Supporting Information (SI)

Alkaloids with Different Carbon Units from *Myrioneuron faberi*

Ming-Ming Cao,[†,‡] Yu Zhang,[†] Sheng-Dian Huang,[†] Ying-Tong Di,[†] Zong-Gen Peng,[§] Jian-Dong Jiang,[§] Chun-Mao Yuan,[†] Duo-Zhi Chen,[†] Shun-Lin Li,[†] Hong-Ping He,[†] and Xiao-Jiang Hao[*,†]

† State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650201, Yunnan, People's Republic of China

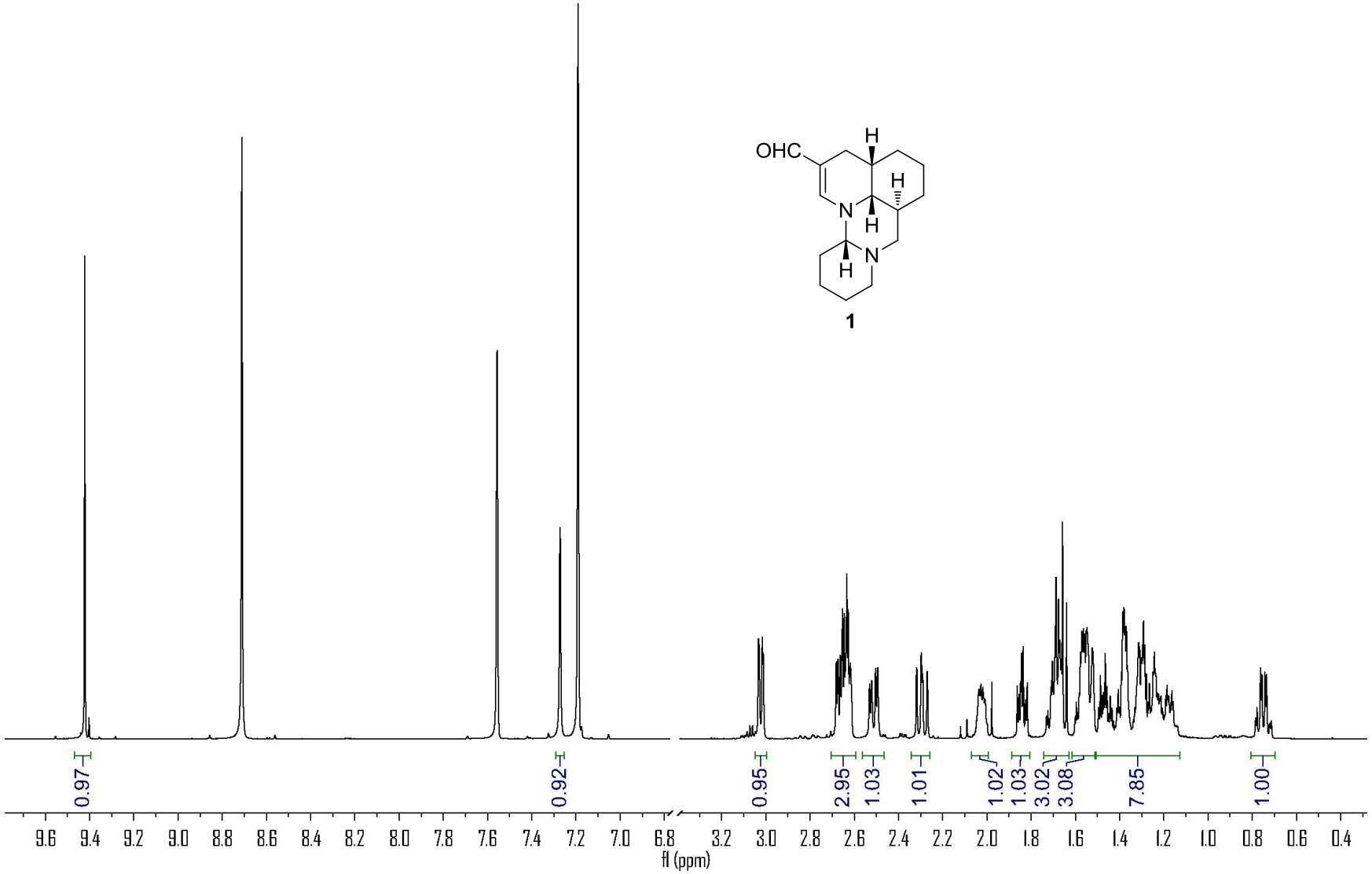
‡ College of Food Science and Technology, Nanjing Agricultural University, Nanjing 210095, Jiangsu, People's Republic of China

§ Institute of Medicinal Biotechnology, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 10050, People's Republic of China

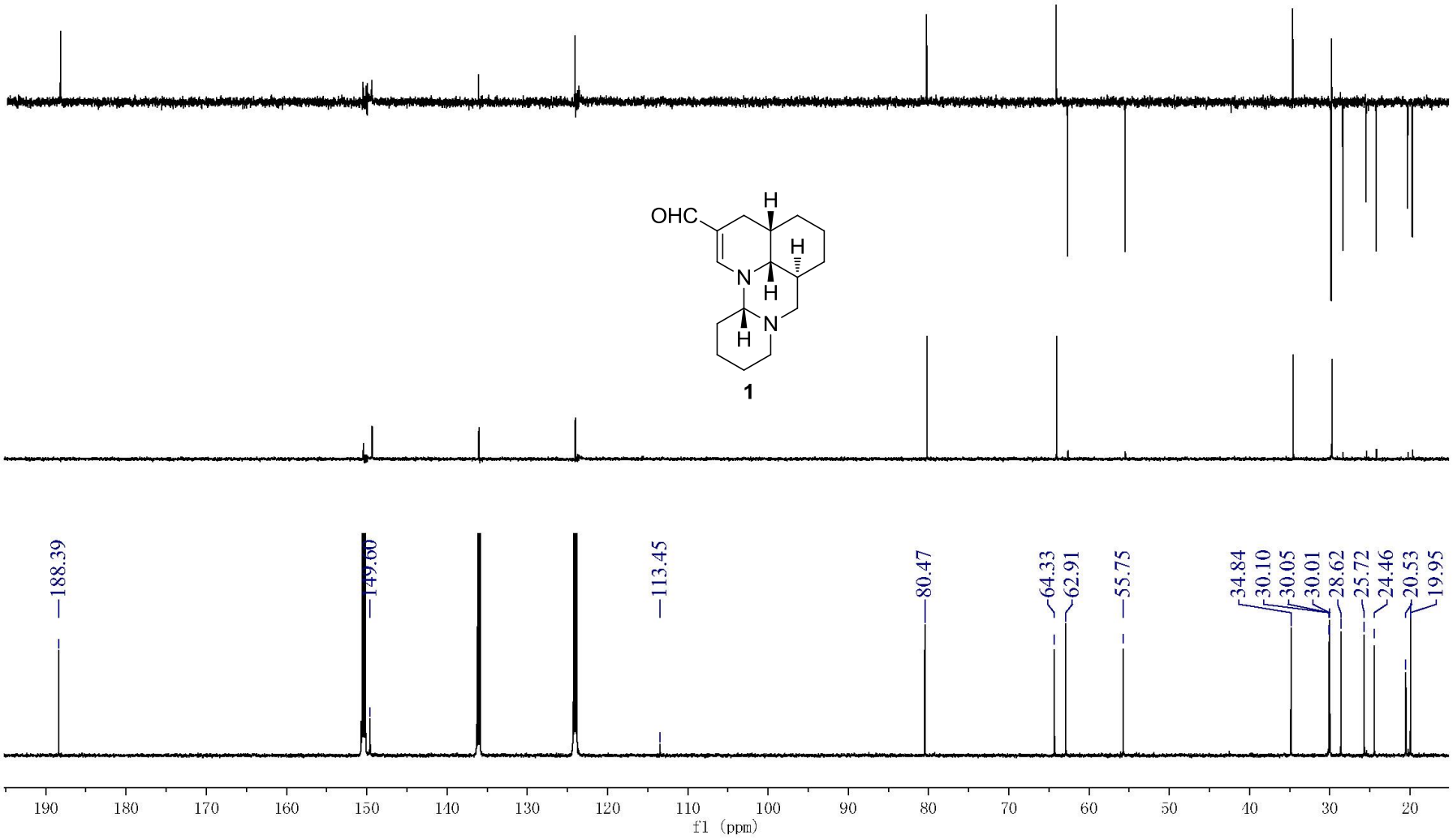
* To whom correspondence should be addressed. Tel: +86-871-65223263. Fax: +86-871-65223070. E-mail: haoxj@mail.kib.ac.cn.

Contents

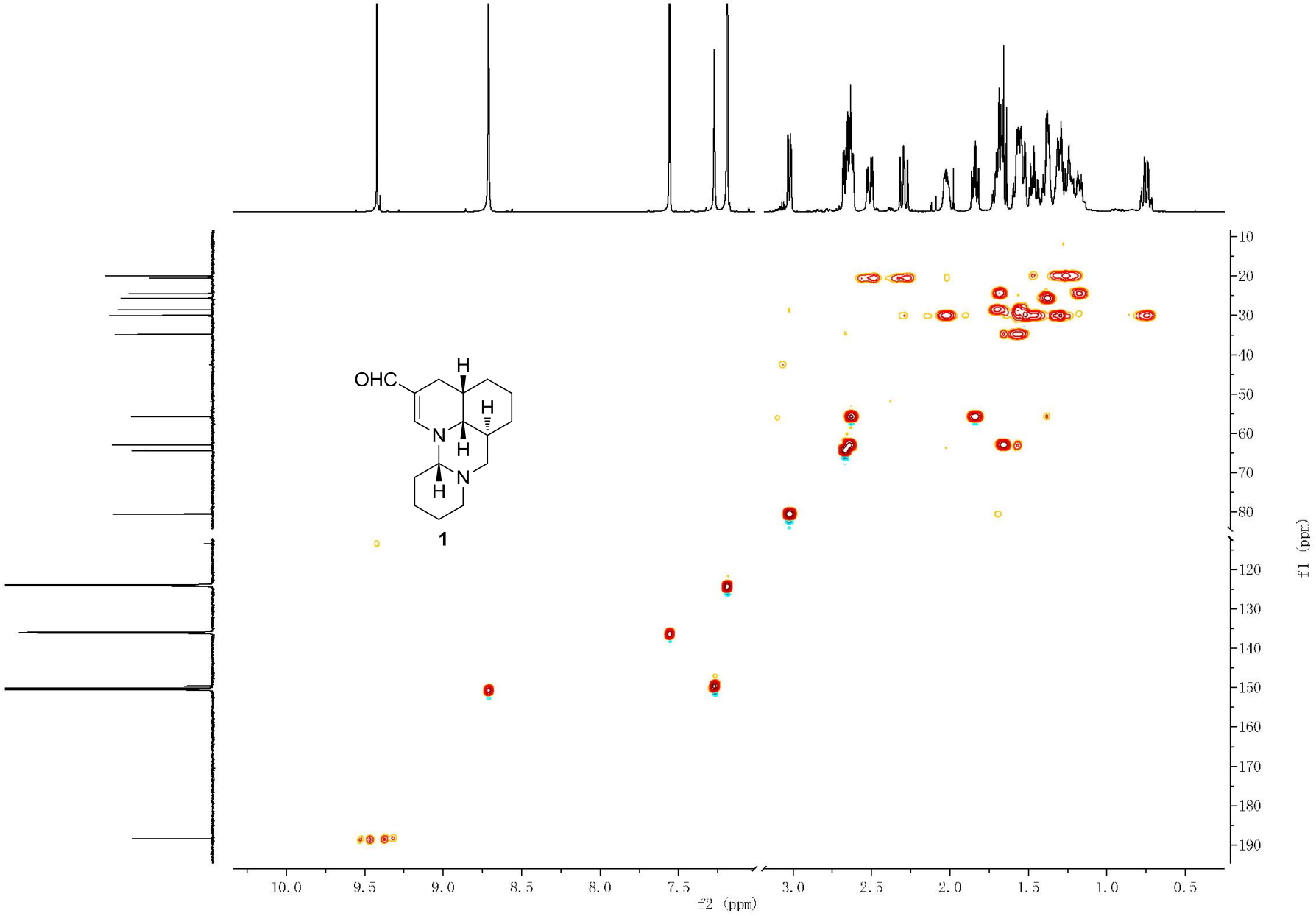
S1.1 ^{1}H NMR spectrum of myrifamine A (**1**) in prydine-d_5 at 294K



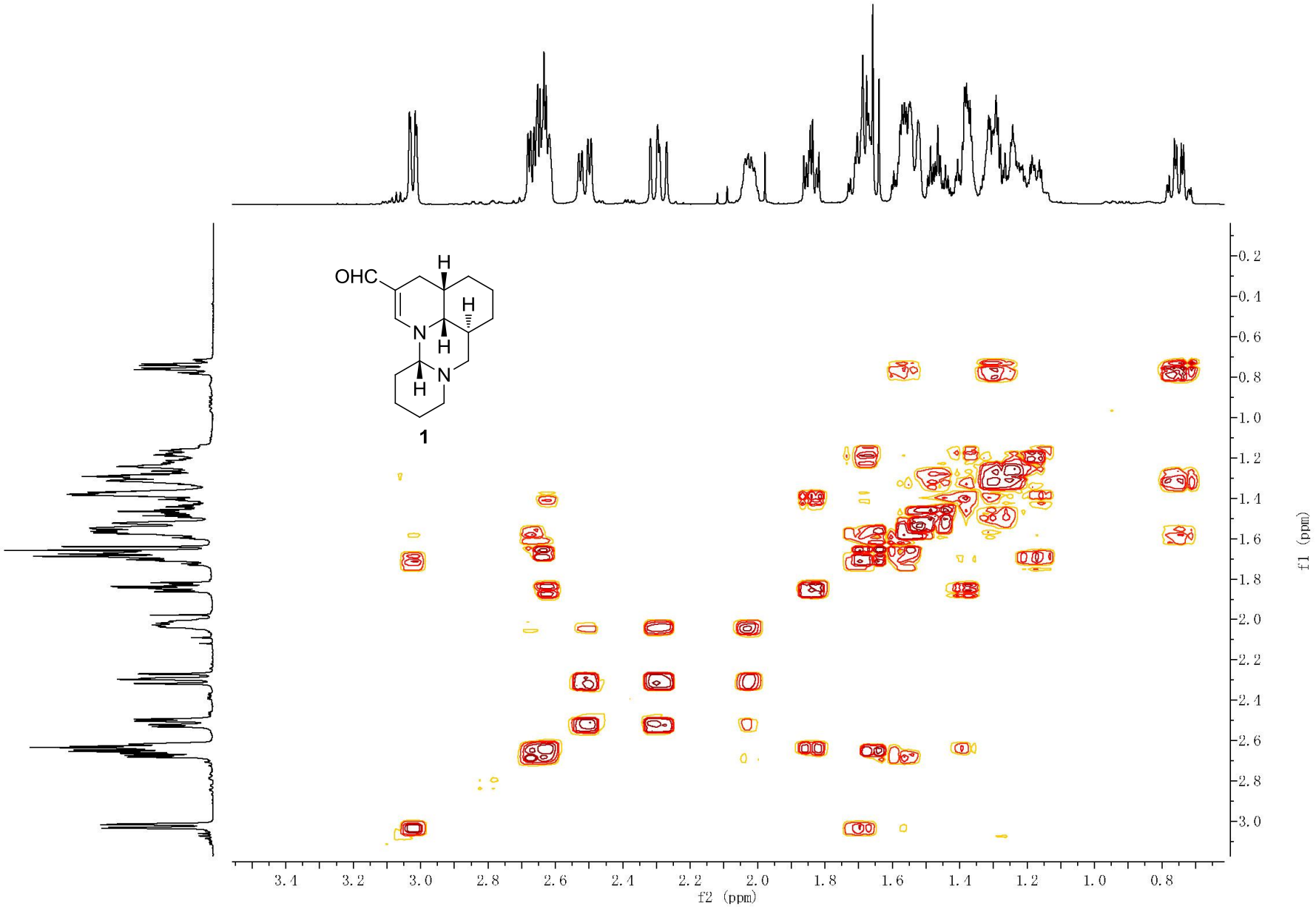
S1.2 ^{13}C NMR spectrum of myrifamine A (**1**) in prydine-d_5 at 294K



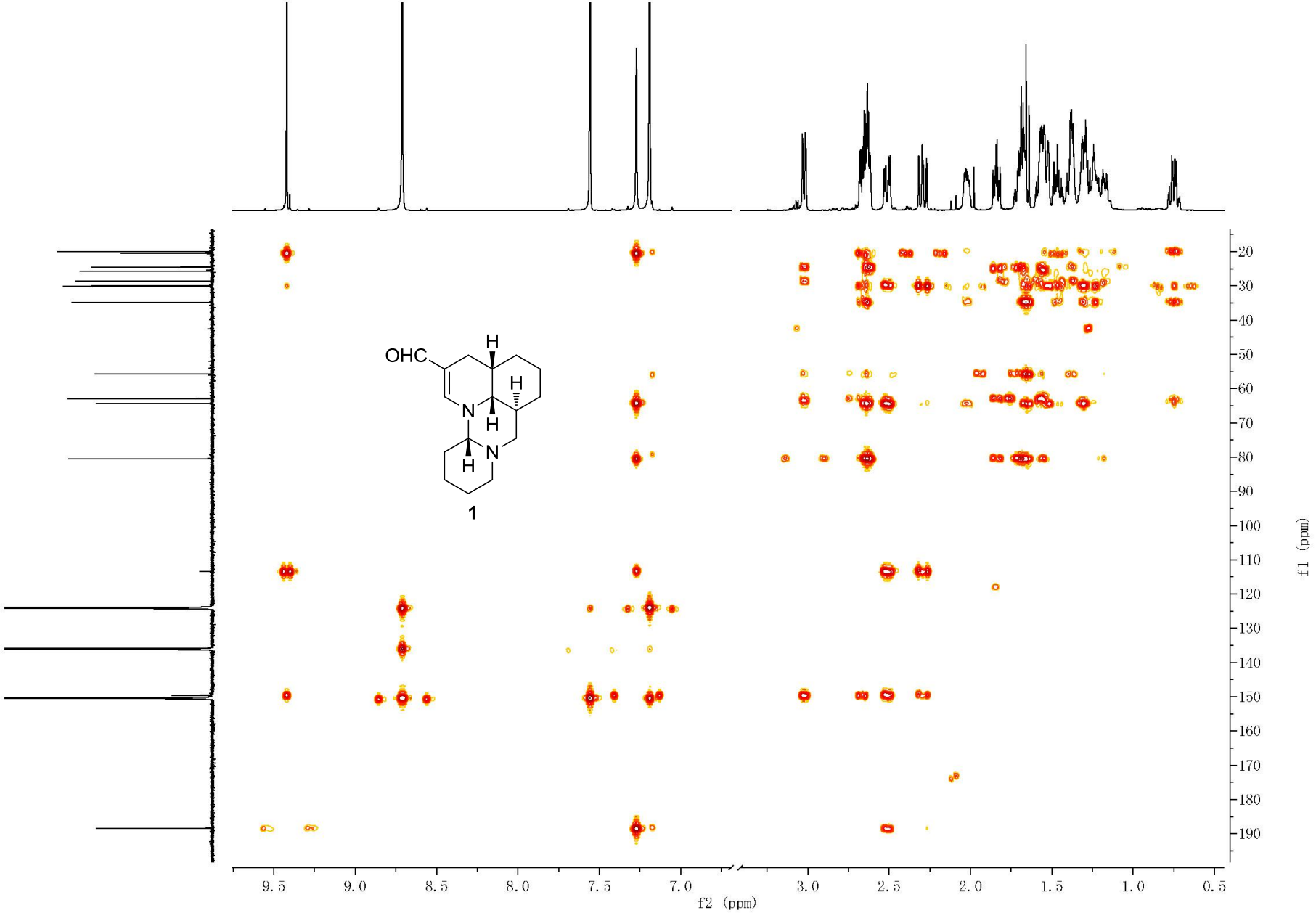
S1.3 HSQC spectrum of myrifamine A (**1**) in prydine-d_5 at 294K



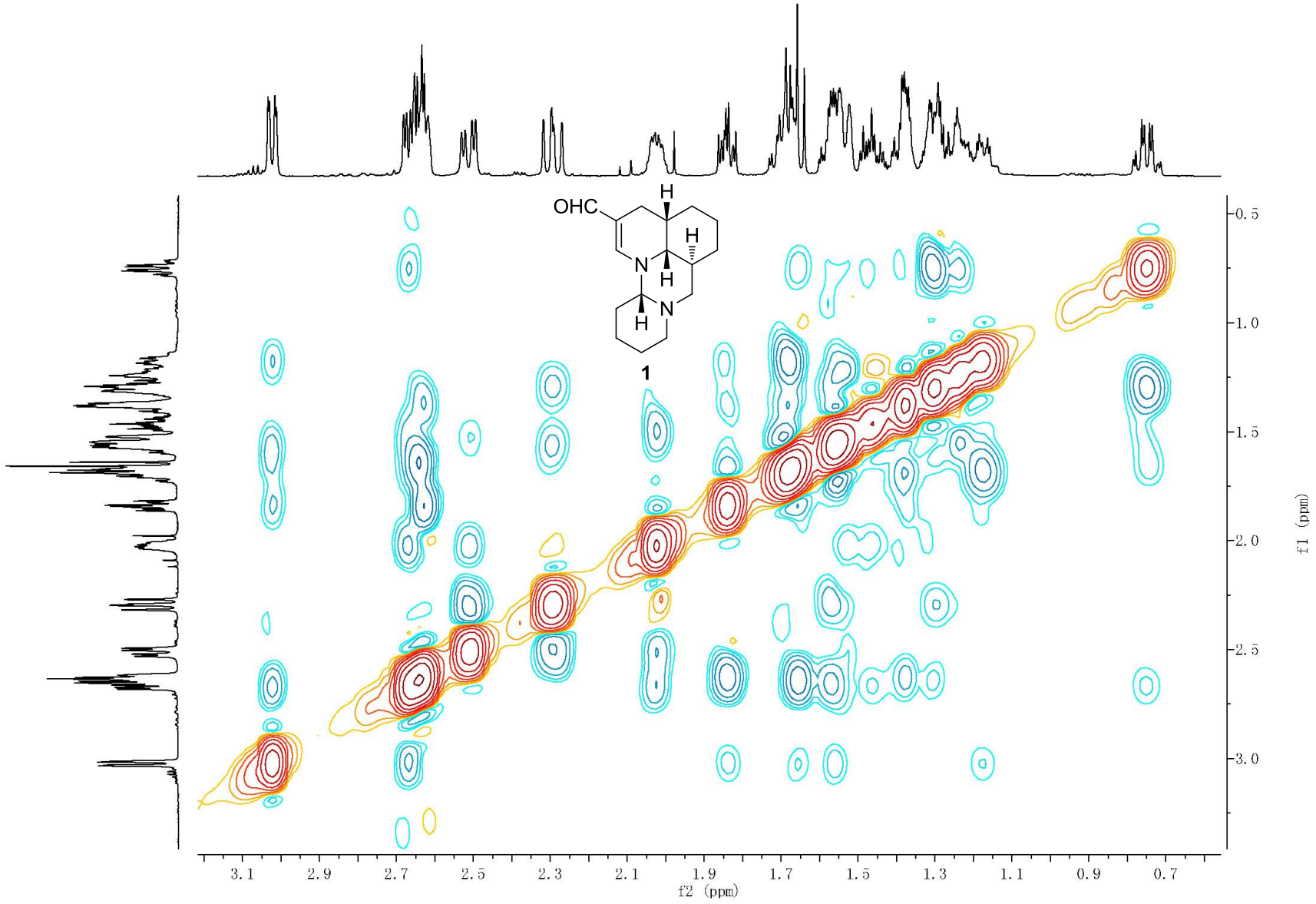
S1.4 COSY spectrum of myrifamine A (**1**) in prydine-d_5 at 294K

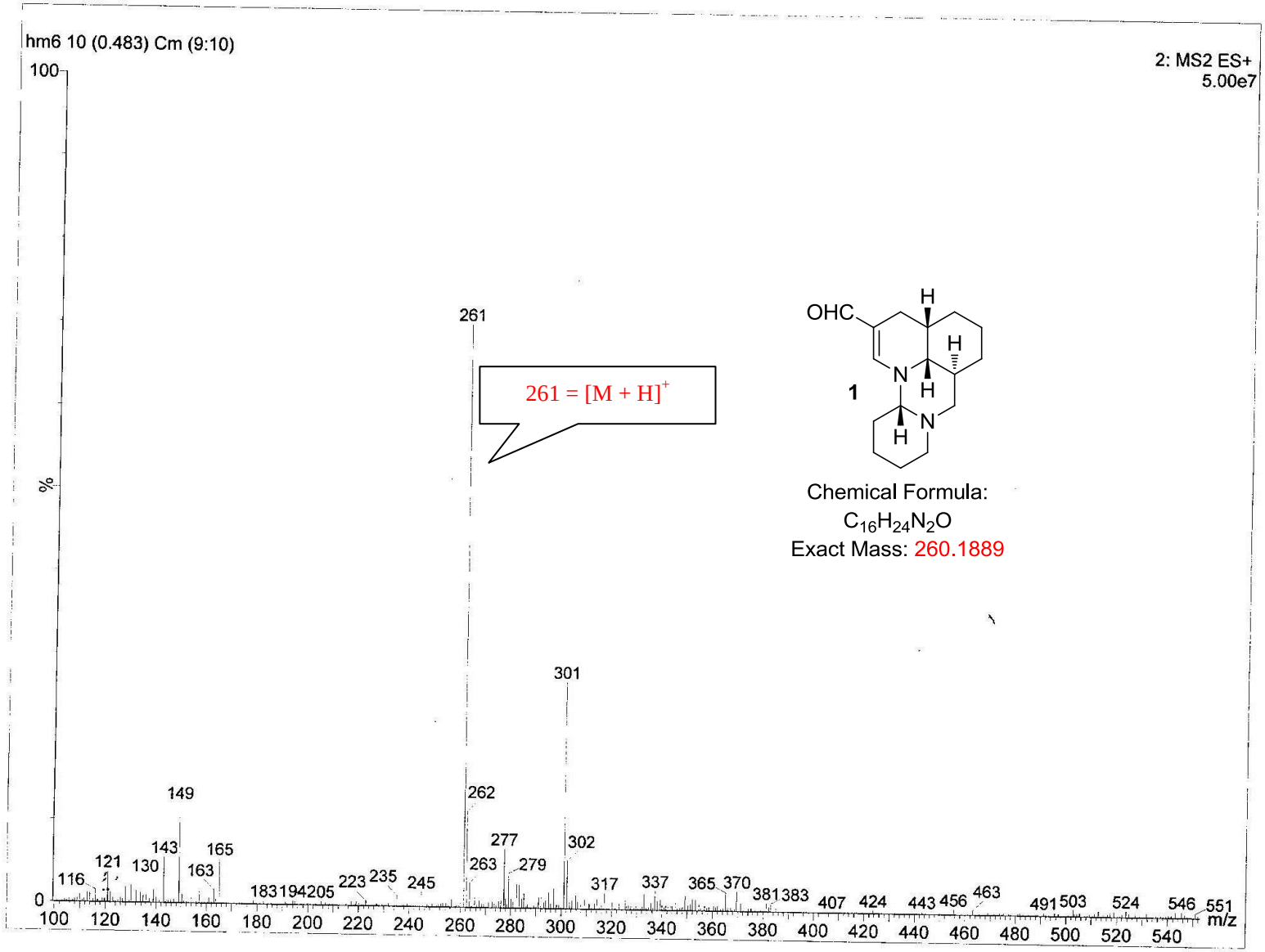


S1.5 HMBC spectrum of myrifamine A (**1**) in prydine-d_5 at 294K



S1.6 ROESY spectrum of myrifamine A (**1**) in prydine-d_5 at 294K




hm6 10 (0.483) Cm (9:10)
2: MS2 ES+
5.00e7
100
%
0
261
261 = [M + H]+
301
149
262
277
302
263
279
121
130
143
165
116
163
183
194
205
223
235
245
317
337
365
370
381
383
407
424
443
456
463
491
503
524
546
551
100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540
m/z
OHC
H
H
N
H
1
H
N
Chemical Formula:
C16H24N2O
Exact Mass: 260.1889

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

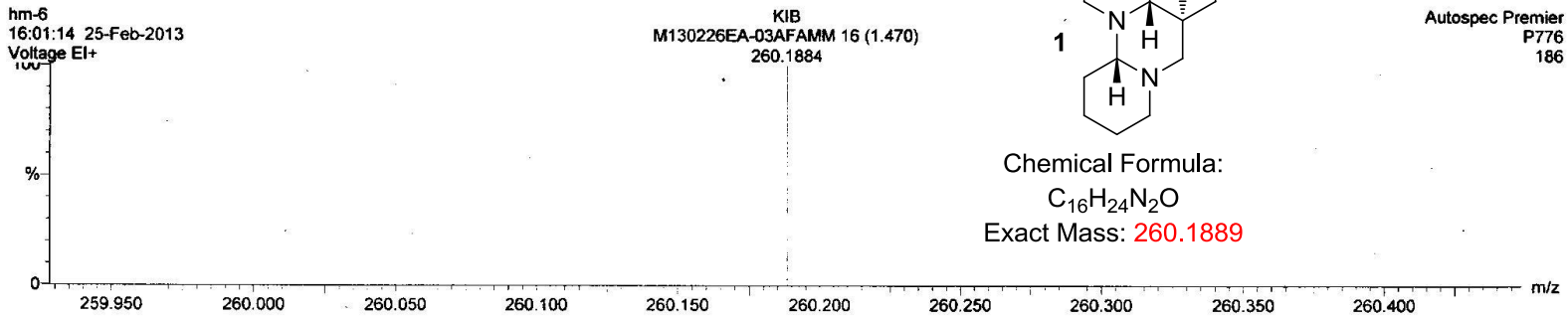
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

14 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 N: 2-2 O: 0-2



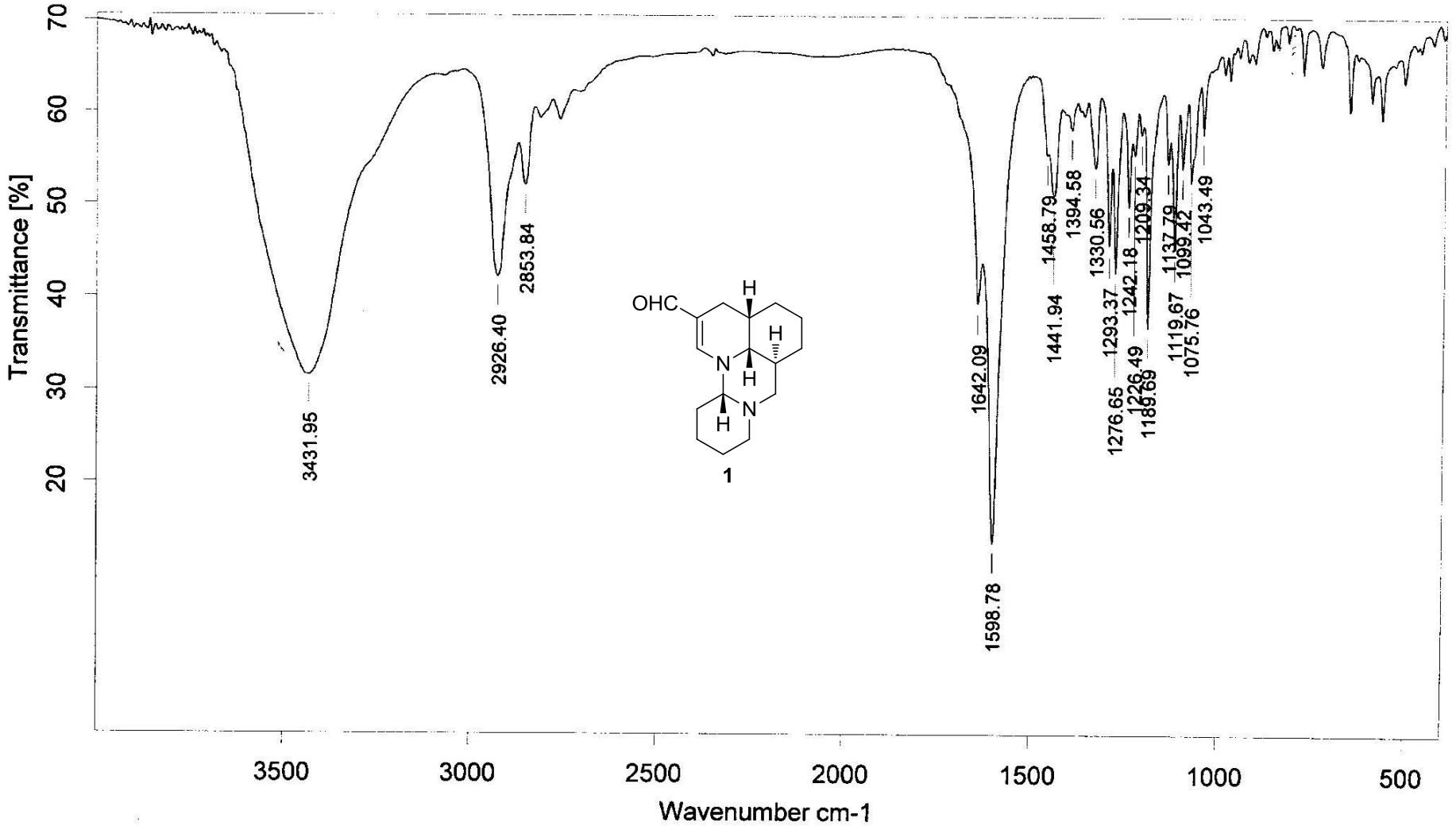
Chemical Formula:

$C_{16}H_{24}N_2O$

Exact Mass: 260.1889

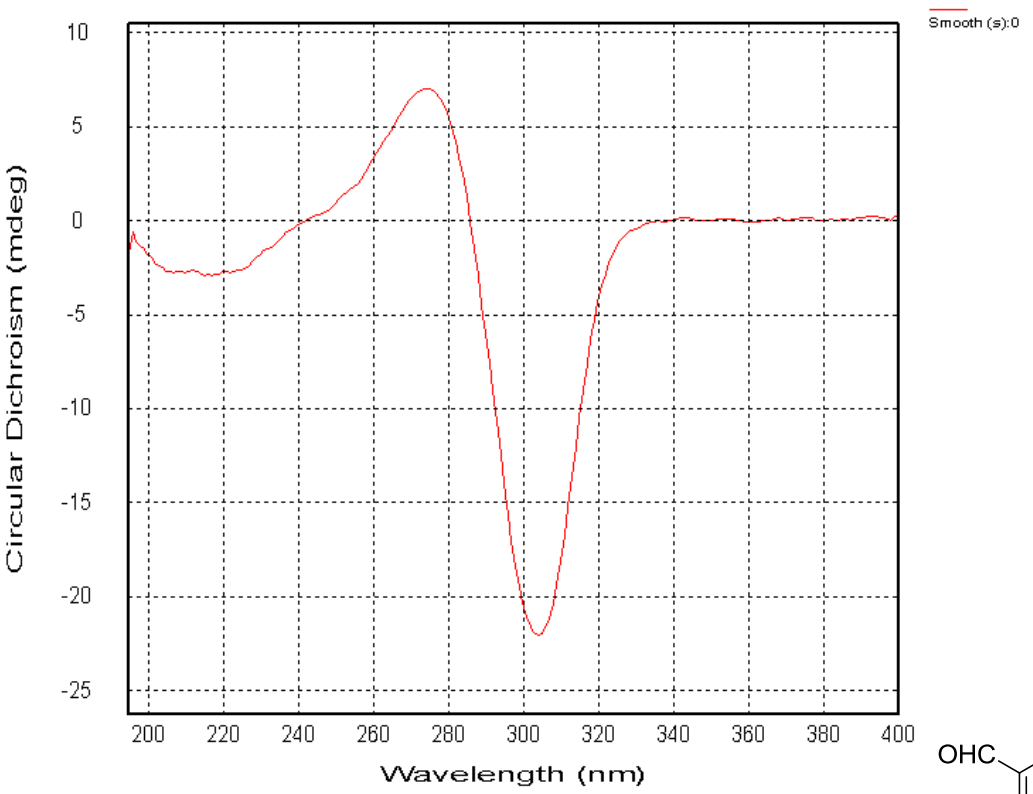
Minimum:				-10.0		
Maximum:		200.0	10.0	120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
260.1884	260.1889	-0.5	-1.9	6.0	5546101.5	C16 H24 N2 O

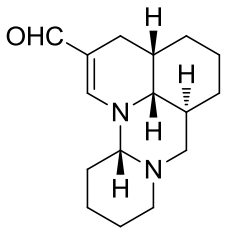
S1.8 IR spectrum of myrifamine A (**1**)



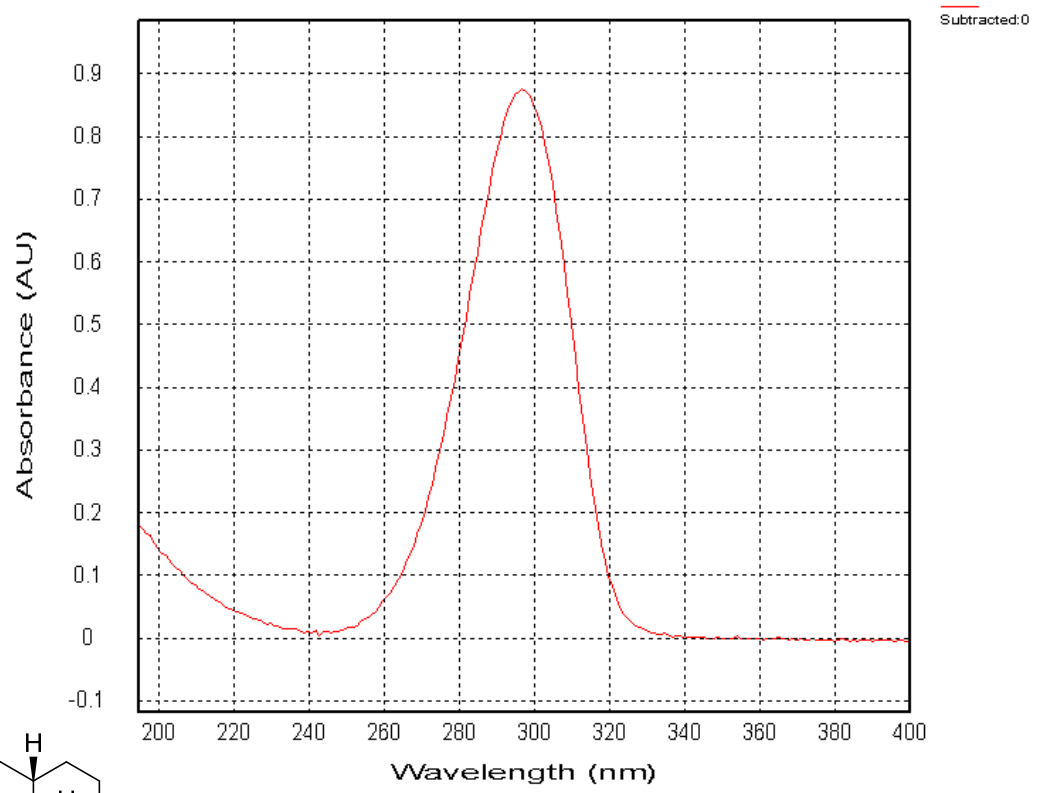
Sample : hm-6	Frequency Range : 399.246 - 3996.32	Measured on : 28/02/2013	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 130228IR0	Zerofilling : 2	Acquisition : Double Sided,For	

