

Supporting Information

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Alkaloids of *Papaver libanoticum* and their Cytotoxic Activity

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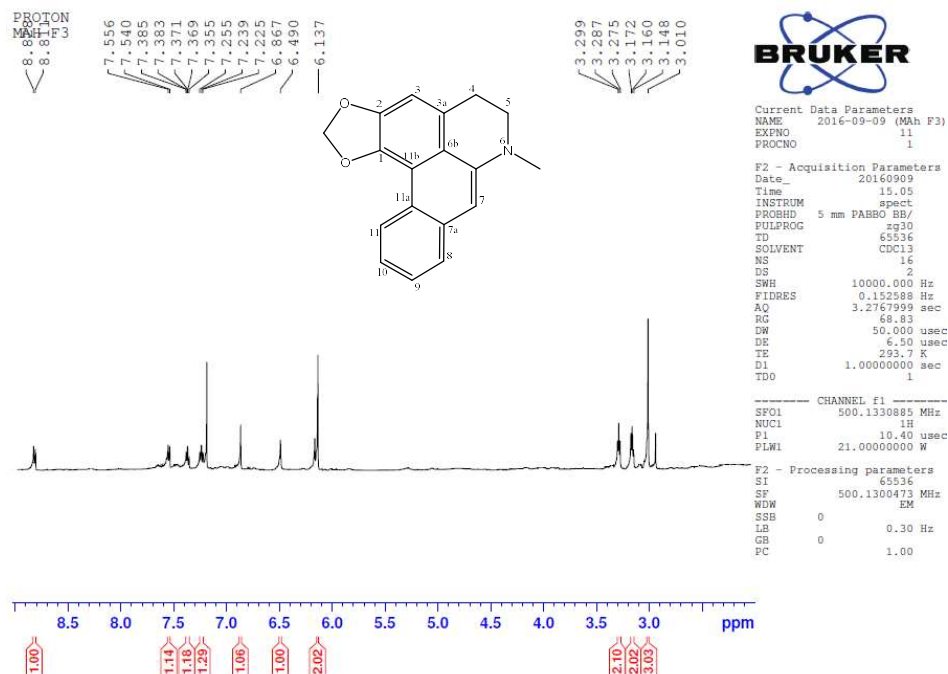
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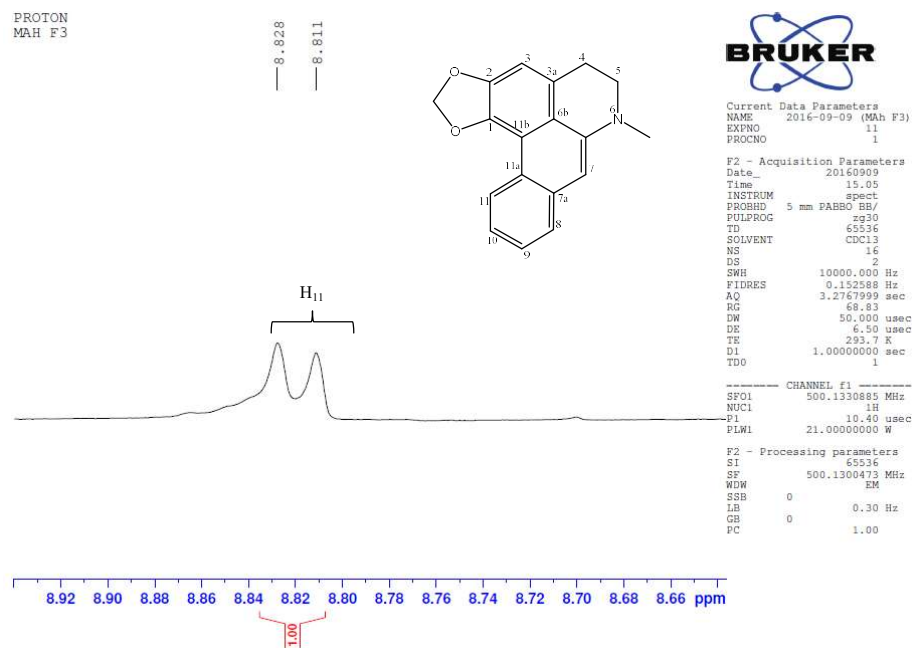
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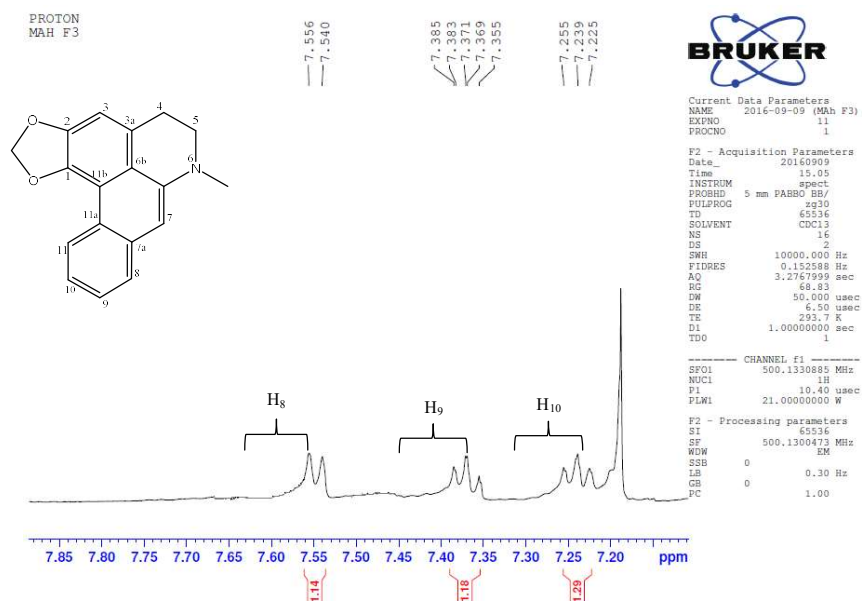
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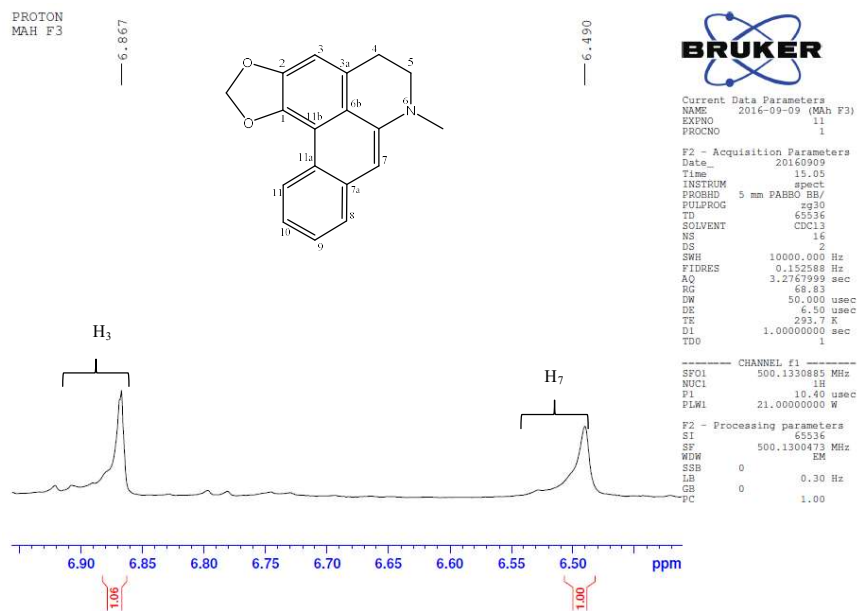
S1: ^1H -NMR (500 MHz, CDCl_3) Spectrum of Compound **1** (dehydroremerine)



S2: Expansion of the ^1H -NMR (500 MHz, CDCl_3) Spectrum of Compound **1** (dehydroremerine)

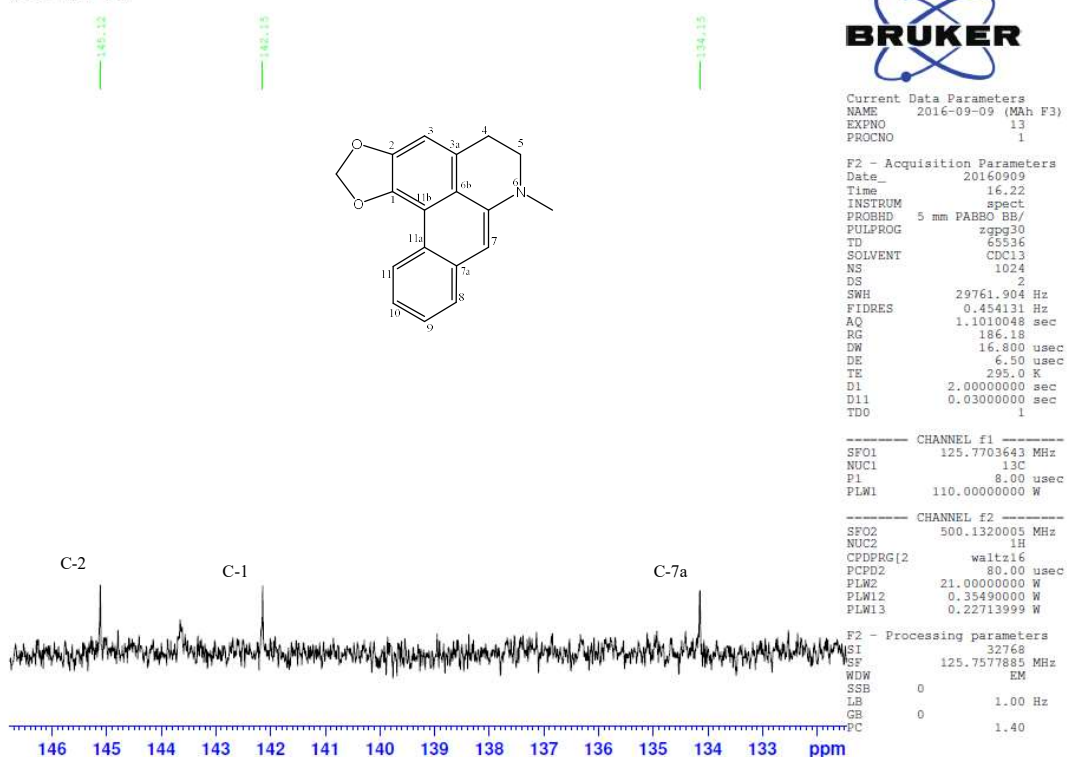


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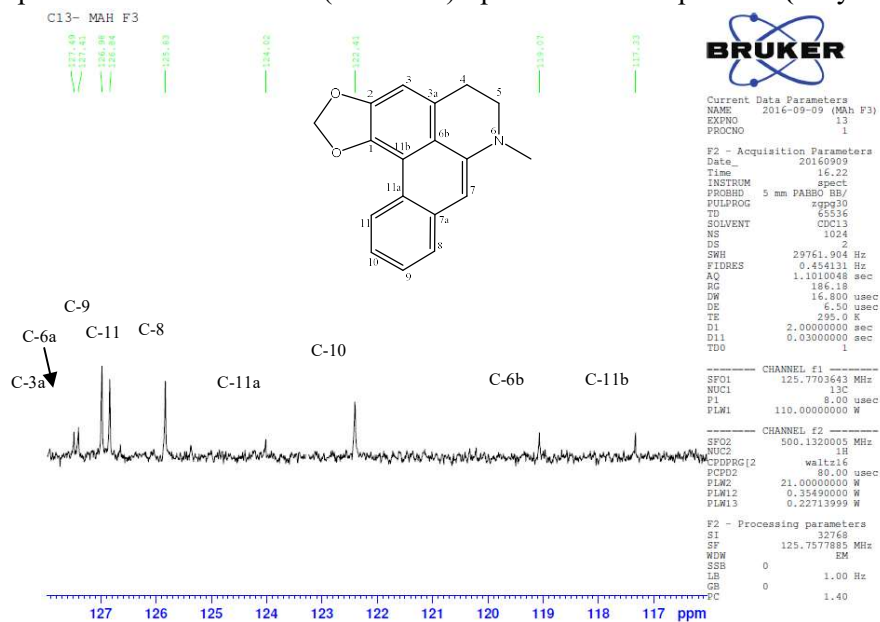


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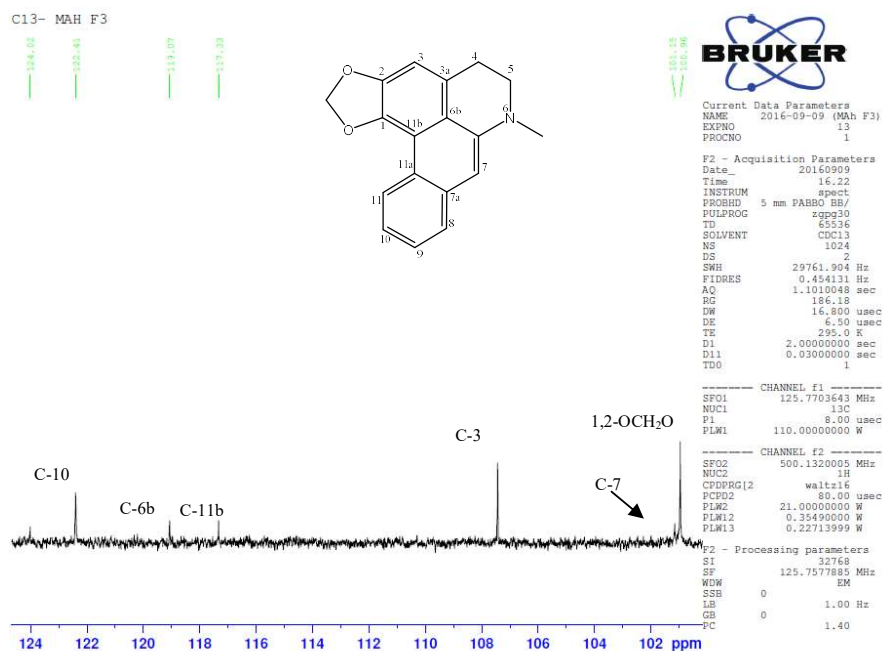
C13- MAH F3



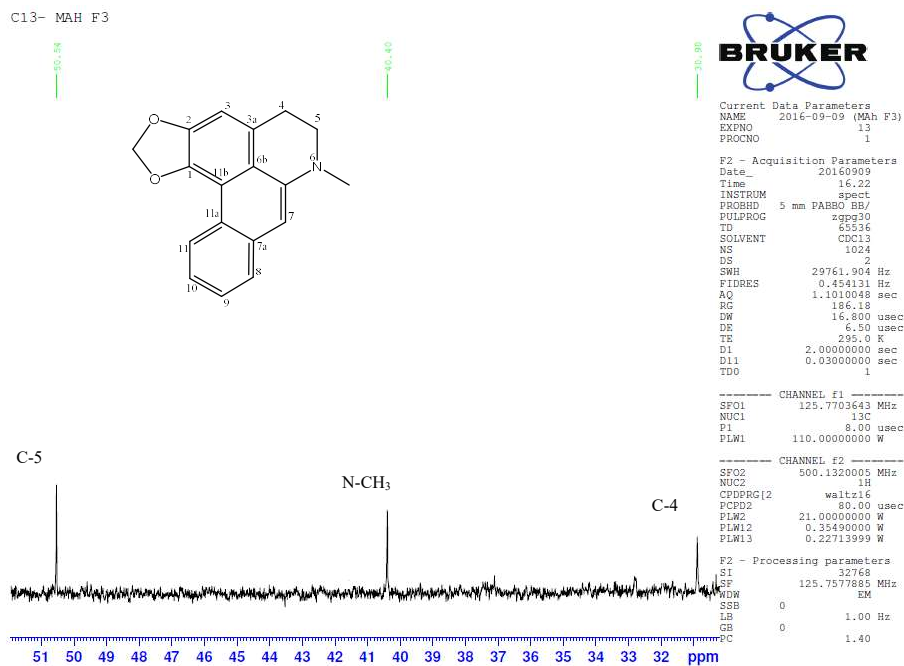
S7: Expansion of the ^{13}C -NMR (500 MHz) Spectrum of Compound 1 (dehydrremeirine)



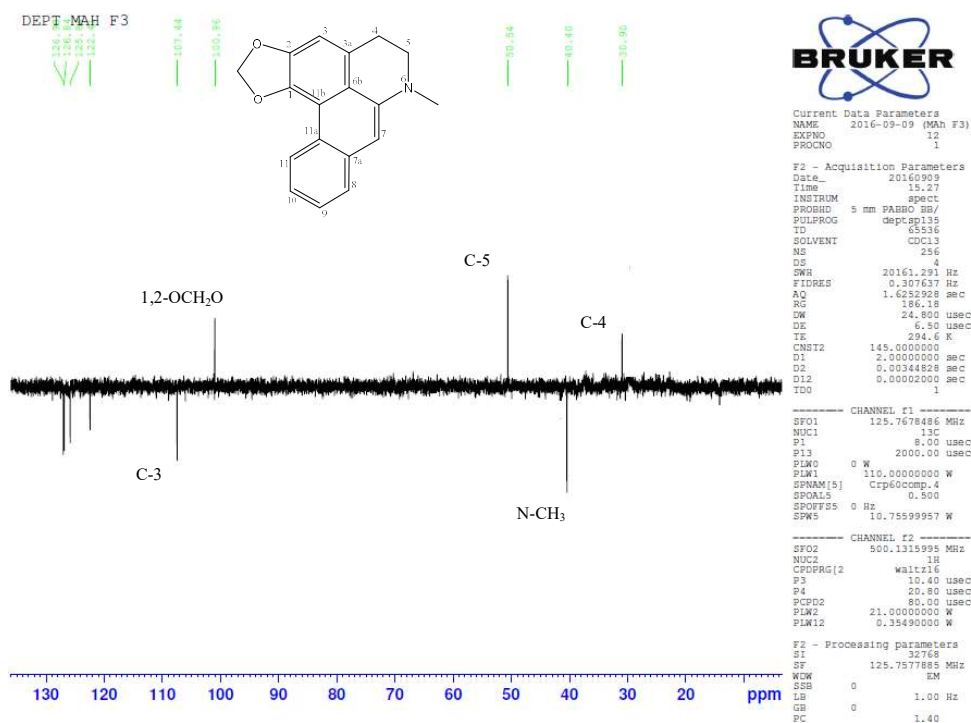
S8: Expansion of the ^{13}C -NMR (500 MHz) Spectrum of Compound 1 (dehydrremeirine)



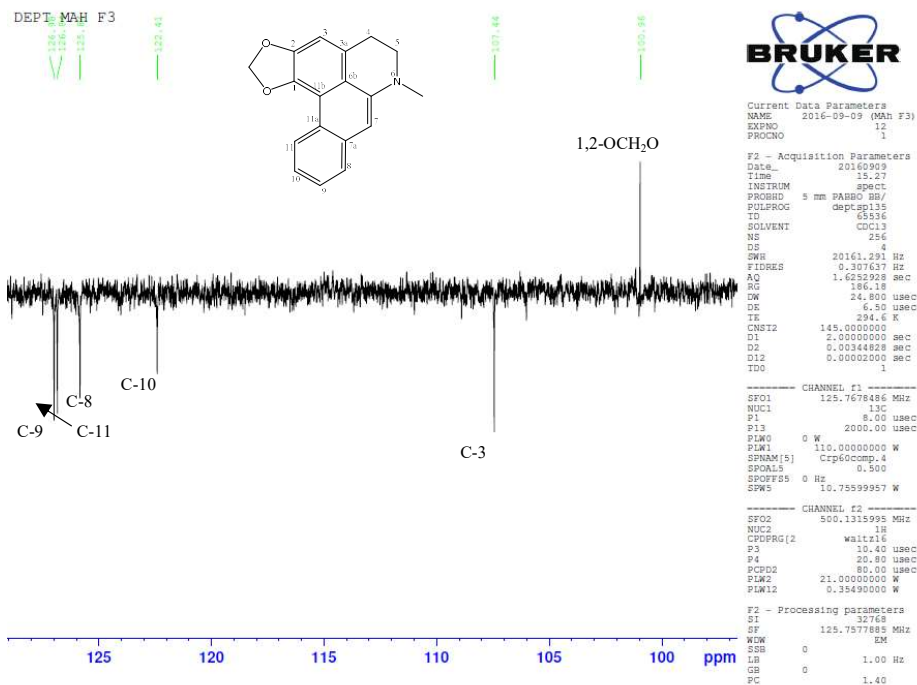
S9: Expansion of the ^{13}C -NMR (500 MHz) Spectrum of Compound **1** (dehydrmerine)



S10: Expansion of the ^{13}C -NMR (500 MHz) Spectrum of Compound **1** (dehydrmerine)

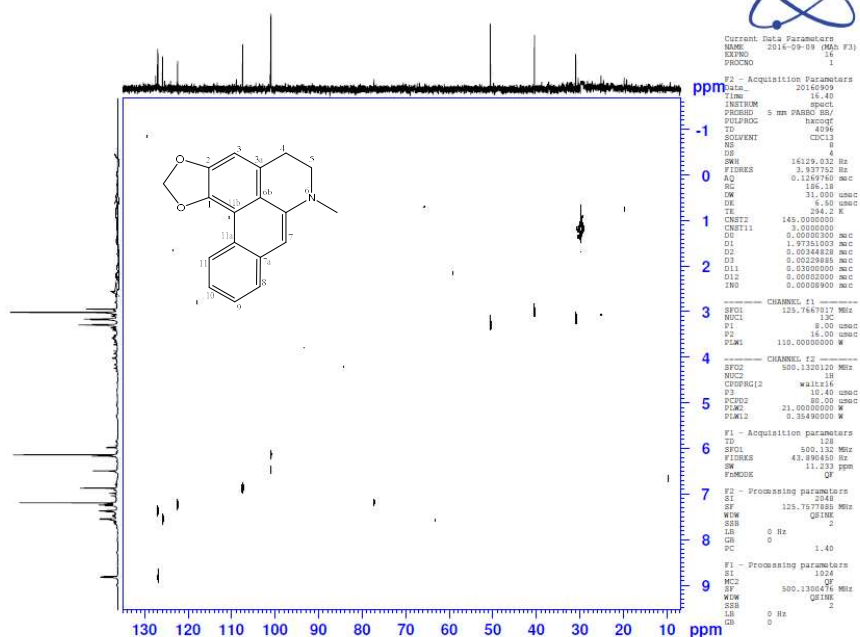


S11: DEPT (500 MHz) Spectrum of Compound 1 (dehydroremerine)



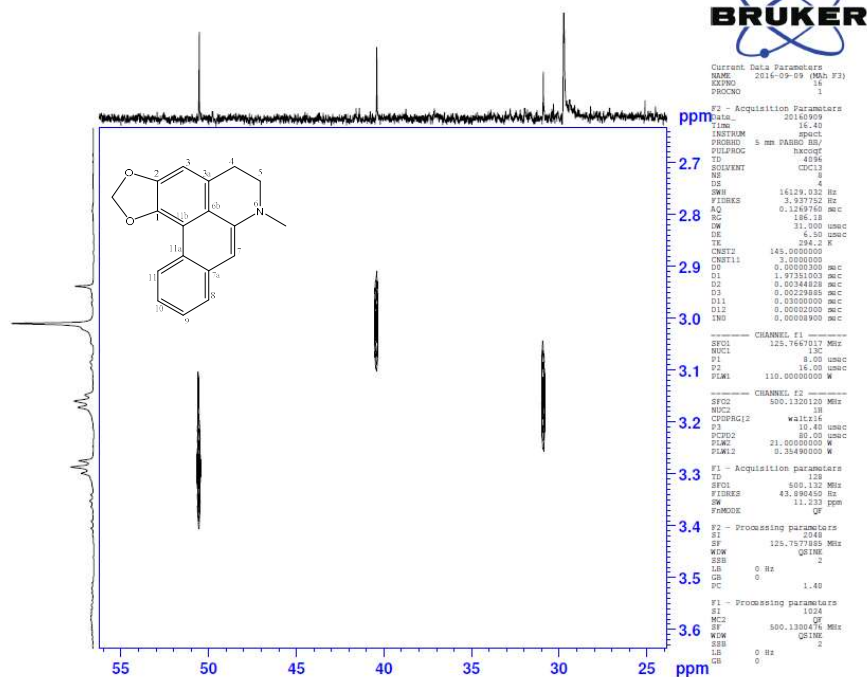
S12: Expansion of the DEPT (500 MHz) Spectrum of Compound 1 (dehydroremerine)

HCCOSW MAH F3



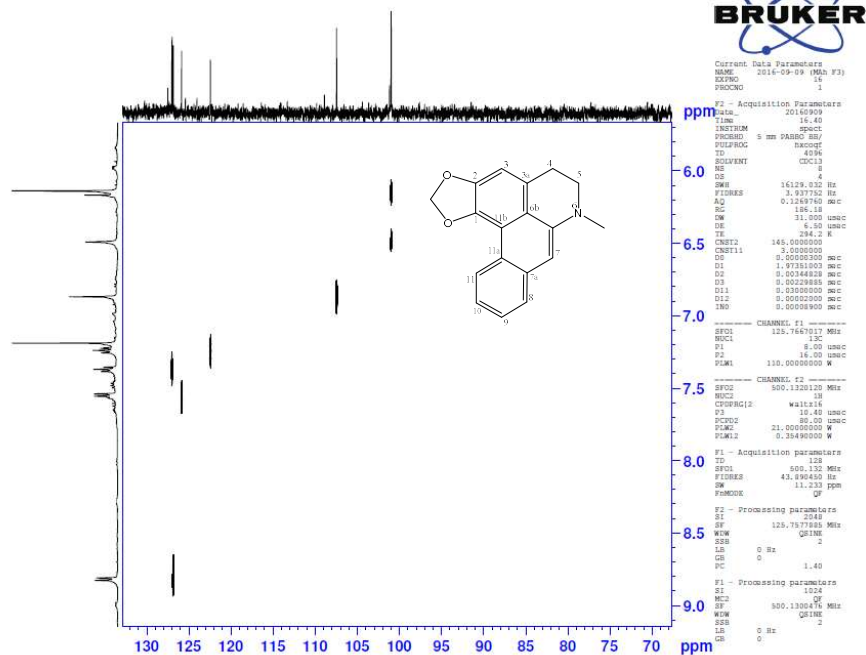
S13: HCCOSW Spectrum of Compound 1 (dehydroremerine)

13COSY MAH F3



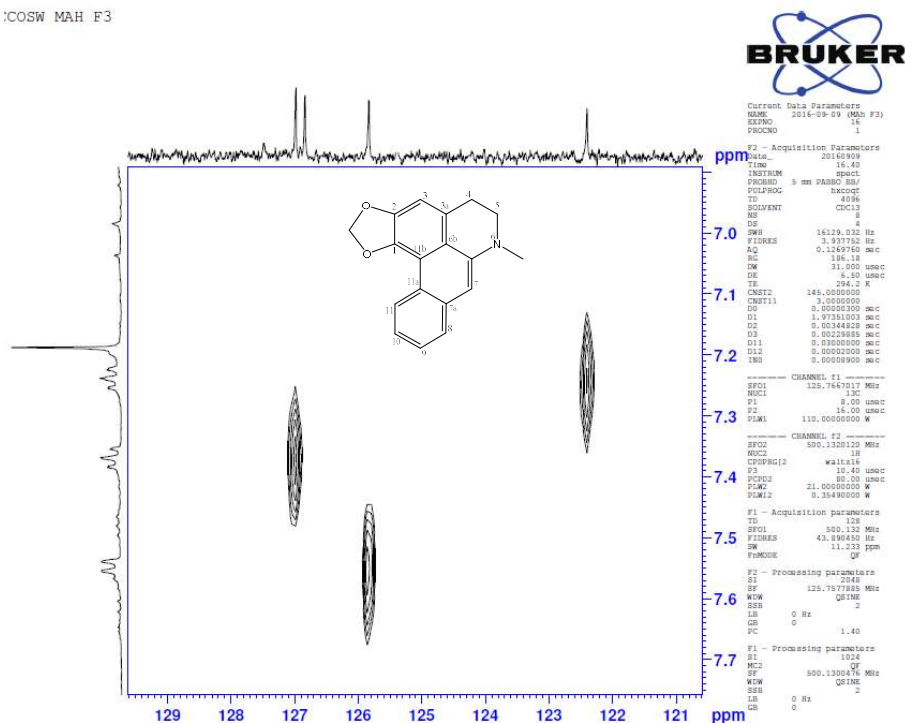
S14: Expansion of the HCCOSW Spectrum of Compound 1 (dehydroremerine)

