

# Supplementary Information

Figure S1. <sup>1</sup>H NMR spectrum of Hainanerectamine A.

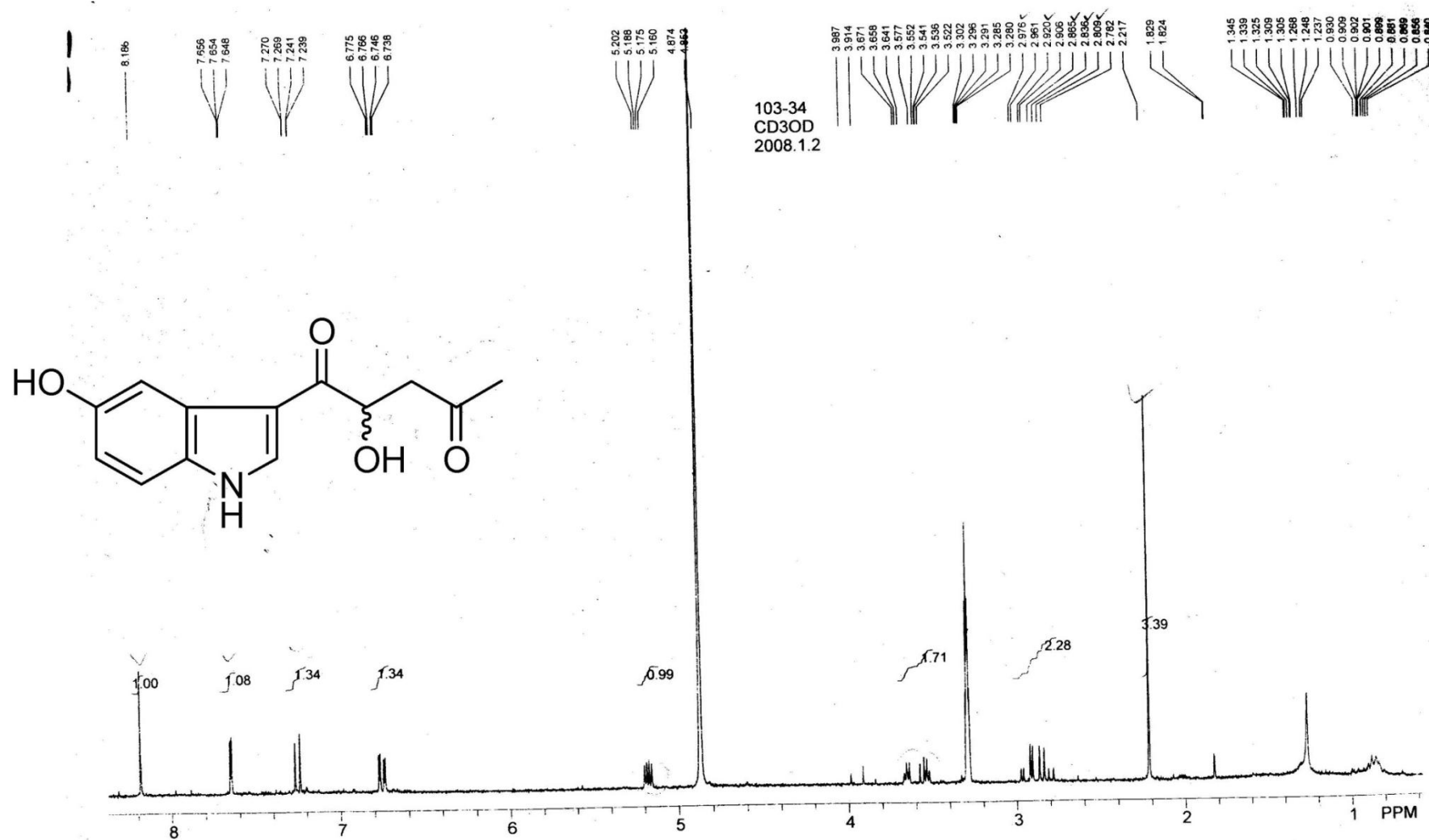


Figure S2.  $^{13}\text{C}$  NMR spectrum of Hainanerectamine A.

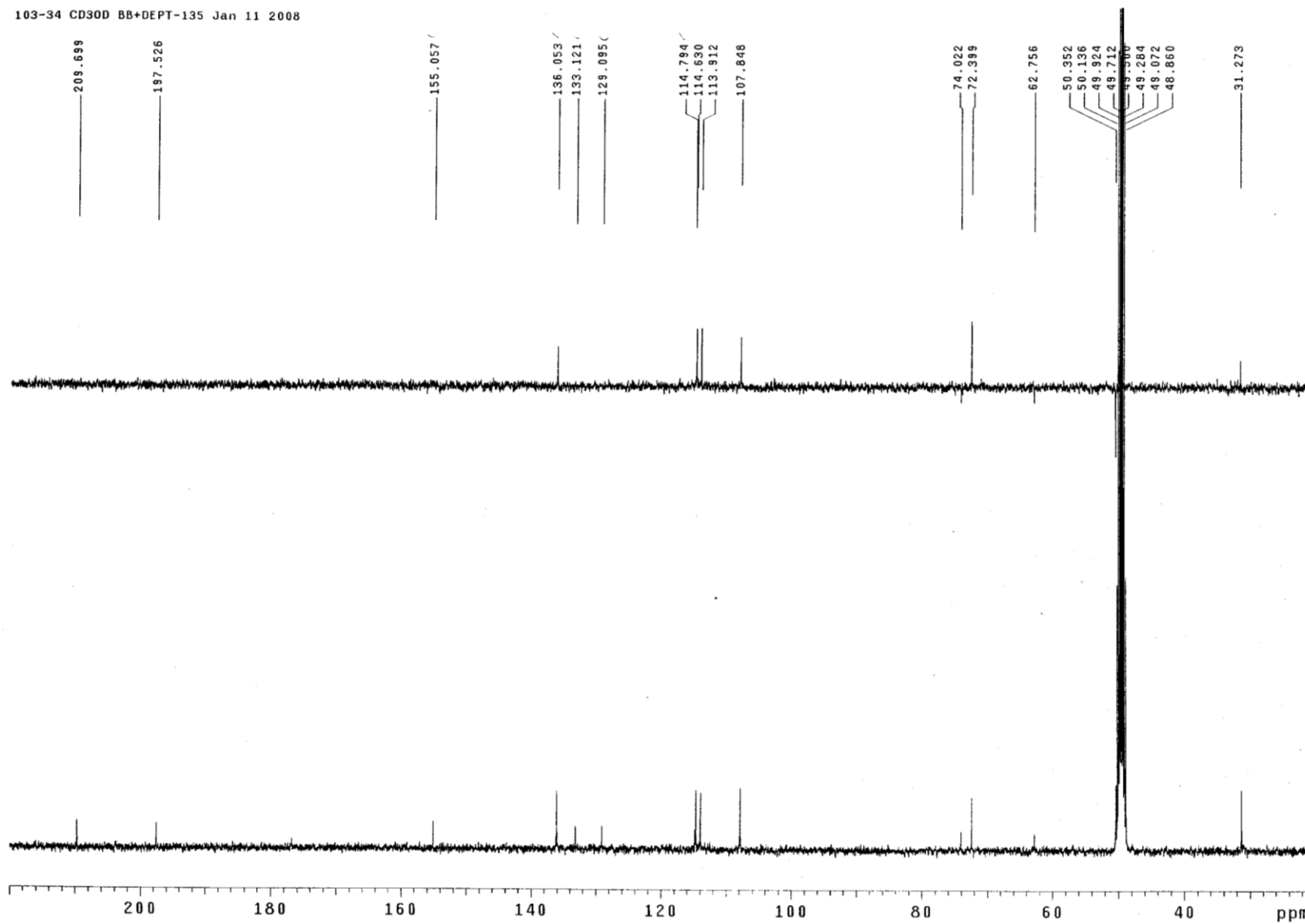


Figure S3. HSQC spectrum of Hainanerectamine A.

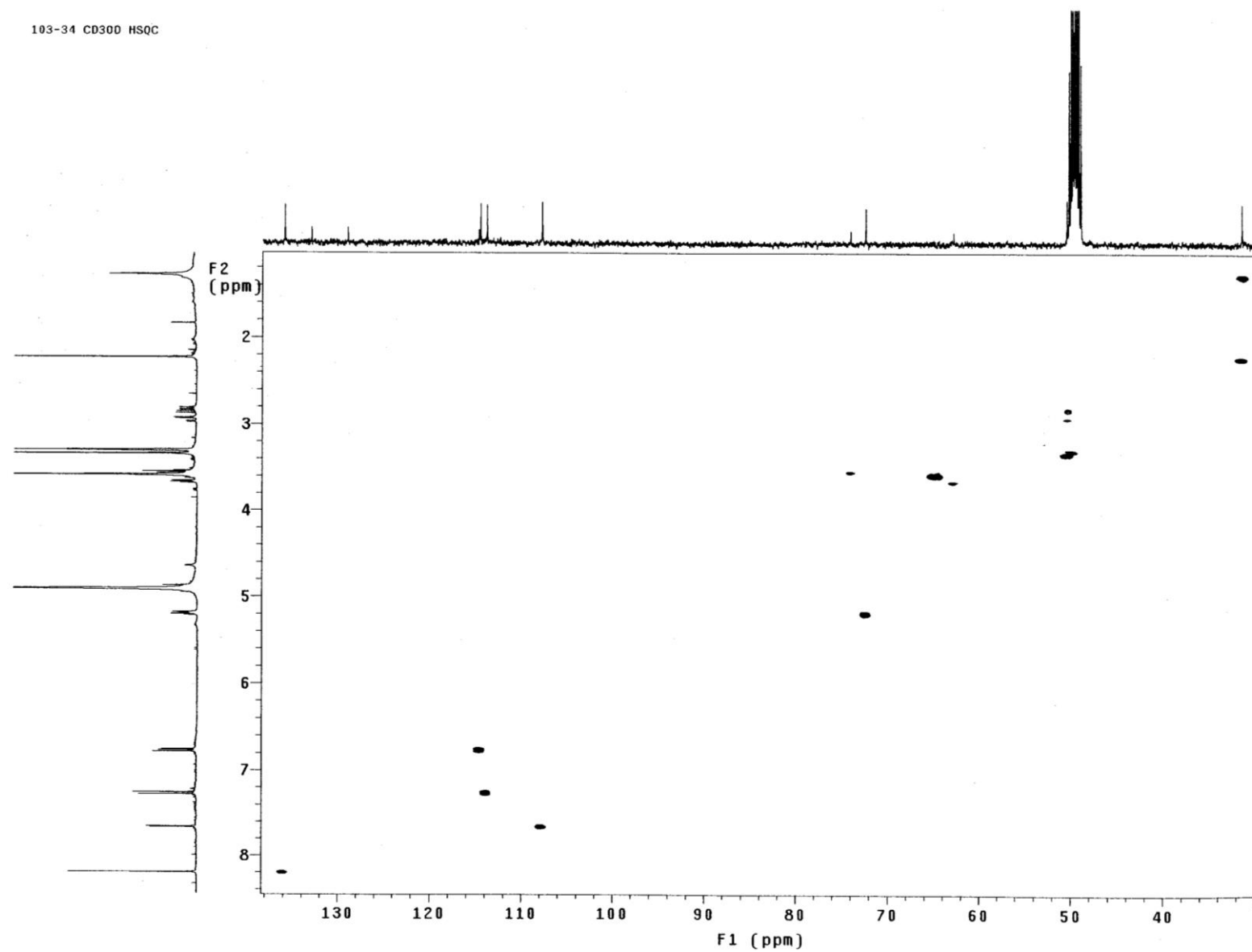


Figure S4. HMBC spectrum of Hainanerectamine A.

