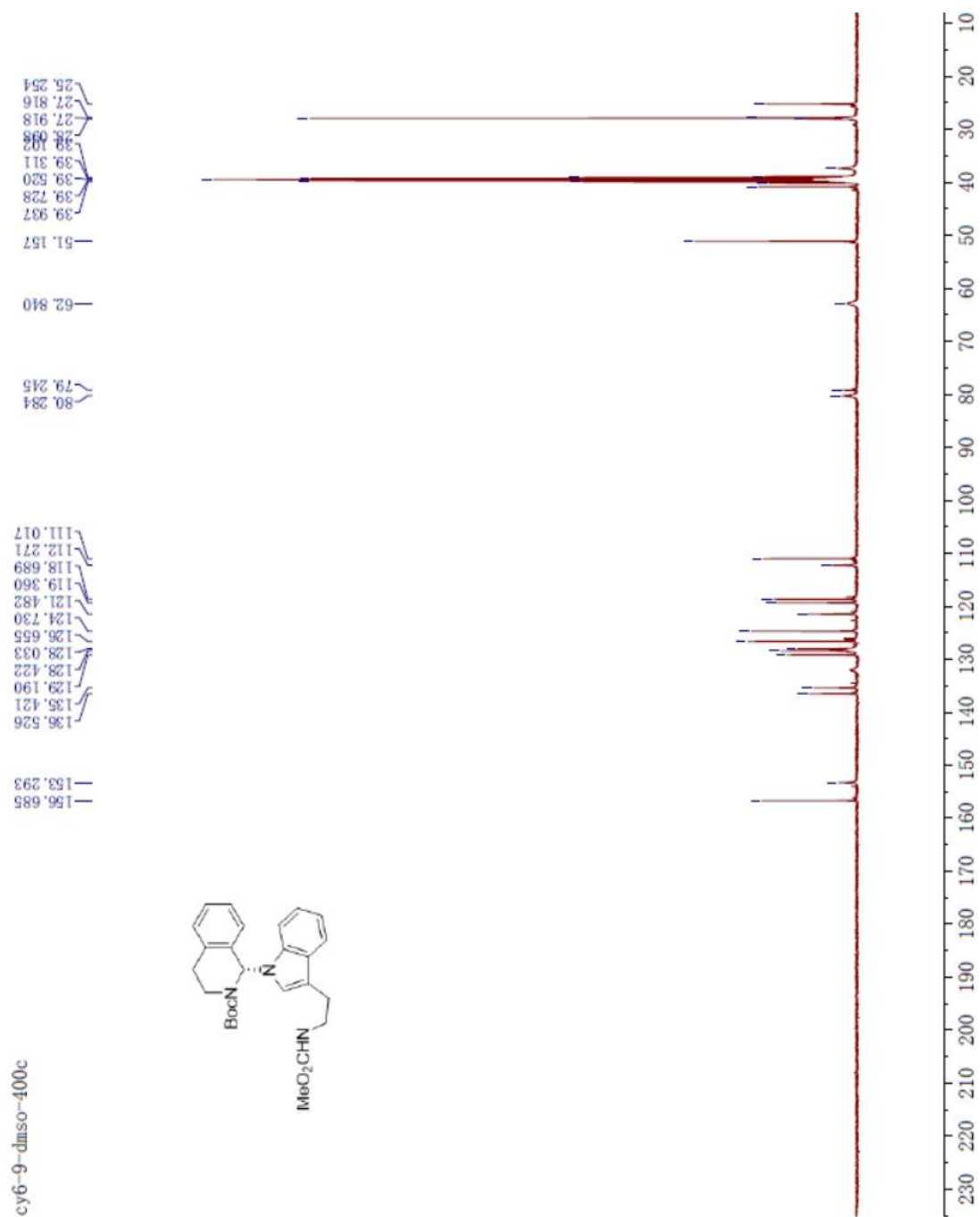


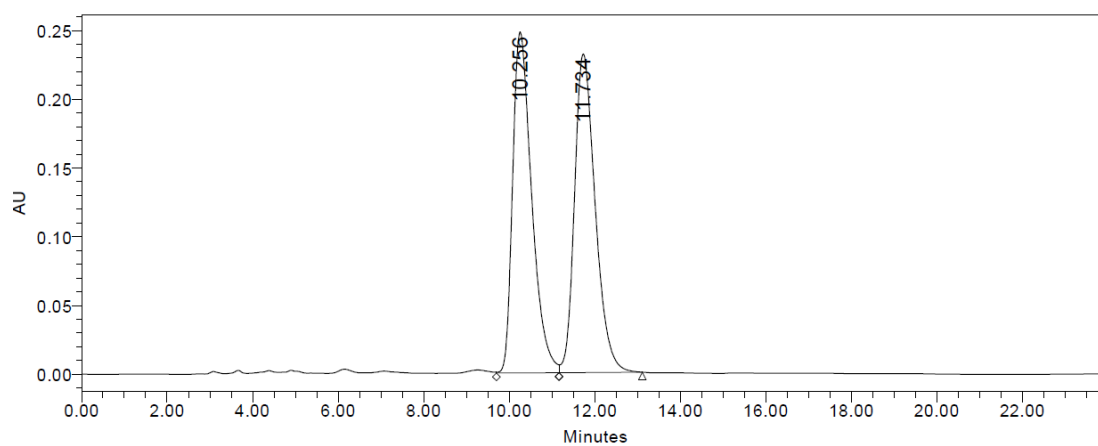
	RT	Area	% Area	Height
1	4.721	1845201	7.40	224744
2	5.378	23081612	92.60	2636319