S1.9 ECD spectrum of myrifamine A (**1**) in methanol

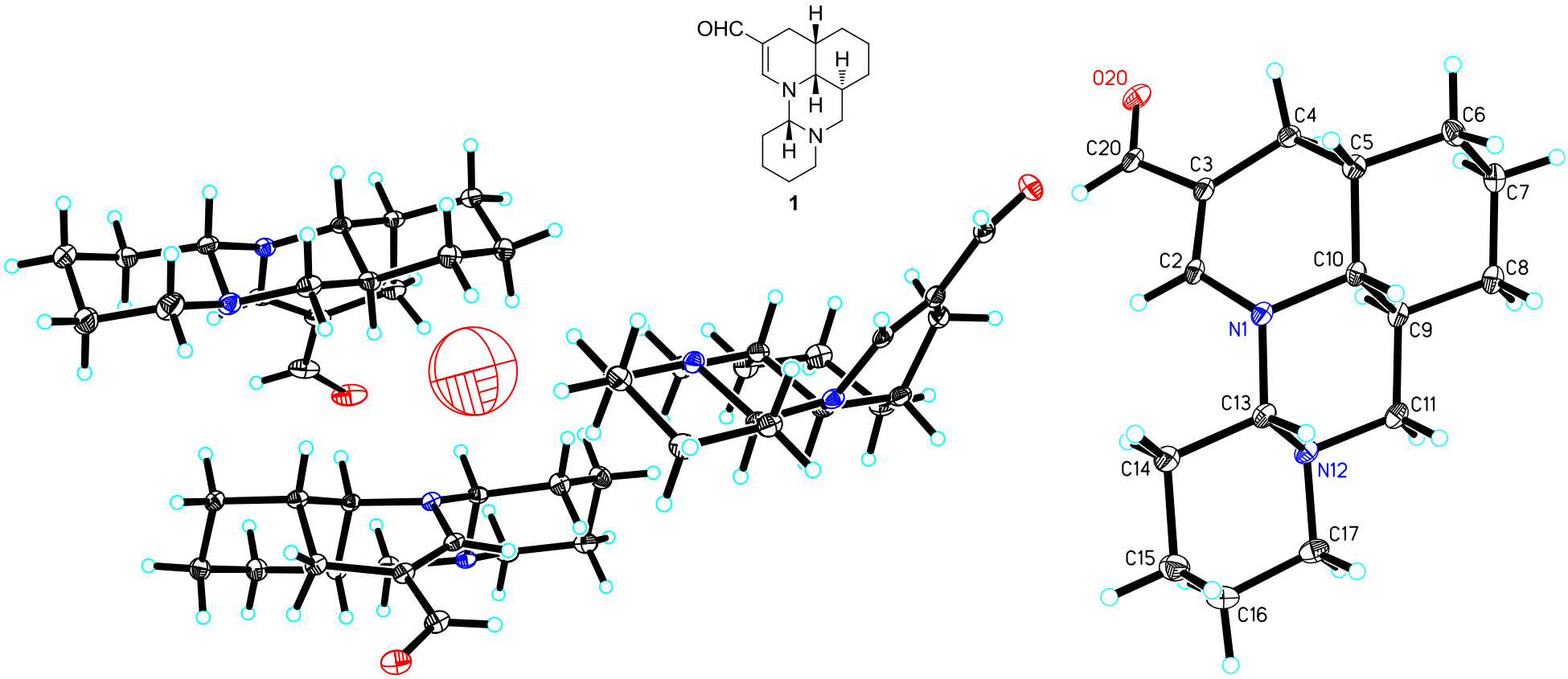




1

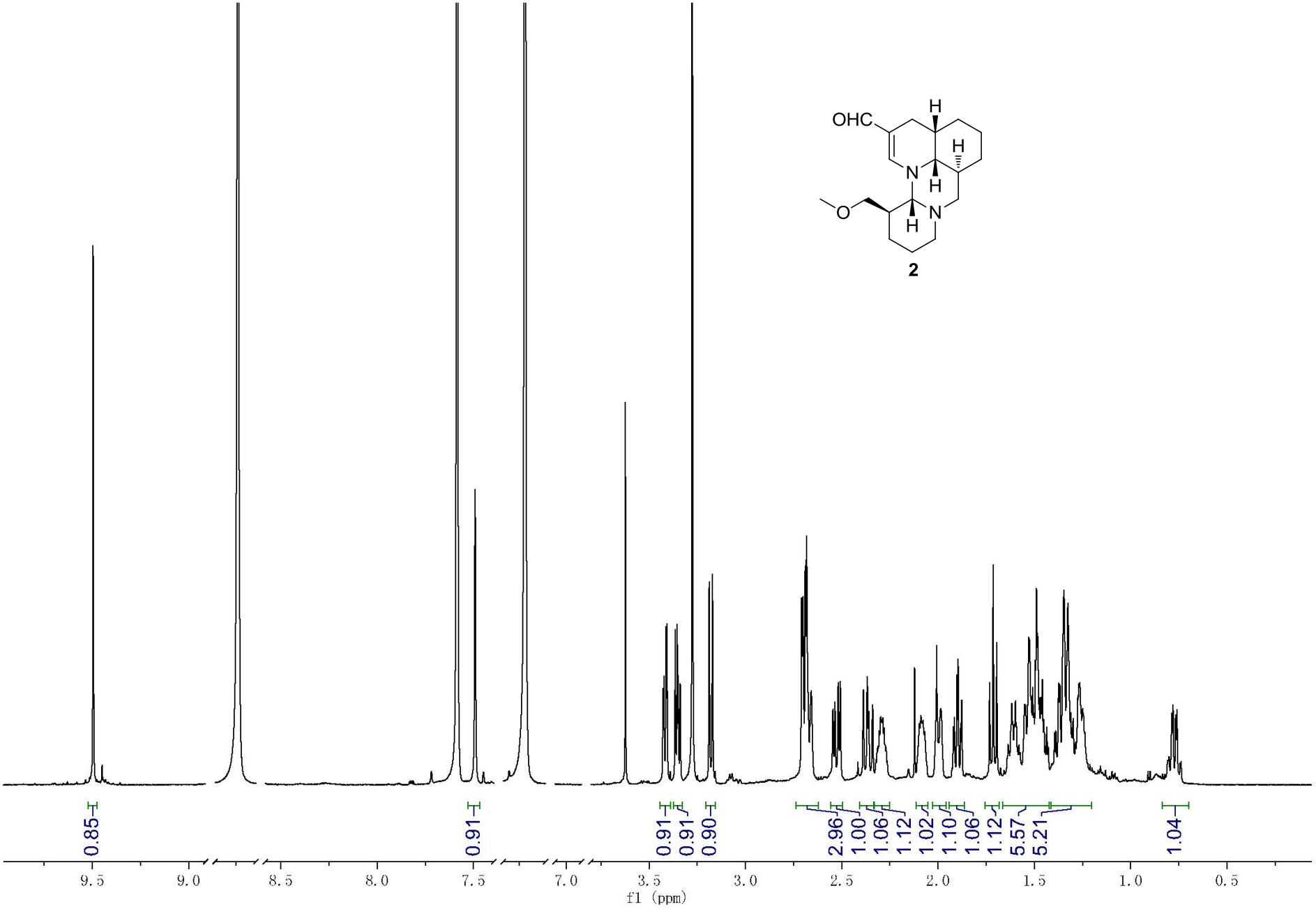


S1.10 X-ray crystal structure of myrifamine A (**1**)

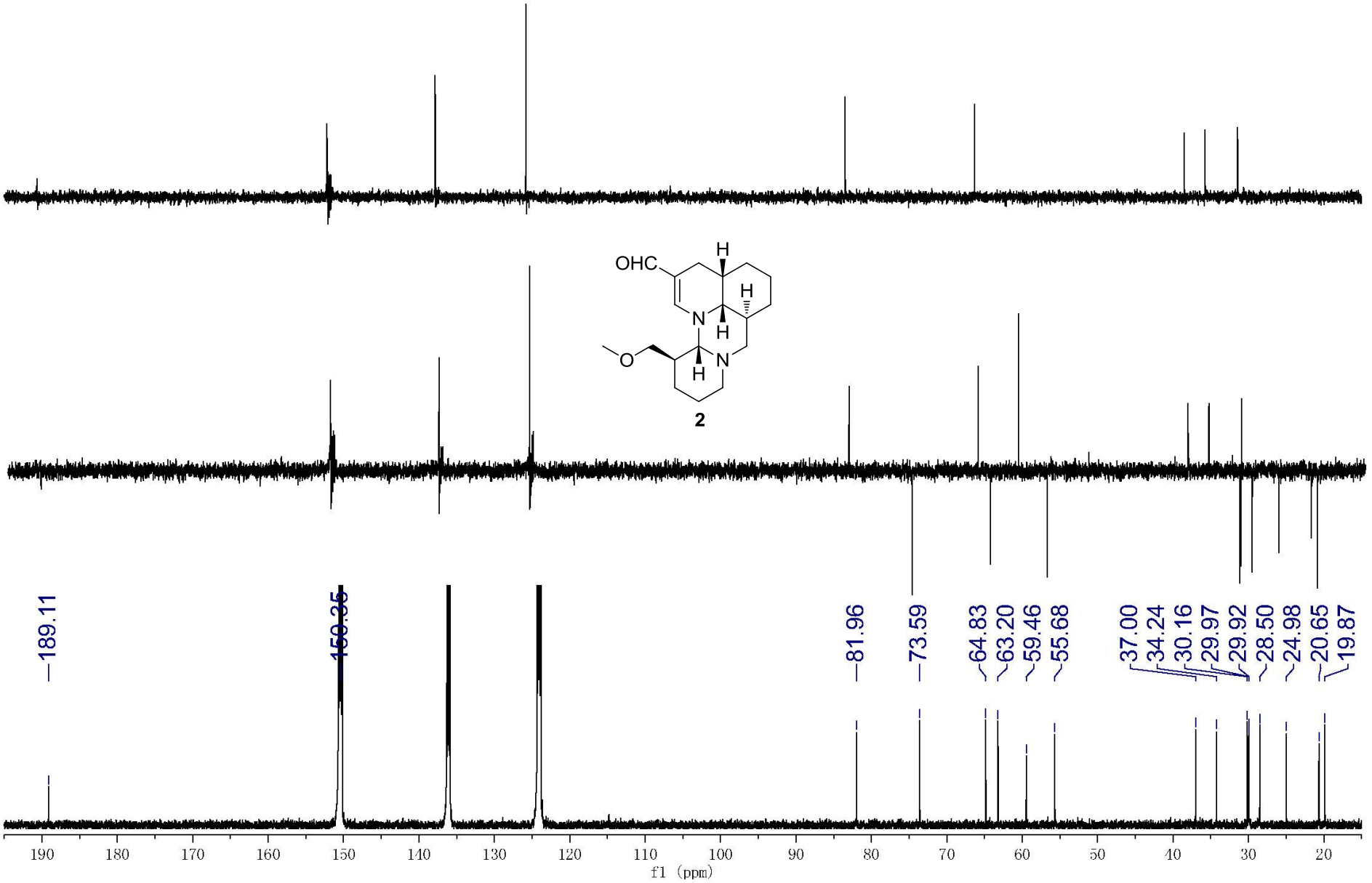


A: View of the molecules in an asymmetric unit. B: View of a molecule of myrifamine A (**2**) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

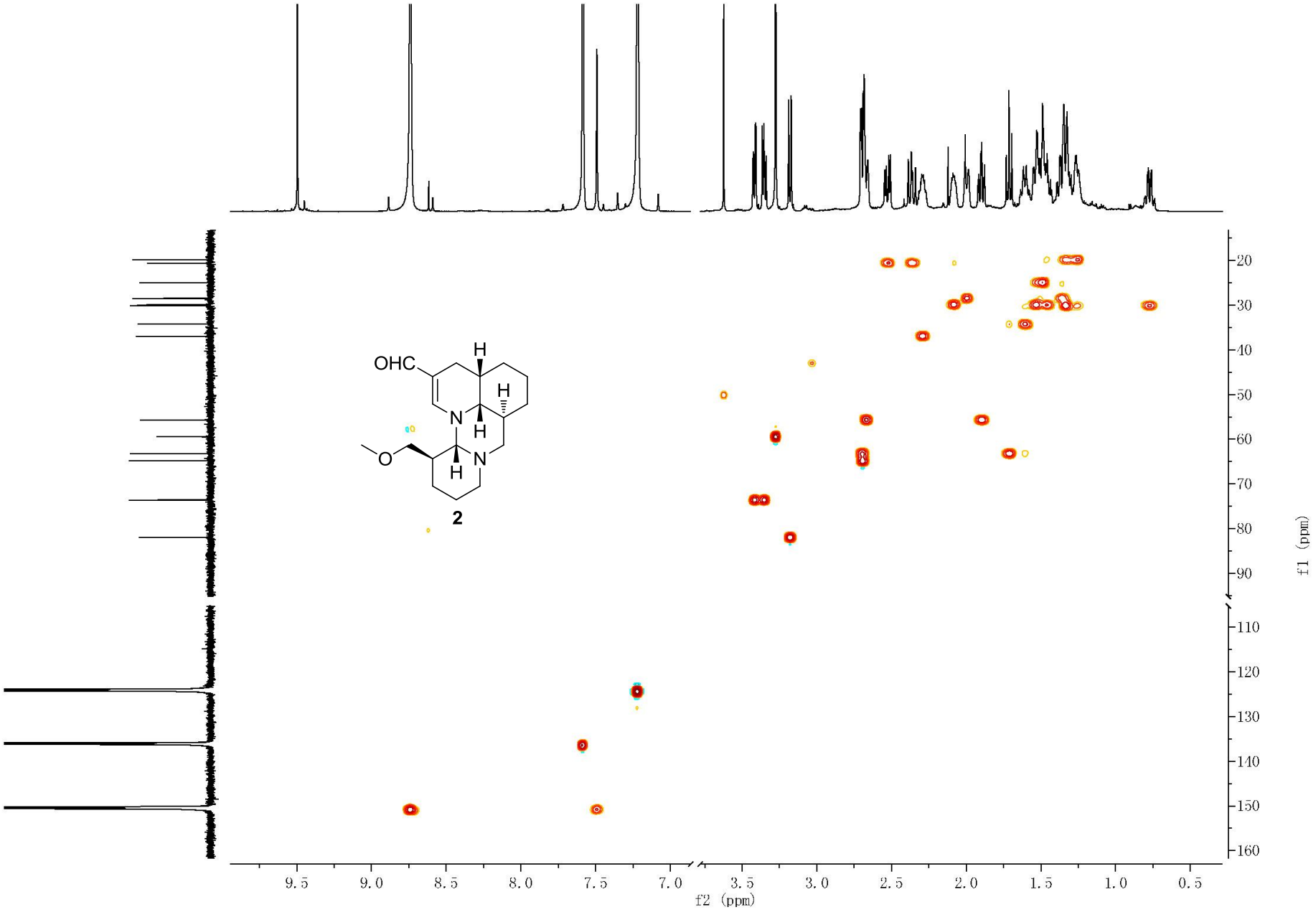
S2.1 ^{1}H NMR spectrum of myrifamine B (**2**) in prydine-d_5 at 294K



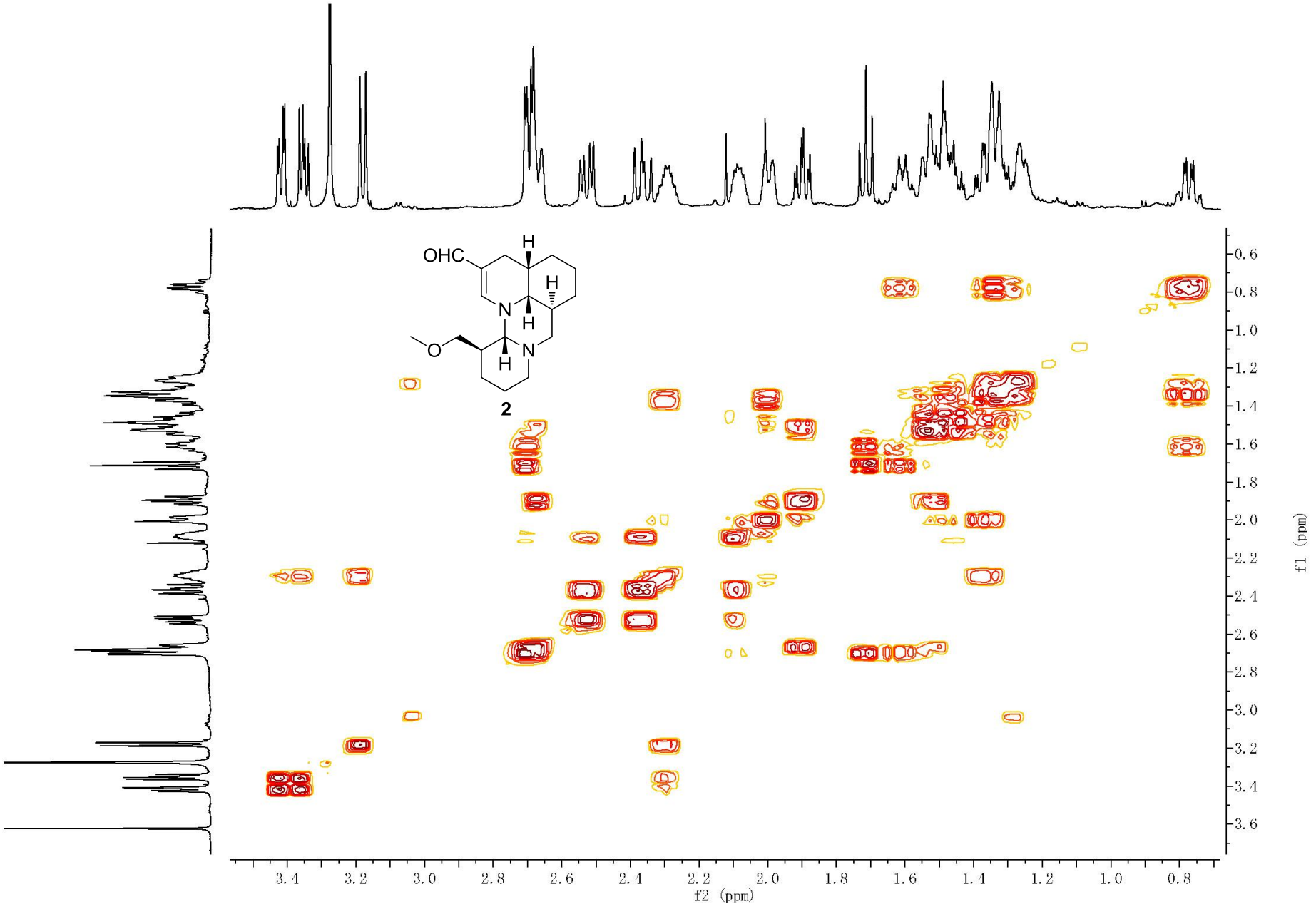
S2.2 ^{13}C NMR spectrum of myrifamine B (**2**) in prydine-d_5 at 294K



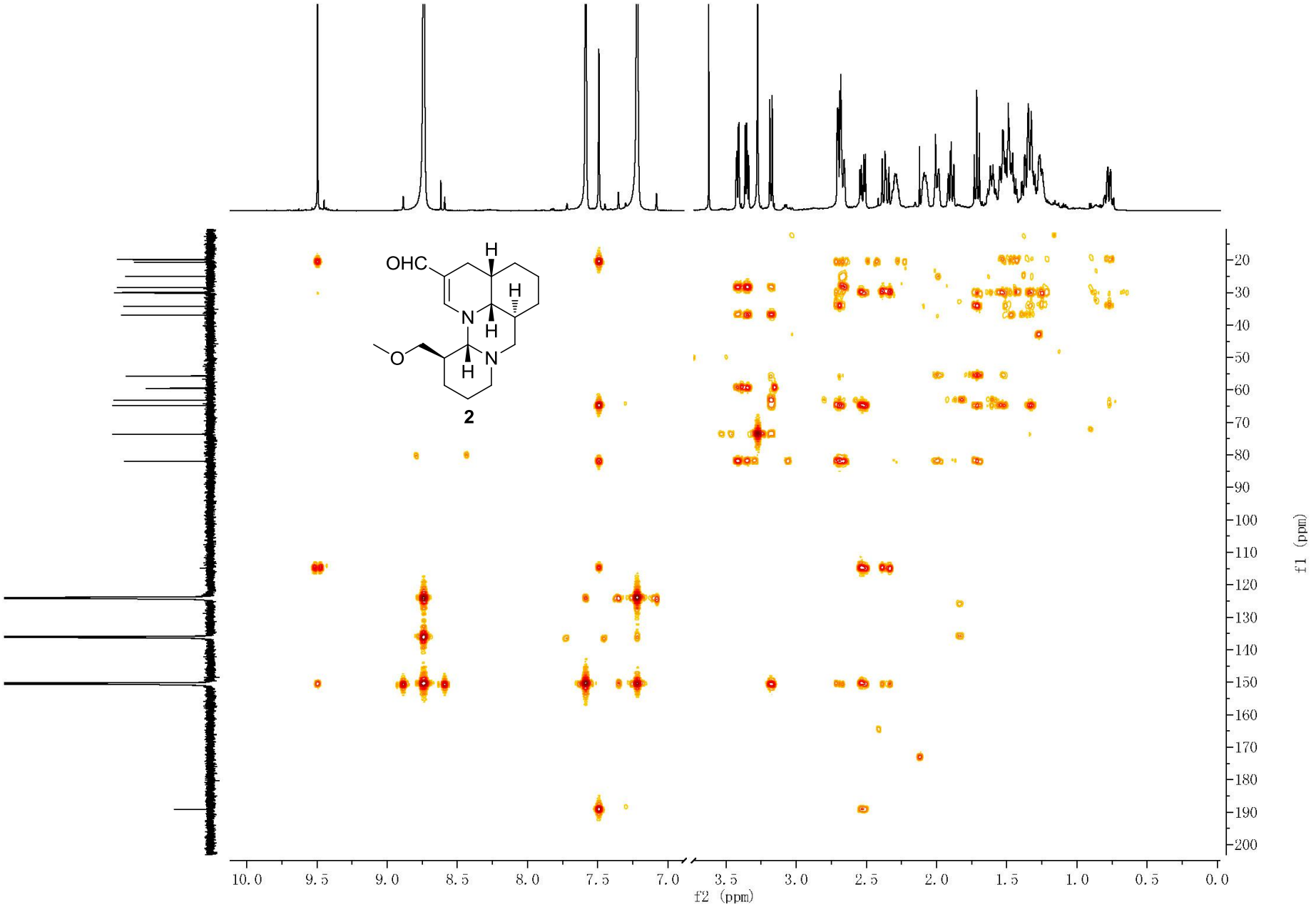
S3.3 HSQC spectrum of myrifamine B (**2**) in prydine-d_5 at 294K



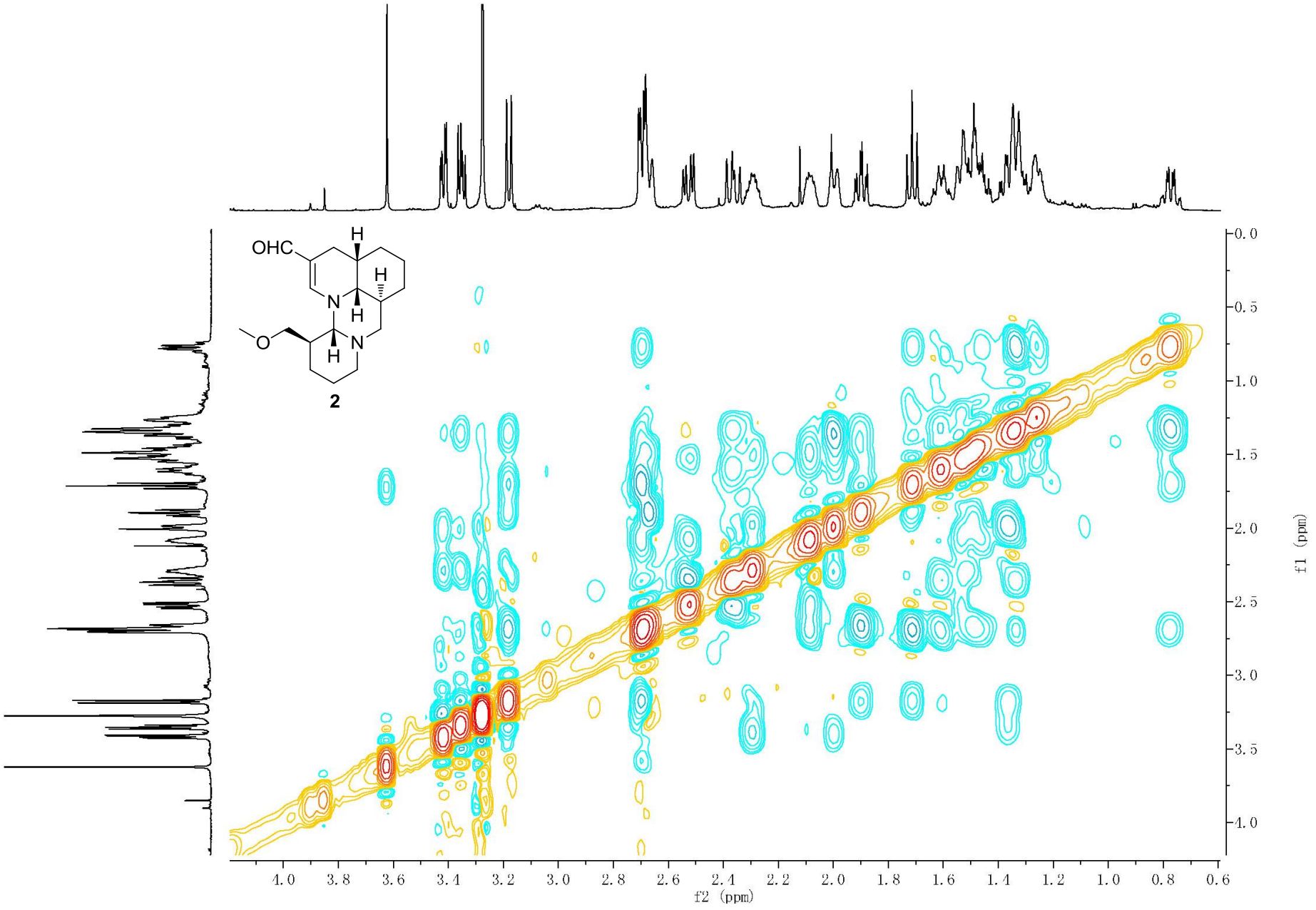
S2.4 COSY spectrum of myrifamine B (**2**) in prydine-d_5 at 294K



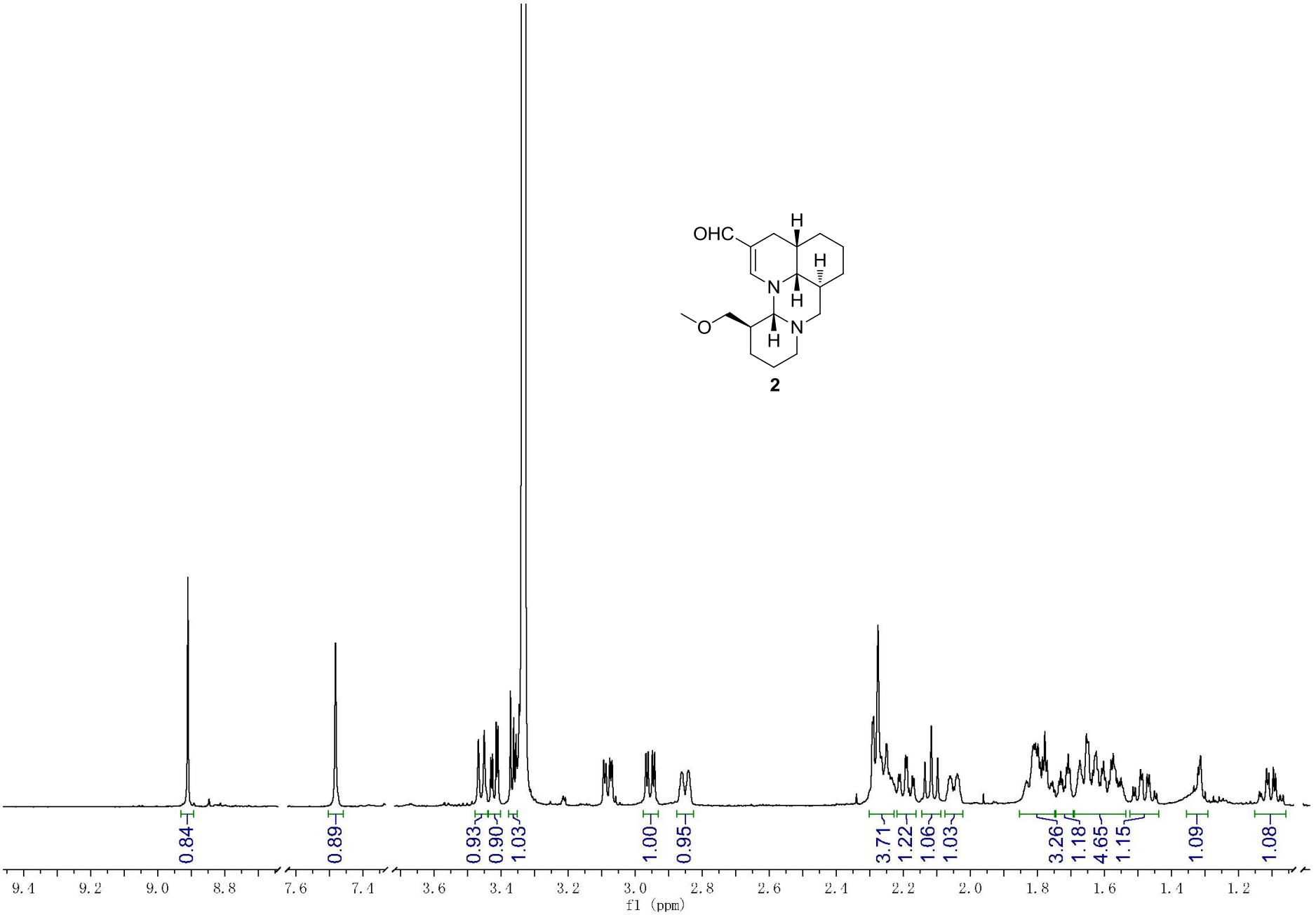
S2.5 HMBC spectrum of myrifamine B (**2**) in prydine-d_5 at 294K



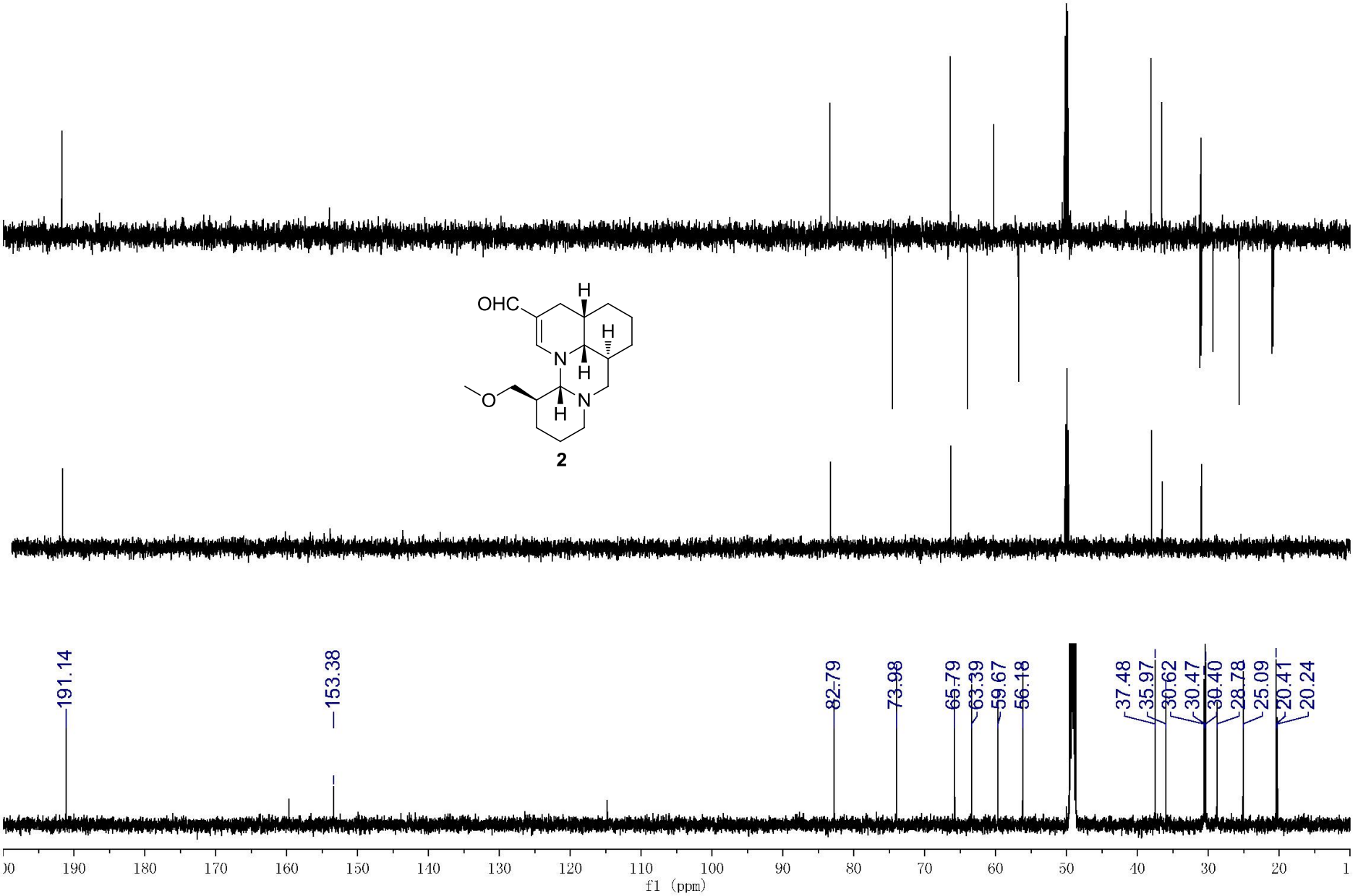
S2.6 ROESY spectrum of myrifamine B (**2**) in prydine-d_5 at 294K



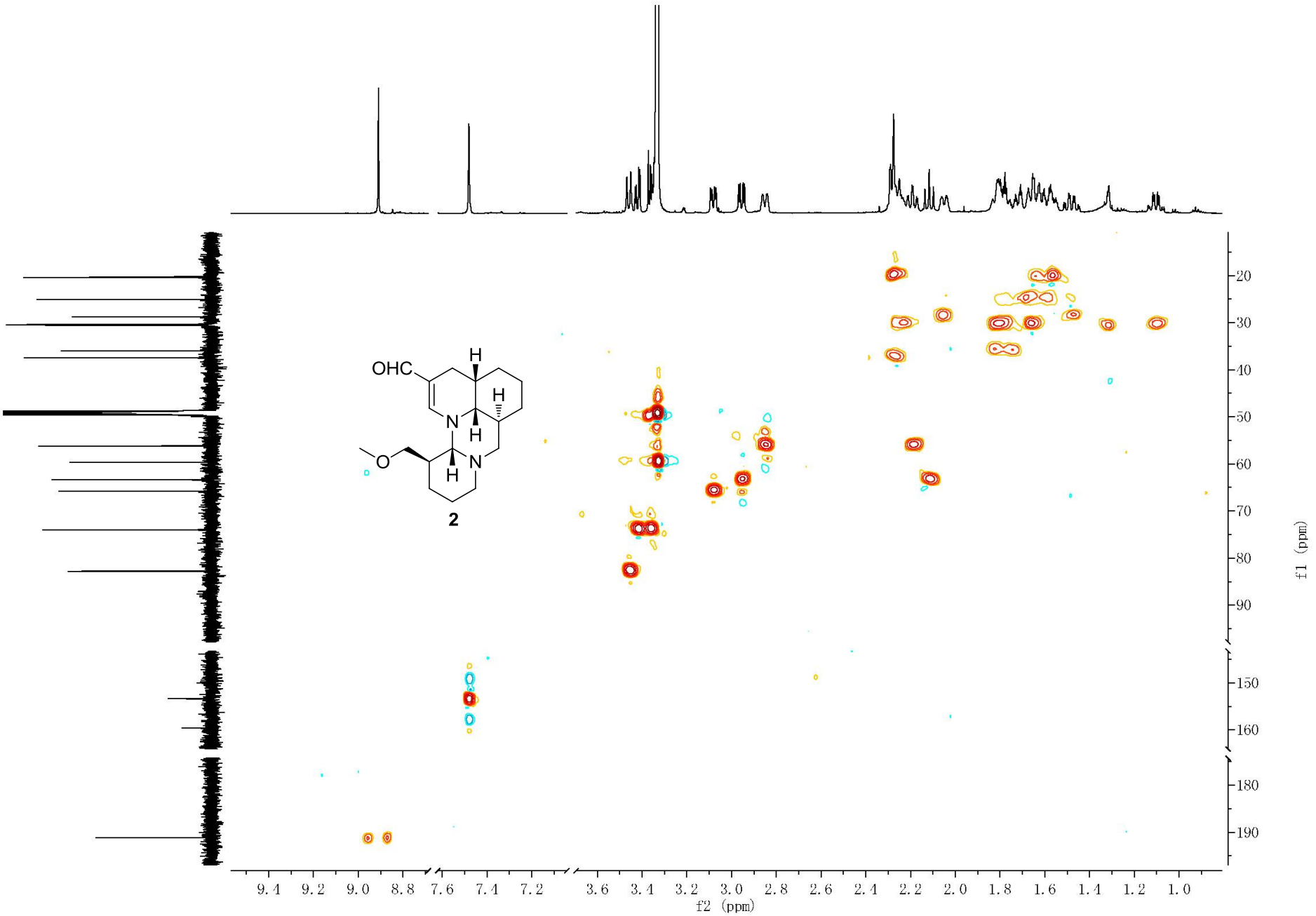
S2.7 ^{1}H NMR spectrum of myrifamine B (**2**) in CD_3OD at 294K