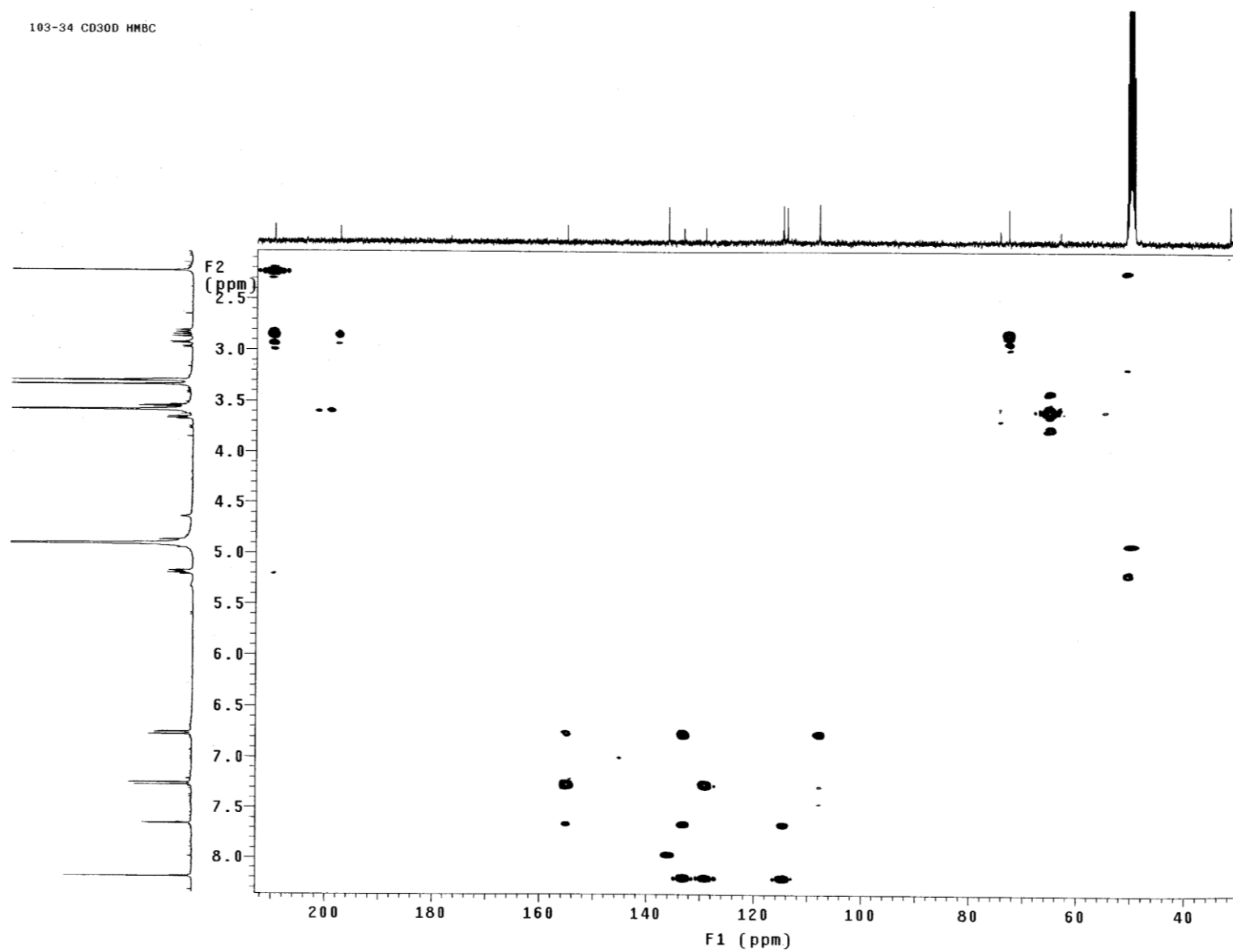


Figure S5.  $^1\text{H}$   $^1\text{H}$  COSY spectrum of Hainanerectamine A.

103-34 CD300 COSY

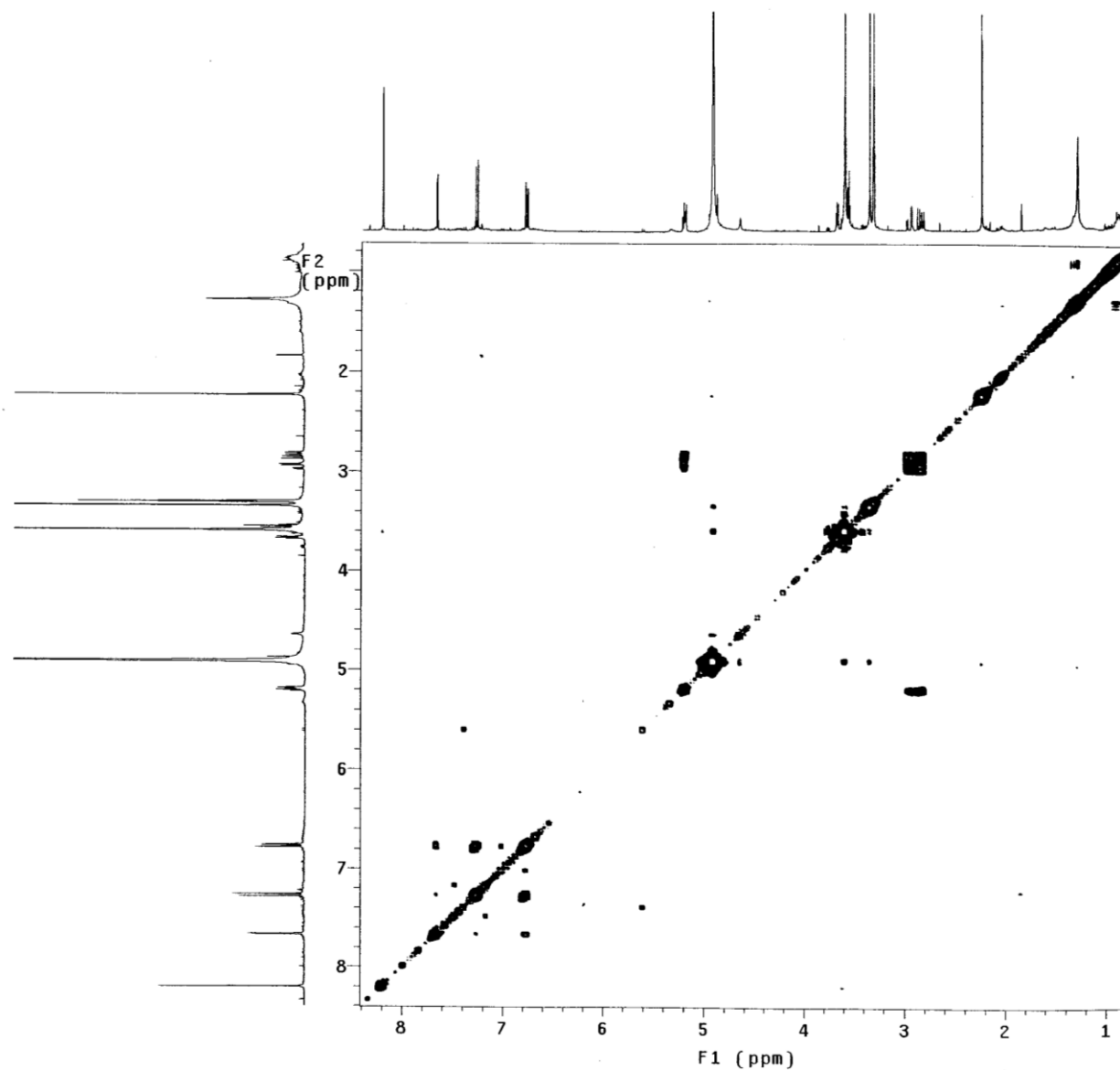
Solvent: CD30D  
Ambient temperature  
Mercury-400BB "simm401"Relax. delay 1.000 sec  
COSY 90-90  
Acq. time 0.171 sec  
Width 6009.6 Hz  
2D Width 6009.6 Hz  
4 repetitions  
320 increments  
OBSERVE H1, 400.1661632 MHz  
DATA PROCESSING  
Sq. sine bell 0.085 sec  
F1 DATA PROCESSING  
Sq. sine bell 0.026 sec  
FT size 2048 x 2048  
Total time 28 min, 44 sec

Figure S6. HREI spectrum of Hainanerectamine A.

LIST: h80151-c1 18-Jan-08 Elapse: 05:22.4 25  
 Samp: 103-34 Start : 14:04:12 27  
 Comm: Finnigan/MAT95//70eV/Tsou:200c/R:10000  
 Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM  
 Oper: WANG\_J@SIMM.CAS Client: S/N:SW01-0001 Inlet :  
 Limt: ( 0)  
 : ( 347) C14.H100.N.O4  
 Peak: 1000.00 mmu R+D: -2.0 > 60.0  
 Data: CMASS : converted

Mass	Intensity	%RA	%RIC	Delta	R+D	Composition
51.02992	*	4939	1.05	0.02	2.1 -1.0	H5.N.O2
76.03226	*	4760	1.01	0.02	-1.0 5.0	C6.H4
77.03959	*	9283	1.97	0.04	-0.5 4.5	C6.H5
103.0400	*	6545	1.39	0.03	-0.5 1.5	C4.H7.O3
					2.2 6.0	C7.H5.N
105.0319	*	18090	3.84	0.08	2.2 5.5	C7.H5.O
131.0386	*	6069	1.29	0.03	-1.5 7.0	C8.H5.N.O
132.0455	*	48498	10.31	0.22	-0.5 6.5	C8.H6.N.O
133.0510	*	7438	1.58	0.03	-0.9 1.5	C5.H9.O4
					1.8 6.0	C8.H7.N.O
146.9877	*	7021	1.49	0.03		
159.0318	*	10889	2.31	0.05	0.3 8.0	C9.H5.N.O2
160.0392	*	470587	100.00	2.15	0.6 7.5	C9.H6.N.O2
161.0425	*	50284	10.69	0.23		
162.9932	*	6783	1.44	0.03	-2.7 8.0	C7.H.N.O4
173.9850	*	31658	6.73	0.14	-2.3 9.5	C8.N.O4
186.0546	*	9461	2.01	0.04	0.9 8.5	C11.H8.N.O2
196.9839	*	4998	1.06	0.02		
229.0736	*	16721	3.55	0.08	0.3 9.0	C13.H11.N.O3
247.0835	*	46237	9.83	0.21	0.9 8.0	C13.H13.N.O4

Figure S7. <sup>1</sup>H NMR spectrum of Hainanerectamine B.

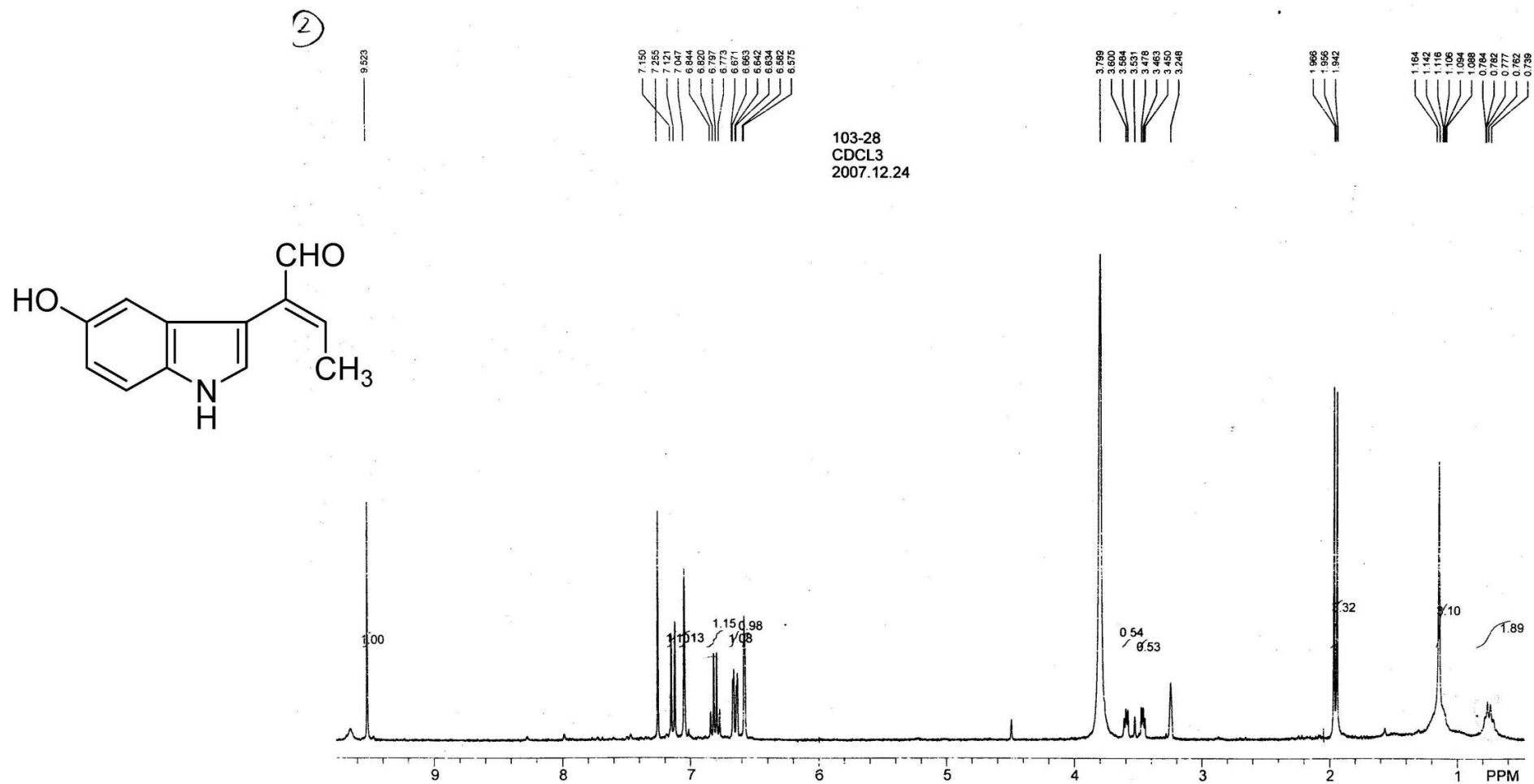


Figure S8.  $^{13}\text{C}$  NMR spectrum of Hainanerectamine B.