NMR Spectra and HPLC Chromatographs of **5aa**

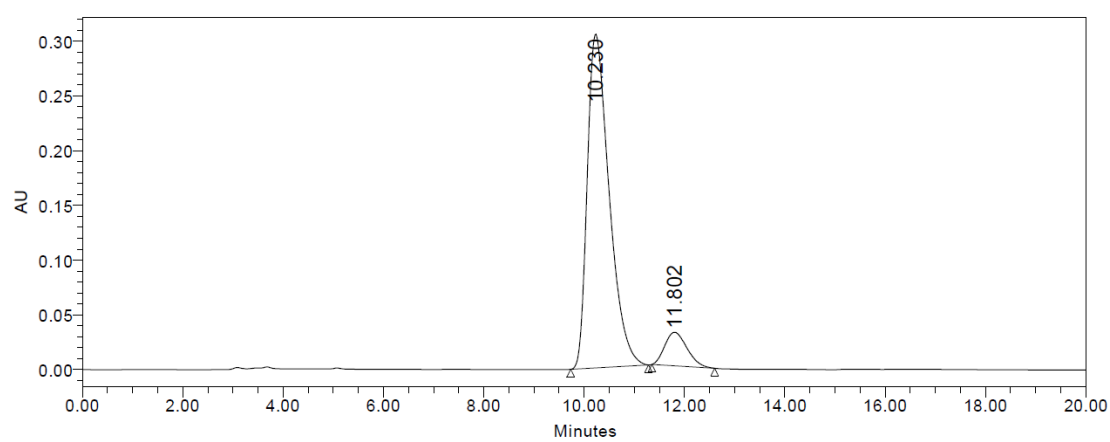


cy6-9-dmsO-400c