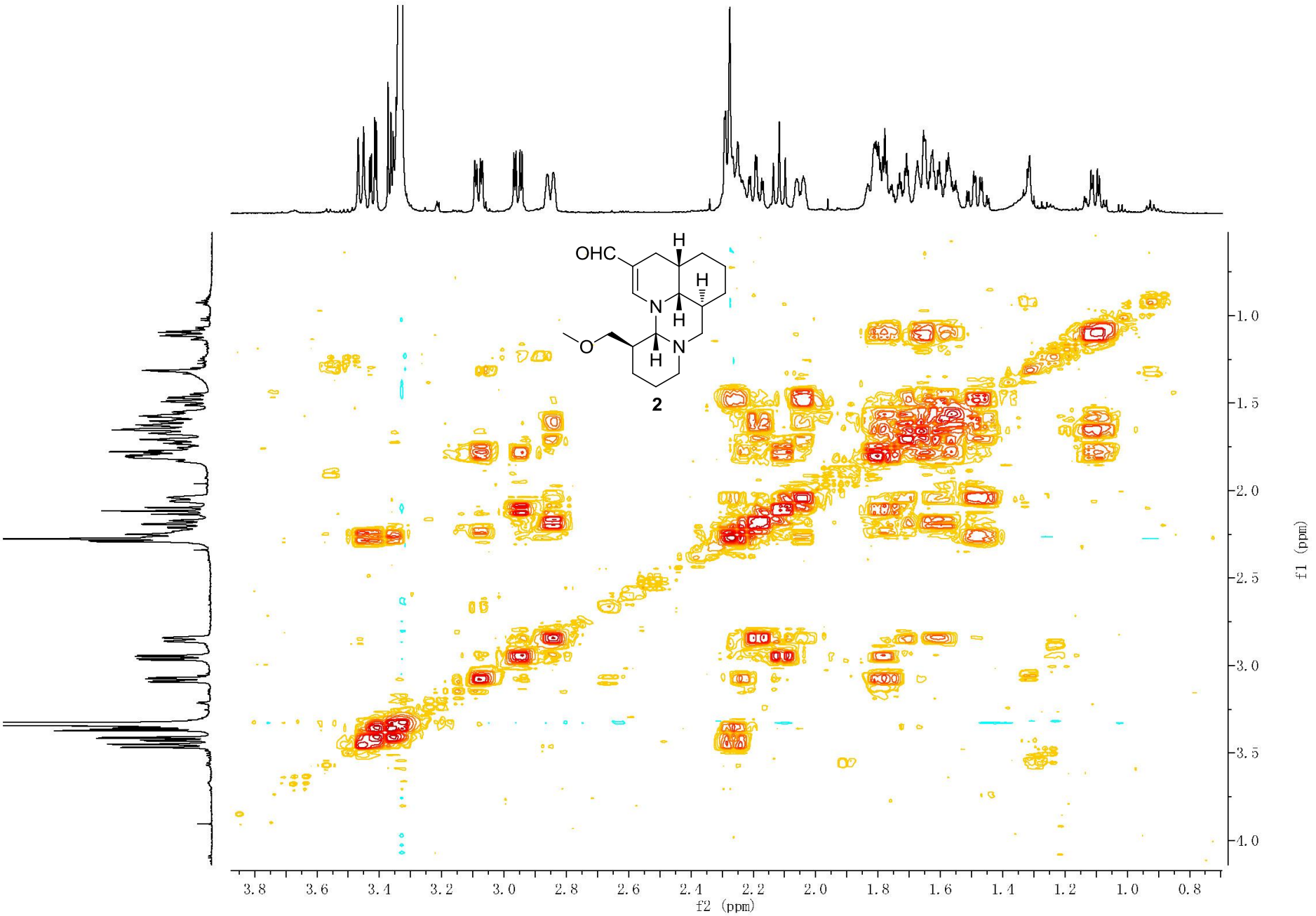
S2.8 ^{13}C NMR spectrum of myrifamine B (**2**) in CD_3OD at 294K



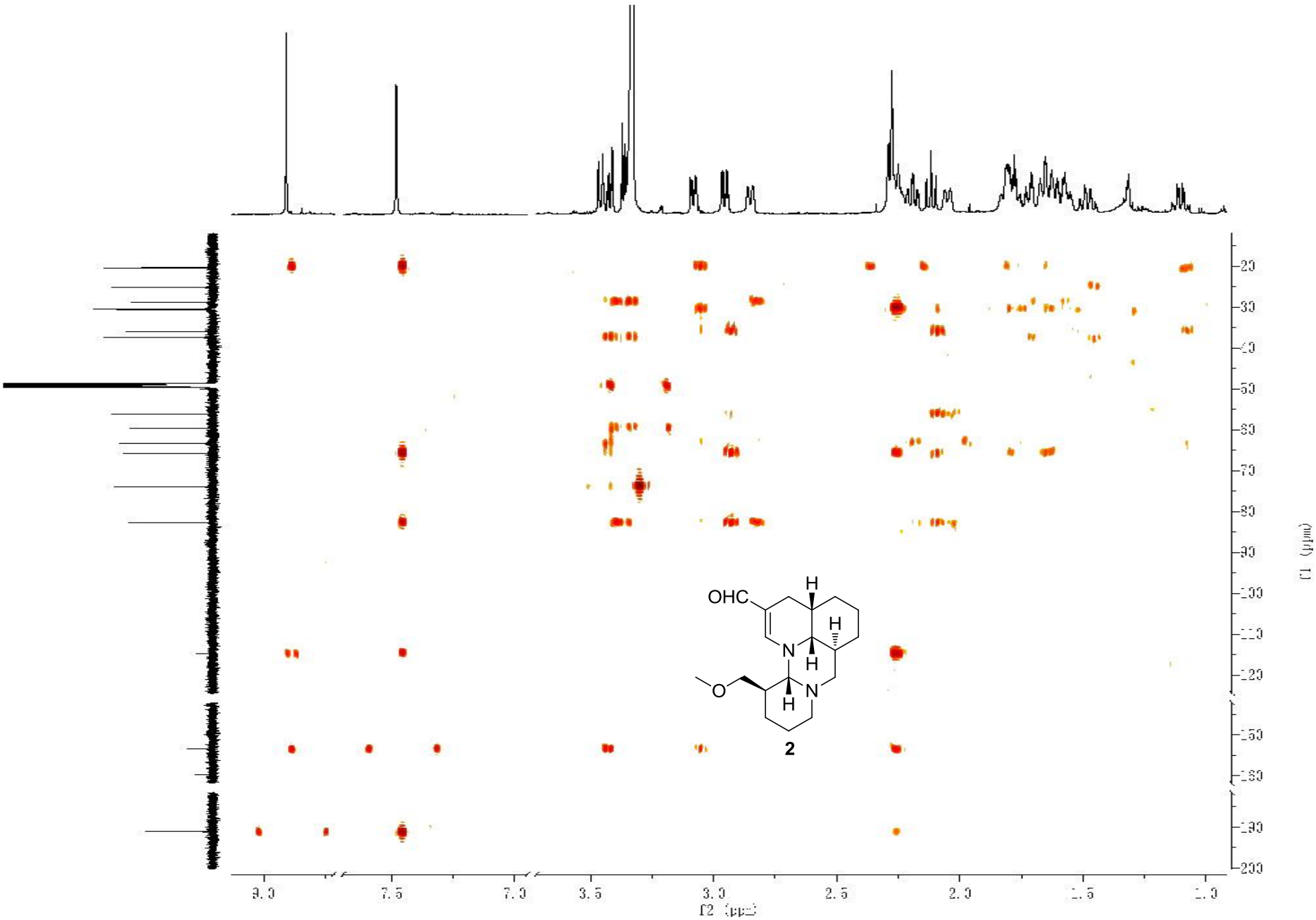
S2.9 HSQC spectrum of myrifamine B (**2**) in CD_3OD at 294K



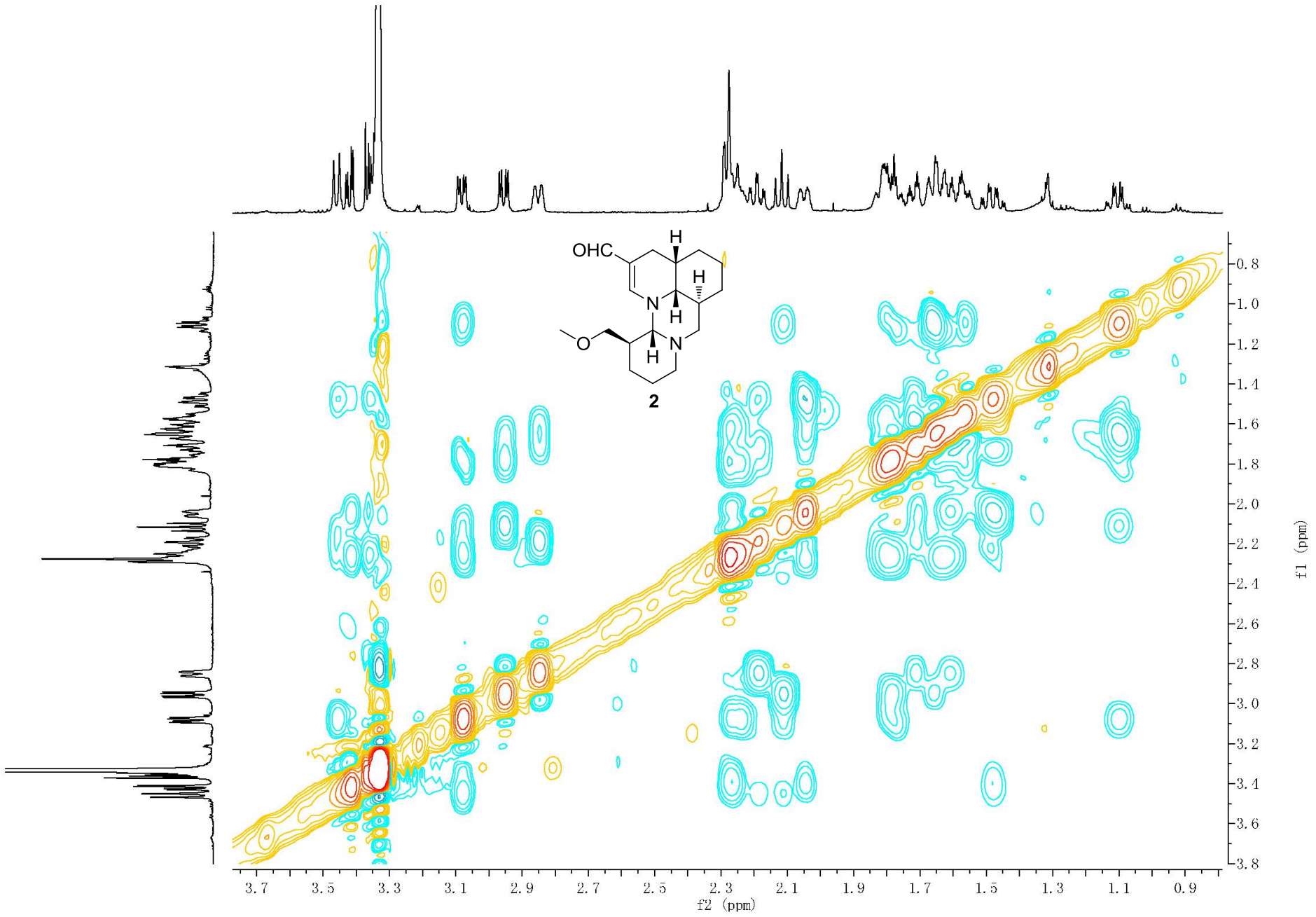
S2.10 COSY spectrum of myrifamine B (**2**) in CD_3OD at 294K



S2.11 HMBC spectrum of myrifamine B (**2**) in CD_3OD at 294K



S2.12 ROESY spectrum of myrifamine B (**2**) in CD_3OD at 294K

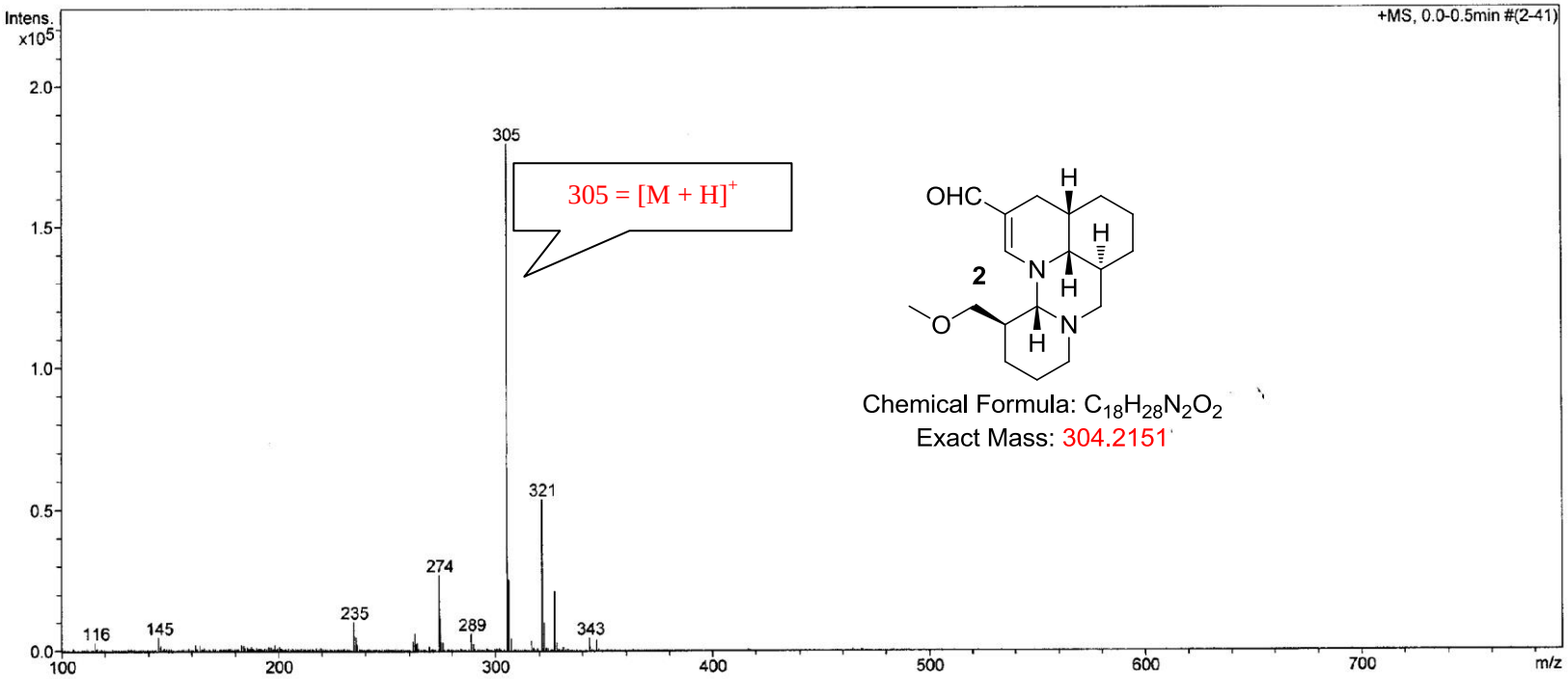


Mass Spectrum List Report

Analysis Info			
Analysis Name	D:\DATA\2012file\1204\120419\hm-6a01.d	Acquisition Date	4/19/2012 11:34:23 AM
Method	ms_ptservice.m	Operator	Bruker
Sample Name	hm-6a	Instrument	HCT

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Ultra Scan	Scan Begin	100 m/z	Scan End	800 m/z
Capillary Exit	40.0 Volt	Skimmer	40.0 Volt	Trap Drive	29.9
Accumulation Time	78119 µs	Averages	5 Spectra	Auto MS/MS	off



Chemical Formula: $C_{18}H_{28}N_2O_2$

Exact Mass: 304.2151

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = 0.5, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

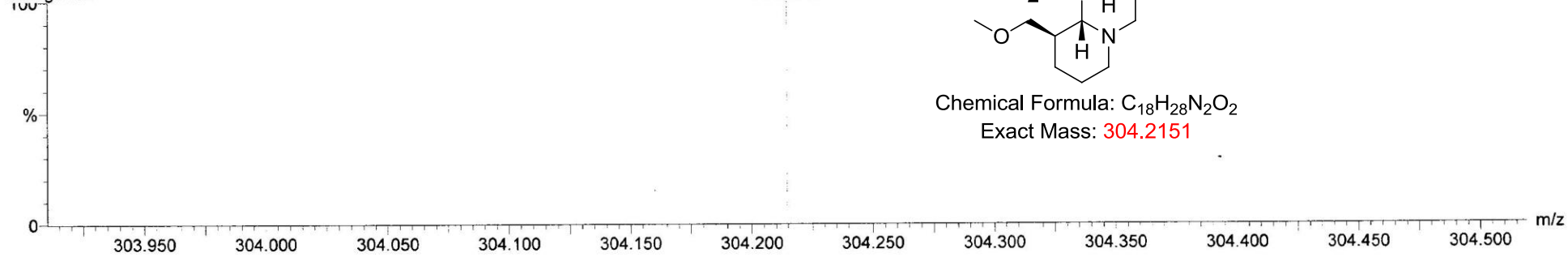
17 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

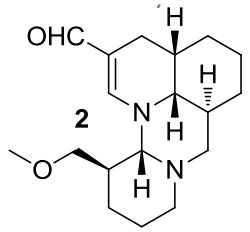
Elements Used:

C: 0-200 H: 0-400 N: 2-2 O: 0-3

hm-6a
09:37:24 25-Apr-2012
Voltage EI+

KIB
M120425EA-01AFAMM 13 (1.194)
304.2146



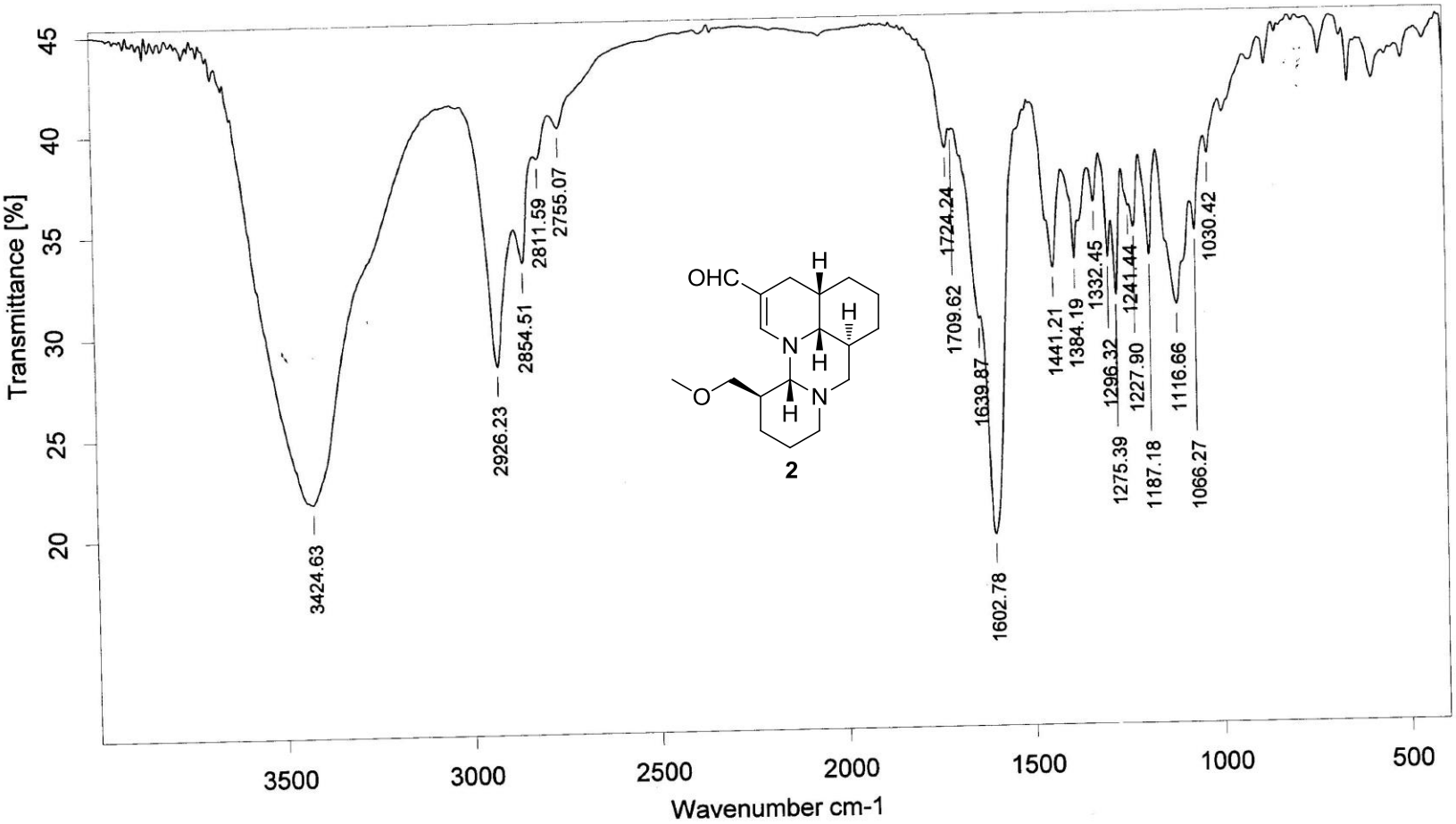


Chemical Formula: $C_{18}H_{28}N_2O_2$
Exact Mass: 304.2151

Autospec Premier
P776
821

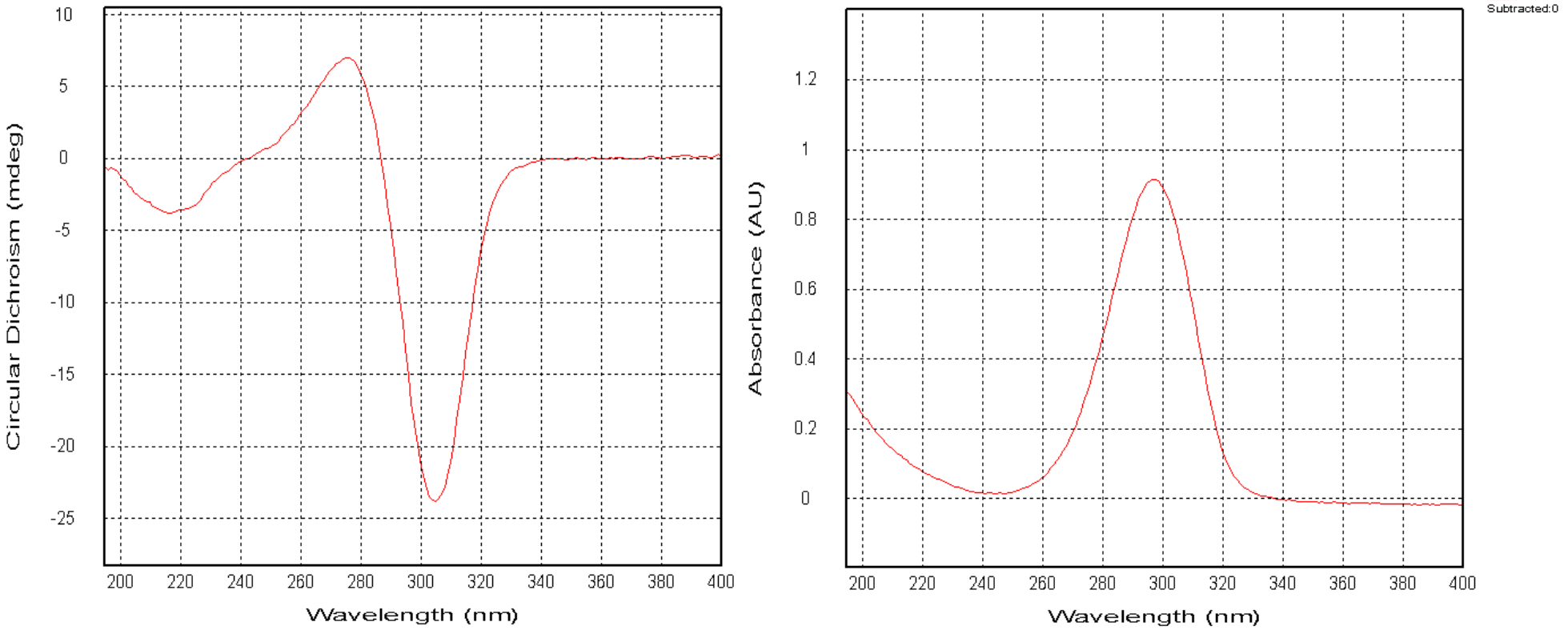
Minimum:				0.5		
Maximum:		160.0	10.0	120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
304.2146	304.2151	-0.5	-1.6	6.0	5546420.5	C18 H28 N2 O2

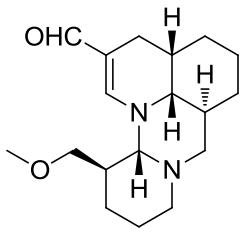
S2.14 IR spectrum of myrifamine B (**2**)



Sample : hm-6a	Frequency Range : 399.246 - 3996.32		Measured on : 07/06/2012
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 120607IR1	Zerofilling : 2	Acquisition : Double Sided,For	

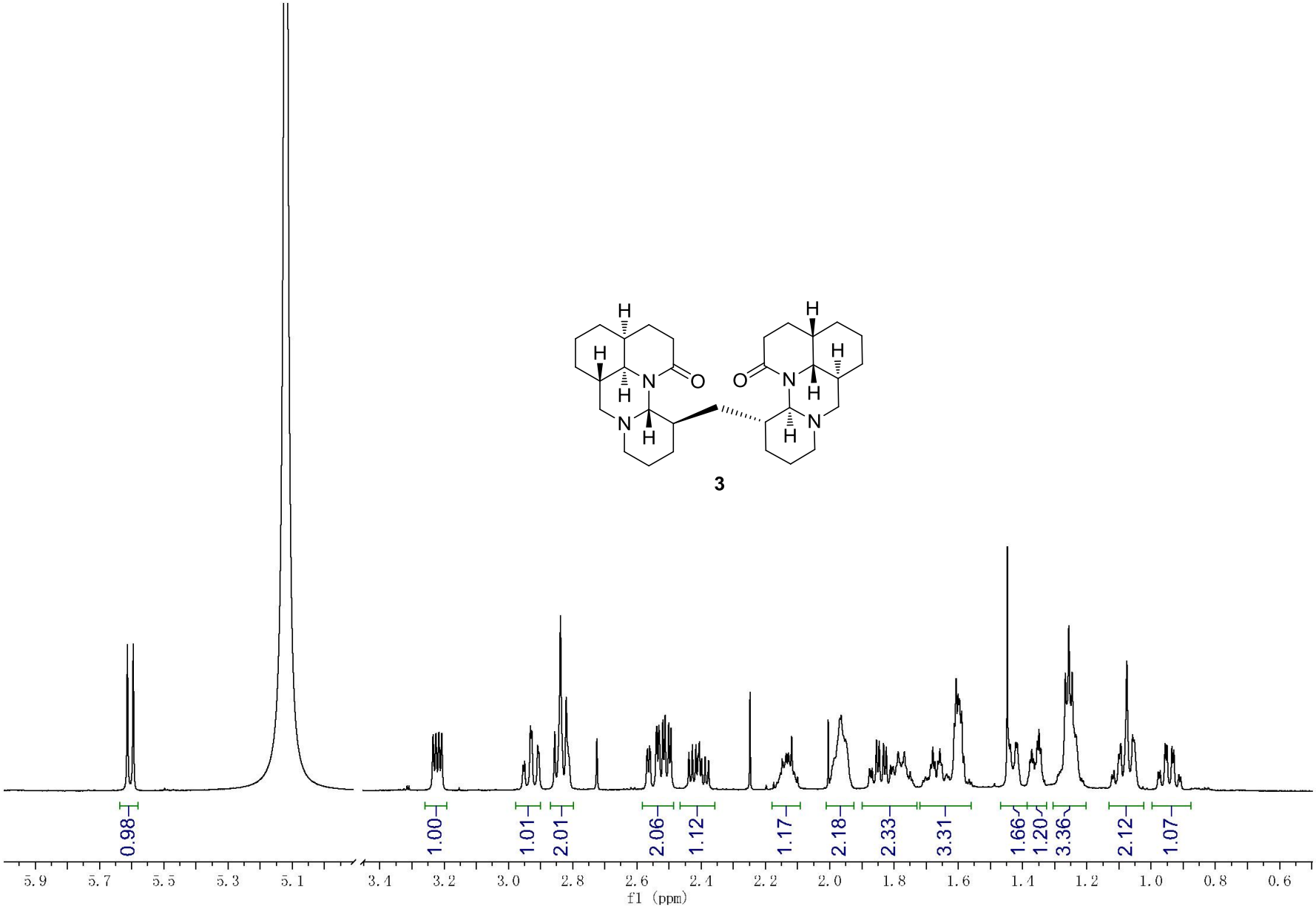
S2.15 ECD spectrum of myrifamine B (**2**) in methanol



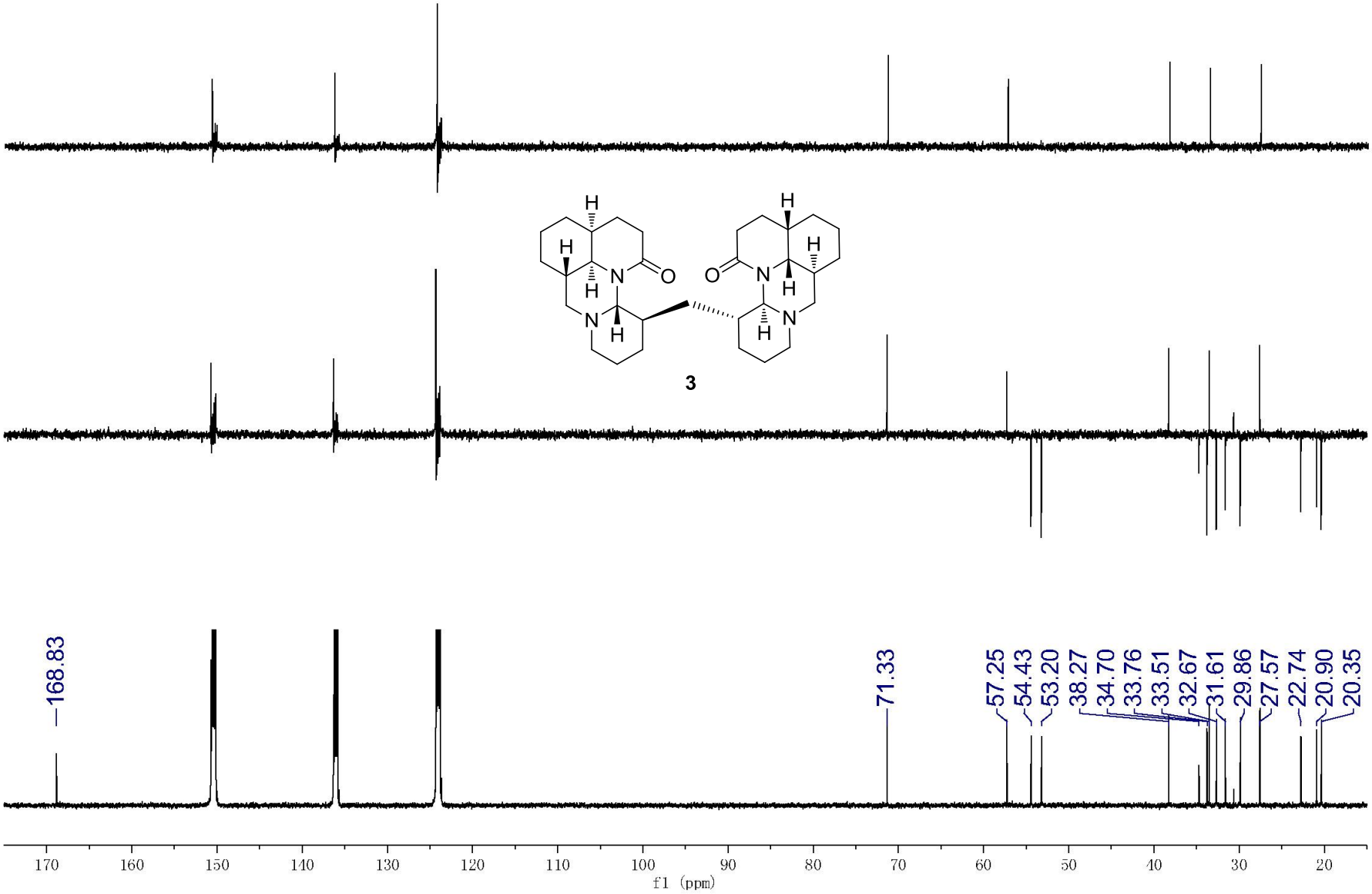


2

3.1 ^{1}H NMR spectrum of myrifamine C (**3**) in prydine-d_5 at 294K

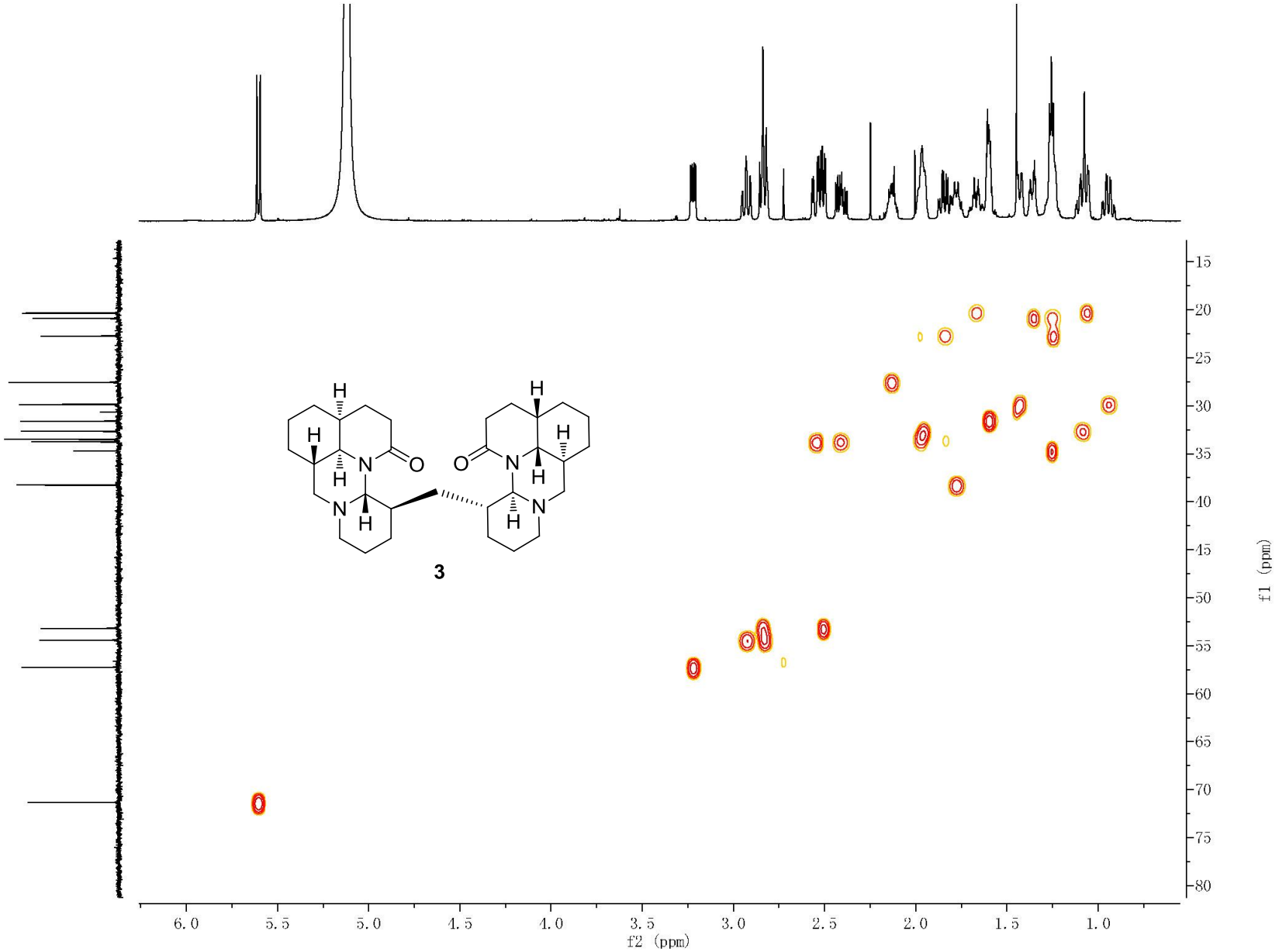


S3.2 ^{13}C NMR spectrum of myrifamine C (**3**) in prydine-d_5 at 294K

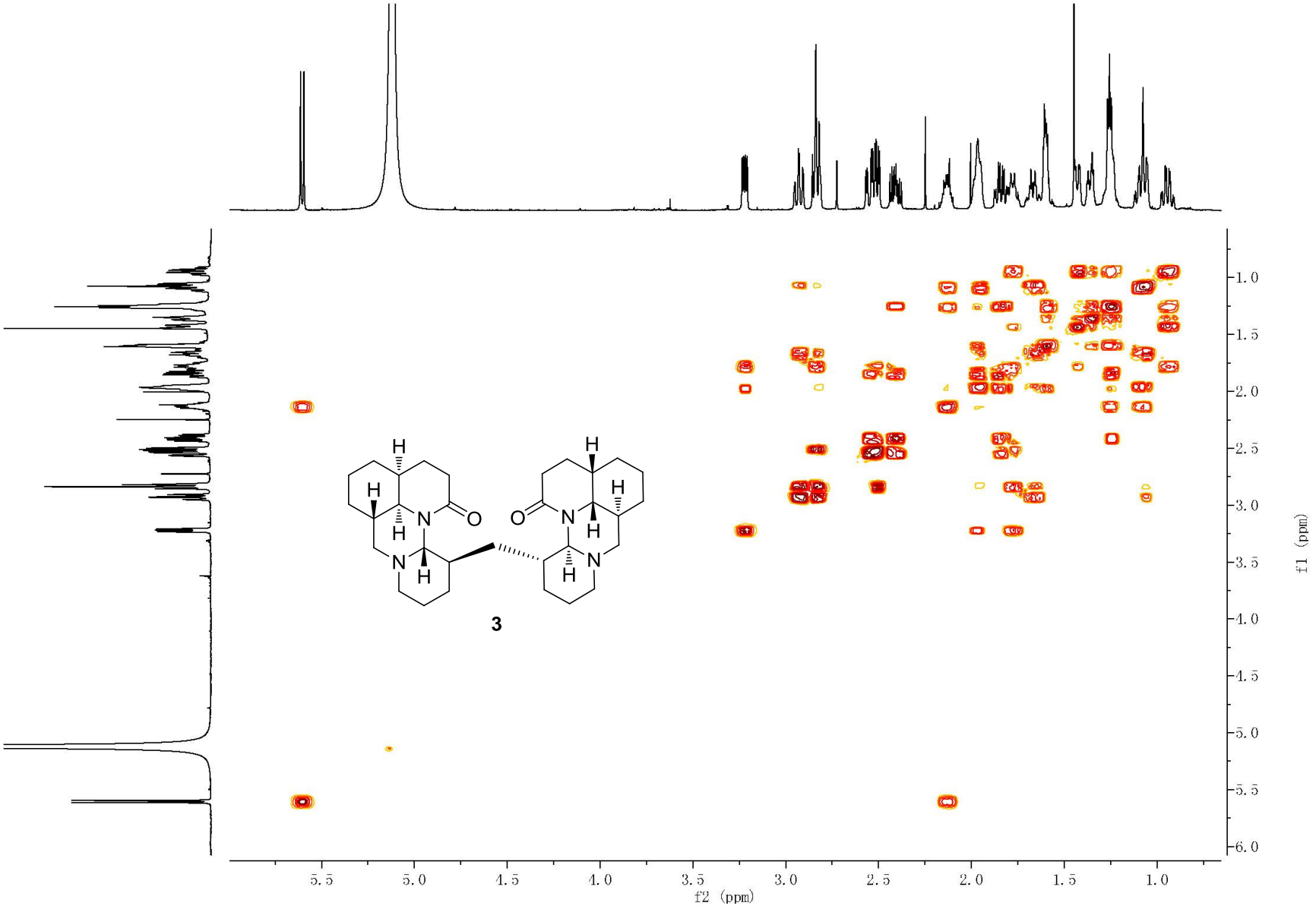


3

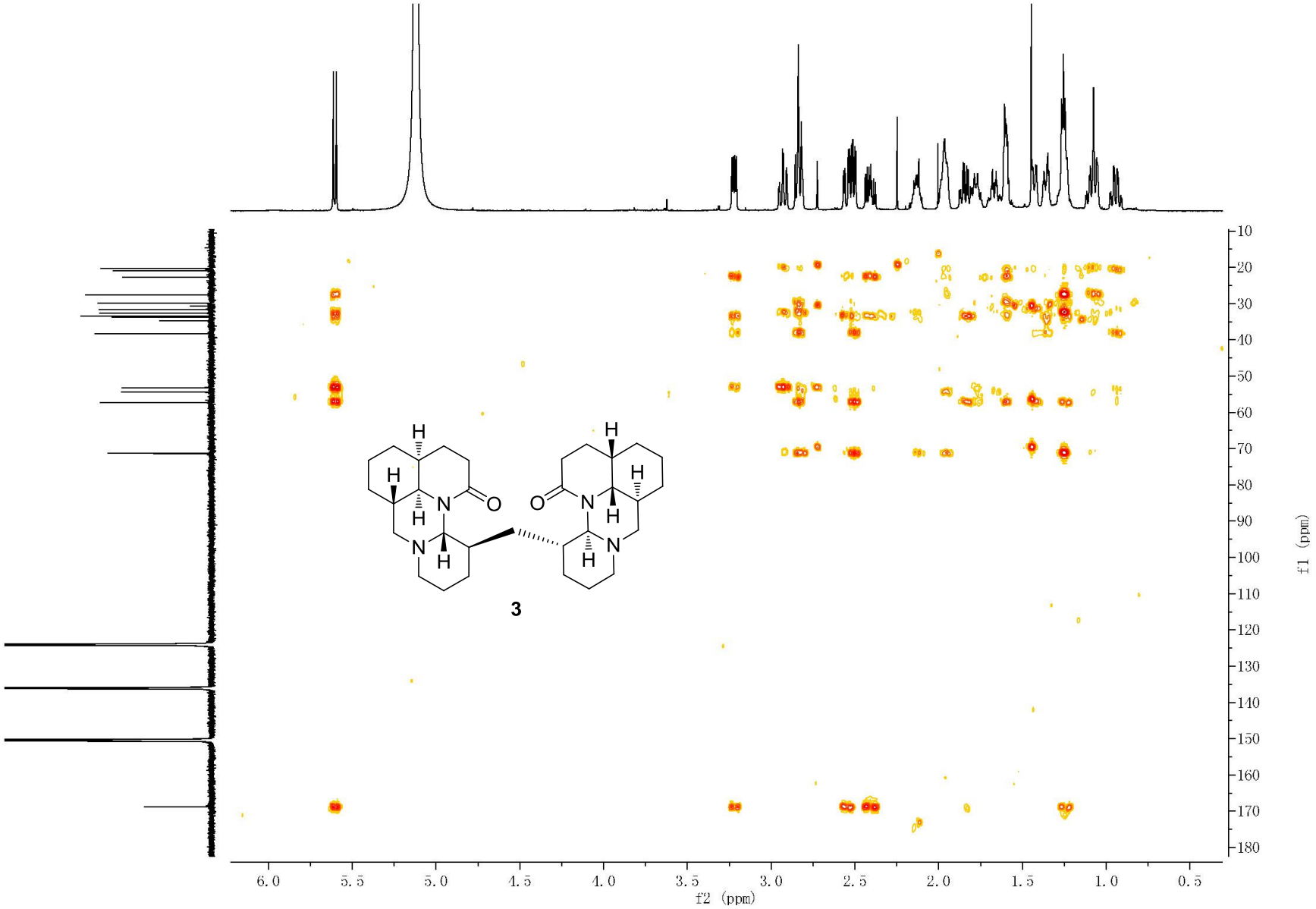
S3.3 HSQC spectrum of myrifamine C (**3**) in prydine-d_5 at 294K



