

Supporting Information

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Alkaloids of *Papaver libanoticum* and their Cytotoxic Activity

Mohamad Ali Hijazi^{1*}, Maha Aboul-Ela¹, Kamal Bouhadir², Maamoun Fatfat³, Hala Gali-Muhtasib^{3,4} and Abdalla Ellakany¹

¹*Department of Pharmaceutical Sciences, Beirut Arab University, Beirut, Lebanon*

²*Department of Chemistry, American University of Beirut, Beirut, Lebanon*

³*Center for Drug Discovery, Faculty of Medicine, American University of Beirut, Beirut, Lebanon*

⁴*Department of Biology, American University of Beirut, Beirut, Lebanon*

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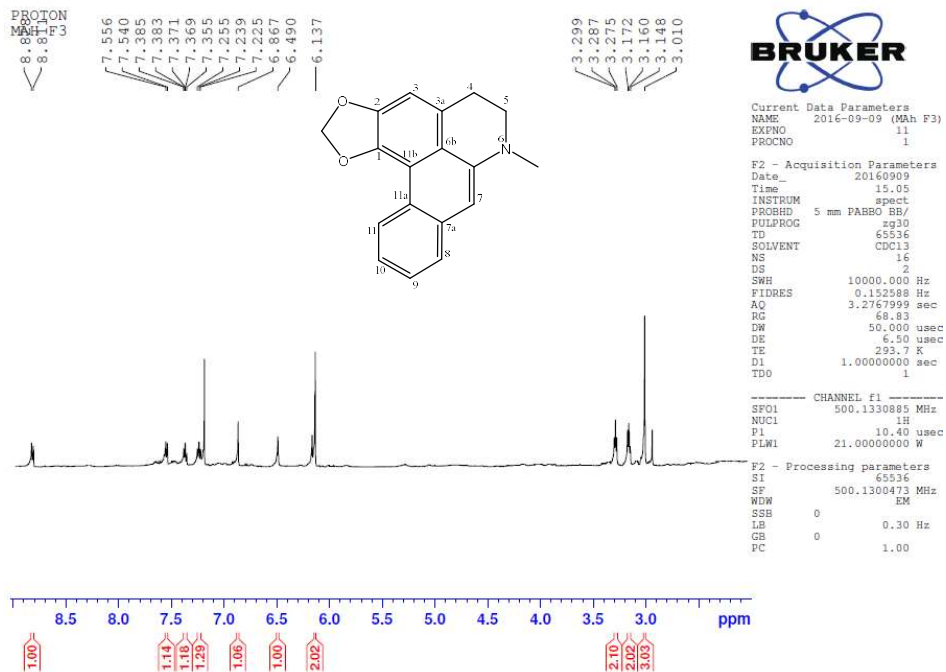
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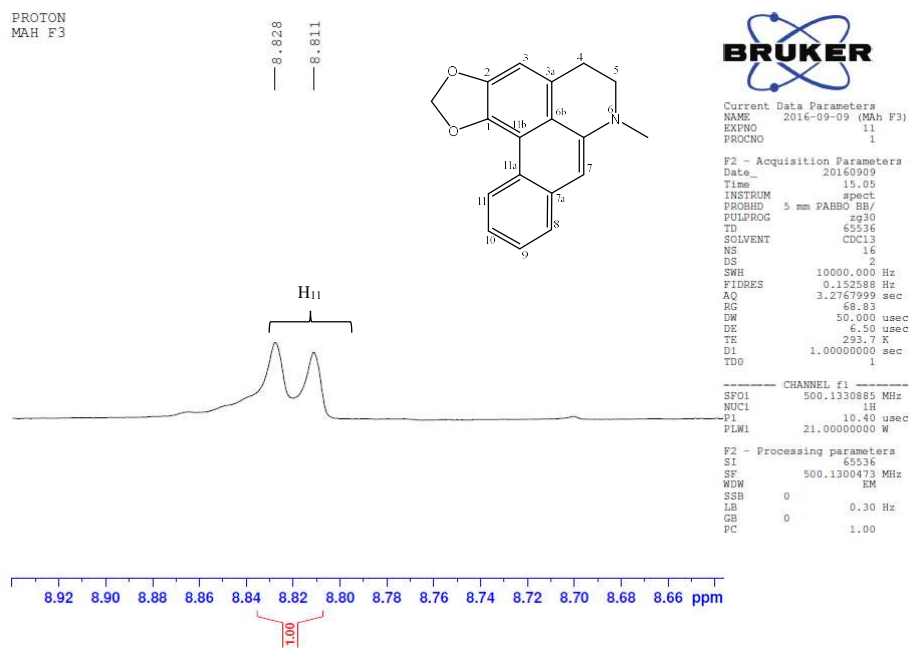
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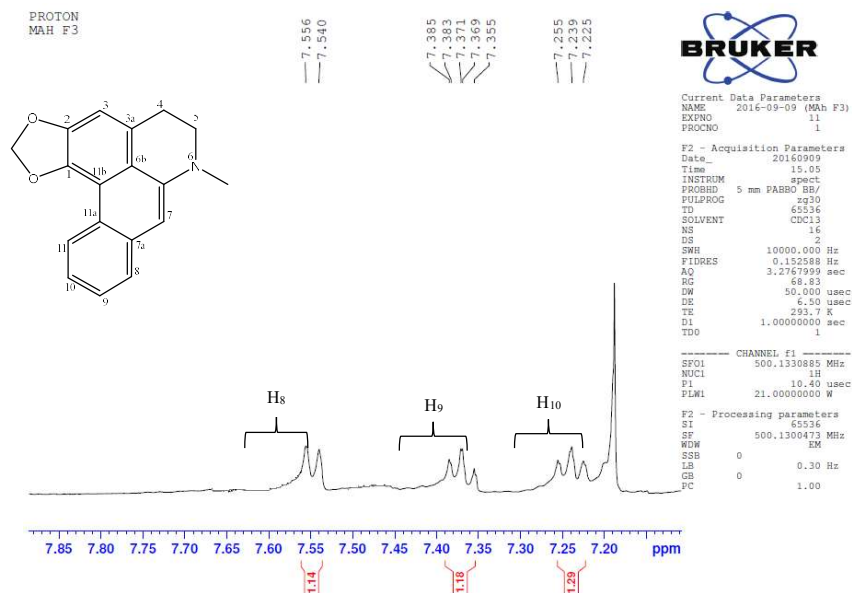
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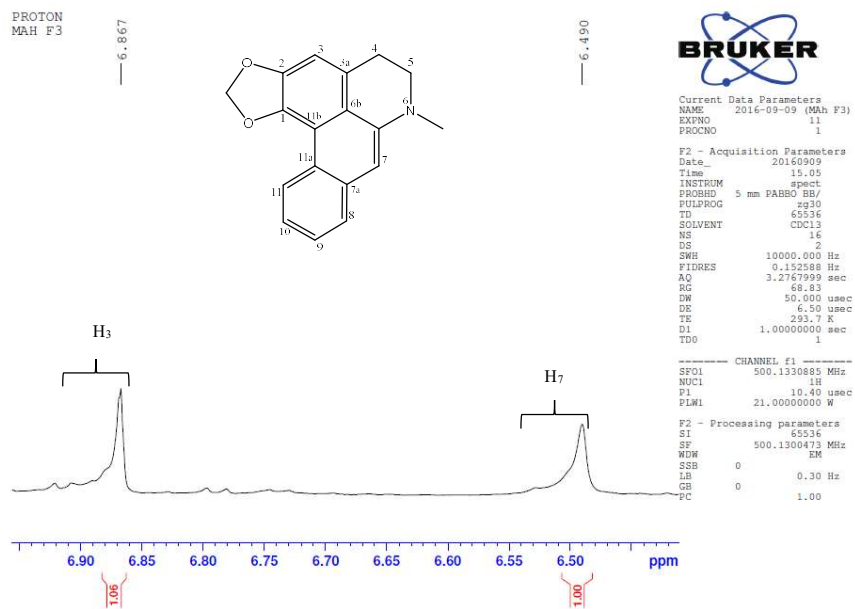
S1: $^1\text{H-NMR}$ (500 MHz, CDCl_3) Spectrum of Compound **1** (dehydroremerine)



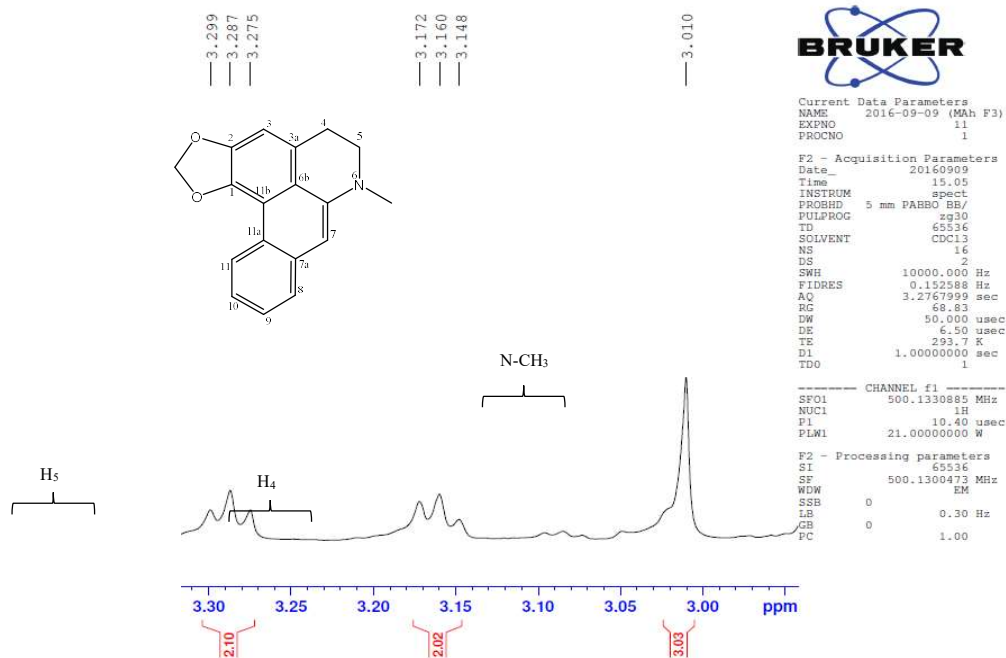
S2: Expansion of the $^1\text{H-NMR}$ (500 MHz, CDCl_3) Spectrum of Compound **1** (dehydroremerine)



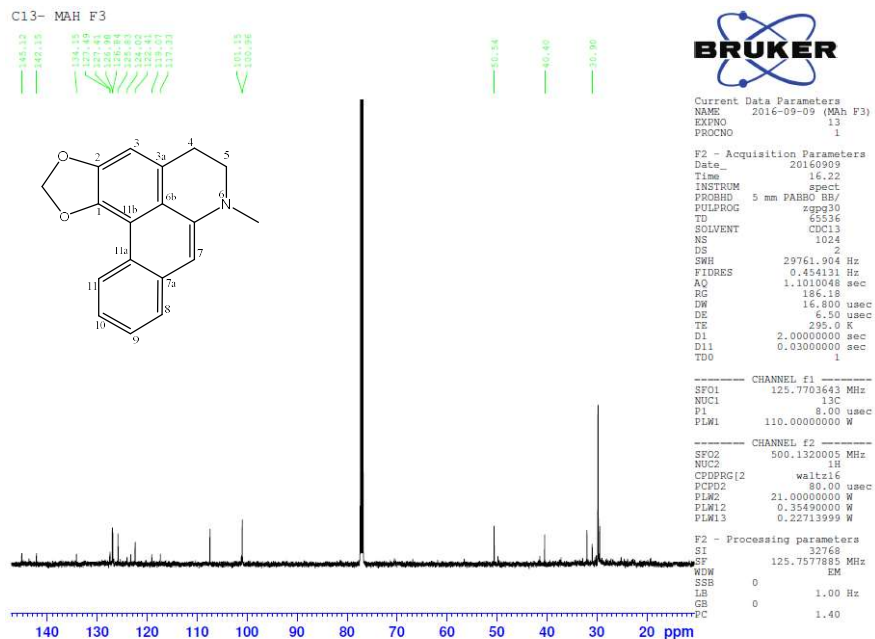
S3: Expansion of the $^1\text{H-NMR}$ (500 MHz, CDCl_3) Spectrum of Compound 1 (dehydroremerine)



S4: Expansion of the $^1\text{H-NMR}$ (500 MHz, CDCl_3) Spectrum of Compound 1 (dehydroremerine)

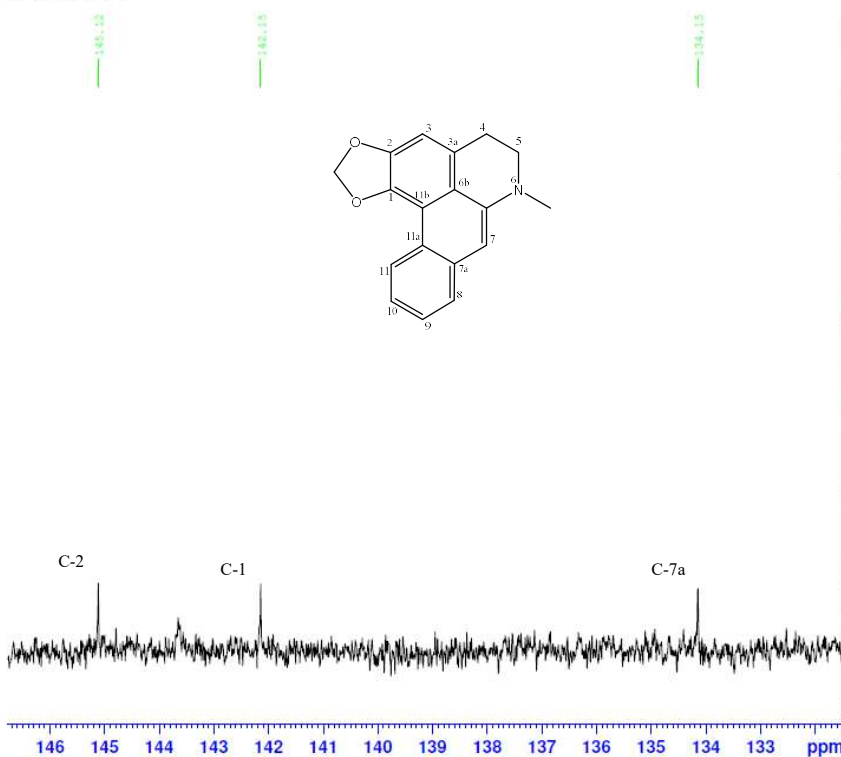


S5: Expansion of the ¹H-NMR (500 MHz, CDCl₃) Spectrum of Compound 1 (dehydremerine)



S6: ¹³C-NMR (500 MHz) Spectrum of Compound 1 (dehydremerine)

C13- MAH F3



Current Data Parameters
NAME 2016-09-09 (MAH F3)
EXPNO 13
PROCNO 1

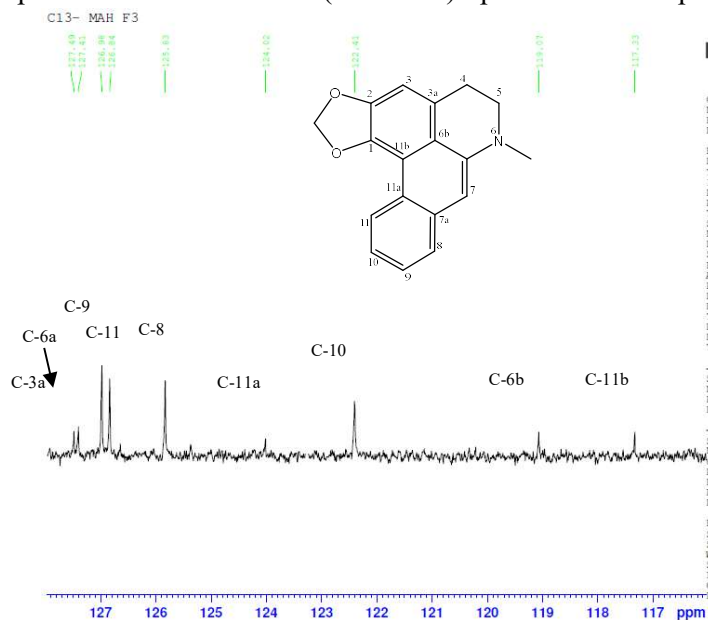
F2 - Acquisition Parameters
Date_ 20160909
Time 16.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 186.18
DW 16.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

----- CHANNEL f1 -----
SF01 125.7703643 MHz
NUC1 13C
P1 8.00 usec
PLW1 110.0000000 W

----- CHANNEL f2 -----
SF02 500.1320005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 21.0000000 W
PLW12 0.35490000 W
PLW13 0.22713999 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S7: Expansion of the ¹³C-NMR (500 MHz) Spectrum of Compound 1 (dehydrremerine)



Current Data Parameters
NAME 2016-09-09 (MAH F3)
EXPNO 13
PROCNO 1

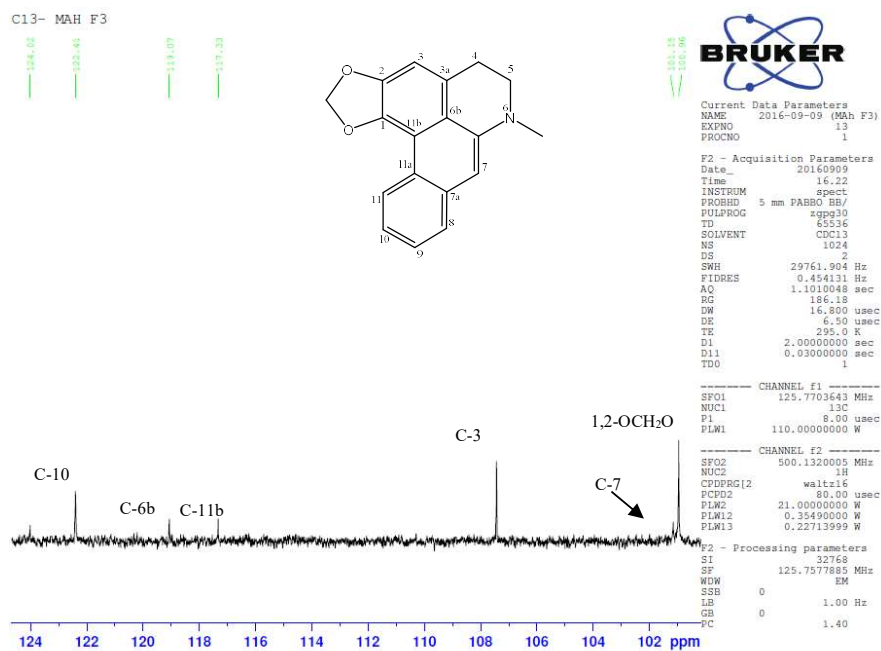
F2 - Acquisition Parameters
Date_ 20160909
Time 16.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 186.18
DW 16.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

----- CHANNEL f1 -----
SF01 125.7703643 MHz
NUC1 13C
P1 8.00 usec
PLW1 110.0000000 W

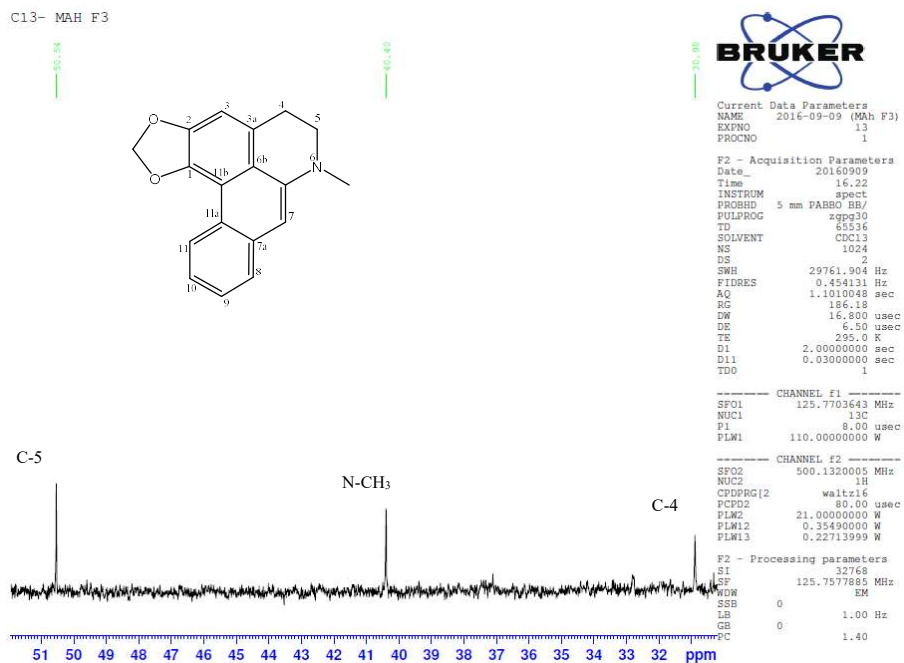
----- CHANNEL f2 -----
SF02 500.1320005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 21.0000000 W
PLW12 0.35490000 W
PLW13 0.22713999 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

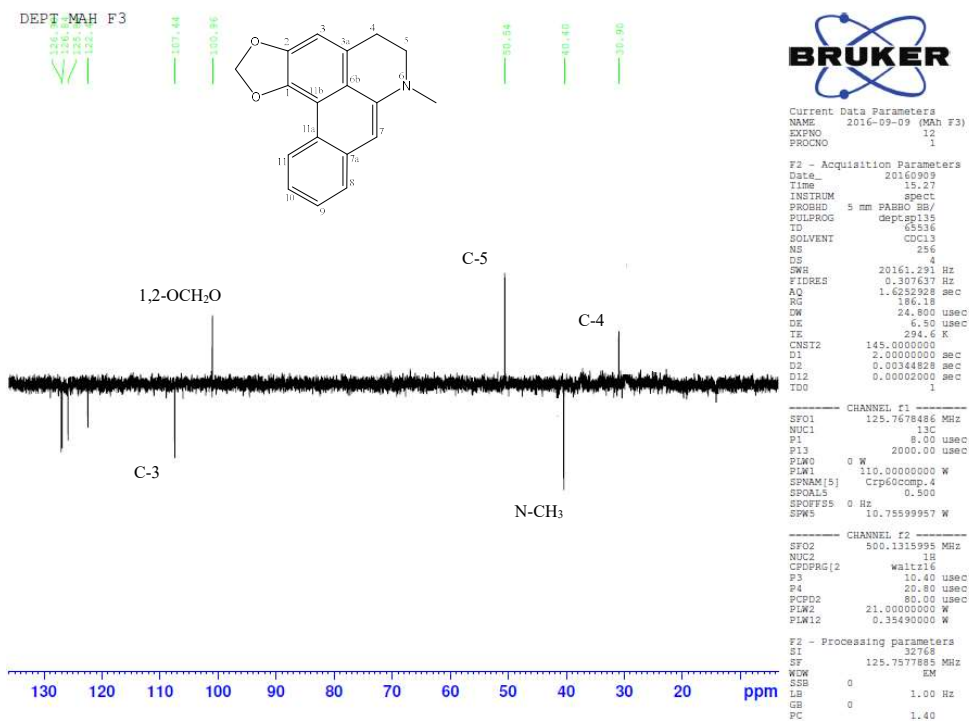
S8: Expansion of the ¹³C-NMR (500 MHz) Spectrum of Compound 1 (dehydrremerine)



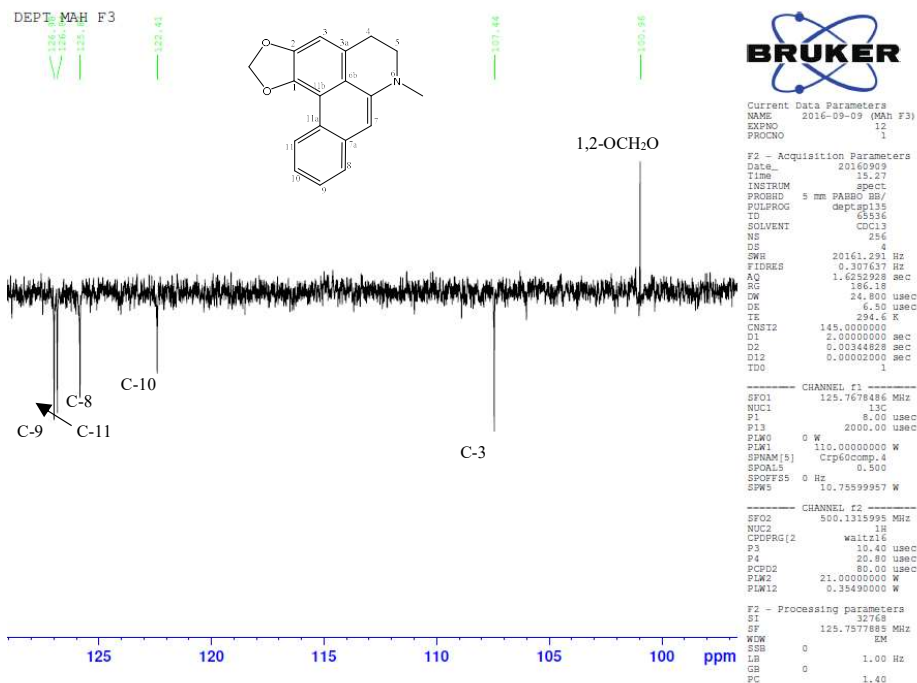
S9: Expansion of the ^{13}C -NMR (500 MHz) Spectrum of Compound 1 (dehydrmerine)



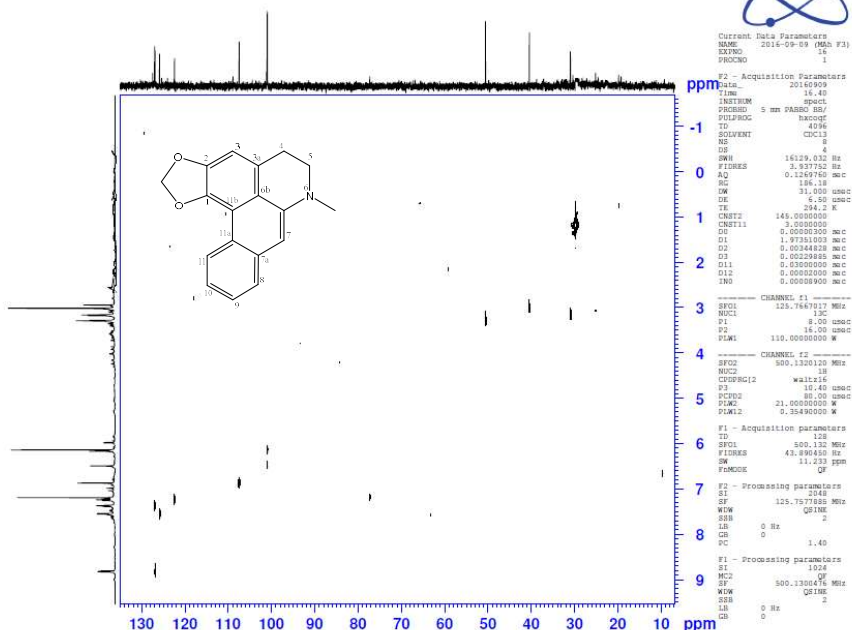
S10: Expansion of the ^{13}C -NMR (500 MHz) Spectrum of Compound 1 (dehydrmerine)