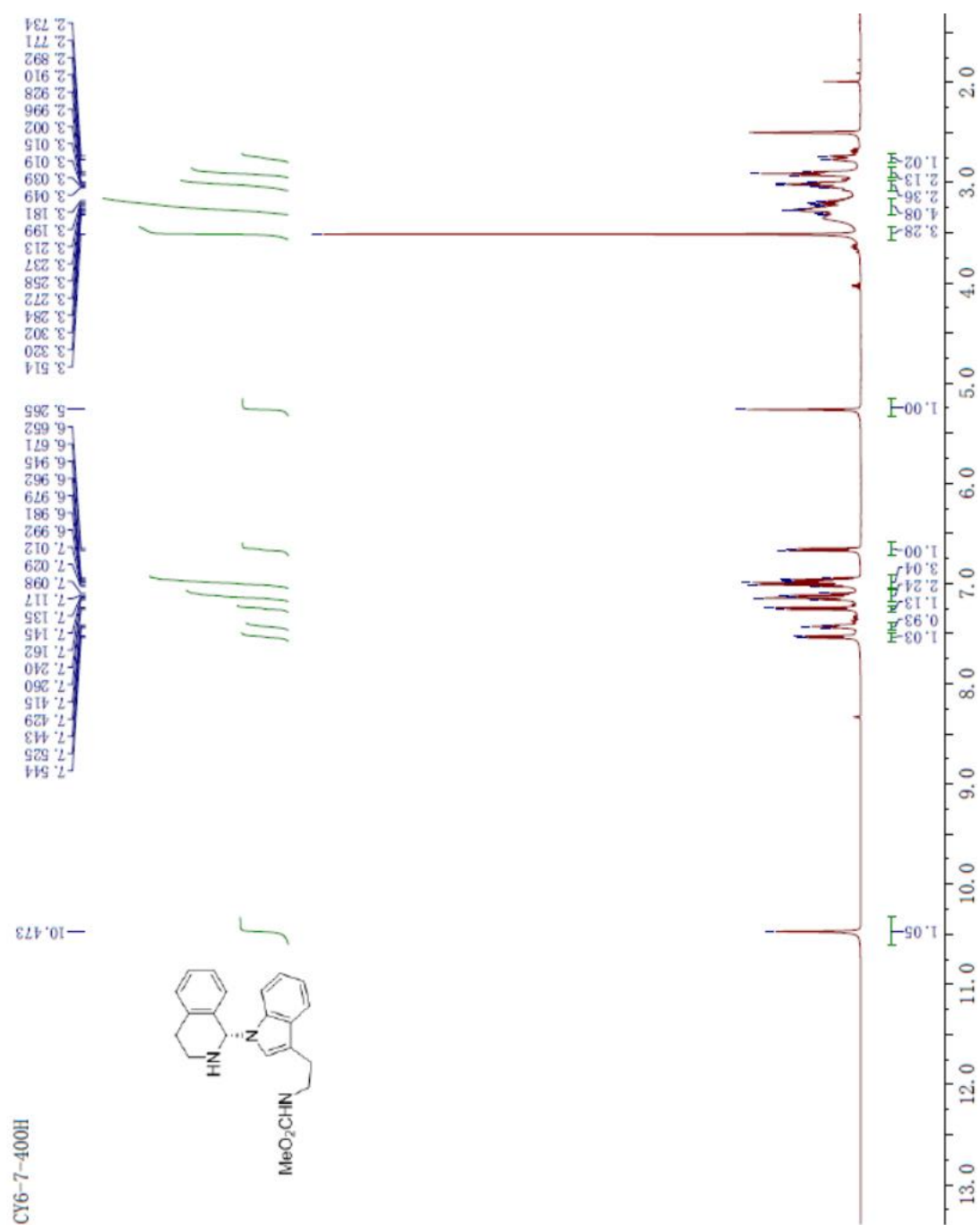


	RT	Area	% Area	Height
1	10.256	7673711	49.60	248101
2	11.734	7796332	50.40	231875