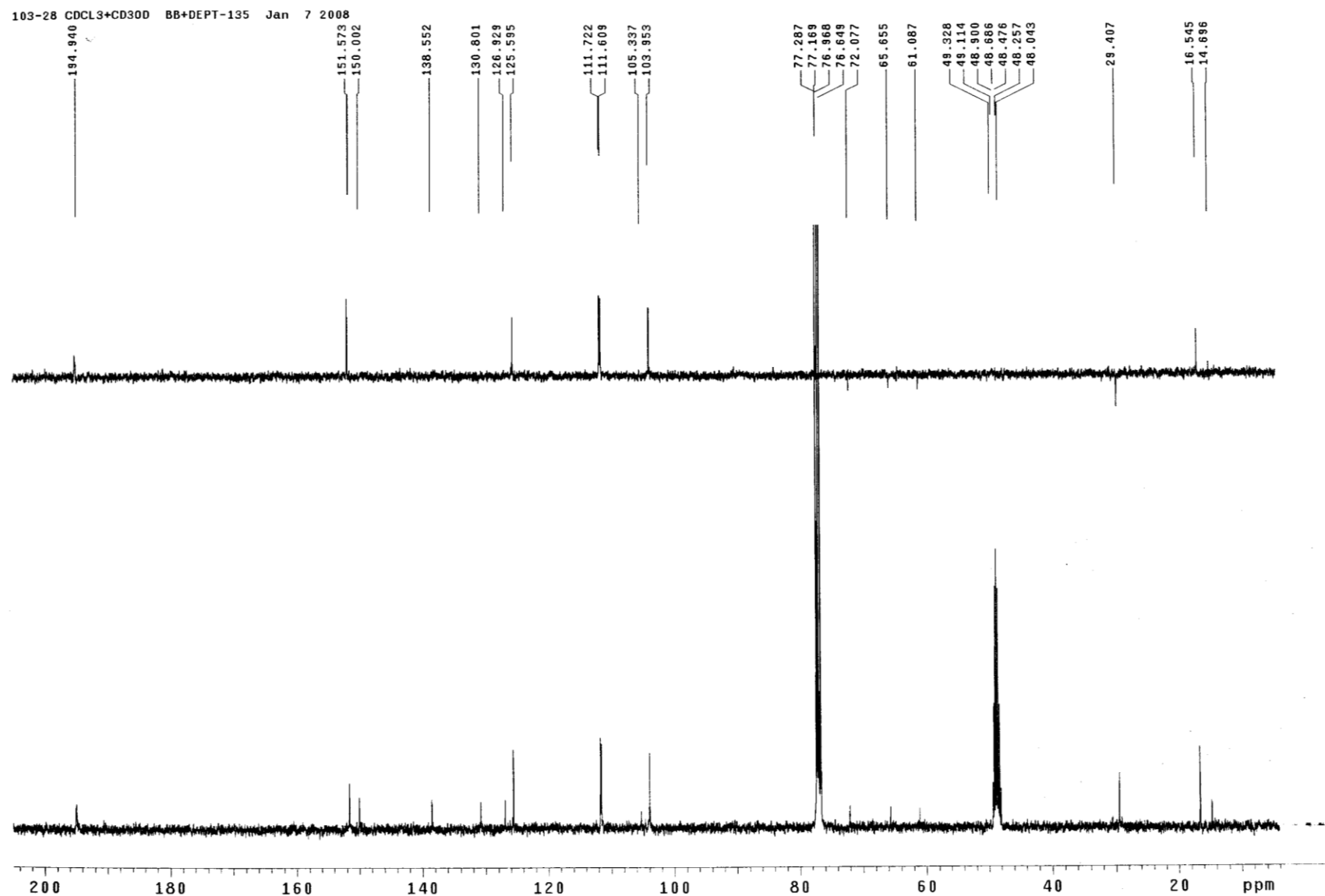




Figure S9. HSQC spectrum of Hainanerectamine B.

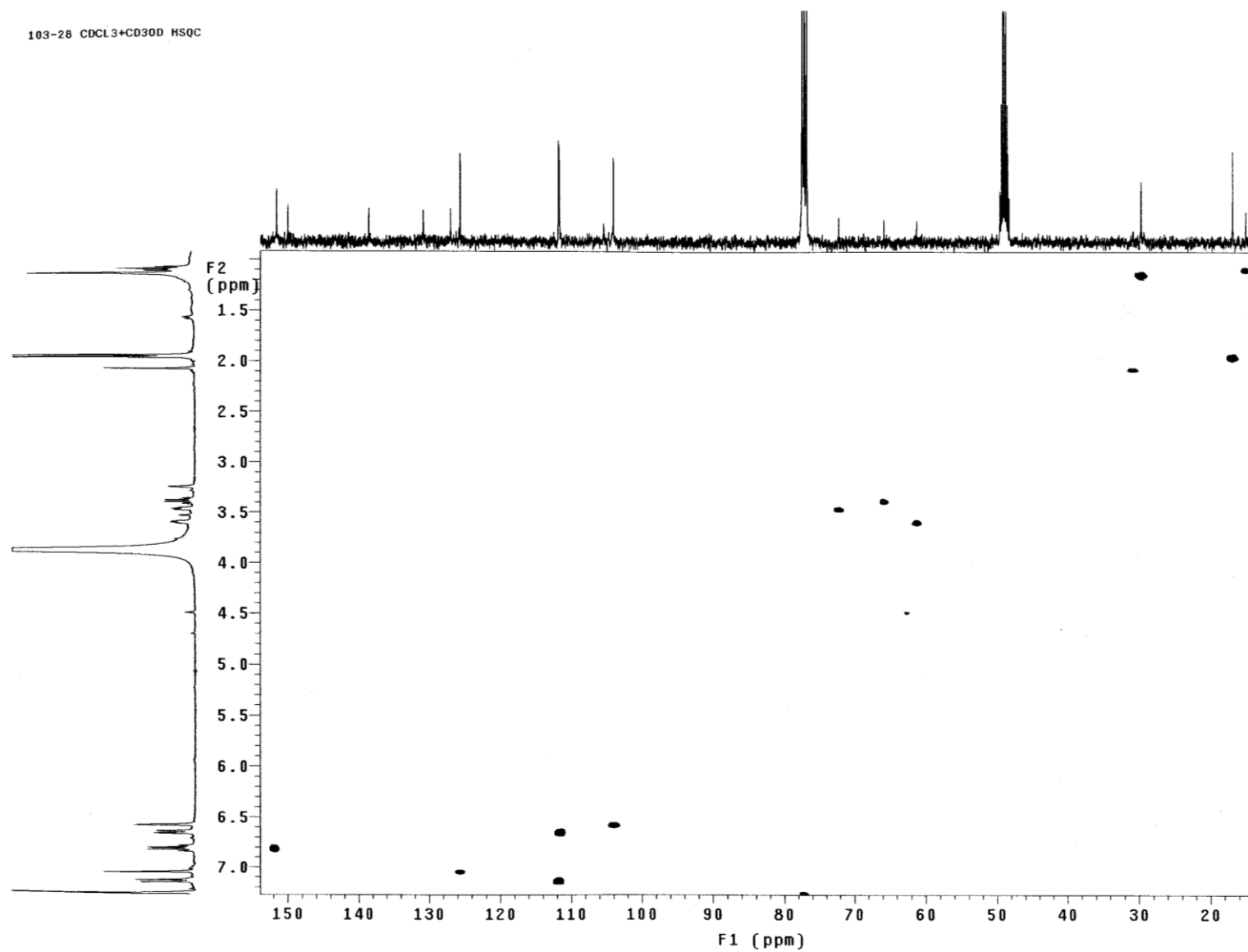


Figure S10. HMBC spectrum of Hainanerectamine B.

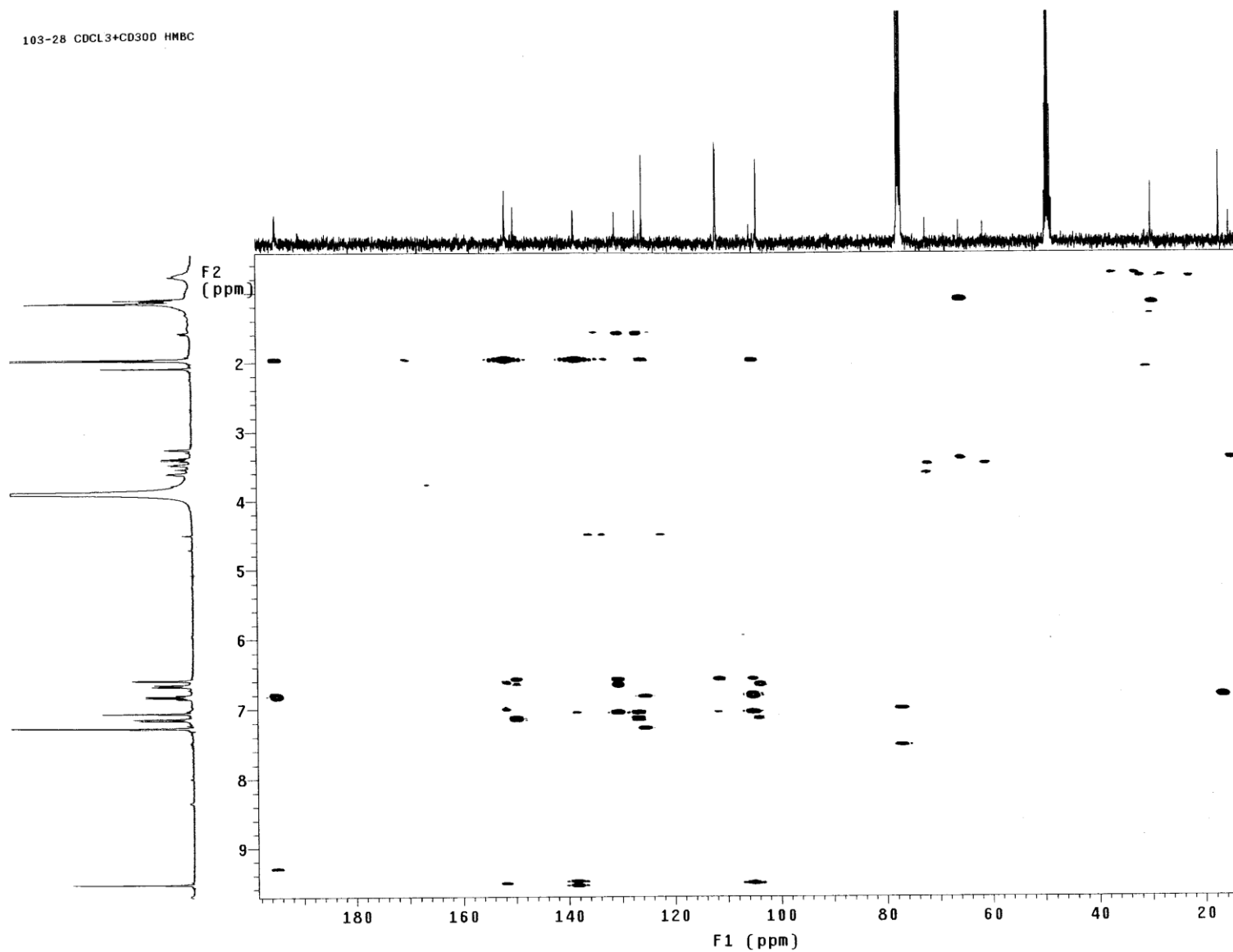


Figure S11. NOE spectrum of Hainanerectamine B.