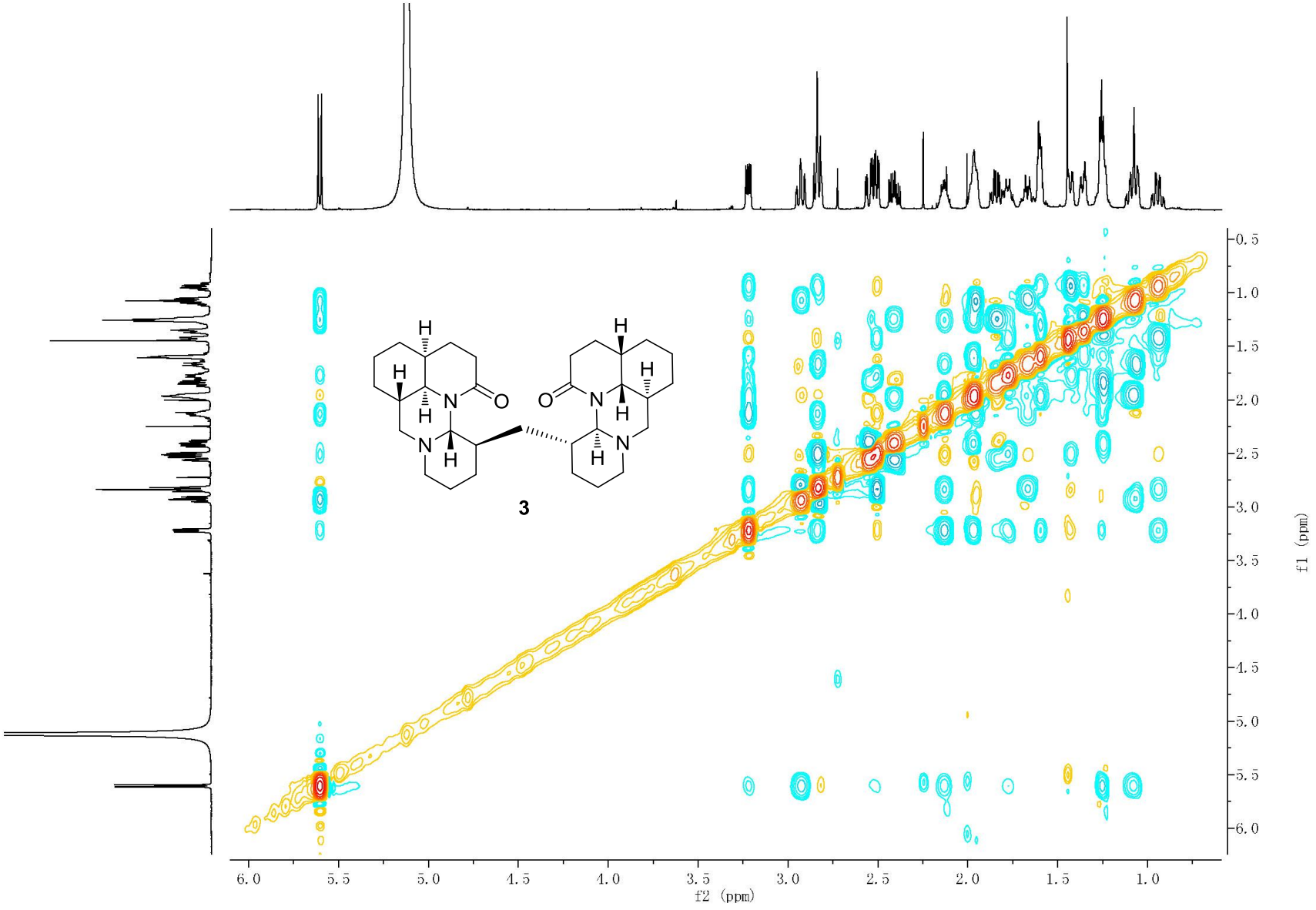
S3.4 COSY spectrum of myrifamine C (**3**) in prydine-d_5 at 294K



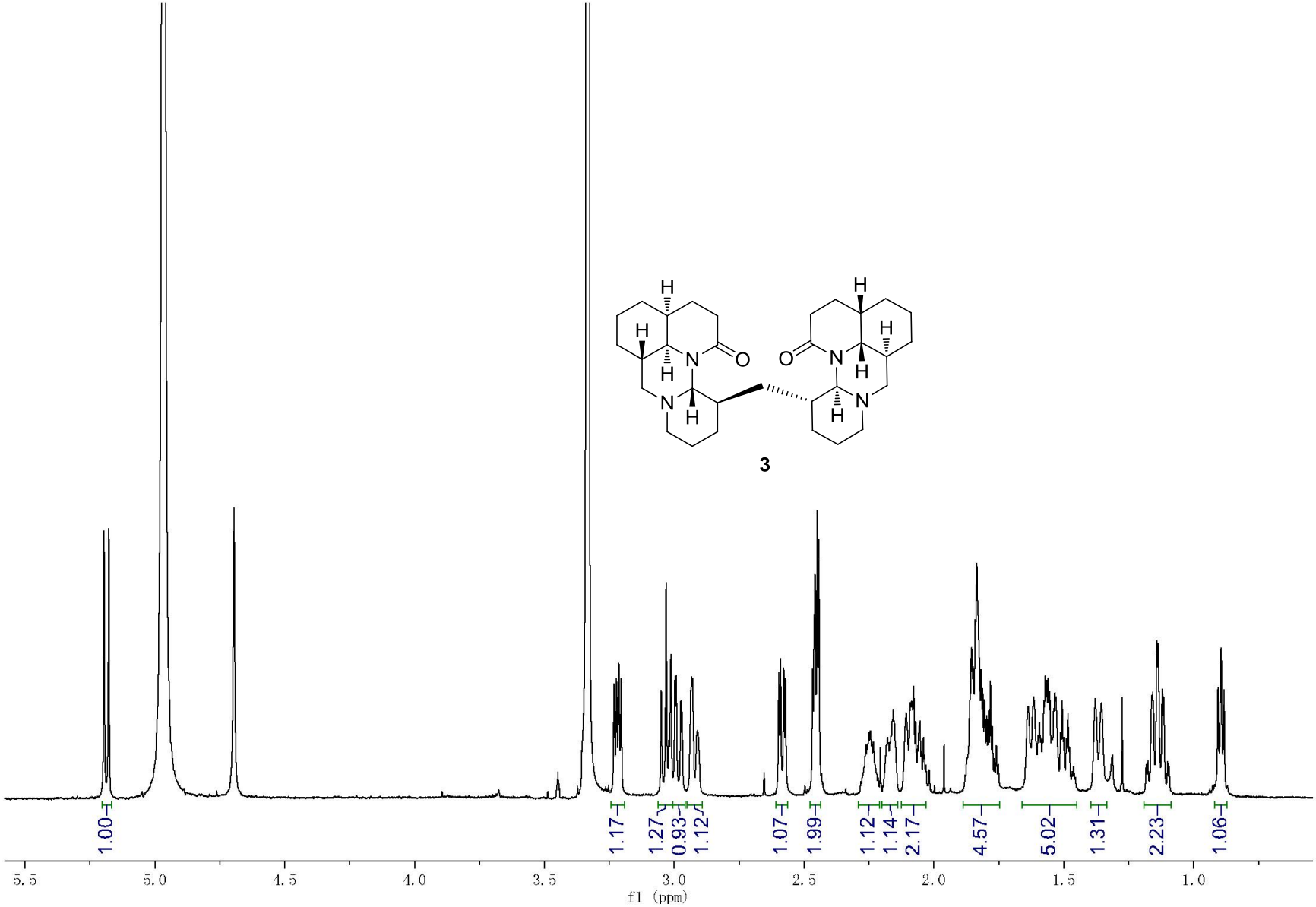
S3.5 HMBC spectrum of myrifamine C (**3**) in prydine-d_5 at 294K



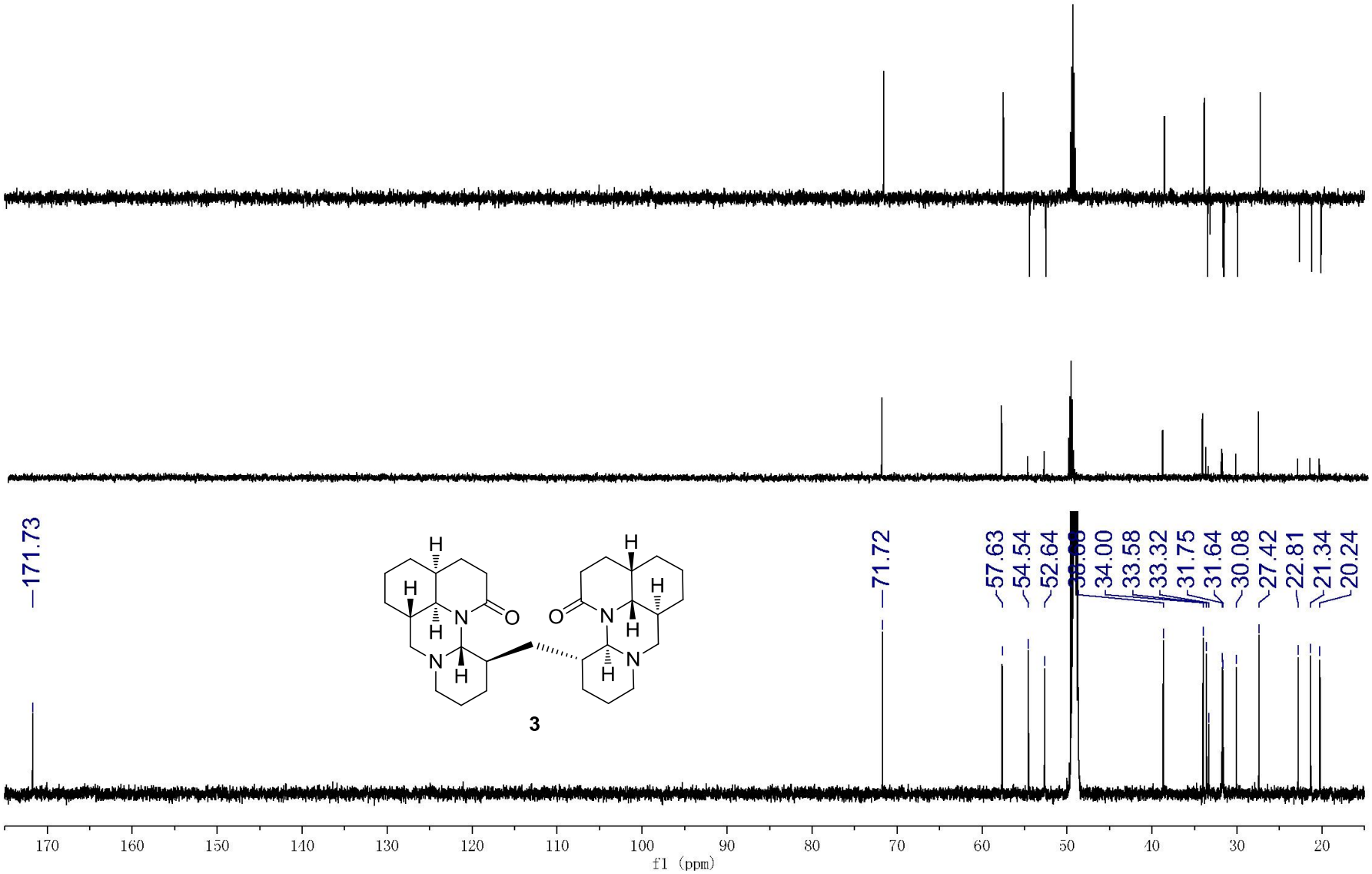
S3.6 ROESY spectrum of myrifamine C (**3**) in prydine-d_5 at 294K



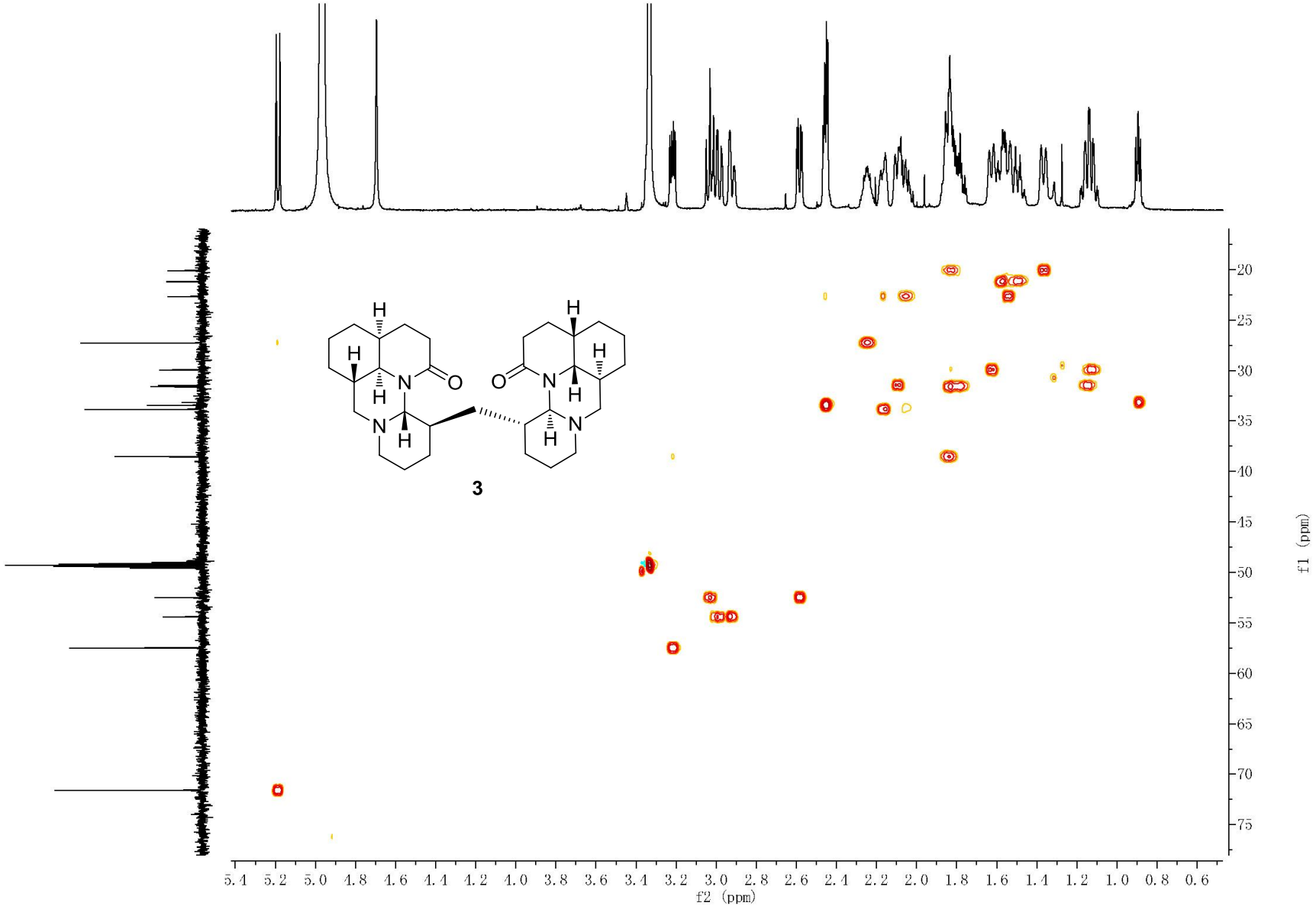
S3.7 ^{1}H NMR spectrum of myrifamine C (**3**) in CD_3OD at 294K



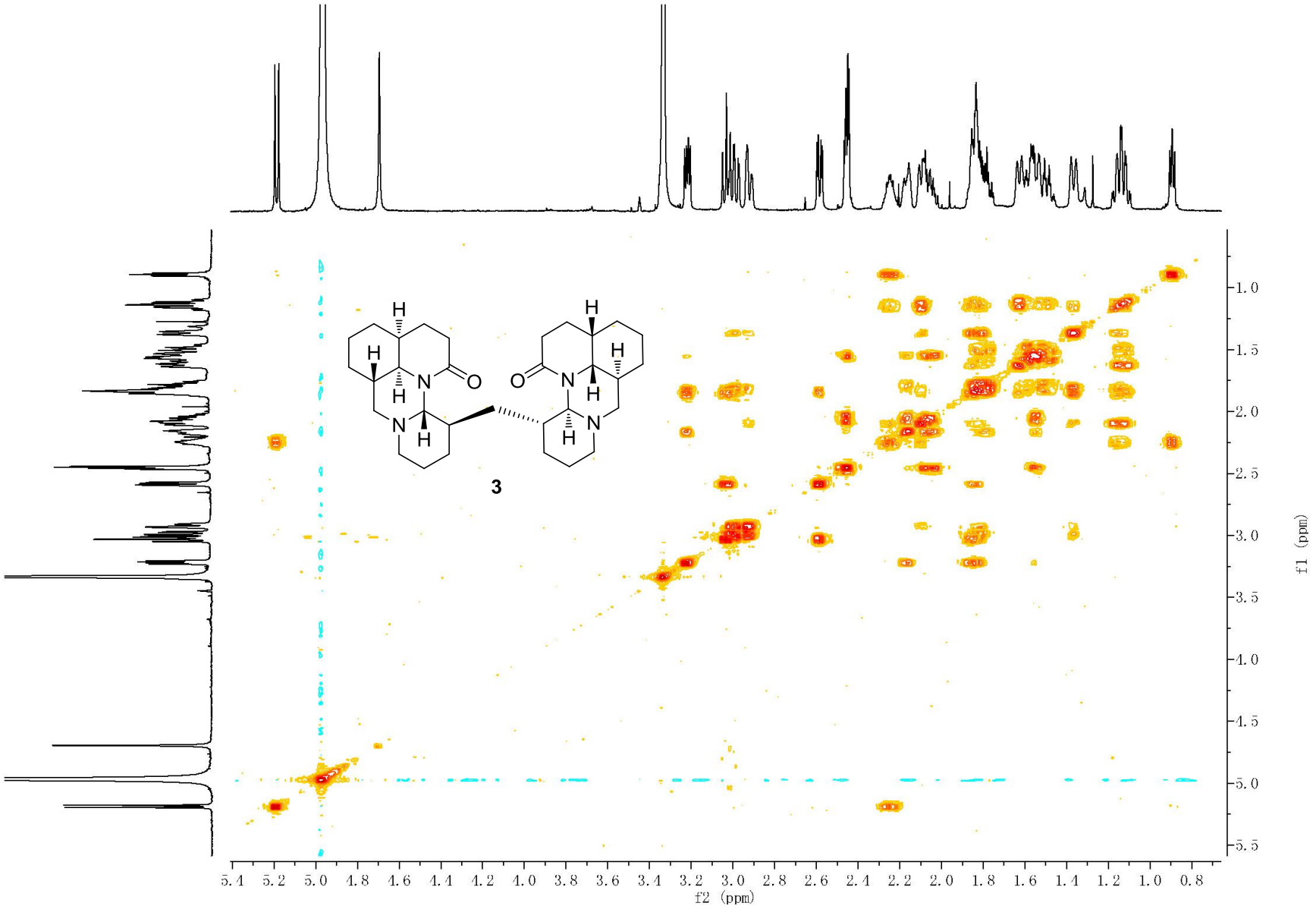
S3.8 ^{13}C NMR spectrum of myrifamine C (**3**) in CD_3OD at 294K



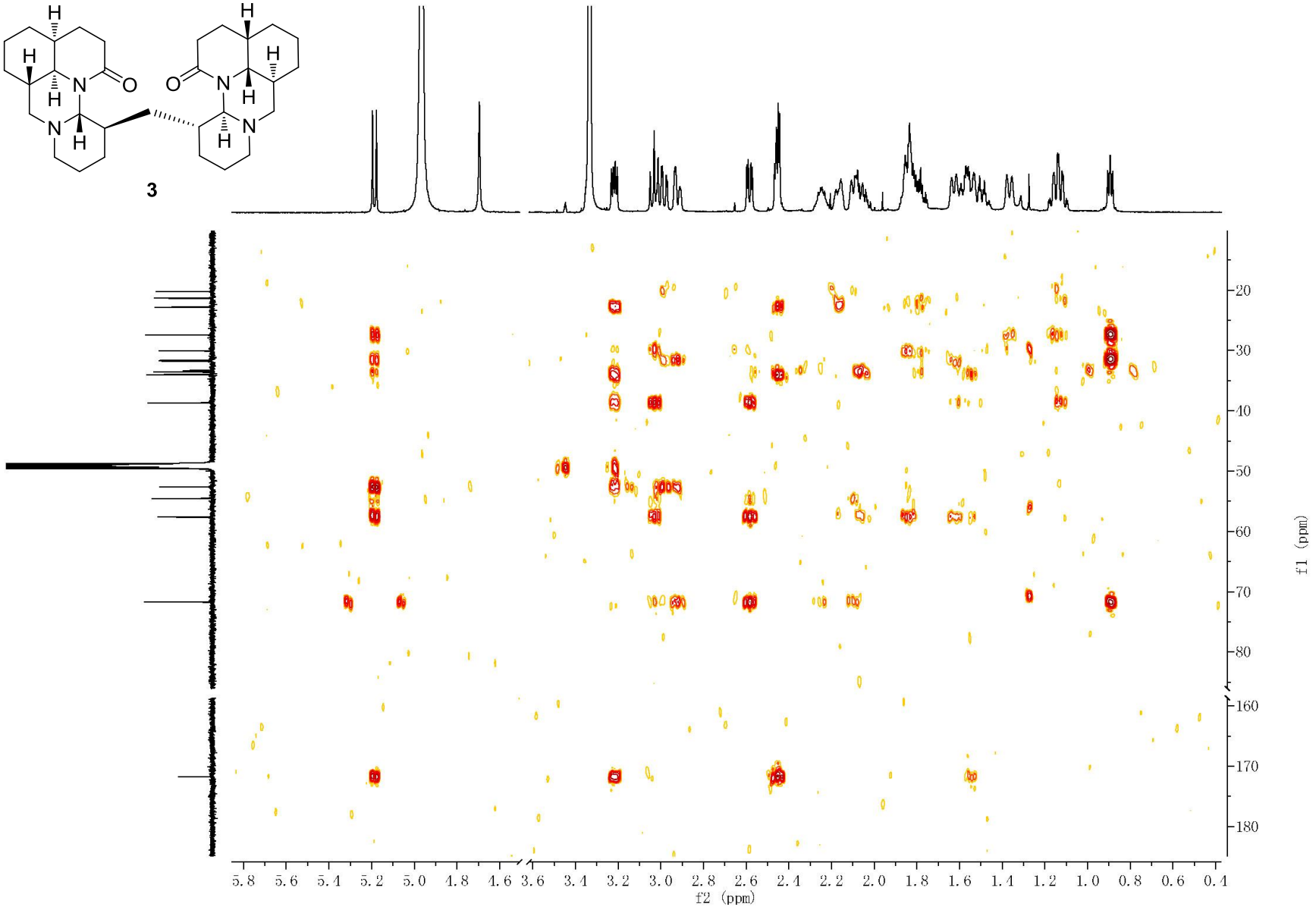
S3.9 HSQC spectrum of myrifamine C (**3**) in CD_3OD at 294K



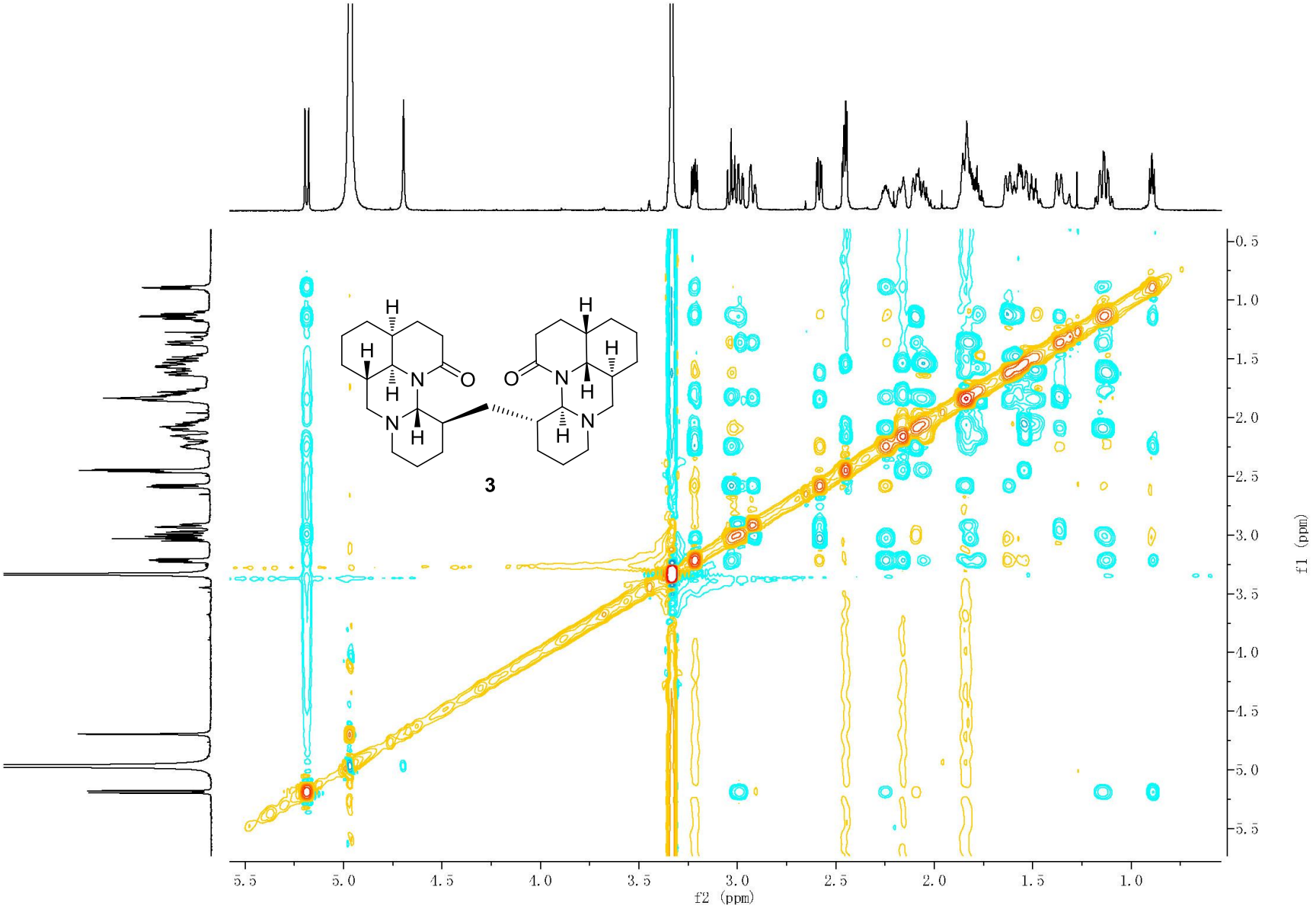
S3.10 COSY spectrum of myrifamine C (**3**) in CD_3OD at 294K



S3.11 HMBC spectrum of myrifamine C (**3**) in CD_3OD at 294K



S3.12 ROESY spectrum of myrifamine C (**3**) in CD_3OD at 294K



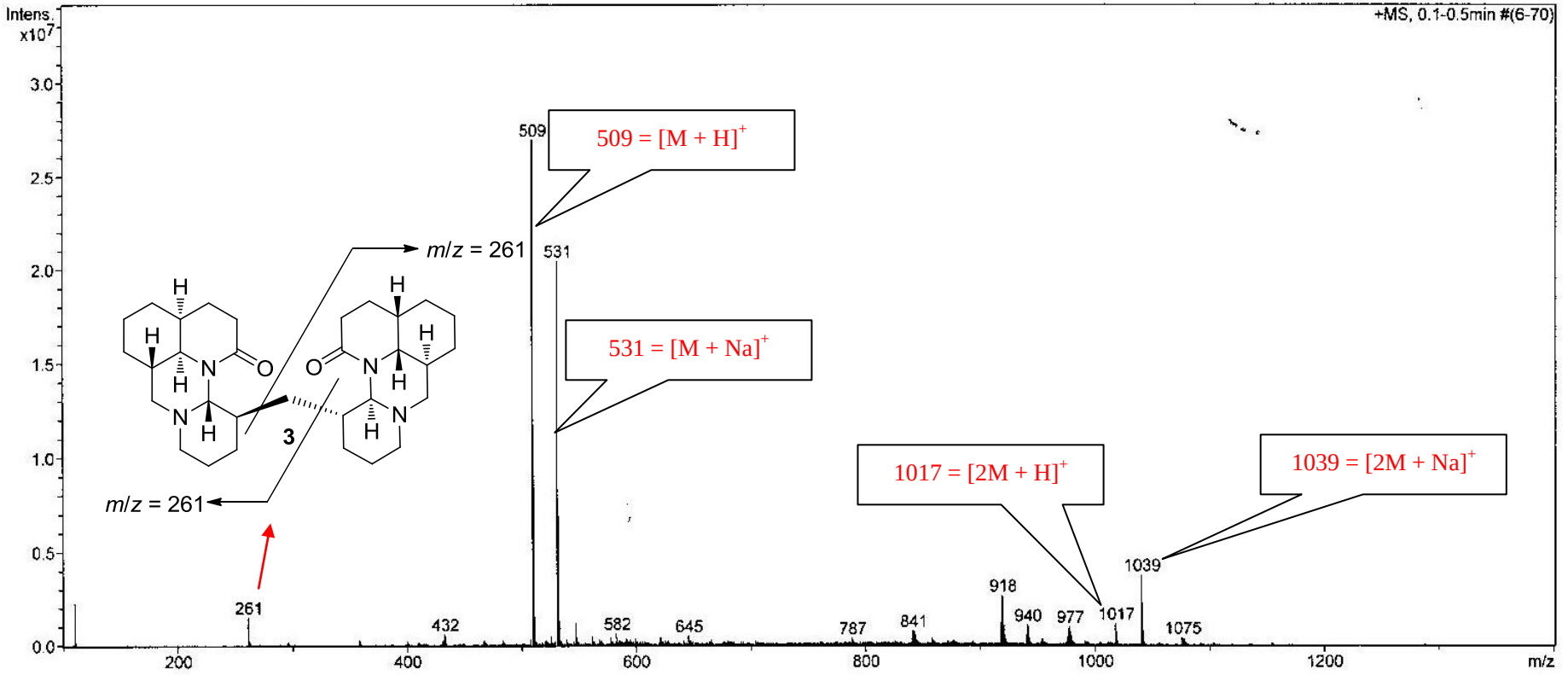
S3.13 ESIMS and HREIMS spectrums of myrifamine C (**3**)

Mass Spectrum List Report

Analysis Info		Acquisition Date	5/2/2012 3:08:58 PM
Analysis Name	D:\DATA\2012file\1205\120502\hm-10b00.d		
Method	ms_ptservice.m	Operator	Bruker
Sample Name	hm-10b	Instrument	HCT

Acquisition Parameter

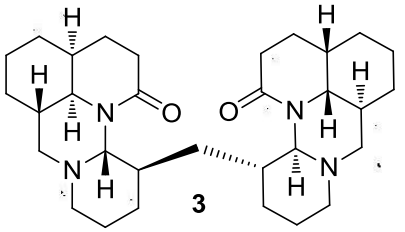
Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Ultra Scan	Scan Begin	100 m/z	Scan End	1400 m/z
Capillary Exit	166.0 Volt	Skimmer	40.0 Volt	Trap Drive	80.4
Accumulation Time	338 µs	Averages	5 Spectra	Auto MS/MS	off



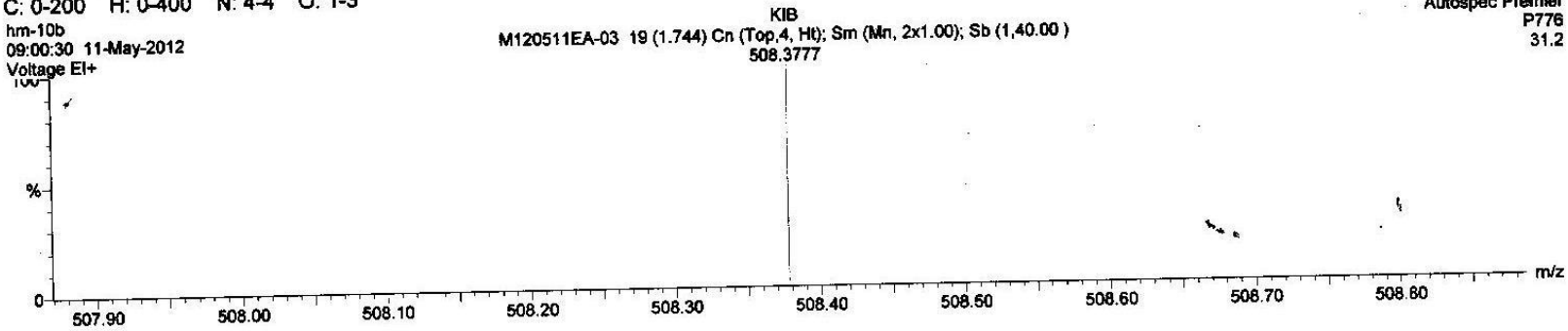
Elemental Composition Report

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = 0.5, max = 120.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
18 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)
Elements Used:
C: 0-200 H: 0-400 N: 4-4 O: 1-3