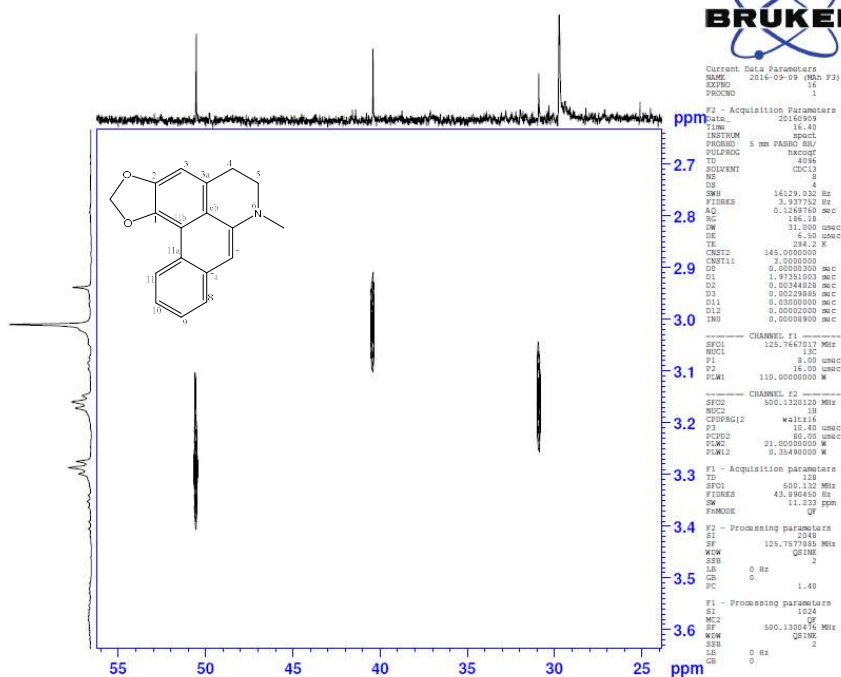
S11: DEPT (500 MHz) Spectrum of Compound 1 (dehydroremerine)



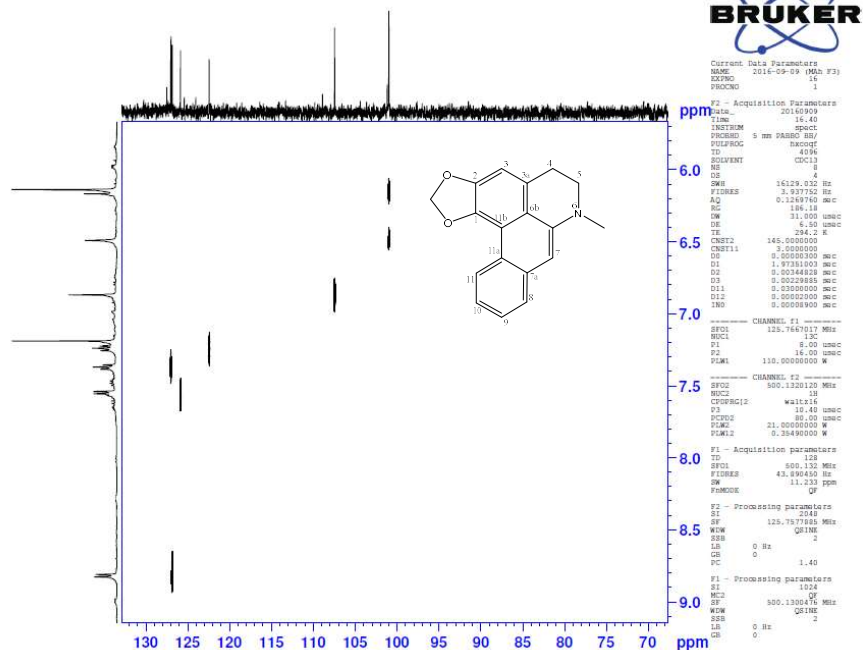
S12: Expansion of the DEPT (500 MHz) Spectrum of Compound 1 (dehydroremerine)



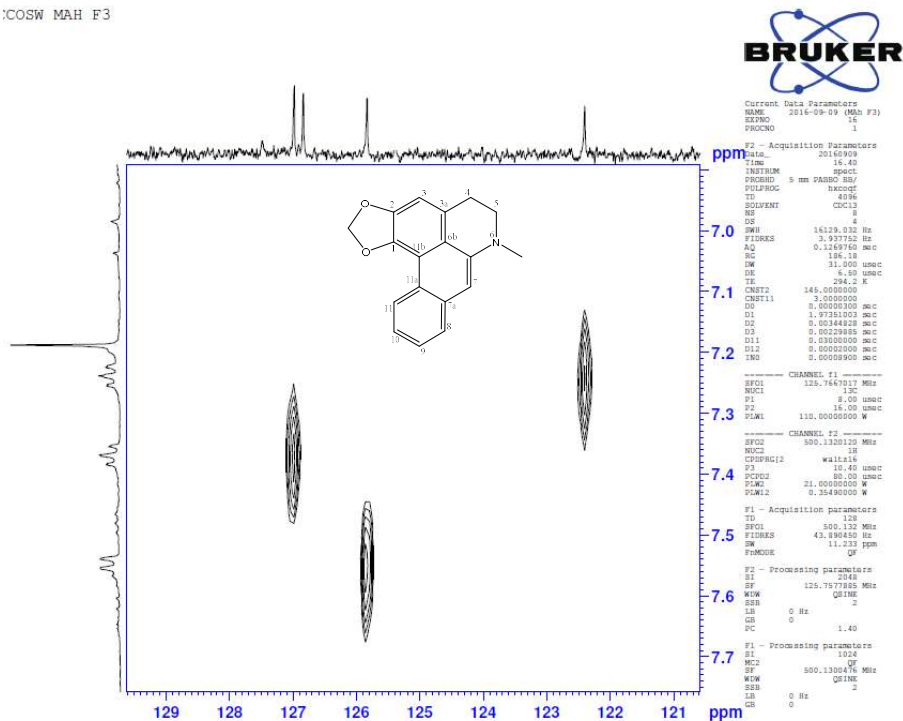
S13: HCCOSW Spectrum of Compound 1 (dehydroremerine)



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

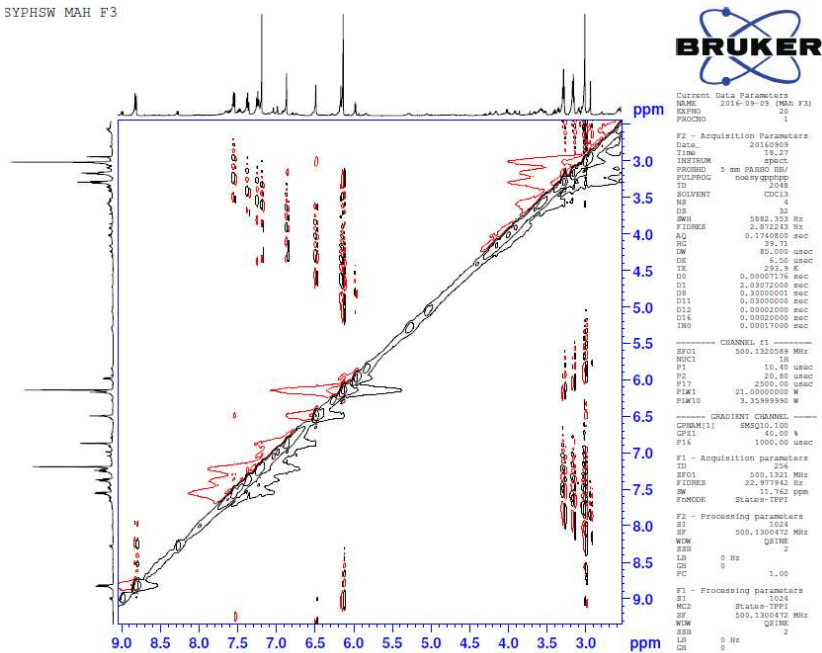


S15: Expansion of the HCCOSY Spectrum of Compound 1 (dehydroremerine)



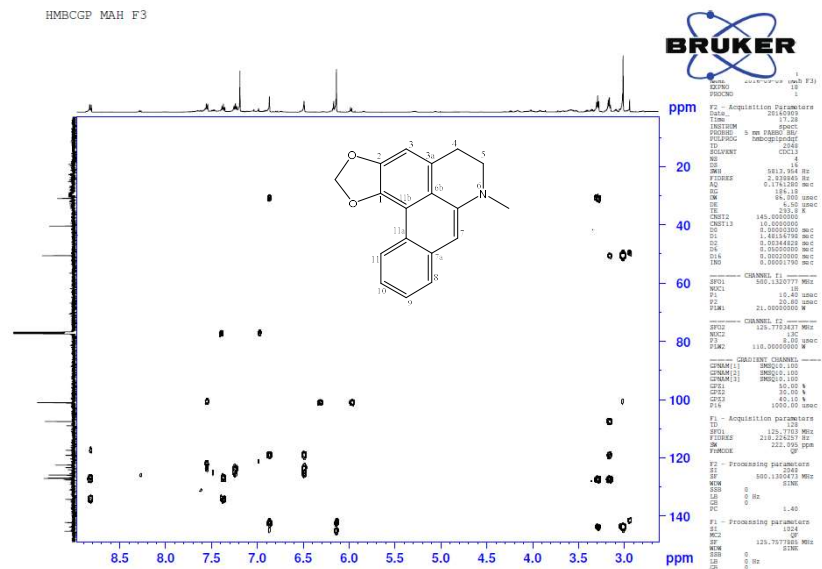
S16: Expansion of the HCCOSY Spectrum of Compound 1 (dehydroremerine)

SYPHSW MAH F3

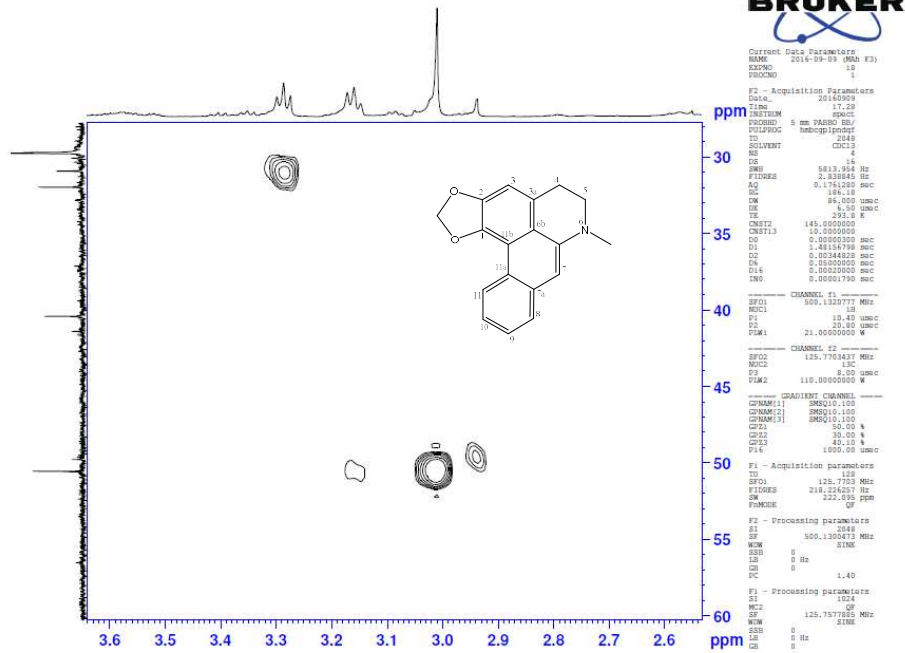


S17: NOSY (500 MHz) Spectrum of Compound 1 (dehydroremerine)

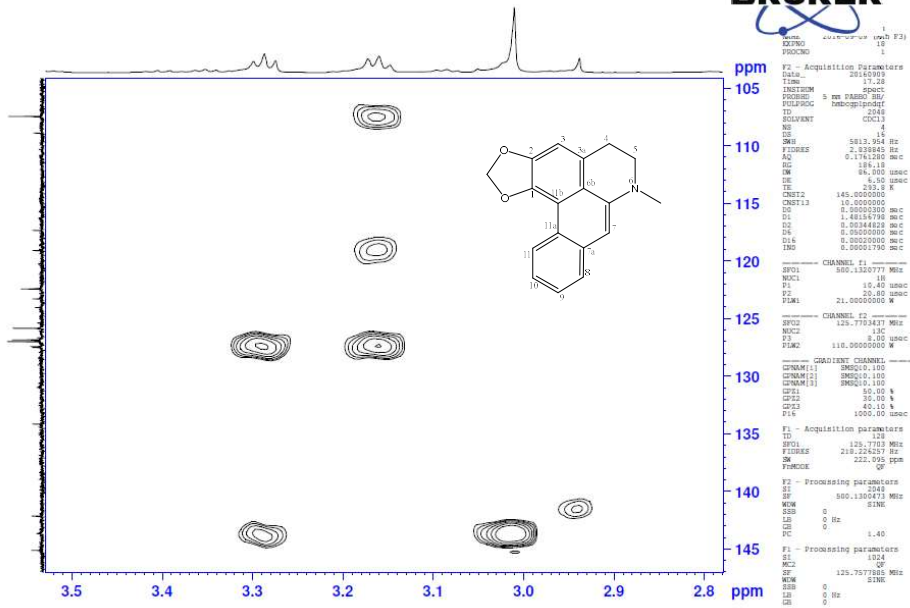
HMBCGP MAH F3



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

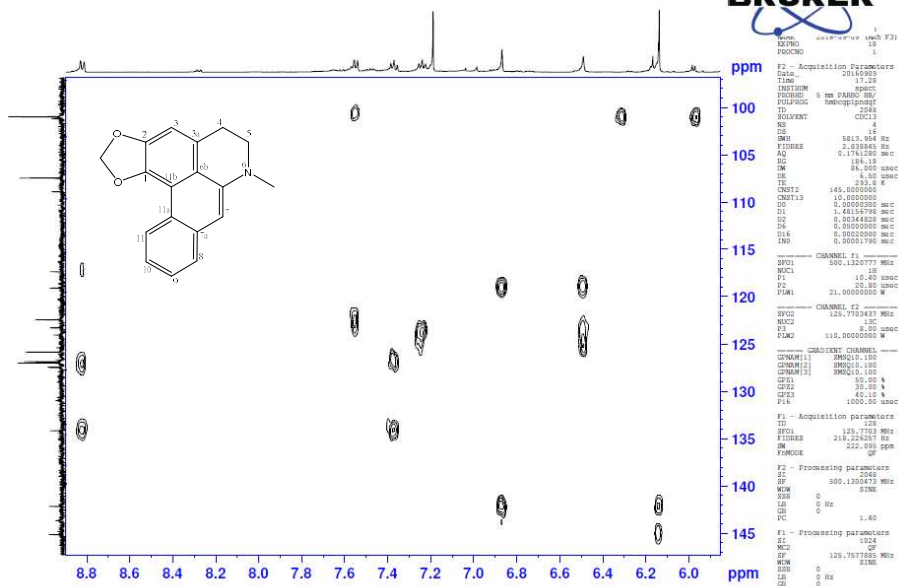


S19: Expansion of the HMBC (500 MHz) Spectrum of Compound 1 (dehydroremerine)



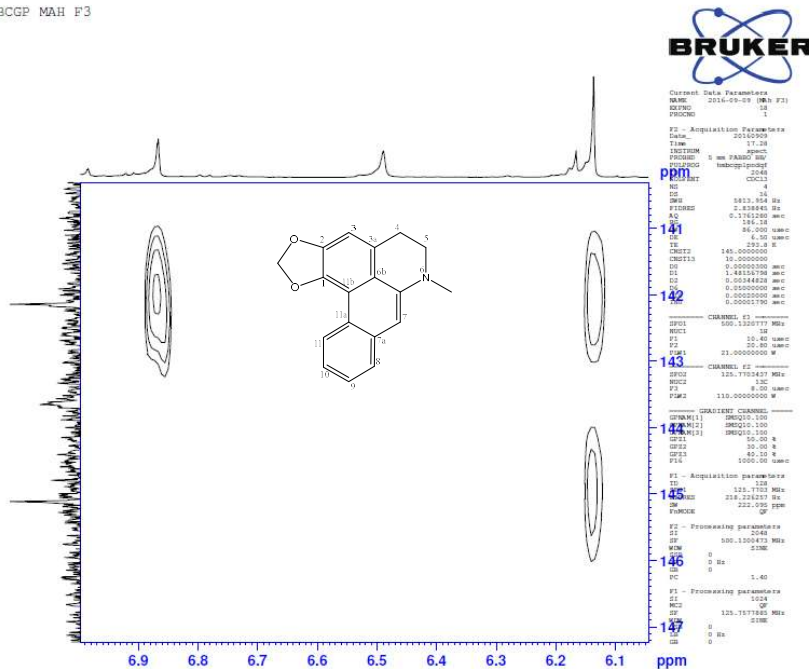
S20: Expansion of the HMBC (500 MHz) Spectrum of Compound 1 (dehydroremerine)

HMBGCP MAH F3

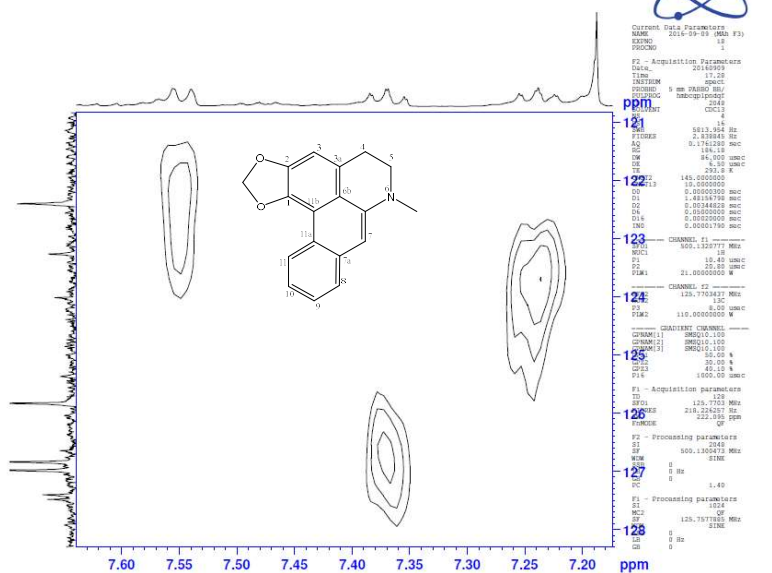


S21: Expansion of the HMBC (500 MHz) Spectrum of Compound 1 (dehydroremerine)

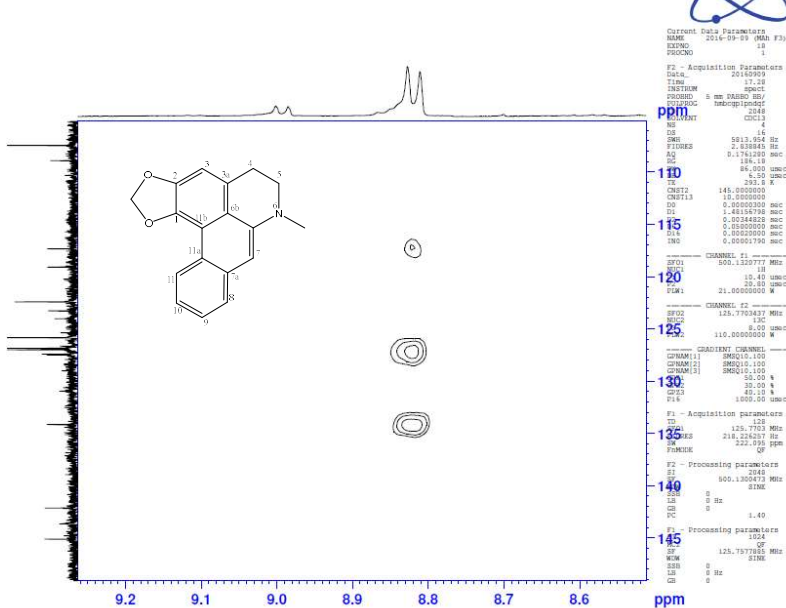
HMBGCP MAH F3



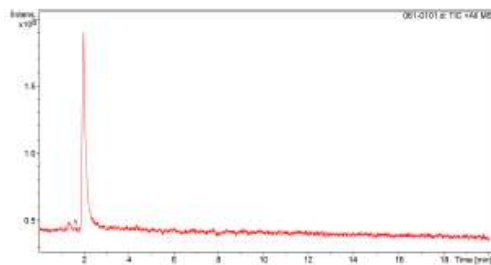
S22: Expansion of the HMBC (500 MHz) Spectrum of Compound 1 (dehydroremerine)



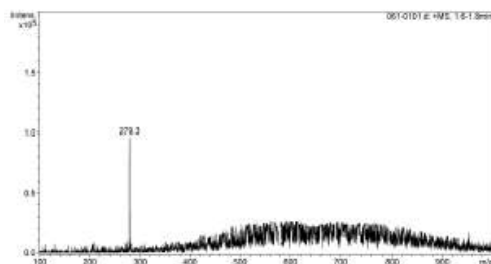
S23: Expansion of the HMBC (500 MHz) Spectrum of Compound 1 (dehydroremerine)



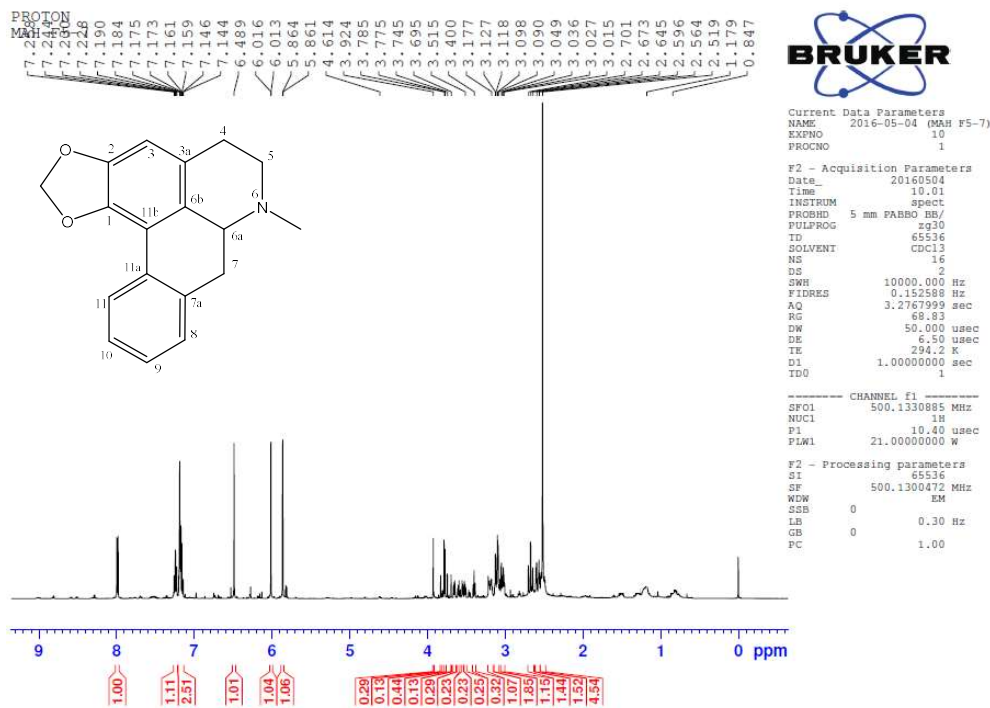
S24: Expansion of the HMBC (500 MHz) Spectrum of Compound 1 (dehydroremerine)



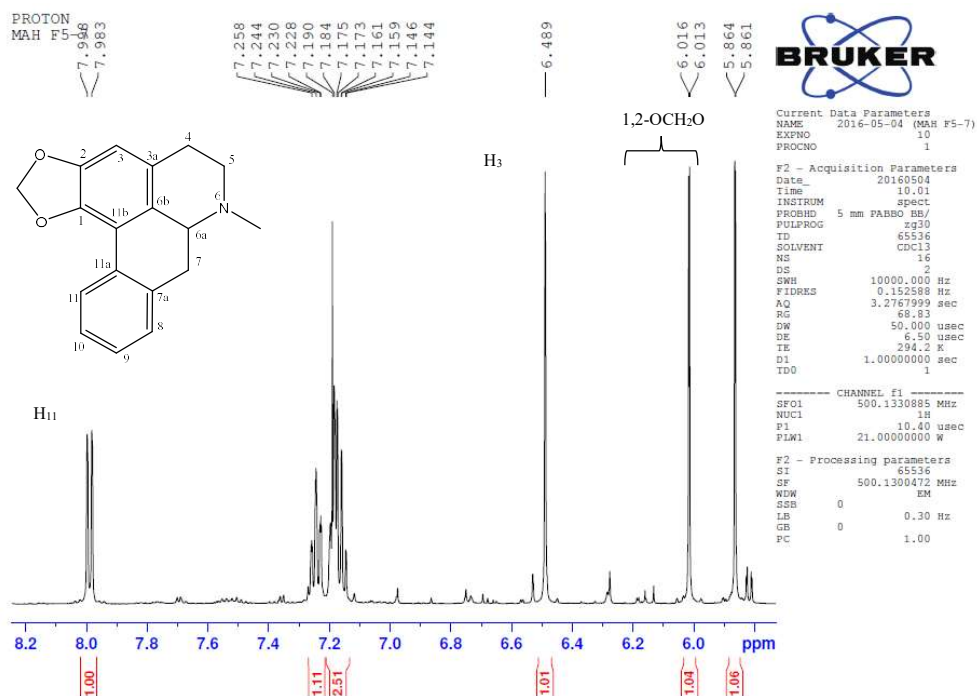
Chrom 1, 1.6 min



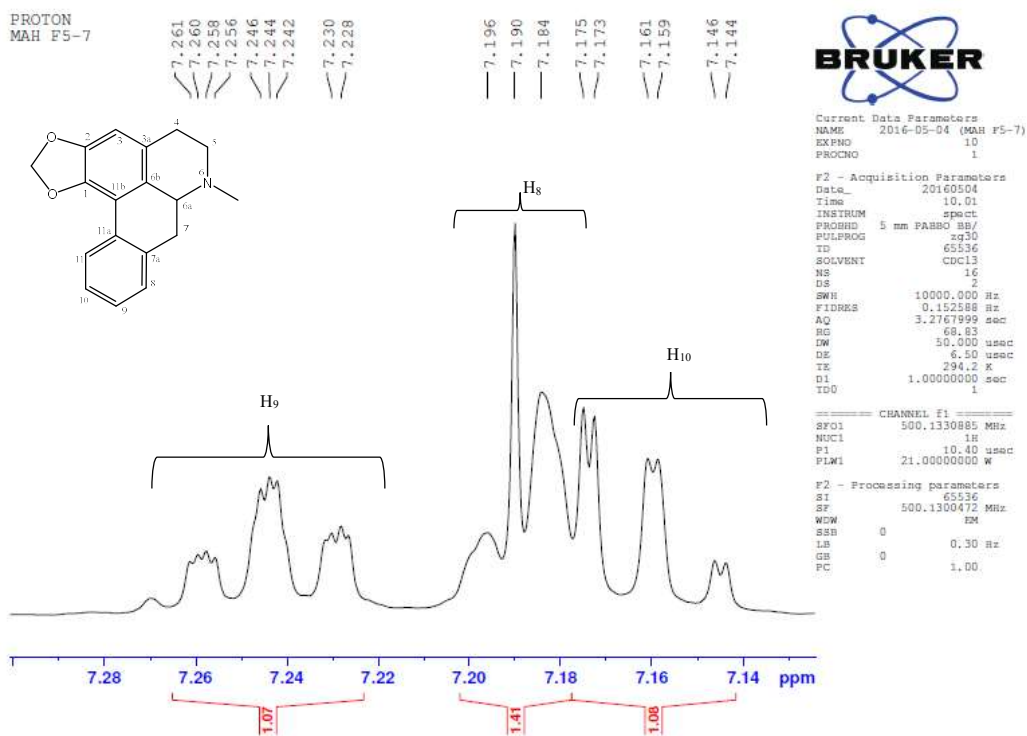
S25: LC-MS Spectrum of Compound 2 (roemerine)