HCCOSW MAH F3



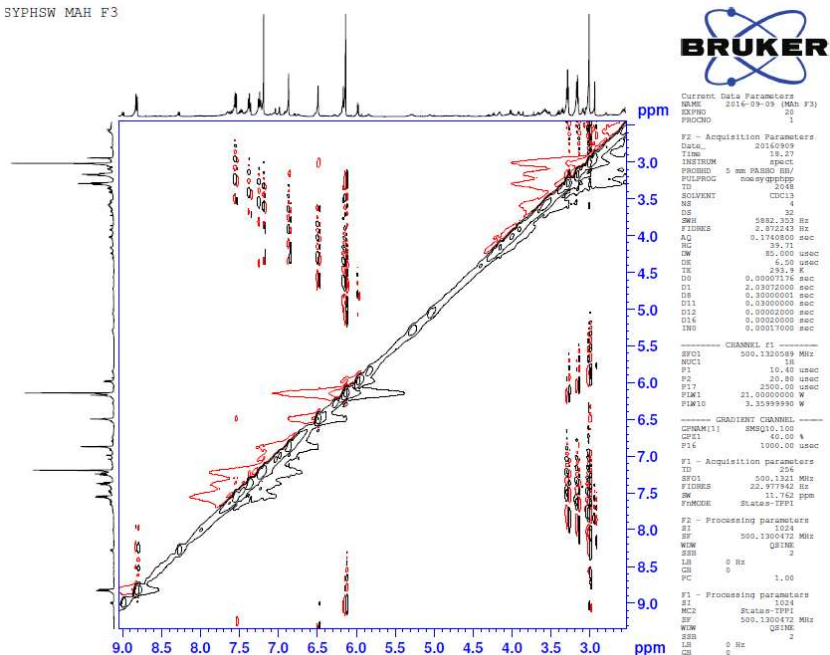
S15: Expansion of the HCCOW Spectrum of Compound **1** (dehydroremerine)

HCCOSW MAH F3



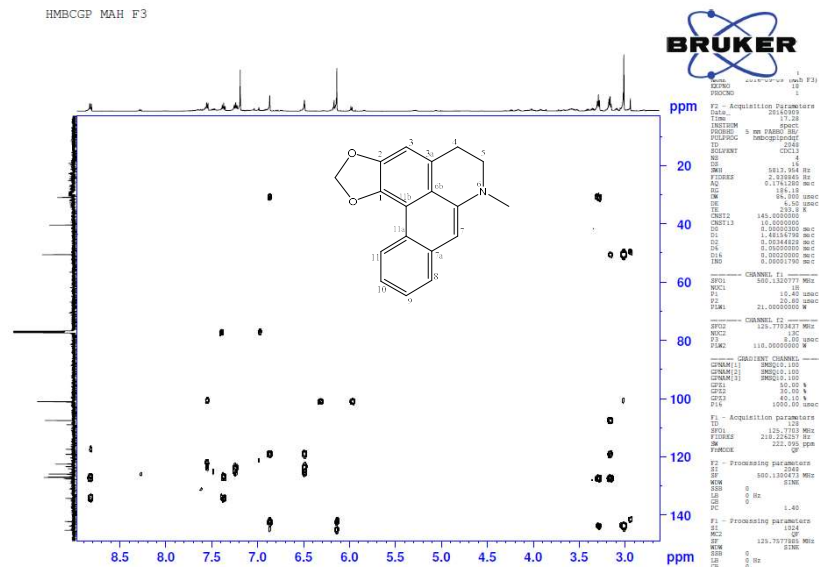
S16: Expansion of the HCCOW Spectrum of Compound **1** (dehydroremerine)

SYPHSW MAH F3



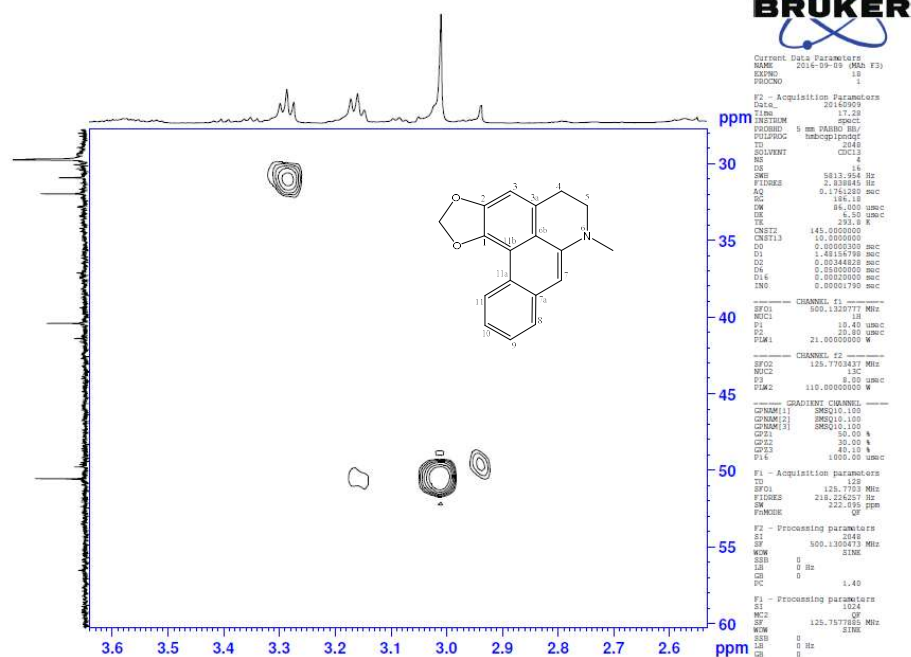
S17: NOSY (500 MHz) Spectrum of Compound 1 (dehydroremerine)

HMBCGP MAH F3



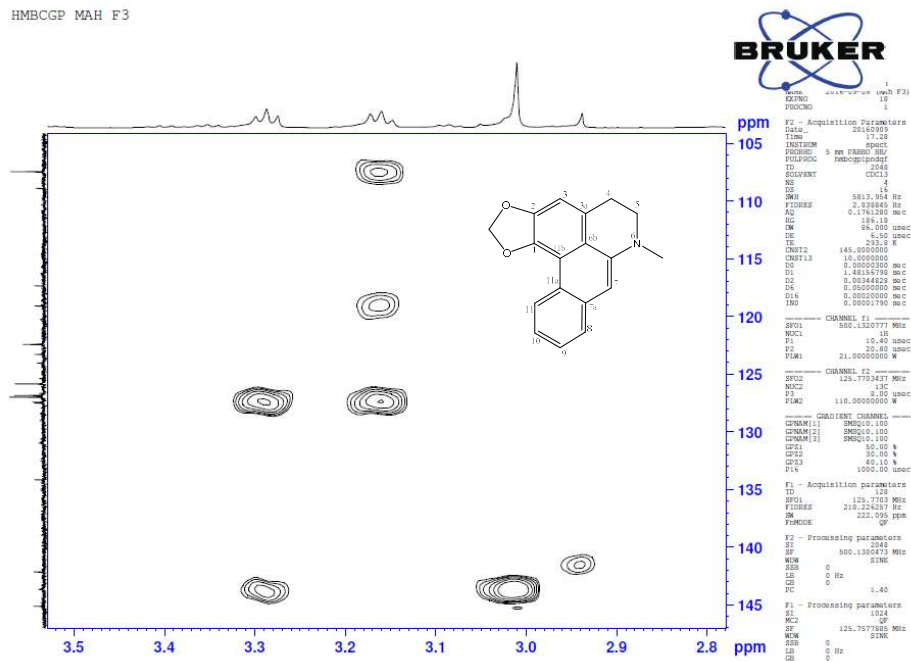
S18: HMBC (500 MHz) Spectrum of Compound 1 (dehydroremerine)

HMBCGP MAH F3



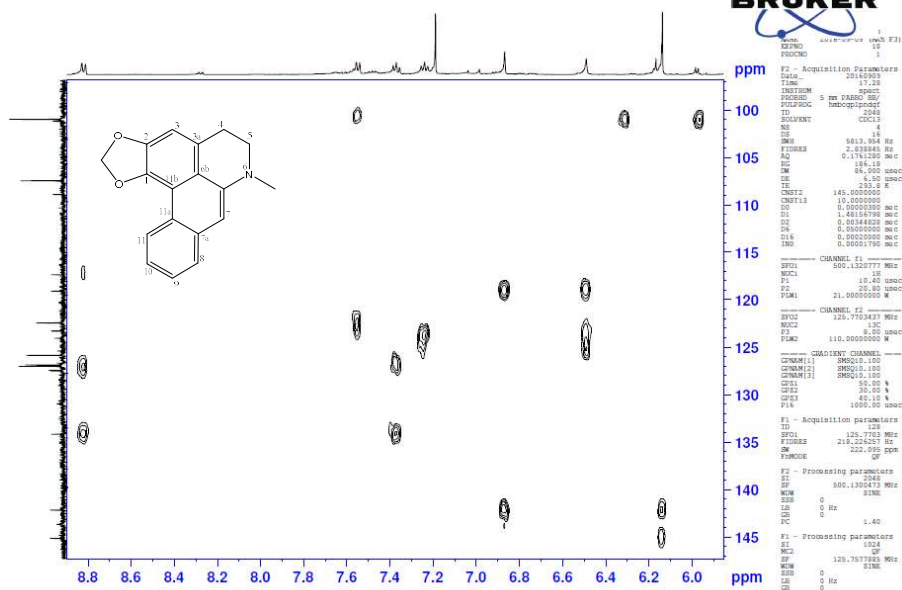
S19: Expansion of the HMBC (500 MHz) Spectrum of Compound **1** (dehydroremerine)

HMBCGP MAH F3



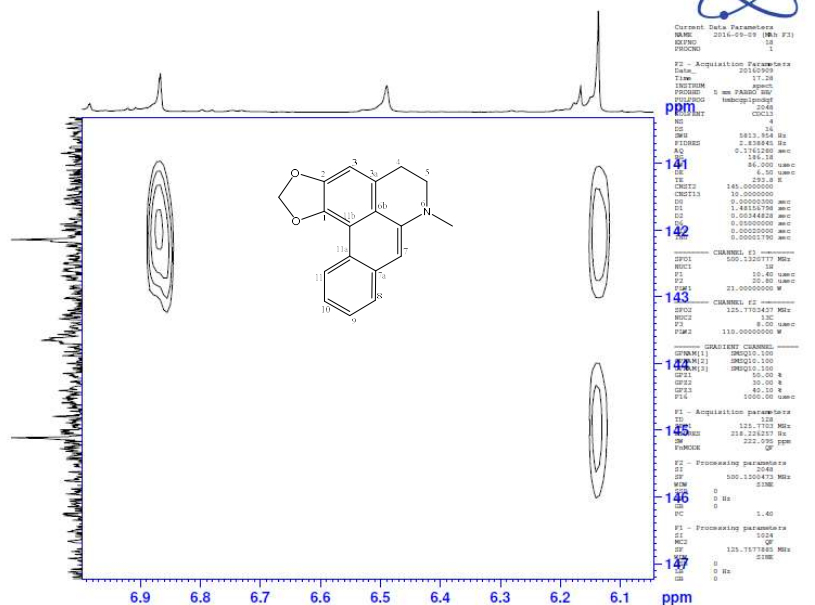
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HMBCGP MAH F3

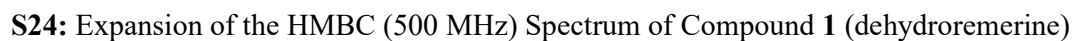


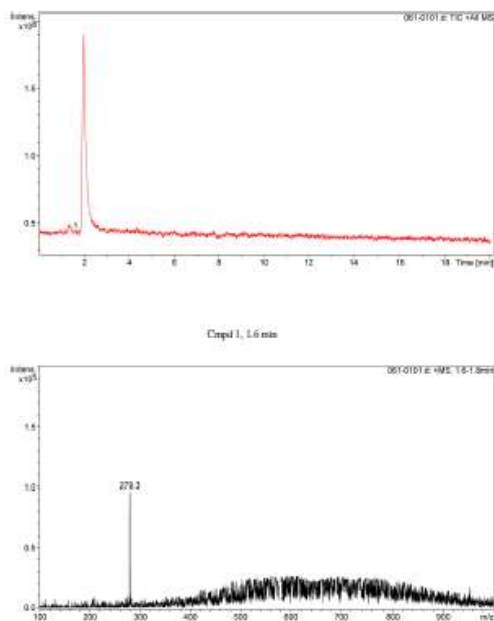
S21: Expansion of the HMBC (500 MHz) Spectrum of Compound **1** (dehydroremerine)

HMBCGP MAH F3

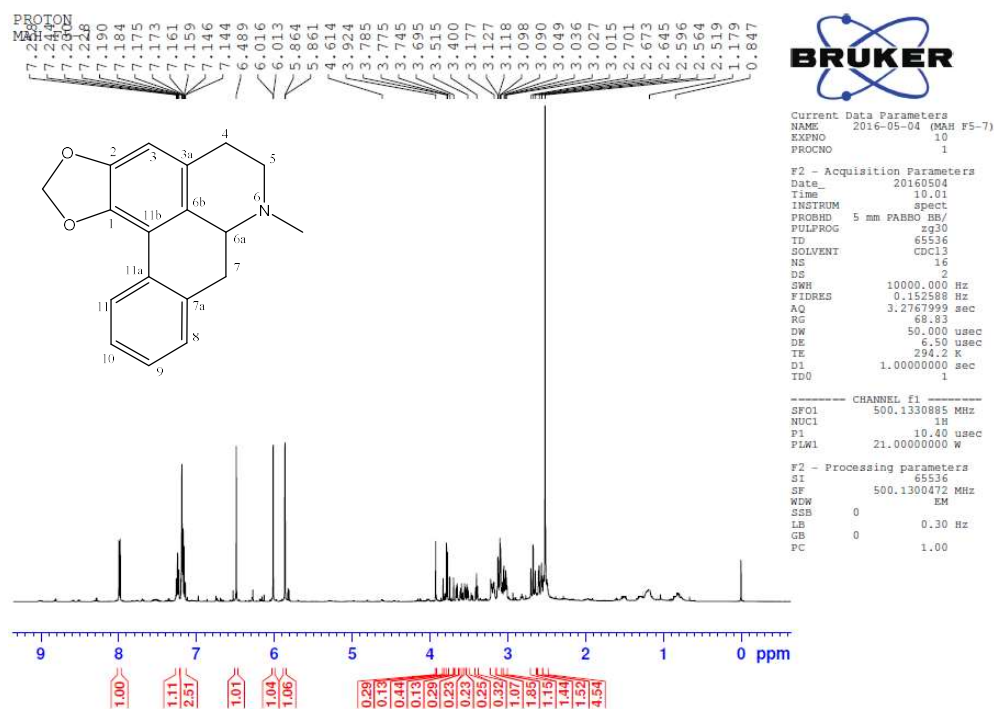


S22: Expansion of the HMBC (500 MHz) Spectrum of Compound **1** (dehydroremerine)

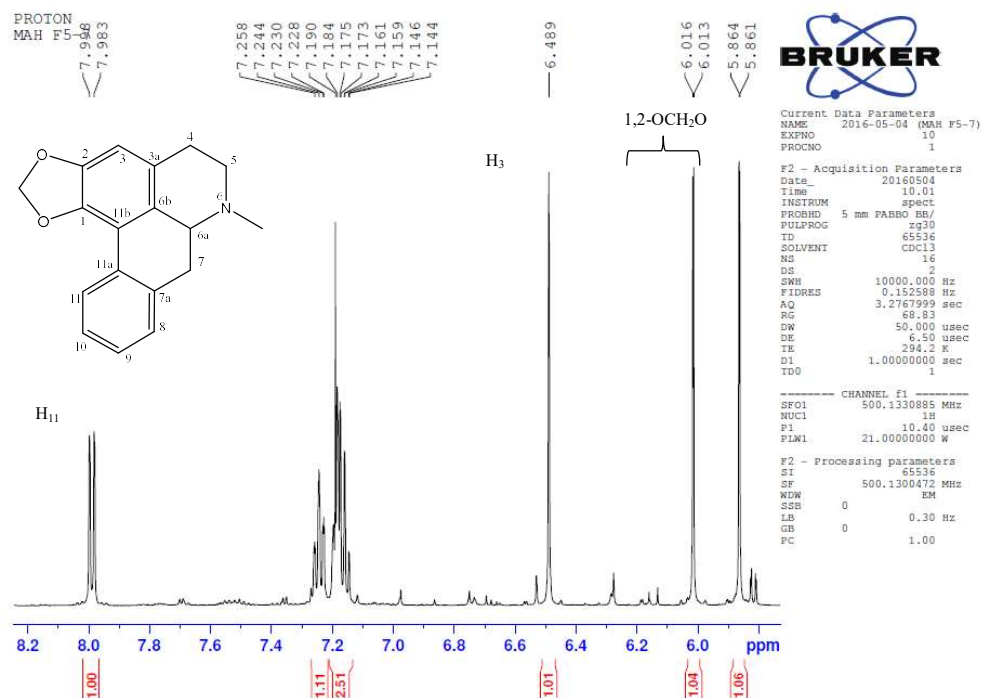




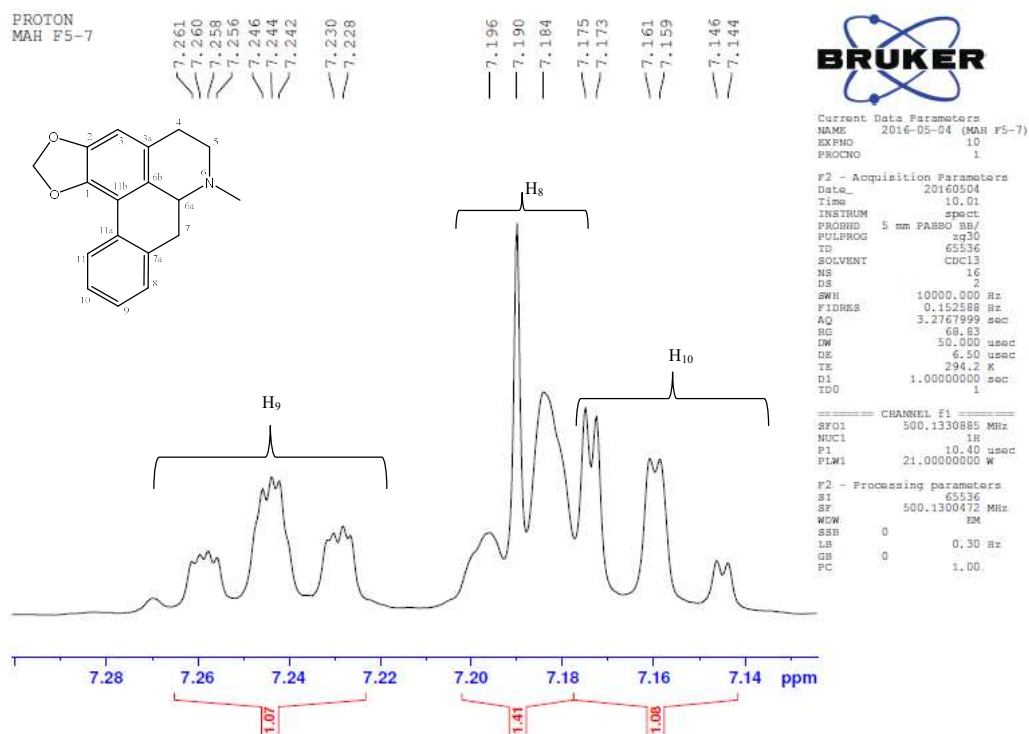
S25: LC-MS Spectrum of Compound **2** (reomerine)



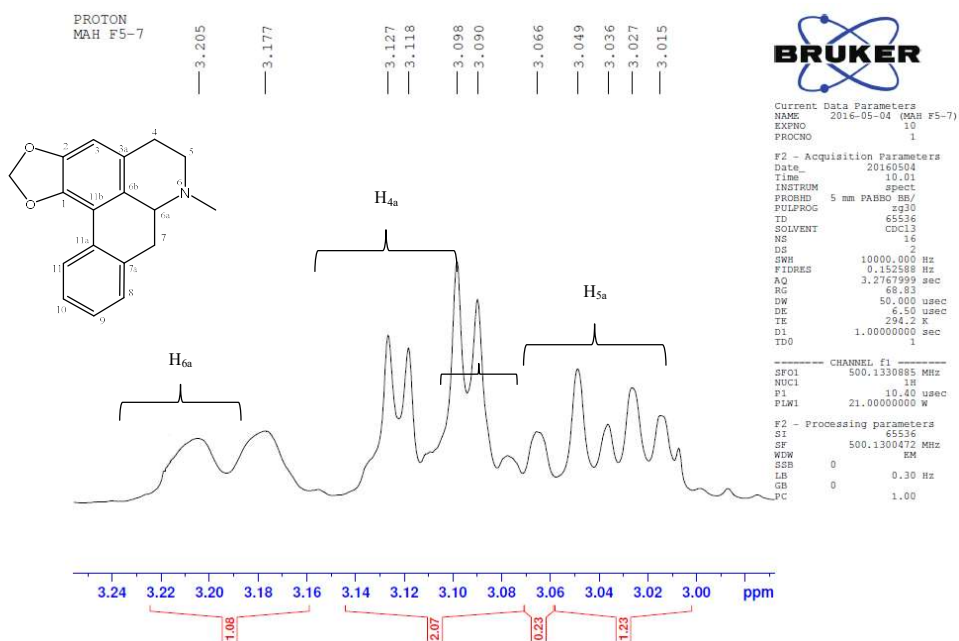
S26: ¹H-NMR (500 MHz, CDCl₃) Spectrum of Compound **2** (reomerine)



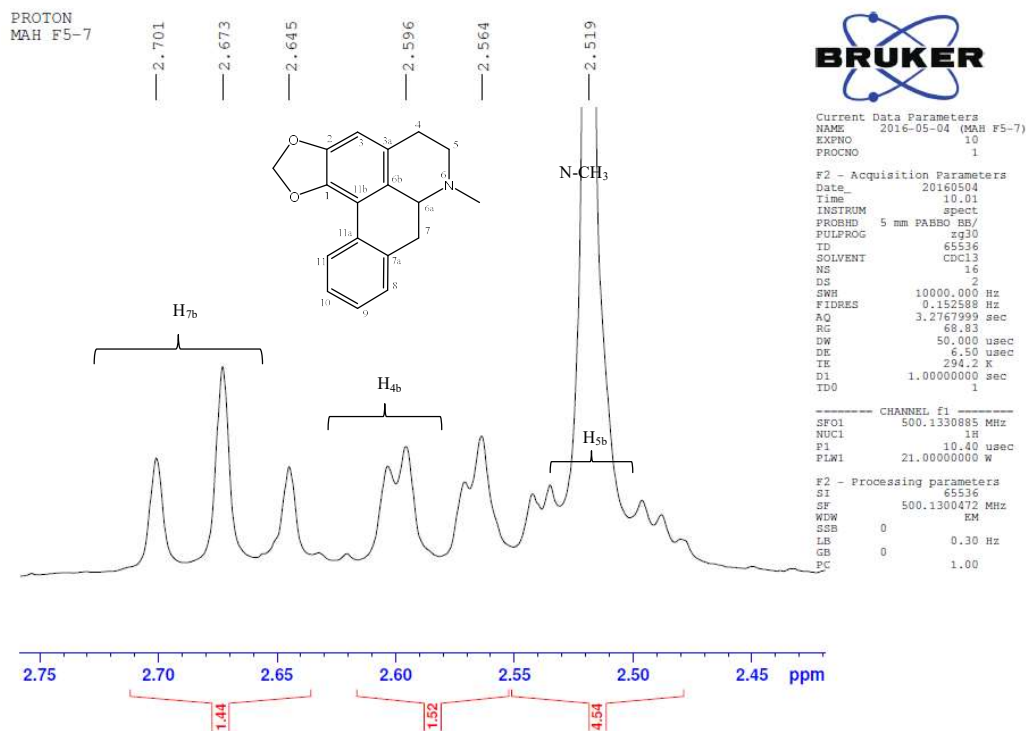
S27: Expansion ¹H-NMR (500 MHz, CDCl₃) Spectrum of Compound 2 (reomerine)



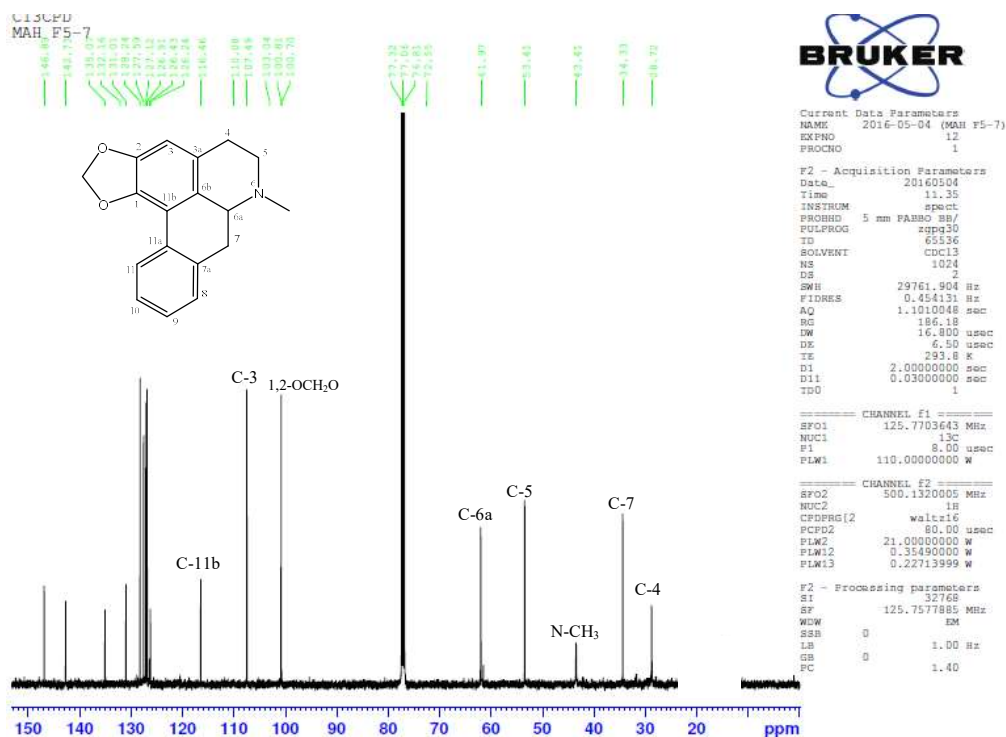
S28: Expansion ¹H-NMR (500 MHz, CDCl₃) Spectrum of Compound 2 (reomerine)



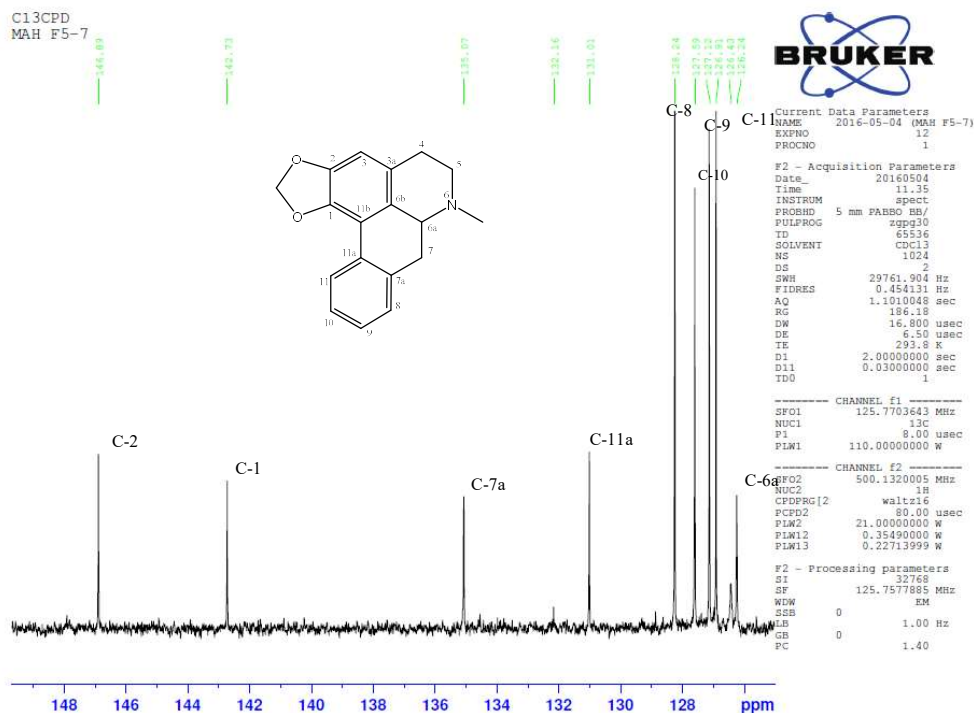
S29: Expansion ^1H -NMR (500 MHz, CDCl_3) Spectrum of Compound 2 (reomerine)