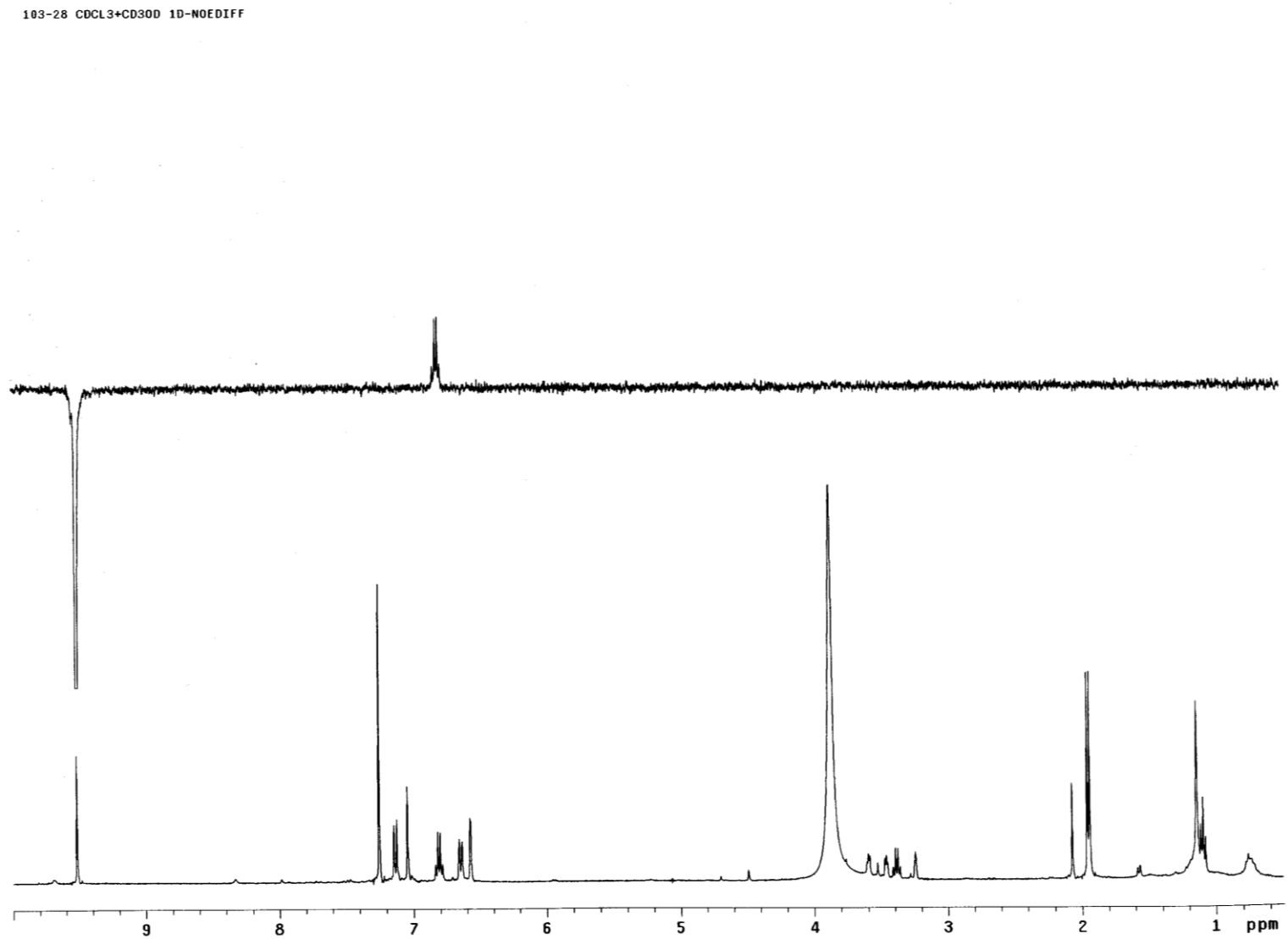


Figure S12. HREI spectrum of Hainanerectamine B.

LIST: h80150-c1 18-Jan-08 Elapse: 08:31.5 41  
 Samp: 103-28 Start : 13:52:28 43  
 Comm: Finnigan/MAT95//70eV/Tsou:200c/R:10000  
 Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM  
 Oper: WANG\_J@SIMM.CAS Client: S/N:SW01-0001 Inlet :  
 Limt: ( 0 )  
 : ( 303 ) C13.H100.N.O2  
 Peak: 1000.00 mmu R+D: -2.0 > 60.0  
 Data: CMASS : converted

Mass	Intensity	%RA	%RIC	Delta	R+D	Composition
51.0307 *	10949	3.89	0.04	1.3	-1.0	H5.N.O2
55.0639 *	8509	3.02	0.03			
57.0785 *	13091	4.65	0.04			
59.0457 *	10175	3.62	0.03			
63.0330 *	15353	5.46	0.05	-1.0	0.0	C.H5.N.O2
65.0486 *	8985	3.19	0.03	-0.9	-1.0	C.H7.N.O2
69.0705 *	7616	2.71	0.02	-0.1	1.5	C5.H9
71.0864 *	7259	2.58	0.02	-0.3	0.5	C5.H11
73.0309 *	6902	2.45	0.02	-2.0	1.5	C3.H5.O2
77.0398 *	9699	3.45	0.03	-0.7	4.5	C6.H5
89.0380 *	11782	4.19	0.04	1.1	5.5	C7.H5
91.0542 *	11068	3.93	0.04	0.5	4.5	C7.H7
102.0485 *	6486	2.30	0.02	-1.6	6.0	C8.H6
108.9938 *	7974	2.83	0.03			
115.0573 *	38799	13.79	0.13	-2.6	6.5	C9.H7
116.0538 *	9402	3.34	0.03			
117.0588 *	7200	2.56	0.02	-1.0	6.0	C8.H7.N
117.0712 *	12080	4.29	0.04	-0.8	5.5	C9.H9
127.0547 *	39334	13.98	0.13	0.0	7.5	C10.H7
128.0499 *	6069	2.16	0.02	0.1	7.5	C9.H6.N
133.0523 *	13091	4.65	0.04	0.4	6.0	C8.H7.N.O
142.0652 *	12080	4.29	0.04	0.5	7.5	C10.H8.N
143.0733 *	13448	4.78	0.04	0.2	7.0	C10.H9.N
144.0456 *	8807	3.13	0.03	-0.6	7.5	C9.H6.N.O
144.0581 *	8033	2.85	0.03	-0.6	7.0	C10.H8.O
144.0815 *	19994	7.10	0.07	-0.2	6.5	C10.H10.N
145.0514 *	9045	3.21	0.03	1.4	7.0	C9.H7.N.O
145.0643 *	26123	9.28	0.09	1.0	6.5	C10.H9.O
146.0623 *	15174	5.39	0.05	-1.7	6.5	C9.H8.N.O
146.9863 *	10175	3.62	0.03			
149.0245 *	13567	4.82	0.04	2.0	11.0	C11.H3.N
154.0653 *	21541	7.65	0.07	0.3	8.5	C11.H8.N
155.0723 *	6843	2.43	0.02	1.2	8.0	C11.H9.N
156.0806 *	13924	4.95	0.05	0.7	7.5	C11.H10.N
157.0530 *	16840	5.98	0.06	-0.2	8.0	C10.H7.N.O
158.0598 *	13270	4.72	0.04	0.8	7.5	C10.H8.N.O
160.0393 *	16483	5.86	0.05	0.5	7.5	C9.H6.N.O2
170.0604 *	27314	9.71	0.09	0.2	8.5	C11.H8.N.O
171.0665 *	15888	5.65	0.05	2.0	8.0	C11.H9.N.O
172.0752 *	193578	68.79	0.63	1.1	7.5	C11.H10.N.O
173.0811 *	44630	15.86	0.15			
173.9852 *	42250	15.01	0.14			
196.9841 *	8390	2.98	0.03			
199.0630 *	6188	2.20	0.02	0.3	9.0	C12.H9.N.O2
200.0705 *	8152	2.90	0.03	0.7	8.5	C12.H10.N.O2
201.0787 *	281412	100.00	0.92	0.3	8.0	C12.H11.N.O2
202.0820 *	29337	10.42	0.10			

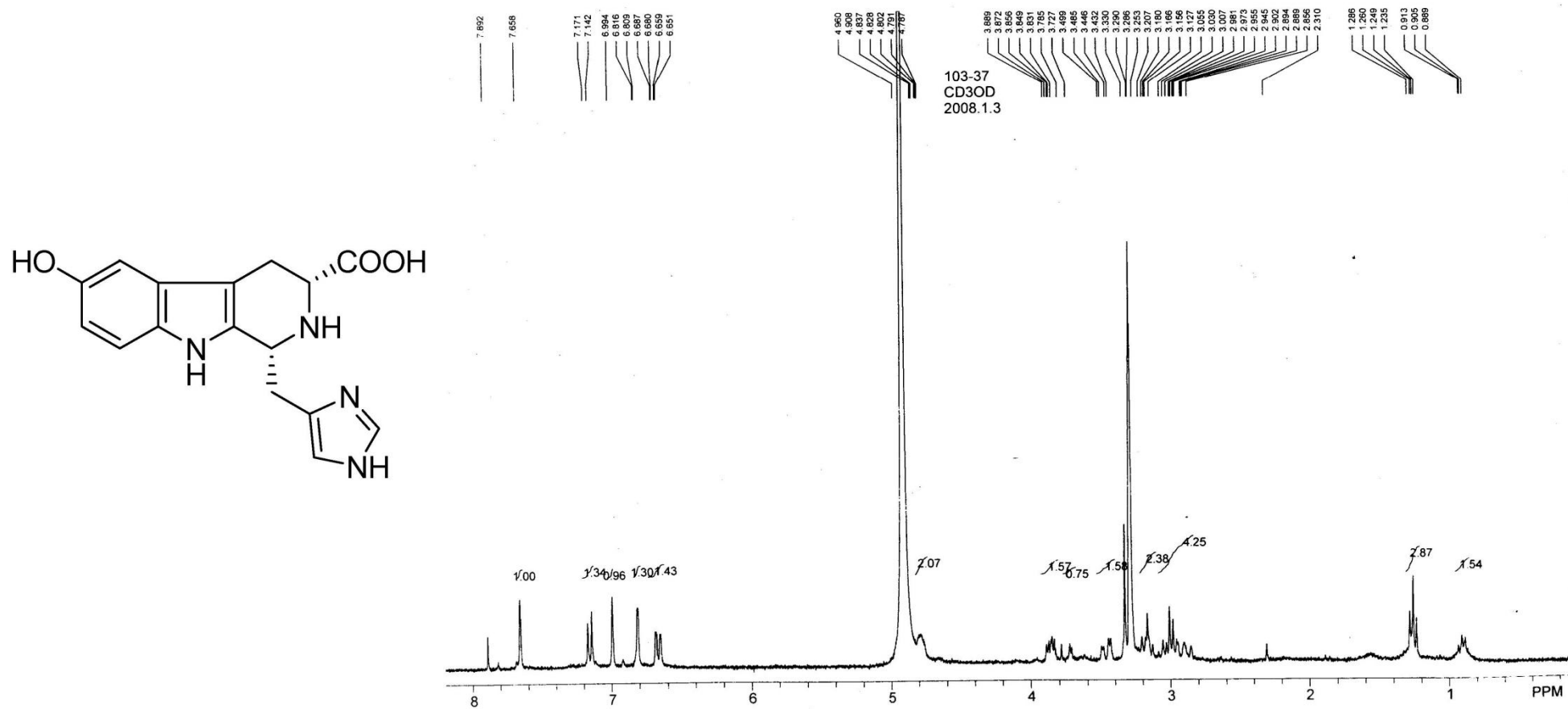
Figure S13.  $^1\text{H}$  NMR spectrum of Compound 3.

Figure S14.  $^{13}\text{C}$  NMR spectrum of Compound 3.