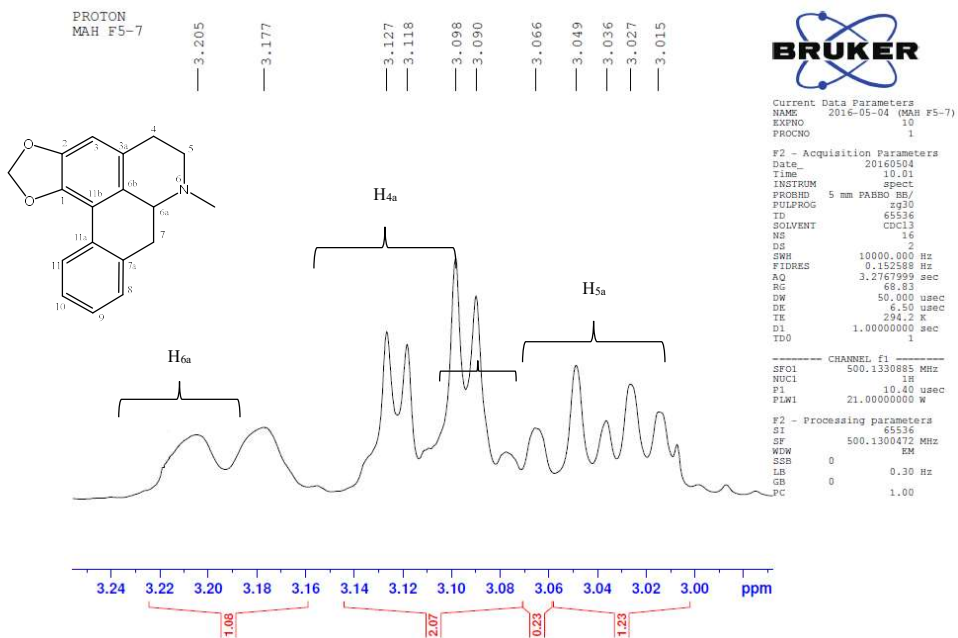
S26: ¹H-NMR (500 MHz, CDCl₃) Spectrum of Compound 2 (roemerine)



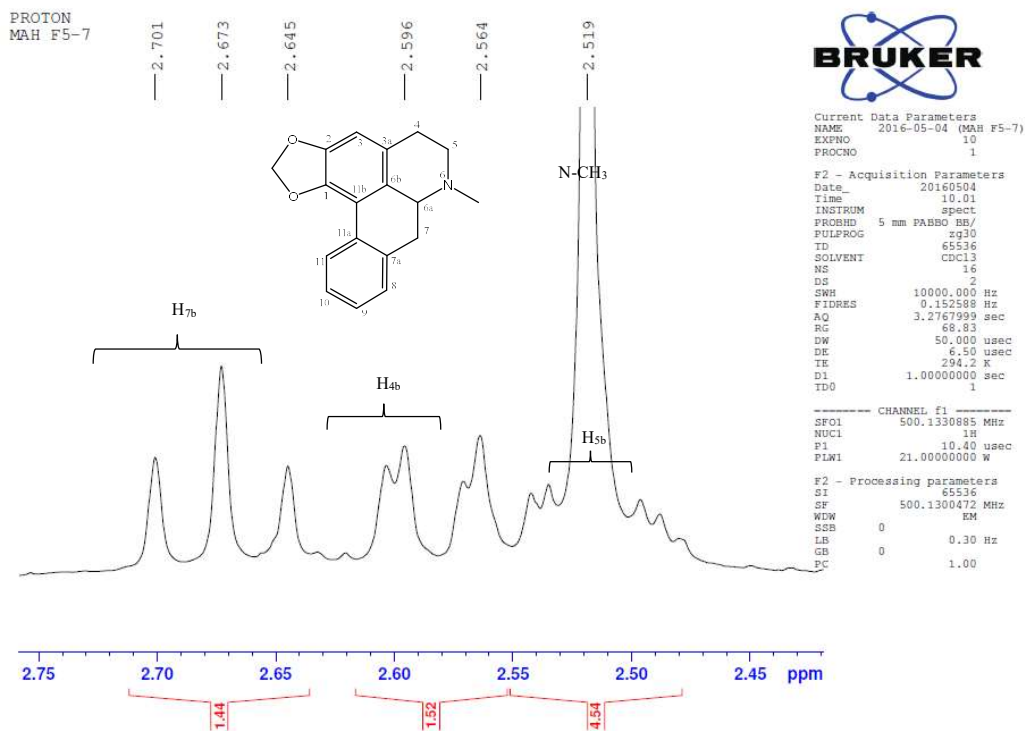
S27: Expansion ¹H-NMR (500 MHz, CDCl₃) Spectrum of Compound 2 (reomerine)



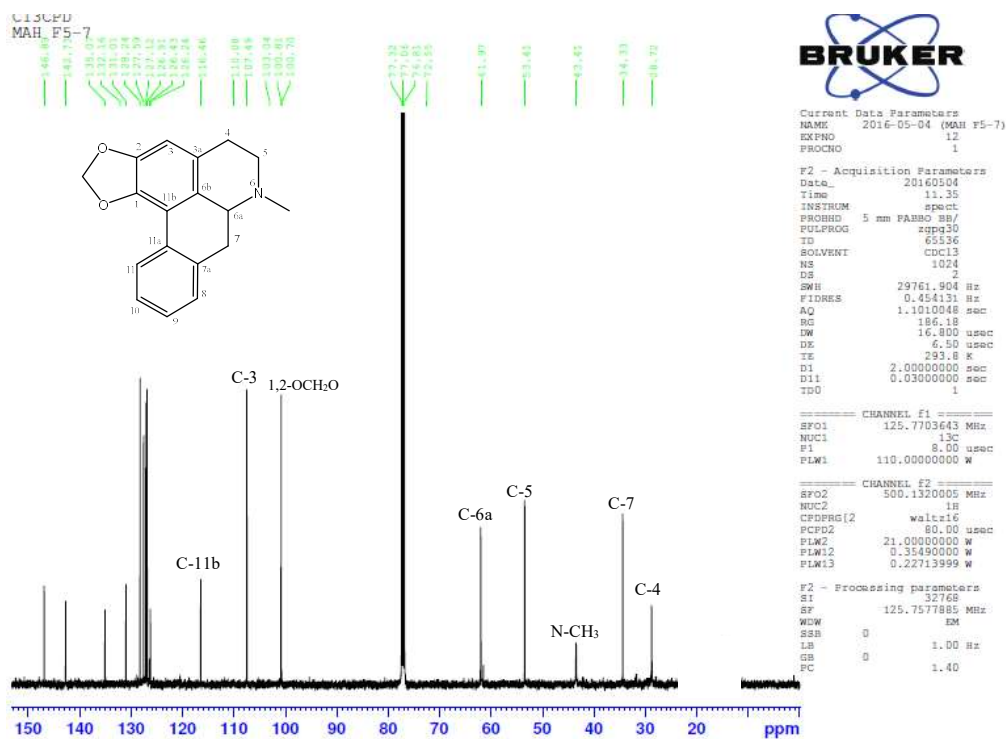
S28: Expansion ¹H-NMR (500 MHz, CDCl₃) Spectrum of Compound 2 (reomerine)



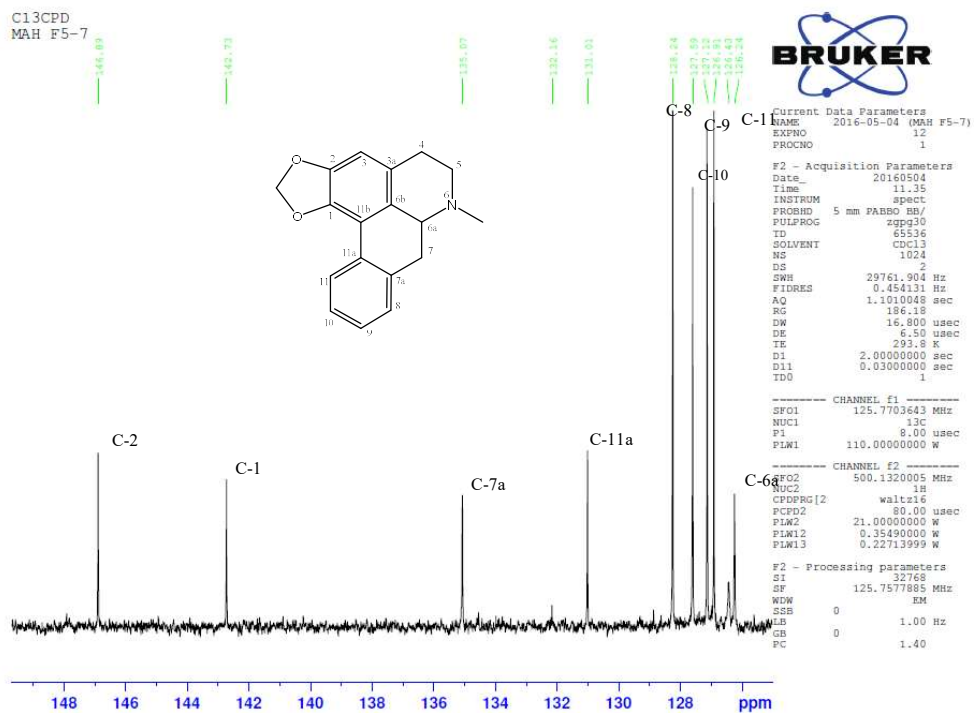
S29: Expansion $^1\text{H-NMR}$ (500 MHz, CDCl_3) Spectrum of Compound 2 (reomerine)



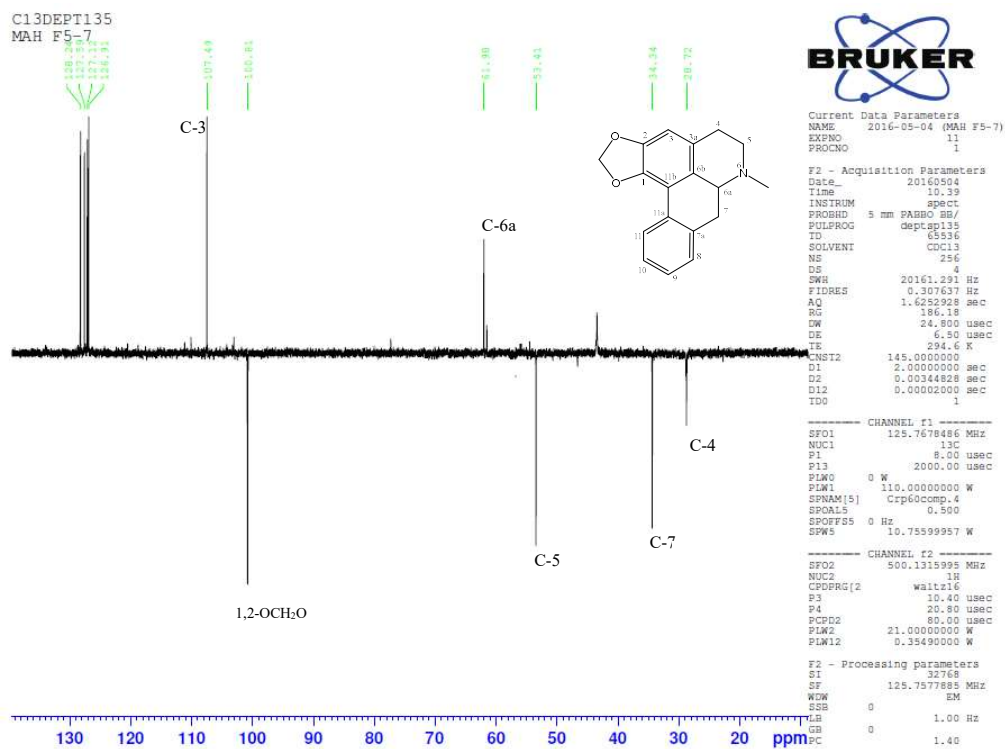
S30: Expansion $^1\text{H-NMR}$ (500 MHz, CDCl_3) Spectrum of Compound 2 (reomerine)



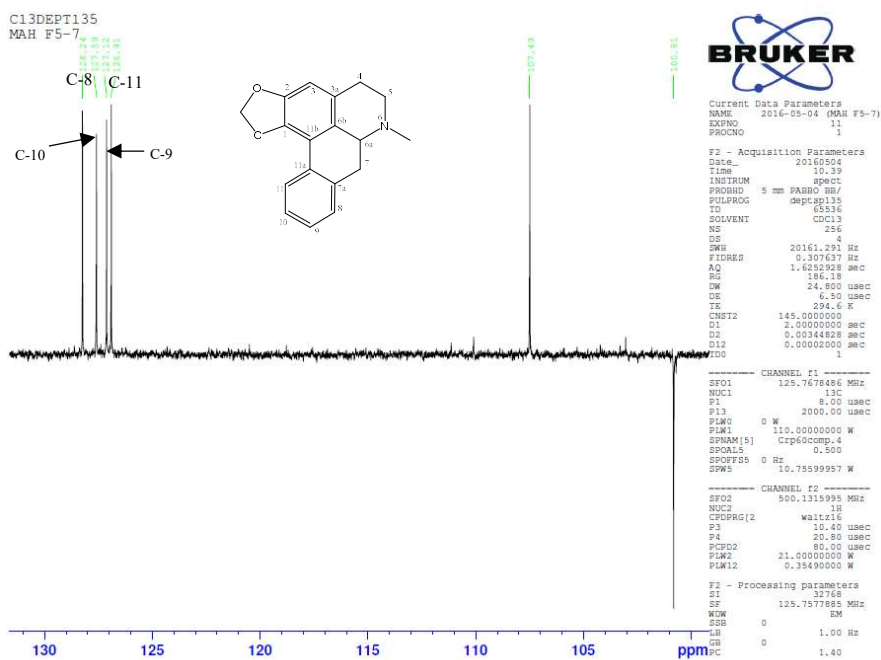
S31: ^{13}C -NMR (500 MHz, CDCl_3) Spectrum of Compound 2 (reomerine)



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

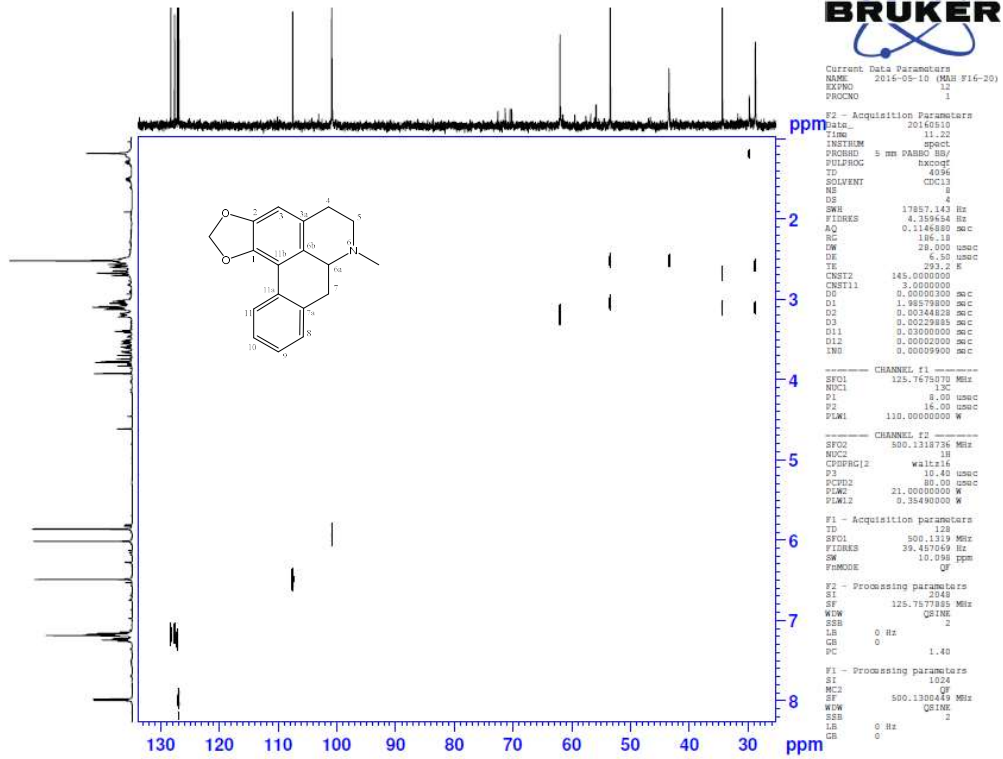


S33: Expansion of the DEPT (500 MHz, CDCl₃) Spectrum of Compound 2 (reomerine)



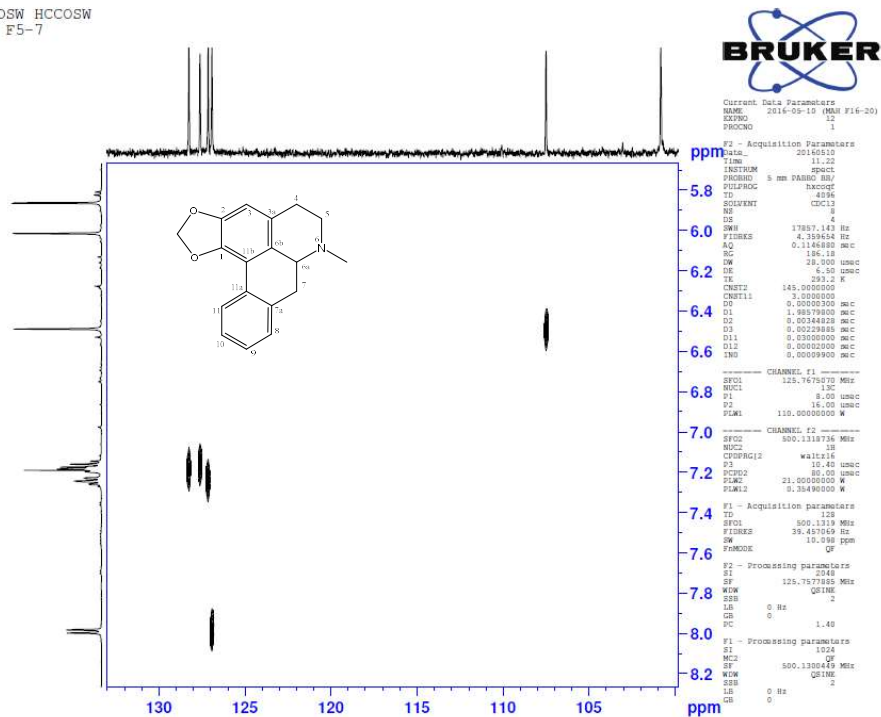
S34: Expansion of the DEPT (500 MHz, CDCl₃) Spectrum of Compound 2 (reomerine)

HCCOSW HCCOSW
MAH F5-7



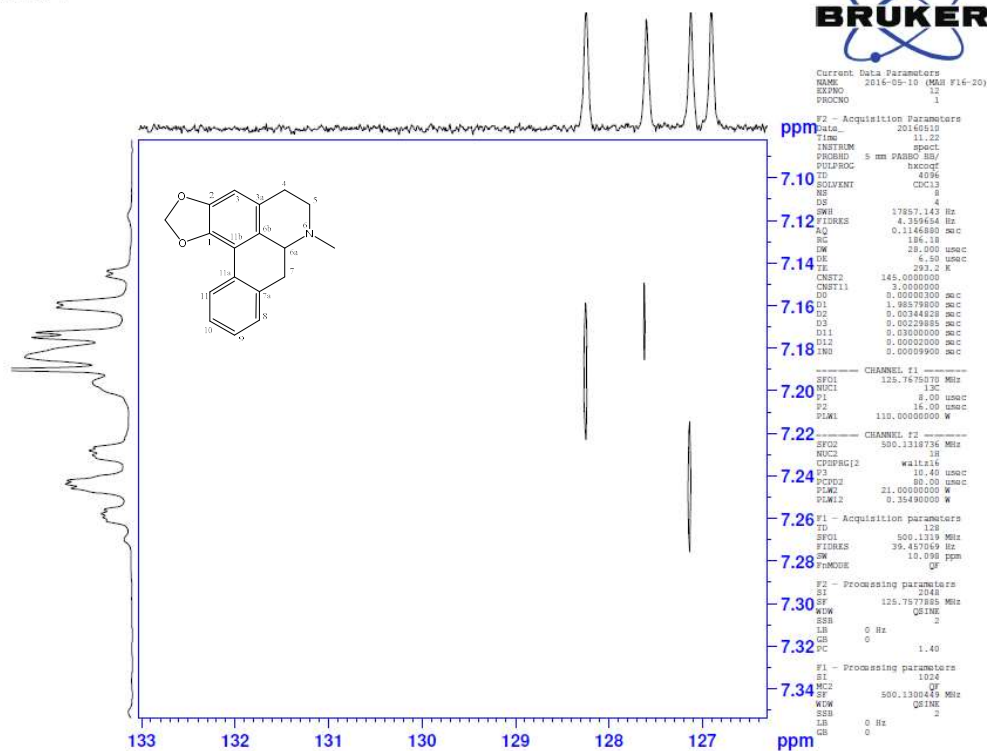
S35: HCCOW Spectrum of Compound 2 (reomerine)

HCCOSW HCCOSW
MAH F5-7



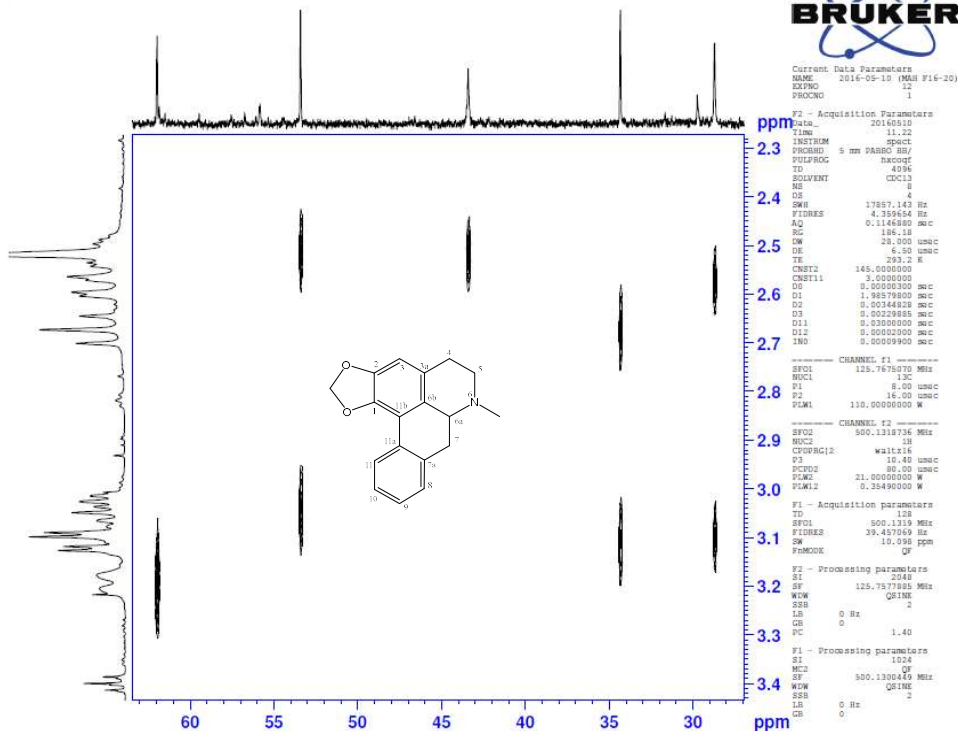
S36: Expansion of the HCCOSW Spectrum of Compound 2 (reomerine)

HCCOSW HCCOSW
MAH F5-7



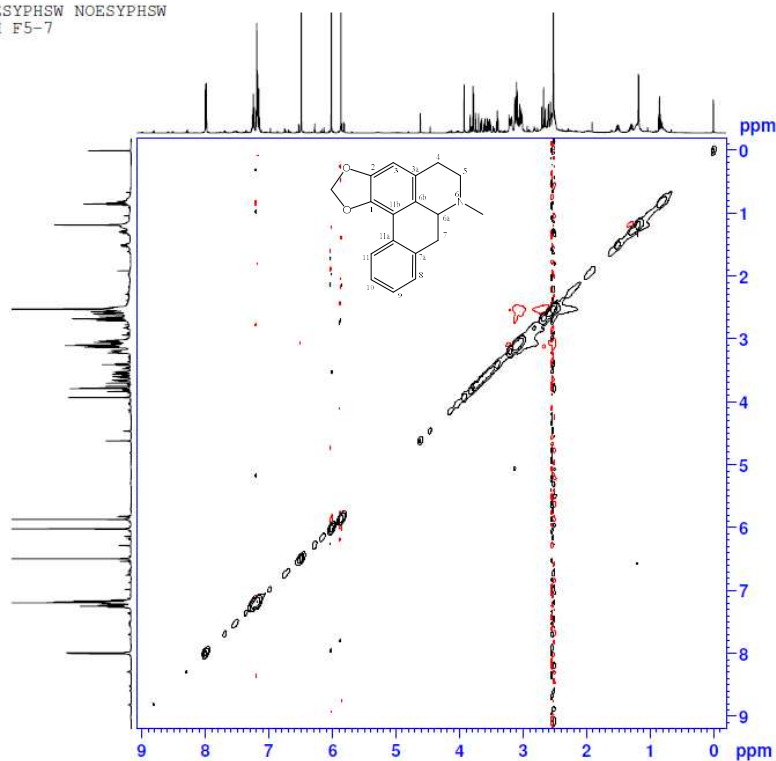
S37: Expansion of the HCCOW Spectrum of Compound 2 (reomerine)

HCCOSW HCCOSW
MAH F5-7



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

NOESYPSHW NOESYPSHW
MAH F5-7



Current Data Parameters
NAME 2016-05-10 MAH F16-20
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160510
Time 12.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG noesypphpp
TD 2048
SOLVENT CDCl3
NS 4
DS 32
SWH 5882.303 Hz
FIDRES 2.872543 Hz
AQ 0.1740800 sec
RG 34.61
DM 85.000 usec
DE 6.50 usec
TE 293.2 K
D0 0.00007176 sec
D1 2.03070000 sec
D2 0.30000001 sec
D3 0.03000000 sec
D12 0.00000000 sec
D14 0.00020000 sec
D16 0.00017000 sec
IN0