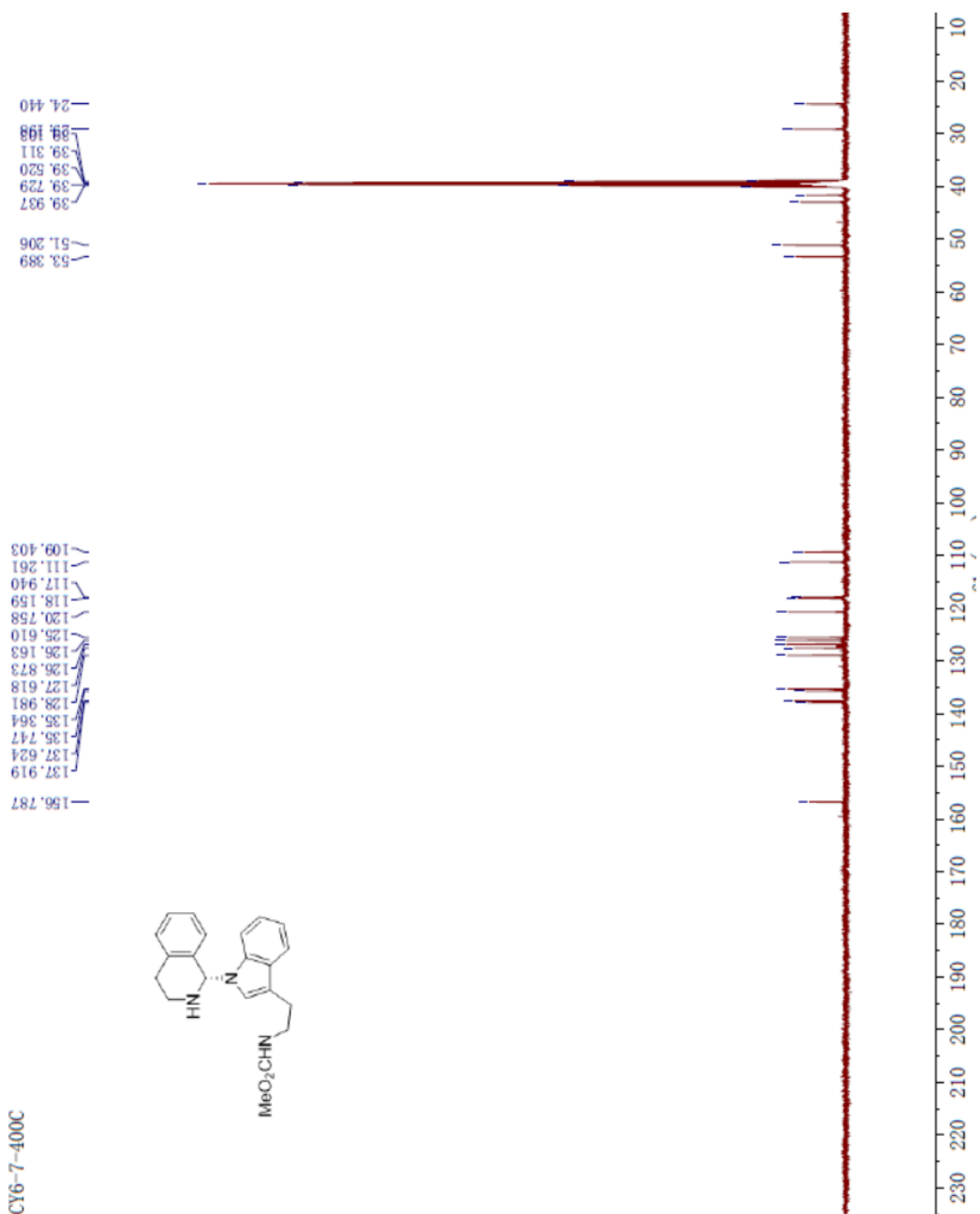


	RT	Area	% Area	Height
1	10.230	9235973	90.74	304700
2	11.802	943031	9.26	30662

NMR Spectra of **6aa**



CY6-7-400C



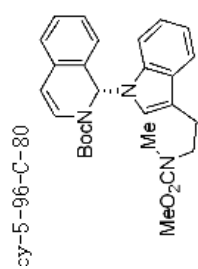
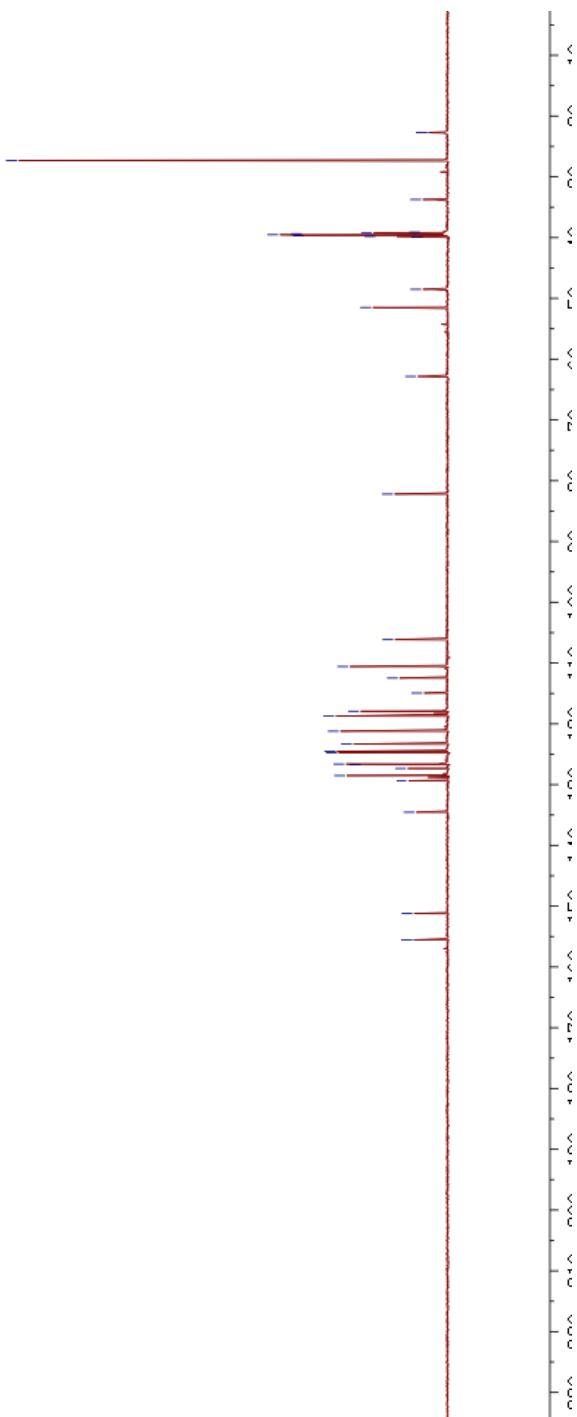
Chemical structure of the compound is shown below:

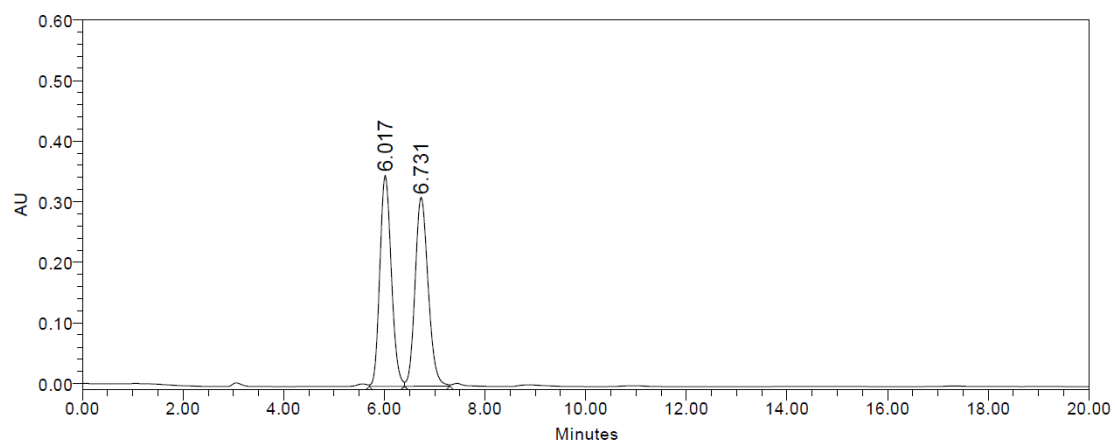
COC(=O)C1=CC=C2C(=C1)N(C2)C[C@H]3C=CC(=C4C(=C3)N(C(=O)OC)C4)C5=CC=CC=C5

The structure is a complex molecule featuring a central chiral center (C[C@H]) connected to a Boc-protected amine (BocN) and a substituted benzene ring (MeO₂CN). The Boc group is a tert-butoxycarbonyl group, and the MeO₂CN group is a methoxycarbonyl group.