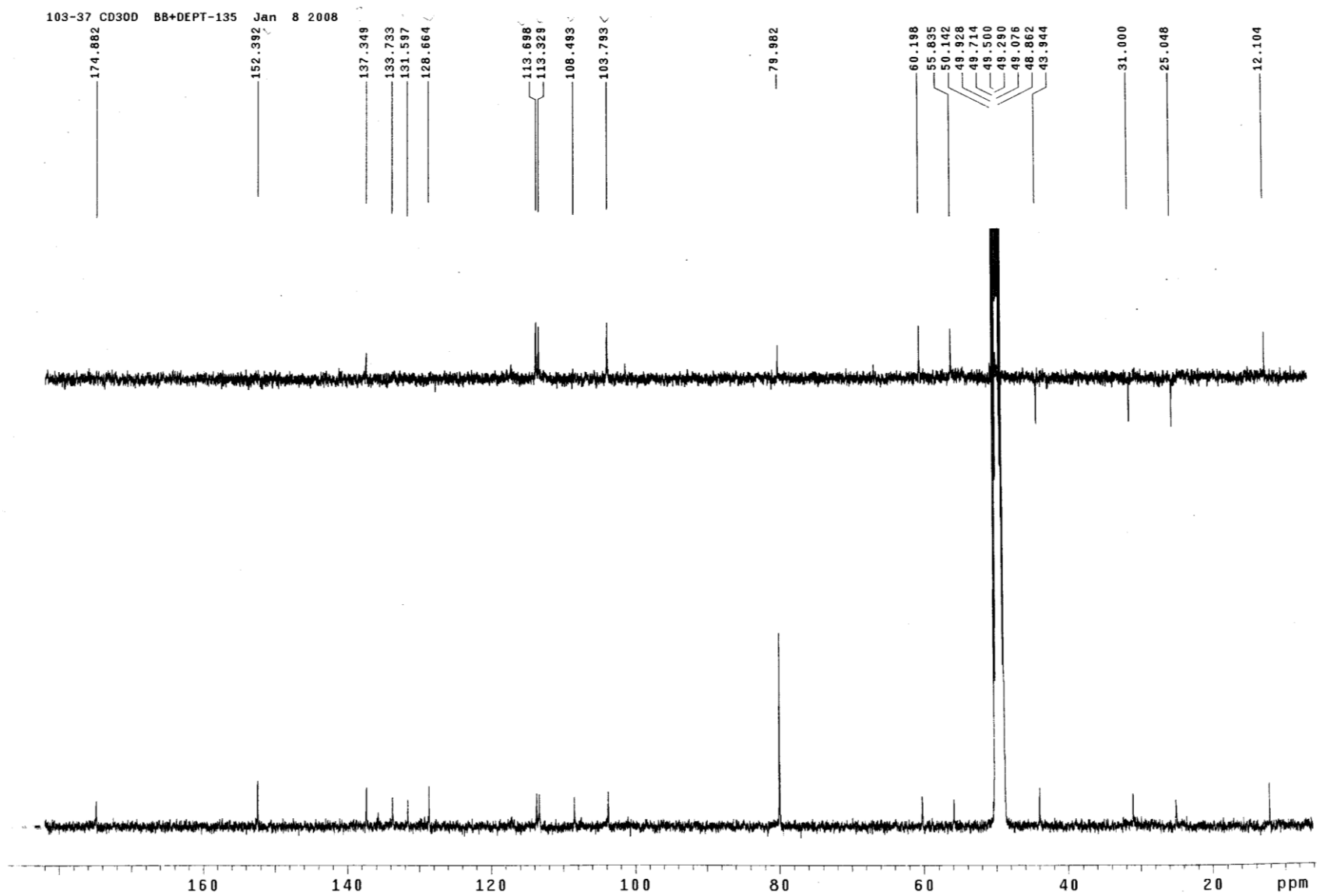


Figure S15.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of Compound 3.

103-37 CD3OD COSY

Solvent: cd3od  
Ambient temperature  
File: 103-37\_cosy  
Mercury-400BB "SIMM400"

Relax. delay 1.000 sec  
Mixing 0.080 sec  
Acq. time 0.128 sec  
Width 8012.8 Hz  
2D Width 8012.8 Hz  
8 repetitions  
320 increments  
OBSERVE H1, 399.7719973 MHz  
DATA PROCESSING  
Sq. sine bell 0.064 sec  
F1 DATA PROCESSING  
Sq. sine bell 0.020 sec  
FT size 2048 x 2048  
Total time 52 min, 58 sec

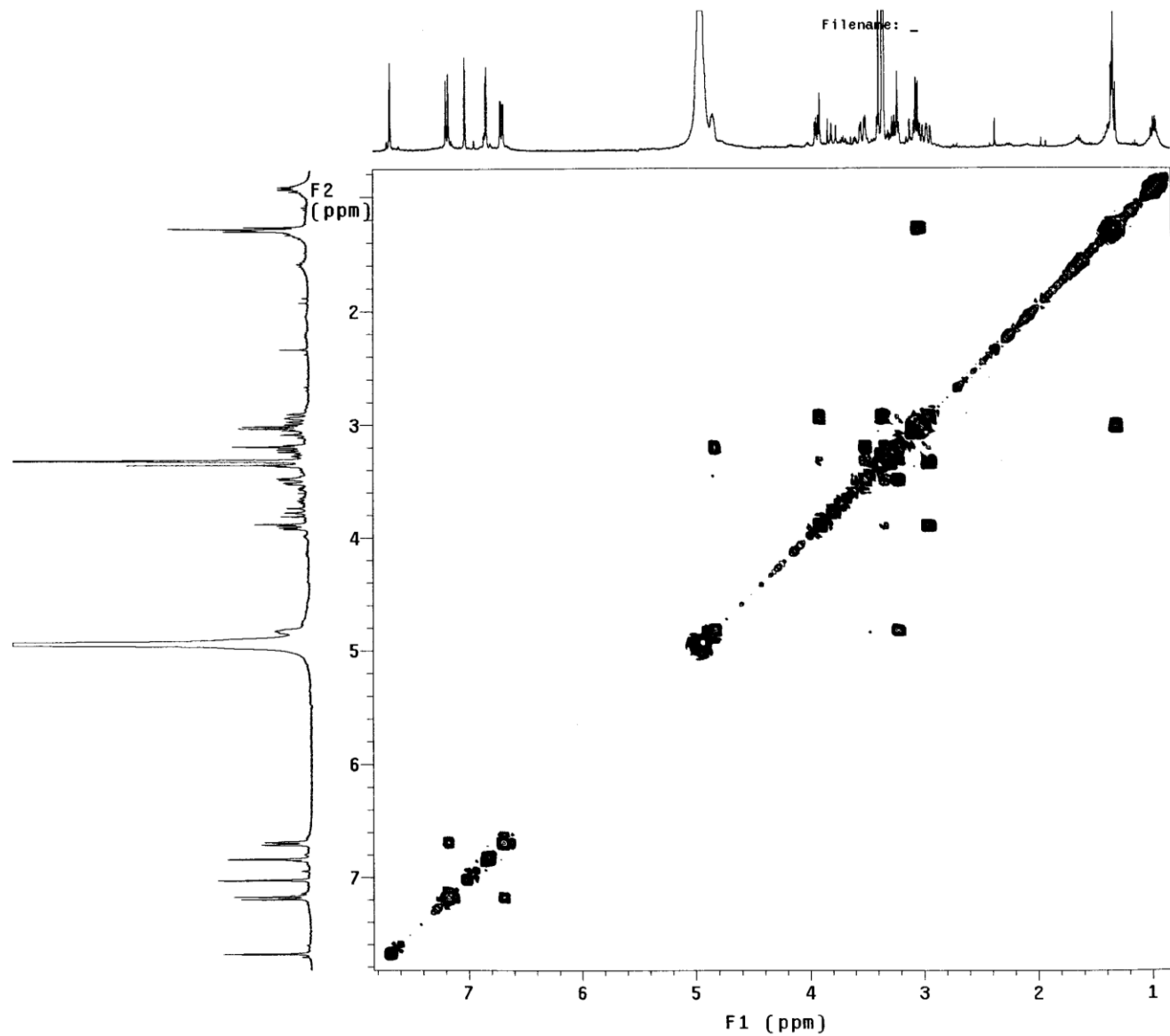


Figure S16. HSQC spectrum of Compound 3.

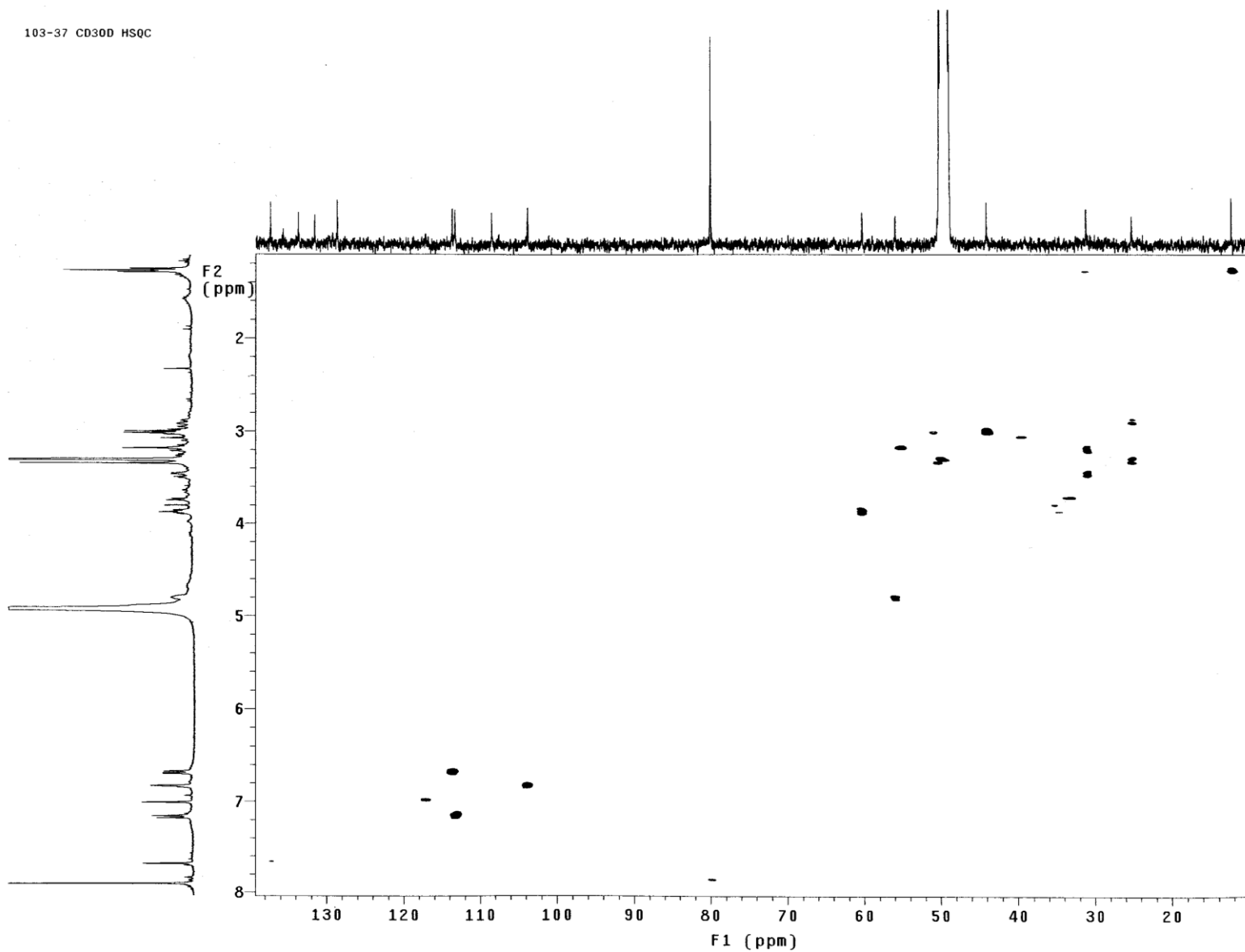




Figure S17. HMBC spectrum of Compound 3.