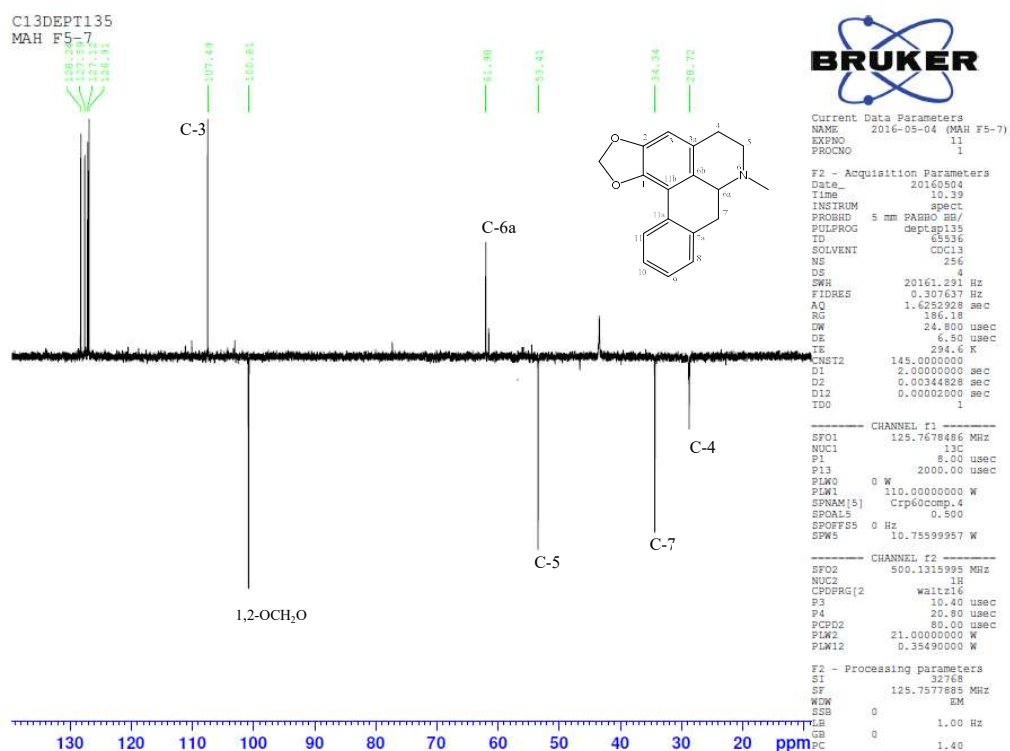
S30: Expansion ^1H -NMR (500 MHz, CDCl_3) Spectrum of Compound 2 (reomerine)



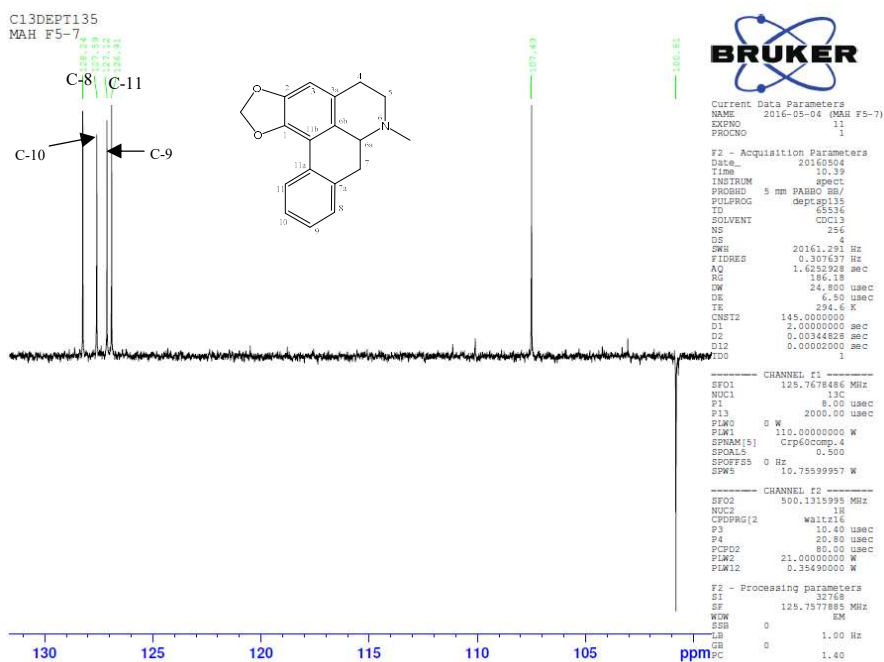
S31: ^{13}C -NMR (500 MHz, CDCl_3) Spectrum of Compound 2 (reomerine)



S32: Expansion of the ^{13}C -NMR (500 MHz, CDCl_3) Spectrum of Compound 2 (reomerine)

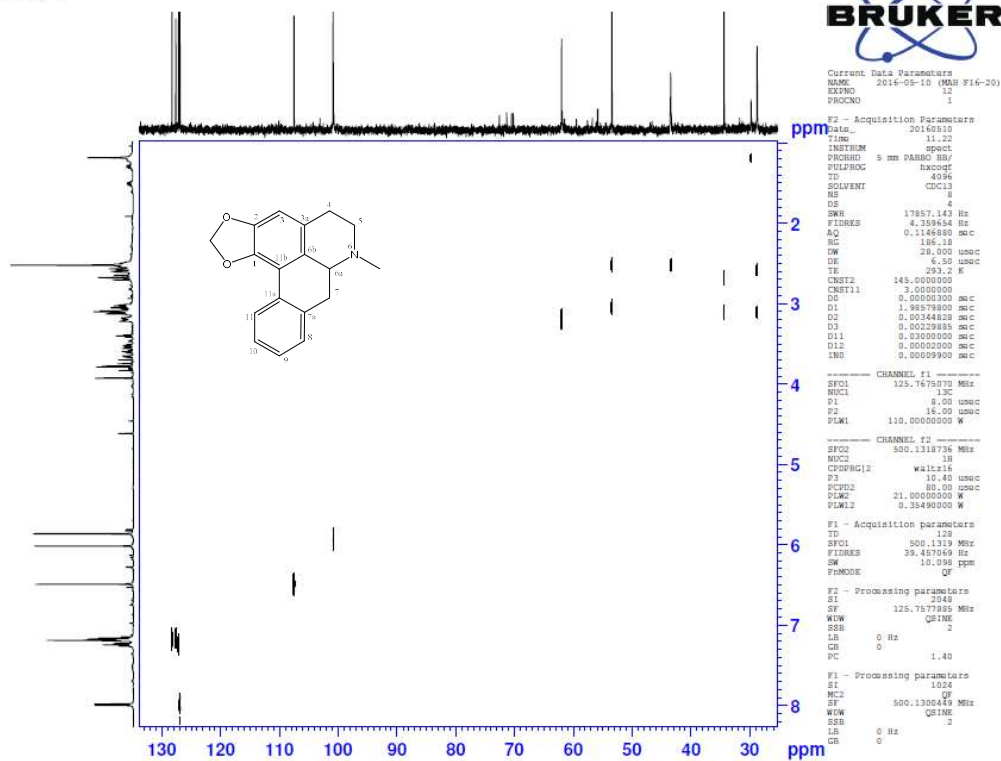


S33: Expansion of the DEPT (500 MHz, CDCl₃) Spectrum of Compound **2** (reomerine)



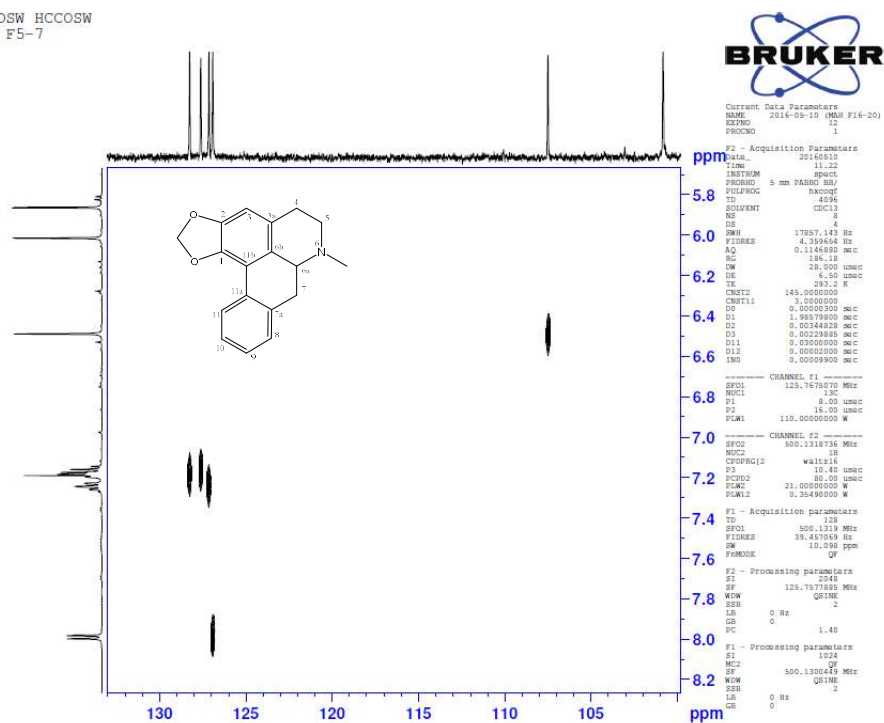
S34: Expansion of the DEPT (500 MHz, CDCl₃) Spectrum of Compound **2** (reomerine)

HCCOSW HCCOSW
MAH F5-7



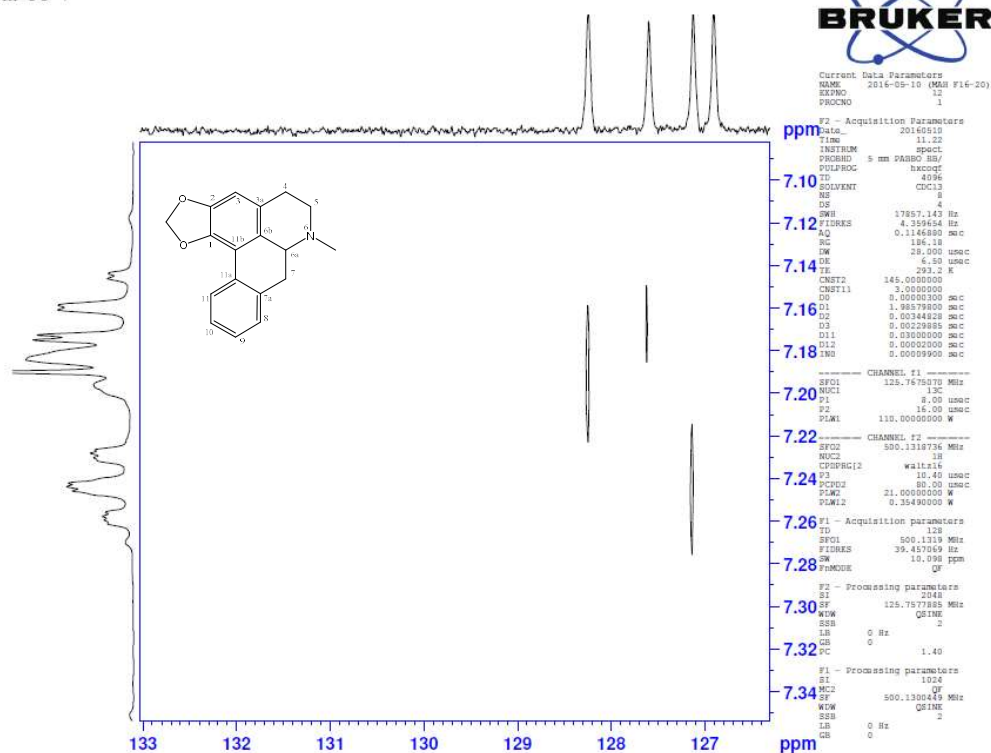
S35: HCCOW Spectrum of Compound 2 (reomerine)

HCCOSW HCCOSW
MAH F5-7



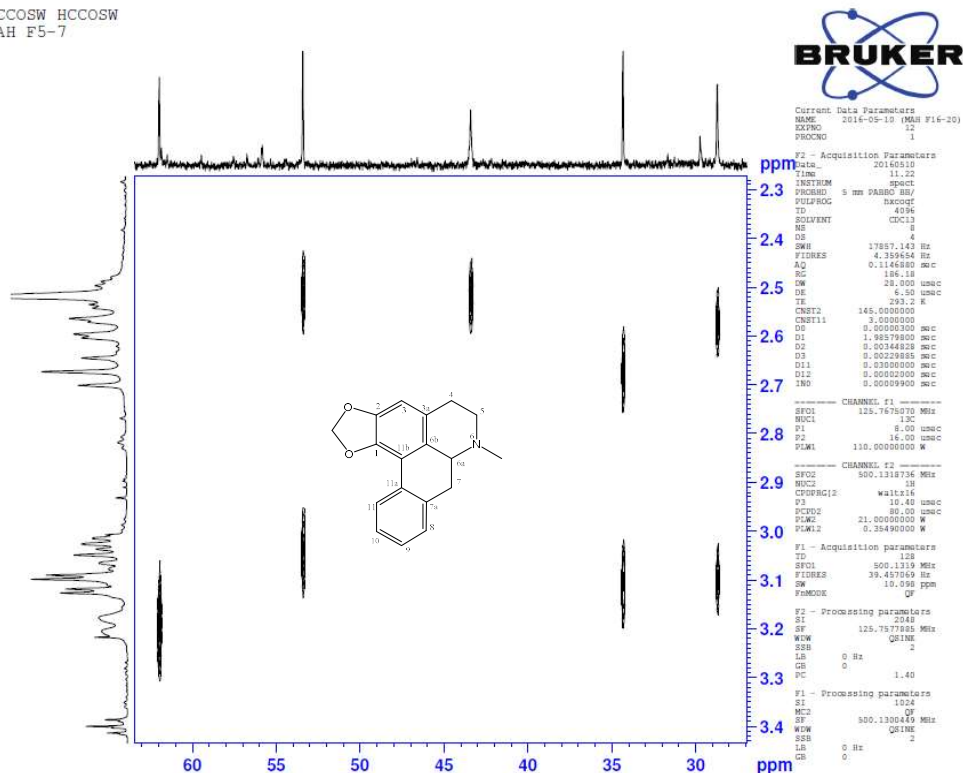
S36: Expansion of the HCCOW Spectrum of Compound 2 (reomerine)

HCCOSW HCCOSW
MAH F5-7



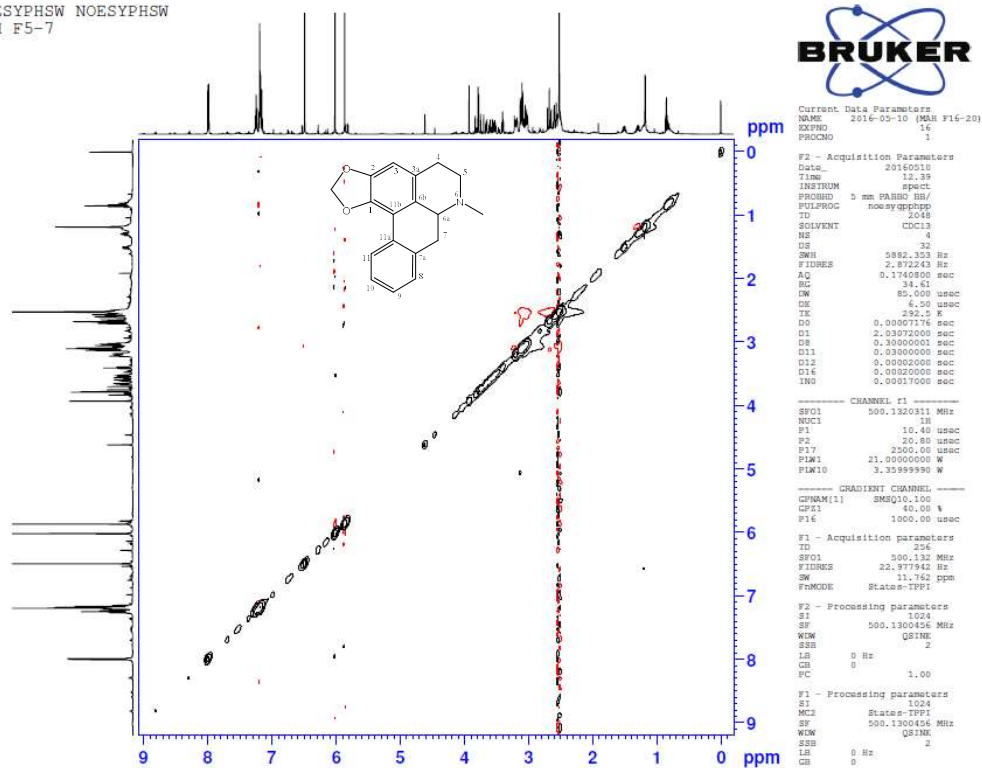
S37: Expansion of the HCCOW Spectrum of Compound 2 (reomerine)

HCCOSW HCCOSW
MAH F5-7



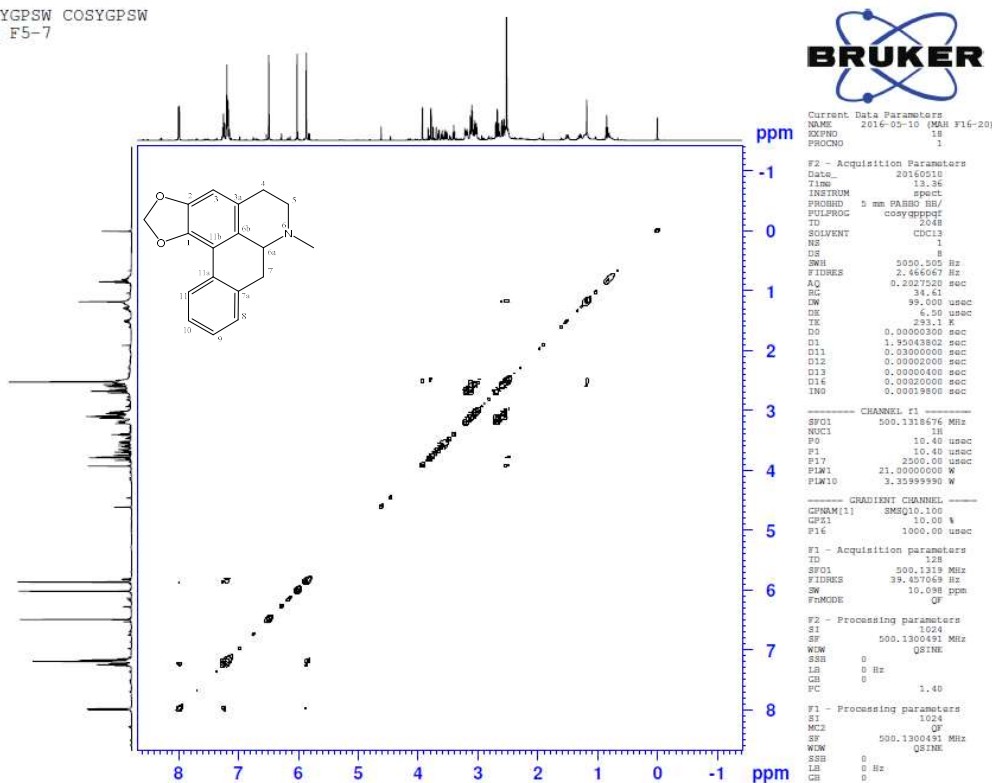
S38: Expansion of the HCCOW Spectrum of Compound 2 (reomerine)

NOESYPSHW NOESYPSHW
MAH F5-7



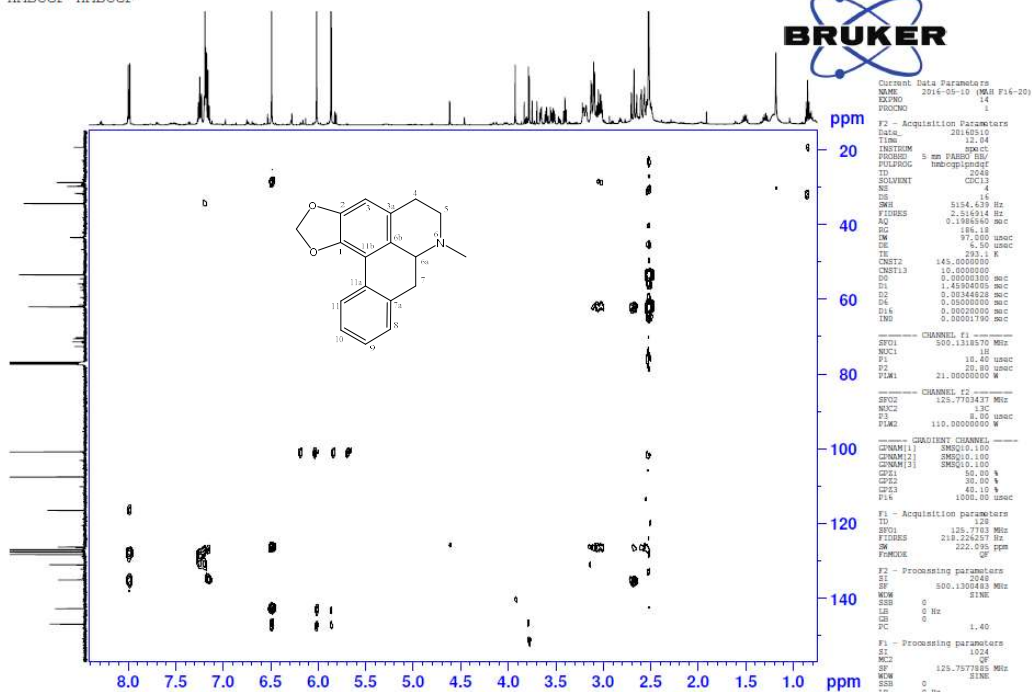
S39: NOSY (500 MHz, CDCl₃) Spectrum of Compound **2** (reomerine)

COSYGPSW COSYGPSW
MAH F5-7



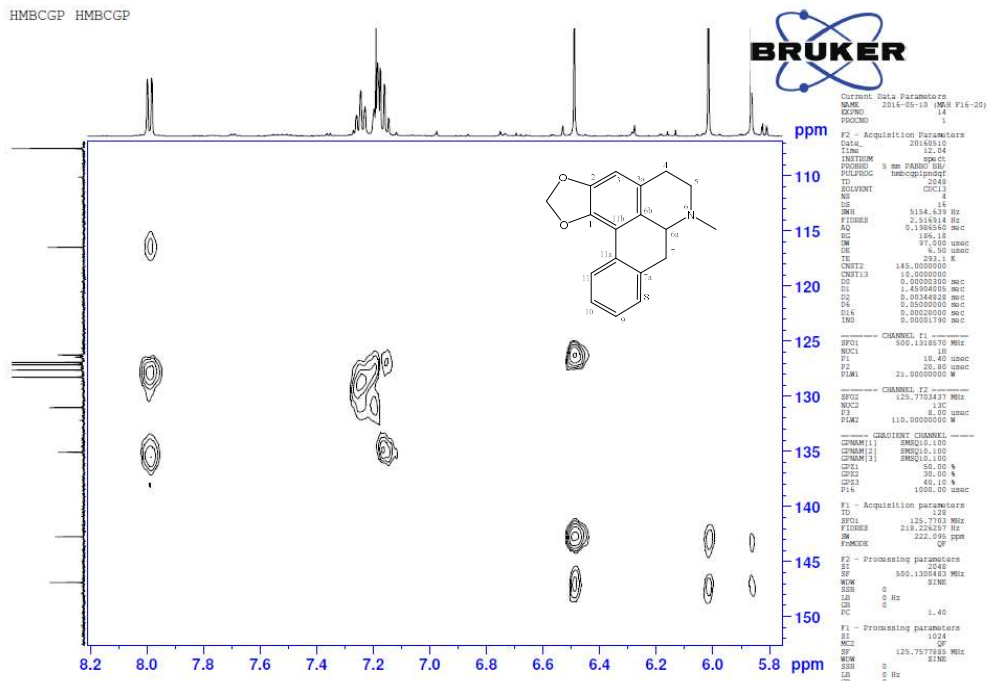
S40: COSY (500 MHz, CDCl₃) Spectrum of Compound **2** (reomerine)

HMBGCP HMBGCP



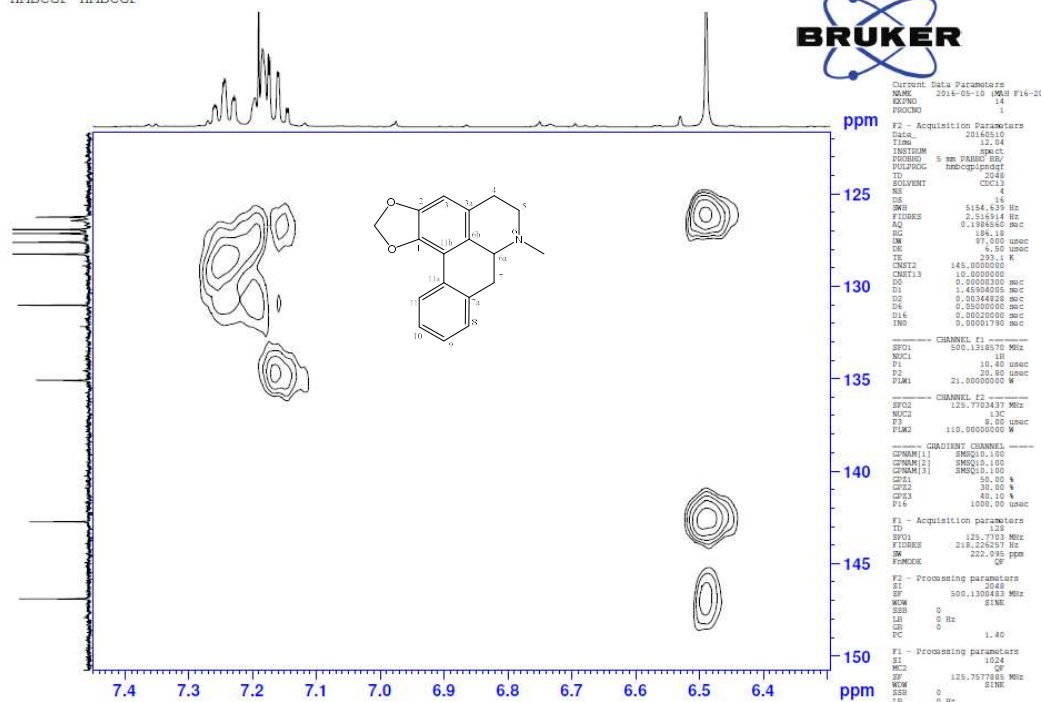
S41: HMBC (500 MHz, CDCl₃) Spectrum of Compound **2** (reomerine)

HMBGCP HMBGCP



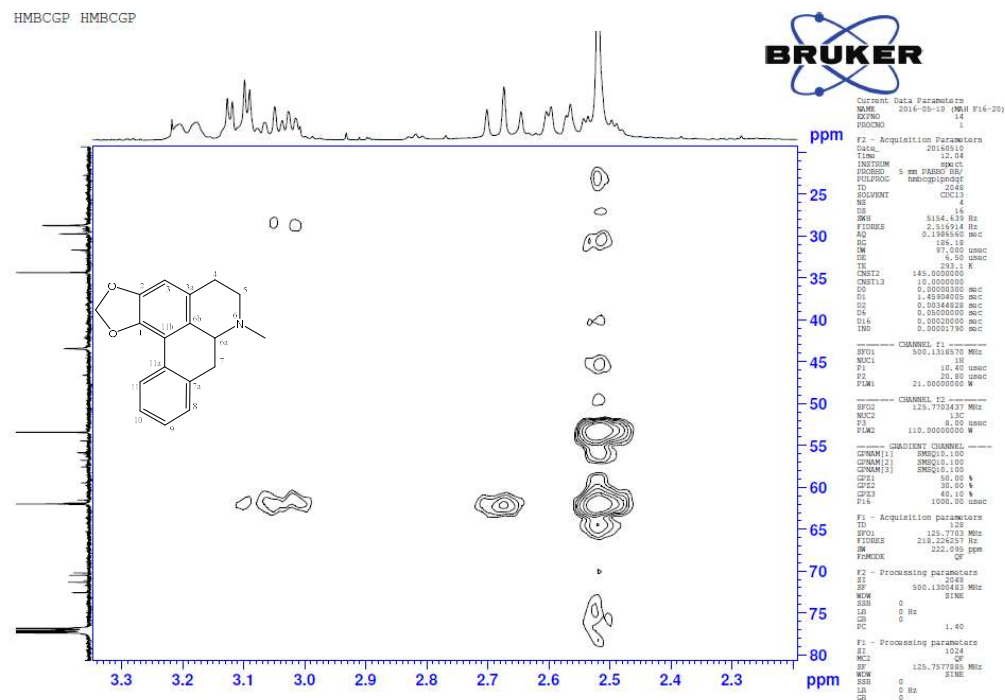
S42: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound **2** (reomerine)