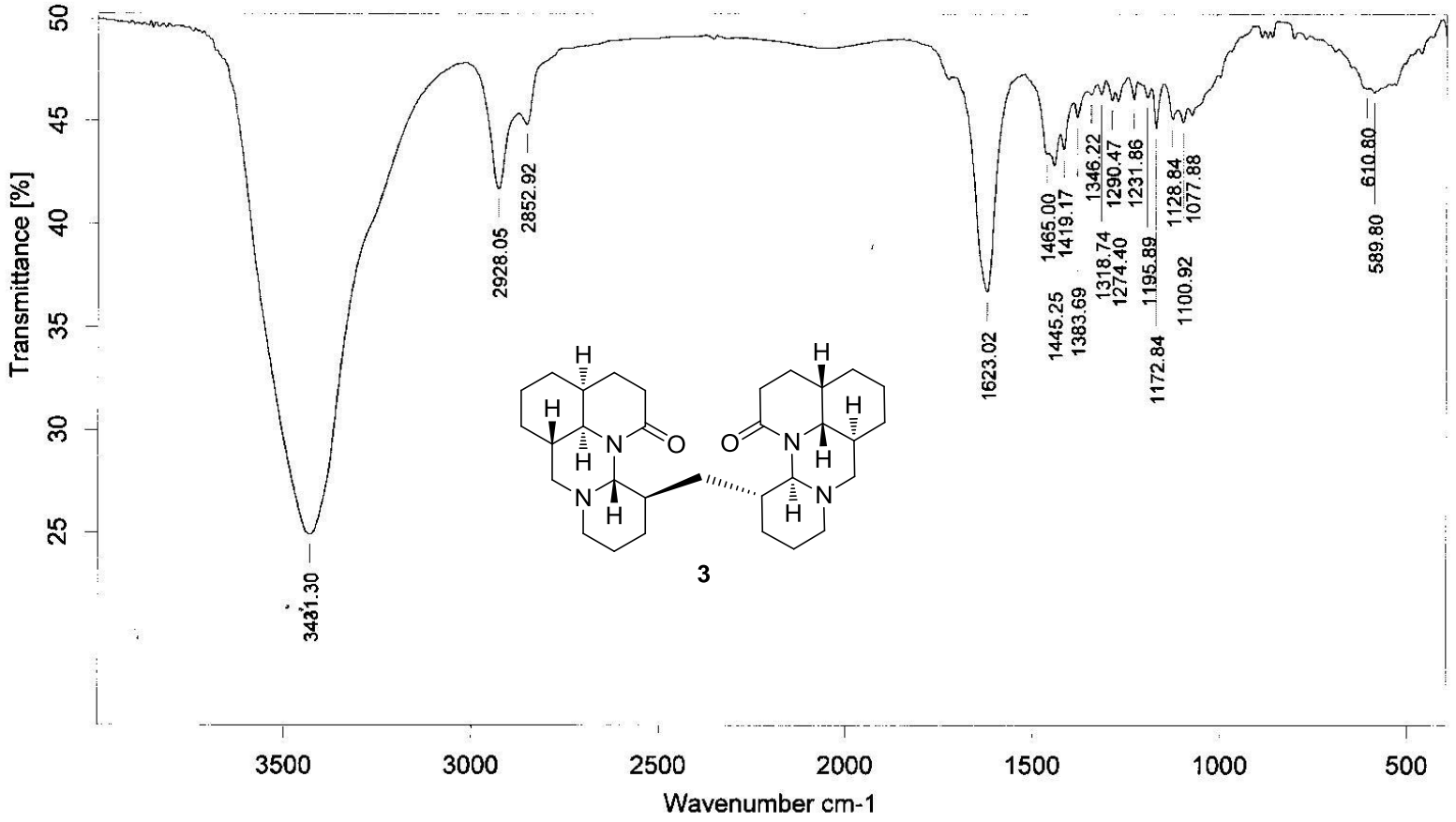


Chemical Formula: $C_{31}H_{48}N_4O_2$
Exact Mass: 508.3777



Minimum:		100.0	10.0	0.5		
Maximum:				120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
508.3777	508.3777	0.0	0.0	10.0	5546035.5	C31 H48 N4 O2

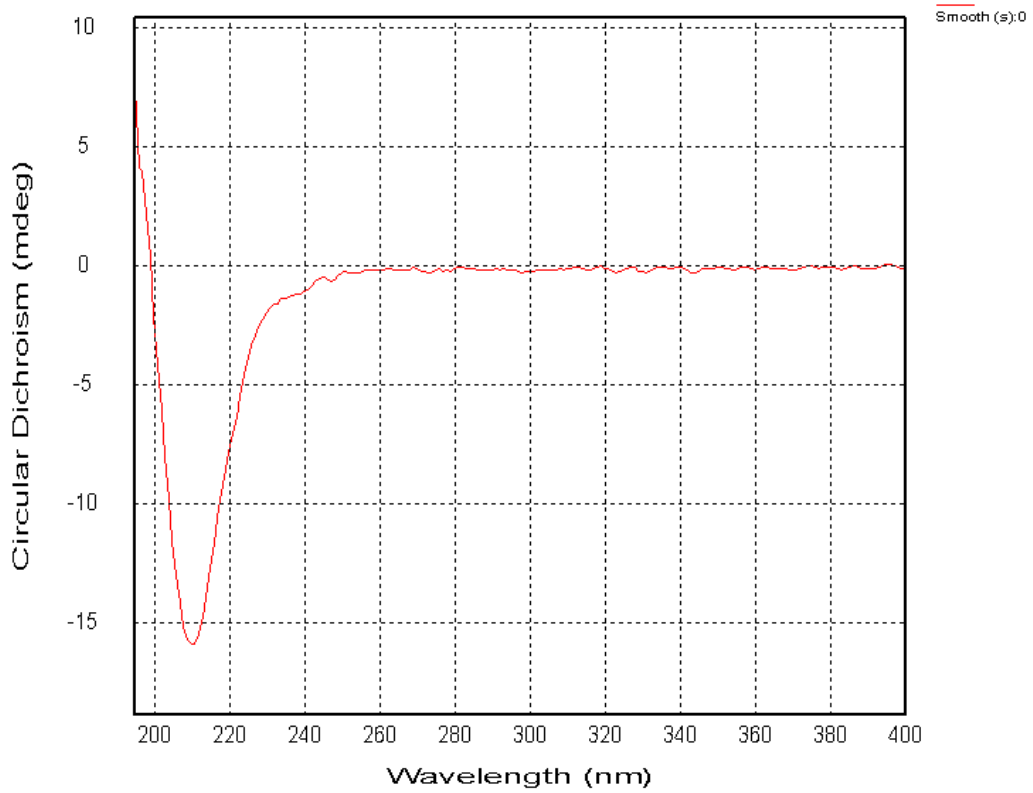
S3.14 IR spectrum of myrifamine C (**3**)

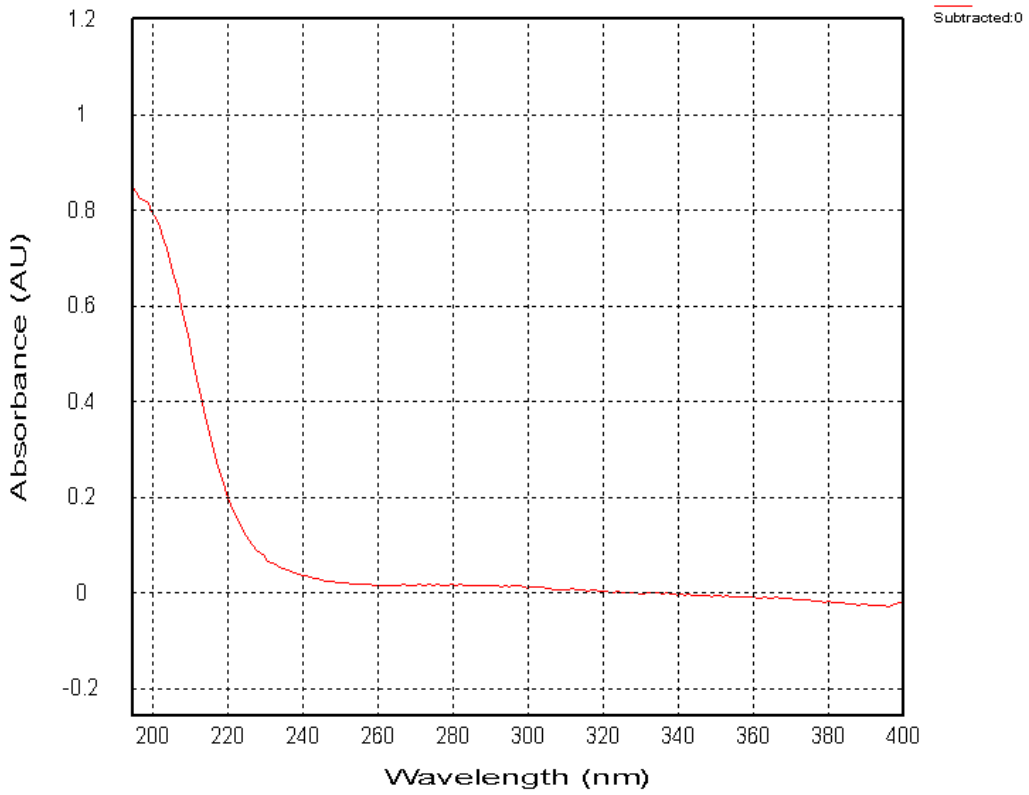


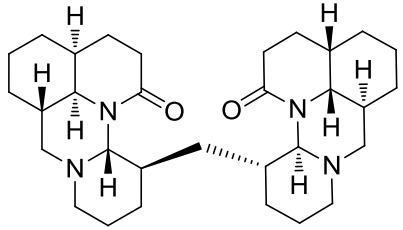
3

Sample : hm-10b	Frequency Range : 399.246 - 3996.32	Measured on : 07/06/2012	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 120607IR0	Zerofilling : 2	Acquisition : Double Sided,For	

S3.15 ECD spectrum of myrifamine C (**3**) in methanol

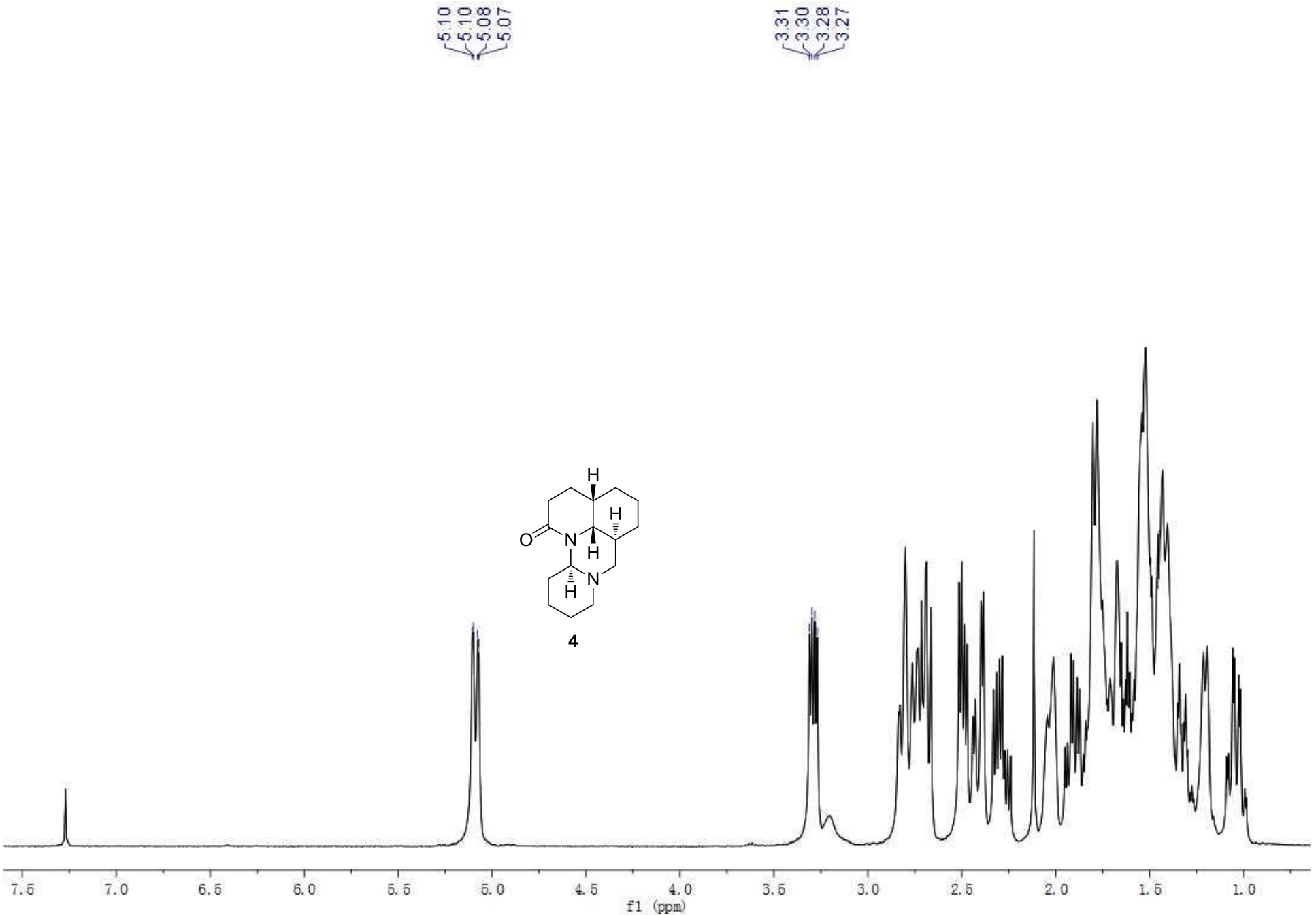




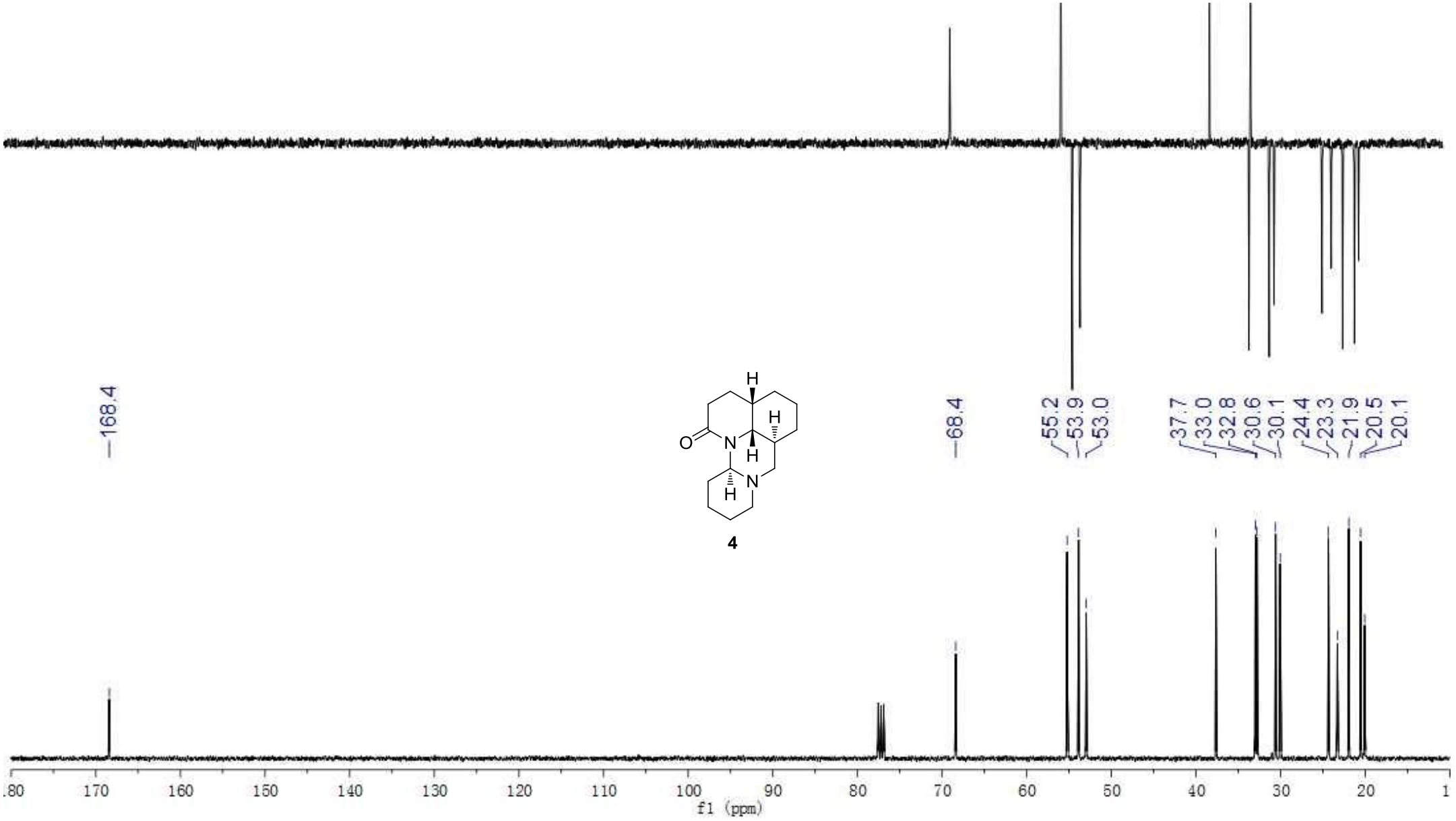


3

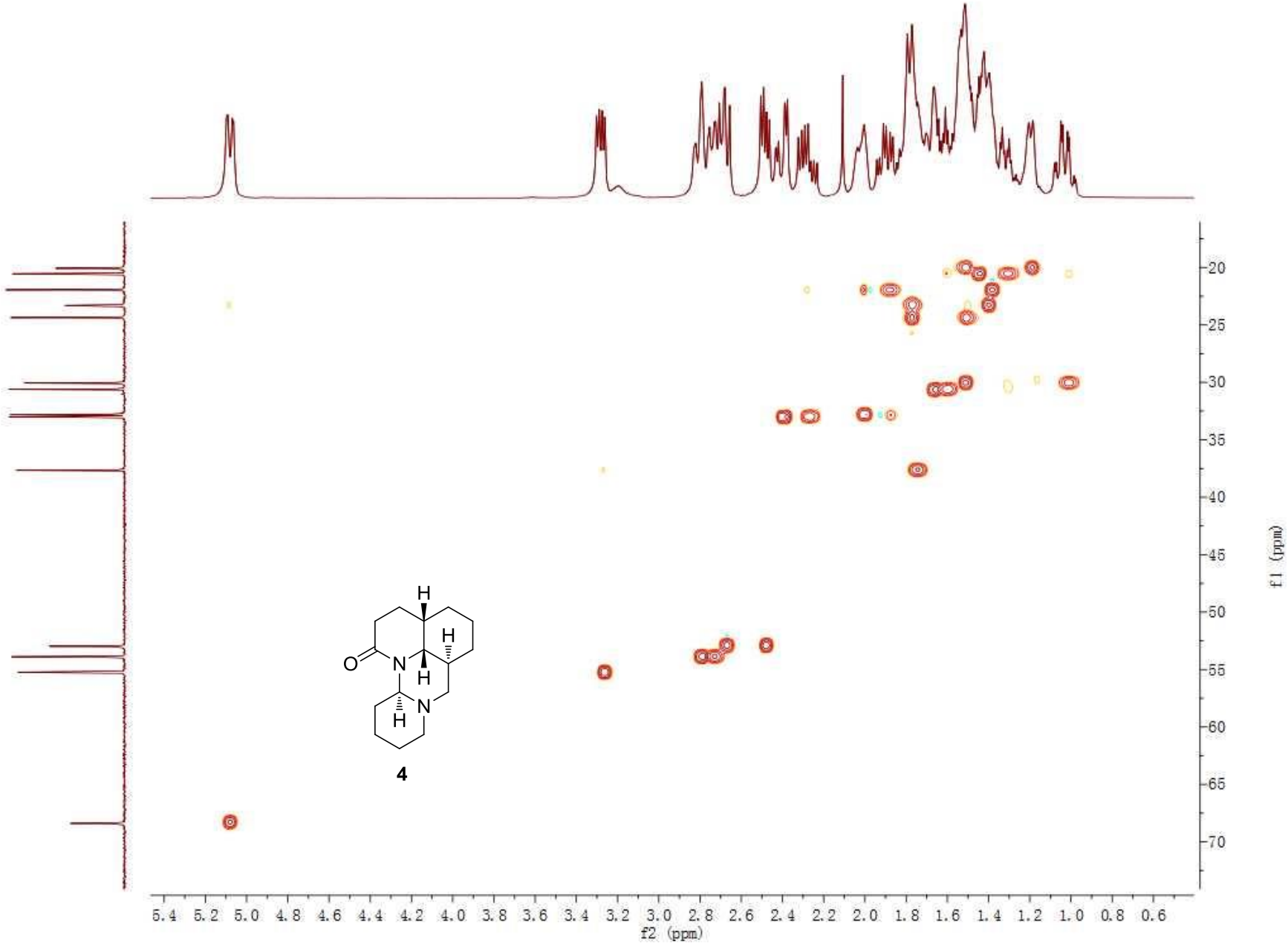
S4.1 ^{1}H NMR spectrum of myrionamide (**4**) in $CDCl_3$ 291K



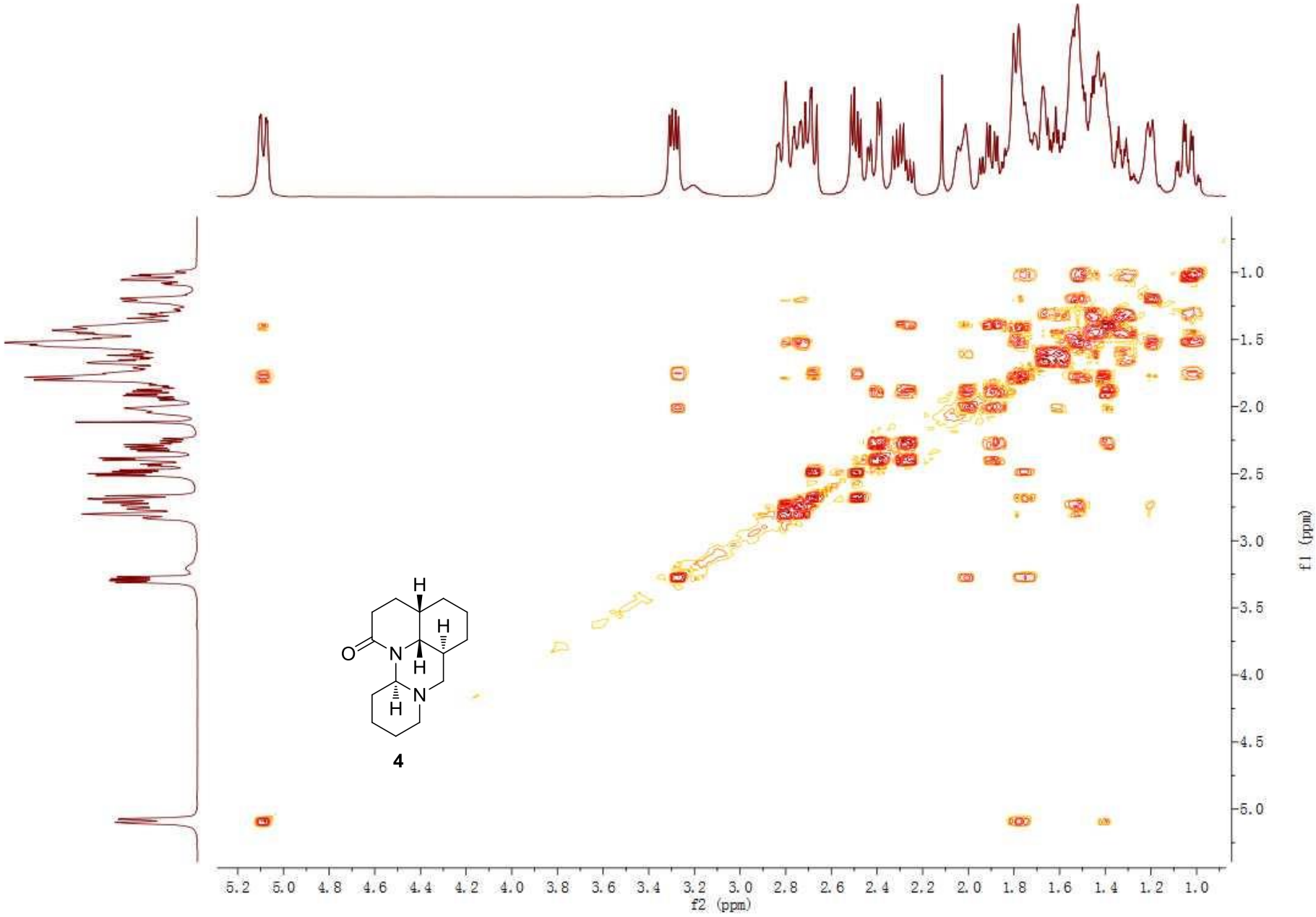
S4.2 ^{13}C NMR spectrum of myrionamide (**4**) in $CDCl_3$ 291K



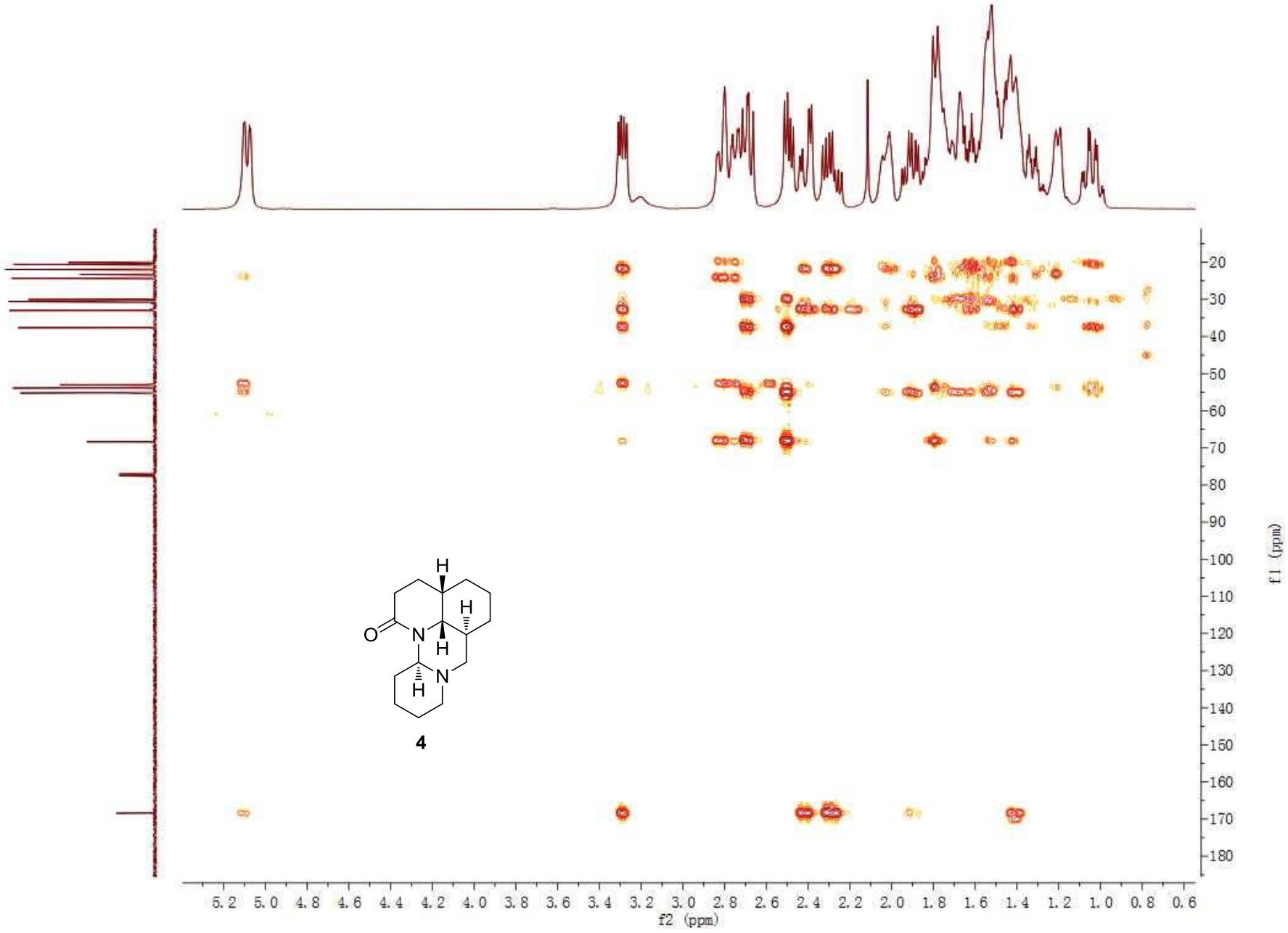
S4.3 HSQC spectrum of myrionamide (**4**) in $CDCl_3$ 291K



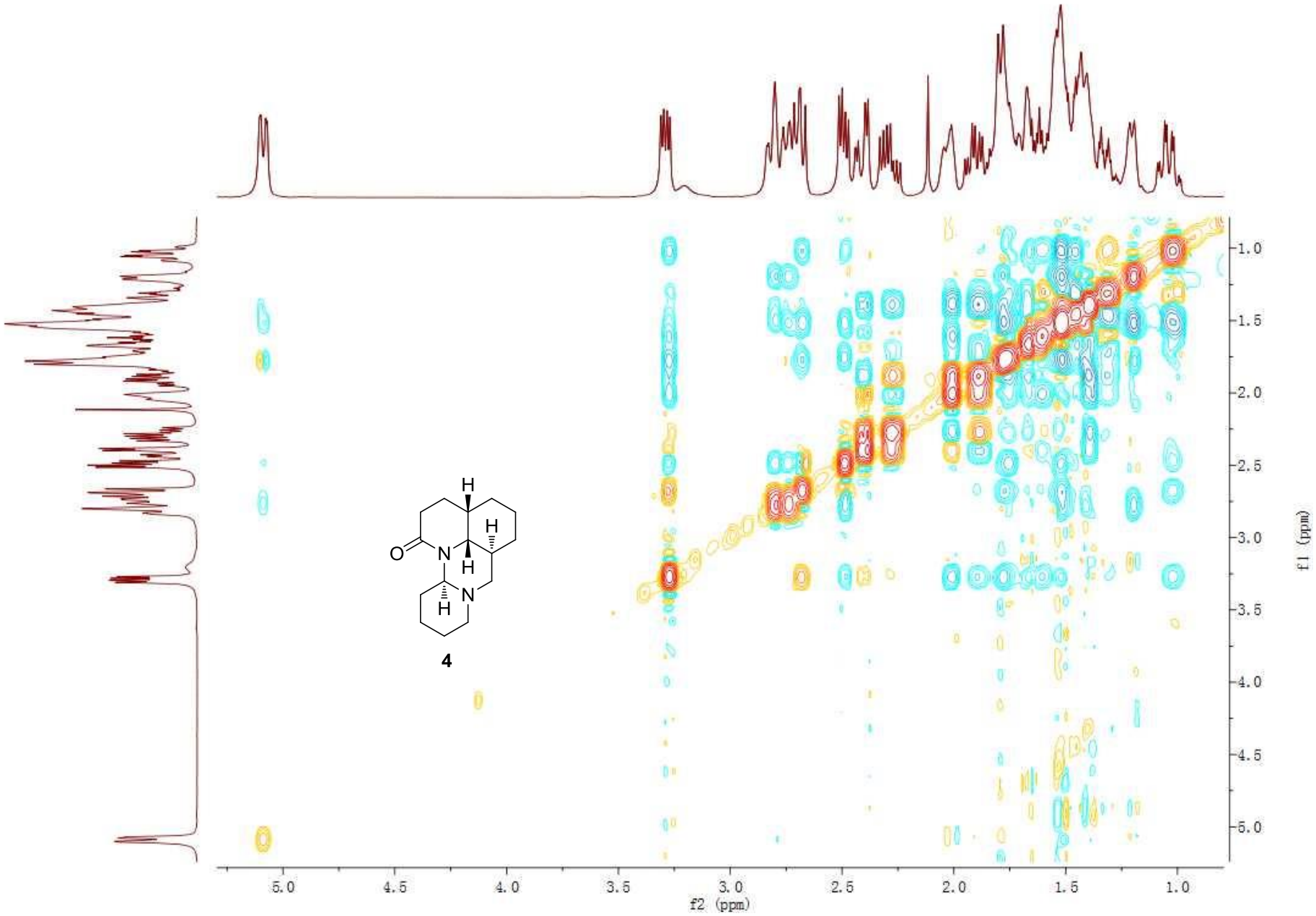
S4.4 COSY spectrum of myrionamide (**4**) in $CDCl_3$ 291K



S4.5 HMBC spectrum of myrionamide (**4**) in $CDCl_3$ 291K



S4.6 ROESY spectrum of myrionamide (**4**) in $CDCl_3$ 291K



S4.7 ESIMS spectrum of myrionamide (**4**)

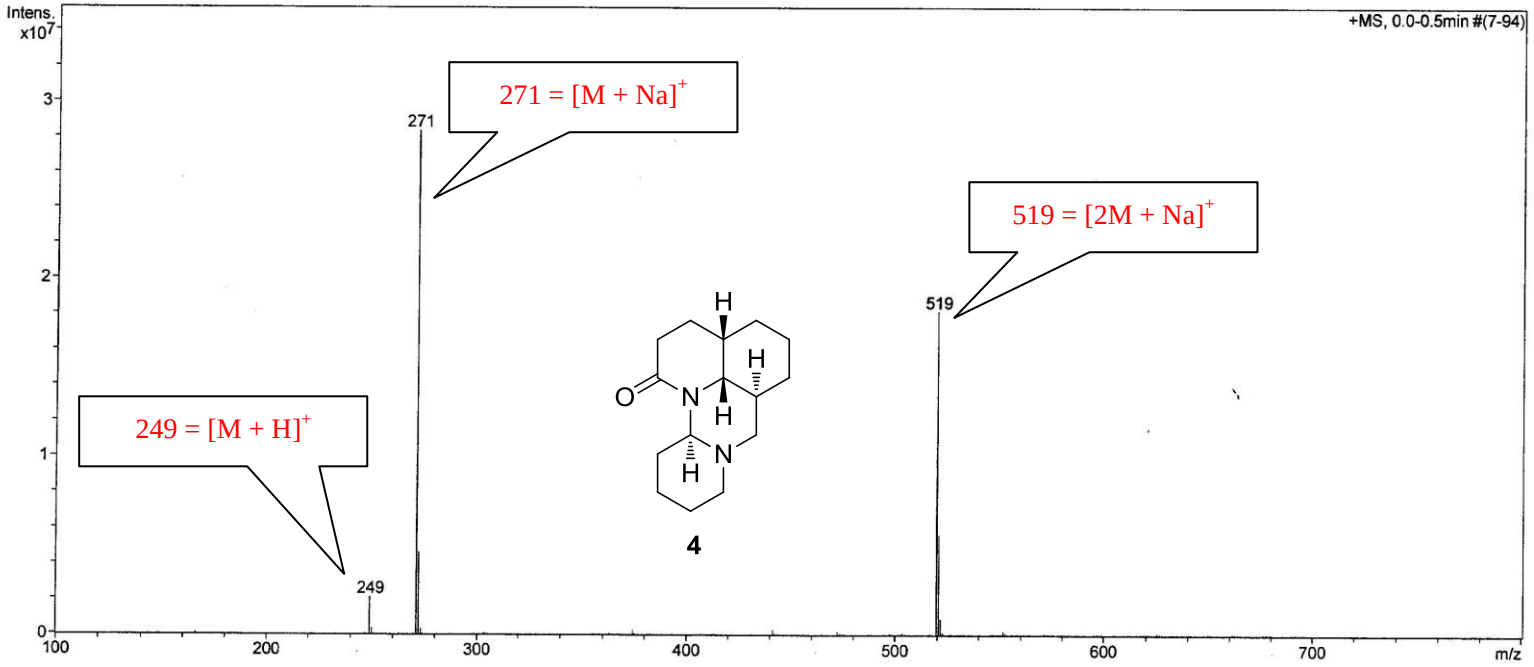
Mass Spectrum List Report

Analysis Info

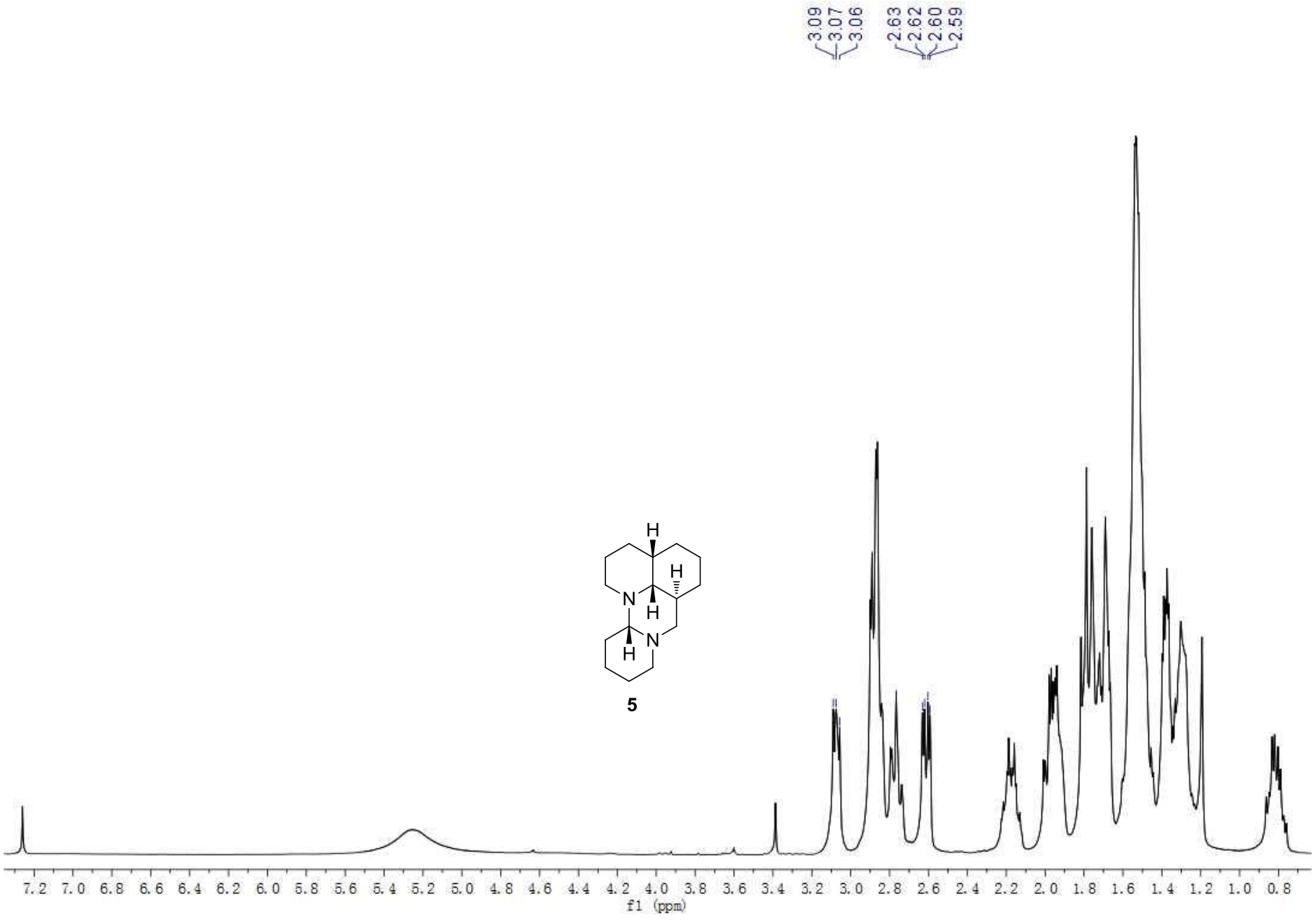
Analysis Name	D:\DATA\2012file\1203\1203012\hm-200.d	Acquisition Date	3/12/2012 4:09:24 PM
Method	ms_ptservice.m	Operator	Bruker
Sample Name	hm-2	Instrument	HCT