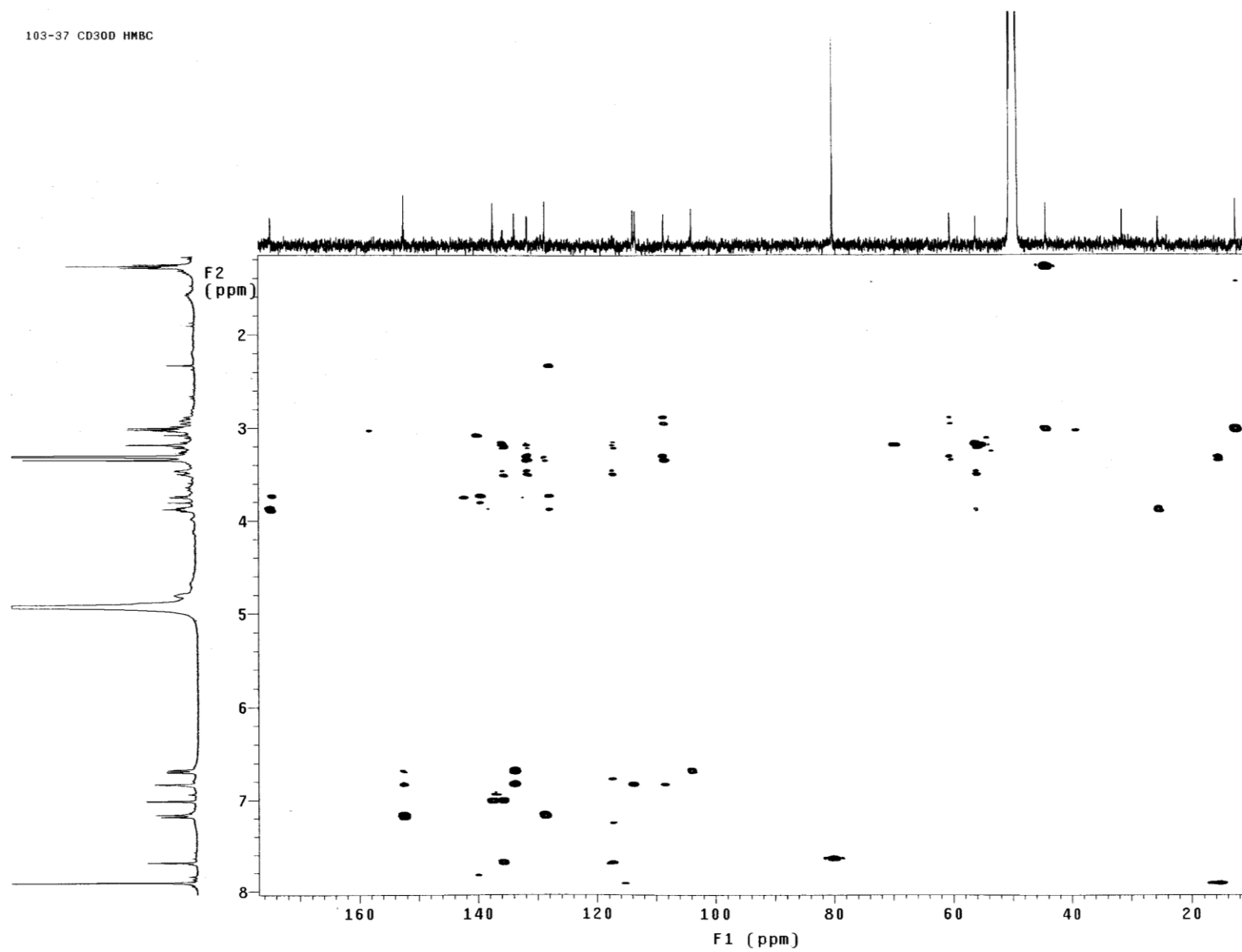


Figure S18. ROESY spectrum of Compound 3.

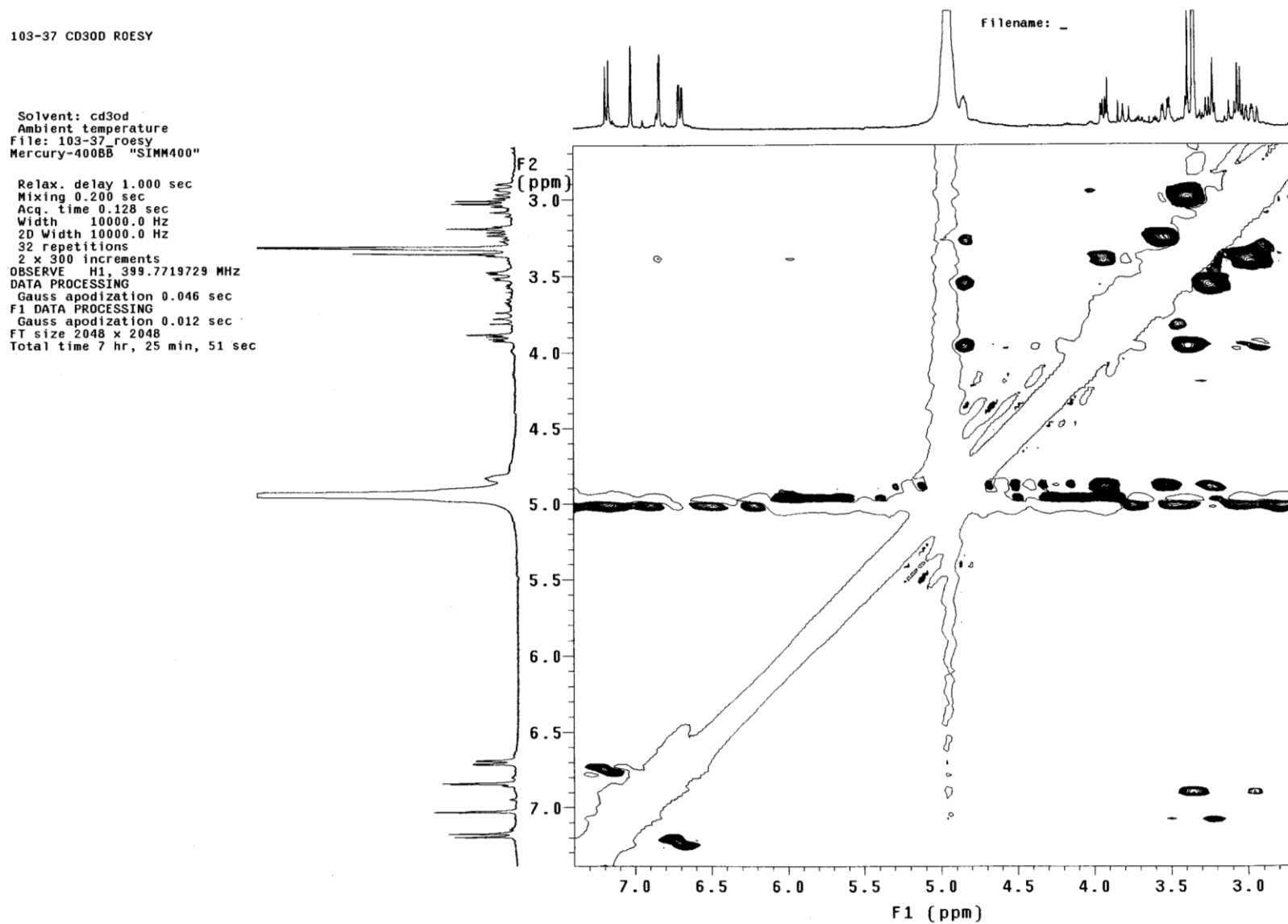


Figure S19. HRESI spectrum of Compound 3.

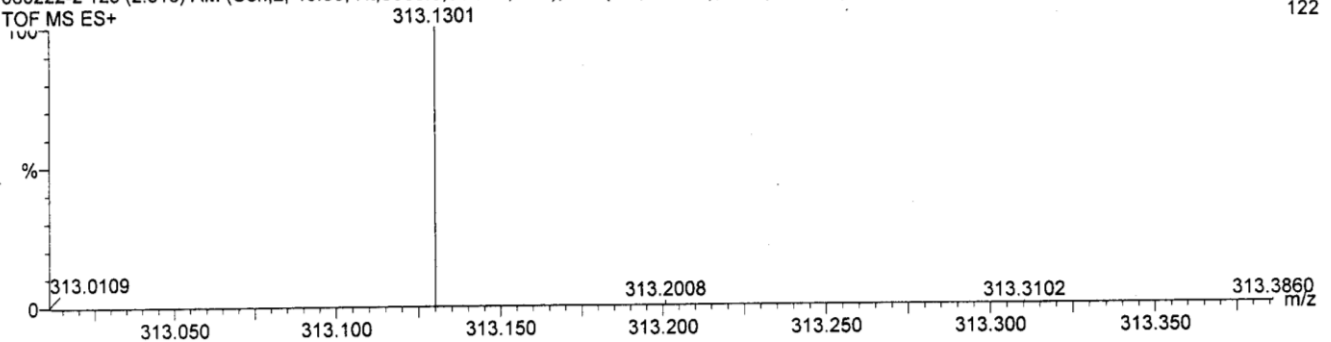
Elemental Composition Report

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0  
 Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions  
 24 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

080222-2 123 (2.316) AM (Cen,2, 40.00, Ht,5000.0,362.93,1.00); Sm (SG, 2x3.00); Cm (117:145)

122



Minimum: 50.00  
 Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
313.1301	100.00	313.1301	0.0	0.1	10.5	1	C16 H17 N4 O3

Figure S20. IR spectrum of Compound 3.