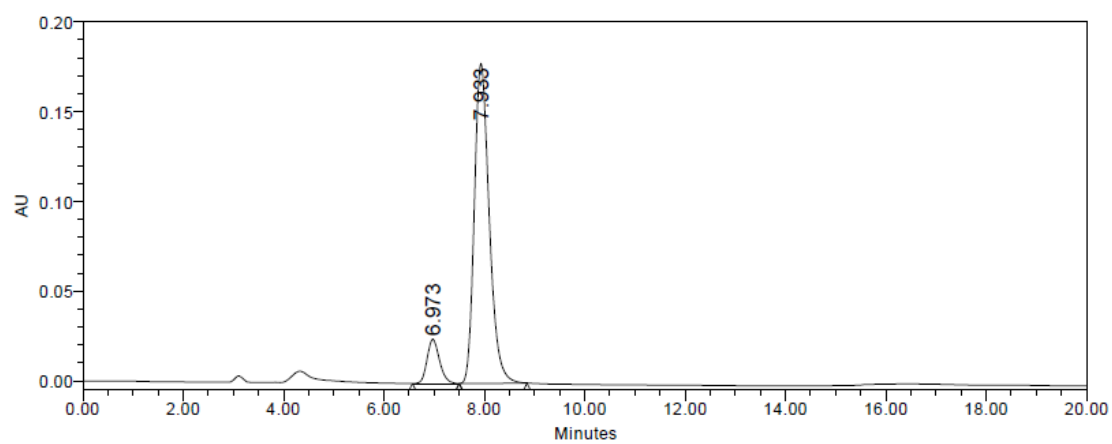
The ¹H NMR spectrum (CDCl₃) shows the following peaks (ppm):

- 9.14 (s, 1H)
- 7.14 (s, 1H)
- 7.09 (s, 1H)
- 7.07 (s, 1H)
- 7.05 (s, 1H)
- 7.03 (s, 1H)
- 7.01 (s, 1H)
- 6.99 (s, 1H)
- 6.97 (s, 1H)
- 6.95 (s, 1H)
- 6.93 (s, 1H)
- 6.91 (s, 1H)
- 6.89 (s, 1H)
- 6.87 (s, 1H)
- 6.85 (s, 1H)
- 6.83 (s, 1H)
- 6.81 (s, 1H)
- 6.79 (s, 1H)
- 6.77 (s, 1H)
- 6.75 (s, 1H)
- 6.73 (s, 1H)
- 6.71 (s, 1H)
- 6.69 (s, 1H)
- 6.67 (s, 1H)
- 6.65 (s, 1H)
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- 6.61 (s, 1H)
- 6.59 (s, 1H)
- 6.57 (s, 1H)
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- 6.47 (s, 1H)
- 6.45 (s, 1H)
- 6.43 (s, 1H)
- 6.41 (s, 1H)
- 6.39 (s, 1H)
- 6.37 (s, 1H)
- 6.35 (s, 1H)
- 6.33 (s, 1H)
- 6.31 (s, 1H)
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- 6.27 (s, 1H)
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- 6.17 (s, 1H)
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- 6.13 (s, 1H)
- 6.11 (s, 1H)
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- 1.97 (s, 1H)
- 1.95 (s





	RT	Area	% Area	Height
1	6.017	5511451	49.51	347761
2	6.731	5619901	50.49	311633



	RT	Area	% Area	Height
1	6.973	423076	10.32	24627
2	7.933	3676066	89.68	178148