CHANNEL f1
SF01 500.132031 MHz
NUC1 1H
P0 10.40 usec
F1 20.80 usec
P17 2500.00 usec
PLM1 21.0000000 W
PLM10 3.35999990 W

GRADIENT CHANNEL
CPGRAM[1] SMSQ10.100
GFS1 40.00 %
P16 1000.00 usec

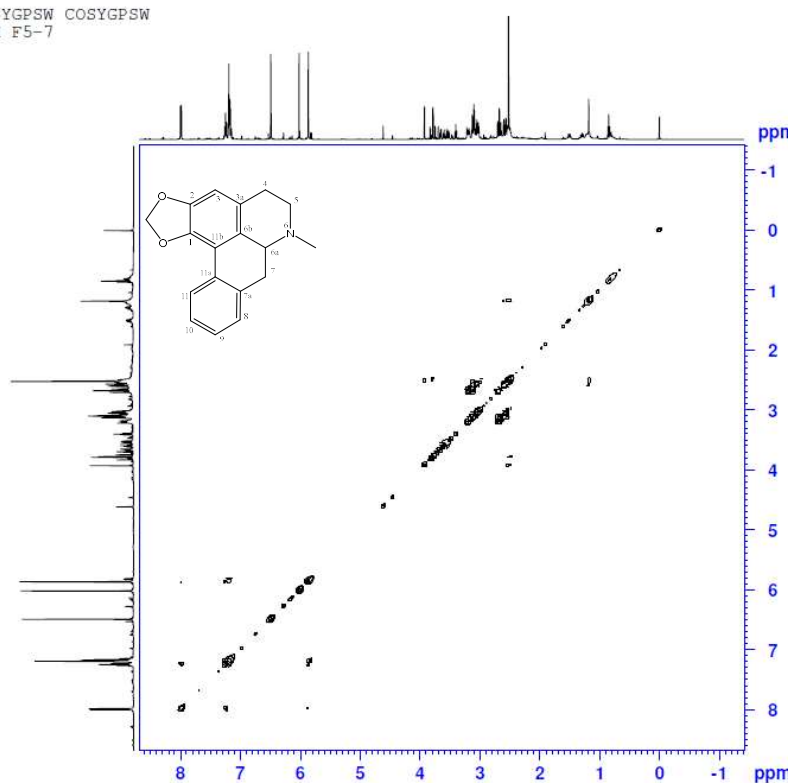
F1 - Acquisition parameters
TD 256
SF01 500.132 MHz
FIDRES 22.977942 Hz
SW 11.762 ppm
FQMODE States-TFPI

F2 - Processing parameters
SI 1024
SF 500.1300454 MHz
WVM Q8INE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TFPI
SF 500.1300454 MHz
WVM Q8INE
SSB 2
LB 0 Hz
GB 0

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

COSYGPSW COSYGPSW
MAH F5-7



Current Data Parameters
NAME 2016-05-10 MAH F16-20
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160510
Time 12.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosyppppqf
TD 2048
SOLVENT CDCl3
NS 1
DS 8
SWH 5050.505 Hz
FIDRES 2.466067 Hz
AQ 0.2027500 sec
RG 34.61
DM 99.000 usec
DE 6.50 usec
TE 293.1 K
D0 0.00000000 sec
D1 1.95043802 sec
D11 0.03000000 sec
D12 0.00000000 sec
D13 0.00000400 sec
D14 0.00020000 sec
D16 0.00018000 sec
IN0

CHANNEL f1
SF01 500.1318676 MHz
NUC1 1H
P0 10.40 usec
F1 20.80 usec
P17 2500.00 usec
PLM1 21.0000000 W
PLM10 3.35999990 W

GRADIENT CHANNEL
CPGRAM[1] SMSQ10.100
GFS1 10.00 %
P16 1000.00 usec

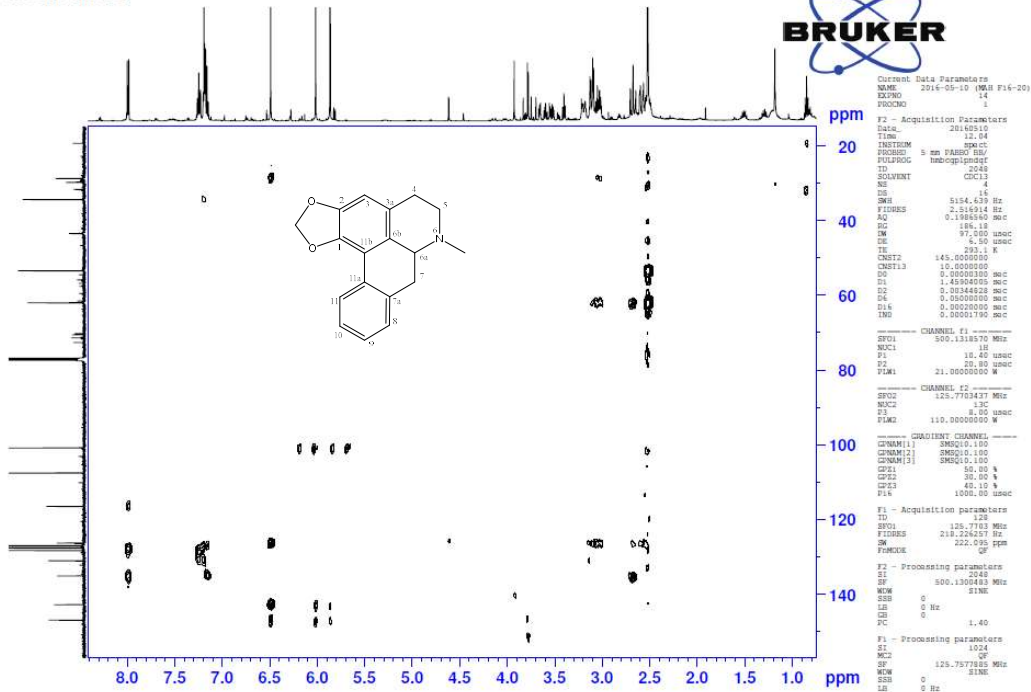
F1 - Acquisition parameters
TD 128
SF01 500.1319 MHz
FIDRES 39.457069 Hz
SW 10.098 ppm
FQMODE OF

F2 - Processing parameters
SI 1024
SF 500.1300491 MHz
WVM Q8INE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 OF
SF 500.1300491 MHz
WVM Q8INE
SSB 0
LB 0 Hz
GB 0

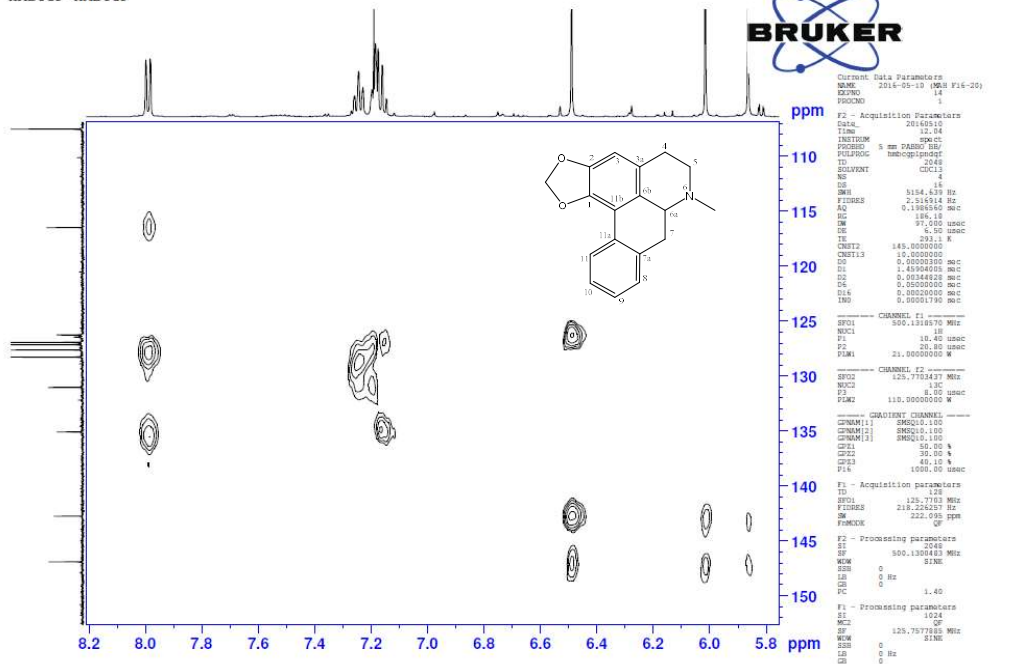
S40: COSY (500 MHz, CDCl₃) Spectrum of Compound 2 (reomerine)

HMBCCP HMBCCP



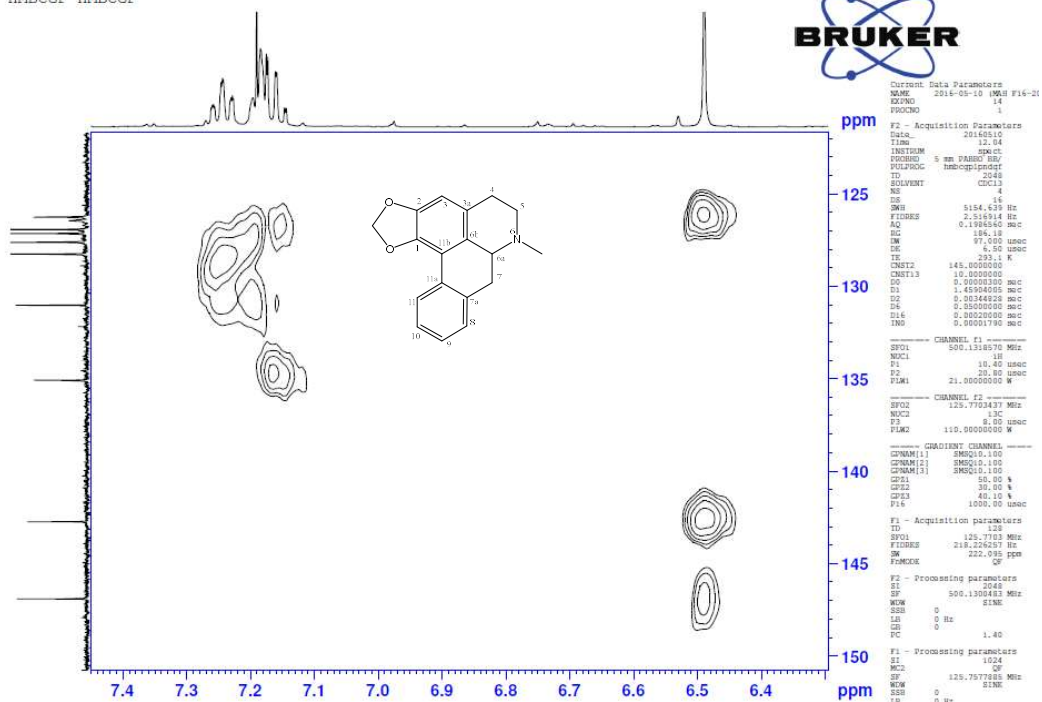
S41: HMBC (500 MHz, CDCl₃) Spectrum of Compound 2 (reomerine)

HMBCCP HMBCCP



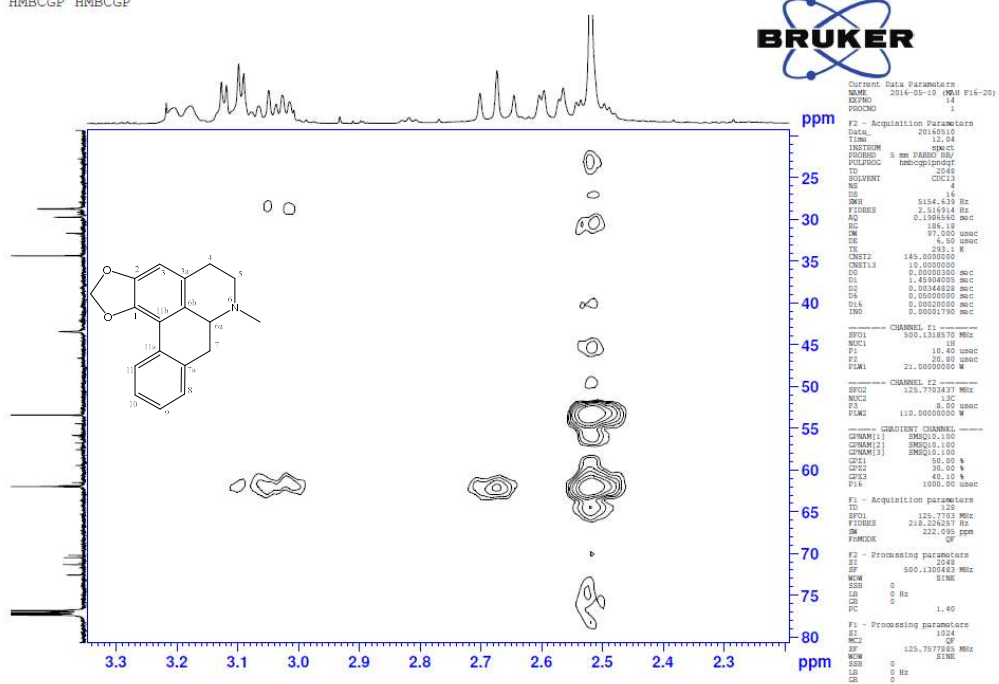
S42: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 2 (reomerine)

HMBCGP HMBCGP



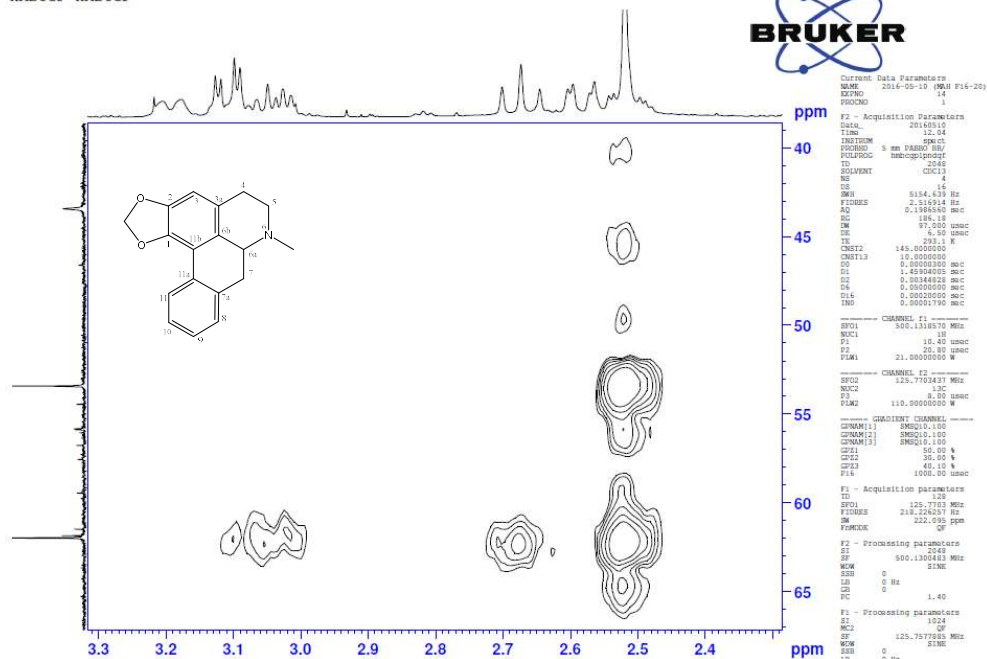
S43: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 2 (reomerine)

HMBCGP HMBCGP

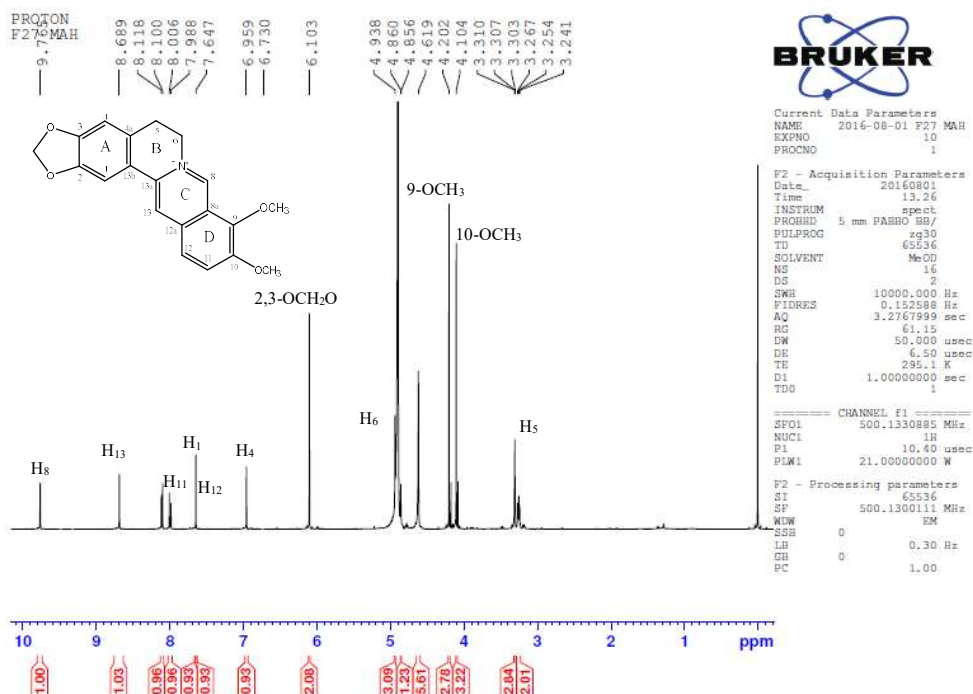


S44: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 2 (reomerine)

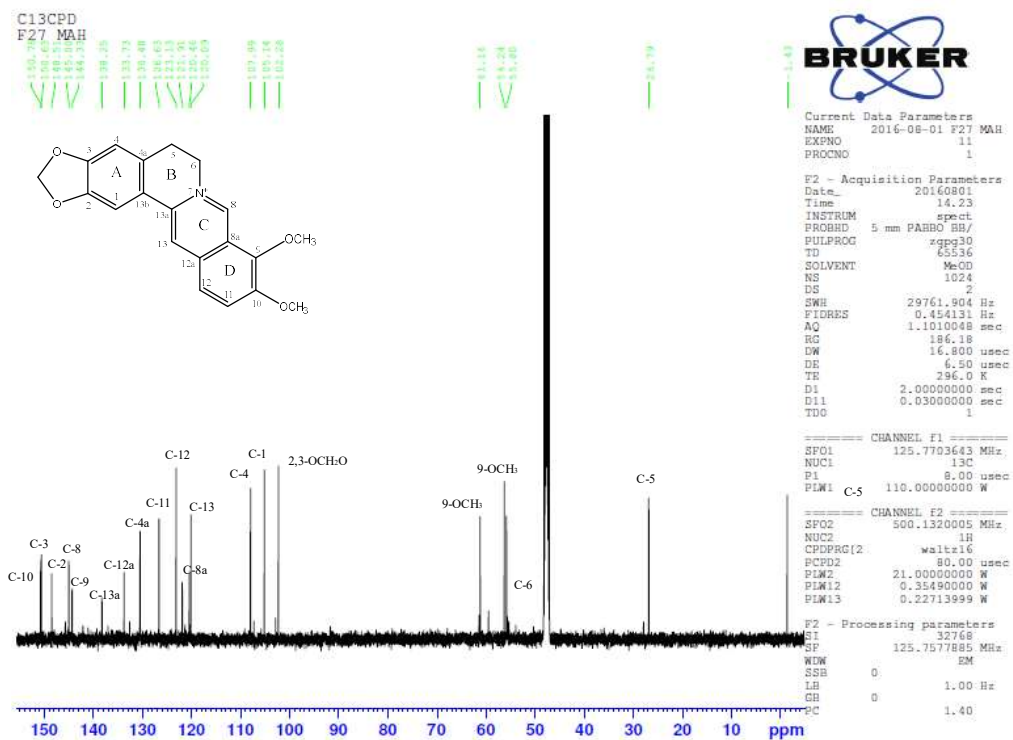
HMBCGP HMBCGP



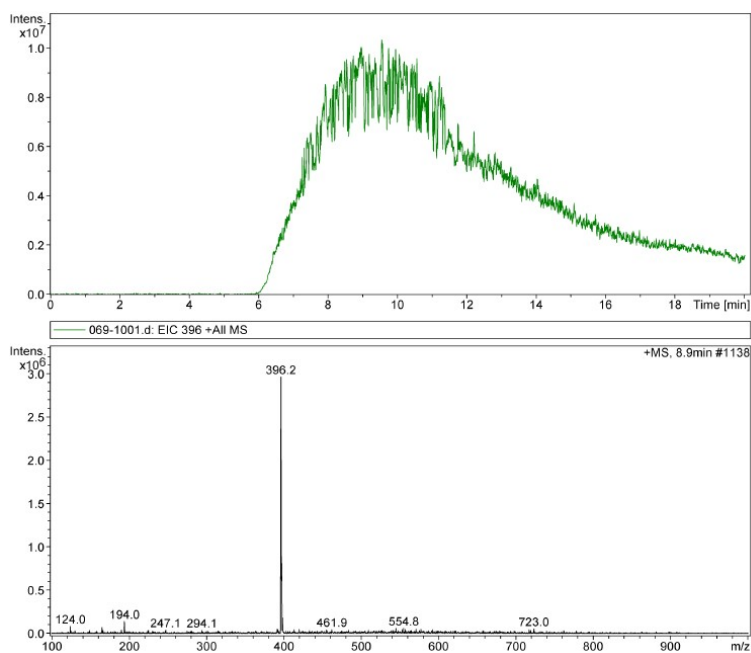
S45: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 2 (reomerine)



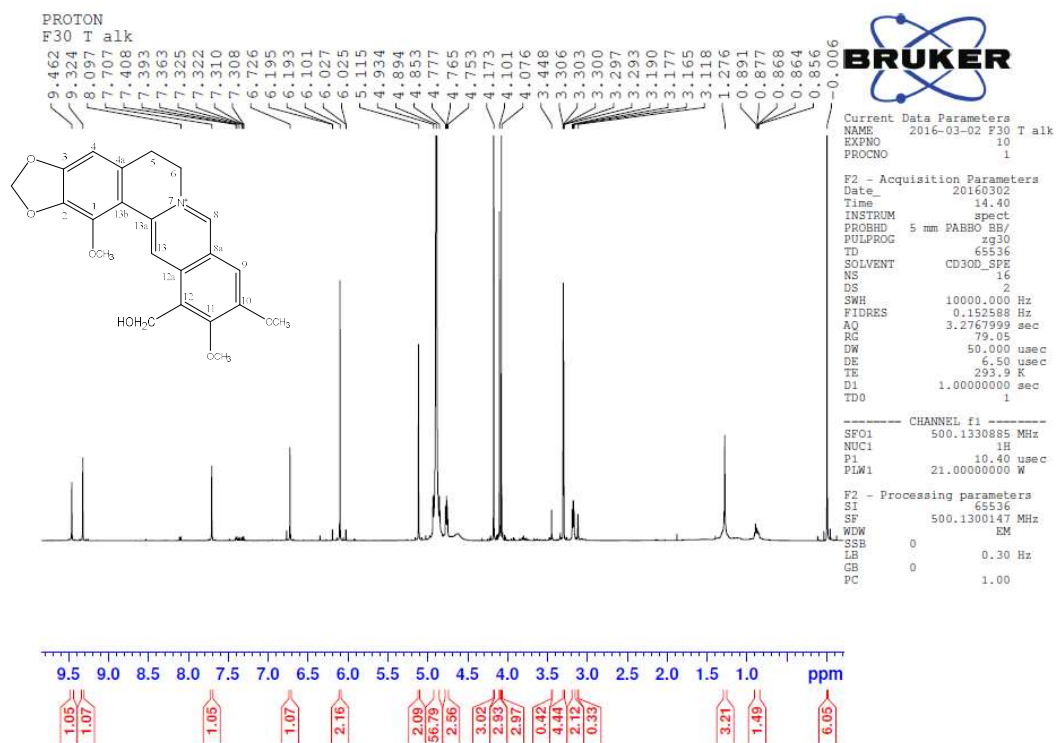
S46: ¹H-NMR (500 MHz, CDCl₃) Spectrum of Compound 3 (berberine)



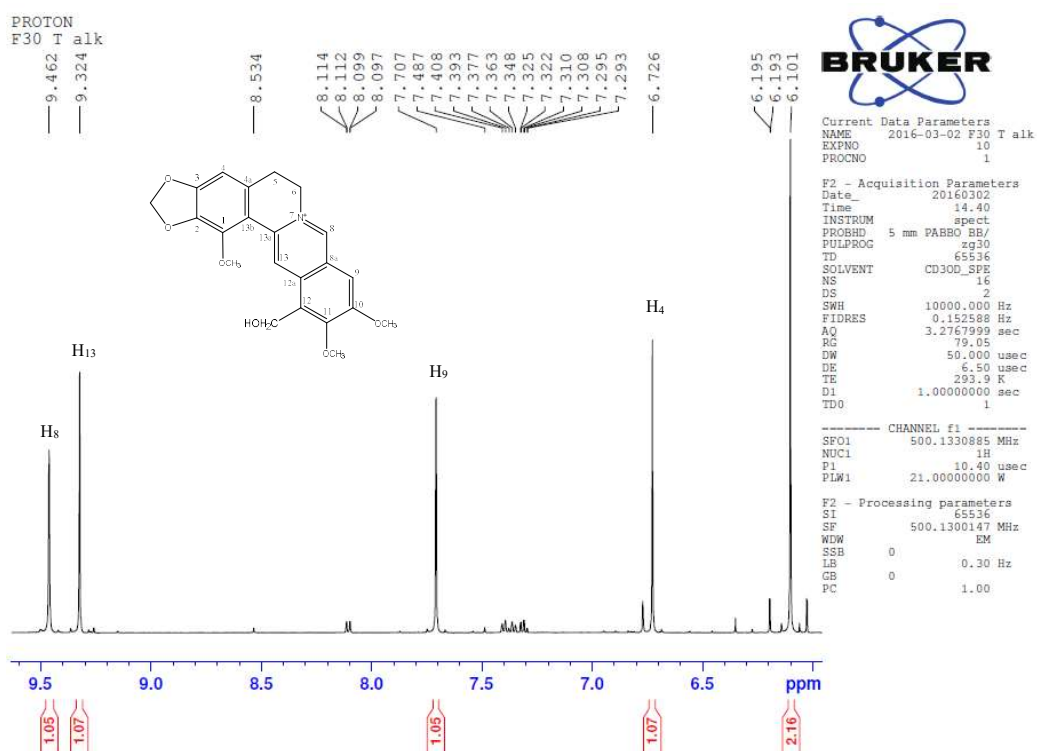
S47: ¹³C-NMR (500 MHz) Spectrum of Compound 3 (berberine)