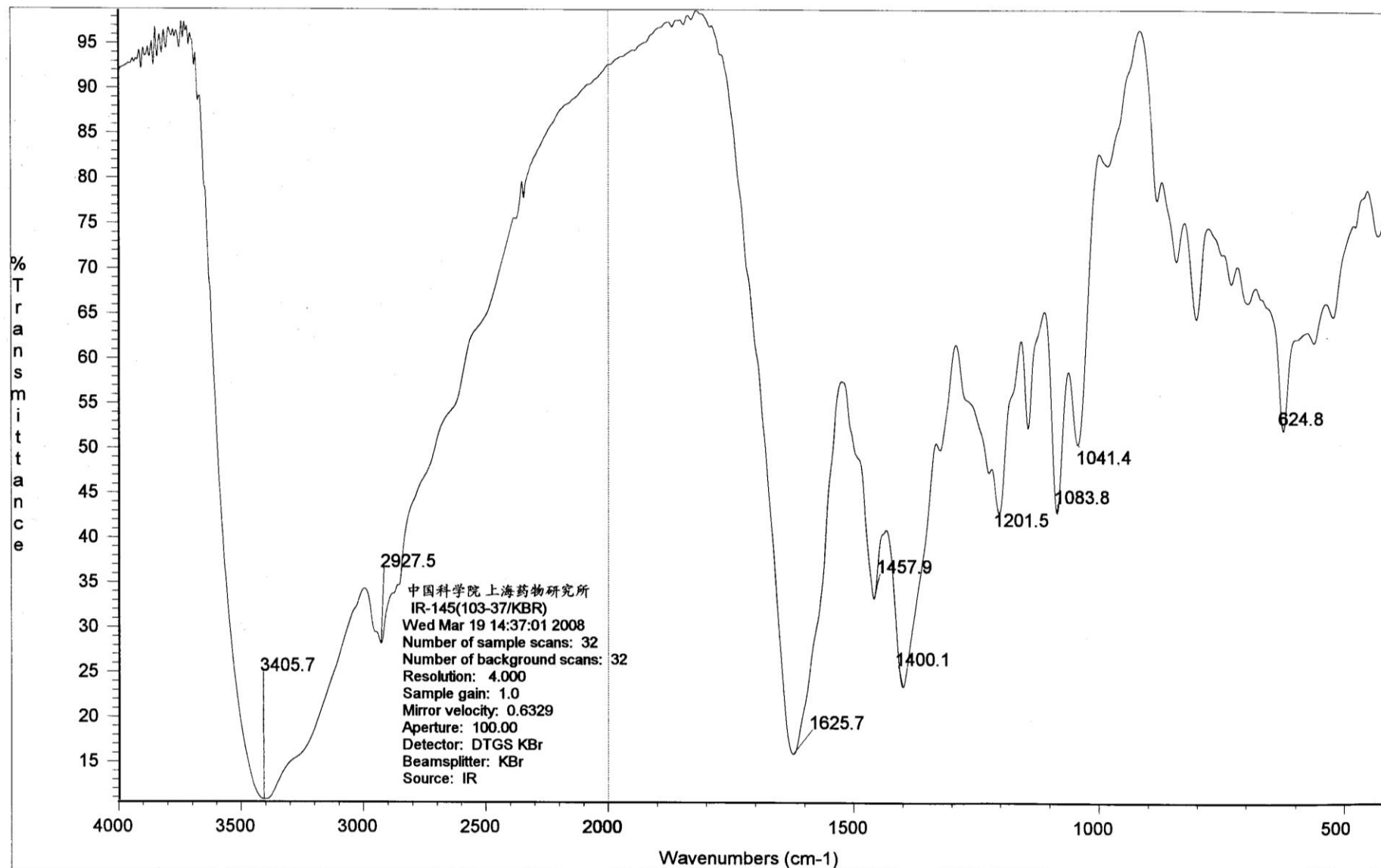


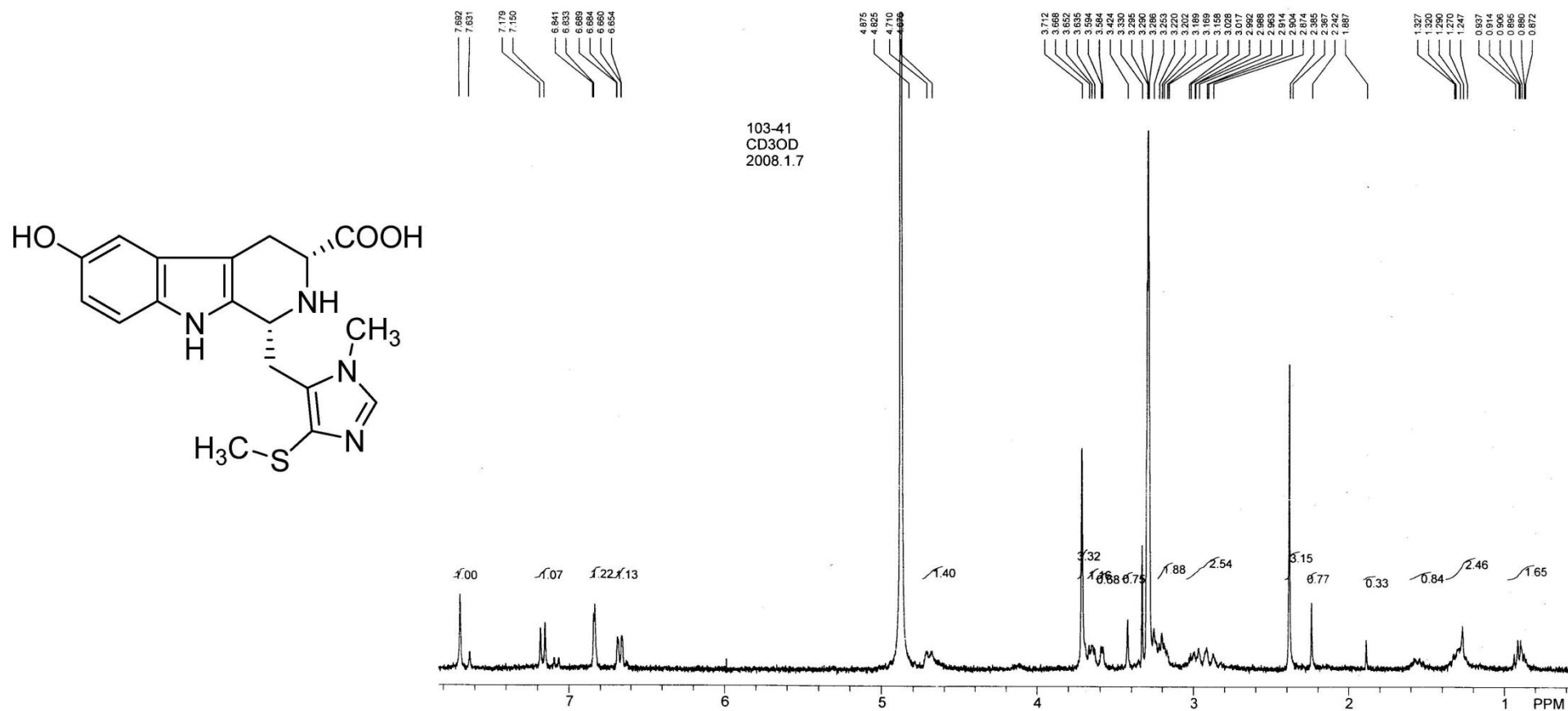
Figure S21.  $^1\text{H}$  NMR spectrum of Hainanerectamine C.

Figure S22. <sup>13</sup>C NMR spectrum of Hainanerectamine C.

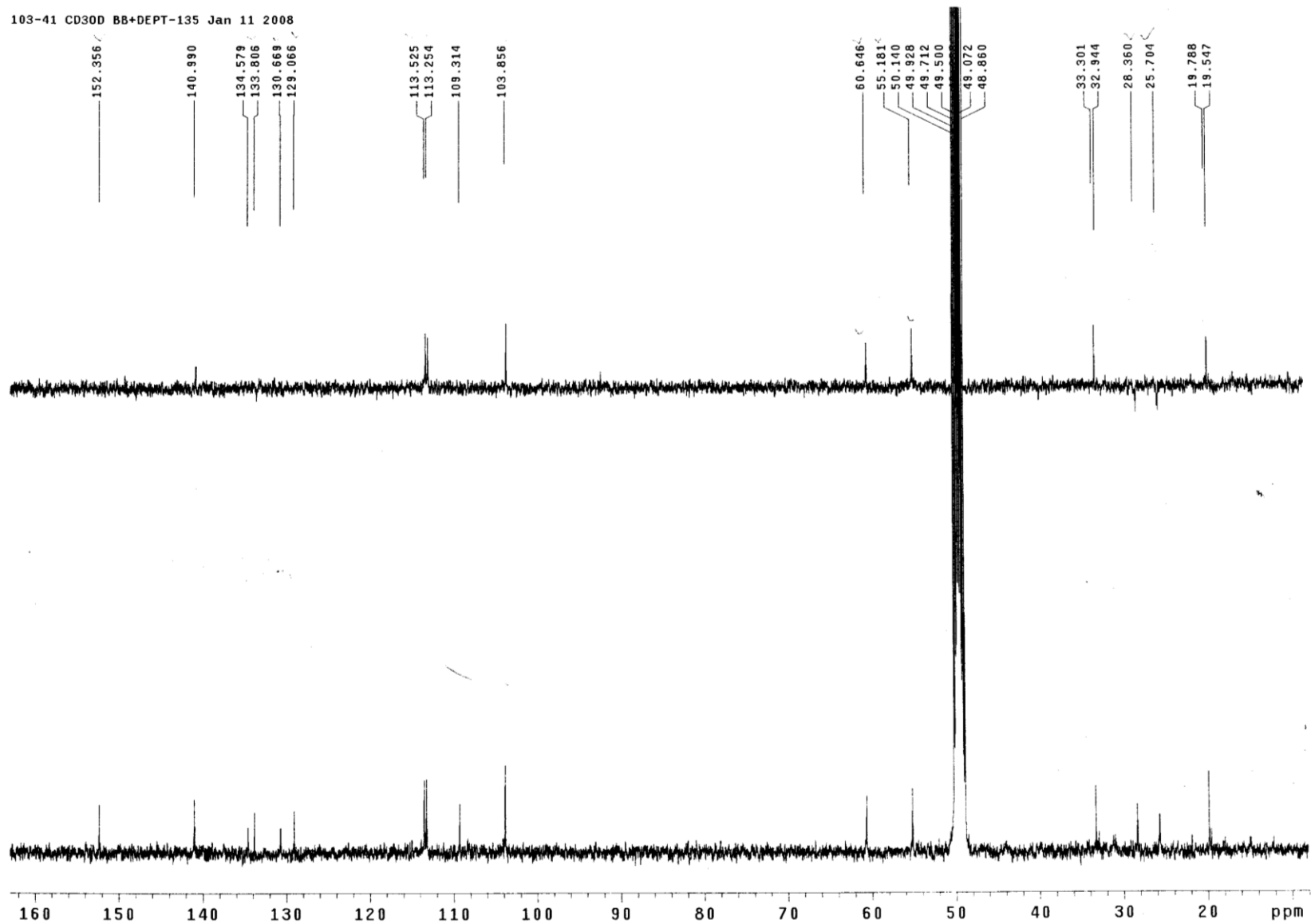


Figure S23. HSQC spectrum of Hainanectamine C.

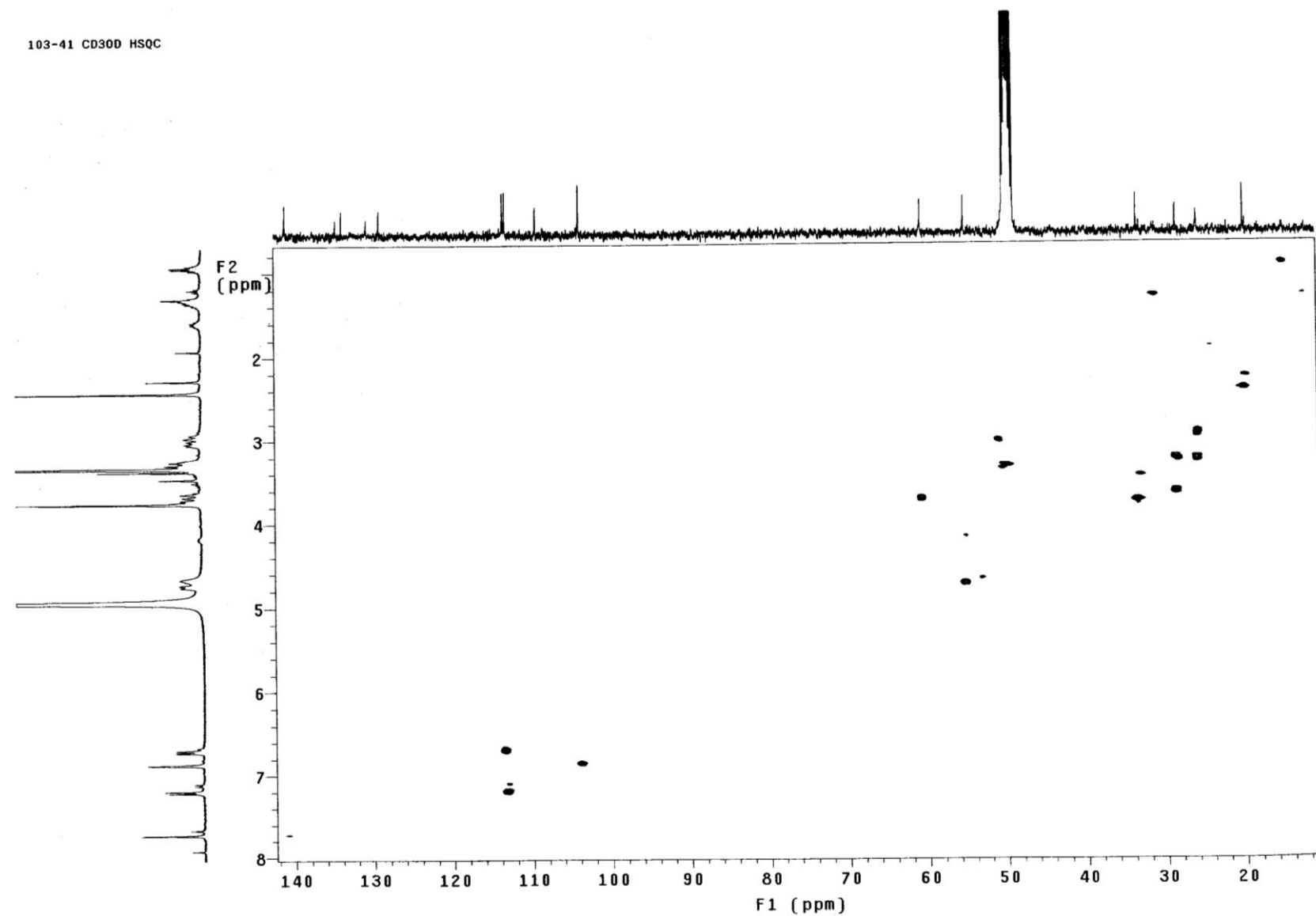


Figure S24. HMBC spectrum of Hainanerectamine C.