Acquisition Parameter

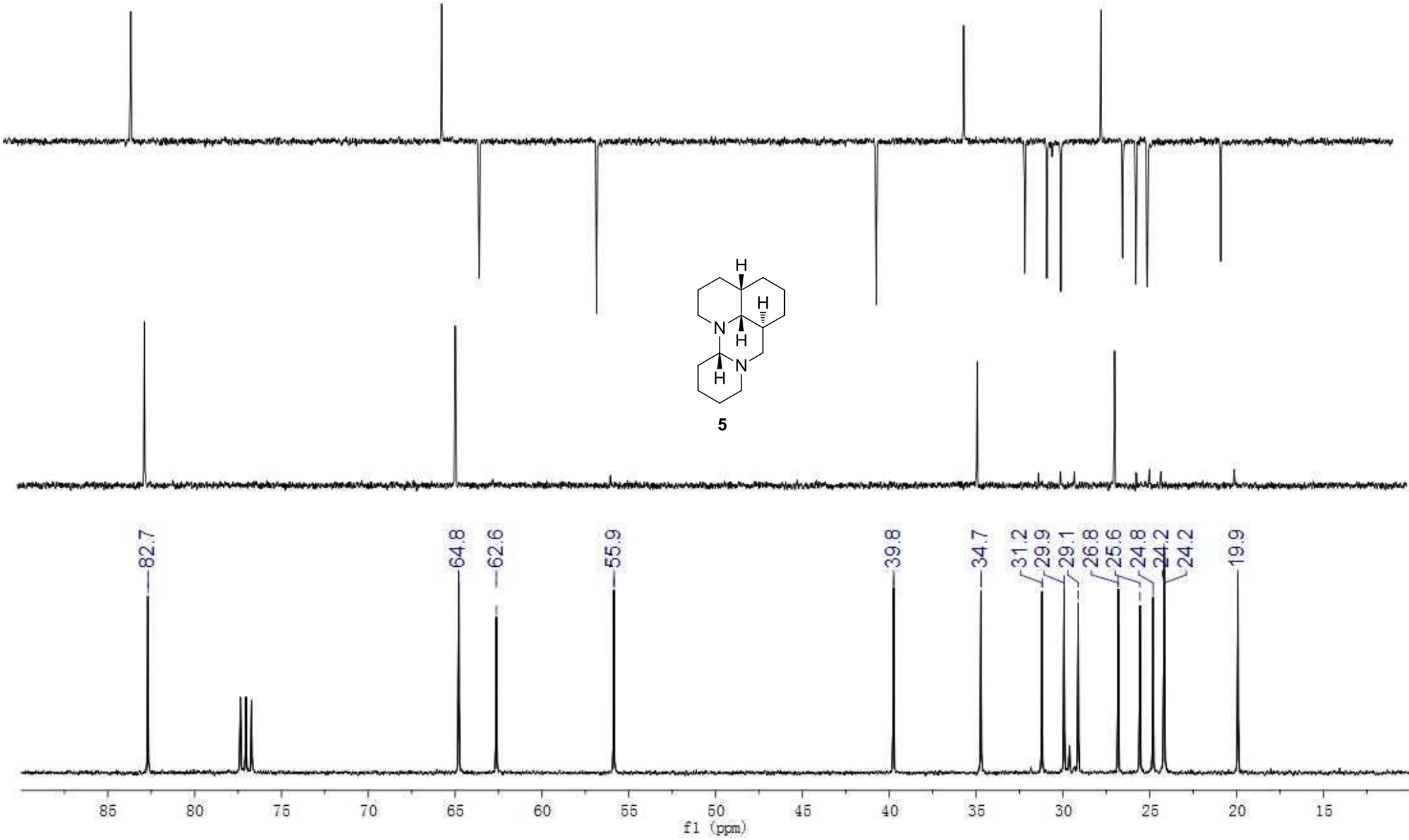
Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Ultra Scan	Scan Begin	100 m/z	Scan End	800 m/z
Capillary Exit	260.0 Volt	Skimmer	40.0 Volt	Trap Drive	60.0
Accumulation Time	395 µs	Averages	5 Spectra	Auto MS/MS	off



S5.1 ^{1}H NMR spectrum of schoberine (**5**) in $CDCl_3$ 291K

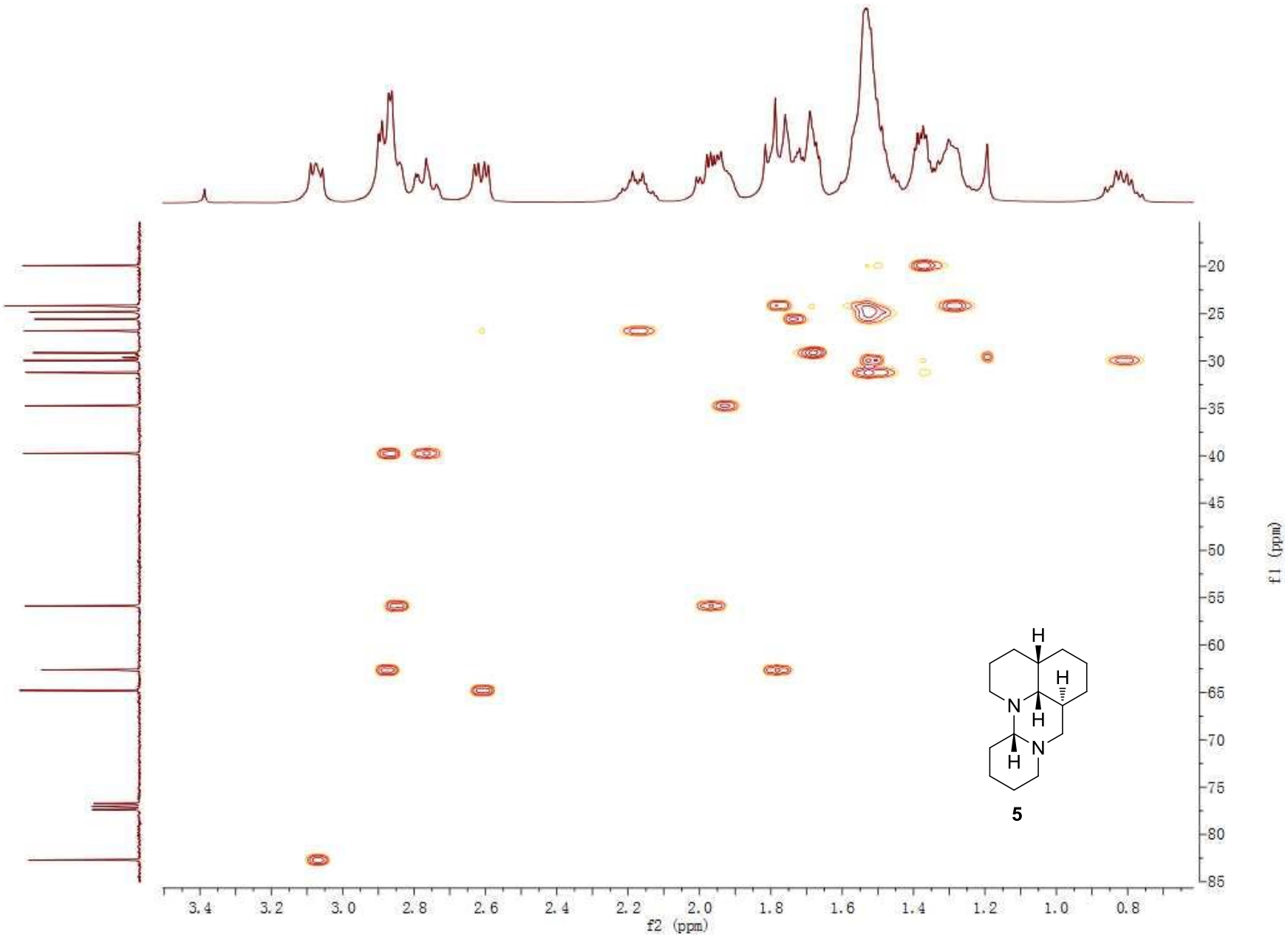


S5.2 ^{13}C NMR spectrum of schoberine (**5**) in $CDCl_3$ 291K

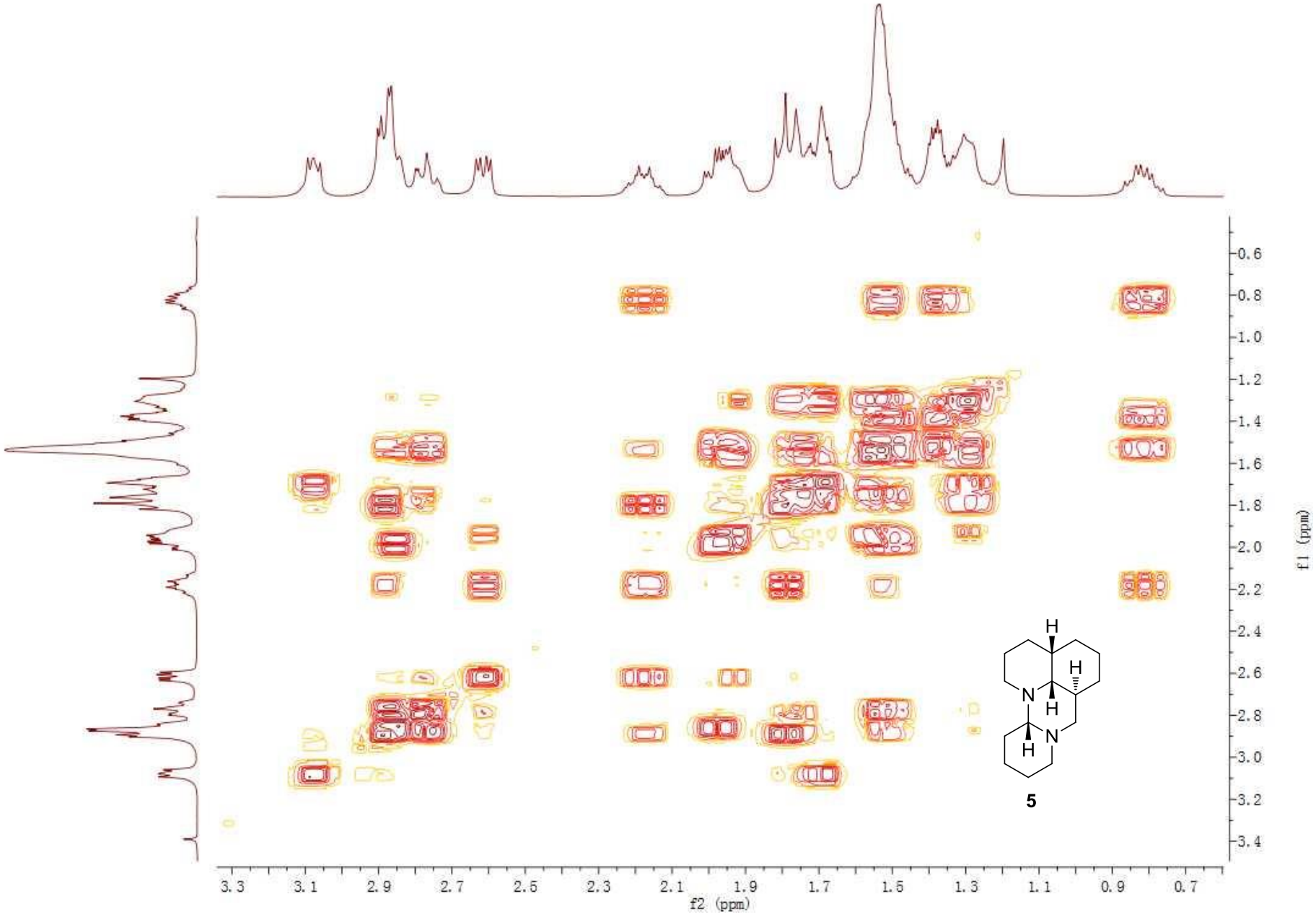


5

S5.3 HSQC spectrum of schoberine (**5**) in $CDCl_3$ 291K

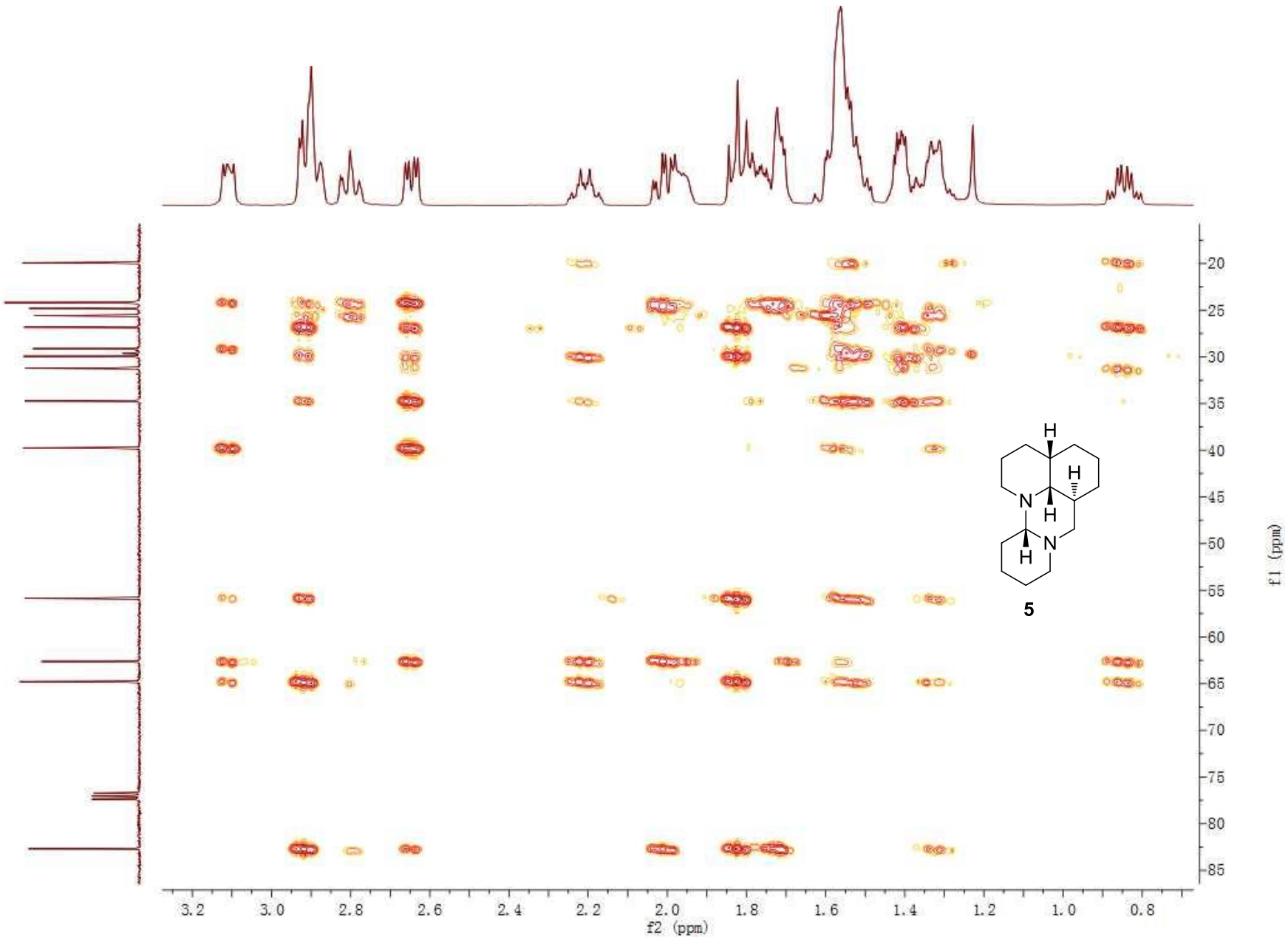


S5.4 COSY spectrum of schoberine (**5**) in $CDCl_3$ 291K

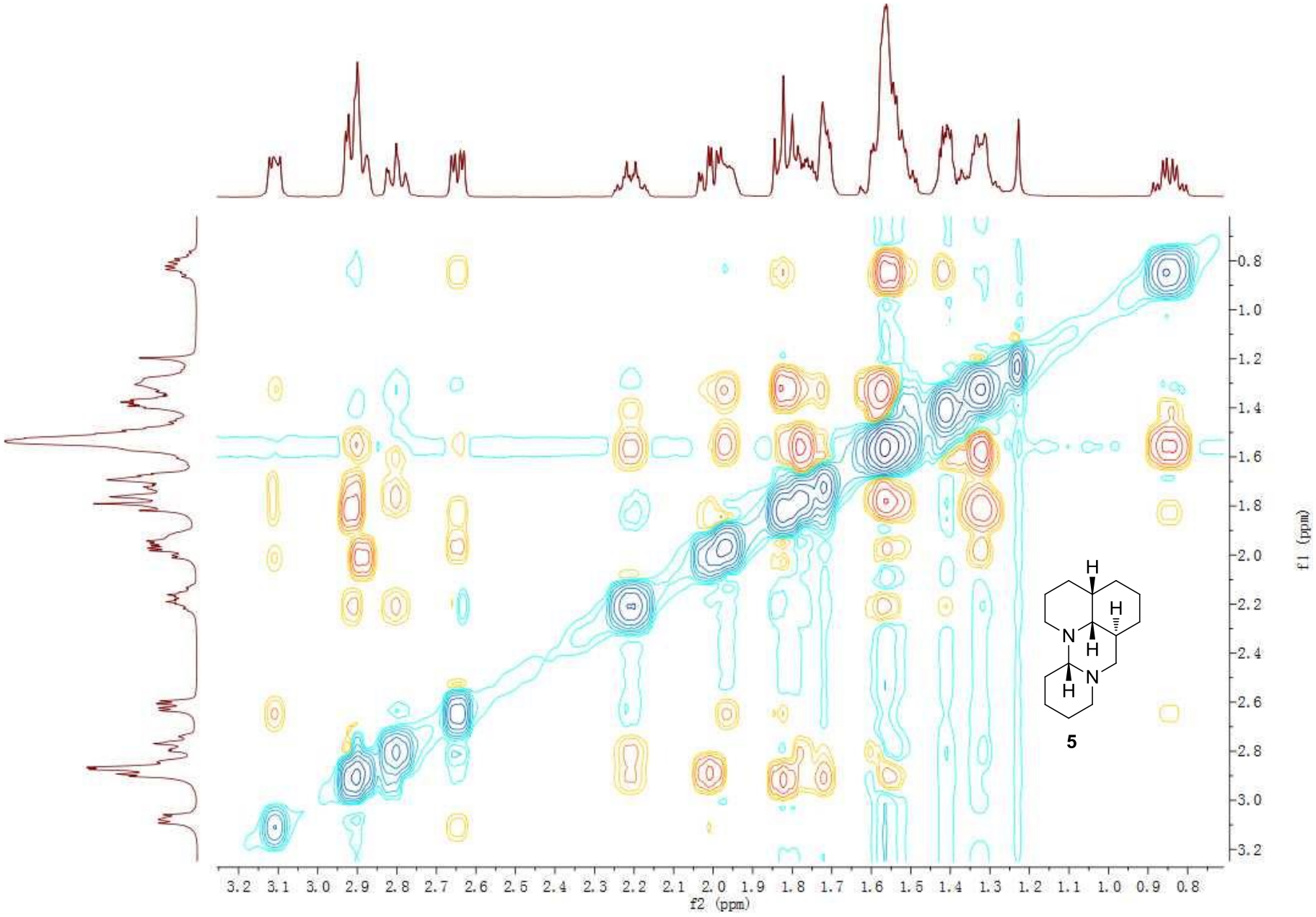


5

S5.5 HMBC spectrum of schoberine (**5**) in $CDCl_3$ 291K



S5.6 ROESY spectrum of schoberine (**5**) in $CDCl_3$ at 291K



S5.7 ESIMS spectrum of schoberine (**5**)

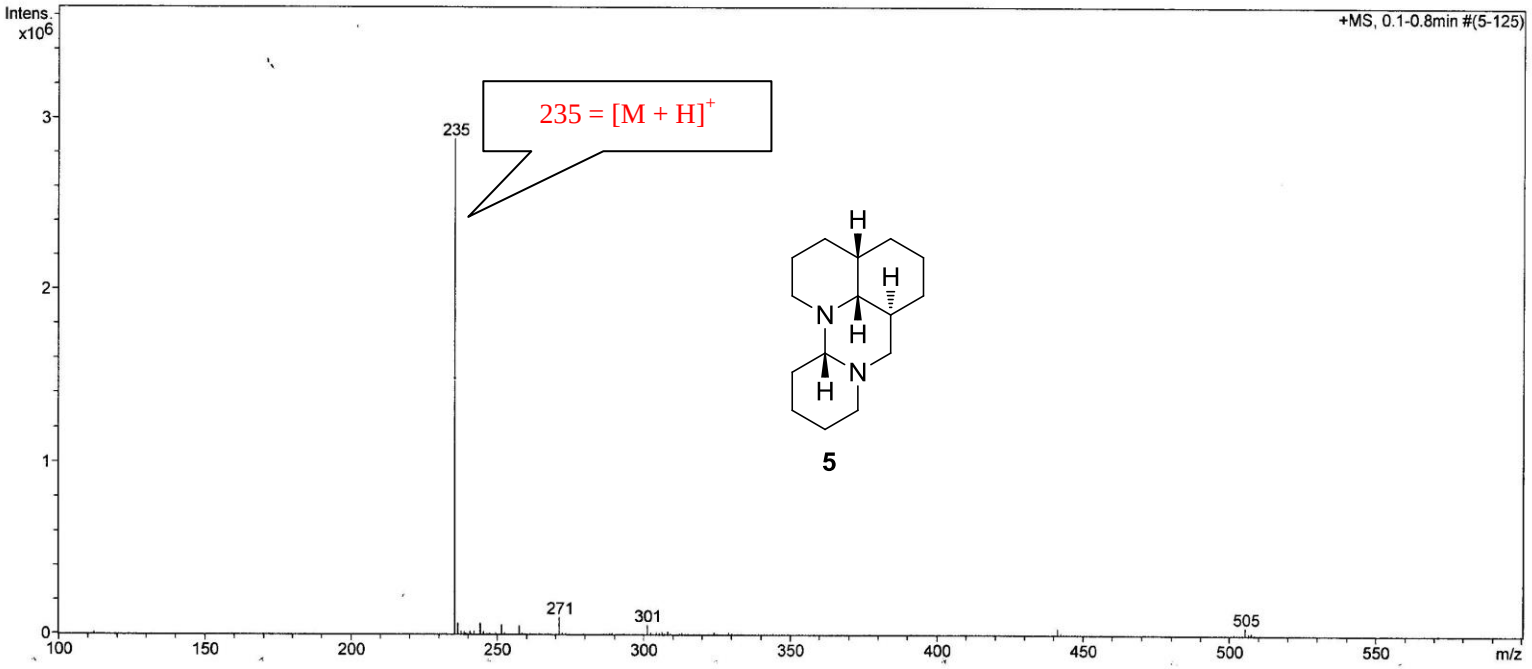
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\DATA\2012file\1210\121017\hm-4a00.d	Acquisition Date	10/17/2012 11:18:36 AM
Method	DEF_MS.M	Operator	Bruker
Sample Name	hm-4a	Instrument	HCT

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Ultra Scan	Scan Begin	100 m/z	Scan End	600 m/z
Capillary Exit	98.5 Volt	Skimmer	40.0 Volt	Trap Drive	28.4
Accumulation Time	11068 µs	Averages	5 Spectra	Auto MS/MS	off



Crystal data and structure refinement for 1.

Identification code	cu_hm6_0m
Empirical formula	C48 H74 N6 O4
Formula weight	799.13
Temperature	100(2) K
Wavelength	1.54178 A
Crystal system, space group	Orthorhombic, P 21 21 21
Unit cell dimensions	a = 9.7135(3) A alpha = 90 deg. b = 13.9213(4) A beta = 90 deg. c = 31.7069(8) A gamma = 90 deg.
Volume	4287.6(2) A^3
Z, Calculated density	4, 1.238 Mg/m^3
Absorption coefficient	0.617 mm^-1
F(000)	1744
Crystal size	1.40 x 0.42 x 0.25 mm
Theta range for data collection	2.79 to 69.37 deg.
Limiting indices	-9<=h<=10, -16<=k<=15, -33<=l<=38
Reflections collected / unique	19888 / 7428 [R(int) = 0.0353]
Completeness to theta = 69.37	93.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8609 and 0.4786
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7428 / 0 / 519

Goodness-of-fit on F^2	1.083
Final R indices [I>2sigma(I)]	R1 = 0.0450, wR2 = 0.1280
R indices (all data)	R1 = 0.0452, wR2 = 0.1283
Absolute structure parameter	0.0(2)
Extinction coefficient	0.00115(13)
Largest diff. peak and hole	0.970 and -0.359 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **1**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(20)	7730(2)	5266(1)	2409(1)	29(1)
O(20A)	2788(2)	9455(1)	-920(1)	35(1)
O(20B)	3123(2)	354(1)	1103(1)	43(1)
N(1)	5426(2)	3197(1)	1451(1)	18(1)
N(12)	6729(2)	2066(1)	1047(1)	20(1)
N(1A)	5380(2)	7952(1)	168(1)	21(1)
N(12A)	4173(2)	7231(1)	738(1)	22(1)
N(1B)	160(2)	2413(1)	1869(1)	21(1)
N(12B)	1108(2)	3433(1)	2397(1)	25(1)
C(20)	7326(2)	5022(1)	2057(1)	22(1)
C(3)	6442(2)	4213(1)	1980(1)	20(1)
C(2)	6191(2)	3966(1)	1570(1)	18(1)
C(13)	5577(2)	2756(1)	1035(1)	19(1)
C(17)	6869(2)	1570(2)	639(1)	27(1)
C(16)	7085(2)	2266(2)	277(1)	28(1)
C(4)	5903(2)	3636(1)	2344(1)	20(1)
C(5)	4740(2)	2968(1)	2202(1)	20(1)
C(6)	4398(2)	2180(2)	2523(1)	24(1)
C(7)	5540(2)	1429(1)	2563(1)	26(1)
C(8)	5871(2)	985(1)	2132(1)	26(1)
C(9)	6247(2)	1759(1)	1809(1)	20(1)
C(11)	6500(2)	1332(1)	1373(1)	24(1)
C(10)	5077(2)	2490(1)	1780(1)	18(1)
C(14)	5765(2)	3485(1)	683(1)	24(1)
C(15)	5895(2)	2971(2)	259(1)	29(1)
C(20A)	3293(2)	9384(2)	-564(1)	28(1)
C(3A)	4156(2)	8615(1)	-424(1)	25(1)
C(2A)	4576(2)	8629(1)	-14(1)	22(1)
C(13A)	5393(2)	7809(1)	626(1)	21(1)
C(17A)	4089(2)	7071(2)	1196(1)	27(1)
C(16A)	4098(2)	8005(2)	1440(1)	27(1)
C(10A)	5537(2)	7044(1)	-64(1)	22(1)
C(5A)	5712(2)	7204(2)	-537(1)	25(1)

C(6A)	5869(2)	6224(2)	-750(1)	28(1)
C(7A)	4697(2)	5531(2)	-646(1)	31(1)
C(8A)	4517(2)	5420(2)	-171(1)	30(1)
C(9A)	4319(2)	6393(1)	45(1)	23(1)
C(11A)	4221(2)	6296(1)	524(1)	25(1)
C(14A)	5450(2)	8750(1)	869(1)	25(1)
C(15A)	5402(2)	8564(2)	1342(1)	28(1)
C(4A)	4530(2)	7808(2)	-718(1)	26(1)
C(20B)	2414(2)	582(2)	1407(1)	33(1)
C(3B)	1561(2)	1416(1)	1425(1)	25(1)
C(2B)	958(2)	1633(1)	1802(1)	23(1)
C(13B)	-59(2)	2798(1)	2293(1)	23(1)
C(14B)	-248(2)	2014(2)	2625(1)	30(1)
C(15B)	-446(3)	2452(2)	3060(1)	38(1)
C(16B)	805(3)	3073(2)	3158(1)	40(1)
C(4B)	1430(2)	2064(2)	1048(1)	25(1)
C(5B)	208(2)	2747(1)	1101(1)	22(1)
C(10B)	149(2)	3164(1)	1544(1)	20(1)
C(17B)	958(3)	3844(2)	2824(1)	37(1)
C(11B)	1193(2)	4226(2)	2091(1)	26(1)
C(9B)	1320(2)	3871(1)	1638(1)	21(1)
C(8B)	1283(2)	4693(1)	1319(1)	28(1)
C(7B)	1359(2)	4312(2)	868(1)	30(1)
C(6B)	225(2)	3576(2)	784(1)	26(1)
O(1S)	3289(19)	761(12)	326(4)	515(9)

O(20)	7730(2)	5266(1)	2409(1)	29(1)
O(20A)	2788(2)	9455(1)	-920(1)	35(1)
O(20B)	3123(2)	354(1)	1103(1)	43(1)
N(1)	5426(2)	3197(1)	1451(1)	18(1)
N(12)	6729(2)	2066(1)	1047(1)	20(1)
N(1A)	5380(2)	7952(1)	168(1)	21(1)
N(12A)	4173(2)	7231(1)	738(1)	22(1)
N(1B)	160(2)	2413(1)	1869(1)	21(1)
N(12B)	1108(2)	3433(1)	2397(1)	25(1)
C(20)	7326(2)	5022(1)	2057(1)	22(1)
C(3)	6442(2)	4213(1)	1980(1)	20(1)
C(2)	6191(2)	3966(1)	1570(1)	18(1)
C(13)	5577(2)	2756(1)	1035(1)	19(1)
C(17)	6869(2)	1570(2)	639(1)	27(1)
C(16)	7085(2)	2266(2)	277(1)	28(1)
C(4)	5903(2)	3636(1)	2344(1)	20(1)
C(5)	4740(2)	2968(1)	2202(1)	20(1)

C(6)	4398(2)	2180(2)	2523(1)	24(1)
C(7)	5540(2)	1429(1)	2563(1)	26(1)
C(8)	5871(2)	985(1)	2132(1)	26(1)
C(9)	6247(2)	1759(1)	1809(1)	20(1)
C(11)	6500(2)	1332(1)	1373(1)	24(1)
C(10)	5077(2)	2490(1)	1780(1)	18(1)
C(14)	5765(2)	3485(1)	683(1)	24(1)
C(15)	5895(2)	2971(2)	259(1)	29(1)
C(20A)	3293(2)	9384(2)	-564(1)	28(1)
C(3A)	4156(2)	8615(1)	-424(1)	25(1)
C(2A)	4576(2)	8629(1)	-14(1)	22(1)
C(13A)	5393(2)	7809(1)	626(1)	21(1)
C(17A)	4089(2)	7071(2)	1196(1)	27(1)
C(16A)	4098(2)	8005(2)	1440(1)	27(1)
C(10A)	5537(2)	7044(1)	-64(1)	22(1)
C(5A)	5712(2)	7204(2)	-537(1)	25(1)
C(6A)	5869(2)	6224(2)	-750(1)	28(1)
C(7A)	4697(2)	5531(2)	-646(1)	31(1)
C(8A)	4517(2)	5420(2)	-171(1)	30(1)
C(9A)	4319(2)	6393(1)	45(1)	23(1)
C(11A)	4221(2)	6296(1)	524(1)	25(1)
C(14A)	5450(2)	8750(1)	869(1)	25(1)
C(15A)	5402(2)	8564(2)	1342(1)	28(1)
C(4A)	4530(2)	7808(2)	-718(1)	26(1)
C(20B)	2414(2)	582(2)	1407(1)	33(1)
C(3B)	1561(2)	1416(1)	1425(1)	25(1)
C(2B)	958(2)	1633(1)	1802(1)	23(1)
C(13B)	-59(2)	2798(1)	2293(1)	23(1)
C(14B)	-248(2)	2014(2)	2625(1)	30(1)
C(15B)	-446(3)	2452(2)	3060(1)	38(1)
C(16B)	805(3)	3073(2)	3158(1)	40(1)
C(4B)	1430(2)	2064(2)	1048(1)	25(1)
C(5B)	208(2)	2747(1)	1101(1)	22(1)
C(10B)	149(2)	3164(1)	1544(1)	20(1)
C(17B)	958(3)	3844(2)	2824(1)	37(1)
C(11B)	1193(2)	4226(2)	2091(1)	26(1)
C(9B)	1320(2)	3871(1)	1638(1)	21(1)
C(8B)	1283(2)	4693(1)	1319(1)	28(1)
C(7B)	1359(2)	4312(2)	868(1)	30(1)
C(6B)	225(2)	3576(2)	784(1)	26(1)
O(1S)	3289(19)	761(12)	326(4)	515(9)

Table 3. Bond lengths [A] and angles [deg] for **1**.

O(20)-C(20)	1.232(3)
O(20A)-C(20A)	1.234(3)
O(20B)-C(20B)	1.227(3)
N(1)-C(2)	1.358(2)
N(1)-C(13)	1.461(2)
N(1)-C(10)	1.473(2)
N(12)-C(11)	1.471(3)
N(12)-C(17)	1.473(2)
N(12)-C(13)	1.476(2)
N(1A)-C(2A)	1.353(3)
N(1A)-C(13A)	1.465(3)
N(1A)-C(10A)	1.470(2)
N(12A)-C(11A)	1.468(2)
N(12A)-C(17A)	1.470(3)
N(12A)-C(13A)	1.476(2)
N(1B)-C(2B)	1.352(3)
N(1B)-C(13B)	1.464(3)
N(1B)-C(10B)	1.468(2)
N(12B)-C(11B)	1.474(3)
N(12B)-C(13B)	1.475(3)
N(12B)-C(17B)	1.476(3)
C(20)-C(3)	1.437(3)
C(20)-H(20)	0.9500
C(3)-C(2)	1.366(3)
C(3)-C(4)	1.499(3)
C(2)-H(2)	0.9500
C(13)-C(14)	1.520(3)
C(13)-H(13)	1.0000
C(17)-C(16)	1.517(3)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(16)-C(15)	1.518(3)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(4)-C(5)	1.531(3)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(10)	1.530(3)
C(5)-C(6)	1.532(3)
C(5)-H(5)	1.0000

C(6)-C(7)	1.531(3)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.534(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.531(3)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(11)	1.522(3)
C(9)-C(10)	1.528(3)
C(9)-H(9)	1.0000
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(10)-H(10)	1.0000
C(14)-C(15)	1.530(3)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(20A)-C(3A)	1.430(3)
C(20A)-H(20A)	0.9500
C(3A)-C(2A)	1.364(3)
C(3A)-C(4A)	1.502(3)
C(2A)-H(2A)	0.9500
C(13A)-C(14A)	1.520(3)
C(13A)-H(13A)	1.0000
C(17A)-C(16A)	1.513(3)
C(17A)-H(17C)	0.9900
C(17A)-H(17D)	0.9900
C(16A)-C(15A)	1.519(3)
C(16A)-H(16C)	0.9900
C(16A)-H(16D)	0.9900
C(10A)-C(5A)	1.525(3)
C(10A)-C(9A)	1.529(3)
C(10A)-H(10A)	1.0000
C(5A)-C(6A)	1.529(3)
C(5A)-C(4A)	1.534(3)
C(5A)-H(5A)	1.0000
C(6A)-C(7A)	1.528(3)
C(6A)-H(6A1)	0.9900
C(6A)-H(6A2)	0.9900
C(7A)-C(8A)	1.526(3)
C(7A)-H(7A1)	0.9900

C(7A)-H(7A2)	0.9900
C(8A)-C(9A)	1.529(3)
C(8A)-H(8A1)	0.9900
C(8A)-H(8A2)	0.9900
C(9A)-C(11A)	1.530(3)
C(9A)-H(9A)	1.0000
C(11A)-H(11C)	0.9900
C(11A)-H(11D)	0.9900
C(14A)-C(15A)	1.525(3)
C(14A)-H(14C)	0.9900
C(14A)-H(14D)	0.9900
C(15A)-H(15C)	0.9900
C(15A)-H(15D)	0.9900
C(4A)-H(4A1)	0.9900
C(4A)-H(4A2)	0.9900
C(20B)-C(3B)	1.427(3)
C(20B)-H(20B)	0.9500
C(3B)-C(2B)	1.363(3)
C(3B)-C(4B)	1.503(3)
C(2B)-H(2B)	0.9500
C(13B)-C(14B)	1.525(3)
C(13B)-H(13B)	1.0000
C(14B)-C(15B)	1.523(3)
C(14B)-H(14E)	0.9900
C(14B)-H(14F)	0.9900
C(15B)-C(16B)	1.523(4)
C(15B)-H(15E)	0.9900
C(15B)-H(15F)	0.9900
C(16B)-C(17B)	1.515(4)
C(16B)-H(16E)	0.9900
C(16B)-H(16F)	0.9900
C(4B)-C(5B)	1.529(3)
C(4B)-H(4B1)	0.9900
C(4B)-H(4B2)	0.9900
C(5B)-C(10B)	1.522(3)
C(5B)-C(6B)	1.530(3)
C(5B)-H(5B)	1.0000
C(10B)-C(9B)	1.533(3)
C(10B)-H(10B)	1.0000
C(17B)-H(17E)	0.9900
C(17B)-H(17F)	0.9900
C(11B)-C(9B)	1.523(3)
C(11B)-H(11E)	0.9900
C(11B)-H(11F)	0.9900

C(9B)-C(8B)	1.528(3)
C(9B)-H(9B)	1.0000
C(8B)-C(7B)	1.528(3)
C(8B)-H(8B1)	0.9900
C(8B)-H(8B2)	0.9900
C(7B)-C(6B)	1.527(3)
C(7B)-H(7B1)	0.9900
C(7B)-H(7B2)	0.9900
C(6B)-H(6B1)	0.9900
C(6B)-H(6B2)	0.9900

C(2)-N(1)-C(13)	121.88(16)
C(2)-N(1)-C(10)	117.12(15)
C(13)-N(1)-C(10)	112.36(14)
C(11)-N(12)-C(17)	107.87(15)
C(11)-N(12)-C(13)	110.77(15)
C(17)-N(12)-C(13)	110.68(15)
C(2A)-N(1A)-C(13A)	121.41(16)
C(2A)-N(1A)-C(10A)	116.48(17)
C(13A)-N(1A)-C(10A)	112.22(15)
C(11A)-N(12A)-C(17A)	108.89(15)
C(11A)-N(12A)-C(13A)	110.23(15)
C(17A)-N(12A)-C(13A)	111.51(16)
C(2B)-N(1B)-C(13B)	121.52(17)
C(2B)-N(1B)-C(10B)	117.75(17)
C(13B)-N(1B)-C(10B)	112.51(15)
C(11B)-N(12B)-C(13B)	110.20(16)
C(11B)-N(12B)-C(17B)	108.66(17)
C(13B)-N(12B)-C(17B)	111.21(17)
O(20)-C(20)-C(3)	124.09(19)
O(20)-C(20)-H(20)	118.0
C(3)-C(20)-H(20)	118.0
C(2)-C(3)-C(20)	117.63(18)
C(2)-C(3)-C(4)	122.38(17)
C(20)-C(3)-C(4)	119.87(17)
N(1)-C(2)-C(3)	124.09(17)
N(1)-C(2)-H(2)	118.0
C(3)-C(2)-H(2)	118.0
N(1)-C(13)-N(12)	109.11(15)
N(1)-C(13)-C(14)	113.16(15)
N(12)-C(13)-C(14)	111.23(16)
N(1)-C(13)-H(13)	107.7
N(12)-C(13)-H(13)	107.7
C(14)-C(13)-H(13)	107.7