HMBCGP HMBCGP



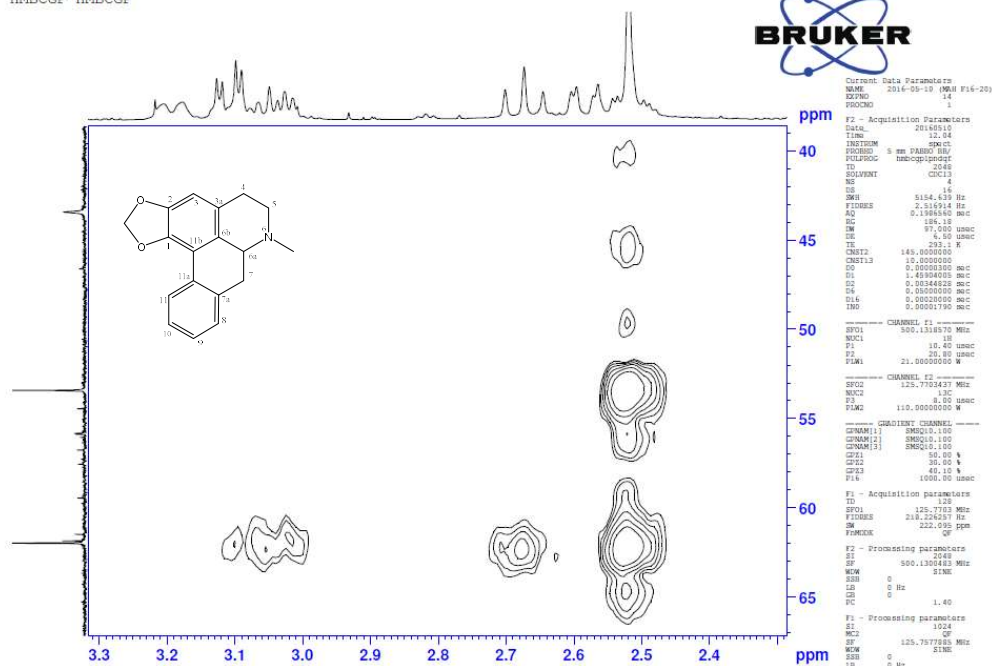
S43: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 2 (reomerine)

HMBCGP HMBCGP

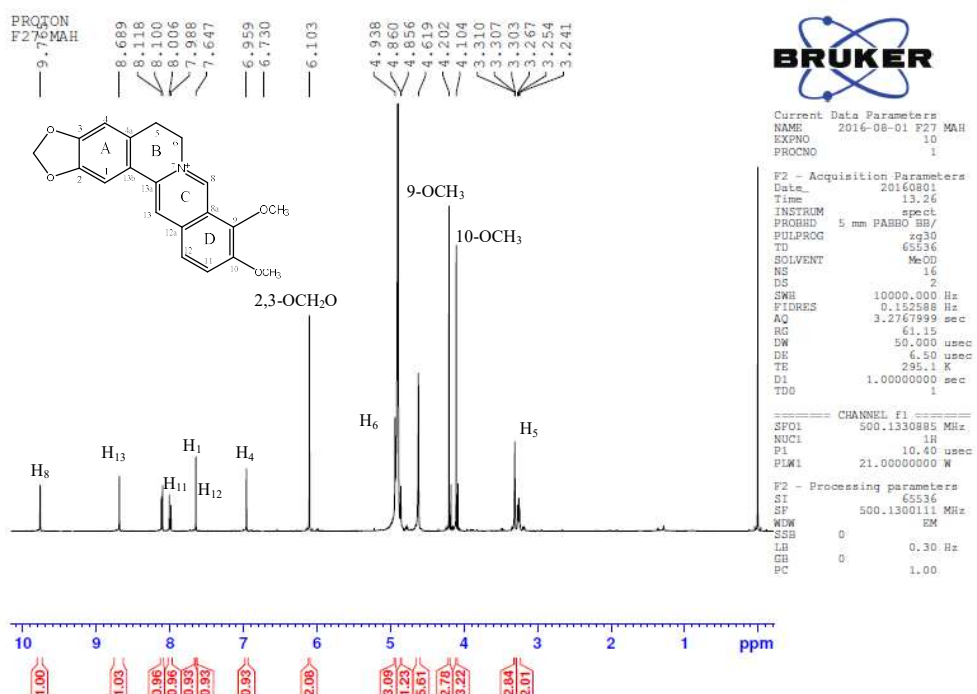


S44: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 2 (reomerine)

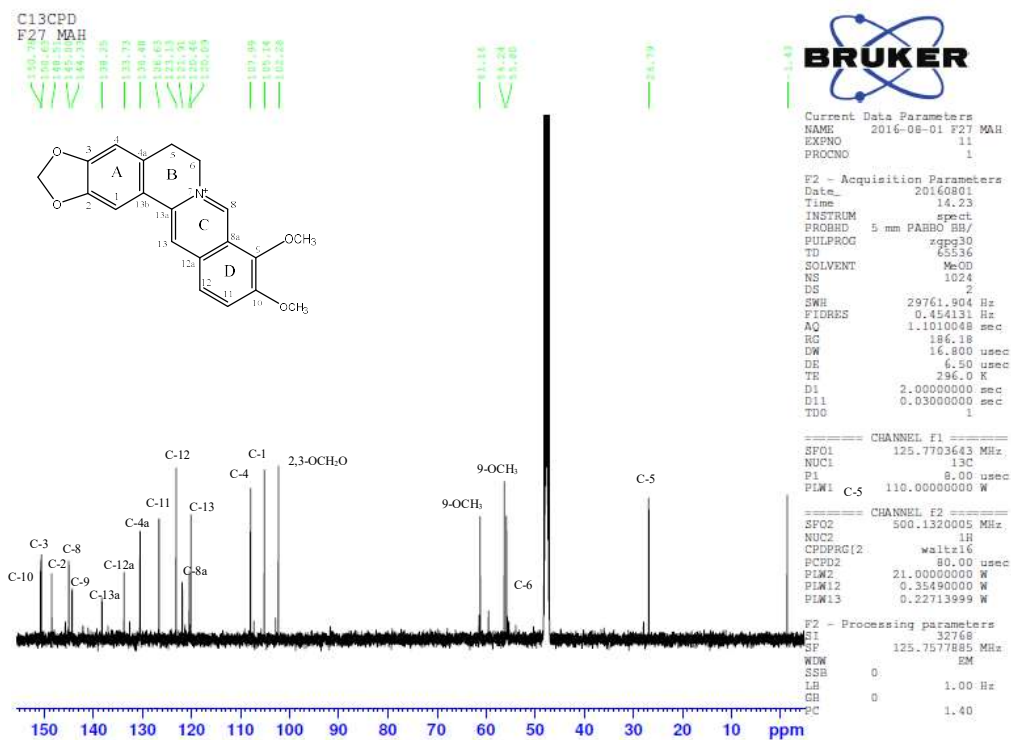
HMBCGP HMBCGP



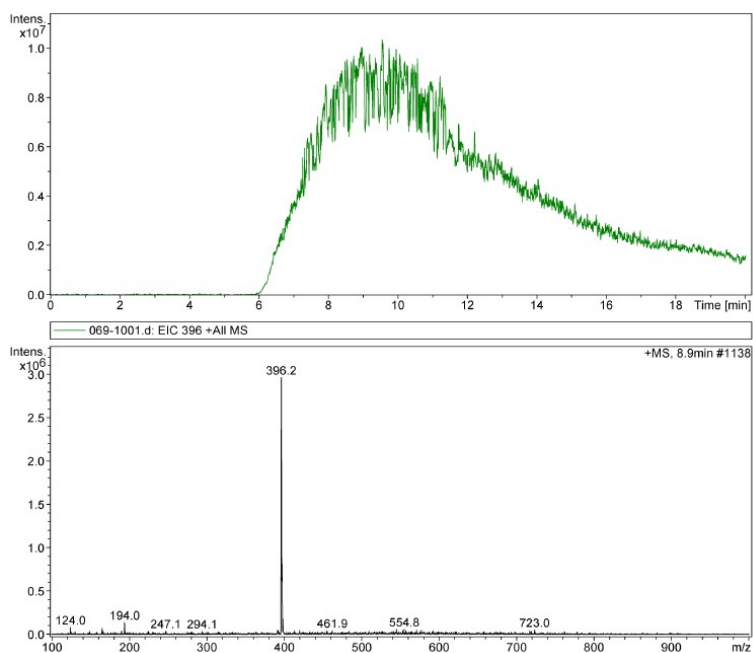
S45: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound **2** (reomerine)



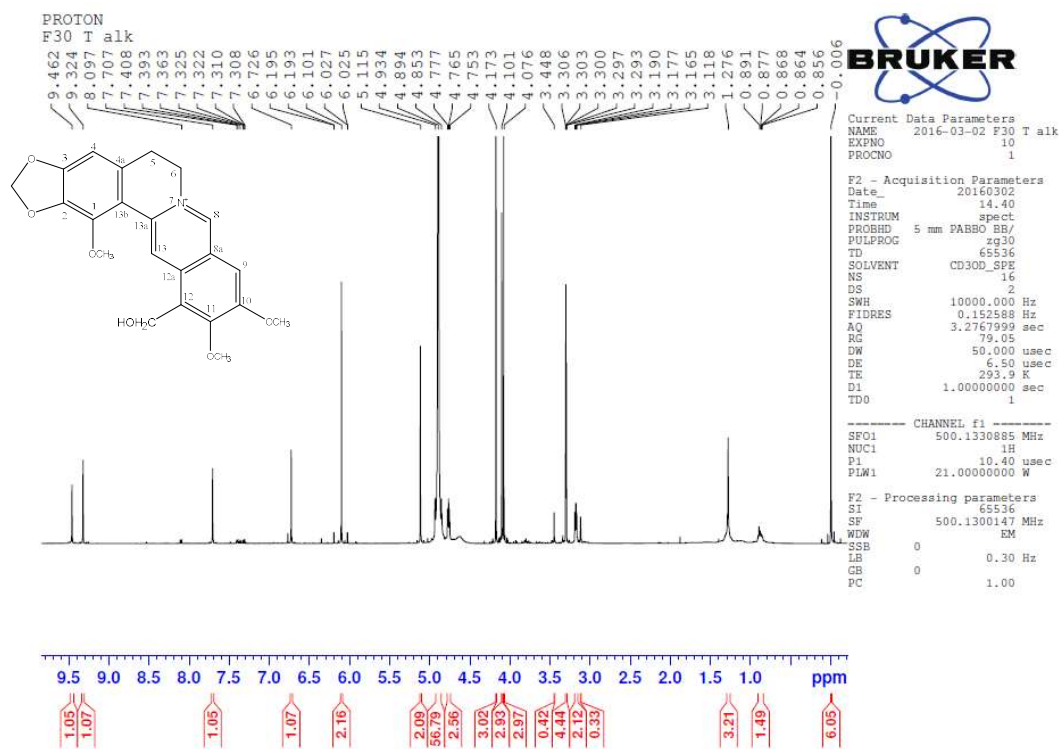
S46: ¹H-NMR (500 MHz, CDCl₃) Spectrum of Compound **3** (berberine)



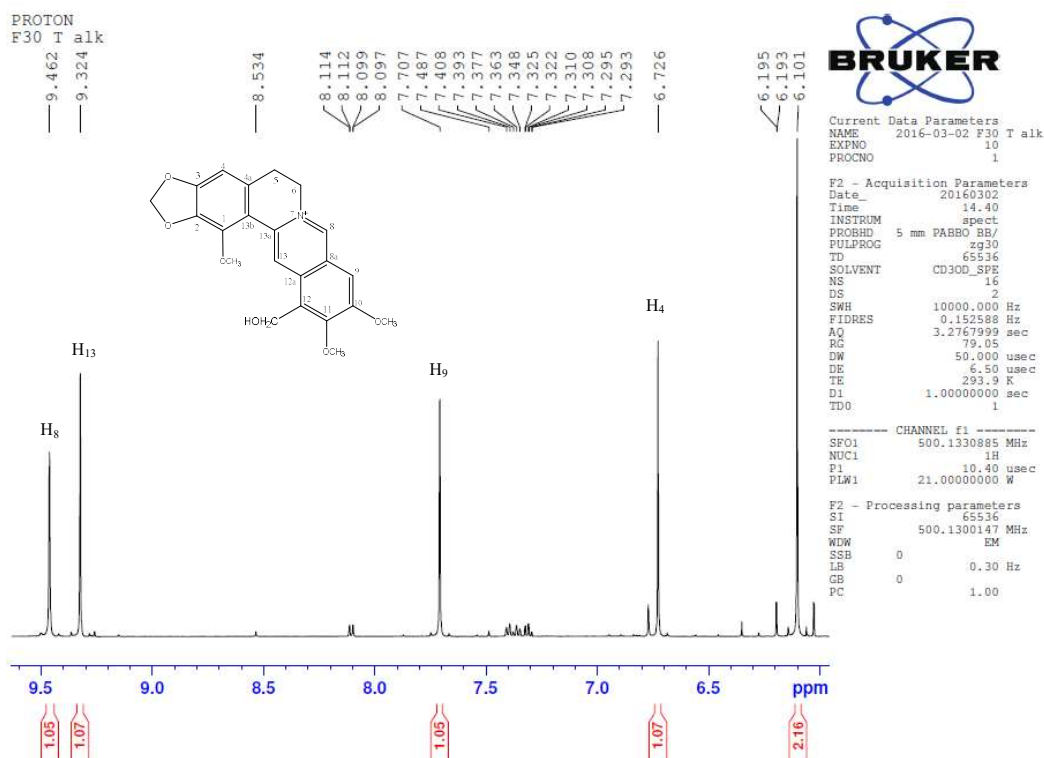
S47: ^{13}C -NMR (500 MHz) Spectrum of Compound **3** (berberine)



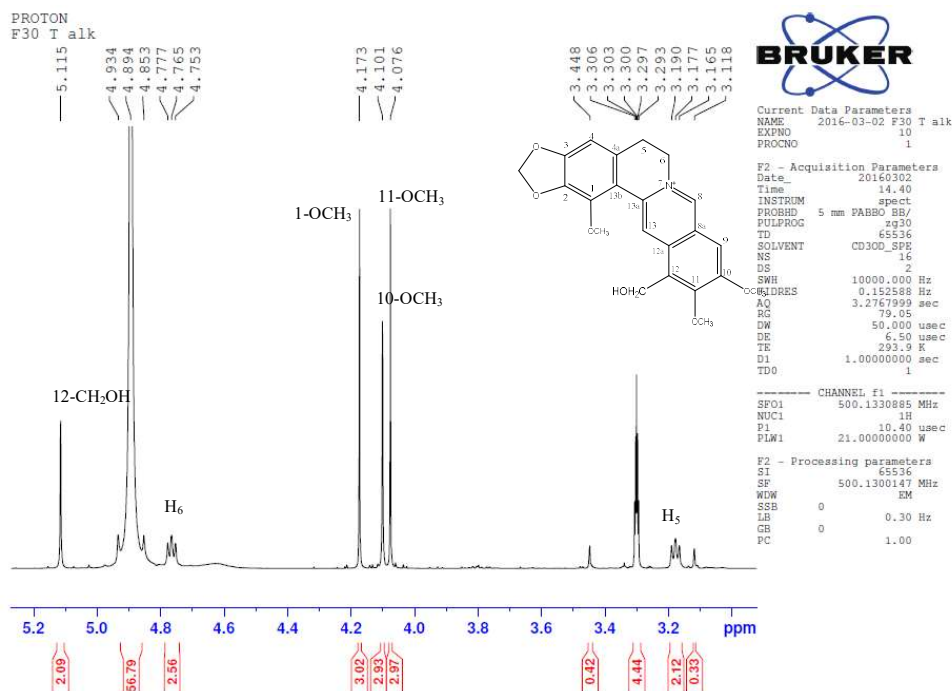
S48: LC-MS Spectrum of Compound **4** (alborine)



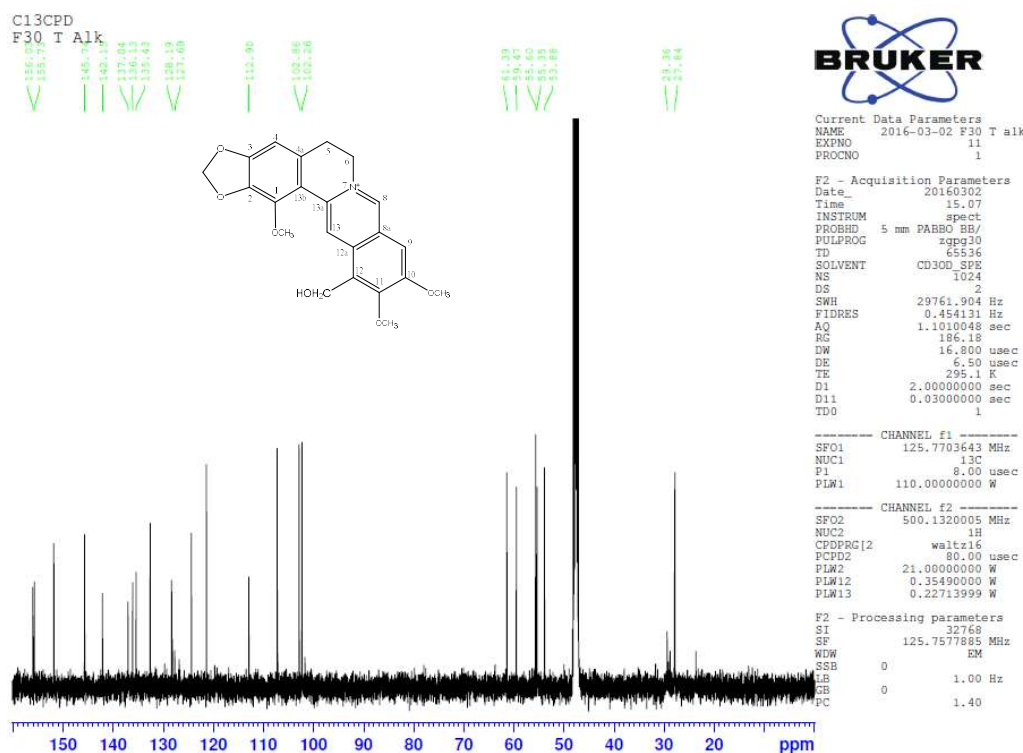
S49: ^1H -NMR (500 MHz, CD_3OD) Spectrum of Compound 4 (alborine)



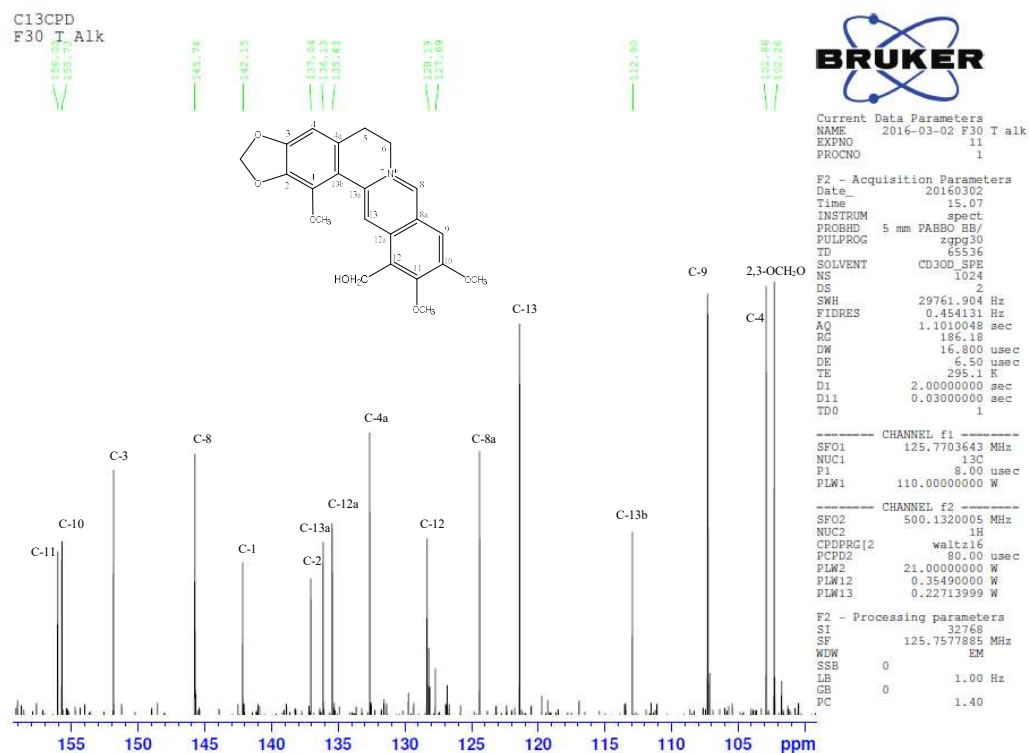
S50: Expansion of the ^1H -NMR (500 MHz, CD_3OD) Spectrum of Compound 4 (alborine)



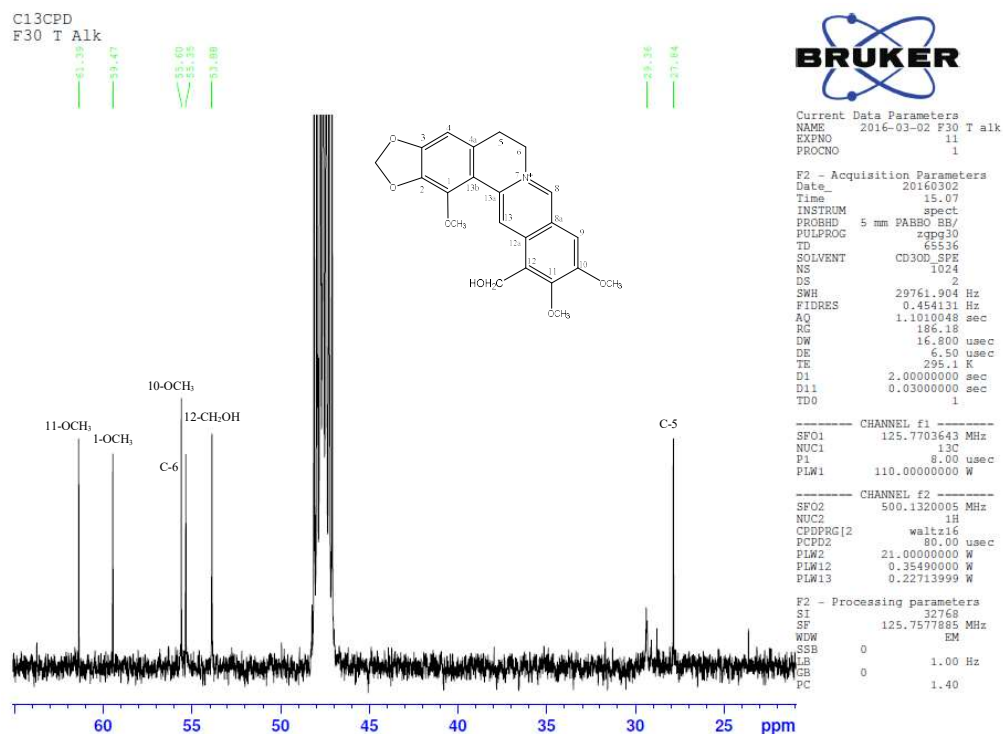
S51: Expansion of the ^1H -NMR (500 MHz, CD_3OD) Spectrum of Compound 4 (alborine)



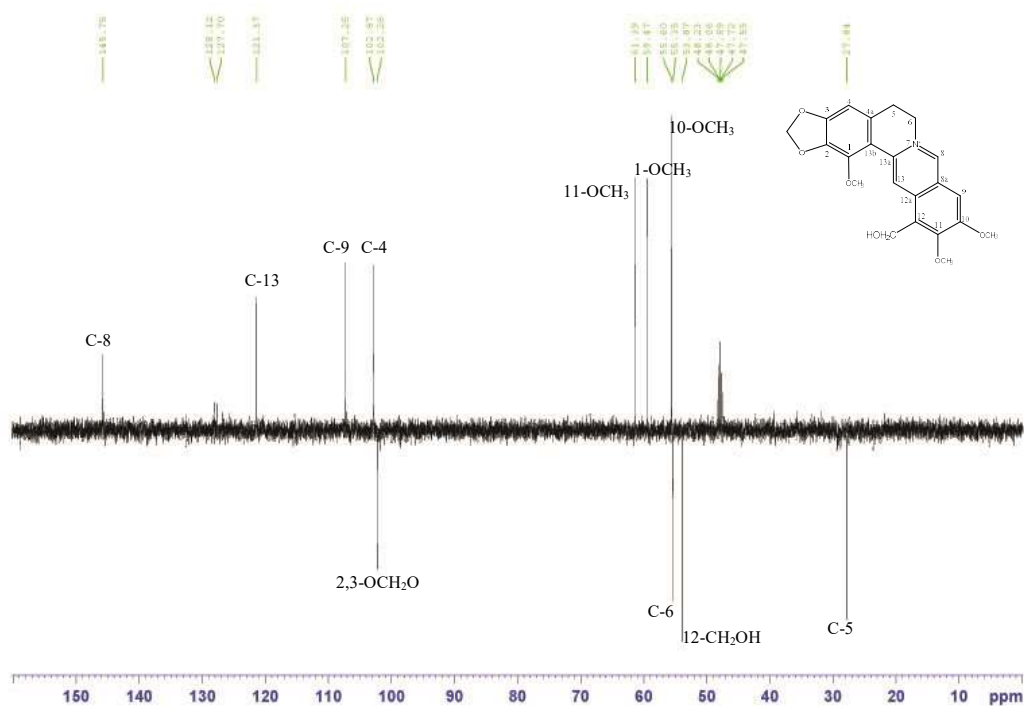
S52: ^{13}C -NMR (500 MHz) Spectrum of Compound 4 (alborine)



S53: Expansion of the ^{13}C -NMR (500 MHz) Spectrum of Compound 4 (alborine)

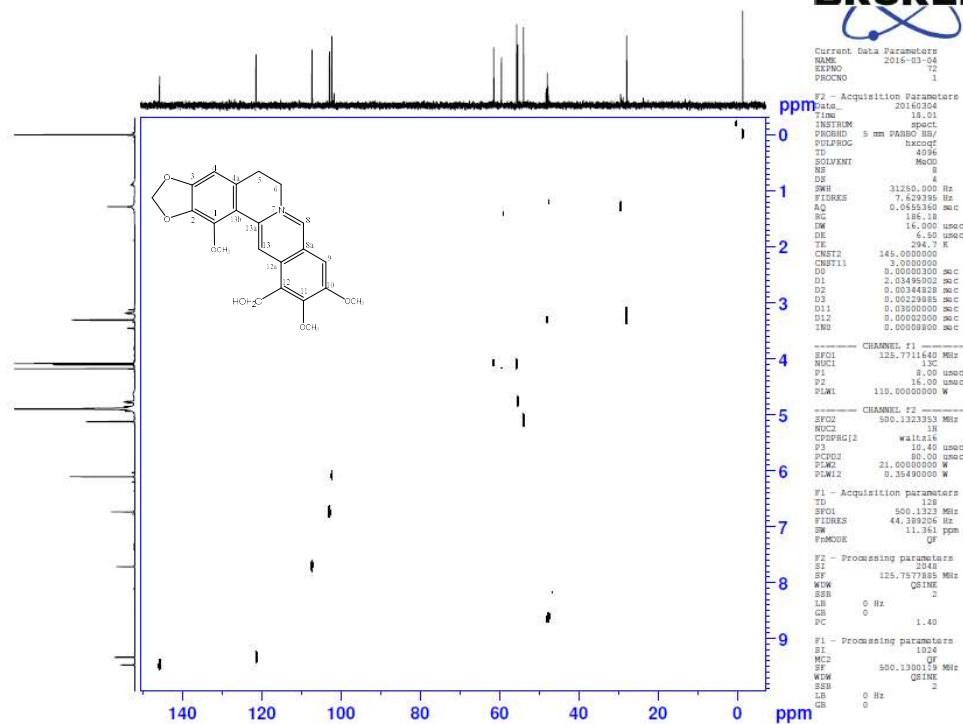


S54: Expansion of the ^{13}C -NMR (500 MHz) Spectrum of Compound 4 (alborine)



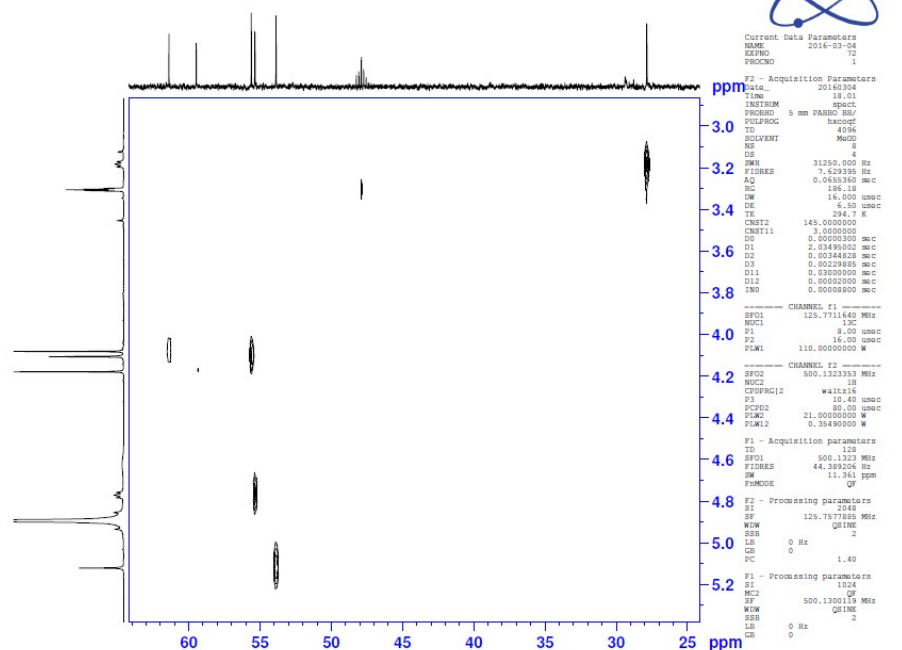
S55: DEPT (500 MHz) Spectrum of Compound 4 (alborine)