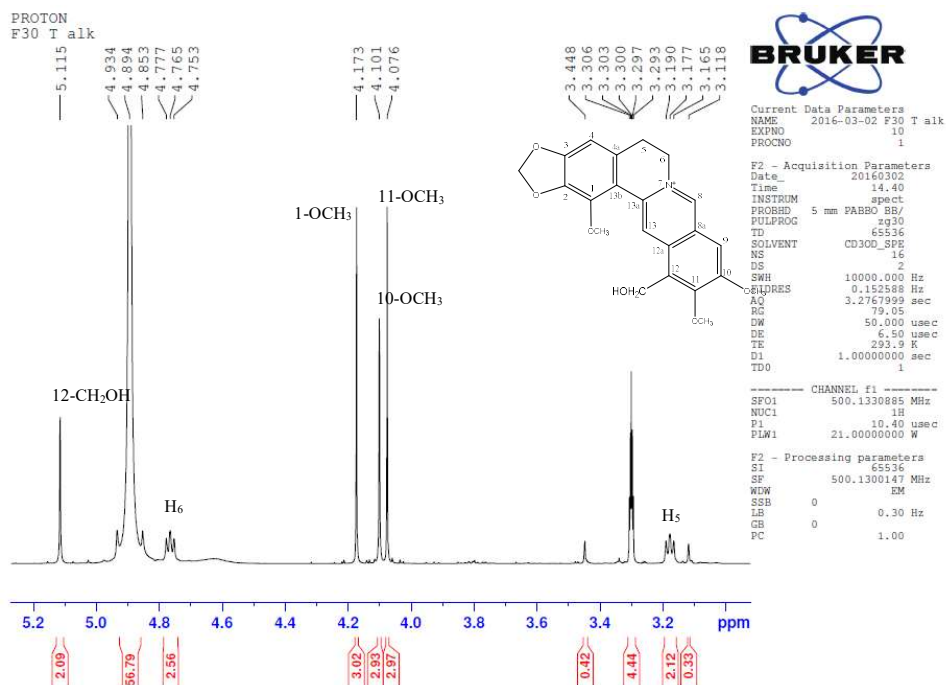
S48: LC-MS Spectrum of Compound 4 (alborine)



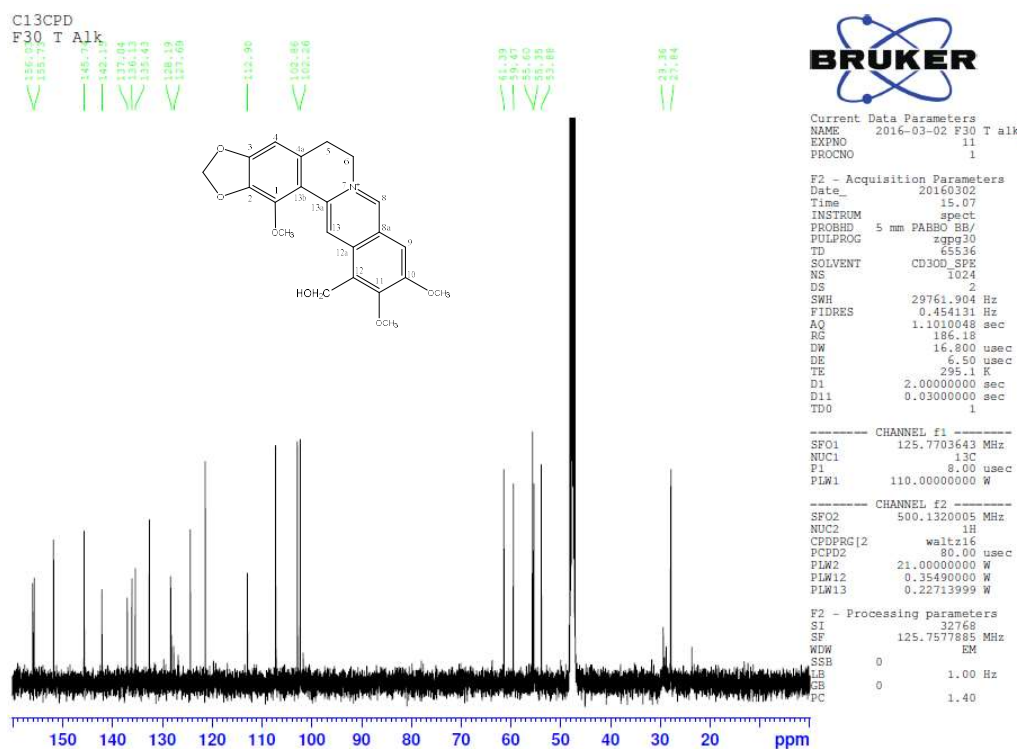
S49: $^1\text{H-NMR}$ (500 MHz, CD_3OD) Spectrum of Compound 4 (alborine)



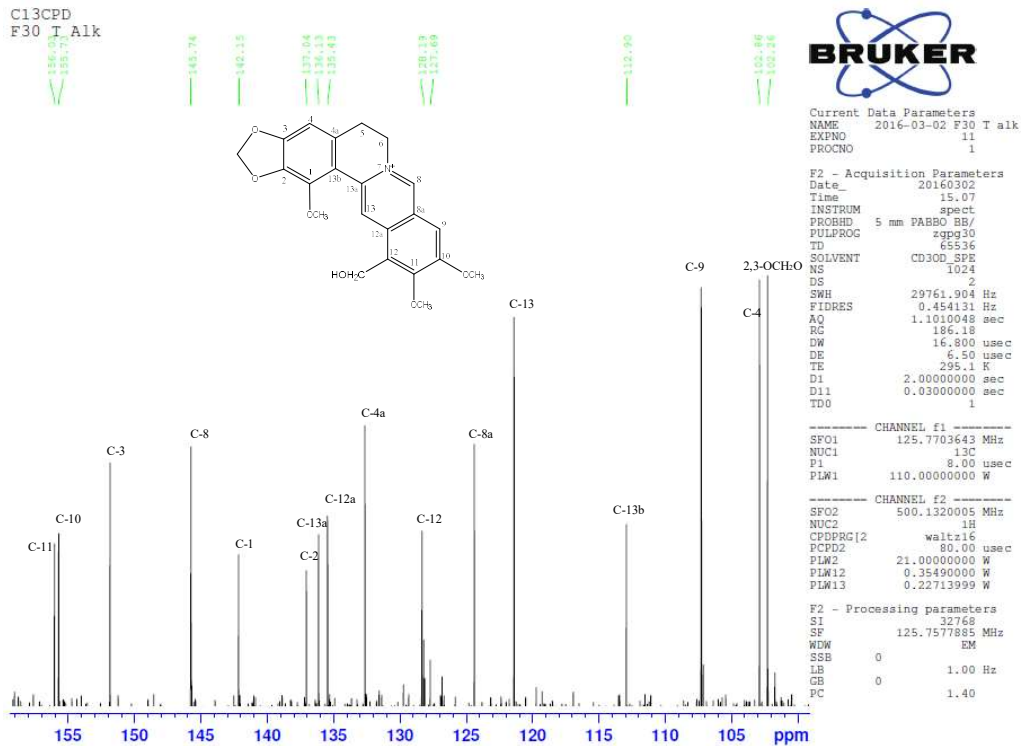
S50: Expansion of the $^1\text{H-NMR}$ (500 MHz, CD_3OD) Spectrum of Compound 4 (alborine)



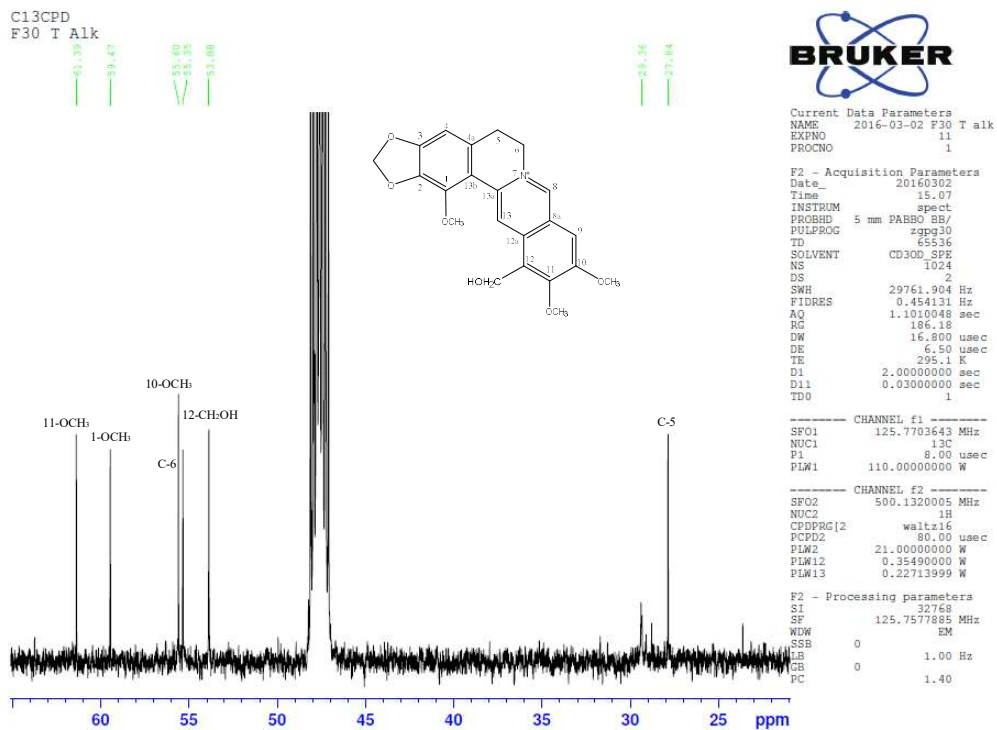
S51: Expansion of the ^1H -NMR (500 MHz, CD_3OD) Spectrum of Compound 4 (alborine)



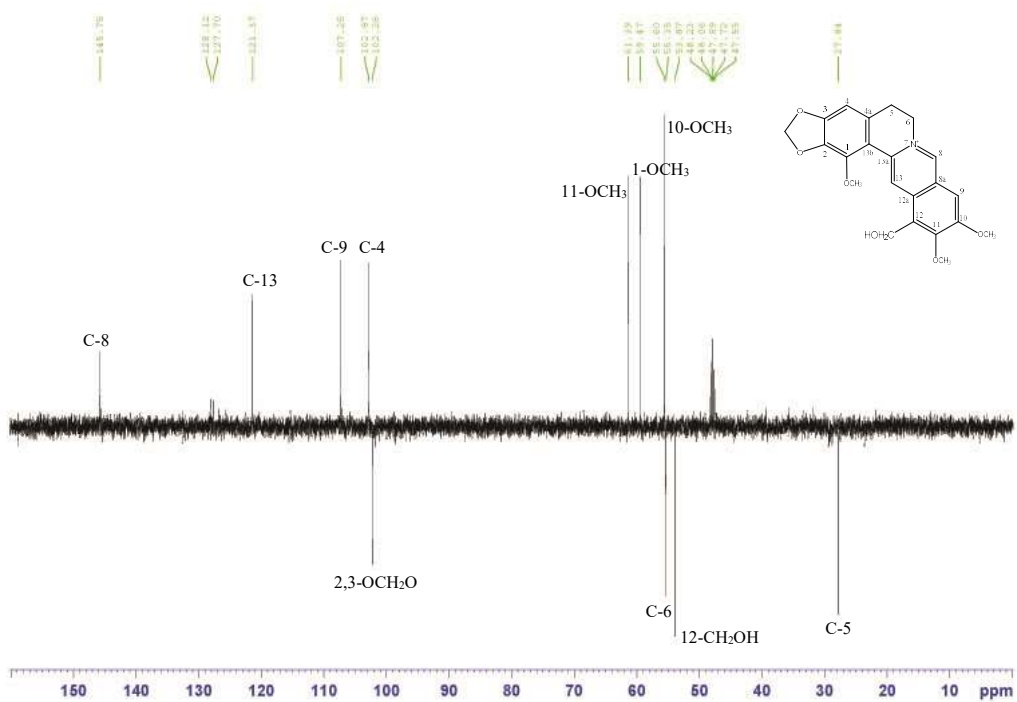
S52: ^{13}C -NMR (500 MHz) Spectrum of Compound 4 (alborine)



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

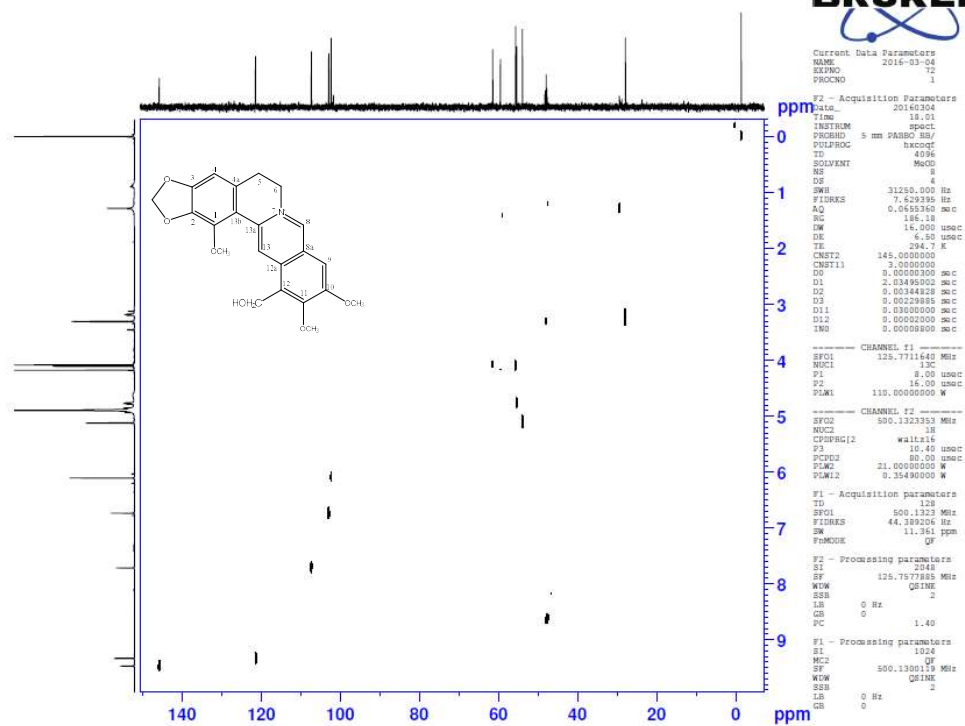


S54: Expansion of the ^{13}C -NMR (500 MHz) Spectrum of Compound 4 (alborine)



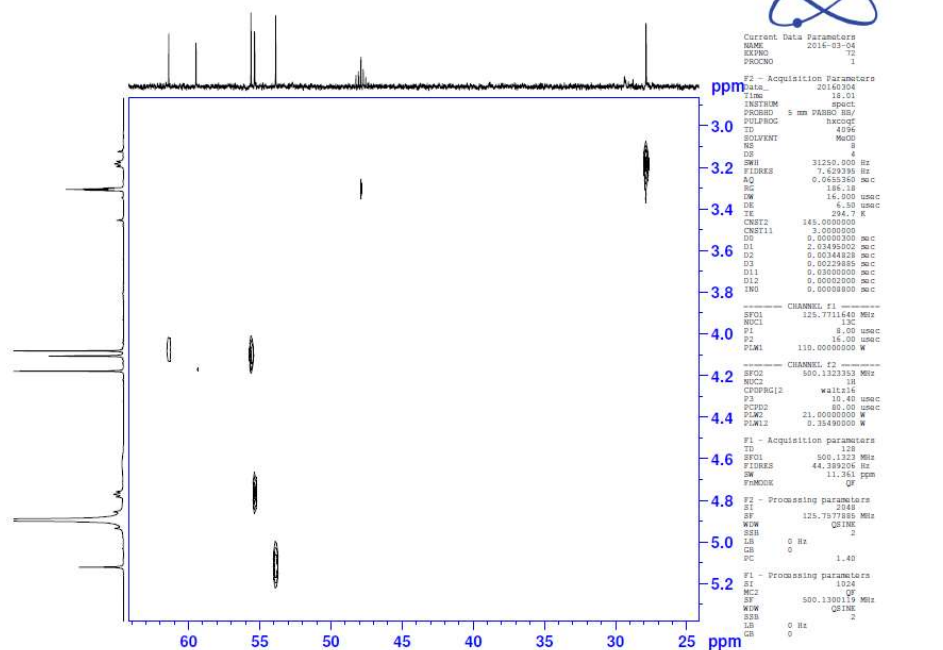
S55: DEPT (500 MHz) Spectrum of Compound 4 (alborine)

HCCOSW MeOD
MAH F30



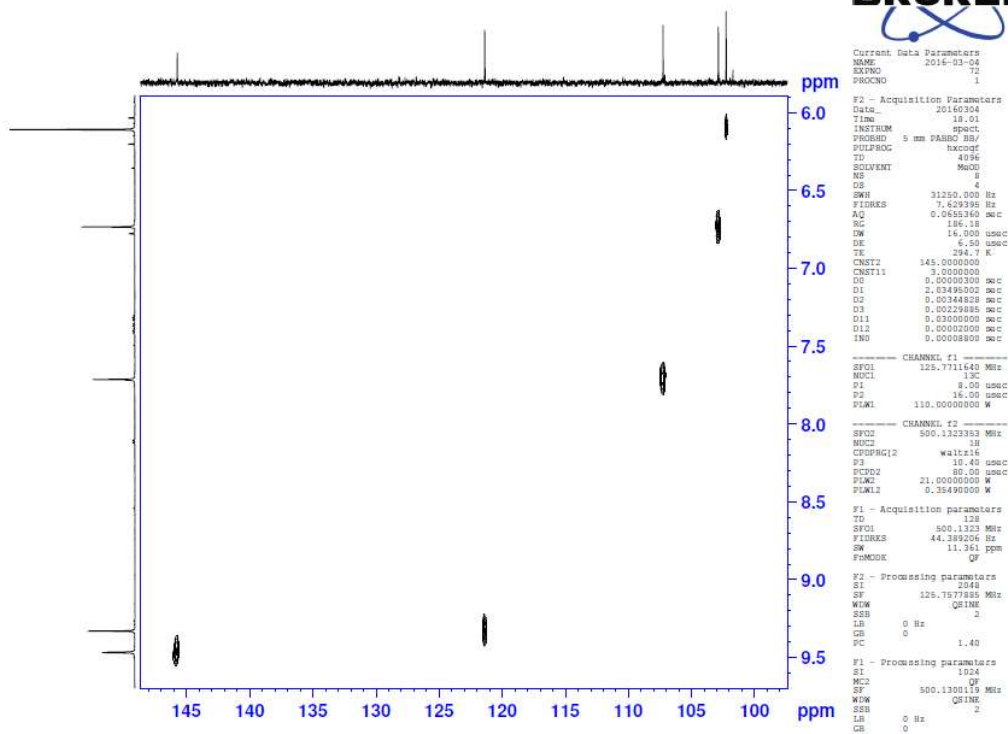
S56: HCCOSW Spectrum of Compound 4 (alborine)

HCCOSW MeOD
MAH F30



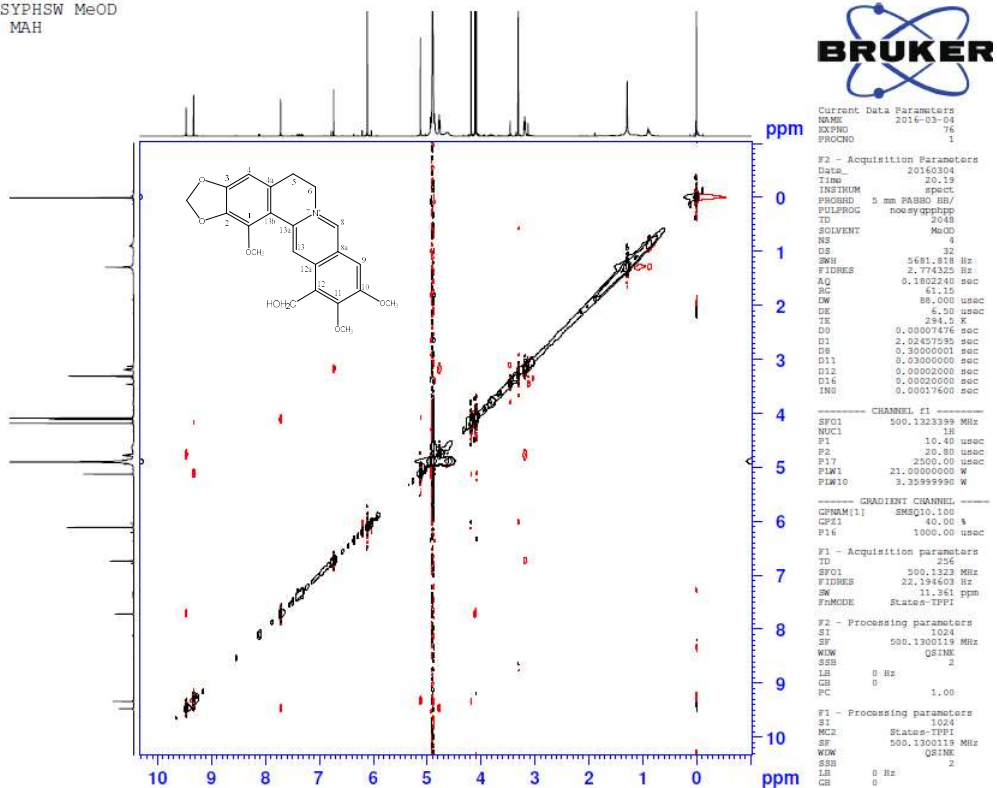
S57: Expansion of the HCCOW Spectrum of Compound 4 (alborine)

HCCOSW MeOD
MAH F30



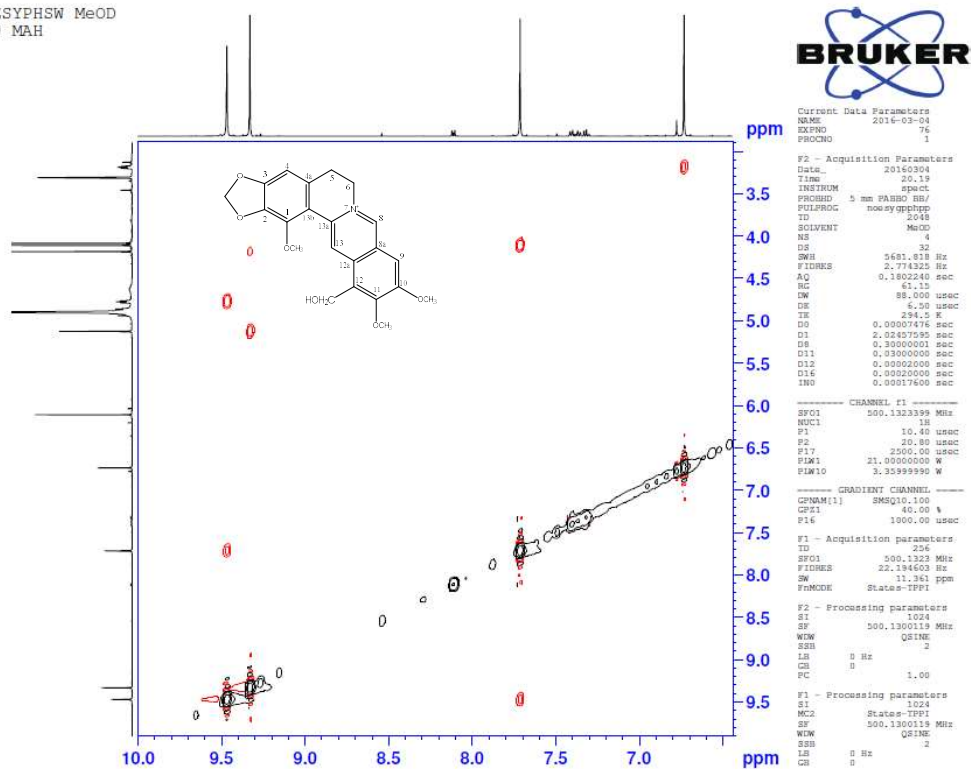
S58: Expansion of the HCCOW Spectrum of Compound 4 (alborine)

NOESYPSHW MeOD
F30 MAH



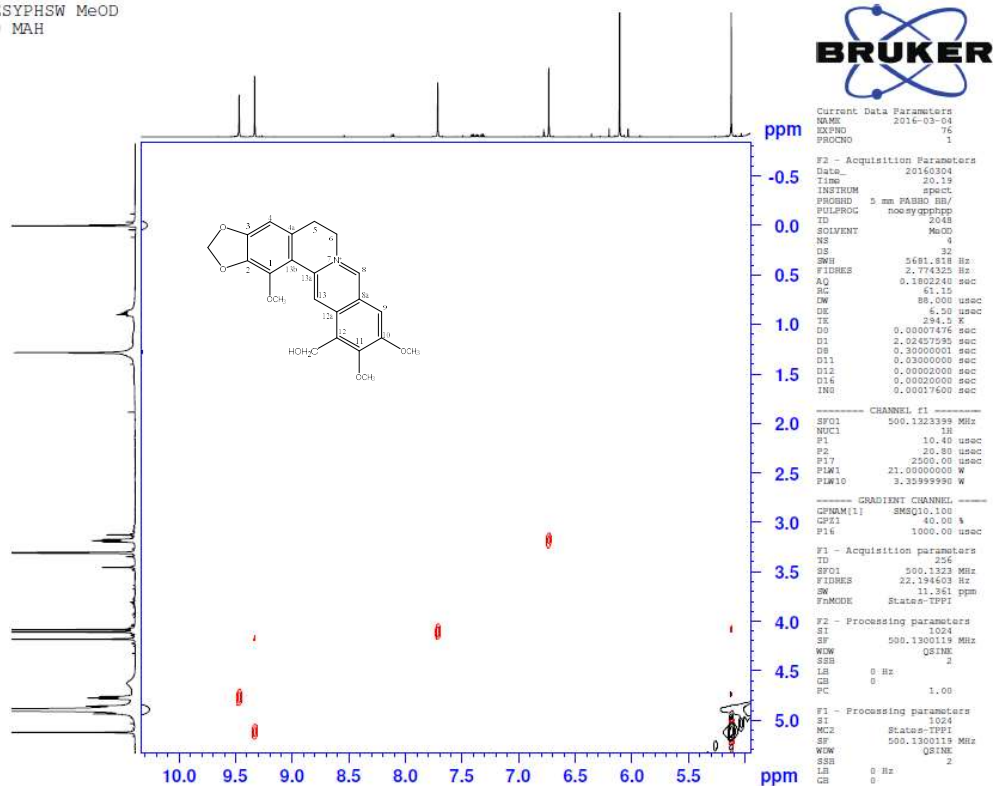
S59: NOSY (500 MHz) Spectrum of Compound 4 (alborine)