N(12)-C(17)-C(16)	112.23(17)
N(12)-C(17)-H(17A)	109.2
C(16)-C(17)-H(17A)	109.2
N(12)-C(17)-H(17B)	109.2
C(16)-C(17)-H(17B)	109.2
H(17A)-C(17)-H(17B)	107.9
C(17)-C(16)-C(15)	109.67(18)
C(17)-C(16)-H(16A)	109.7
C(15)-C(16)-H(16A)	109.7
C(17)-C(16)-H(16B)	109.7
C(15)-C(16)-H(16B)	109.7
H(16A)-C(16)-H(16B)	108.2
C(3)-C(4)-C(5)	110.90(16)
C(3)-C(4)-H(4A)	109.5
C(5)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
C(5)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	108.0
C(10)-C(5)-C(4)	111.28(16)
C(10)-C(5)-C(6)	108.43(15)
C(4)-C(5)-C(6)	113.58(16)
C(10)-C(5)-H(5)	107.8
C(4)-C(5)-H(5)	107.8
C(6)-C(5)-H(5)	107.8
C(7)-C(6)-C(5)	112.83(16)
C(7)-C(6)-H(6A)	109.0
C(5)-C(6)-H(6A)	109.0
C(7)-C(6)-H(6B)	109.0
C(5)-C(6)-H(6B)	109.0
H(6A)-C(6)-H(6B)	107.8
C(6)-C(7)-C(8)	110.57(17)
C(6)-C(7)-H(7A)	109.5
C(8)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
C(8)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	108.1
C(9)-C(8)-C(7)	111.34(16)
C(9)-C(8)-H(8A)	109.4
C(7)-C(8)-H(8A)	109.4
C(9)-C(8)-H(8B)	109.4
C(7)-C(8)-H(8B)	109.4
H(8A)-C(8)-H(8B)	108.0
C(11)-C(9)-C(10)	109.01(16)
C(11)-C(9)-C(8)	111.77(16)

C(10)-C(9)-C(8)	109.34(16)
C(11)-C(9)-H(9)	108.9
C(10)-C(9)-H(9)	108.9
C(8)-C(9)-H(9)	108.9
N(12)-C(11)-C(9)	113.03(16)
N(12)-C(11)-H(11A)	109.0
C(9)-C(11)-H(11A)	109.0
N(12)-C(11)-H(11B)	109.0
C(9)-C(11)-H(11B)	109.0
H(11A)-C(11)-H(11B)	107.8
N(1)-C(10)-C(9)	108.45(15)
N(1)-C(10)-C(5)	112.23(15)
C(9)-C(10)-C(5)	113.34(16)
N(1)-C(10)-H(10)	107.5
C(9)-C(10)-H(10)	107.5
C(5)-C(10)-H(10)	107.5
C(13)-C(14)-C(15)	110.11(16)
C(13)-C(14)-H(14A)	109.6
C(15)-C(14)-H(14A)	109.6
C(13)-C(14)-H(14B)	109.6
C(15)-C(14)-H(14B)	109.6
H(14A)-C(14)-H(14B)	108.2
C(16)-C(15)-C(14)	109.40(17)
C(16)-C(15)-H(15A)	109.8
C(14)-C(15)-H(15A)	109.8
C(16)-C(15)-H(15B)	109.8
C(14)-C(15)-H(15B)	109.8
H(15A)-C(15)-H(15B)	108.2
O(20A)-C(20A)-C(3A)	125.1(2)
O(20A)-C(20A)-H(20A)	117.4
C(3A)-C(20A)-H(20A)	117.4
C(2A)-C(3A)-C(20A)	117.35(19)
C(2A)-C(3A)-C(4A)	121.98(19)
C(20A)-C(3A)-C(4A)	120.63(19)
N(1A)-C(2A)-C(3A)	124.65(19)
N(1A)-C(2A)-H(2A)	117.7
C(3A)-C(2A)-H(2A)	117.7
N(1A)-C(13A)-N(12A)	107.91(15)
N(1A)-C(13A)-C(14A)	112.69(16)
N(12A)-C(13A)-C(14A)	112.09(16)
N(1A)-C(13A)-H(13A)	108.0
N(12A)-C(13A)-H(13A)	108.0
C(14A)-C(13A)-H(13A)	108.0
N(12A)-C(17A)-C(16A)	111.96(16)

N(12A)-C(17A)-H(17C)	109.2
C(16A)-C(17A)-H(17C)	109.2
N(12A)-C(17A)-H(17D)	109.2
C(16A)-C(17A)-H(17D)	109.2
H(17C)-C(17A)-H(17D)	107.9
C(17A)-C(16A)-C(15A)	109.96(18)
C(17A)-C(16A)-H(16C)	109.7
C(15A)-C(16A)-H(16C)	109.7
C(17A)-C(16A)-H(16D)	109.7
C(15A)-C(16A)-H(16D)	109.7
H(16C)-C(16A)-H(16D)	108.2
N(1A)-C(10A)-C(5A)	112.21(16)
N(1A)-C(10A)-C(9A)	108.45(16)
C(5A)-C(10A)-C(9A)	113.24(17)
N(1A)-C(10A)-H(10A)	107.6
C(5A)-C(10A)-H(10A)	107.6
C(9A)-C(10A)-H(10A)	107.6
C(10A)-C(5A)-C(6A)	108.33(16)
C(10A)-C(5A)-C(4A)	111.32(16)
C(6A)-C(5A)-C(4A)	113.58(17)
C(10A)-C(5A)-H(5A)	107.8
C(6A)-C(5A)-H(5A)	107.8
C(4A)-C(5A)-H(5A)	107.8
C(7A)-C(6A)-C(5A)	113.17(17)
C(7A)-C(6A)-H(6A1)	108.9
C(5A)-C(6A)-H(6A1)	108.9
C(7A)-C(6A)-H(6A2)	108.9
C(5A)-C(6A)-H(6A2)	108.9
H(6A1)-C(6A)-H(6A2)	107.8
C(8A)-C(7A)-C(6A)	111.23(18)
C(8A)-C(7A)-H(7A1)	109.4
C(6A)-C(7A)-H(7A1)	109.4
C(8A)-C(7A)-H(7A2)	109.4
C(6A)-C(7A)-H(7A2)	109.4
H(7A1)-C(7A)-H(7A2)	108.0
C(7A)-C(8A)-C(9A)	111.46(18)
C(7A)-C(8A)-H(8A1)	109.3
C(9A)-C(8A)-H(8A1)	109.3
C(7A)-C(8A)-H(8A2)	109.3
C(9A)-C(8A)-H(8A2)	109.3
H(8A1)-C(8A)-H(8A2)	108.0
C(8A)-C(9A)-C(10A)	109.09(17)
C(8A)-C(9A)-C(11A)	111.98(16)
C(10A)-C(9A)-C(11A)	108.96(16)

C(8A)-C(9A)-H(9A)	108.9
C(10A)-C(9A)-H(9A)	108.9
C(11A)-C(9A)-H(9A)	108.9
N(12A)-C(11A)-C(9A)	112.56(16)
N(12A)-C(11A)-H(11C)	109.1
C(9A)-C(11A)-H(11C)	109.1
N(12A)-C(11A)-H(11D)	109.1
C(9A)-C(11A)-H(11D)	109.1
H(11C)-C(11A)-H(11D)	107.8
C(13A)-C(14A)-C(15A)	110.64(16)
C(13A)-C(14A)-H(14C)	109.5
C(15A)-C(14A)-H(14C)	109.5
C(13A)-C(14A)-H(14D)	109.5
C(15A)-C(14A)-H(14D)	109.5
H(14C)-C(14A)-H(14D)	108.1
C(16A)-C(15A)-C(14A)	108.26(17)
C(16A)-C(15A)-H(15C)	110.0
C(14A)-C(15A)-H(15C)	110.0
C(16A)-C(15A)-H(15D)	110.0
C(14A)-C(15A)-H(15D)	110.0
H(15C)-C(15A)-H(15D)	108.4
C(3A)-C(4A)-C(5A)	111.08(18)
C(3A)-C(4A)-H(4A1)	109.4
C(5A)-C(4A)-H(4A1)	109.4
C(3A)-C(4A)-H(4A2)	109.4
C(5A)-C(4A)-H(4A2)	109.4
H(4A1)-C(4A)-H(4A2)	108.0
O(20B)-C(20B)-C(3B)	124.6(2)
O(20B)-C(20B)-H(20B)	117.7
C(3B)-C(20B)-H(20B)	117.7
C(2B)-C(3B)-C(20B)	117.7(2)
C(2B)-C(3B)-C(4B)	121.76(18)
C(20B)-C(3B)-C(4B)	120.4(2)
N(1B)-C(2B)-C(3B)	124.27(19)
N(1B)-C(2B)-H(2B)	117.9
C(3B)-C(2B)-H(2B)	117.9
N(1B)-C(13B)-N(12B)	108.28(16)
N(1B)-C(13B)-C(14B)	112.86(17)
N(12B)-C(13B)-C(14B)	111.55(17)
N(1B)-C(13B)-H(13B)	108.0
N(12B)-C(13B)-H(13B)	108.0
C(14B)-C(13B)-H(13B)	108.0
C(15B)-C(14B)-C(13B)	110.70(19)
C(15B)-C(14B)-H(14E)	109.5

C(13B)-C(14B)-H(14E)	109.5
C(15B)-C(14B)-H(14F)	109.5
C(13B)-C(14B)-H(14F)	109.5
H(14E)-C(14B)-H(14F)	108.1
C(14B)-C(15B)-C(16B)	108.08(19)
C(14B)-C(15B)-H(15E)	110.1
C(16B)-C(15B)-H(15E)	110.1
C(14B)-C(15B)-H(15F)	110.1
C(16B)-C(15B)-H(15F)	110.1
H(15E)-C(15B)-H(15F)	108.4
C(17B)-C(16B)-C(15B)	109.8(2)
C(17B)-C(16B)-H(16E)	109.7
C(15B)-C(16B)-H(16E)	109.7
C(17B)-C(16B)-H(16F)	109.7
C(15B)-C(16B)-H(16F)	109.7
H(16E)-C(16B)-H(16F)	108.2
C(3B)-C(4B)-C(5B)	110.65(17)
C(3B)-C(4B)-H(4B1)	109.5
C(5B)-C(4B)-H(4B1)	109.5
C(3B)-C(4B)-H(4B2)	109.5
C(5B)-C(4B)-H(4B2)	109.5
H(4B1)-C(4B)-H(4B2)	108.1
C(10B)-C(5B)-C(4B)	111.53(16)
C(10B)-C(5B)-C(6B)	108.57(16)
C(4B)-C(5B)-C(6B)	112.90(17)
C(10B)-C(5B)-H(5B)	107.9
C(4B)-C(5B)-H(5B)	107.9
C(6B)-C(5B)-H(5B)	107.9
N(1B)-C(10B)-C(5B)	112.03(15)
N(1B)-C(10B)-C(9B)	108.40(15)
C(5B)-C(10B)-C(9B)	113.37(16)
N(1B)-C(10B)-H(10B)	107.6
C(5B)-C(10B)-H(10B)	107.6
C(9B)-C(10B)-H(10B)	107.6
N(12B)-C(17B)-C(16B)	112.1(2)
N(12B)-C(17B)-H(17E)	109.2
C(16B)-C(17B)-H(17E)	109.2
N(12B)-C(17B)-H(17F)	109.2
C(16B)-C(17B)-H(17F)	109.2
H(17E)-C(17B)-H(17F)	107.9
N(12B)-C(11B)-C(9B)	112.49(16)
N(12B)-C(11B)-H(11E)	109.1
C(9B)-C(11B)-H(11E)	109.1
N(12B)-C(11B)-H(11F)	109.1

C(9B)-C(11B)-H(11F)	109.1
H(11E)-C(11B)-H(11F)	107.8
C(11B)-C(9B)-C(8B)	112.24(16)
C(11B)-C(9B)-C(10B)	109.38(16)
C(8B)-C(9B)-C(10B)	109.52(16)
C(11B)-C(9B)-H(9B)	108.5
C(8B)-C(9B)-H(9B)	108.5
C(10B)-C(9B)-H(9B)	108.5
C(9B)-C(8B)-C(7B)	111.05(17)
C(9B)-C(8B)-H(8B1)	109.4
C(7B)-C(8B)-H(8B1)	109.4
C(9B)-C(8B)-H(8B2)	109.4
C(7B)-C(8B)-H(8B2)	109.4
H(8B1)-C(8B)-H(8B2)	108.0
C(6B)-C(7B)-C(8B)	111.16(17)
C(6B)-C(7B)-H(7B1)	109.4
C(8B)-C(7B)-H(7B1)	109.4
C(6B)-C(7B)-H(7B2)	109.4
C(8B)-C(7B)-H(7B2)	109.4
H(7B1)-C(7B)-H(7B2)	108.0
C(7B)-C(6B)-C(5B)	113.55(17)
C(7B)-C(6B)-H(6B1)	108.9
C(5B)-C(6B)-H(6B1)	108.9
C(7B)-C(6B)-H(6B2)	108.9
C(5B)-C(6B)-H(6B2)	108.9
H(6B1)-C(6B)-H(6B2)	107.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **1**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(20)	27(1)	24(1)	36(1)	-10(1)	-3(1)	-2(1)
O(20A)	34(1)	30(1)	40(1)	12(1)	-4(1)	4(1)
O(20B)	29(1)	28(1)	72(1)	-20(1)	-4(1)	9(1)
N(1)	17(1)	15(1)	23(1)	-1(1)	1(1)	0(1)
N(12)	17(1)	18(1)	24(1)	-3(1)	0(1)	2(1)
N(1A)	16(1)	16(1)	30(1)	1(1)	2(1)	1(1)
N(12A)	20(1)	18(1)	28(1)	3(1)	0(1)	-3(1)
N(1B)	18(1)	16(1)	28(1)	2(1)	0(1)	1(1)
N(12B)	21(1)	28(1)	26(1)	-2(1)	-1(1)	-4(1)
C(20)	21(1)	14(1)	33(1)	-4(1)	2(1)	0(1)
C(3)	19(1)	14(1)	26(1)	-1(1)	2(1)	0(1)
C(2)	14(1)	13(1)	28(1)	1(1)	2(1)	0(1)
C(13)	16(1)	17(1)	24(1)	-2(1)	-2(1)	1(1)
C(17)	26(1)	26(1)	28(1)	-8(1)	-1(1)	6(1)
C(16)	24(1)	37(1)	23(1)	-8(1)	0(1)	2(1)
C(4)	21(1)	18(1)	23(1)	-3(1)	2(1)	0(1)
C(5)	16(1)	19(1)	25(1)	-1(1)	0(1)	1(1)
C(6)	20(1)	26(1)	24(1)	2(1)	1(1)	-5(1)
C(7)	27(1)	22(1)	29(1)	5(1)	-1(1)	-3(1)
C(8)	28(1)	18(1)	32(1)	3(1)	-1(1)	0(1)
C(9)	20(1)	15(1)	26(1)	0(1)	-1(1)	-1(1)
C(11)	26(1)	16(1)	30(1)	-2(1)	-1(1)	4(1)
C(10)	16(1)	15(1)	23(1)	0(1)	-1(1)	-3(1)
C(14)	28(1)	21(1)	24(1)	-1(1)	0(1)	2(1)
C(15)	32(1)	31(1)	24(1)	-1(1)	-2(1)	3(1)
C(20A)	26(1)	20(1)	39(1)	8(1)	6(1)	0(1)
C(3A)	20(1)	21(1)	34(1)	8(1)	6(1)	0(1)
C(2A)	18(1)	13(1)	36(1)	4(1)	6(1)	-2(1)
C(13A)	15(1)	18(1)	31(1)	0(1)	-1(1)	2(1)
C(17A)	30(1)	24(1)	28(1)	6(1)	0(1)	-4(1)
C(16A)	27(1)	29(1)	26(1)	2(1)	-2(1)	2(1)
C(10A)	18(1)	16(1)	32(1)	-1(1)	0(1)	2(1)
C(5A)	17(1)	25(1)	32(1)	2(1)	4(1)	0(1)
C(6A)	19(1)	32(1)	32(1)	-3(1)	2(1)	6(1)

C(7A)	30(1)	26(1)	38(1)	-7(1)	0(1)	1(1)
C(8A)	33(1)	19(1)	39(1)	-2(1)	-1(1)	-3(1)
C(9A)	19(1)	17(1)	32(1)	1(1)	-2(1)	0(1)
C(11A)	24(1)	17(1)	33(1)	3(1)	-2(1)	-3(1)
C(14A)	22(1)	18(1)	34(1)	-1(1)	2(1)	0(1)
C(15A)	27(1)	23(1)	34(1)	-4(1)	-4(1)	1(1)
C(4A)	24(1)	27(1)	29(1)	5(1)	4(1)	2(1)
C(20B)	24(1)	18(1)	58(1)	-8(1)	-12(1)	1(1)
C(3B)	20(1)	16(1)	40(1)	-6(1)	-8(1)	-1(1)
C(2B)	17(1)	18(1)	35(1)	2(1)	-7(1)	-3(1)
C(13B)	16(1)	24(1)	28(1)	1(1)	1(1)	0(1)
C(14B)	21(1)	37(1)	34(1)	9(1)	-1(1)	0(1)
C(15B)	25(1)	59(2)	31(1)	9(1)	3(1)	-4(1)
C(16B)	31(1)	64(2)	25(1)	-1(1)	0(1)	-8(1)
C(4B)	23(1)	22(1)	31(1)	-7(1)	-1(1)	2(1)
C(5B)	16(1)	22(1)	28(1)	0(1)	-1(1)	1(1)
C(10B)	15(1)	16(1)	30(1)	3(1)	0(1)	2(1)
C(17B)	31(1)	48(1)	32(1)	-9(1)	3(1)	-9(1)
C(11B)	22(1)	21(1)	34(1)	-4(1)	0(1)	-2(1)
C(9B)	19(1)	14(1)	30(1)	1(1)	-2(1)	1(1)
C(8B)	27(1)	18(1)	39(1)	4(1)	-2(1)	-3(1)
C(7B)	26(1)	28(1)	34(1)	10(1)	-1(1)	-3(1)
C(6B)	20(1)	29(1)	29(1)	2(1)	0(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **1**.

	x	y	z	U(eq)
H(20)	7616	5391	1821	27
H(2)	6576	4358	1355	22
H(13)	4716	2386	975	23
H(17A)	6029	1186	585	32
H(17B)	7660	1122	653	32
H(16A)	7144	1907	8	34
H(16B)	7960	2619	317	34
H(4A)	5557	4076	2565	25
H(4B)	6660	3250	2466	25
H(5)	3895	3368	2161	24
H(6A)	4238	2480	2802	28
H(6B)	3535	1857	2436	28
H(7A)	5244	918	2761	31
H(7B)	6378	1734	2680	31
H(8A)	6648	531	2162	31
H(8B)	5061	621	2030	31
H(9)	7102	2095	1904	24
H(11A)	7314	905	1387	28
H(11B)	5697	935	1293	28
H(10)	4235	2139	1684	22
H(14A)	6603	3871	737	29
H(14B)	4966	3926	677	29
H(15A)	5030	2624	195	35
H(15B)	6058	3447	32	35
H(20A)	3093	9880	-367	34
H(2A)	4283	9152	157	26
H(13A)	6232	7428	699	26
H(17C)	4878	6672	1287	33
H(17D)	3233	6714	1261	33
H(16C)	4050	7869	1746	33
H(16D)	3282	8393	1362	33
H(10A)	6391	6724	42	26
H(5A)	6587	7568	-581	30
H(6A1)	5910	6316	-1059	33
H(6A2)	6752	5933	-660	33

H(7A1)	3830	5775	-771	38
H(7A2)	4895	4896	-773	38
H(8A1)	5338	5098	-51	36
H(8A2)	3707	5008	-113	36
H(9A)	3454	6694	-63	27
H(11C)	3382	5927	597	30
H(11D)	5026	5930	628	30
H(14C)	4662	9160	786	29
H(14D)	6309	9096	797	29
H(15C)	6220	8191	1431	34
H(15D)	5401	9181	1498	34
H(4A1)	4809	8076	-994	32
H(4A2)	3715	7394	-763	32
H(20B)	2434	175	1647	40
H(2B)	1109	1208	2031	28
H(13B)	-914	3197	2288	28
H(14E)	-1060	1618	2552	37
H(14F)	572	1591	2627	37
H(15E)	-539	1938	3274	46
H(15F)	-1293	2848	3066	46
H(16E)	694	3376	3438	48
H(16F)	1642	2669	3165	48
H(4B1)	1300	1671	791	30
H(4B2)	2287	2442	1015	30
H(5B)	-654	2369	1054	26
H(10B)	-738	3524	1571	24
H(17E)	141	4268	2830	44
H(17F)	1777	4241	2889	44
H(11E)	2001	4632	2159	31
H(11F)	359	4631	2116	31
H(9B)	2217	3524	1608	25
H(8B1)	2068	5131	1371	34
H(8B2)	422	5064	1356	34
H(7B1)	1264	4853	667	35
H(7B2)	2269	4010	820	35
H(6B1)	349	3310	497	31
H(6B2)	-677	3905	792	31

Table 6. Torsion angles [deg] for **1**.

O(20)-C(20)-C(3)-C(2)	-173.37(19)
O(20)-C(20)-C(3)-C(4)	2.9(3)
C(13)-N(1)-C(2)-C(3)	-157.47(18)
C(10)-N(1)-C(2)-C(3)	-12.2(3)
C(20)-C(3)-C(2)-N(1)	177.11(17)
C(4)-C(3)-C(2)-N(1)	1.0(3)
C(2)-N(1)-C(13)-N(12)	84.2(2)
C(10)-N(1)-C(13)-N(12)	-62.57(19)
C(2)-N(1)-C(13)-C(14)	-40.2(2)
C(10)-N(1)-C(13)-C(14)	173.02(17)
C(11)-N(12)-C(13)-N(1)	57.55(19)
C(17)-N(12)-C(13)-N(1)	177.16(15)
C(11)-N(12)-C(13)-C(14)	-176.91(16)
C(17)-N(12)-C(13)-C(14)	-57.3(2)
C(11)-N(12)-C(17)-C(16)	178.97(17)
C(13)-N(12)-C(17)-C(16)	57.6(2)
N(12)-C(17)-C(16)-C(15)	-57.6(2)
C(2)-C(3)-C(4)-C(5)	-17.0(3)
C(20)-C(3)-C(4)-C(5)	166.95(17)
C(3)-C(4)-C(5)-C(10)	42.2(2)
C(3)-C(4)-C(5)-C(6)	164.91(16)
C(10)-C(5)-C(6)-C(7)	55.0(2)
C(4)-C(5)-C(6)-C(7)	-69.2(2)
C(5)-C(6)-C(7)-C(8)	-55.8(2)
C(6)-C(7)-C(8)-C(9)	55.7(2)
C(7)-C(8)-C(9)-C(11)	-176.87(17)
C(7)-C(8)-C(9)-C(10)	-56.1(2)
C(17)-N(12)-C(11)-C(9)	-176.33(17)
C(13)-N(12)-C(11)-C(9)	-55.1(2)
C(10)-C(9)-C(11)-N(12)	53.3(2)
C(8)-C(9)-C(11)-N(12)	174.32(17)
C(2)-N(1)-C(10)-C(9)	-87.1(2)
C(13)-N(1)-C(10)-C(9)	61.33(19)
C(2)-N(1)-C(10)-C(5)	38.8(2)
C(13)-N(1)-C(10)-C(5)	-172.69(16)
C(11)-C(9)-C(10)-N(1)	-54.5(2)
C(8)-C(9)-C(10)-N(1)	-176.95(15)
C(11)-C(9)-C(10)-C(5)	-179.82(16)
C(8)-C(9)-C(10)-C(5)	57.7(2)
C(4)-C(5)-C(10)-N(1)	-54.2(2)

C(6)-C(5)-C(10)-N(1)	-179.78(16)
C(4)-C(5)-C(10)-C(9)	69.1(2)
C(6)-C(5)-C(10)-C(9)	-56.5(2)
N(1)-C(13)-C(14)-C(15)	-179.21(17)
N(12)-C(13)-C(14)-C(15)	57.5(2)
C(17)-C(16)-C(15)-C(14)	56.5(2)
C(13)-C(14)-C(15)-C(16)	-57.0(2)
O(20A)-C(20A)-C(3A)-C(2A)	-177.1(2)
O(20A)-C(20A)-C(3A)-C(4A)	0.5(3)
C(13A)-N(1A)-C(2A)-C(3A)	-157.70(19)
C(10A)-N(1A)-C(2A)-C(3A)	-14.6(3)
C(20A)-C(3A)-C(2A)-N(1A)	179.28(18)
C(4A)-C(3A)-C(2A)-N(1A)	1.7(3)
C(2A)-N(1A)-C(13A)-N(12A)	80.1(2)
C(10A)-N(1A)-C(13A)-N(12A)	-64.41(19)
C(2A)-N(1A)-C(13A)-C(14A)	-44.2(2)
C(10A)-N(1A)-C(13A)-C(14A)	171.29(16)
C(11A)-N(12A)-C(13A)-N(1A)	60.19(19)
C(17A)-N(12A)-C(13A)-N(1A)	-178.73(16)
C(11A)-N(12A)-C(13A)-C(14A)	-175.15(16)
C(17A)-N(12A)-C(13A)-C(14A)	-54.1(2)
C(11A)-N(12A)-C(17A)-C(16A)	177.54(17)
C(13A)-N(12A)-C(17A)-C(16A)	55.7(2)
N(12A)-C(17A)-C(16A)-C(15A)	-58.7(2)
C(2A)-N(1A)-C(10A)-C(5A)	41.1(2)
C(13A)-N(1A)-C(10A)-C(5A)	-172.54(16)
C(2A)-N(1A)-C(10A)-C(9A)	-84.7(2)
C(13A)-N(1A)-C(10A)-C(9A)	61.6(2)
N(1A)-C(10A)-C(5A)-C(6A)	179.86(16)
C(9A)-C(10A)-C(5A)-C(6A)	-57.0(2)
N(1A)-C(10A)-C(5A)-C(4A)	-54.6(2)
C(9A)-C(10A)-C(5A)-C(4A)	68.6(2)
C(10A)-C(5A)-C(6A)-C(7A)	54.2(2)
C(4A)-C(5A)-C(6A)-C(7A)	-70.0(2)
C(5A)-C(6A)-C(7A)-C(8A)	-54.4(2)
C(6A)-C(7A)-C(8A)-C(9A)	54.7(2)
C(7A)-C(8A)-C(9A)-C(10A)	-56.0(2)
C(7A)-C(8A)-C(9A)-C(11A)	-176.70(18)
N(1A)-C(10A)-C(9A)-C(8A)	-176.22(16)
C(5A)-C(10A)-C(9A)-C(8A)	58.5(2)
N(1A)-C(10A)-C(9A)-C(11A)	-53.7(2)
C(5A)-C(10A)-C(9A)-C(11A)	-178.93(16)
C(17A)-N(12A)-C(11A)-C(9A)	-179.63(17)
C(13A)-N(12A)-C(11A)-C(9A)	-57.0(2)

C(8A)-C(9A)-C(11A)-N(12A)	174.13(17)
C(10A)-C(9A)-C(11A)-N(12A)	53.4(2)
N(1A)-C(13A)-C(14A)-C(15A)	177.67(17)
N(12A)-C(13A)-C(14A)-C(15A)	55.7(2)
C(17A)-C(16A)-C(15A)-C(14A)	58.6(2)
C(13A)-C(14A)-C(15A)-C(16A)	-57.4(2)
C(2A)-C(3A)-C(4A)-C(5A)	-15.7(3)
C(20A)-C(3A)-C(4A)-C(5A)	166.78(18)
C(10A)-C(5A)-C(4A)-C(3A)	40.9(2)
C(6A)-C(5A)-C(4A)-C(3A)	163.46(17)
O(20B)-C(20B)-C(3B)-C(2B)	-172.6(2)
O(20B)-C(20B)-C(3B)-C(4B)	3.0(3)
C(13B)-N(1B)-C(2B)-C(3B)	-158.12(19)
C(10B)-N(1B)-C(2B)-C(3B)	-12.0(3)
C(20B)-C(3B)-C(2B)-N(1B)	177.98(19)
C(4B)-C(3B)-C(2B)-N(1B)	2.5(3)
C(2B)-N(1B)-C(13B)-N(12B)	83.8(2)
C(10B)-N(1B)-C(13B)-N(12B)	-63.9(2)
C(2B)-N(1B)-C(13B)-C(14B)	-40.2(3)
C(10B)-N(1B)-C(13B)-C(14B)	172.08(17)
C(11B)-N(12B)-C(13B)-N(1B)	59.8(2)
C(17B)-N(12B)-C(13B)-N(1B)	-179.66(17)
C(11B)-N(12B)-C(13B)-C(14B)	-175.44(17)
C(17B)-N(12B)-C(13B)-C(14B)	-54.9(2)
N(1B)-C(13B)-C(14B)-C(15B)	179.05(18)
N(12B)-C(13B)-C(14B)-C(15B)	56.9(2)
C(13B)-C(14B)-C(15B)-C(16B)	-58.0(3)
C(14B)-C(15B)-C(16B)-C(17B)	58.4(3)
C(2B)-C(3B)-C(4B)-C(5B)	-19.1(3)
C(20B)-C(3B)-C(4B)-C(5B)	165.57(18)
C(3B)-C(4B)-C(5B)-C(10B)	43.6(2)
C(3B)-C(4B)-C(5B)-C(6B)	166.12(17)
C(2B)-N(1B)-C(10B)-C(5B)	37.7(2)
C(13B)-N(1B)-C(10B)-C(5B)	-173.30(16)
C(2B)-N(1B)-C(10B)-C(9B)	-88.2(2)
C(13B)-N(1B)-C(10B)-C(9B)	60.8(2)
C(4B)-C(5B)-C(10B)-N(1B)	-53.8(2)
C(6B)-C(5B)-C(10B)-N(1B)	-178.77(16)
C(4B)-C(5B)-C(10B)-C(9B)	69.3(2)
C(6B)-C(5B)-C(10B)-C(9B)	-55.7(2)
C(11B)-N(12B)-C(17B)-C(16B)	177.67(19)
C(13B)-N(12B)-C(17B)-C(16B)	56.2(3)
C(15B)-C(16B)-C(17B)-N(12B)	-58.5(3)
C(13B)-N(12B)-C(11B)-C(9B)	-56.8(2)

C(17B)-N(12B)-C(11B)-C(9B)	-178.83(18)
N(12B)-C(11B)-C(9B)-C(8B)	175.05(17)
N(12B)-C(11B)-C(9B)-C(10B)	53.3(2)
N(1B)-C(10B)-C(9B)-C(11B)	-53.4(2)
C(5B)-C(10B)-C(9B)-C(11B)	-178.49(16)
N(1B)-C(10B)-C(9B)-C(8B)	-176.82(16)
C(5B)-C(10B)-C(9B)-C(8B)	58.1(2)
C(11B)-C(9B)-C(8B)-C(7B)	-177.91(17)
C(10B)-C(9B)-C(8B)-C(7B)	-56.2(2)
C(9B)-C(8B)-C(7B)-C(6B)	54.9(2)
C(8B)-C(7B)-C(6B)-C(5B)	-54.4(2)
C(10B)-C(5B)-C(6B)-C(7B)	53.5(2)
C(4B)-C(5B)-C(6B)-C(7B)	-70.7(2)

Symmetry transformations used to generate equivalent atoms:

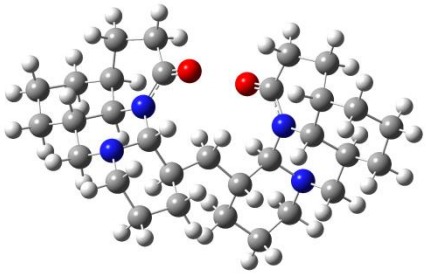
Table 7. Hydrogen bonds for **1** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

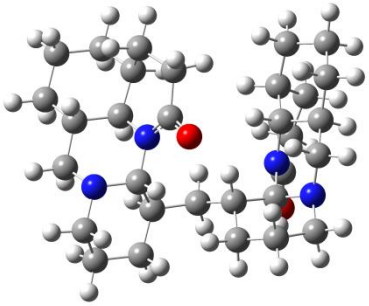
Computational methods for ECD of myrifamine C (**3**).

The CONFLEX[1, 2] searches based on molecular mechanics with MMFF94S force fields were performed for **3** which gave 50 stable conformers, respectively. Selected conformers (3) with distributions higher than 1% were further optimized by the density functional theory method at the B3LYP/6-31G** level in Gaussian 09 program package,[3] leading to 2 stable geometries, respectively, which were in good agreement with the ROESY data. The optimized geometries were further checked by frequency calculation and resulted in no imaginary frequencies. The ECD was calculated using TD-DFT-B3LYP/6-311G+(2d,p) of theory on B3LYP/6-31G(d,p) optimized geometries through the IEFPCM model (in MeOH). The overall calculated ECD curve was generated using SpecDis 1.50[4] with σ=0.16 ev, UV shifts -33 nm.

S4.1 Two stable conformers of optimized geometries of compound **3** at the B3LYP/6-31G** level in the gas phase.

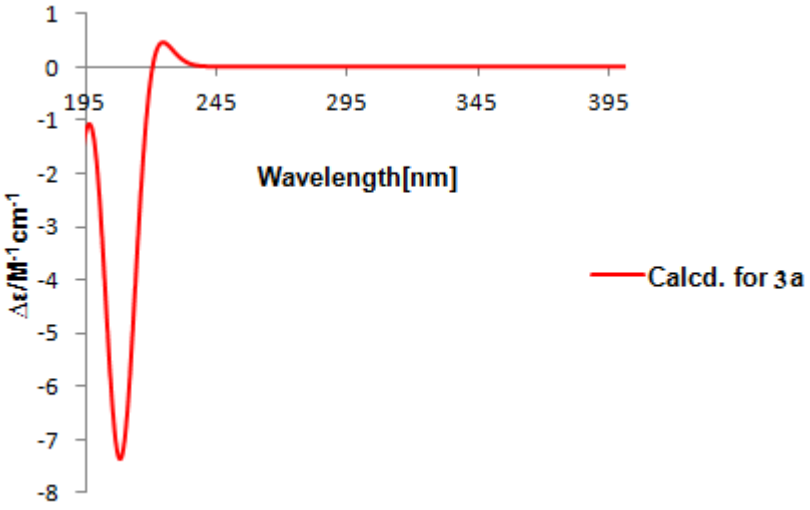


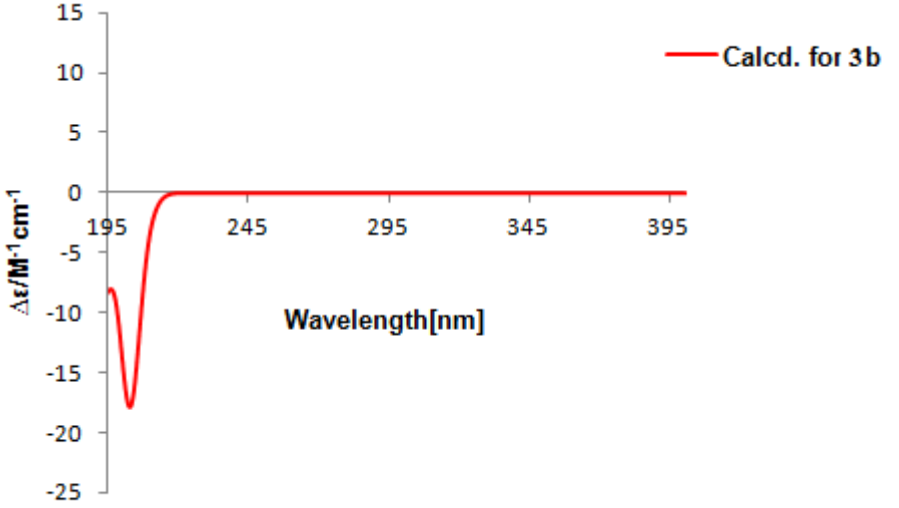
3a (79.87%)

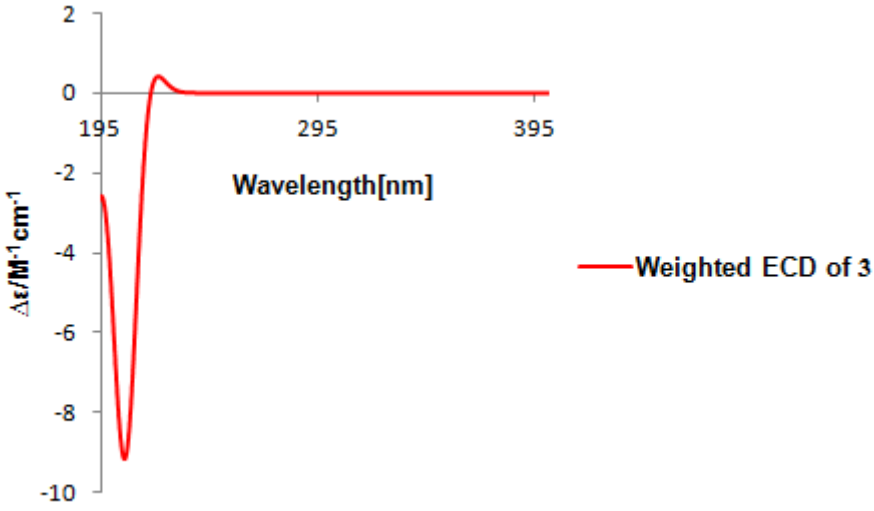


3b (20.13%)

S4.2 Calculated ECD spectra of **3** in the MeOH at the B3LYP/6-311G+(2d,p) level (**a** and **b**) and weighted ECD (red) in MeOH (σ=0.16 ev, UV shift= -33 nm).