HCCOSW MeOD
MAH F30



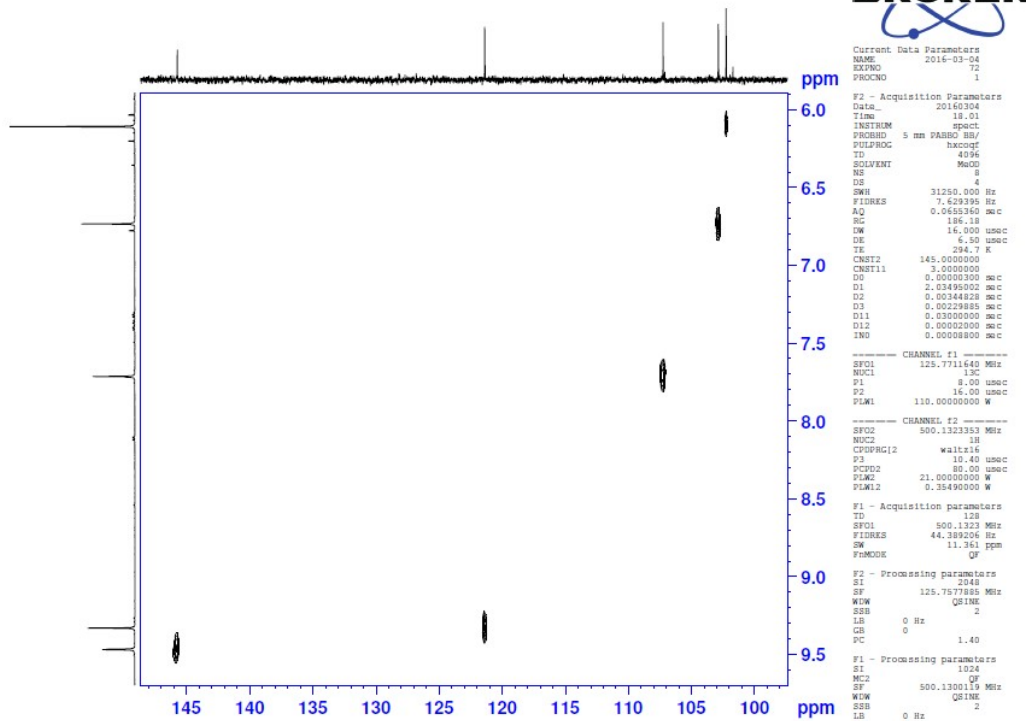
S56: HCCOW Spectrum of Compound 4 (alborine)

HCCOSW MeOD
MAH F30



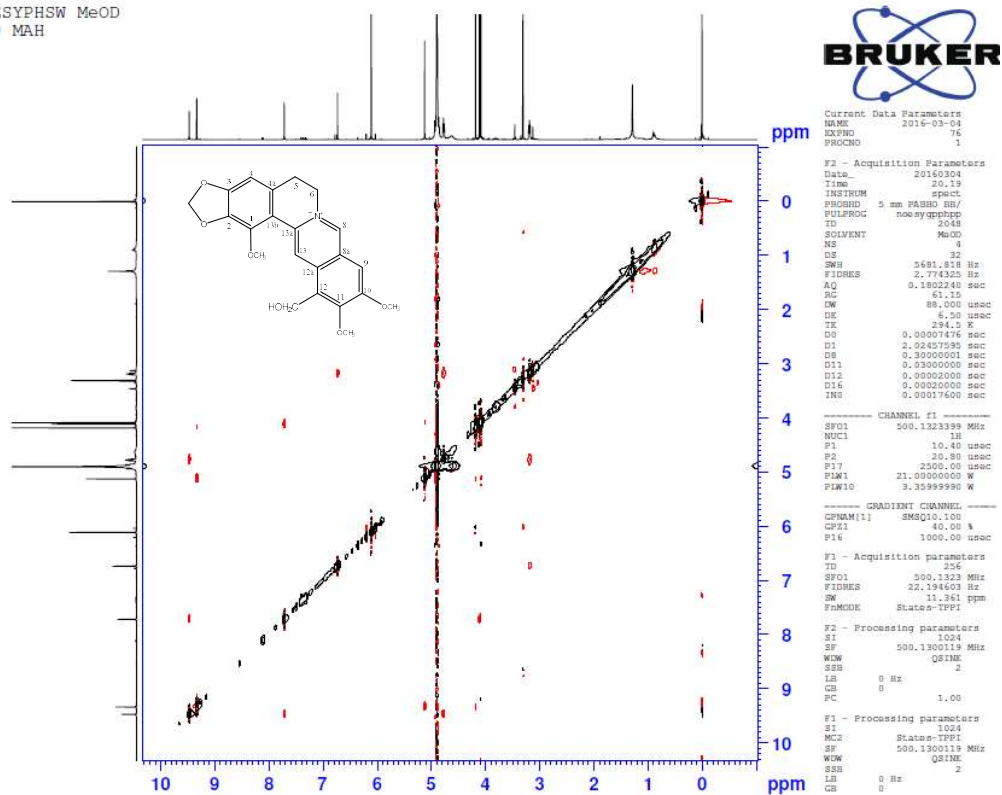
S57: Expansion of the HCCOW Spectrum of Compound **4** (alborine)

HCCOSW MeOD
MAH F30



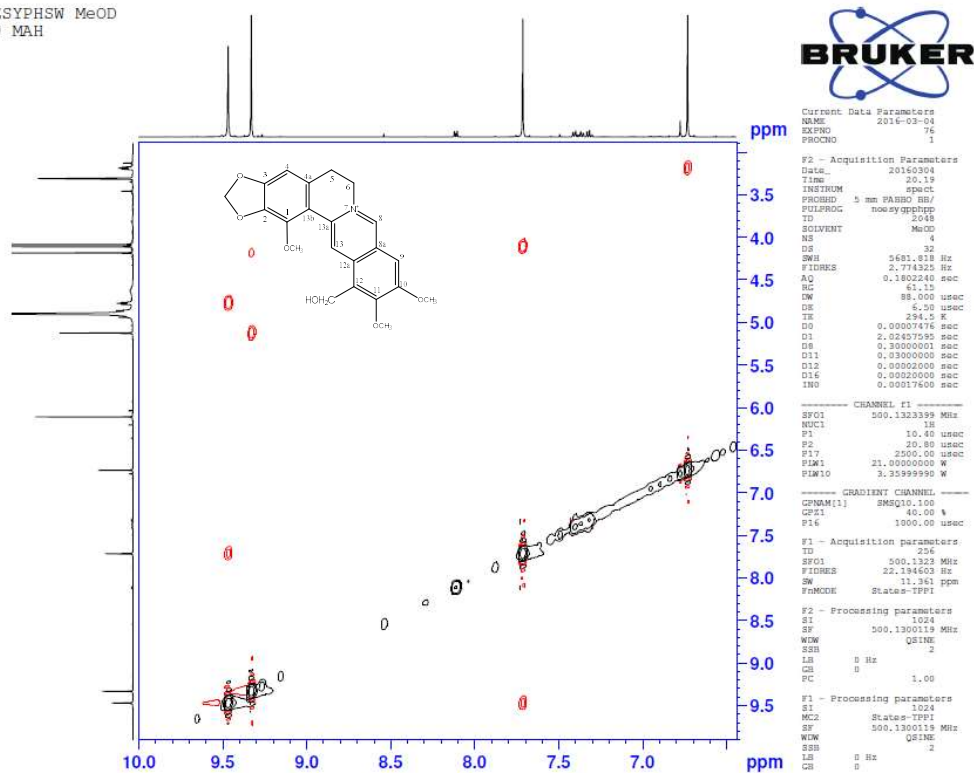
S58: Expansion of the HCCOW Spectrum of Compound **4** (alborine)

NOESYPSHW MeOD
F30 MAH



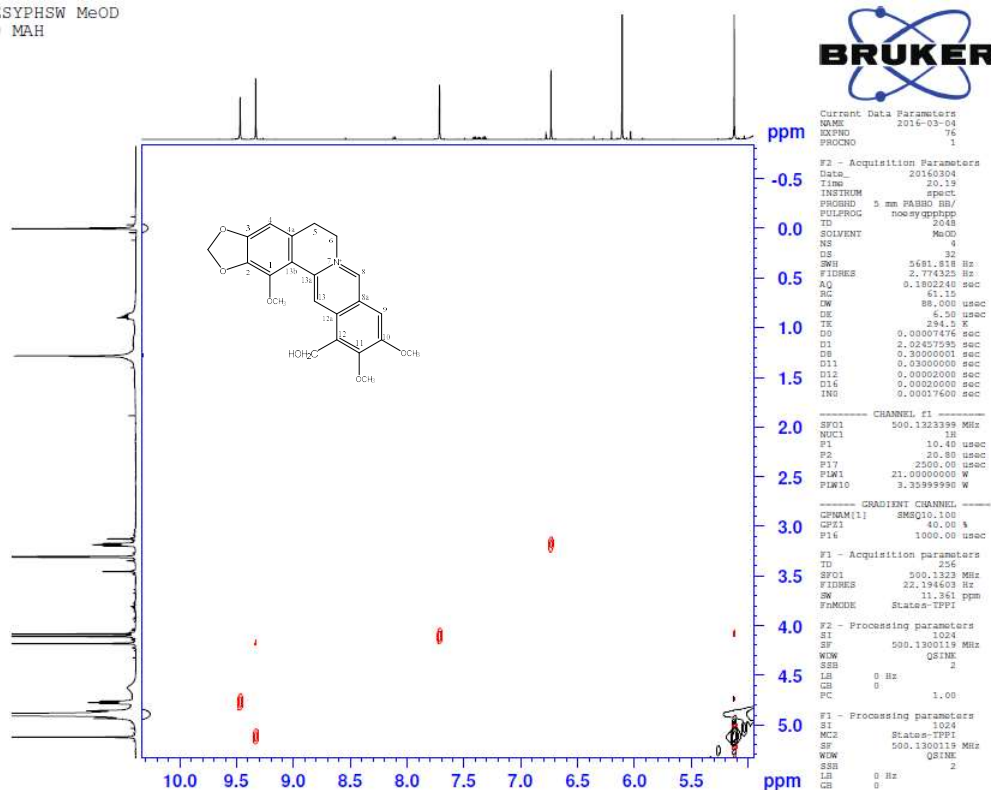
S59: NOSY (500 MHz) Spectrum of Compound 4 (alborine)

NOESYPSHW MeOD
F30 MAH



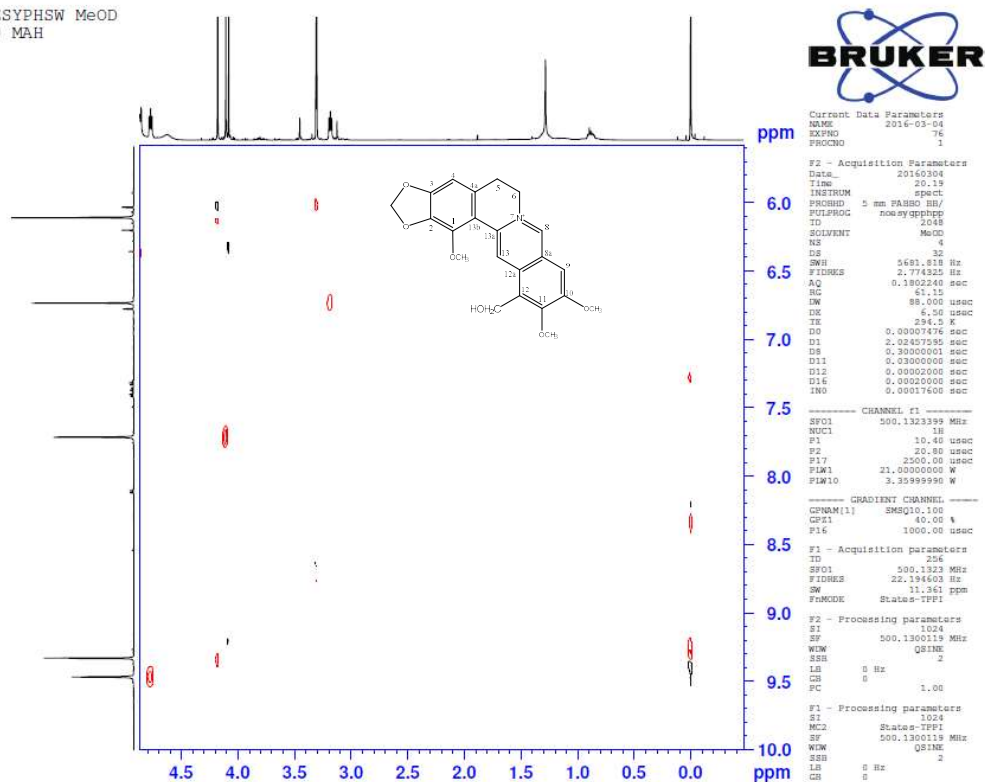
S60: Expansion of the NOSY (500 MHz) Spectrum of Compound 4 (alborine)

ESYPHSW MeOD
0 MAH



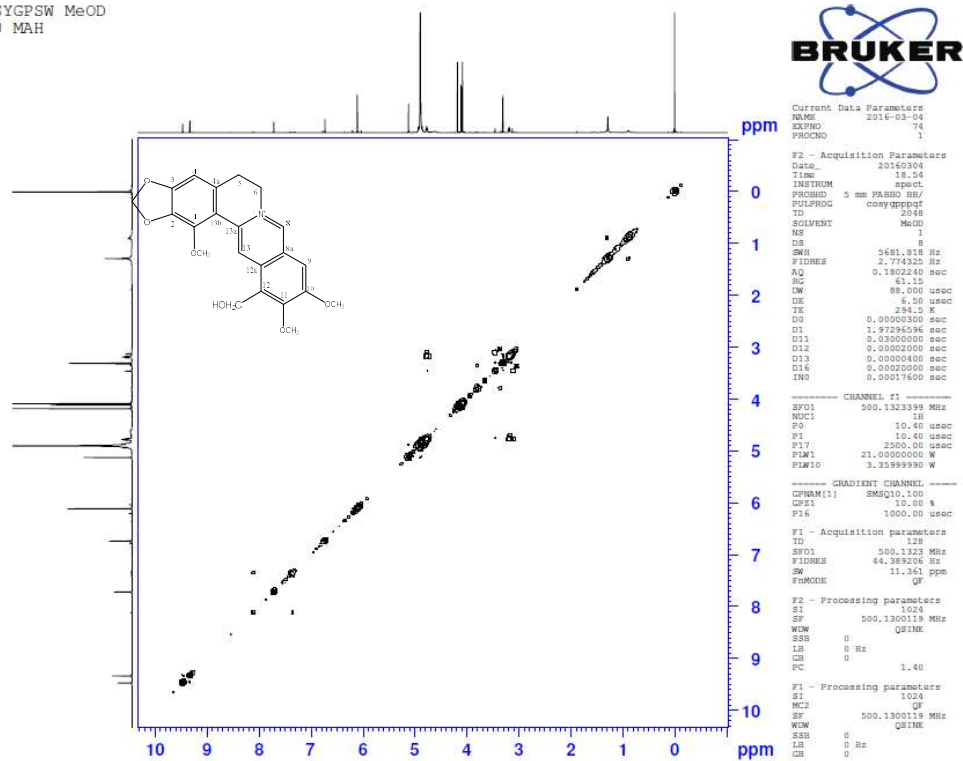
S61: Expansion of the NOSY (500 MHz) Spectrum of Compound 4 (alborine)

ESYPHSW MeOD
0 MAH



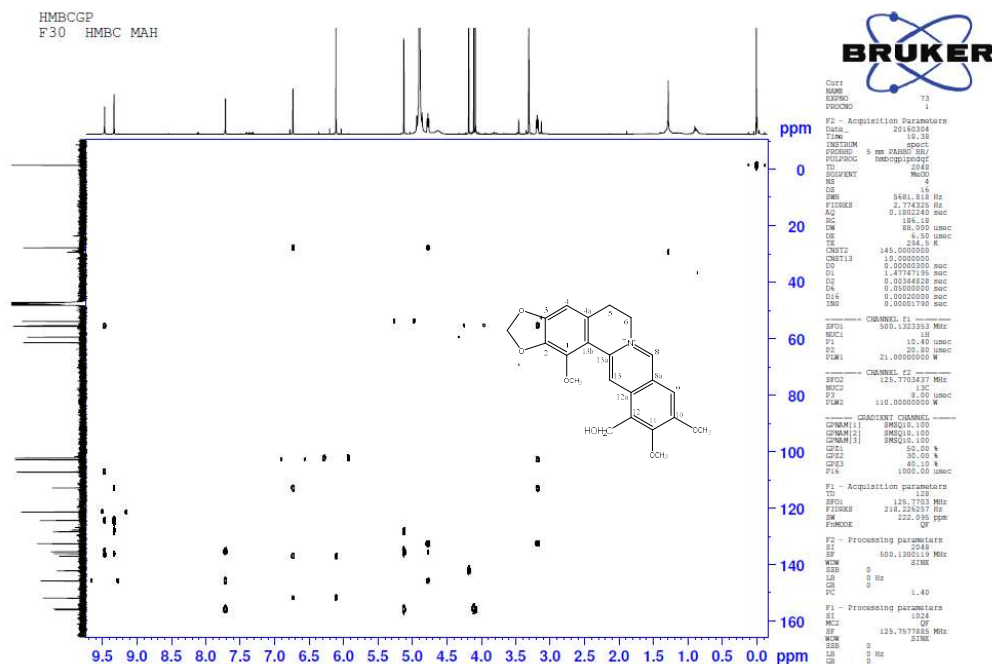
S62: Expansion of the NOSY (500 MHz) Spectrum of Compound 4 (alborine)

COSYGPSW MeOD
F30 MAH

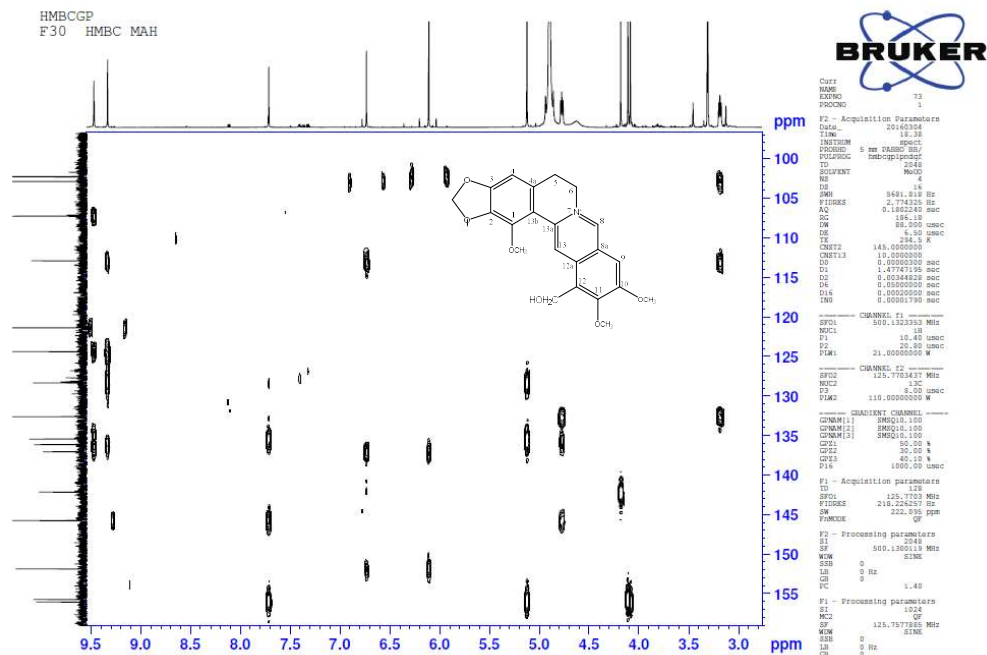


S63: COSY (500 MHz) Spectrum of Compound 4 (alborine)

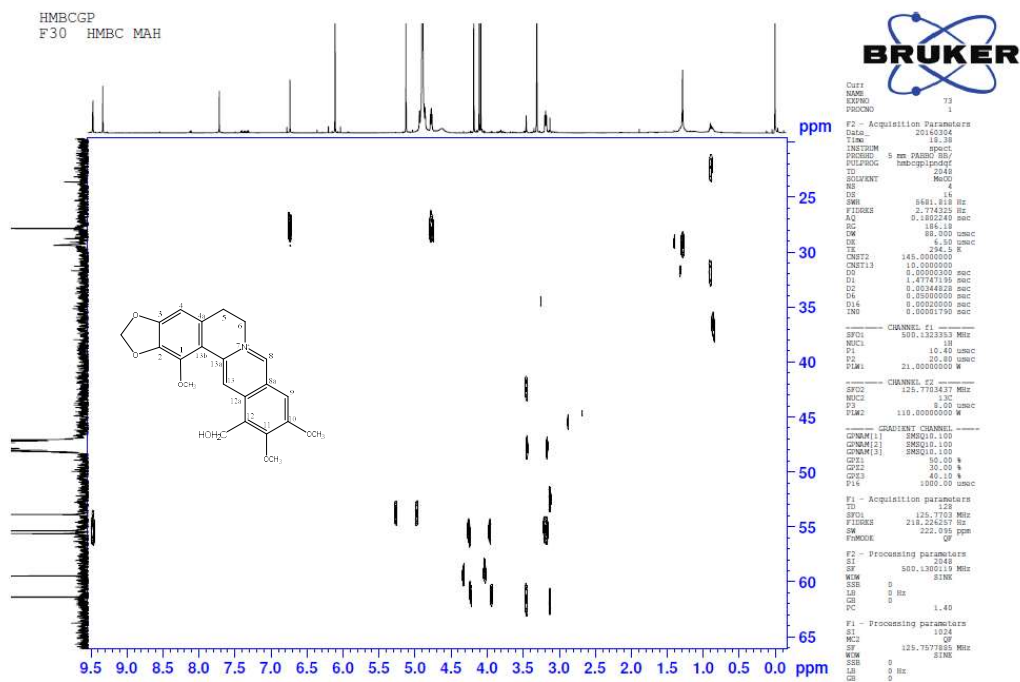
HMBGCP
F30 HMBC MAH



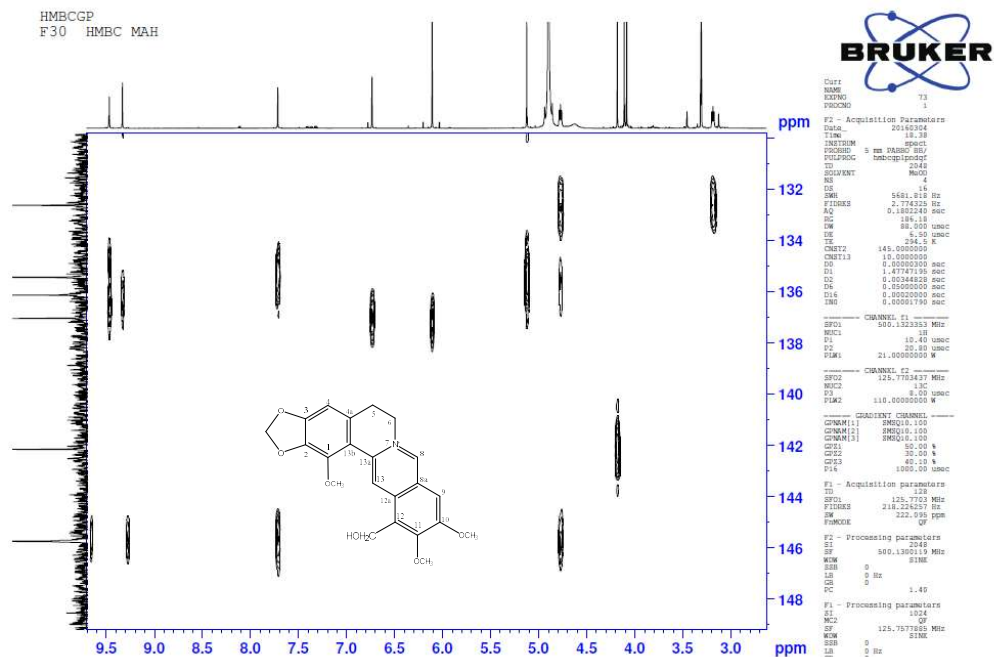
S64: HMBC (500 MHz, CDCl₃) Spectrum of Compound 4 (alborine)



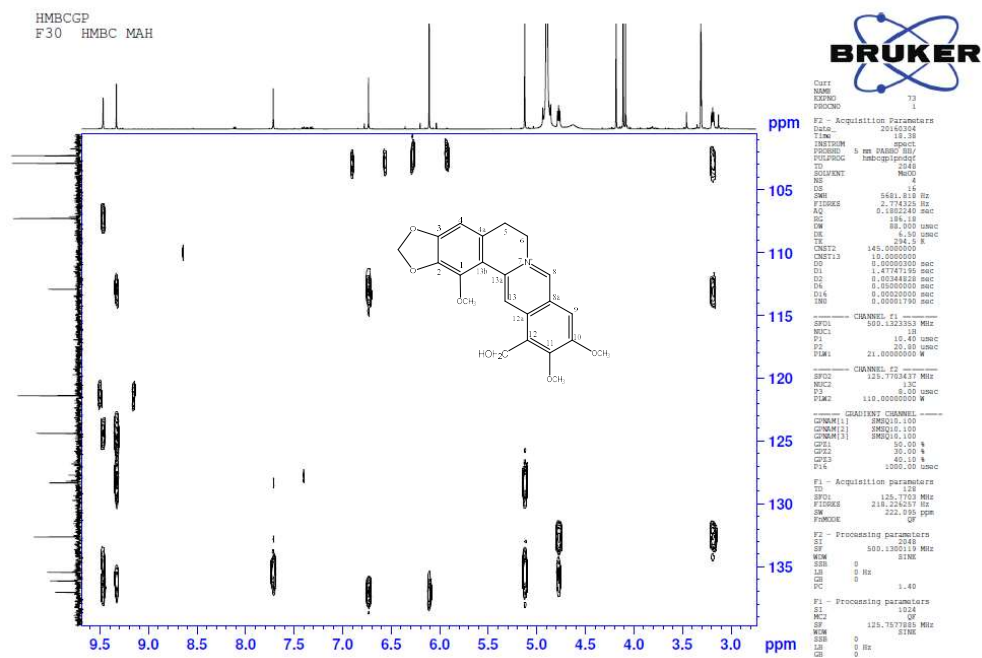
S65: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 4 (alborine)



S66: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 4 (alborine)

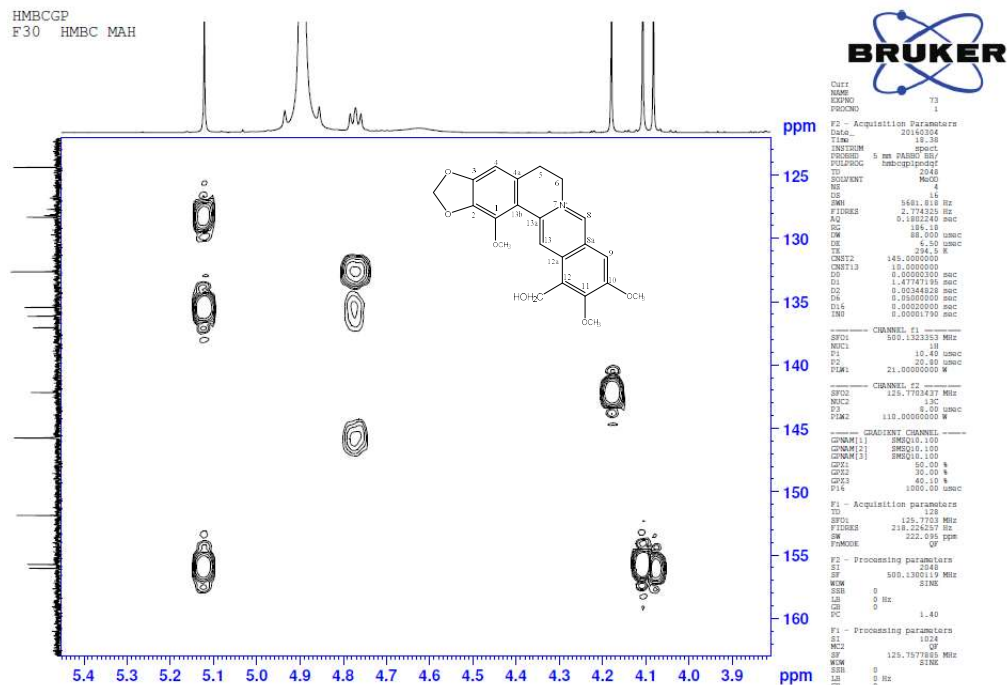


S67: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 4 (alborine)