NOESYPSHW MeOD
F30 MAH



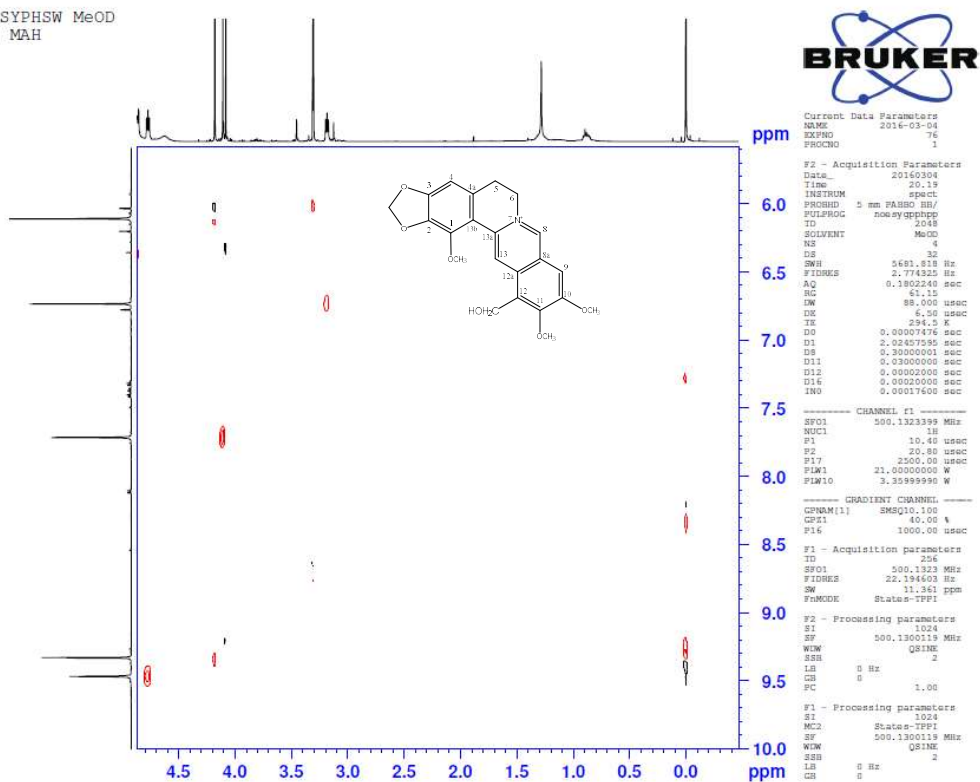
S60: Expansion of the NOSY (500 MHz) Spectrum of Compound 4 (alborine)

ESYPHSW MeOD
0 MAH



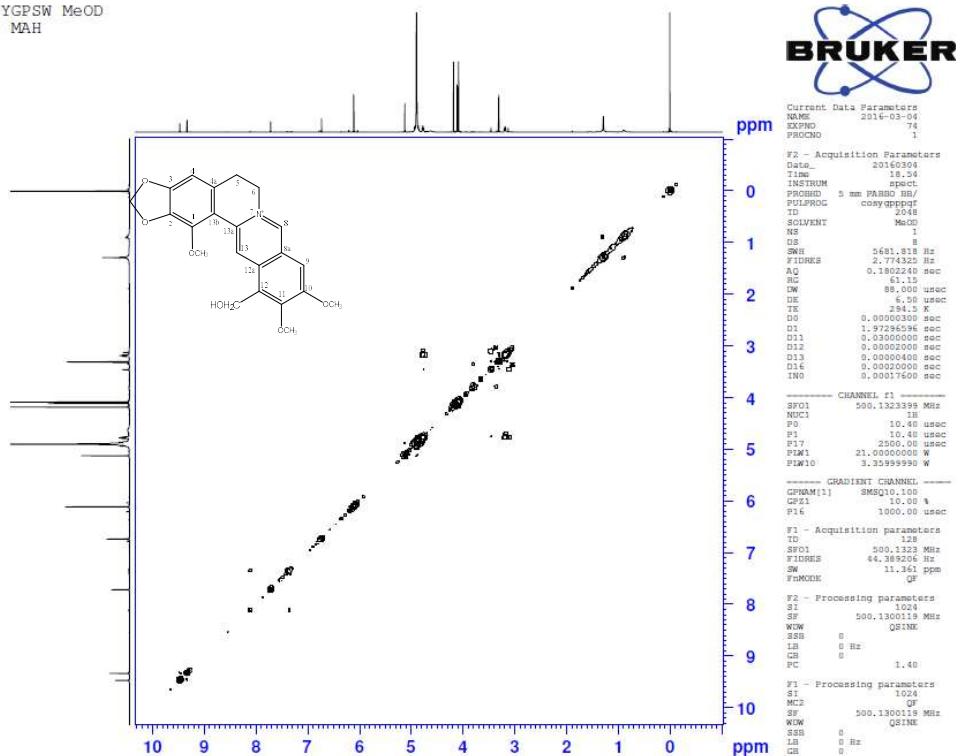
S61: Expansion of the NOSY (500 MHz) Spectrum of Compound 4 (alborine)

ESYPHSW MeOD
0 MAH



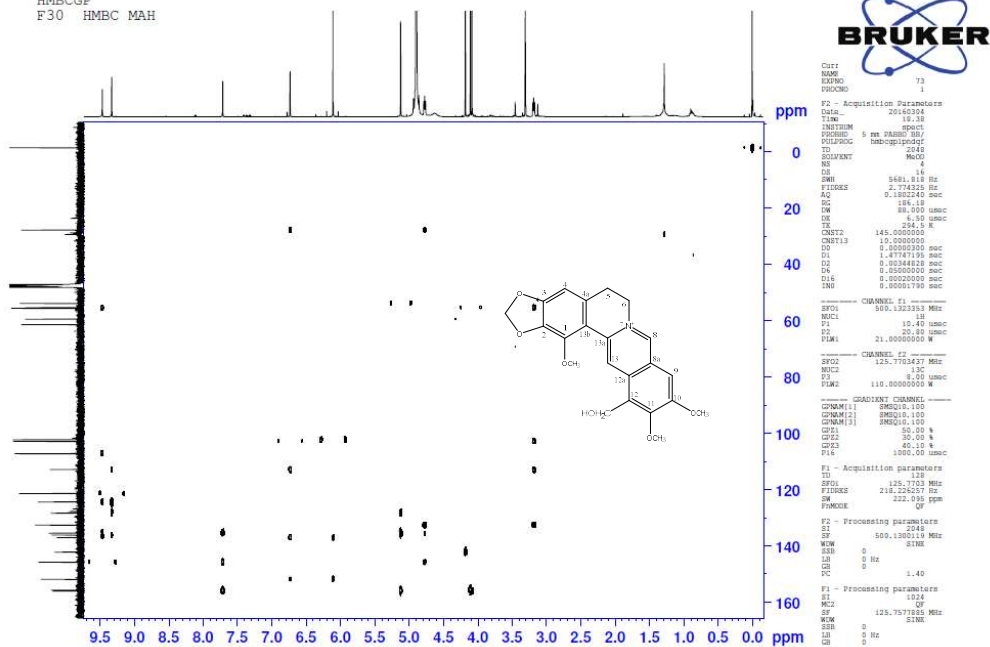
S62: Expansion of the NOSY (500 MHz) Spectrum of Compound 4 (alborine)

COSYGPSW MeOD
F30 MAH

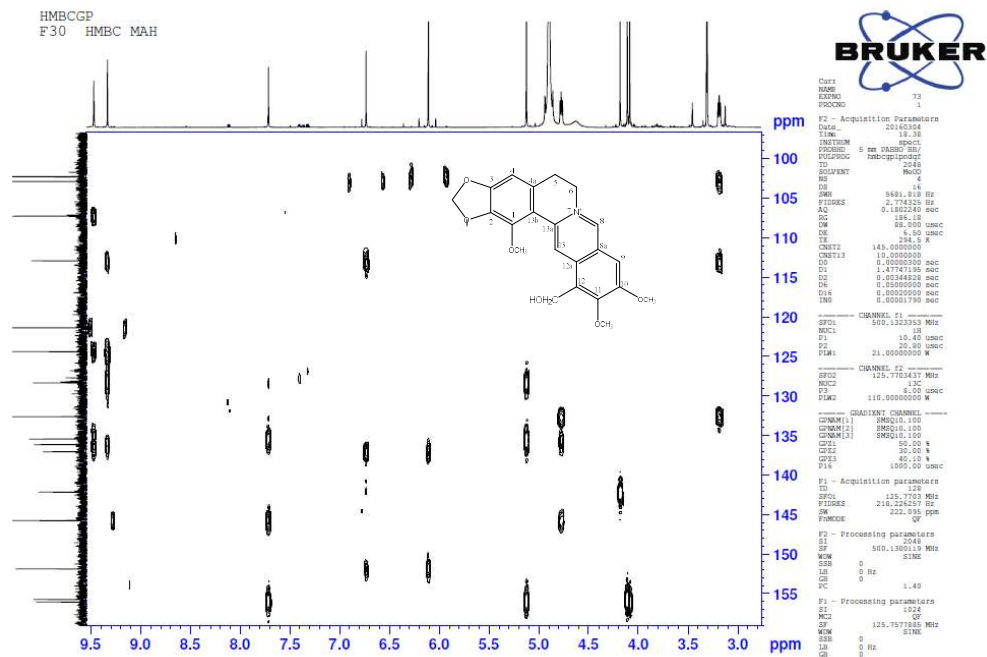


S63: COSY (500 MHz) Spectrum of Compound 4 (alborine)

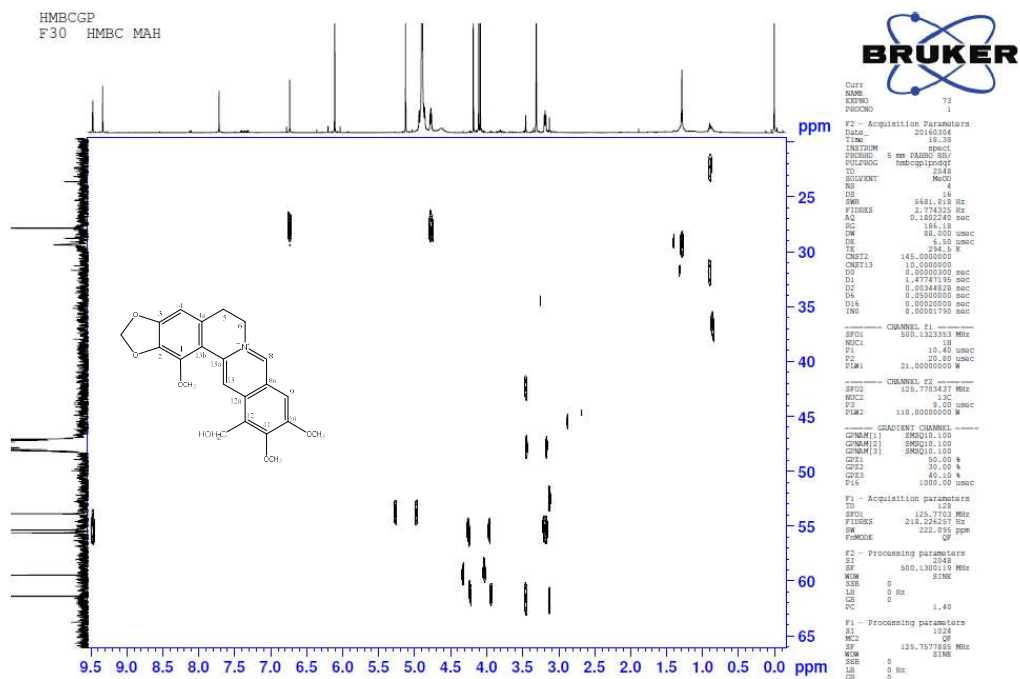
HMBGCP
F30 HMBG MAH



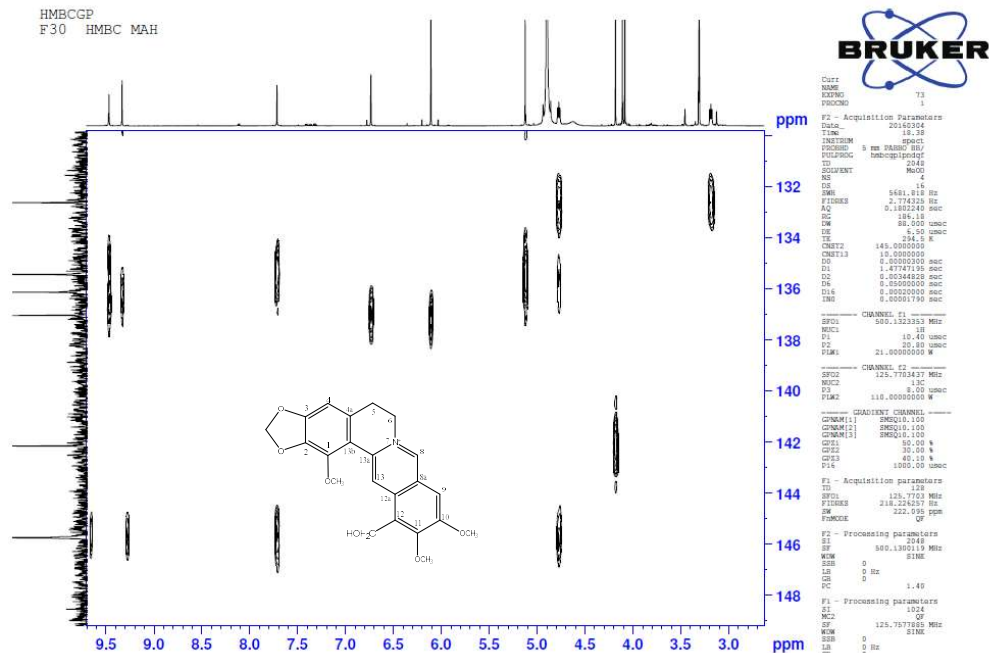
S64: HMBC (500 MHz, CDCl₃) Spectrum of Compound 4 (alborine)



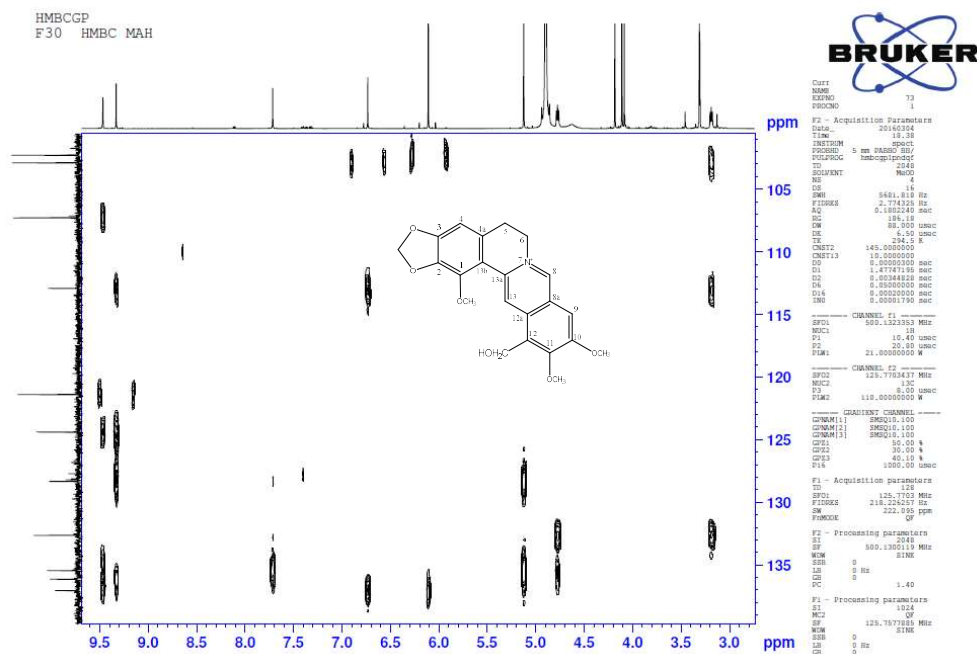
S65: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 4 (alborine)



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

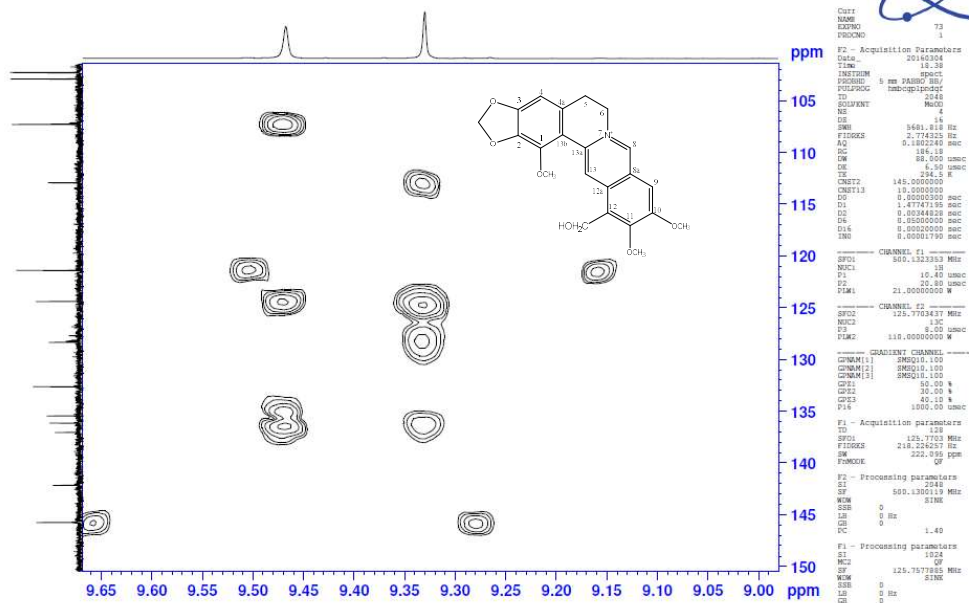


S67: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 4 (alborine)



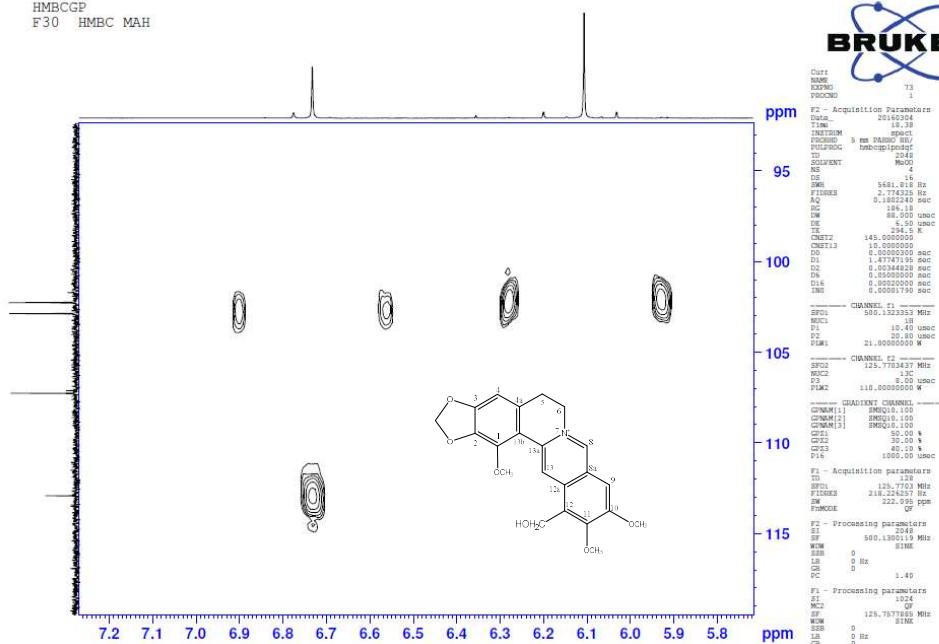
S68: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 4 (alborine)

HMBCGP
F30 HMBC MAH

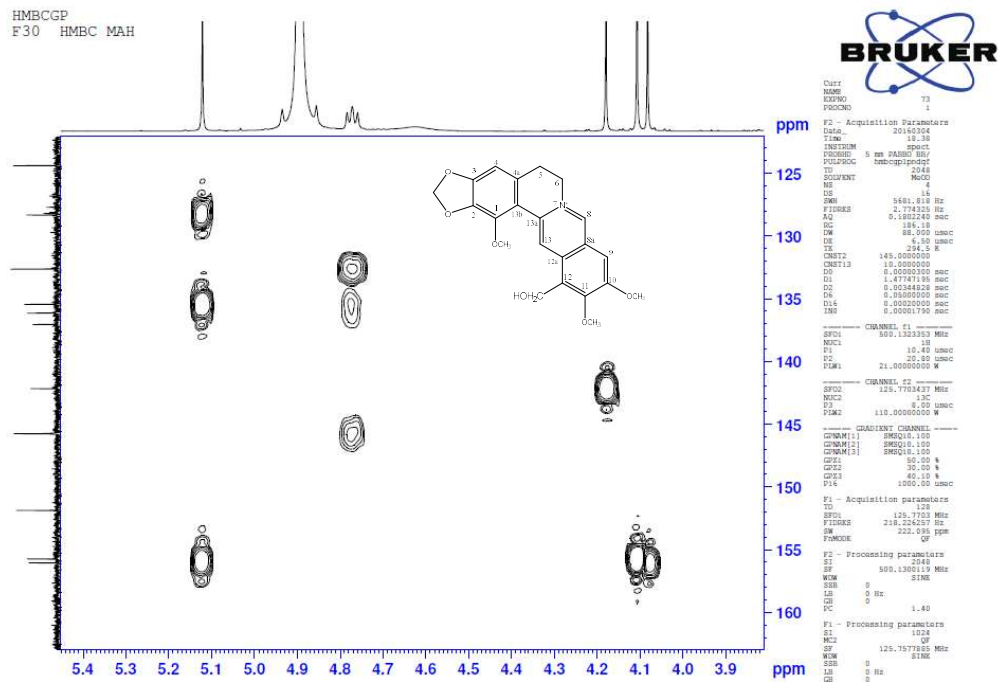


S69: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 4 (alborine)

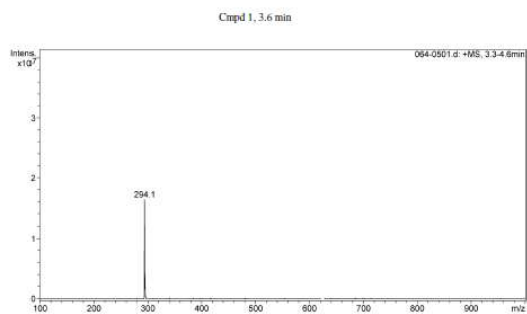
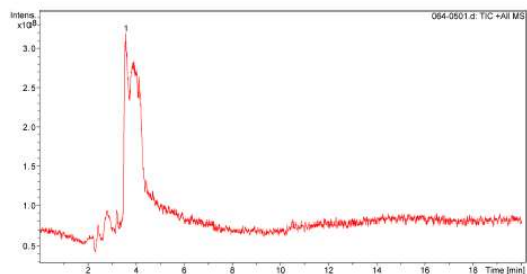
HMBCGP
F30 HMBC MAH



S70: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 4 (alborine)

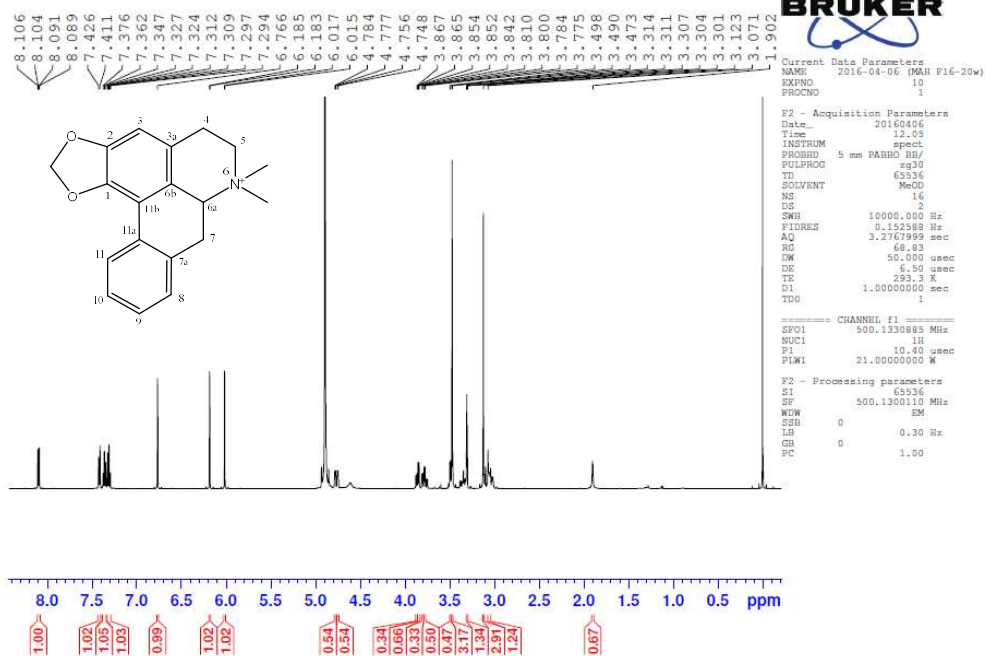


S71: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound **4** (alborine)



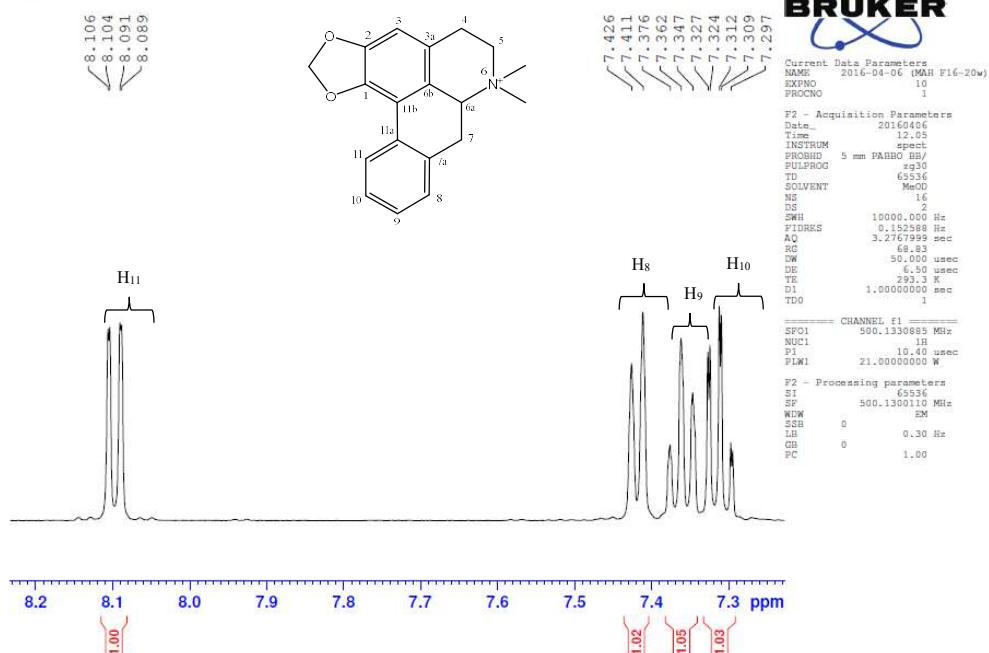
S72: LC-MS Spectrum of Compound **5** (remrefidine)