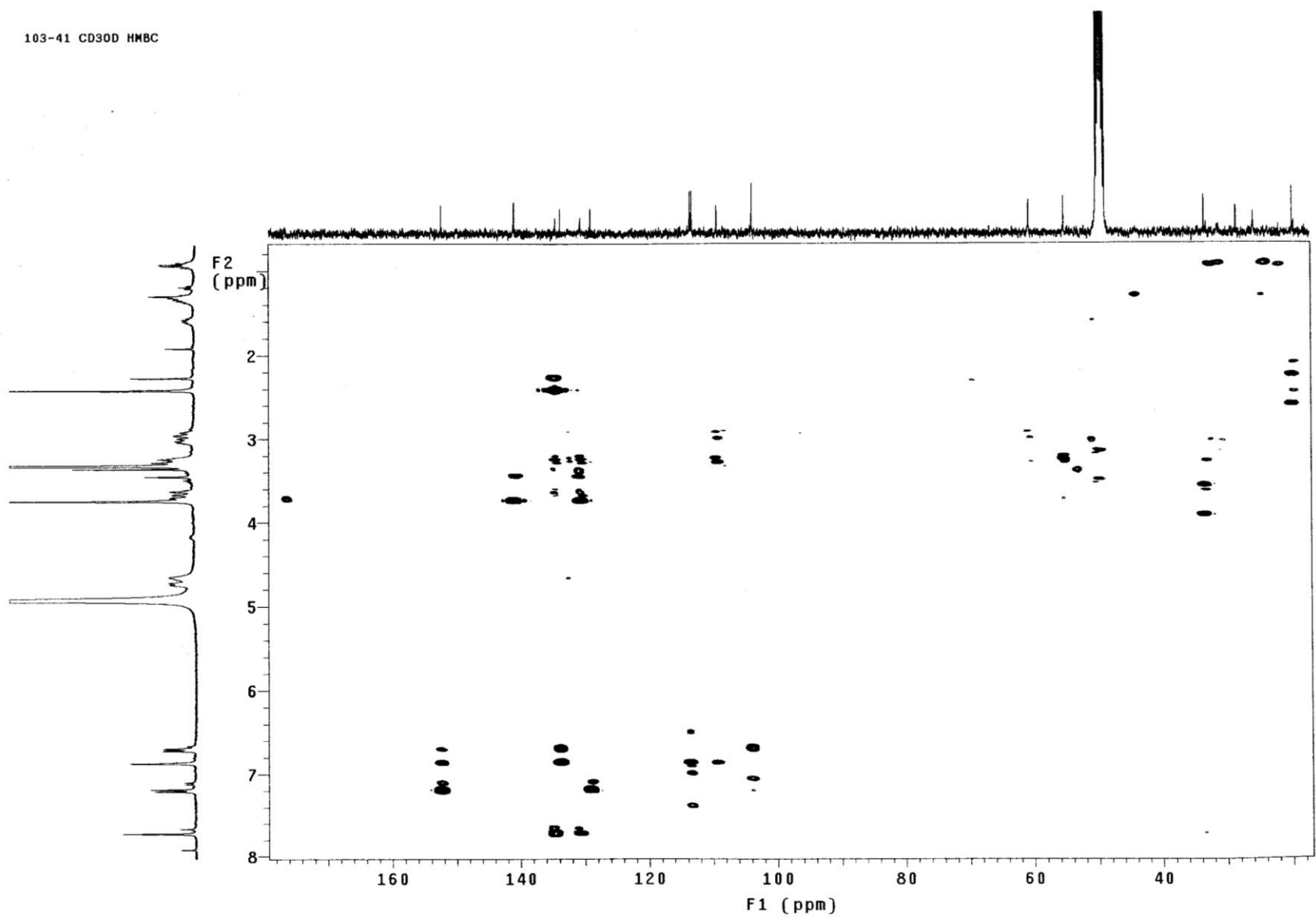




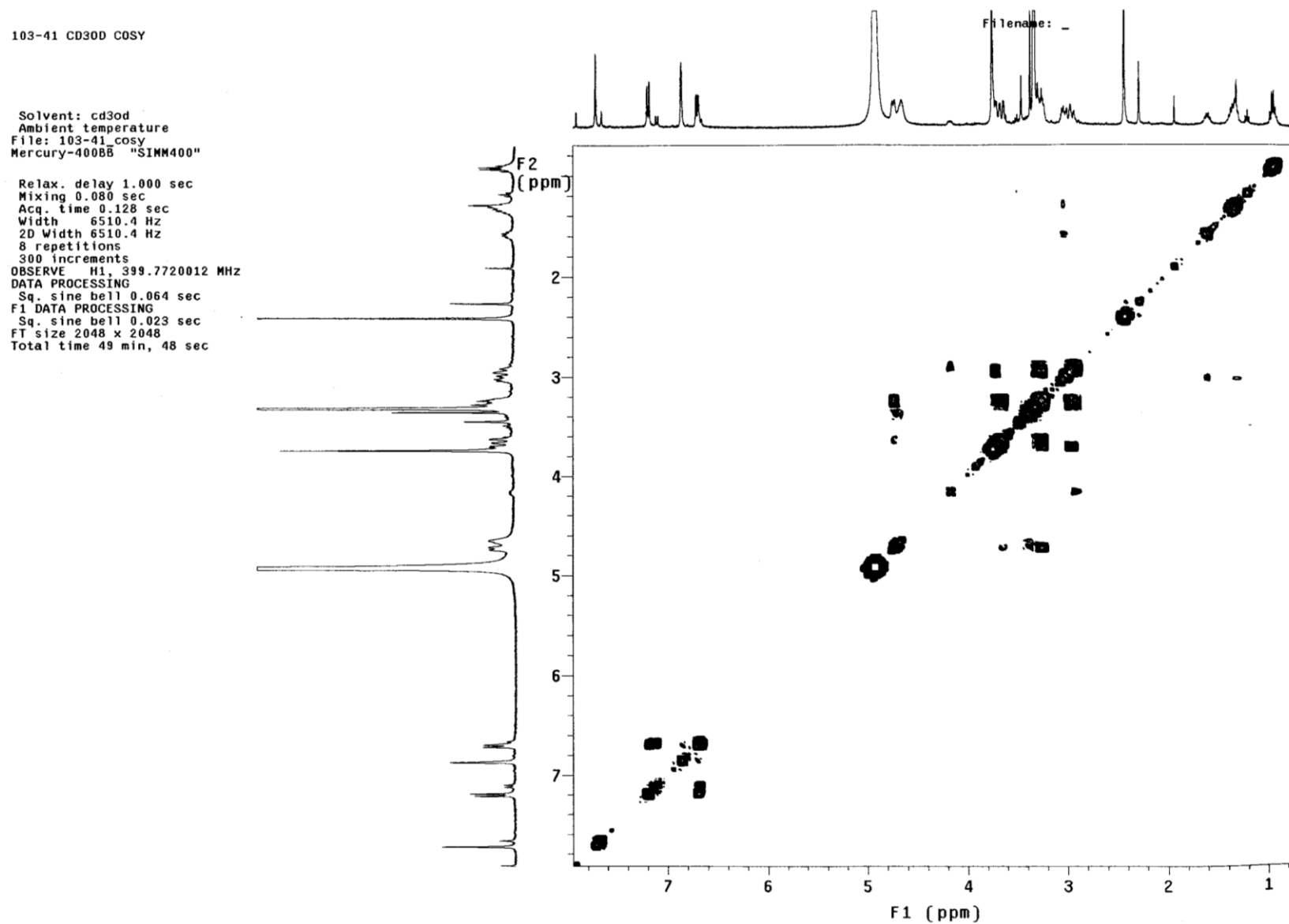
Figure S25.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of Hainanerectamine C.

Figure S26. ROESY spectrum of Hainanerectamine C.

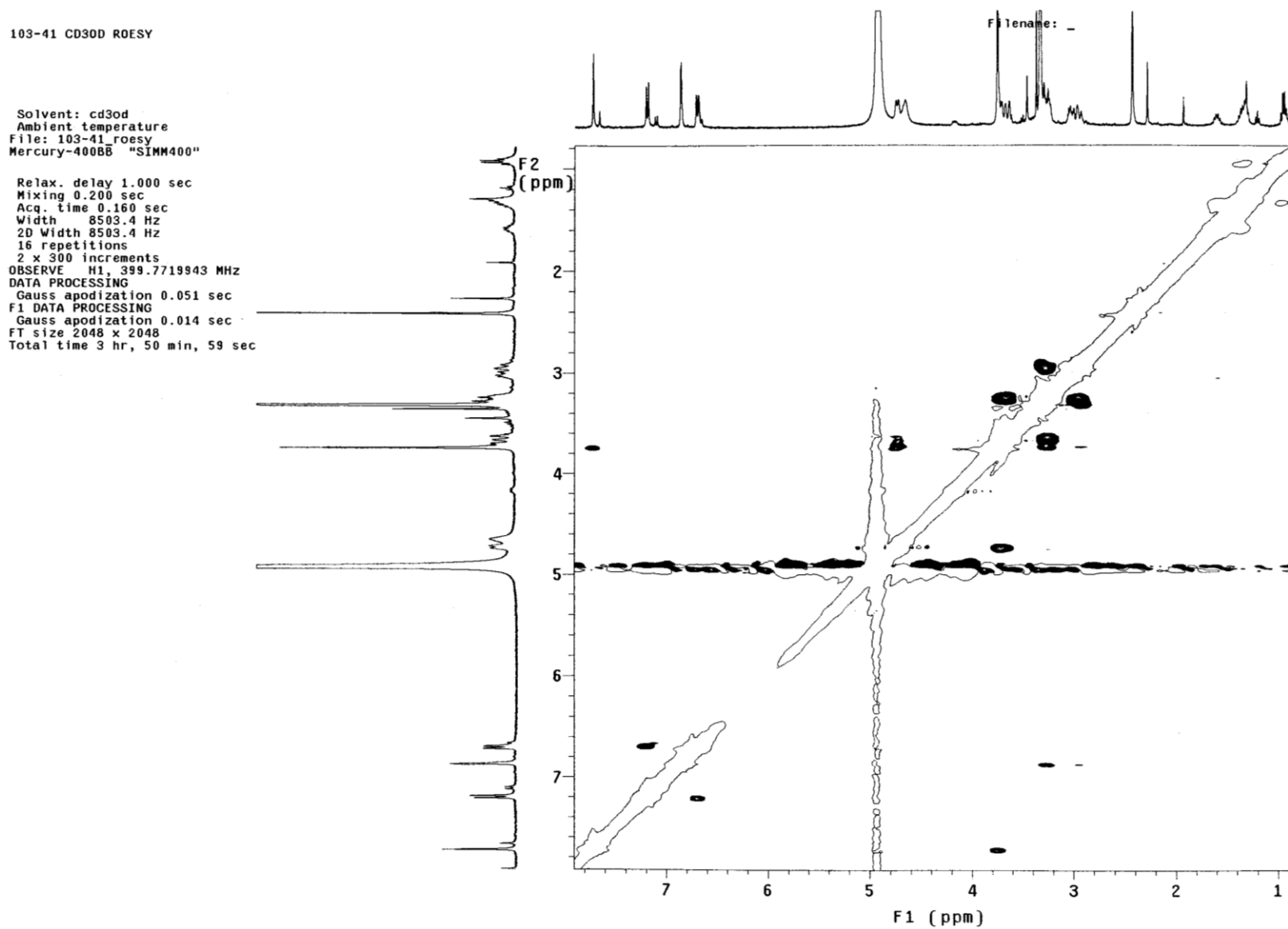


Figure S27. HRESI spectrum of Hainanerectamine C.

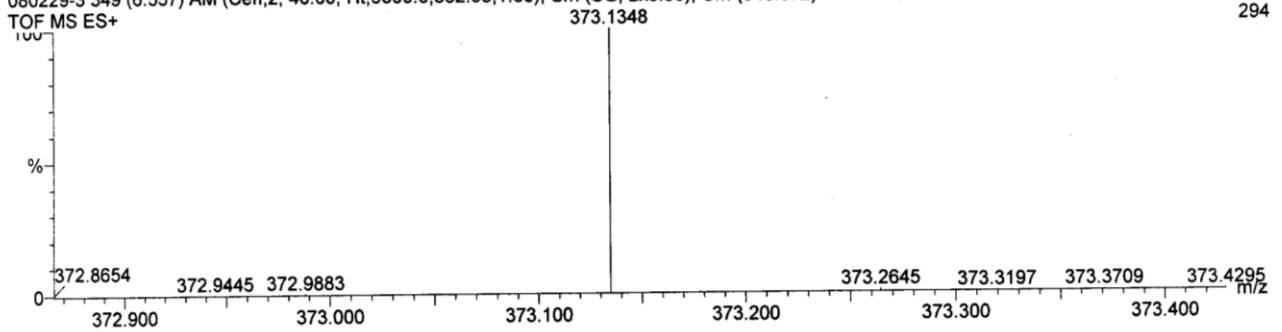
Elemental Composition Report

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0  
 Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions  
 36 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

080229-3 349 (6.557) AM (Cen,2, 40.00, Ht,5000.0,362.93,1.00); Sm (SG, 2x3.00); Cm (346:372)  
 TOF MS ES+

294



Minimum: 50.00  
 Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
373.1348	100.00	373.1334	1.4	3.7	10.5	1	C18 H21 N4 O3 S

Figure S28. IR spectrum of Hainanerectamine C.