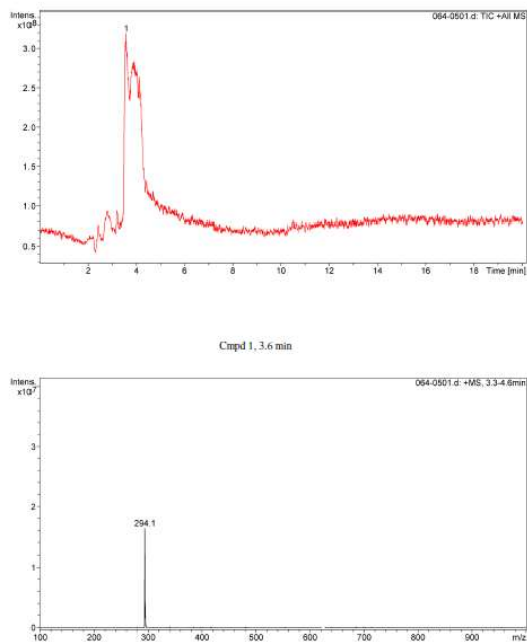


S68: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 4 (alborine)

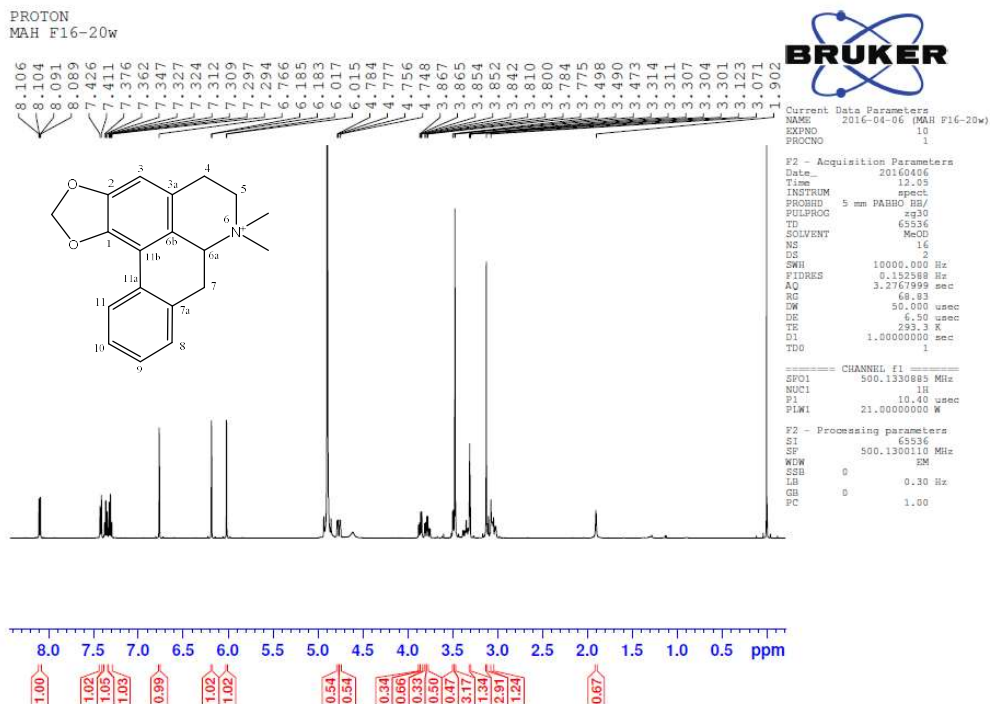




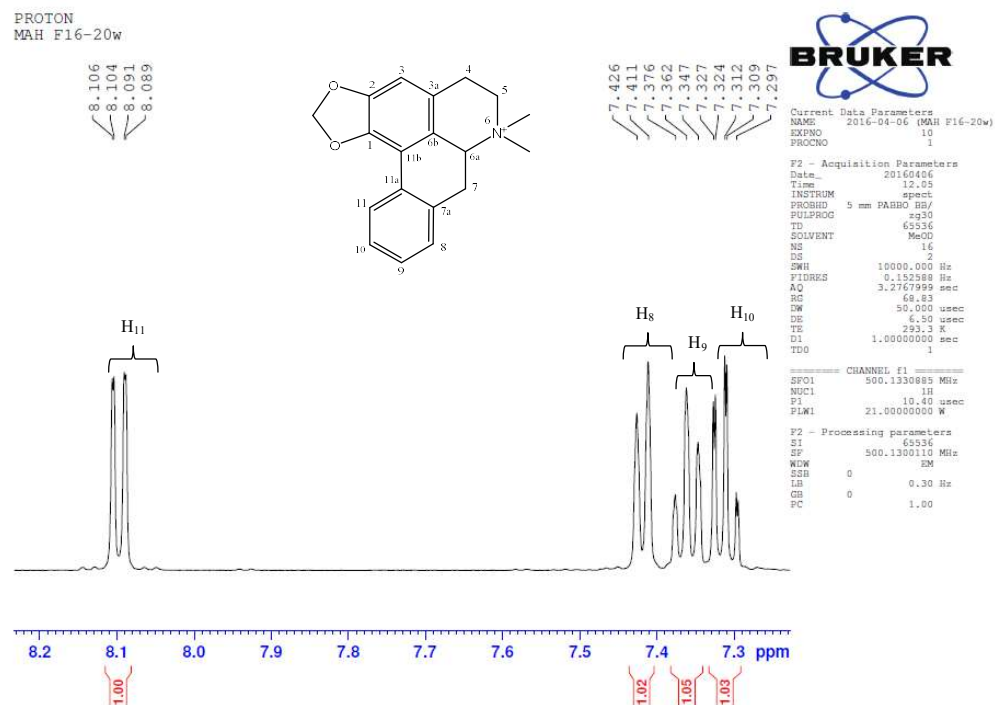
S71: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound **4** (alborine)



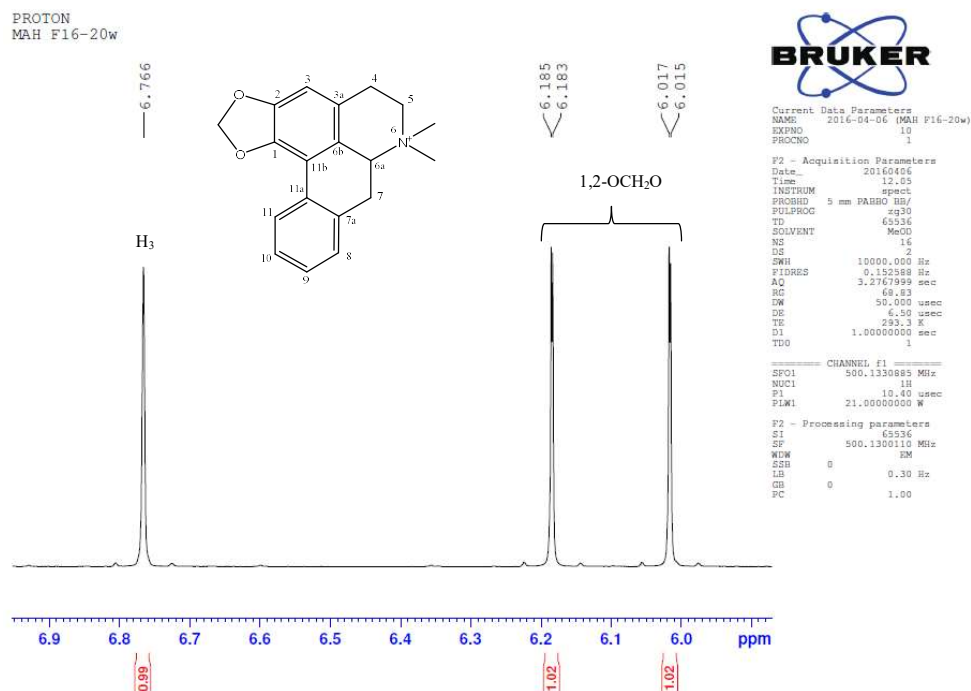
S72: LC-MS Spectrum of Compound **5** (remrefidine)



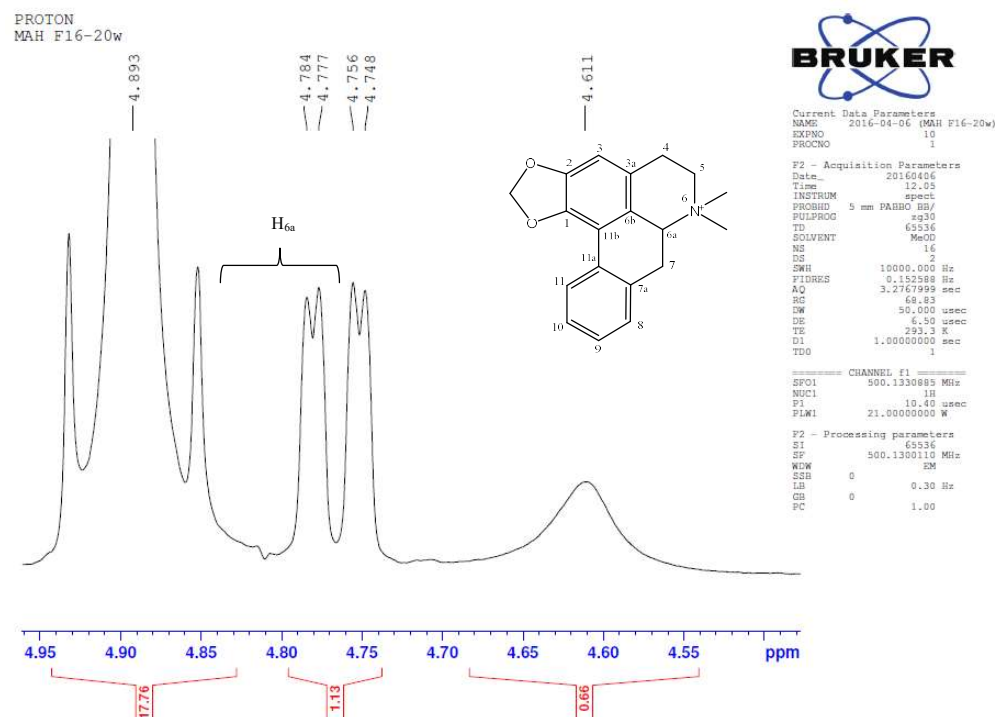
S73: ^1H -NMR (500 MHz, CD_3OD) Spectrum of Compound **5** (remrefidine)



S74: Expansion of the ^1H -NMR (500 MHz) Spectrum of Compound **5** (remrefidine)

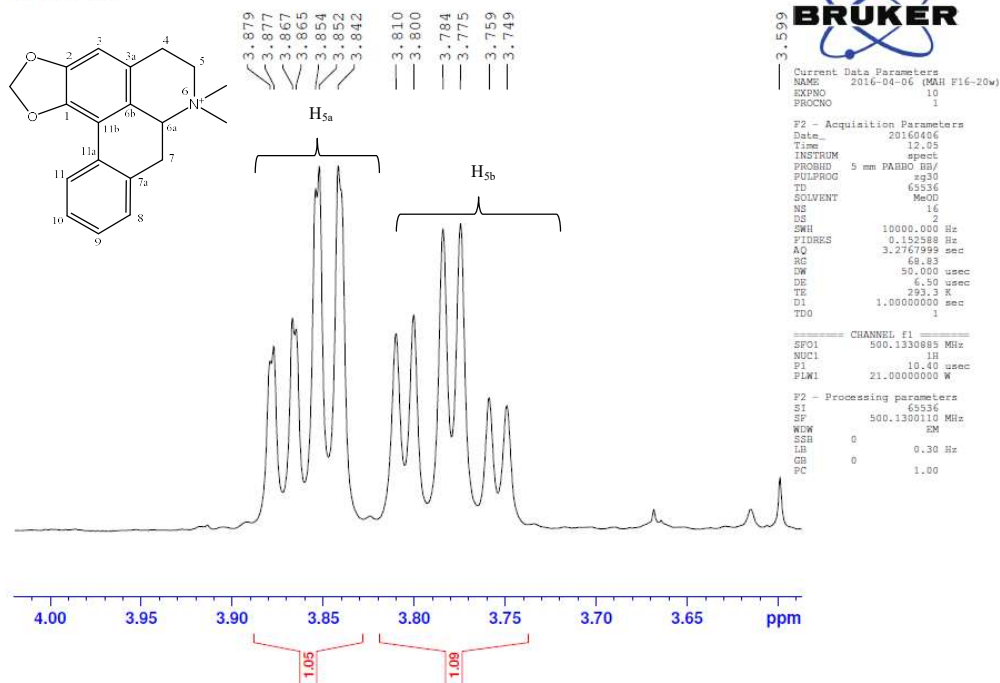


S75: Expansion of the ¹H-NMR (500 MHz) Spectrum of Compound **5** (remrefidine)



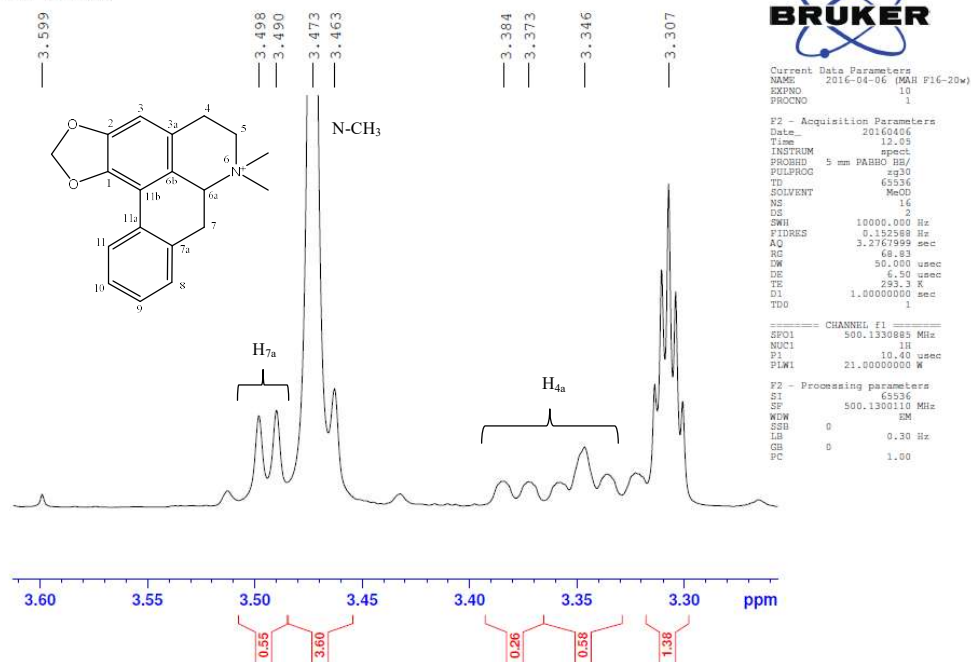
S76: Expansion of the ¹H-NMR (500 MHz) Spectrum of Compound **5** (remrefidine)

PROTON
MAH F16-20w

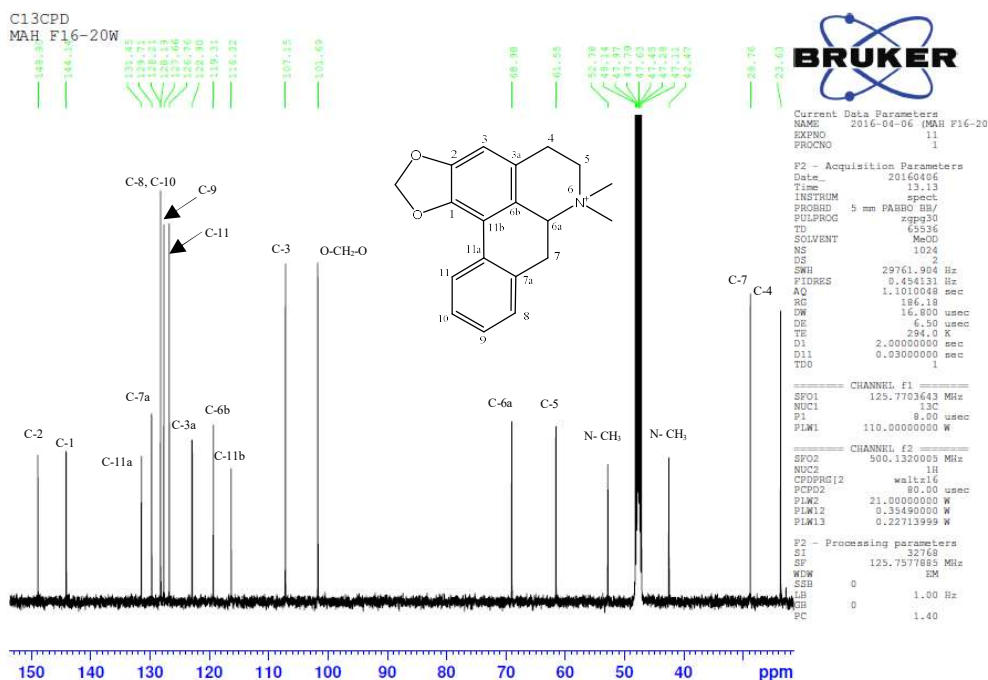


S77: Expansion of the ¹H-NMR (500 MHz) Spectrum of Compound 5 (remrefidine)

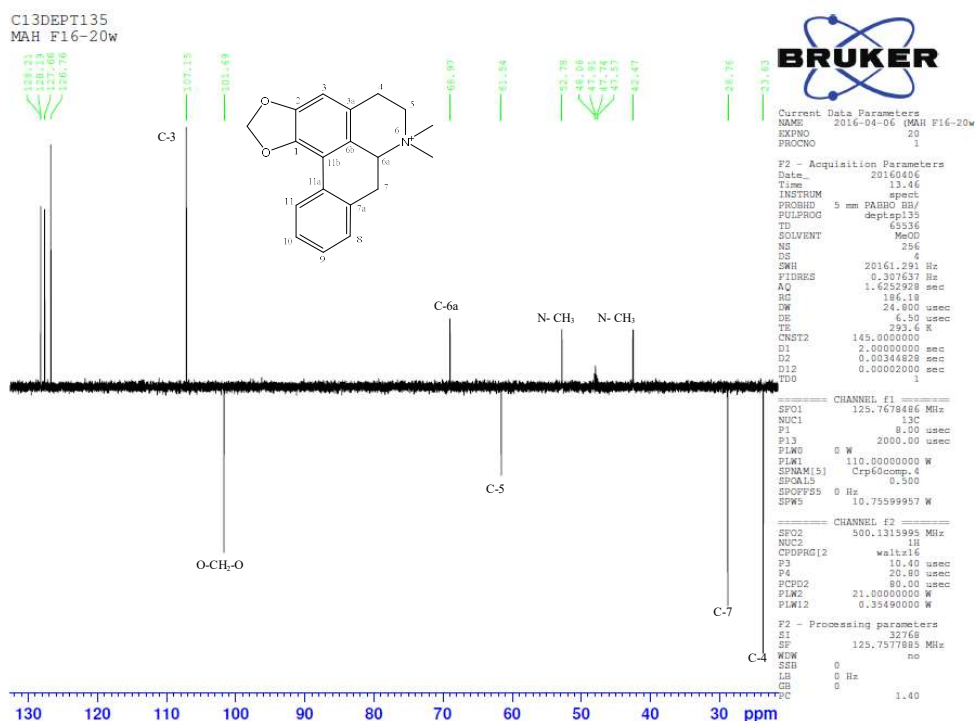
PROTON
MAH F16-20w



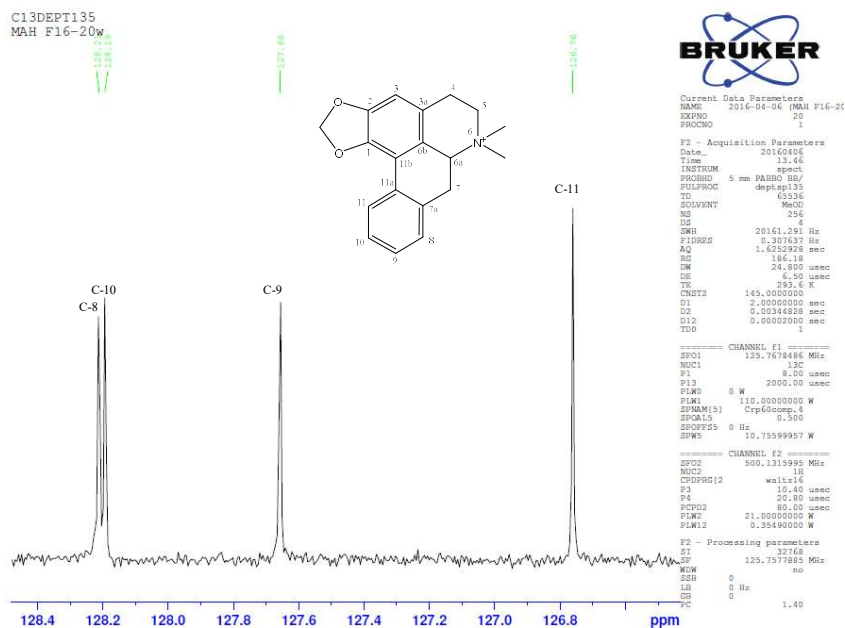
S78: Expansion of the ¹H-NMR (500 MHz) Spectrum of Compound 5 (remrefidine)



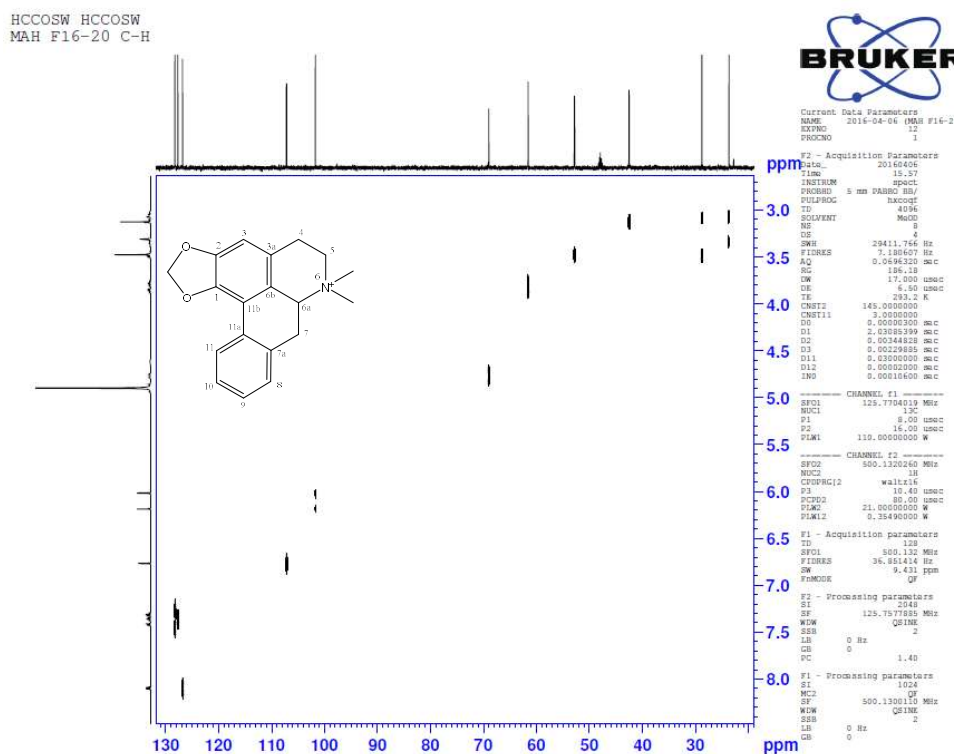
S79: ^{13}C -NMR (500 MHz) Spectrum of Compound **5** (remrefidine)



S80: DEPT (500 MHz) Spectrum of Compound **5** (remrefidine)

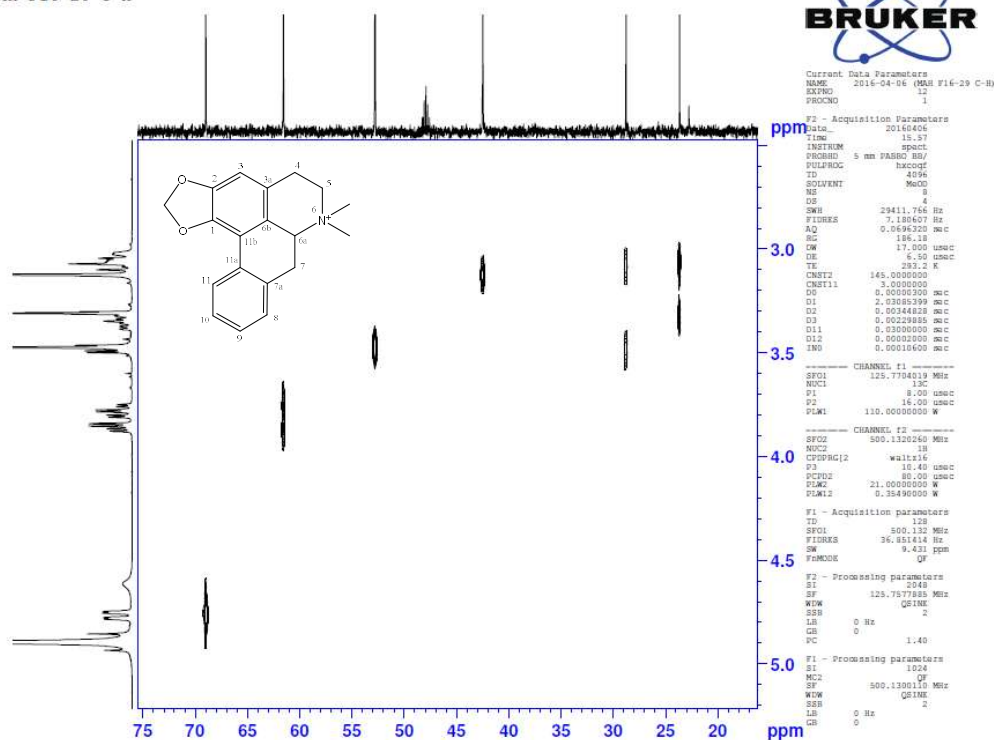


S81: Expansion of the DEPT (500 MHz) Spectrum of Compound **5** (remrefidine)



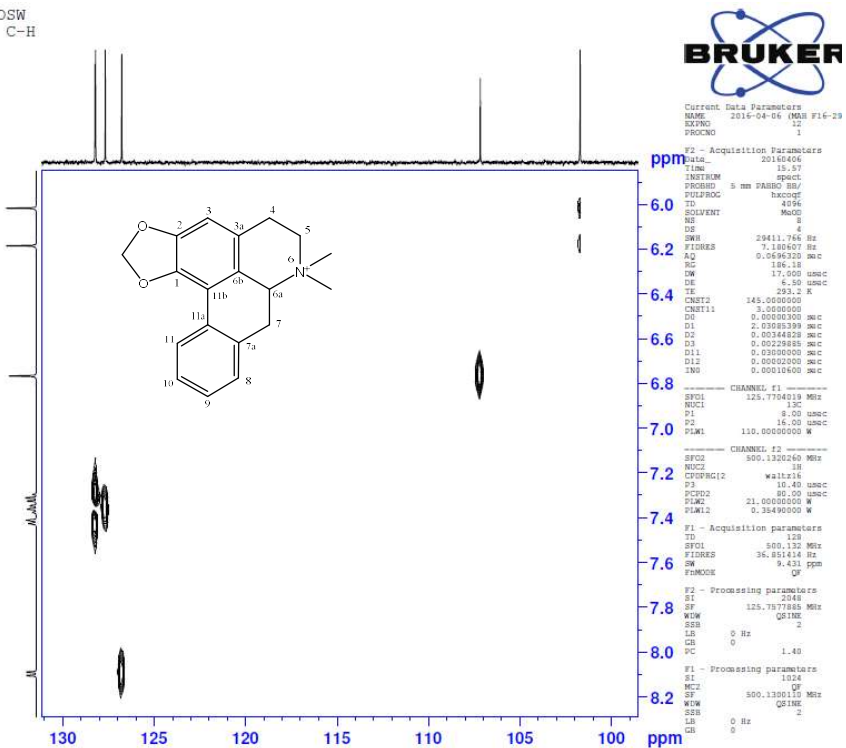
S82: HCCOW Spectrum of Compound **5** (remrefidine)

HCCOSW HCCOSW
MAH F16-20 C-H



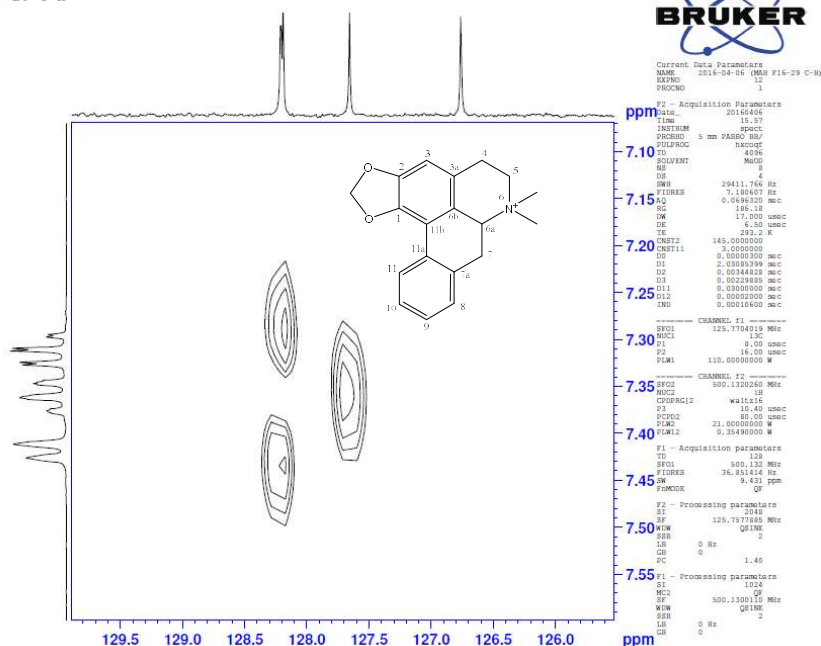
S83: Expansion of the HCCOW Spectrum of Compound **5** (remrefidine)