PROTON
MAH F16-20w



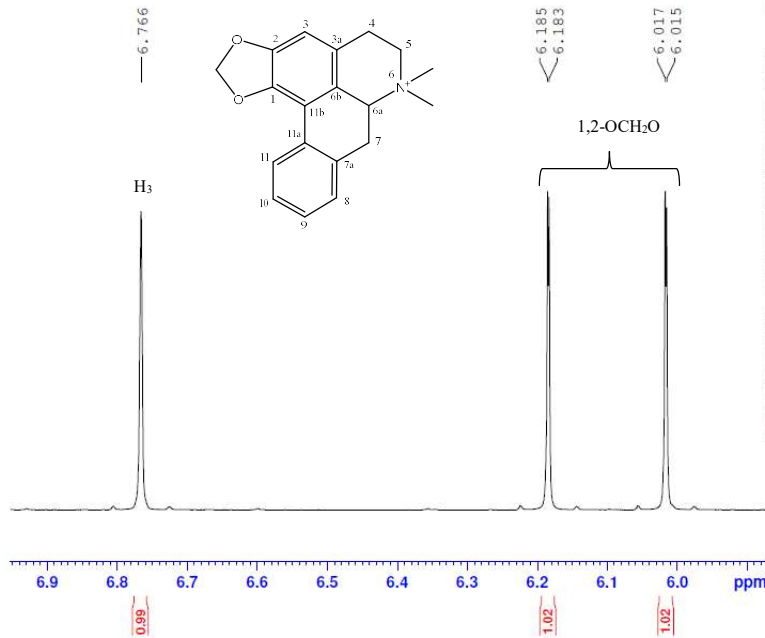
S73: $^1\text{H-NMR}$ (500 MHz, CD_3OD) Spectrum of Compound 5 (remrefidine)

PROTON
MAH F16-20w



S74: Expansion of the $^1\text{H-NMR}$ (500 MHz) Spectrum of Compound 5 (remrefidine)

PROTON
MAH F16-20w



Current Data Parameters
NAME: 2016-04-06 (MAH F16-20w)
EXPNO: 10
PROCNO: 1

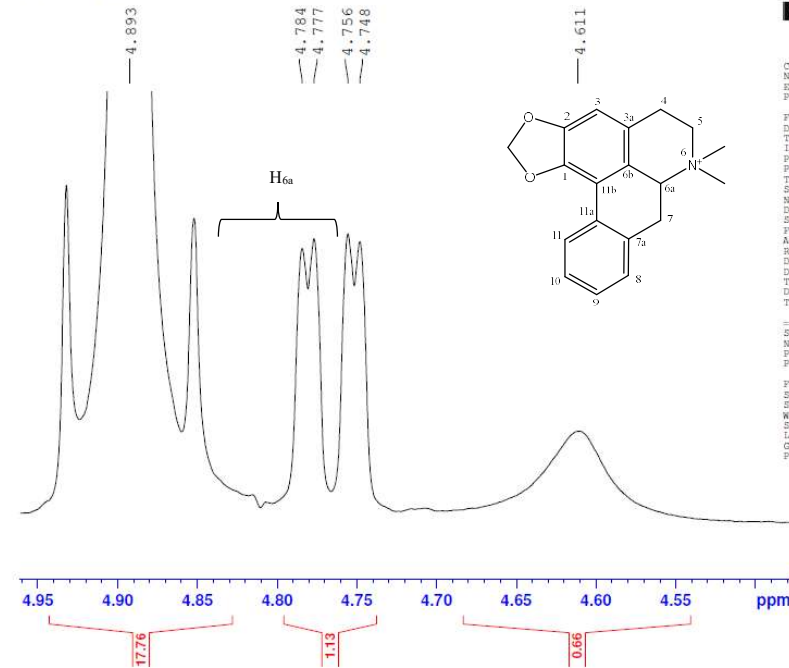
F2 - Acquisition Parameters
Date_: 20160406
Time: 12.05
INSTRUM: spect
PROBHD: 5 mm PABBO BB/
PULPROG: zg30
TD: 65536
SOLVENT: MeOD
NS: 16
DS: 2
SWH: 10000.000 Hz
FIDRES: 0.152589 Hz
AQ: 3.2767999 sec
RG: 68.83
DW: 50.000 usec
DE: 6.30 usec
TE: 293.3 K
D1: 1.00000000 sec
TD0: 1

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

F2 - Processing parameters
S1: 65536
SF: 500.1300110 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

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

PROTON
MAH F16-20w



Current Data Parameters
NAME: 2016-04-06 (MAH F16-20w)
EXPNO: 10
PROCNO: 1

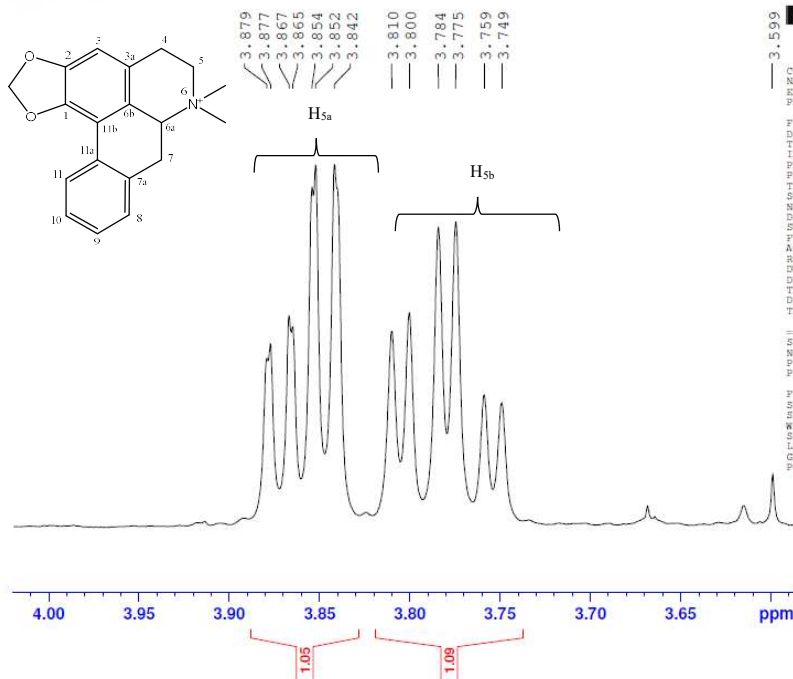
F2 - Acquisition Parameters
Date_: 20160406
Time: 12.05
INSTRUM: spect
PROBHD: 5 mm PABBO BB/
PULPROG: zg30
TD: 65536
SOLVENT: MeOD
NS: 16
DS: 2
SWH: 10000.000 Hz
FIDRES: 0.152589 Hz
AQ: 3.2767999 sec
RG: 68.83
DW: 50.000 usec
DE: 6.30 usec
TE: 293.3 K
D1: 1.00000000 sec
TD0: 1

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

F2 - Processing parameters
S1: 65536
SF: 500.1300110 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

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

PROTON
MAH F16-20w



Current Data Parameters
NAME: 2016-04-06 (MAH F16-20w)
EXPNO: 10
PROCNO: 1

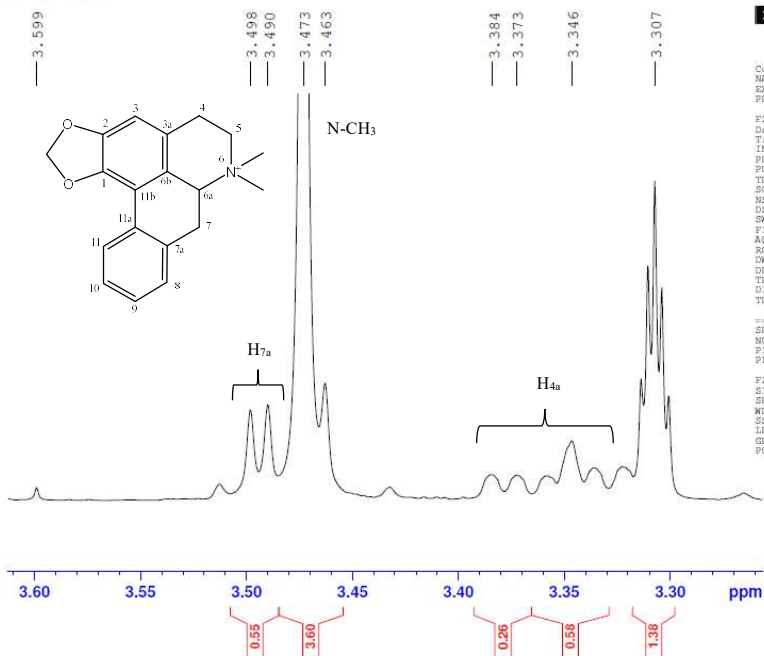
F2 - Acquisition Parameters
Date_: 20160406
Time: 12.03
INSTRUM: spect
PROBHD: 5 mm PABBO BB/
PULPROG: zg30
TD: 65536
SOLVENT: MeOD
NS: 16
DS: 2
SWH: 10000.000 Hz
FIDRES: 0.152588 Hz
AQ: 3.2767999 sec
RC: 68.93
DW: 50.000 usec
DE: 6.50 usec
TE: 293.3 K
D1: 1.00000000 sec
TDO: 1

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

F2 - Processing parameters
SI: 65536
SF: 500.1300110 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

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

PROTON
MAH F16-20w



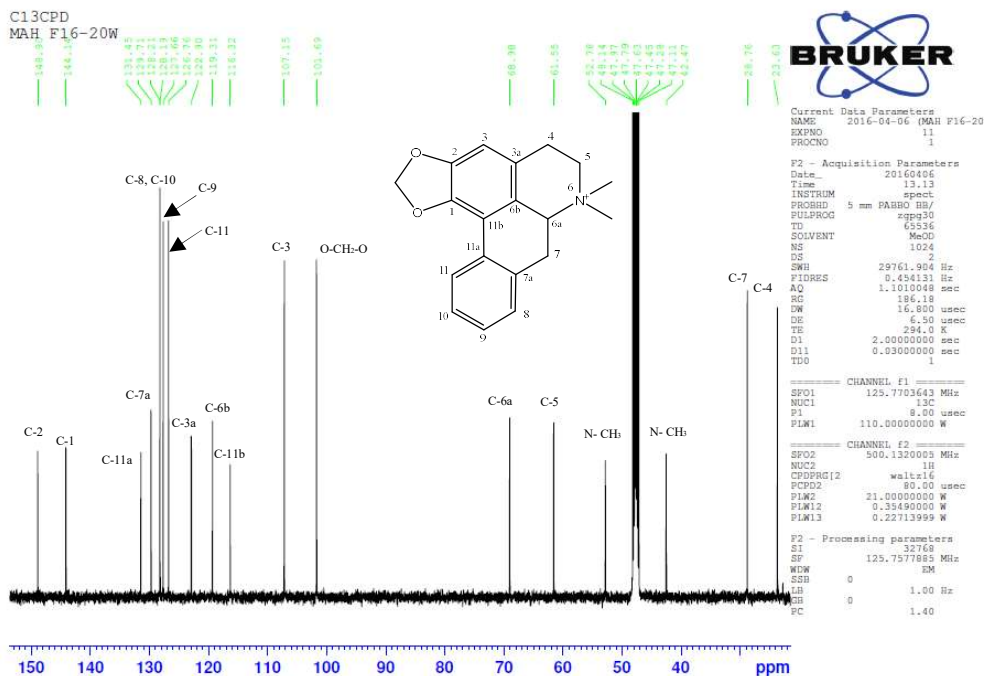
Current Data Parameters
NAME: 2016-04-06 (MAH F16-20w)
EXPNO: 10
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20160406
Time: 12.03
INSTRUM: spect
PROBHD: 5 mm PABBO BB/
PULPROG: zg30
TD: 65536
SOLVENT: MeOD
NS: 16
DS: 2
SWH: 10000.000 Hz
FIDRES: 0.152588 Hz
AQ: 3.2767999 sec
RC: 68.93
DW: 50.000 usec
DE: 6.50 usec
TE: 293.3 K
D1: 1.00000000 sec
TDO: 1

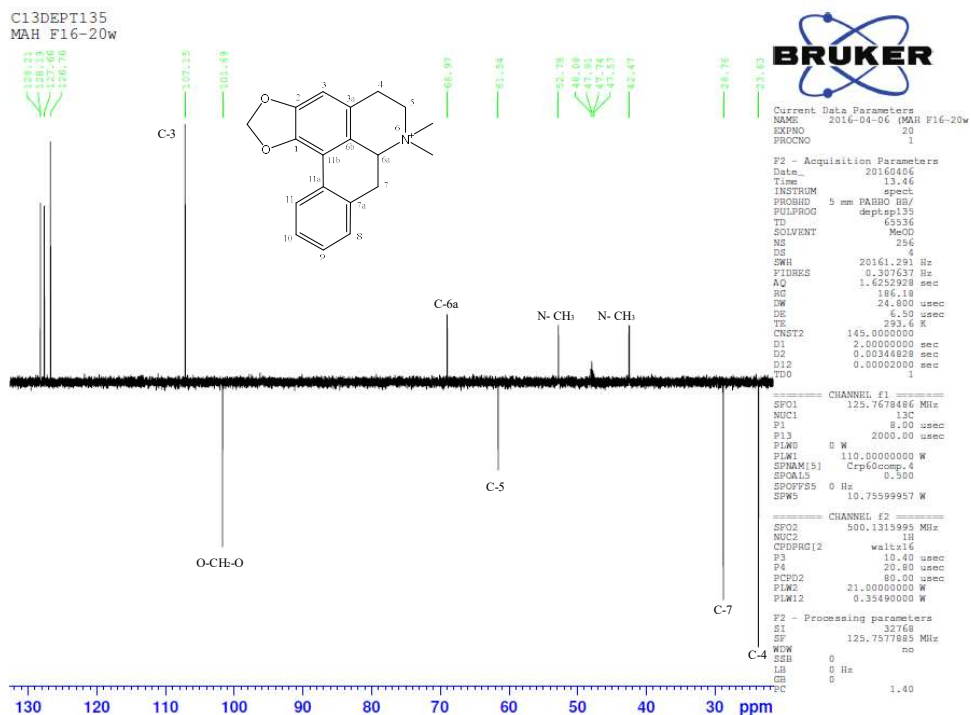
==== CHANNEL f1 =====
SFO1: 500.1330885 MHz
NUC1: 1H
P1: 10.40 usec
PLW1: 21.00000000 W

F2 - Processing parameters
SI: 65536
SF: 500.1300110 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

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

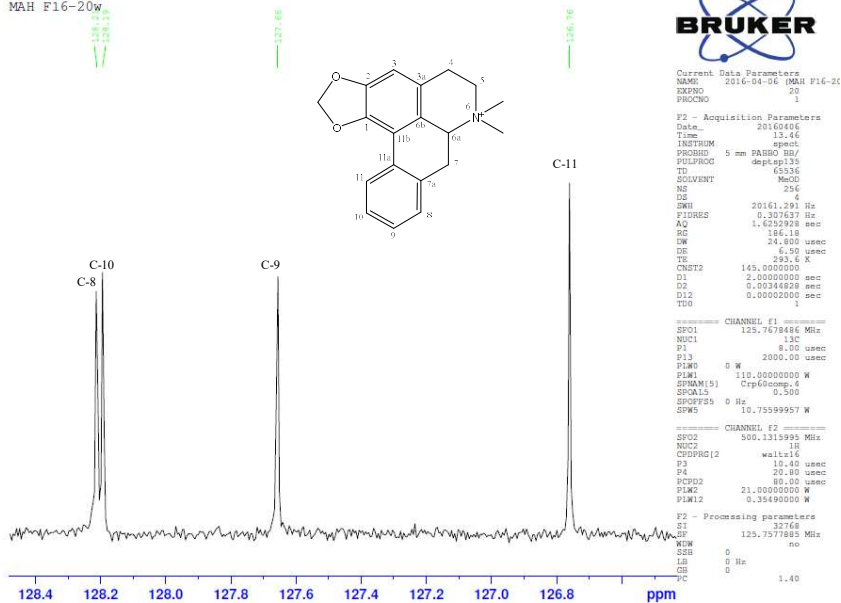


S79: ¹³C-NMR (500 MHz) Spectrum of Compound 5 (remrefidine)



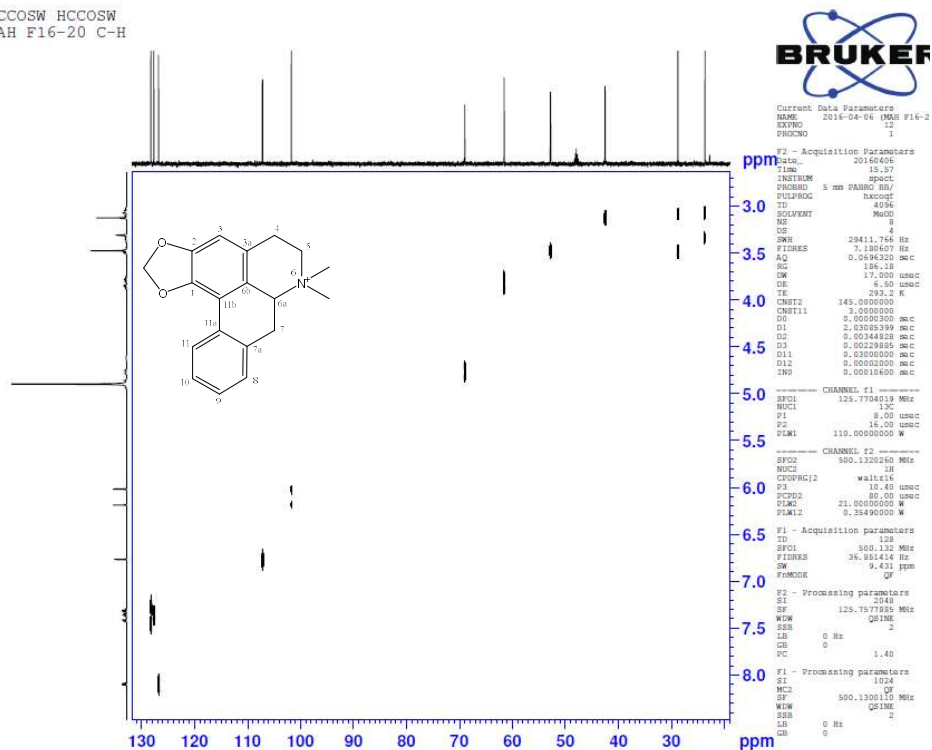
S80: DEPT (500 MHz) Spectrum of Compound 5 (remrefidine)

C13DEPT135
MAH F16-20W



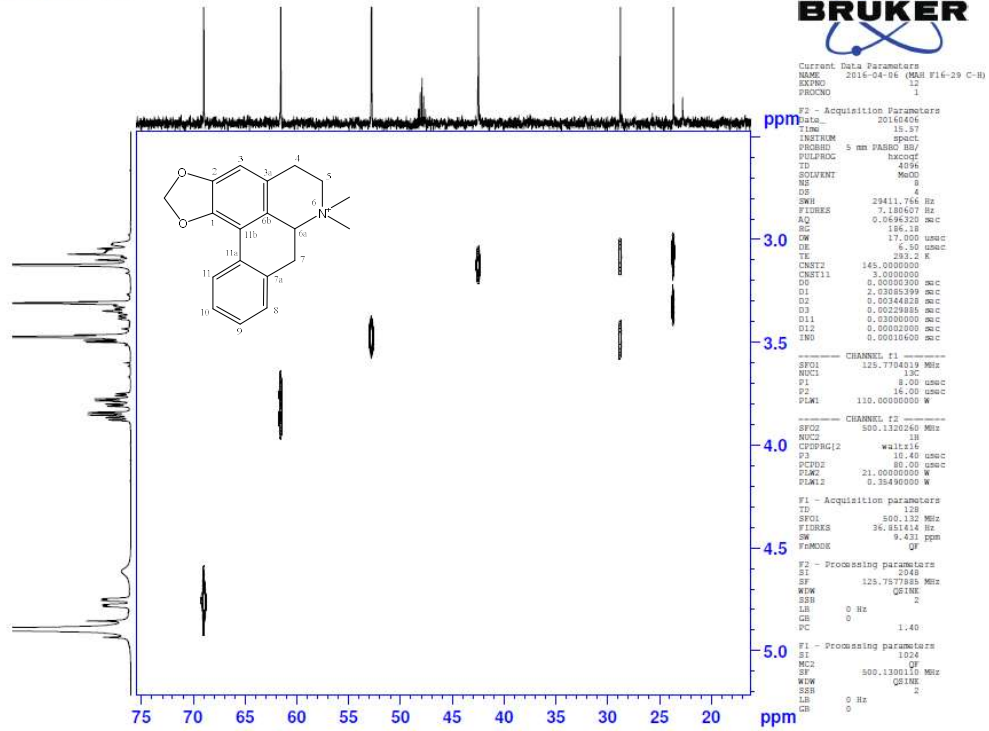
S81: Expansion of the DEPT (500 MHz) Spectrum of Compound 5 (remrefidine)

HCCOSW HCCOSW
MAH F16-20 C-H



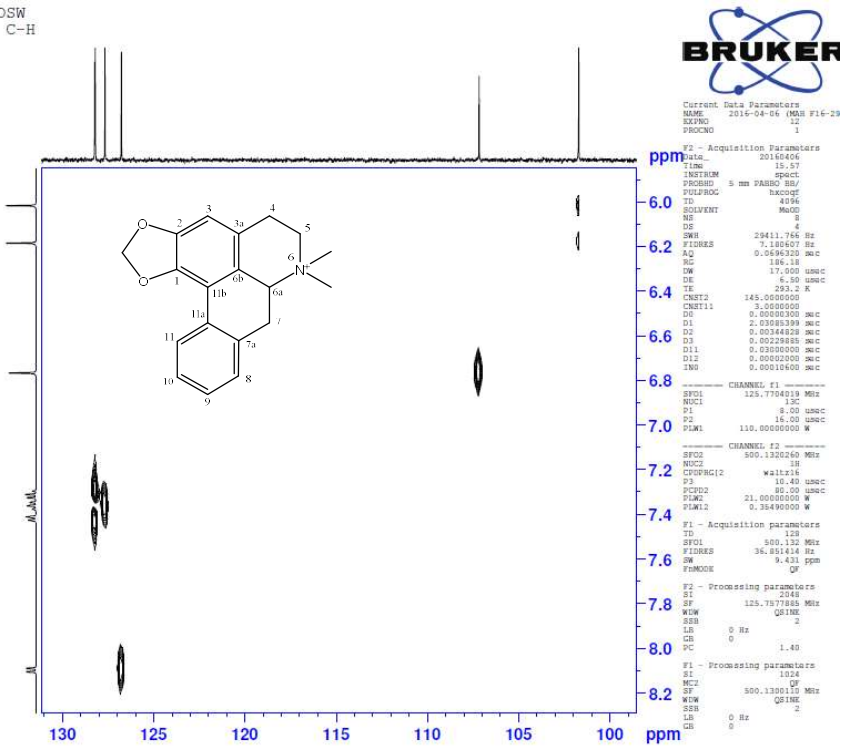
S82: HCCOW Spectrum of Compound 5 (remrefidine)

HCCOSW HCCOSW
MAH F16-20 C-H



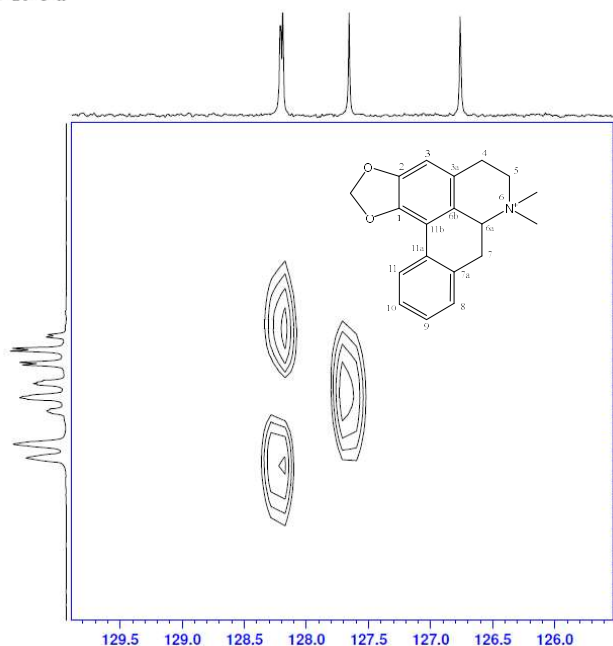
S83: Expansion of the HCCOSW Spectrum of Compound 5 (remrefidine)

HCCOSW
6-20 C-H



S84: Expansion of the HCCOSW Spectrum of Compound 5 (remrefidine)

W HCCOSW
16-20 C-H



Current Data Parameters
NAME 2016-04-06 (MNH F16-29 C-H)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160406
Time 15:37
INSTRUM spect
PROBHD 5 mm QNP800 BBO
PULPROG zgpg30
SOLVENT MeOH
NS 4
DS 4
SWH 29411.746 Hz
FIDRES 7.180607 Hz
AQ 0.0696202 sec
RG 186.18
DM 173.000 usec
DE 4.50 usec
TE 300.2 K
DO 145.000000
CSTRT1 3.000000
CSTRT2 0.000000 sec
D1 0.0000000 sec
D2 2.0000000 sec
D3 0.00348023 sec
D4 0.00228000 sec
D5 0.03000000 sec
D6 0.00000000 sec
D7 0.00016000 sec

7.10
7.15
7.20
7.25

CHANNEL f1
SFO1 125.770010 MHz
NUC1 13C
P1 10.00 usec
P2 16.00 usec
PLW1 110.0000000 W

7.30
7.35

CHANNEL f2
SFO2 300.1320260 MHz
NUC2 1H
CPOPRG2 zgpg30
D1 10.40 usec
D2 21.0000000 sec
D3 0.03490000 W

7.40
7.45

F1 - Acquisition parameters
TD 128
SFO1 500.132 MHz
FIDRES 36.891414 Hz
SW 9.431 ppm
FHMNDR 0

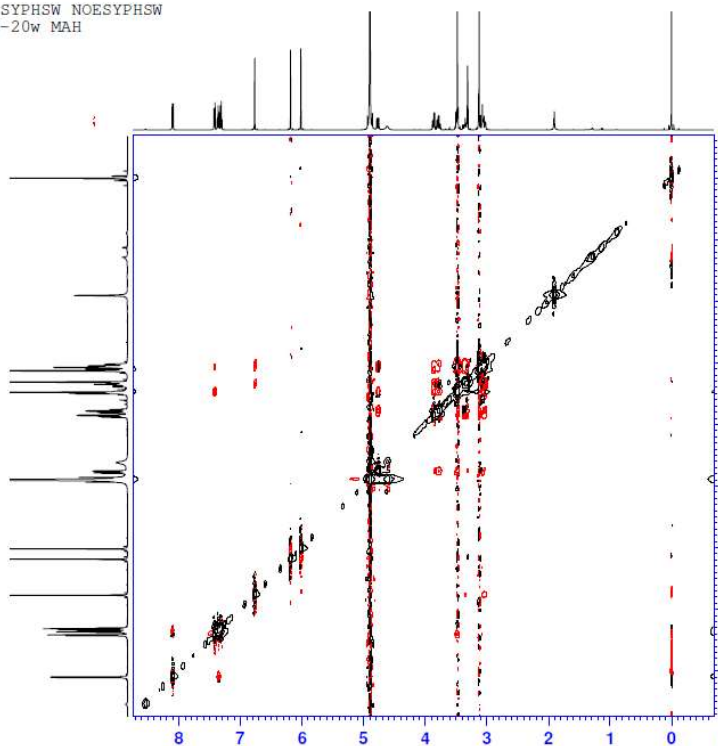
7.50
7.55

F2 - Processing parameters
SI 3204
SF 125.777788 MHz
WDW EM
SSB 2
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 0
SF 500.130010 MHz
WDW EM
SSB 2
GB 0
PC 0