1
0
-1
-2
-3
-4
-5
-6
-7
-8
195
245
295
345
395
Wavelength[nm]
Δε/M-1cm-1
Calcd. for 3a


15
10
5
0
-5
-10
-15
-20
-25
195
245
295
345
395
Wavelength[nm]
Δε/M-1cm-1
Calcd. for 3b


2
0
-2
-4
-6
-8
-10
195
295
395
Wavelength[nm]
Δε/M-1cm-1
Weighted ECD of 3

Standard orientation of **3a** at B3LYP/6-31G(d,p) level in gas phase:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.664382	-1.530901	1.397856
2	6	0	-3.452727	-0.341267	0.441720
3	6	0	-4.723558	0.152398	-0.285090
4	6	0	-5.875766	0.392954	0.699070
5	6	0	-6.153932	-0.864678	1.533445
6	6	0	-4.894169	-1.294517	2.298788
7	7	0	-2.417937	-0.598644	-0.573426
8	6	0	-2.058631	0.556694	-1.397019
9	7	0	-3.265319	1.122412	-2.015295
10	6	0	-4.356589	1.410259	-1.086966
11	6	0	-1.170747	1.591976	-0.638222
12	6	0	-0.774238	2.680464	-1.653411
13	6	0	-2.021480	3.304205	-2.301094
14	6	0	-2.912131	2.213171	-2.926347
15	6	0	-3.673719	-2.848761	0.615968
16	6	0	-2.307227	-3.019918	-0.050524
17	6	0	-1.845508	-1.816184	-0.860745
18	6	0	2.021481	3.304188	2.301120
19	6	0	0.774237	2.680450	1.653438
20	6	0	1.170744	1.591971	0.638238
21	6	0	2.058632	0.556685	1.397024
22	7	0	3.265322	1.122399	2.015297
23	6	0	2.912137	2.213151	2.926359
24	7	0	2.417934	-0.598648	0.573421
25	6	0	3.452720	-0.341265	-0.441728
26	6	0	4.723553	0.152401	0.285077
27	6	0	4.356586	1.410256	1.086964
28	6	0	3.664374	-1.530895	-1.397866
29	6	0	4.894154	-1.294502	-2.298807
30	6	0	6.153920	-0.864661	-1.533471
31	6	0	5.875754	0.392967	-0.699089
32	6	0	1.845508	-1.816191	0.860735
33	6	0	2.307241	-3.019925	0.050523
34	6	0	3.673727	-2.848755	-0.615978
35	8	0	-0.967254	-1.946052	-1.715068
36	8	0	0.967284	-1.946071	1.715088
37	1	0	-5.025489	-0.622710	-1.002627
38	1	0	-2.783470	-1.571930	2.054682

39	1	0	-3.097302	0.499407	1.059176
40	1	0	-1.447193	0.153094	-2.208892
41	1	0	1.447197	0.153079	2.208897
42	1	0	2.783458	-1.571931	-2.054686
43	1	0	3.097289	0.499411	-1.059179
44	1	0	5.025492	-0.622711	1.002608
45	6	0	-0.000002	0.827880	0.000006
46	1	0	-6.774680	0.701527	0.149346
47	1	0	-5.620013	1.225701	1.372169
48	1	0	-6.971665	-0.679764	2.241152
49	1	0	-6.491990	-1.674948	0.872790
50	1	0	-4.648300	-0.507847	3.026859
51	1	0	-5.088210	-2.203421	2.882655
52	1	0	-4.132505	2.227950	-0.372084
53	1	0	-5.219762	1.741007	-1.679011
54	1	0	-1.763074	2.077177	0.151507
55	1	0	-0.167019	3.457618	-1.173401
56	1	0	-0.142597	2.229112	-2.434644
57	1	0	-1.734688	4.029867	-3.073582
58	1	0	-2.588572	3.861309	-1.542451
59	1	0	-3.840031	2.644000	-3.321298
60	1	0	-2.377017	1.768875	-3.778973
61	1	0	-3.873983	-3.689833	1.291563
62	1	0	-4.469113	-2.854889	-0.140778
63	1	0	-1.530805	-3.190314	0.708872
64	1	0	-2.276622	-3.877522	-0.729516
65	1	0	1.734691	4.029843	3.073616
66	1	0	2.588568	3.861301	1.542480
67	1	0	0.167015	3.457607	1.173436
68	1	0	0.142601	2.229091	2.434669
69	1	0	1.763070	2.077180	-0.151488
70	1	0	2.377029	1.768848	3.778985
71	1	0	3.840038	2.643979	3.321308
72	1	0	5.219762	1.741002	1.679006
73	1	0	4.132495	2.227951	0.372089
74	1	0	4.648276	-0.507831	-3.026874
75	1	0	5.088195	-2.203404	-2.882678
76	1	0	6.491987	-1.674932	-0.872822
77	1	0	6.971648	-0.679740	-2.241183
78	1	0	5.619994	1.225716	-1.372182
79	1	0	6.774671	0.701540	-0.149368
80	1	0	1.530817	-3.190336	-0.708867
81	1	0	2.276651	-3.877525	0.729521
82	1	0	4.469126	-2.854875	0.140763

83	1	0	3.873995	-3.689826	-1.291573
84	1	0	-0.414487	0.159769	0.763874
85	1	0	0.414484	0.159774	-0.763867

Standard orientation of **3b** at B3LYP/6-31G(d,p) level in gas phase:

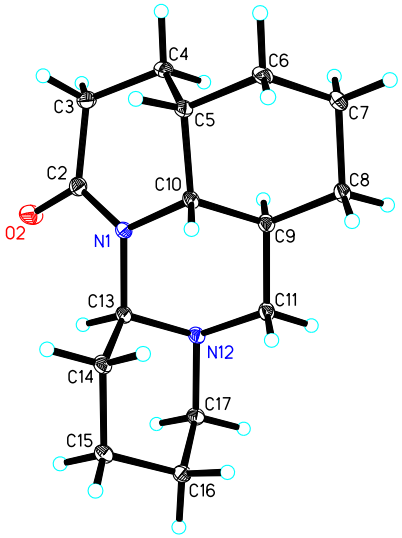
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.643280	-2.216326	0.791763
2	6	0	2.569345	-0.840685	0.103939
3	6	0	3.706244	-0.580602	-0.908466
4	6	0	3.811754	-1.720030	-1.930558
5	6	0	3.985375	-3.075360	-1.233074
6	6	0	2.832163	-3.334530	-0.252662
7	7	0	2.517356	0.275645	1.064359
8	6	0	2.331694	1.605709	0.468813
9	7	0	3.381672	1.824826	-0.540454
10	6	0	3.465030	0.783555	-1.564627
11	6	0	0.880674	1.869501	-0.041494
12	6	0	0.843778	3.312246	-0.594499
13	6	0	1.943570	3.561265	-1.637290
14	6	0	3.319524	3.188606	-1.068156
15	6	0	3.697529	-2.197689	1.903368
16	6	0	3.294641	-1.155322	2.946444
17	6	0	2.915422	0.211539	2.382693
18	6	0	-3.585140	3.471823	0.958482
19	6	0	-2.066514	3.287883	1.084494
20	6	0	-1.638343	1.809285	0.920162
21	6	0	-2.242343	1.251000	-0.398413
22	7	0	-3.708854	1.420867	-0.486318
23	6	0	-4.082868	2.830051	-0.347131
24	7	0	-1.915955	-0.161376	-0.653734
25	6	0	-2.609091	-1.132098	0.214699
26	6	0	-4.134725	-0.941153	0.070217
27	6	0	-4.477363	0.520463	0.372535
28	6	0	-2.143995	-2.581411	-0.015376
29	6	0	-2.974122	-3.553475	0.847229
30	6	0	-4.491069	-3.372762	0.687848
31	6	0	-4.900617	-1.921548	0.969053
32	6	0	-1.326072	-0.477614	-1.858224
33	6	0	-1.181350	-1.952490	-2.224479

34	6	0	-2.141889	-2.904602	-1.512760
35	8	0	2.929401	1.196504	3.116446
36	8	0	-0.862674	0.377286	-2.612128
37	1	0	4.648344	-0.513187	-0.348486
38	1	0	1.673704	-2.384937	1.283677
39	1	0	1.627214	-0.814209	-0.464273
40	1	0	2.524450	2.310954	1.282093
41	1	0	-1.814895	1.800567	-1.239909
42	1	0	-1.099852	-2.645416	0.324452
43	1	0	-2.348792	-0.871918	1.251328
44	1	0	-4.402322	-1.131125	-0.977503
45	6	0	-0.117679	1.573335	1.103221
46	1	0	4.646930	-1.527325	-2.614610
47	1	0	2.903137	-1.742214	-2.549739
48	1	0	4.029492	-3.883313	-1.972244
49	1	0	4.944580	-3.092722	-0.699670
50	1	0	1.902879	-3.435395	-0.830905
51	1	0	2.974655	-4.289670	0.267012
52	1	0	2.567591	0.712311	-2.208014
53	1	0	4.305631	1.031575	-2.224244
54	1	0	0.660719	1.204536	-0.883062
55	1	0	-0.128777	3.515851	-1.050289
56	1	0	0.961878	4.022731	0.237192
57	1	0	1.940156	4.613099	-1.948745
58	1	0	1.733859	2.967110	-2.535148
59	1	0	4.105092	3.301451	-1.824185
60	1	0	3.566614	3.874491	-0.245319
61	1	0	3.781375	-3.187693	2.366877
62	1	0	4.687009	-1.958442	1.497362
63	1	0	2.425545	-1.511270	3.515739
64	1	0	4.083268	-0.969440	3.679772
65	1	0	-3.844241	4.537372	0.973172
66	1	0	-4.094562	3.016148	1.817222
67	1	0	-1.713187	3.655683	2.055051
68	1	0	-1.578407	3.907429	0.325754
69	1	0	-2.110571	1.273938	1.756483
70	1	0	-3.655396	3.373620	-1.201225
71	1	0	-5.172777	2.905445	-0.435407
72	1	0	-5.541210	0.699989	0.174351
73	1	0	-4.328897	0.695355	1.455513
74	1	0	-2.712747	-3.395911	1.902596
75	1	0	-2.682202	-4.583162	0.608828
76	1	0	-4.799691	-3.650524	-0.328126
77	1	0	-5.016778	-4.054800	1.365584

78	1	0	-4.696413	-1.684914	2.023562
79	1	0	-5.979850	-1.790016	0.825706
80	1	0	-0.143321	-2.227489	-1.993172
81	1	0	-1.271673	-2.001593	-3.312451
82	1	0	-3.148259	-2.804765	-1.934551
83	1	0	-1.837525	-3.944674	-1.677952
84	1	0	0.017816	0.519426	1.368157
85	1	0	0.195989	2.135615	1.993764

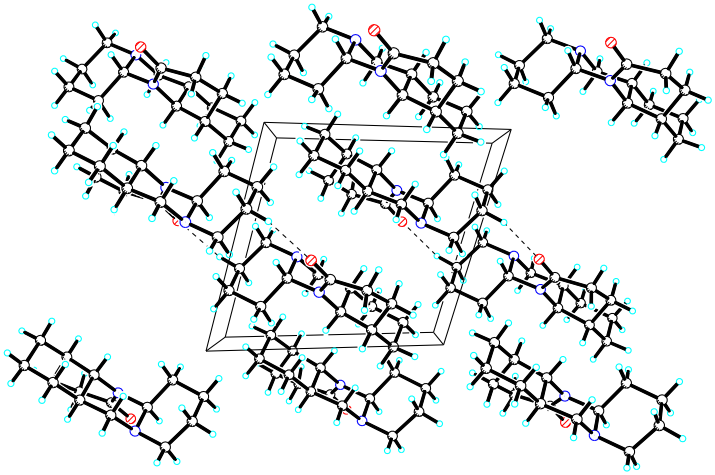
Crystal data for 4:

$C_{15}H_{24}N_2O$, M = 248.36, triclinic, a = 8.8466(2) Å, b = 9.1188(2) Å, c = 9.5971(2) Å, α = 95.0940(10)°, β = 112.7170(10)°, γ = 112.0040(10)°, V = 636.97(2) Å^3, T = 100(2) K, space group $P\bar{1}$, Z = 2, μ(CuKα) = 0.632 mm^{-1}, 8830 reflections measured, 2193 independent reflections (R_{int} = 0.0390). The final R_1 values were 0.0514 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1481 ($I > 2\sigma(I)$). The final R_1 values were 0.0515 (all data). The final $wR(F^2)$ values were 0.1483 (all data). The goodness of fit on F^2 was 1.054.



View of the molecule of **4** with the atom-labelling scheme.

Displacement ellipsoids are drawn at the 30% probability level.



View of the hydrogen-bonded motif of hm2.

Hydrogen-bonds are shown as dashed lines.

Table 1. Crystal data and structure refinement for **4**.

Identification code	cu_hm2_0m
Empirical formula	C15 H24 N2 O
Formula weight	248.36
Temperature	100(2) K
Wavelength	1.54178 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 8.8466(2) A alpha = 95.0940(10) deg. b = 9.1188(2) A beta = 112.7170(10) deg. c = 9.5971(2) A gamma = 112.0040(10) deg.
Volume	636.97(2) A^3
Z, Calculated density	2, 1.295 Mg/m^3
Absorption coefficient	0.632 mm^-1
F(000)	272
Crystal size	0.30 x 0.26 x 0.20 mm
Theta range for data collection	5.19 to 69.55 deg.
Limiting indices	-10<=h<=10, -11<=k<=11, -11<=l<=11
Reflections collected / unique	8830 / 2193 [R(int) = 0.0390]
Completeness to theta = 69.55	91.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8839 and 0.8329
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2193 / 0 / 164
Goodness-of-fit on F^2	1.054

Final R indices [I>2sigma(I)]	R1 = 0.0514, wR2 = 0.1481
R indices (all data)	R1 = 0.0515, wR2 = 0.1483
Extinction coefficient	0.072(5)
Largest diff. peak and hole	0.413 and -0.330 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **4**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(2)	8656(2)	5932(2)	3239(1)	29(1)
N(1)	7408(2)	7459(2)	3922(1)	15(1)
N(12)	4172(2)	5815(1)	2462(1)	16(1)
C(6)	8628(2)	10139(2)	7855(2)	18(1)
C(5)	8966(2)	9248(2)	6658(2)	16(1)
C(10)	7221(2)	8434(2)	5096(2)	15(1)
C(13)	5852(2)	6815(2)	2351(2)	16(1)
C(14)	5748(2)	8172(2)	1537(2)	17(1)
C(15)	4101(2)	7436(2)	-96(2)	18(1)
C(16)	2349(2)	6399(2)	-1(2)	18(1)
C(17)	2609(2)	5129(2)	879(2)	17(1)
C(11)	3866(2)	6703(2)	3599(2)	16(1)
C(9)	5502(2)	7344(2)	5229(2)	16(1)
C(2)	8645(2)	6832(2)	4261(2)	19(1)
C(3)	10092(2)	7328(2)	5951(2)	19(1)
C(4)	9625(2)	7978(2)	7170(2)	18(1)
C(7)	6953(2)	9032(2)	8026(2)	20(1)
C(8)	5235(2)	8290(2)	6438(2)	18(1)

Table 3. Bond lengths [A] and angles [deg] for **4**.

O(2)-C(2)	1.2276(19)
N(1)-C(2)	1.3624(19)
N(1)-C(13)	1.4650(17)
N(1)-C(10)	1.4715(17)
N(12)-C(11)	1.4683(17)
N(12)-C(17)	1.4735(17)
N(12)-C(13)	1.4742(18)
C(6)-C(7)	1.529(2)
C(6)-C(5)	1.5335(19)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(5)-C(4)	1.520(2)
C(5)-C(10)	1.5285(18)
C(5)-H(5)	1.0000
C(10)-C(9)	1.5345(19)
C(10)-H(10)	1.0000
C(13)-C(14)	1.5341(19)
C(13)-H(13)	1.0000
C(14)-C(15)	1.5316(19)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.5266(19)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.527(2)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(11)-C(9)	1.5293(19)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(9)-C(8)	1.5273(19)
C(9)-H(9)	1.0000
C(2)-C(3)	1.519(2)
C(3)-C(4)	1.5245(19)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900

C(7)-C(8)	1.5322(19)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900

C(2)-N(1)-C(13)	118.93(11)
C(2)-N(1)-C(10)	124.89(12)
C(13)-N(1)-C(10)	114.38(11)
C(11)-N(12)-C(17)	112.83(11)
C(11)-N(12)-C(13)	113.26(10)
C(17)-N(12)-C(13)	109.12(10)
C(7)-C(6)-C(5)	112.99(11)
C(7)-C(6)-H(6A)	109.0
C(5)-C(6)-H(6A)	109.0
C(7)-C(6)-H(6B)	109.0
C(5)-C(6)-H(6B)	109.0
H(6A)-C(6)-H(6B)	107.8
C(4)-C(5)-C(10)	109.54(11)
C(4)-C(5)-C(6)	114.77(12)
C(10)-C(5)-C(6)	109.48(11)
C(4)-C(5)-H(5)	107.6
C(10)-C(5)-H(5)	107.6
C(6)-C(5)-H(5)	107.6
N(1)-C(10)-C(5)	112.38(11)
N(1)-C(10)-C(9)	108.46(11)
C(5)-C(10)-C(9)	114.39(11)
N(1)-C(10)-H(10)	107.1
C(5)-C(10)-H(10)	107.1
C(9)-C(10)-H(10)	107.1
N(1)-C(13)-N(12)	108.87(11)
N(1)-C(13)-C(14)	112.31(11)
N(12)-C(13)-C(14)	114.49(11)
N(1)-C(13)-H(13)	106.9
N(12)-C(13)-H(13)	106.9
C(14)-C(13)-H(13)	106.9
C(15)-C(14)-C(13)	110.17(11)
C(15)-C(14)-H(14A)	109.6
C(13)-C(14)-H(14A)	109.6
C(15)-C(14)-H(14B)	109.6
C(13)-C(14)-H(14B)	109.6
H(14A)-C(14)-H(14B)	108.1
C(16)-C(15)-C(14)	110.80(11)
C(16)-C(15)-H(15A)	109.5

C(14)-C(15)-H(15A)	109.5
C(16)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	108.1
C(15)-C(16)-C(17)	110.13(11)
C(15)-C(16)-H(16A)	109.6
C(17)-C(16)-H(16A)	109.6
C(15)-C(16)-H(16B)	109.6
C(17)-C(16)-H(16B)	109.6
H(16A)-C(16)-H(16B)	108.1
N(12)-C(17)-C(16)	114.86(11)
N(12)-C(17)-H(17A)	108.6
C(16)-C(17)-H(17A)	108.6
N(12)-C(17)-H(17B)	108.6
C(16)-C(17)-H(17B)	108.6
H(17A)-C(17)-H(17B)	107.5
N(12)-C(11)-C(9)	110.69(11)
N(12)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11A)	109.5
N(12)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	108.1
C(8)-C(9)-C(11)	112.03(11)
C(8)-C(9)-C(10)	110.96(11)
C(11)-C(9)-C(10)	108.16(11)
C(8)-C(9)-H(9)	108.5
C(11)-C(9)-H(9)	108.5
C(10)-C(9)-H(9)	108.5
O(2)-C(2)-N(1)	122.04(13)
O(2)-C(2)-C(3)	119.58(13)
N(1)-C(2)-C(3)	118.33(12)
C(2)-C(3)-C(4)	114.80(11)
C(2)-C(3)-H(3A)	108.6
C(4)-C(3)-H(3A)	108.6
C(2)-C(3)-H(3B)	108.6
C(4)-C(3)-H(3B)	108.6
H(3A)-C(3)-H(3B)	107.5
C(5)-C(4)-C(3)	108.89(12)
C(5)-C(4)-H(4A)	109.9
C(3)-C(4)-H(4A)	109.9
C(5)-C(4)-H(4B)	109.9
C(3)-C(4)-H(4B)	109.9
H(4A)-C(4)-H(4B)	108.3
C(6)-C(7)-C(8)	110.82(11)

C(6)-C(7)-H(7A)	109.5
C(8)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
C(8)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	108.1
C(9)-C(8)-C(7)	110.85(11)
C(9)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8A)	109.5
C(9)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	108.1

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **4**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(2)	32(1)	39(1)	18(1)	-3(1)	7(1)	24(1)
N(1)	15(1)	18(1)	12(1)	0(1)	6(1)	7(1)
N(12)	16(1)	16(1)	12(1)	-1(1)	6(1)	5(1)
C(6)	20(1)	18(1)	13(1)	-1(1)	5(1)	7(1)
C(5)	15(1)	16(1)	13(1)	1(1)	6(1)	5(1)
C(10)	17(1)	14(1)	13(1)	1(1)	8(1)	8(1)
C(13)	15(1)	18(1)	13(1)	0(1)	6(1)	7(1)
C(14)	16(1)	18(1)	14(1)	1(1)	7(1)	5(1)
C(15)	20(1)	20(1)	14(1)	3(1)	7(1)	8(1)
C(16)	16(1)	20(1)	12(1)	-1(1)	5(1)	8(1)
C(17)	16(1)	17(1)	14(1)	-1(1)	5(1)	4(1)
C(11)	16(1)	17(1)	16(1)	1(1)	8(1)	6(1)
C(9)	17(1)	16(1)	15(1)	2(1)	8(1)	6(1)
C(2)	18(1)	20(1)	18(1)	2(1)	9(1)	9(1)
C(3)	17(1)	22(1)	17(1)	2(1)	6(1)	10(1)
C(4)	17(1)	19(1)	13(1)	1(1)	4(1)	7(1)
C(7)	22(1)	22(1)	14(1)	1(1)	9(1)	10(1)
C(8)	19(1)	21(1)	16(1)	1(1)	9(1)	8(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **4**.

	x	y	z	U(eq)
H(6A)	9722	10569	8890	22
H(6B)	8461	11090	7529	22
H(5)	9928	10097	6475	19
H(10)	7000	9337	4673	18
H(13)	6053	6054	1706	19
H(14A)	5631	8998	2177	21
H(14B)	6886	8733	1439	21
H(15A)	3965	8332	-563	22
H(15B)	4310	6742	-785	22
H(16A)	1328	5833	-1073	21
H(16B)	2034	7121	551	21
H(17A)	1479	4512	971	21
H(17B)	2772	4336	246	21
H(11A)	2749	5959	3649	20
H(11B)	3677	7638	3250	20
H(9)	5654	6385	5576	19
H(3A)	11255	8186	6061	23
H(3B)	10296	6362	6181	23
H(4A)	8657	7062	7268	21
H(4B)	10721	8485	8206	21
H(7A)	6771	9681	8776	23
H(7B)	7161	8137	8451	23
H(8A)	4180	7539	6566	22
H(8B)	4962	9180	6059	22

Table 6. Torsion angles [deg] for **4**.

C(7)-C(6)-C(5)-C(4)	-70.48(15)
C(7)-C(6)-C(5)-C(10)	53.15(15)
C(2)-N(1)-C(10)-C(5)	22.44(18)
C(13)-N(1)-C(10)-C(5)	-173.10(10)
C(2)-N(1)-C(10)-C(9)	-105.02(15)
C(13)-N(1)-C(10)-C(9)	59.44(14)
C(4)-C(5)-C(10)-N(1)	-49.38(15)
C(6)-C(5)-C(10)-N(1)	-176.04(10)
C(4)-C(5)-C(10)-C(9)	74.86(14)
C(6)-C(5)-C(10)-C(9)	-51.79(15)
C(2)-N(1)-C(13)-N(12)	108.44(13)
C(10)-N(1)-C(13)-N(12)	-57.02(14)
C(2)-N(1)-C(13)-C(14)	-123.70(13)
C(10)-N(1)-C(13)-C(14)	70.85(14)
C(11)-N(12)-C(13)-N(1)	54.88(14)
C(17)-N(12)-C(13)-N(1)	-178.53(10)
C(11)-N(12)-C(13)-C(14)	-71.74(15)
C(17)-N(12)-C(13)-C(14)	54.85(15)
N(1)-C(13)-C(14)-C(15)	-179.98(10)
N(12)-C(13)-C(14)-C(15)	-55.16(15)
C(13)-C(14)-C(15)-C(16)	52.89(15)
C(14)-C(15)-C(16)-C(17)	-52.95(15)
C(11)-N(12)-C(17)-C(16)	71.67(14)
C(13)-N(12)-C(17)-C(16)	-55.16(15)
C(15)-C(16)-C(17)-N(12)	55.52(15)
C(17)-N(12)-C(11)-C(9)	178.31(10)
C(13)-N(12)-C(11)-C(9)	-57.10(15)
N(12)-C(11)-C(9)-C(8)	179.45(10)
N(12)-C(11)-C(9)-C(10)	56.85(14)
N(1)-C(10)-C(9)-C(8)	179.86(10)
C(5)-C(10)-C(9)-C(8)	53.55(15)
N(1)-C(10)-C(9)-C(11)	-56.89(14)
C(5)-C(10)-C(9)-C(11)	176.80(10)
C(13)-N(1)-C(2)-O(2)	11.1(2)
C(10)-N(1)-C(2)-O(2)	174.90(13)
C(13)-N(1)-C(2)-C(3)	-171.36(11)
C(10)-N(1)-C(2)-C(3)	-7.6(2)
O(2)-C(2)-C(3)-C(4)	-161.86(14)
N(1)-C(2)-C(3)-C(4)	20.52(18)
C(10)-C(5)-C(4)-C(3)	62.30(14)

C(6)-C(5)-C(4)-C(3)	-174.10(11)
C(2)-C(3)-C(4)-C(5)	-47.87(16)
C(5)-C(6)-C(7)-C(8)	-56.73(15)
C(11)-C(9)-C(8)-C(7)	-175.54(11)
C(10)-C(9)-C(8)-C(7)	-54.54(15)
C(6)-C(7)-C(8)-C(9)	56.55(15)

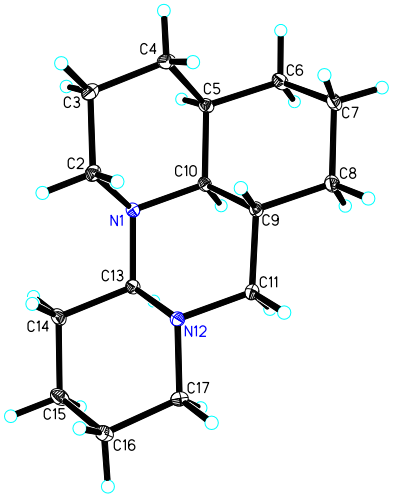
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **4** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

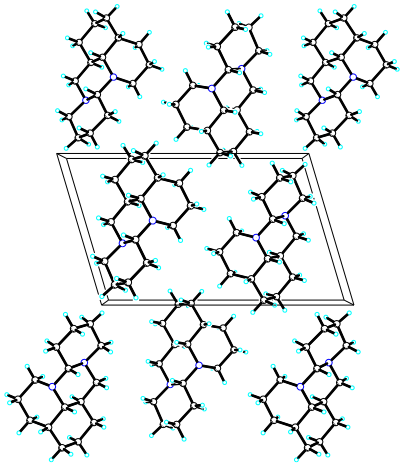
Crystal data for 5:

$C_{15}H_{26}N_2$, M = 234.38, monoclinic, a = 9.1535(15) Å, b = 5.1702(9) Å, c = 14.568(2) Å, α = 90.00°, β = 106.495(2)°, γ = 90.00°, V = 661.05(19) Å^3, T = 100(2) K, space group $P21$, Z = 2, μ(MoKα) = 0.069 mm^{-1}, 6946 reflections measured, 3538 independent reflections (R_{int} = 0.0225). The final R_1 values were 0.0352 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0994 ($I > 2\sigma(I)$). The final R_1 values were 0.0375 (all data). The final $wR(F^2)$ values were 0.1019 (all data). The goodness of fit on F^2 was 1.073. Flack parameter = 0.6(16).



View of a molecule of **5** with the atom-labelling scheme.

Displacement ellipsoids are drawn at the 30% probability level.



View of the hydrogen-bonded motif of **5**.

Hydrogen-bonds are shown as dashed lines.

Table 1. Crystal data and structure refinement for **5**.

Identification code	mo_hm4a_0m
Empirical formula	C15 H26 N2
Formula weight	234.38
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21
Unit cell dimensions	a = 9.1535(15) A alpha = 90 deg. b = 5.1702(9) A beta = 106.495(2) deg. c = 14.568(2) A gamma = 90 deg.
Volume	661.05(19) A^3
Z, Calculated density	2, 1.177 Mg/m^3
Absorption coefficient	0.069 mm^-1
F(000)	260
Crystal size	0.94 x 0.22 x 0.15 mm
Theta range for data collection	1.46 to 30.07 deg.
Limiting indices	-12<=h<=12, -7<=k<=7, -17<=l<=20
Reflections collected / unique	6946 / 3538 [R(int) = 0.0225]
Completeness to theta = 30.07	95.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9897 and 0.9380
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3538 / 1 / 154
Goodness-of-fit on F^2	1.073

Final R indices [I>2sigma(I)]	R1 = 0.0352, wR2 = 0.0994
R indices (all data)	R1 = 0.0375, wR2 = 0.1019
Absolute structure parameter	0.6(16)
Largest diff. peak and hole	0.333 and -0.277 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	5561(1)	2604(2)	3054(1)	13(1)
N(12)	4075(1)	524(2)	1568(1)	13(1)
C(4)	8032(1)	160(2)	4510(1)	18(1)
C(5)	8347(1)	1882(2)	3734(1)	14(1)
C(10)	6987(1)	1932(2)	2830(1)	12(1)
C(13)	4325(1)	2896(2)	2168(1)	13(1)
C(14)	2841(1)	3735(2)	2357(1)	18(1)
C(15)	1596(1)	4201(2)	1422(1)	20(1)
C(16)	1383(1)	1772(2)	809(1)	18(1)
C(3)	6535(1)	963(3)	4695(1)	20(1)
C(2)	5235(1)	851(2)	3769(1)	16(1)
C(6)	9805(1)	1139(2)	3475(1)	18(1)
C(7)	9646(1)	-1335(2)	2881(1)	18(1)
C(8)	8297(1)	-1138(2)	1978(1)	17(1)
C(9)	6821(1)	-562(2)	2234(1)	13(1)
C(11)	5482(1)	-204(2)	1342(1)	14(1)
C(17)	2896(1)	975(2)	658(1)	17(1)

Table 3. Bond lengths [A] and angles [deg] for **5**.

N(1)-C(13)	1.4624(12)
N(1)-C(2)	1.4740(13)
N(1)-C(10)	1.4751(12)
N(12)-C(11)	1.4661(12)
N(12)-C(17)	1.4709(12)
N(12)-C(13)	1.4859(13)
C(4)-C(3)	1.5272(15)
C(4)-C(5)	1.5290(15)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(10)	1.5346(13)
C(5)-C(6)	1.5359(14)
C(5)-H(5)	1.0000
C(10)-C(9)	1.5376(13)
C(10)-H(10)	1.0000
C(13)-C(14)	1.5240(13)
C(13)-H(13)	1.0000
C(14)-C(15)	1.5268(15)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.5214(16)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.5195(14)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(3)-C(2)	1.5253(14)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(6)-C(7)	1.5278(15)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.5307(14)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.5295(13)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900

C(9)-C(11)	1.5236(13)
C(9)-H(9)	1.0000
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900

C(13)-N(1)-C(2)	115.26(8)
C(13)-N(1)-C(10)	109.88(7)
C(2)-N(1)-C(10)	112.40(8)
C(11)-N(12)-C(17)	107.75(7)
C(11)-N(12)-C(13)	110.24(7)
C(17)-N(12)-C(13)	110.51(8)
C(3)-C(4)-C(5)	109.82(9)
C(3)-C(4)-H(4A)	109.7
C(5)-C(4)-H(4A)	109.7
C(3)-C(4)-H(4B)	109.7
C(5)-C(4)-H(4B)	109.7
H(4A)-C(4)-H(4B)	108.2
C(4)-C(5)-C(10)	111.56(8)
C(4)-C(5)-C(6)	113.31(9)
C(10)-C(5)-C(6)	110.03(8)
C(4)-C(5)-H(5)	107.2
C(10)-C(5)-H(5)	107.2
C(6)-C(5)-H(5)	107.2
N(1)-C(10)-C(5)	111.52(8)
N(1)-C(10)-C(9)	111.73(7)
C(5)-C(10)-C(9)	113.37(8)
N(1)-C(10)-H(10)	106.6
C(5)-C(10)-H(10)	106.6
C(9)-C(10)-H(10)	106.6
N(1)-C(13)-N(12)	112.67(8)
N(1)-C(13)-C(14)	112.04(8)
N(12)-C(13)-C(14)	110.19(8)
N(1)-C(13)-H(13)	107.2
N(12)-C(13)-H(13)	107.2
C(14)-C(13)-H(13)	107.2
C(13)-C(14)-C(15)	111.17(8)
C(13)-C(14)-H(14A)	109.4
C(15)-C(14)-H(14A)	109.4
C(13)-C(14)-H(14B)	109.4
C(15)-C(14)-H(14B)	109.4
H(14A)-C(14)-H(14B)	108.0
C(16)-C(15)-C(14)	109.42(9)

C(16)-C(15)-H(15A)	109.8
C(14)-C(15)-H(15A)	109.8
C(16)-C(15)-H(15B)	109.8
C(14)-C(15)-H(15B)	109.8
H(15A)-C(15)-H(15B)	108.2
C(17)-C(16)-C(15)	109.80(9)
C(17)-C(16)-H(16A)	109.7
C(15)-C(16)-H(16A)	109.7
C(17)-C(16)-H(16B)	109.7
C(15)-C(16)-H(16B)	109.7
H(16A)-C(16)-H(16B)	108.2
C(2)-C(3)-C(4)	110.31(8)
C(2)-C(3)-H(3A)	109.6
C(4)-C(3)-H(3A)	109.6
C(2)-C(3)-H(3B)	109.6
C(4)-C(3)-H(3B)	109.6
H(3A)-C(3)-H(3B)	108.1
N(1)-C(2)-C(3)	109.78(8)
N(1)-C(2)-H(2A)	109.7
C(3)-C(2)-H(2A)	109.7
N(1)-C(2)-H(2B)	109.7
C(3)-C(2)-H(2B)	109.7
H(2A)-C(2)-H(2B)	108.2
C(7)-C(6)-C(5)	113.51(8)
C(7)-C(6)-H(6A)	108.9
C(5)-C(6)-H(6A)	108.9
C(7)-C(6)-H(6B)	108.9
C(5)-C(6)-H(6B)	108.9
H(6A)-C(6)-H(6B)	107.7
C(6)-C(7)-C(8)	110.79(9)
C(6)-C(7)-H(7A)	109.5
C(8)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
C(8)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	108.1
C(9)-C(8)-C(7)	110.89(8)
C(9)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8A)	109.5
C(9)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	108.1
C(11)-C(9)-C(8)	111.56(8)
C(11)-C(9)-C(10)	107.85(8)
C(8)-C(9)-C(10)	110.35(8)

C(11)-C(9)-H(9)	109.0
C(8)-C(9)-H(9)	109.0
C(10)-C(9)-H(9)	109.0
N(12)-C(11)-C(9)	112.59(8)
N(12)-C(11)-H(11A)	109.1
C(9)-C(11)-H(11A)	109.1
N(12)-C(11)-H(11B)	109.1
C(9)-C(11)-H(11B)	109.1
H(11A)-C(11)-H(11B)	107.8
N(12)-C(17)-C(16)	112.24(8)
N(12)-C(17)-H(17A)	109.2
C(16)-C(17)-H(17A)	109.2
N(12)-C(17)-H(17B)	109.2
C(16)-C(17)-H(17B)	109.2
H(17A)-C(17)-H(17B)	107.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **5**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	12(1)	14(1)	13(1)	0(1)	4(1)	1(1)
N(12)	12(1)	13(1)	13(1)	-1(1)	3(1)	1(1)
C(4)	18(1)	19(1)	15(1)	1(1)	1(1)	1(1)
C(5)	13(1)	12(1)	16(1)	-1(1)	2(1)	1(1)
C(10)	12(1)	11(1)	14(1)	0(1)	4(1)	0(1)
C(13)	12(1)	12(1)	14(1)	-1(1)	3(1)	0(1)
C(14)	13(1)	20(1)	21(1)	-5(1)	4(1)	3(1)
C(15)	15(1)	18(1)	25(1)	-2(1)	2(1)	4(1)
C(16)	14(1)	20(1)	20(1)	0(1)	1(1)	1(1)
C(3)	21(1)	25(1)	13(1)	0(1)	5(1)	0(1)
C(2)	17(1)	19(1)	14(1)	1(1)	6(1)	-1(1)
C(6)	13(1)	16(1)	22(1)	-3(1)	3(1)	1(1)
C(7)	14(1)	17(1)	22(1)	-3(1)	4(1)	3(1)
C(8)	15(1)	17(1)	18(1)	-3(1)	5(1)	2(1)
C(9)	12(1)	12(1)	14(1)	-1(1)	4(1)	1(1)
C(11)	15(1)	16(1)	13(1)	-2(1)	5(1)	1(1)
C(17)	15(1)	20(1)	13(1)	-1(1)	1(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5.**

	x	y	z	U(eq)
H(4A)	7969	-1670	4302	22
H(4B)	8876	321	5108	22
H(5)	8491	3684	3993	17
H(10)	7189	3358	2418	15
H(13)	4630	4304	1789	16
H(14A)	3016	5343	2742	22
H(14B)	2503	2379	2731	22
H(15A)	629	4645	1561	24
H(15B)	1886	5667	1073	24
H(16A)	988	356	1129	22
H(16B)	632	2106	182	22
H(3A)	6311	-207	5176	24
H(3B)	6630	2744	4955	24
H(2A)	5118	-940	3519	20
H(2B)	4270	1367	3897	20
H(6A)	10091	2577	3111	21
H(6B)	10642	909	4072	21
H(7A)	9494	-2826	3270	21
H(7B)	10594	-1634	2697	21
H(8A)	8491	255	1561	20
H(8B)	8187	-2785	1618	20
H(9)	6595	-2034	2618	15
H(11A)	5740	1153	934	17
H(11B)	5309	-1837	971	17
H(17A)	2749	-626	270	20
H(17B)	3246	2347	296	20

Table 6. Torsion angles [deg] for **5**.

C(3)-C(4)-C(5)-C(10)	-52.96(11)
C(3)-C(4)-C(5)-C(6)	-177.80(9)
C(13)-N(1)-C(10)-C(5)	174.15(8)
C(2)-N(1)-C(10)-C(5)	-56.06(11)
C(13)-N(1)-C(10)-C(9)	-57.81(10)
C(2)-N(1)-C(10)-C(9)	71.97(10)
C(4)-C(5)-C(10)-N(1)	52.55(11)
C(6)-C(5)-C(10)-N(1)	179.20(9)
C(4)-C(5)-C(10)-C(9)	-74.61(10)
C(6)-C(5)-C(10)-C(9)	52.04(11)
C(2)-N(1)-C(13)-N(12)	-70.07(10)
C(10)-N(1)-C(13)-N(12)	58.15(10)
C(2)-N(1)-C(13)-C(14)	54.86(11)
C(10)-N(1)-C(13)-C(14)	-176.92(8)
C(11)-N(12)-C(13)-N(1)	-57.13(10)
C(17)-N(12)-C(13)-N(1)	-176.13(8)
C(11)-N(12)-C(13)-C(14)	176.94(8)
C(17)-N(12)-C(13)-C(14)	57.93(10)
N(1)-C(13)-C(14)-C(15)	176.24(9)
N(12)-C(13)-C(14)-C(15)	-57.47(11)
C(13)-C(14)-C(15)-C(16)	56.22(12)
C(14)-C(15)-C(16)-C(17)	-55.20(12)
C(5)-C(4)-C(3)-C(2)	56.61(12)
C(13)-N(1)-C(2)-C(3)	-173.53(8)
C(10)-N(1)-C(2)-C(3)	59.51(10)
C(4)-C(3)-C(2)-N(1)	-59.61(11)
C(4)-C(5)-C(6)-C(7)	73.84(11)
C(10)-C(5)-C(6)-C(7)	-51.82(12)
C(5)-C(6)-C(7)-C(8)	54.94(12)
C(6)-C(7)-C(8)-C(9)	-56.77(12)
C(7)-C(8)-C(9)-C(11)	176.69(8)
C(7)-C(8)-C(9)-C(10)	56.82(11)
N(1)-C(10)-C(9)-C(11)	55.48(10)
C(5)-C(10)-C(9)-C(11)	-177.48(8)
N(1)-C(10)-C(9)-C(8)	177.56(8)
C(5)-C(10)-C(9)-C(8)	-55.39(10)
C(17)-N(12)-C(11)-C(9)	176.47(8)
C(13)-N(12)-C(11)-C(9)	55.79(10)
C(8)-C(9)-C(11)-N(12)	-176.08(9)
C(10)-C(9)-C(11)-N(12)	-54.75(10)

C(11)-N(12)-C(17)-C(16)	-179.44(9)
C(13)-N(12)-C(17)-C(16)	-58.94(11)
C(15)-C(16)-C(17)-N(12)	57.69(12)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **5** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

[1] Goto, H.; Osawa, E.; *J. Am. Chem. Soc.* **1989**, *111*, 8950–8951.

[2] Goto, H.; Osawa, E.; *J. Chem. Soc., Perkin Trans. 2*, **1993**, 187–198.

[3] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Jr., Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J.; Gaussian *09*, Revision B.01,Gaussian, Inc., Wallingford CT, 2010.

[4]. Bruhn, T.; Hemberger, Y.; Schaumlöffel, A.; Bringmann, G. *Spec Dis*, version 1.50, University of Würzburg, Germany, 2010.