HCCOSW
6-20 C-H



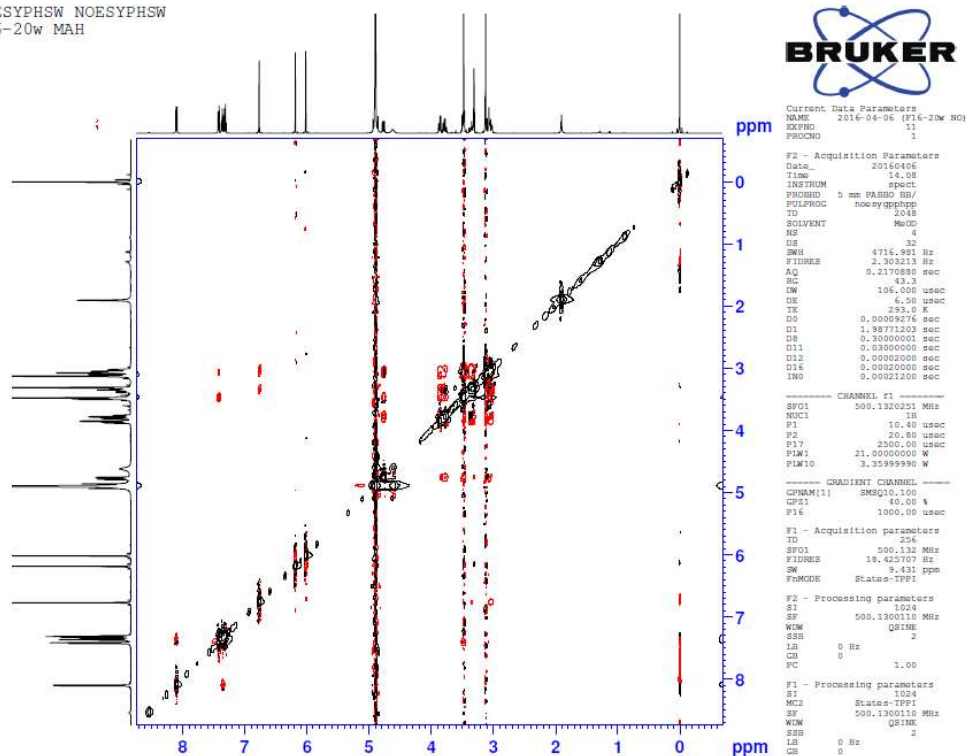
S84: Expansion of the HCCOW Spectrum of Compound **5** (remrefidine)

¹³C HCCOSW
16-20 C-H



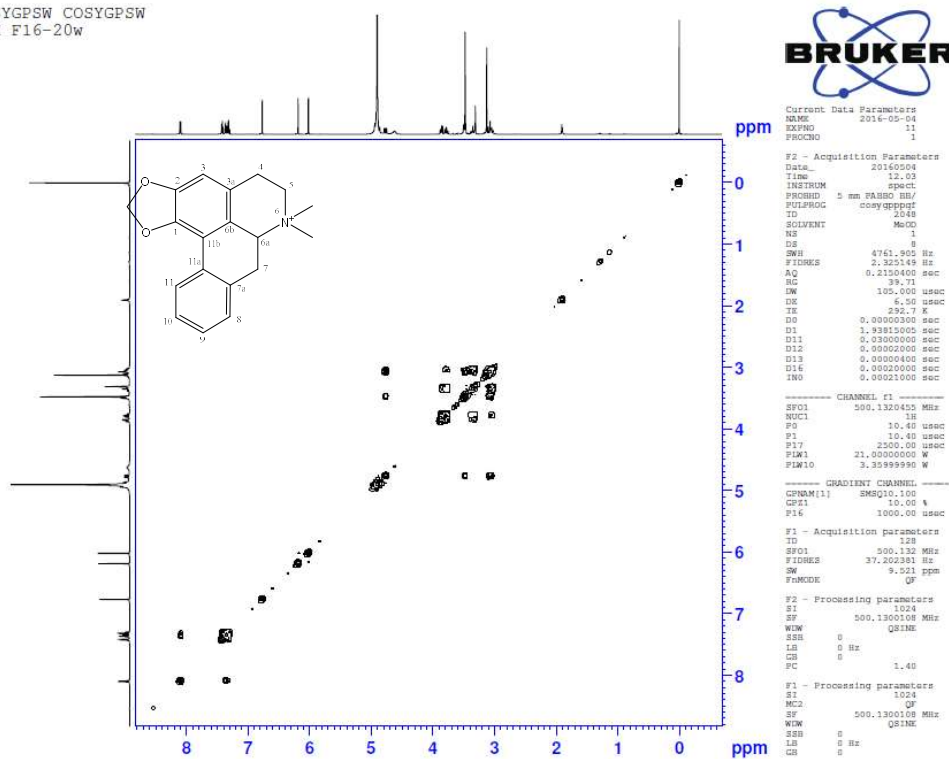
S85: Expansion of the HCCOW Spectrum of Compound **5** (remrefidine)

OESYPSHW NOESYPSHW
16-20w MAH



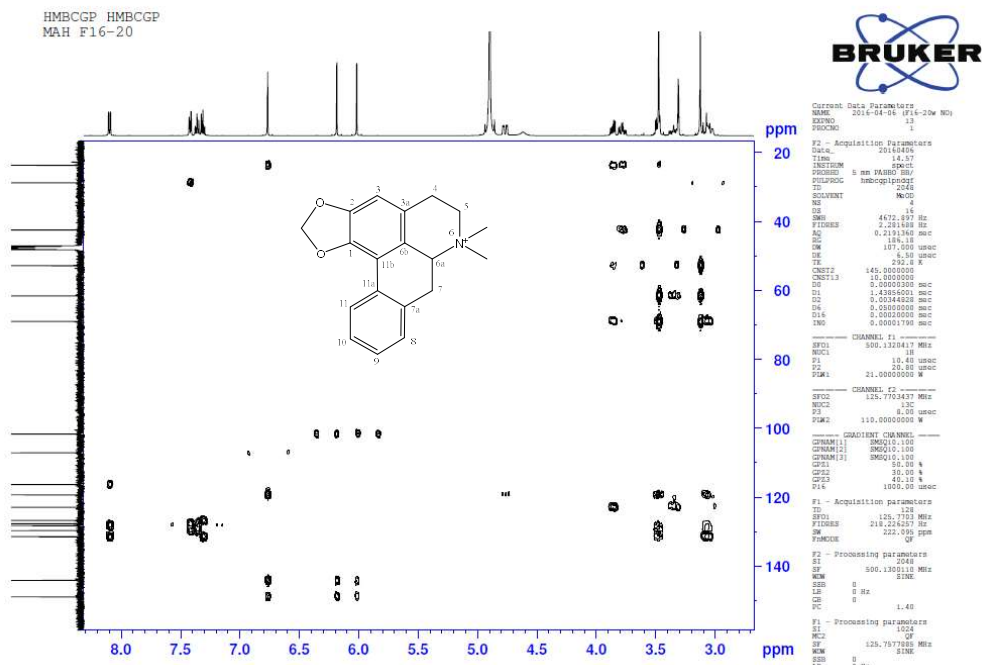
S86: NOSY (500 MHz) Spectrum of Compound **5** (remrefidine)

COSYGPW COSYGPW
MAH F16-20w

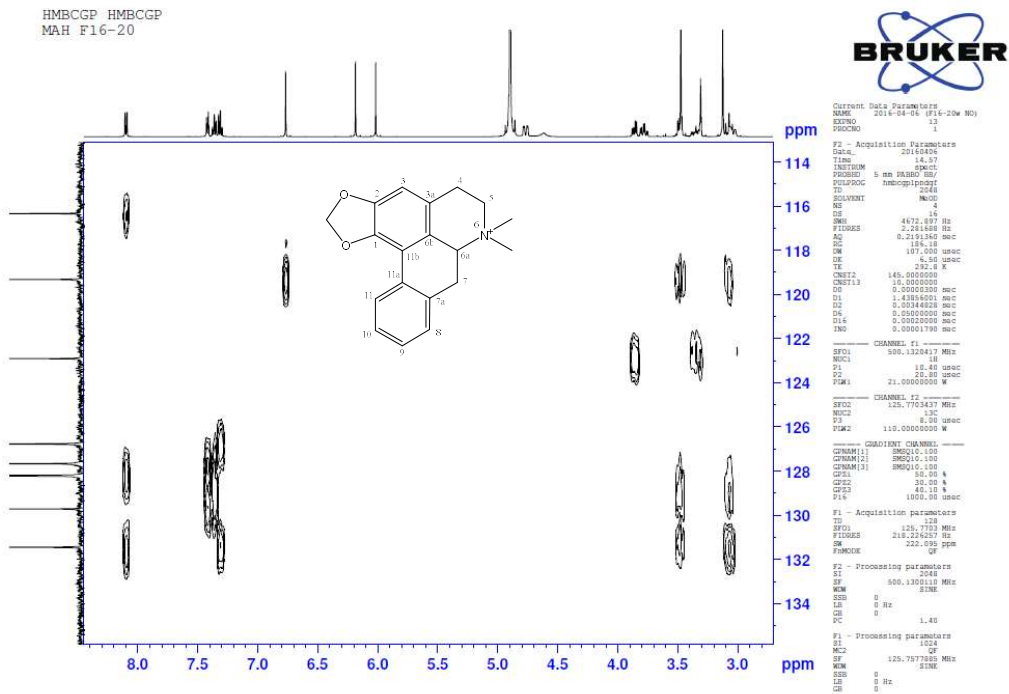


S87: COSY (500 MHz) Spectrum of Compound 5 (remrefidine)

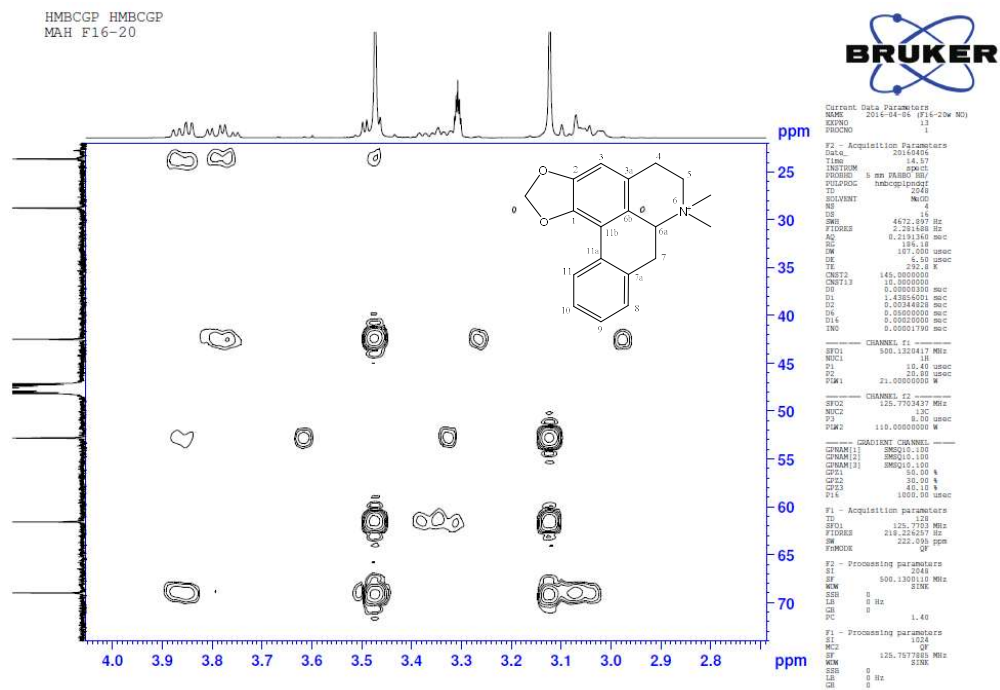
HMBCGP HMBCGP
MAH F16-20



S88: HMBC (500 MHz, CDCl₃) Spectrum of Compound 5 remrefidine)

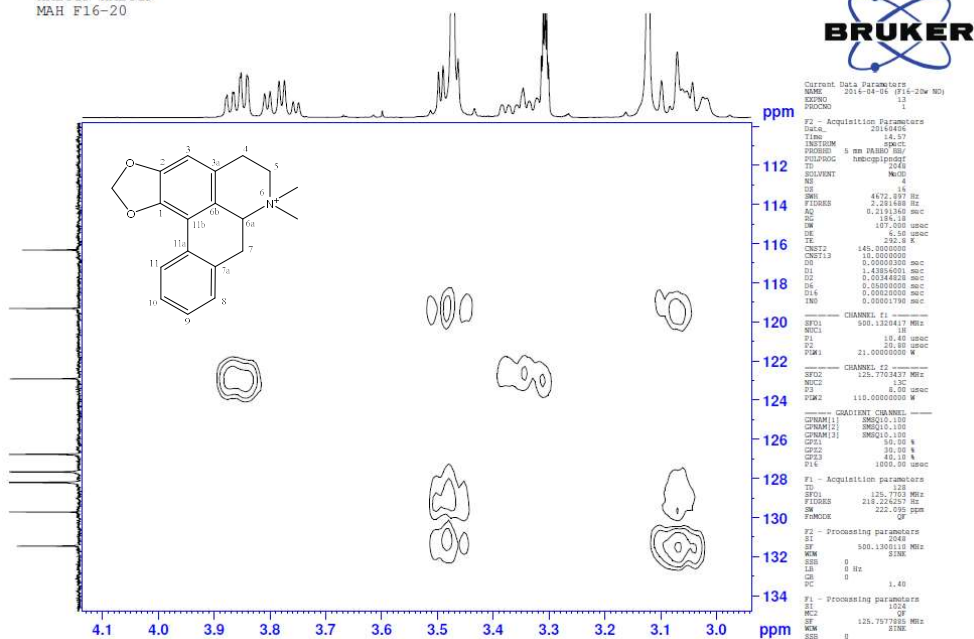


S89: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound **5** (remrefidine)

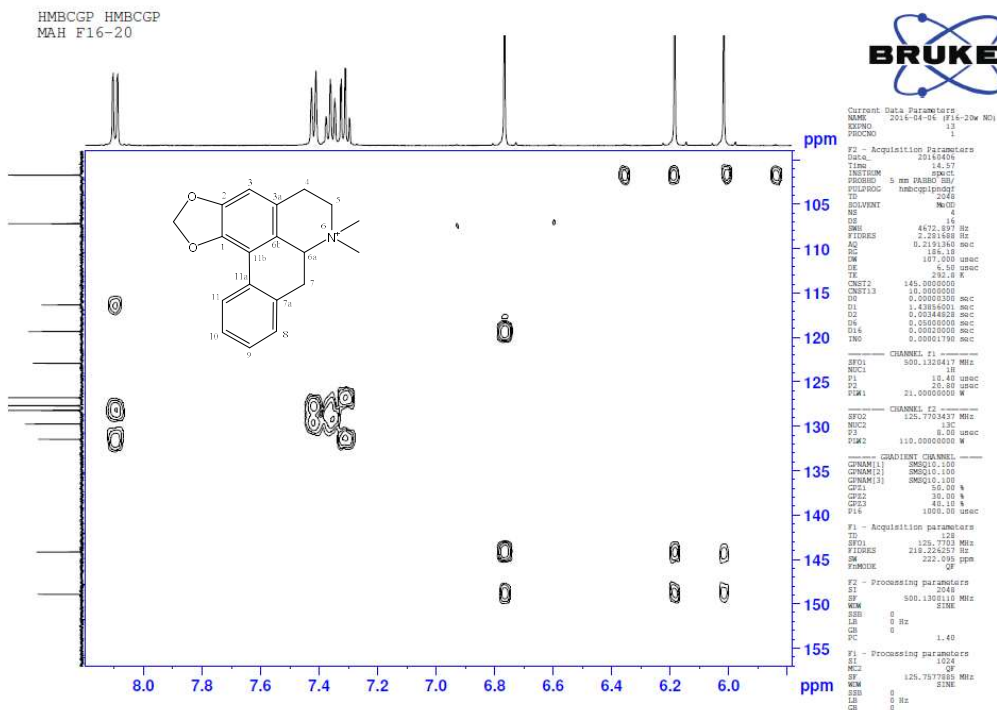


S90: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound **5** (remrefidine)

HMBGCP HMBGCP
MAH F16-20

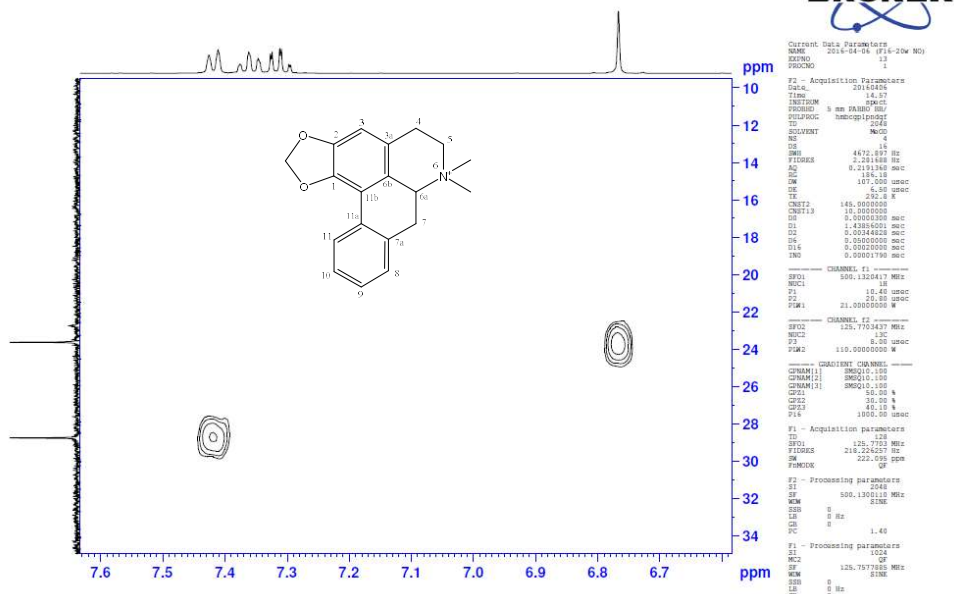


S91: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 5 (remrefidine)



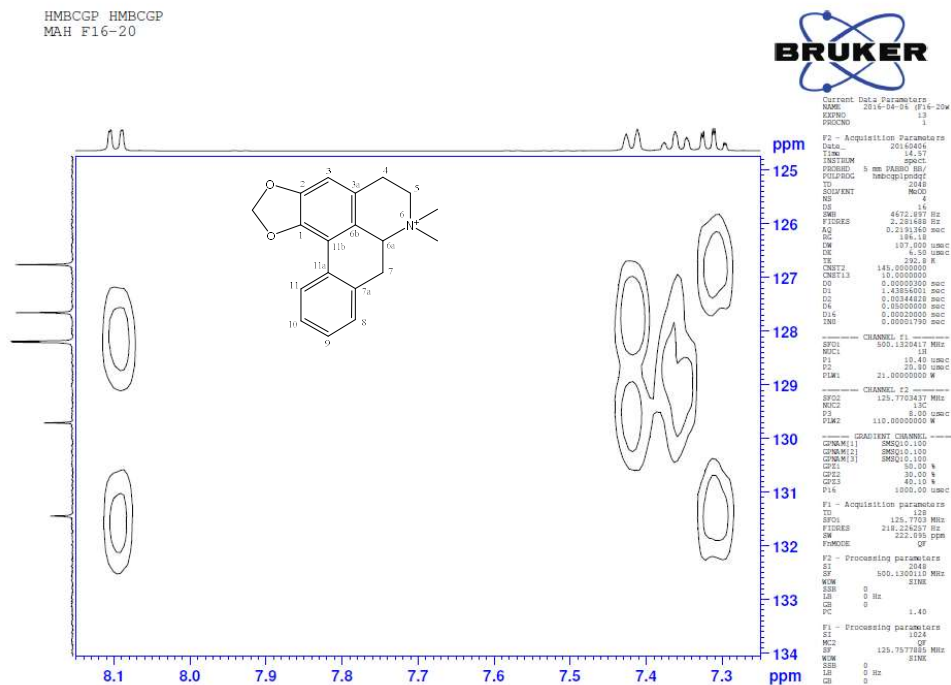
S92: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 5 (remrefidine)

HMBGCP HMBGCP
MAH F16-20

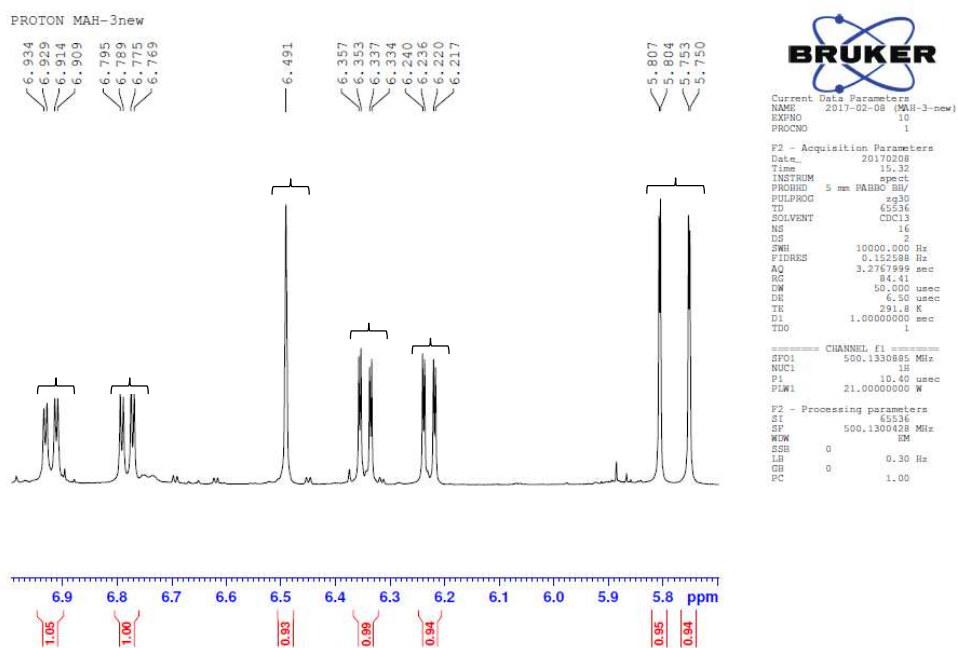
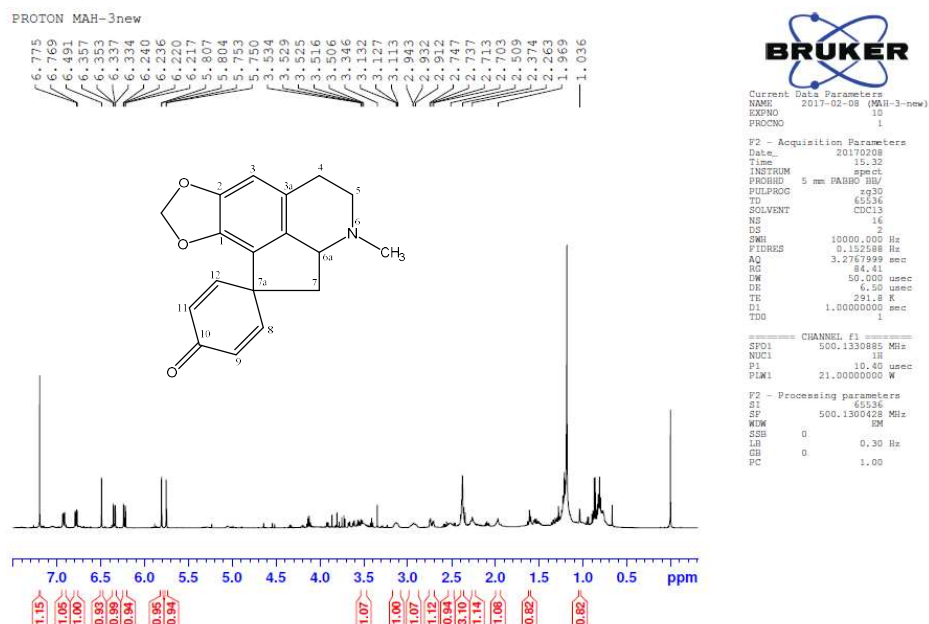


S93: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound **5** (remrefidine)

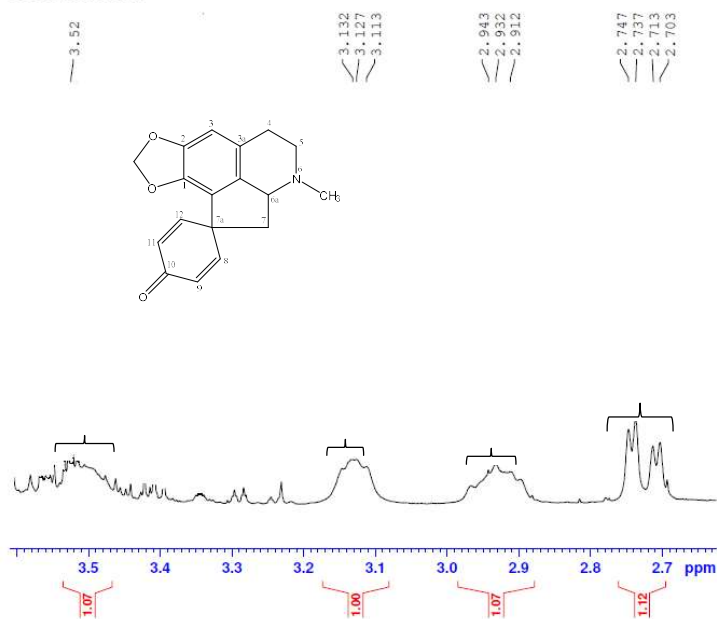
HMBGCP HMBGCP
MAH F16-20



S94: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound **5** (remrefidine)



PROTON MAH-3new



BRUKER

Current Data Parameters
NAME 2017-02-08 (MAH-3-new)
EXPNO 10
PROCNO 1

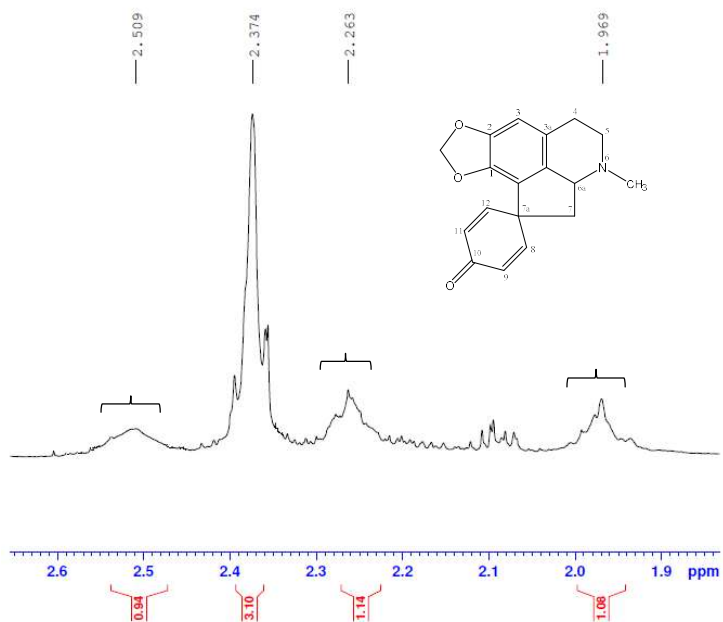
F2 - Acquisition Parameters
Date_ 20170208
Time 15.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 84.41
DW 50.000 usec
DE 6.50 usec
TE 291.8 K
D1 1.0000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 10.40 usec
PLW1 21.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300428 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S97: Expansion of the ^1H -NMR (500 MHz) Spectrum of Compound 6 (mecambrine)

PROTON MAH-3new



BRUKER

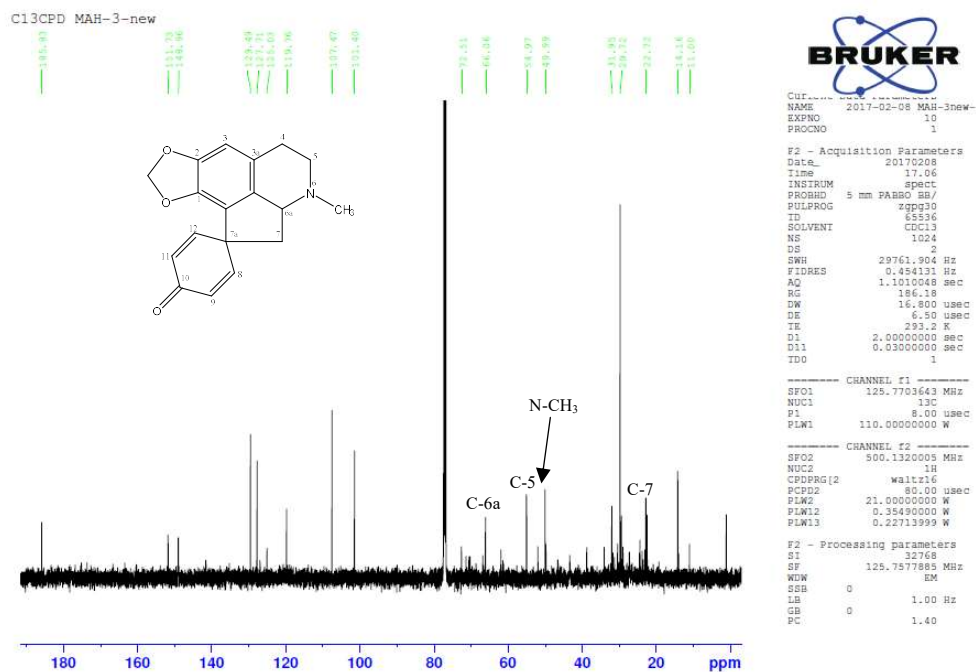
Current Data Parameters
NAME 2017-02-08 (MAH-3-new)
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170208
Time 15.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 84.41
DW 50.000 usec
DE 6.50 usec
TE 291.8 K
D1 1.0000000 sec
TDO 1

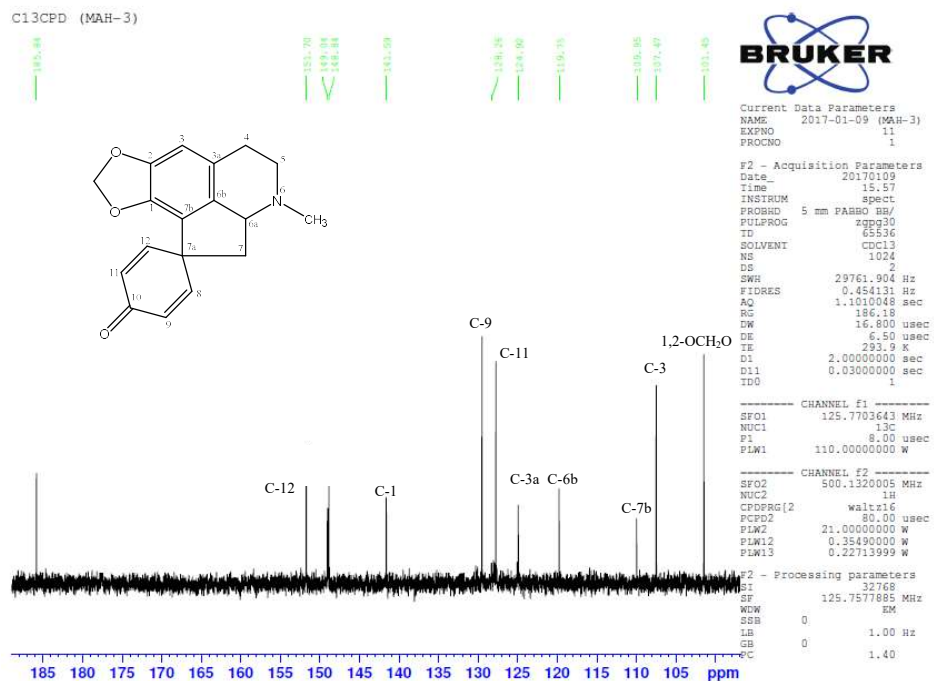
==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 10.40 usec
PLW1 21.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300428 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

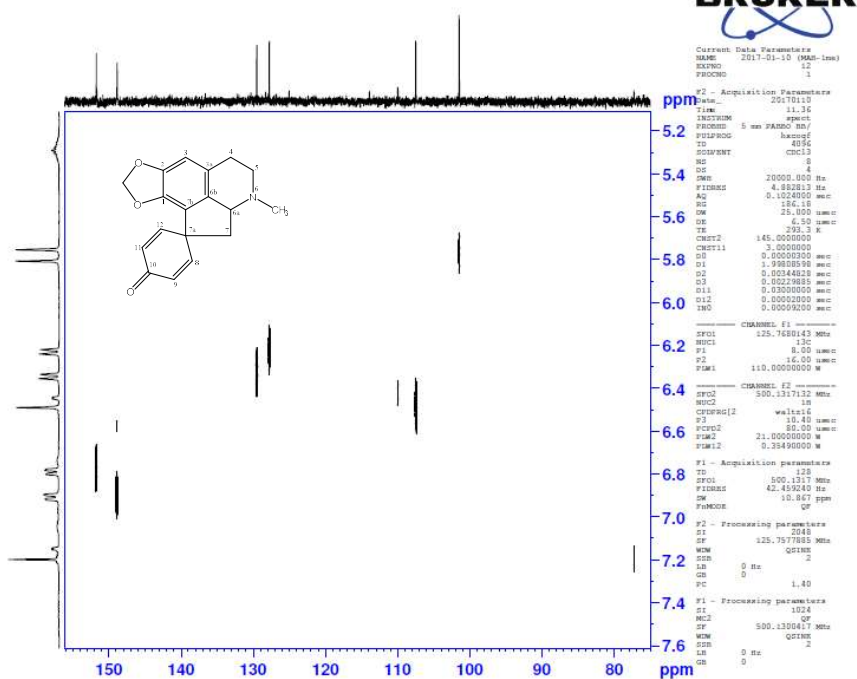
S98: Expansion of the ^1H -NMR (500 MHz) Spectrum of Compound 6 (mecambrine)



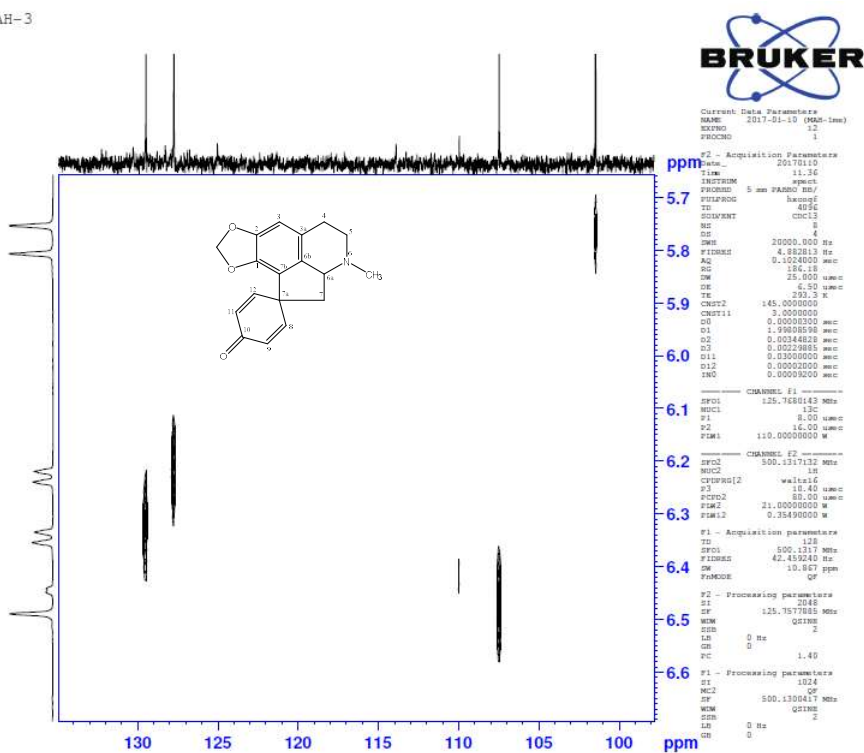
S99: ¹³C-NMR (500 MHz) Spectrum of Compound 6 (mecambrine)



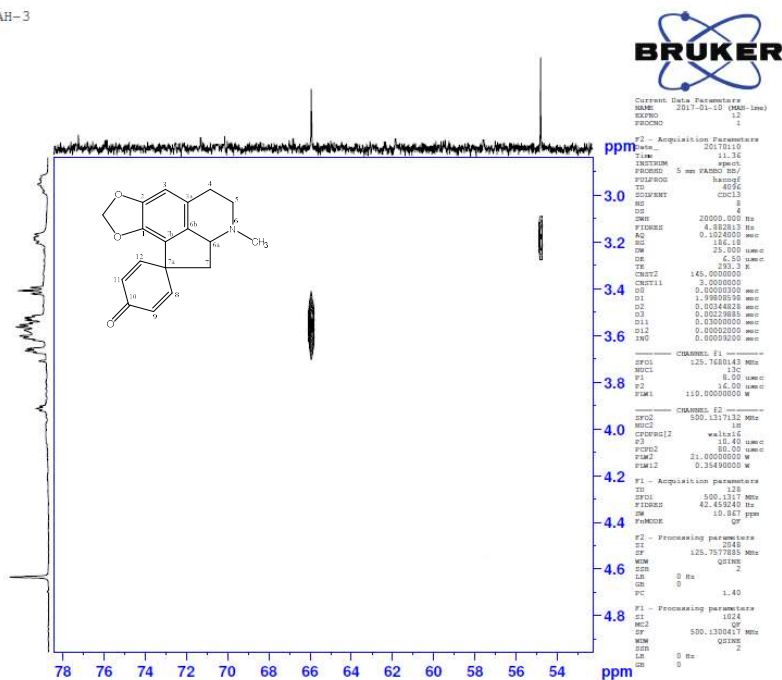
S100: Expansion of the ¹³C-NMR (500 MHz) Spectrum of Compound 6 (mecambrine)



S103: Expansion of the HCCOW Spectrum of Compound 6 (mecambrine)

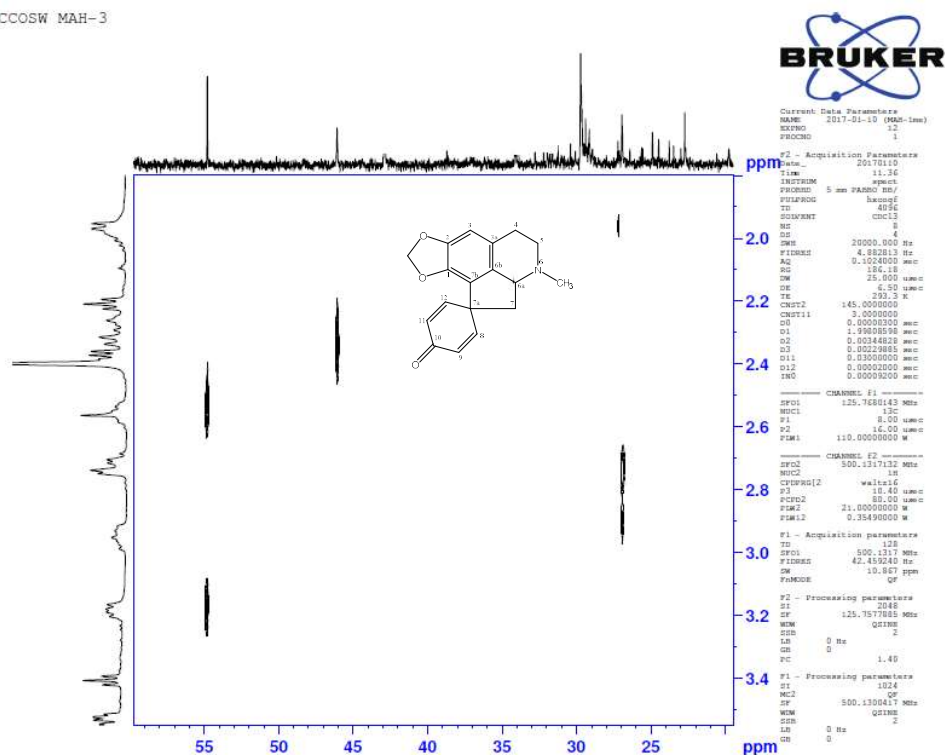


S104: Expansion of the HCCOW Spectrum of Compound 6 (mecambrine)



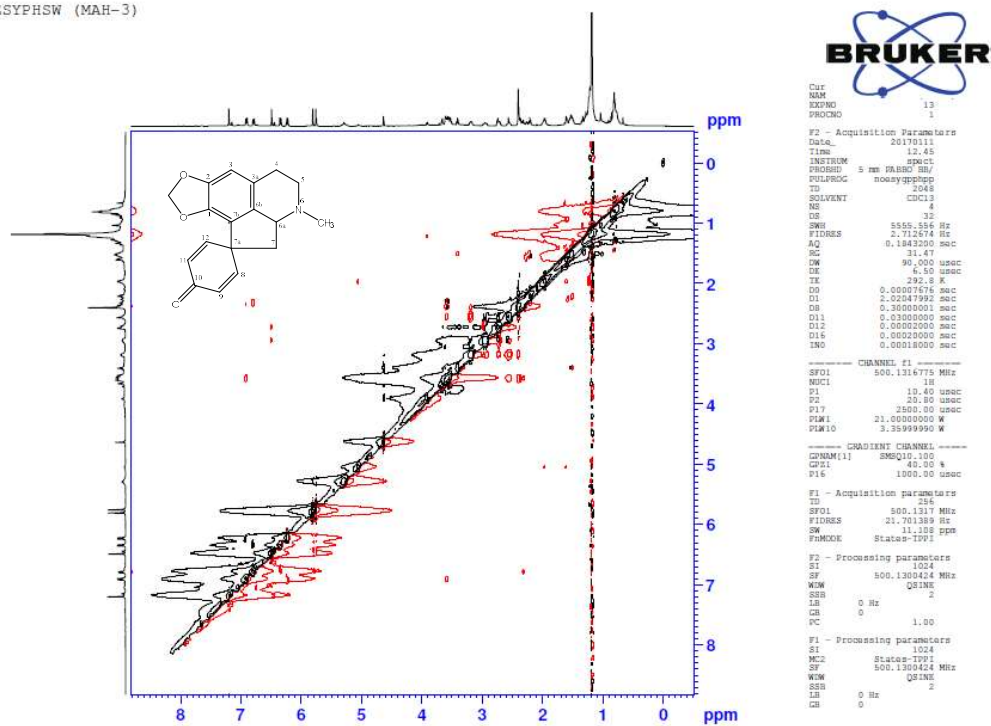
S105: Expansion of the HCCOW Spectrum of Compound 6 (mecambrine)

HCCOSW MAH-3



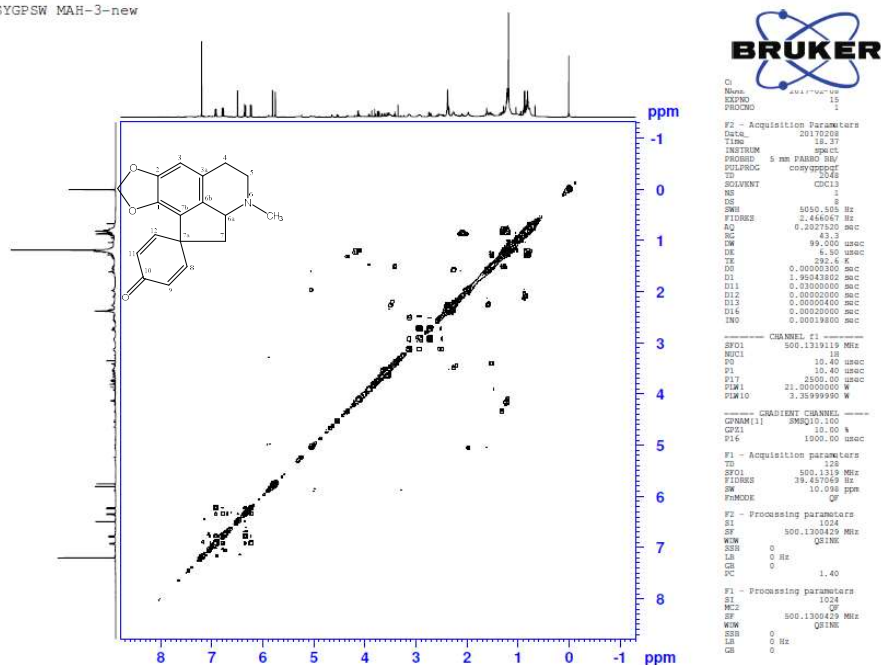
S106: Expansion of the HCCOW Spectrum of Compound 6 (mecambrine)

NOESYPSHW (MAH-3)

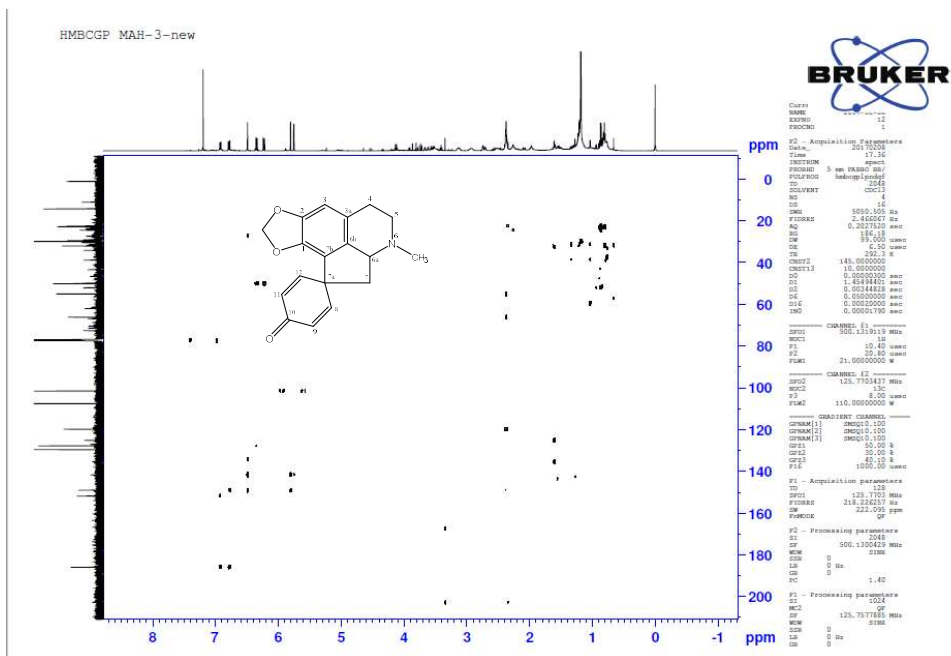


S107: NOSY (500 MHz) Spectrum of Compound 6 (mecambrine)

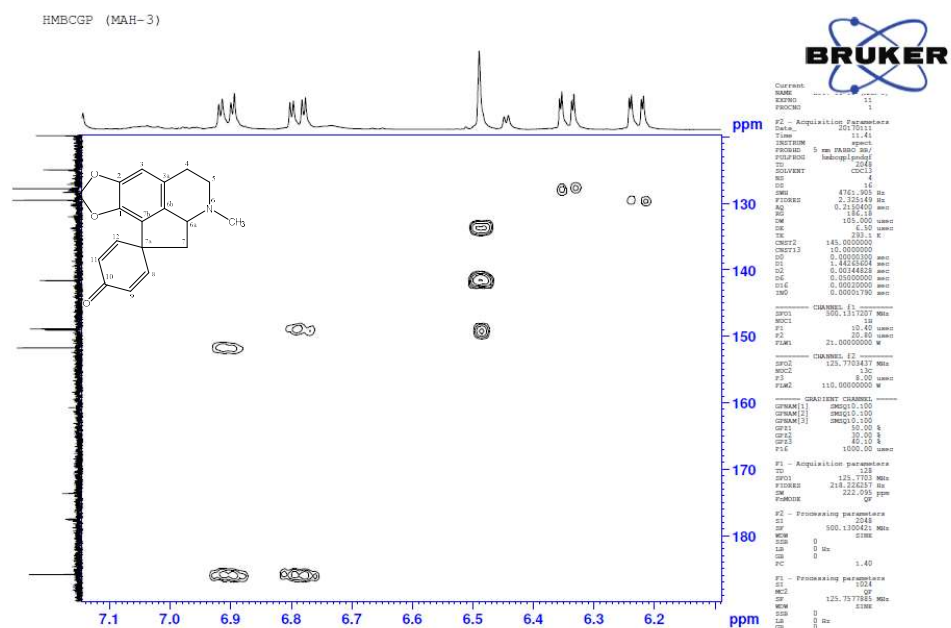
ISYGPSW MAH-3-new



S108: COSY (500 MHz) Spectrum of Compound 6 (mecambrine)

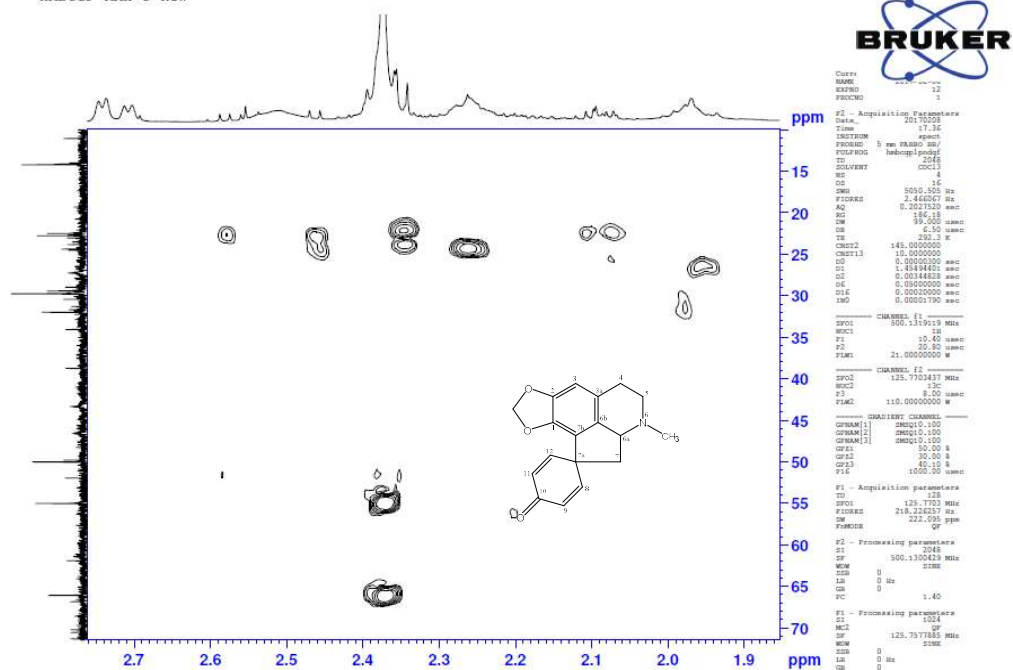


S109: HMBC (500 MHz, CDCl₃) Spectrum of Compound **6** (mecambrine)



S110: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound **6** (mecambrine)

HMBCGP MAH-3-new



S111: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound **6** (mecambrine)

S112: ¹H NMR (500MHz) data of isolated compounds (CDCl₃, δ in ppm, J in Hz)

Position (H)	Dehydro- remerine	Roemerine	Alborine	Remrefidine	Mecambrine
1-OCH ₃	--	--	4.17 (3H, s)	--	--
1,2-OCH ₂ O	6.137 (2H, s)	6.01 (1H, d, <i>J</i> =1) 5.864 (1H, d, <i>J</i> =1)	--	6.18 (1H, d, <i>J</i> =1) 6.01 (1H, d, <i>J</i> =1)	5.8 (1H, d, <i>J</i> =1.5) 5.75 (1H, d, <i>J</i> =1.5)
3	6.86 (1H, s)	6.48 (1H, s) ~3.09 (1H, m)	--	6.76 (1H, s) ~3.34 (1H, m)	6.49 (1H, s) ~2.9 (1H, m)
4	3.16 (2H, t, <i>J</i> = 6)	~2.58 (1H, dd, <i>J</i> = 16, 3.5)	6.72 (1H, s)	~3.05 (1H, m) ~3.86 (1H, ddd, <i>J</i> =12.5, 6, 1)	~2.7 (1H, dd, <i>J</i> =17, 5) ~2.5 (1H, m)
5	3.28 (2H, t, <i>J</i> = 6)	~3.04 (1H, m) ~2.51 (1H, m)	3.17 (2H, t, <i>J</i> =6)	~3.78 (1H, dt, <i>J</i> =12.5, 5)	~3.12 (1H, m)
6	3.01 (3H, s)	2.51 (3H,s)	4.76 (2H, t, <i>J</i> =6)	3.47 (3H,s) 3.12 (3H, s)	2.37 (3H, s)
6a	--	3.19 (1H, br.d, <i>J</i> =14)	--	4.76 (1H, dd, <i>J</i> =14, 4)	3.52 (1H, m)
7	6.49 (1H, s)	~3.10 (1H, dd, <i>J</i> =18, 4.5) ~2.67 (1H, t, <i>J</i> = 14)	--	~3.48 (1H, dd, <i>J</i> =14, 4) ~3.06 (1H, m)	~2.2 (1H, m) ~1.96 (1H, m)
8	7.54 (1H, d, <i>J</i> =8)	7.19 (1H, m)	9.46 (1H, s)	7.48 (1H, br.d, <i>J</i> =7.5)	6.93 (1H, dd, <i>J</i> =10, 2.5)
9	7.37 (1H, dt, <i>J</i> = 1, 7)	7.24 (1H, t, <i>J</i> = 7)	7.7 (1H, d, <i>J</i> =15)	7.36 (1H, br.t, <i>J</i> =7.5)	6.35 (1H, dd, <i>J</i> =10, 2.5)
10	7.24 (1H, t, <i>J</i> = 7.5)	7.16 (1H, t, <i>J</i> = 7)	--	7.31 (1H, dt, <i>J</i> =7.5, 1.5)	--
11	8.82 (1H, d, <i>J</i> = 8.5)	7.99 (1H, d, <i>J</i> = 7.5)	--	8.09 (1H, dd, <i>J</i> =7.5, 1)	6.23 (1H, dd, <i>J</i> =10, 3)
12	--	--	--	--	6.79 (1H, dd, <i>J</i> =10, 3)

10-OCH ₃	--	--	4.1 (3H, s)	--	--
11-OCH ₃	--	--	4.07 (3H, s)	--	--
12-CH ₂ OH	--	--	5.11 (2H, s)	--	--
13	--	--	9.32 (1H, s)	--	--
2,3-OCH ₂ O	--	--	6.1 (2H, s)	--	--

S113: ¹³C NMR (500MHz) data of isolated compounds (CDCl₃, δ in ppm)

Position (C)	Dehydroremerine	Roemerine	Alborine	Remrefidine	Mecambrine
1	142.15 (C)	142.73 (C)	142.15 (C)	144.14 (C)	141.59 (C)
1a	--	--	--	--	109.9 (C)
1b	--	--	--	--	119.75 (C)
2	145.12 (C)	146.89 (C)	137.04 (C)	148.9 (C)	149.05 (C)
3	107.43 (CH)	107.49 (CH)	151.94 (C)	107.15 (CH)	107.47 (CH)
3a	127.49 (C)	126.43 (C)	--	122.9 (C)	124.9 (C)
4	30.9 (CH ₂)	28.72 (CH)	102.86 (CH)	23.63 (CH)	27.72 (CH)
4a	--	--	132.8 (C)	--	--
5	50.42 (CH ₂)	53.41 (CH ₂)	27.84 (CH ₂)	61.54 (CH ₂)	54.8 (CH ₂)
6	40.4 (N-CH ₃)	43.42 (N-CH ₃)	55.35 (CH ₂)	52.78 (N-CH ₃) 42.77 (N-CH ₃)	49.9 (N-CH ₃)
6a	127.41 (C)	61.98 (CH)	--	68.97 (CH)	65.9 (CH)
6b	119.07 (C)	126.24 (C)	--	119.3 (C)	
7	101.15 (CH)	34.34 (CH ₂)	--	28.76 (CH ₂)	22.7 (CH ₂)
7a	134.15 (C)	135.07 (C)	--	129.7 (C)	46.1 (C)
8	125.83 (CH)	128.24 (CH)	145.75 (CH)	128.19 (CH)	149.96 (CH)
8a	--	--	124.3 (C)	--	--
9	126.98 (CH)	127.12 (CH)	107.25 (CH)	127.66 (CH)	129.6 (CH)
10	122.41 (CH)	127.59 (CH)	155.73 (C)	128.21 (CH)	185.8 (CO)
11	126.84 (CH)	126.91 (CH)	156.03 (C)	126.76 (CH)	128.26 (CH)
11a	124.02 (C)	131.01 (C)	--	131.45 (C)	--
11b	117.33 (C)	116.46 (C)	--	116.32 (C)	--
12	--	--	128.19 (C)	--	151.73 (CH)

12a	--	--	135.43 (C)	--	--
13	--	--	121.4 (CH)	--	--
13a	--	--	136.13 (C)	--	--
13b	--	--	112.9 (C)	--	--
1, 2-OCH ₂ O	100.98 (CH ₂)	101.81 (CH ₂)	--	101.69 (CH ₂)	101.4 (CH ₂)
2, 3-OCH ₂ O	--	--	102.26 (CH ₂)	--	--
1-OCH ₃	--	--	59.47 (C)	--	--
10-OCH ₃	--	--	55.6 (C)	--	--
11-OCH ₃	--	--	61.39 (C)	--	--
12-CH ₂ OH	--	--	53.88 (C)	--	--