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

OESYPSHW NOESYPSHW
16-20w MAH



Current Data Parameters
NAME 2016-04-06 (F16-20w NO)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160406
Time 14:08
INSTRUM spect
PROBHD 5 mm PARBO BBI
PULPROG noesypppp
TD 2048
SOLVENT MeOH
NS 4
DS 32
SWH 4716.901 Hz
FIDRES 2.303213 Hz
AQ 0.2170880 sec
RG 43.3
DM 105.000 usec
DE 6.50 usec
TE 300.2 K
DO 0.00009276 sec
D1 1.98771203 sec
D2 0.10000001 sec
D3 0.03000000 sec
D4 0.00020000 sec
D5 0.00020000 sec
D6 0.00021200 sec

0
1
2
3
4
5
6
7
8

CHANNEL f1
SFO1 500.1320260 MHz
NUC1 1H
P1 10.40 usec
P2 10.80 usec
P3 2500.00 usec
PLW1 21.0000000 W
PLW2 3.35999990 W

GRADIENT CHANNEL
CHANAM[1] SMO10.100
CPC1 40.00 %
P16 1000.00 usec

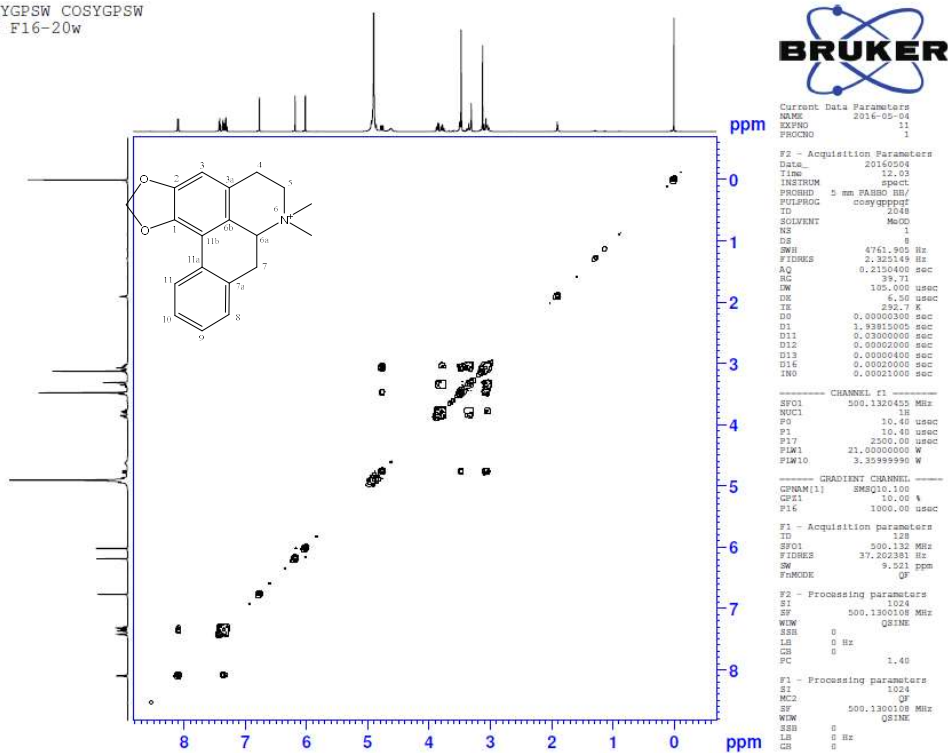
F1 - Acquisition parameters
TD 256
SFO1 500.132 MHz
FIDRES 18.425707 Hz
SW 9.431 ppm
FHMNDR States-TFPI

F2 - Processing parameters
SI 1024
SF 500.130010 MHz
WDW EM
SSB 2
GB 0
PC 1.00

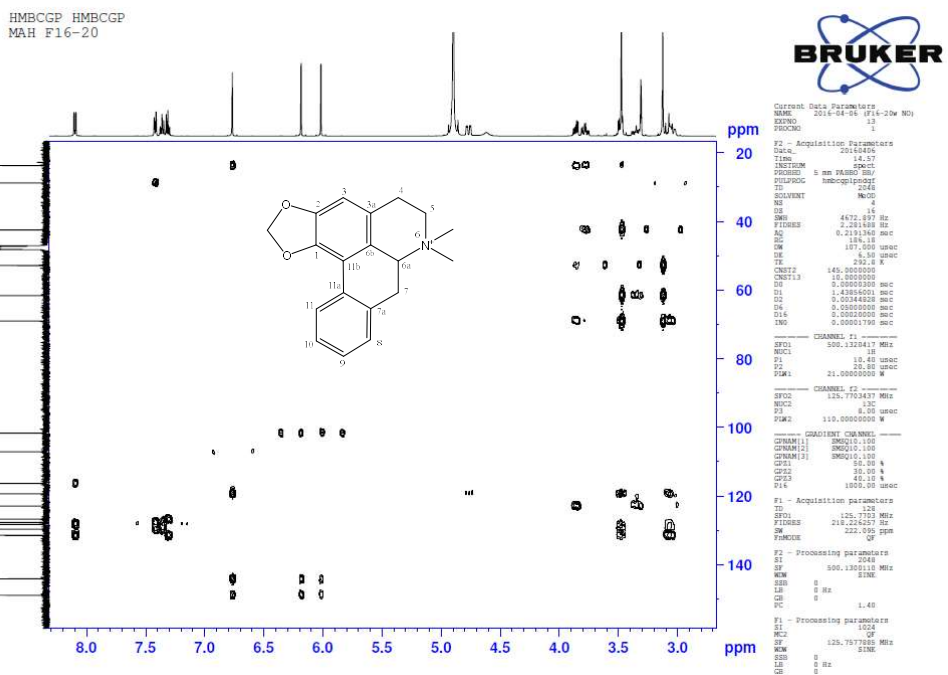
F1 - Processing parameters
SI 1024
MC2 States-TFPI
SF 500.130010 MHz
WDW EM
SSB 2
GB 0
PC 0

S86: NOESY (500 MHz) Spectrum of Compound 5 (remrefidine)

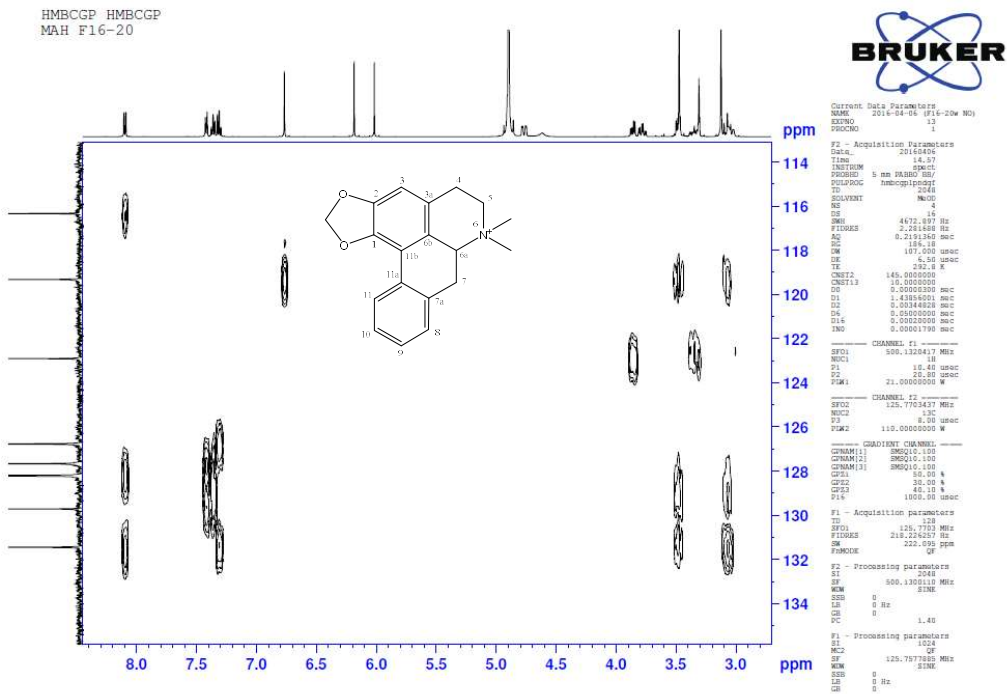
COSYGPW COSYGPW
MAH F16-20w



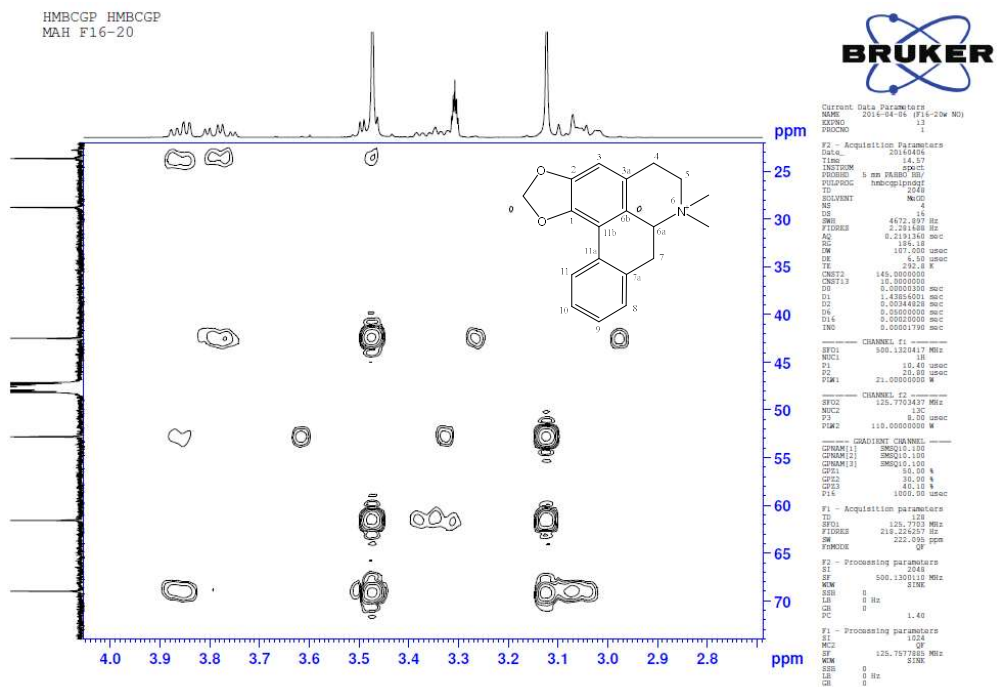
S87: COSY (500 MHz) Spectrum of Compound 5 (remrefidine)



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

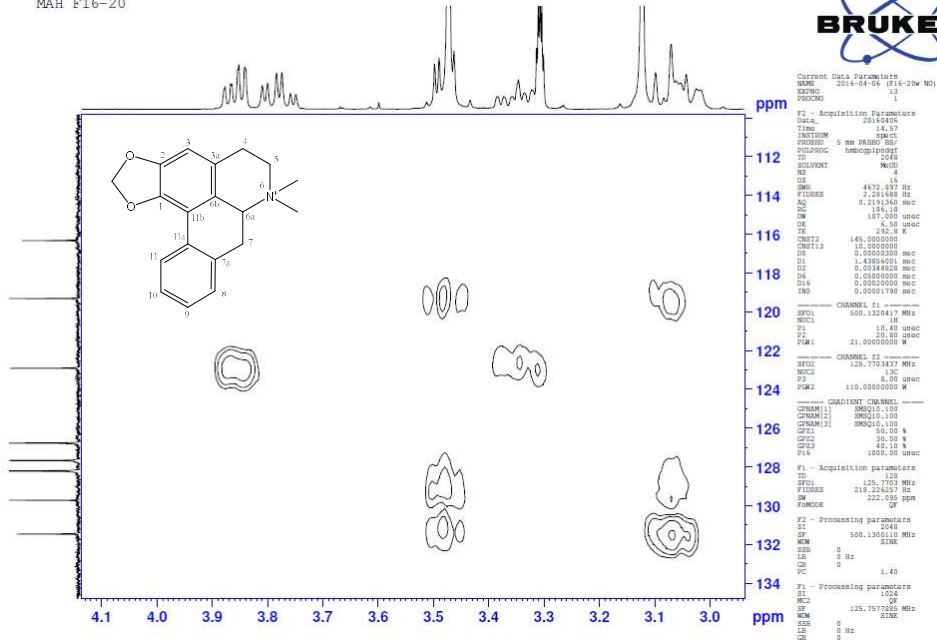


S89: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound **5** (remrefidine)



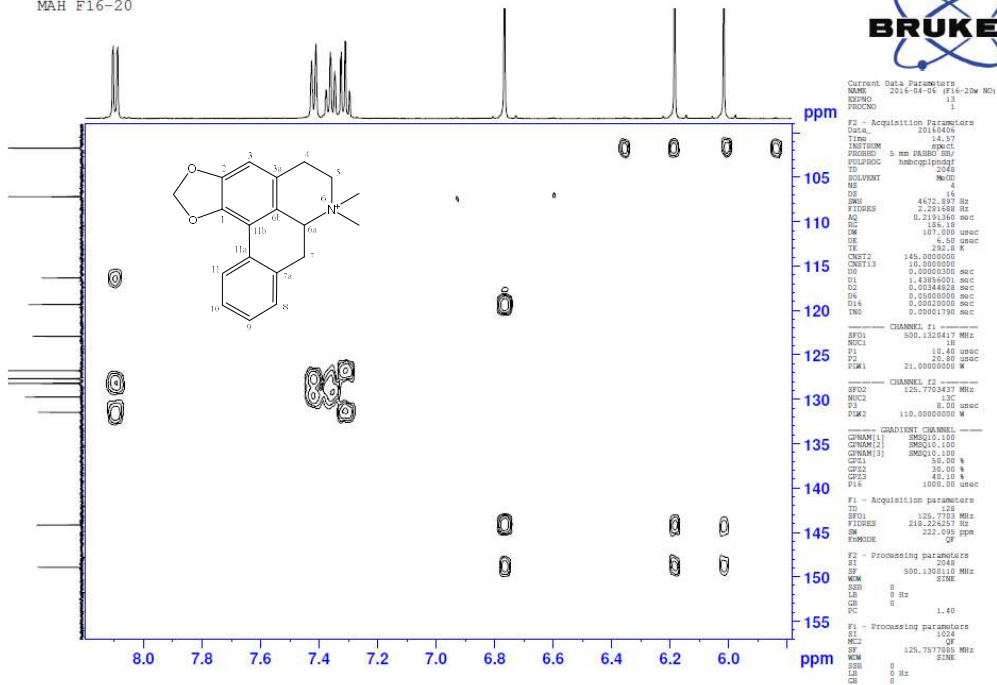
S90: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound **5** (remrefidine)

HMBCCG HMBCCG
MAH F16-20



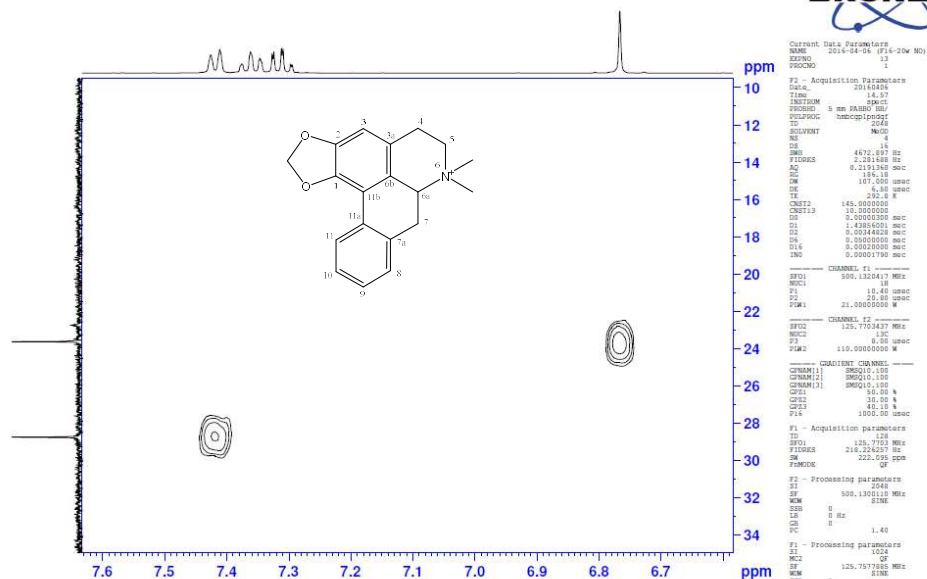
S91: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 5 (remrefidine)

HMBCCG HMBCCG
MAH F16-20



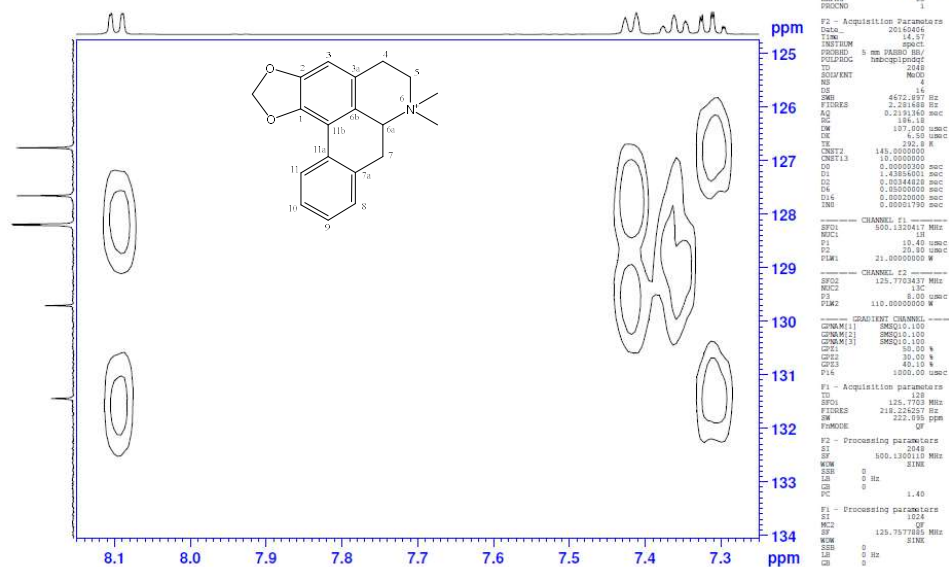
S92: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 5 (remrefidine)

HMBCGP HMBCGP
MAH F16-20

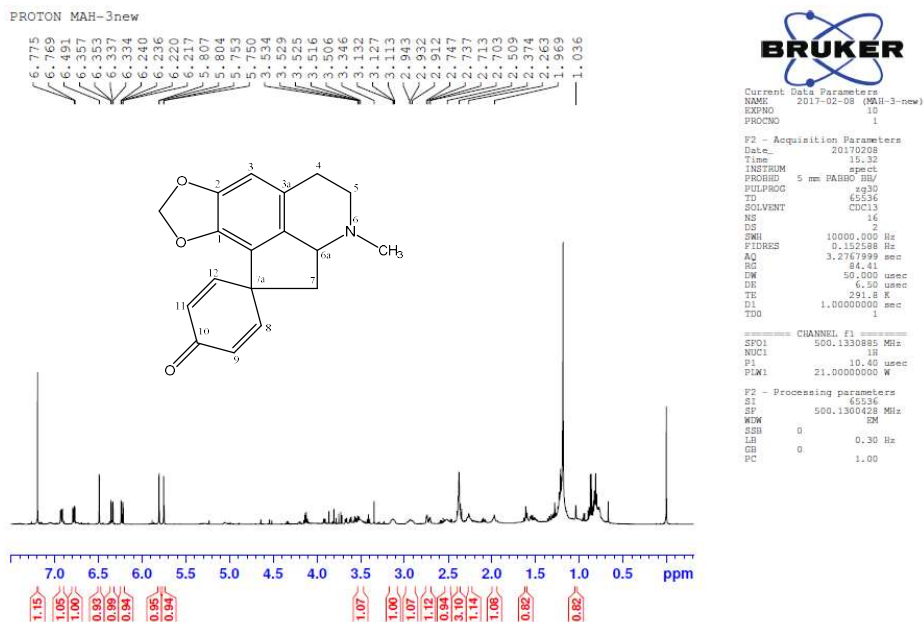


S93: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 5 (remrefidine)

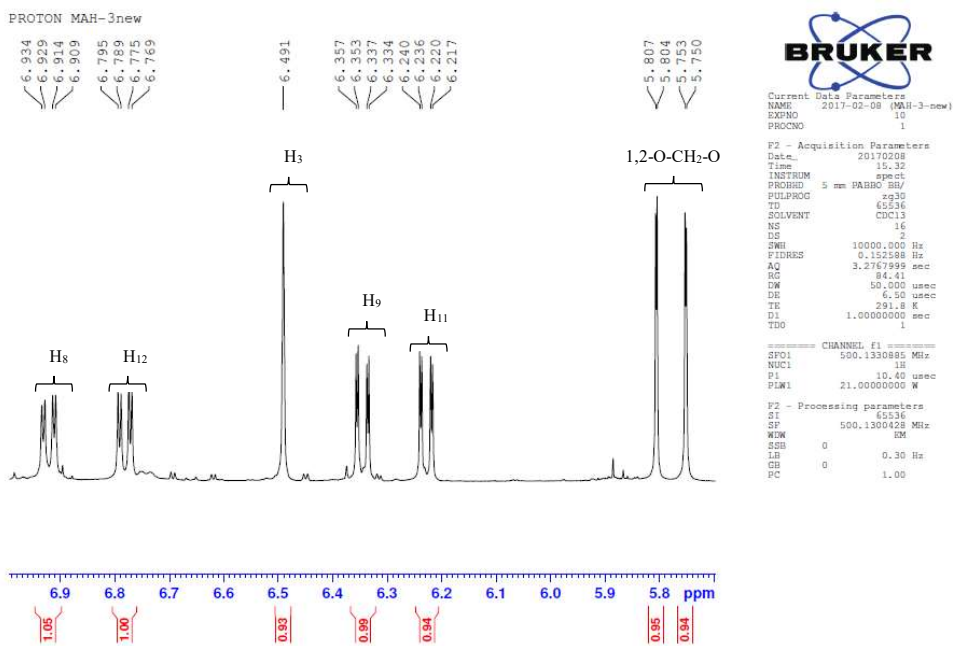
HMBCGP HMBCGP
MAH F16-20



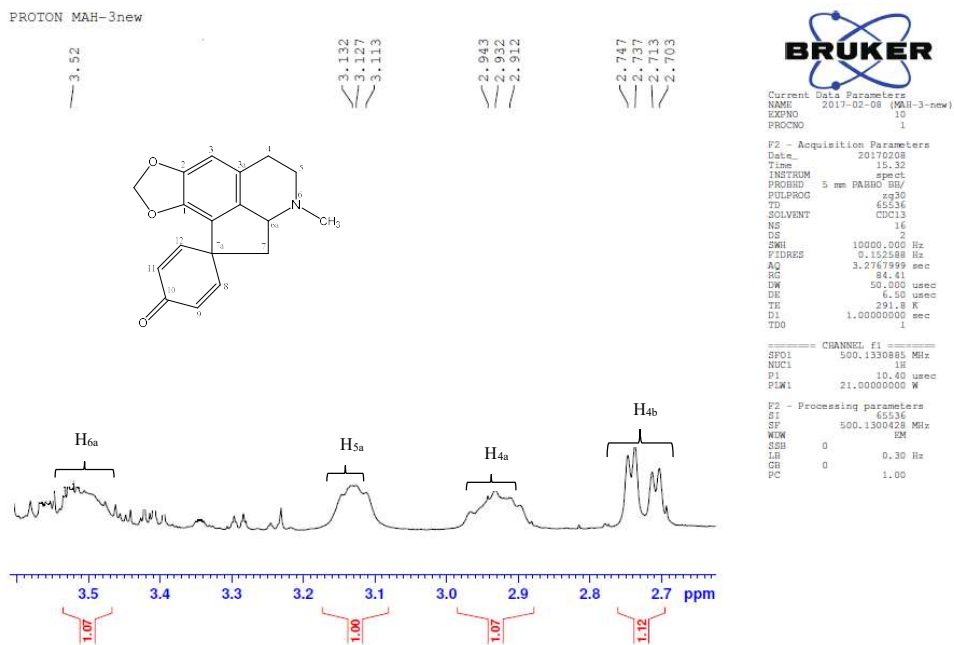
S94: Expansion of the HMBC (500 MHz, CDCl₃) Spectrum of Compound 5 (remrefidine)



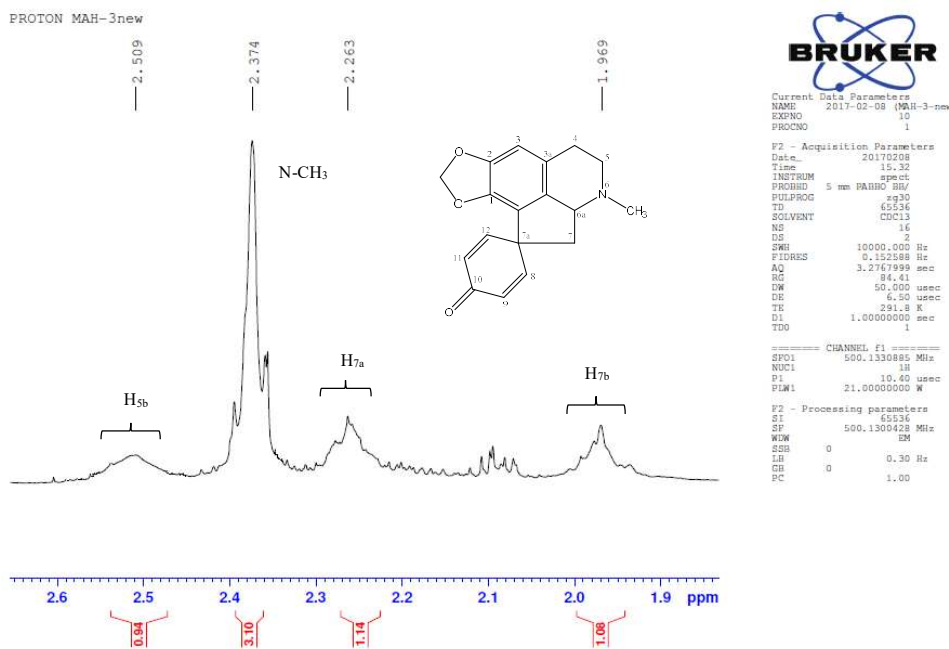
S95: $^1\text{H-NMR}$ (500 MHz, CD_3OD) Spectrum of Compound 6 (mecambrine)



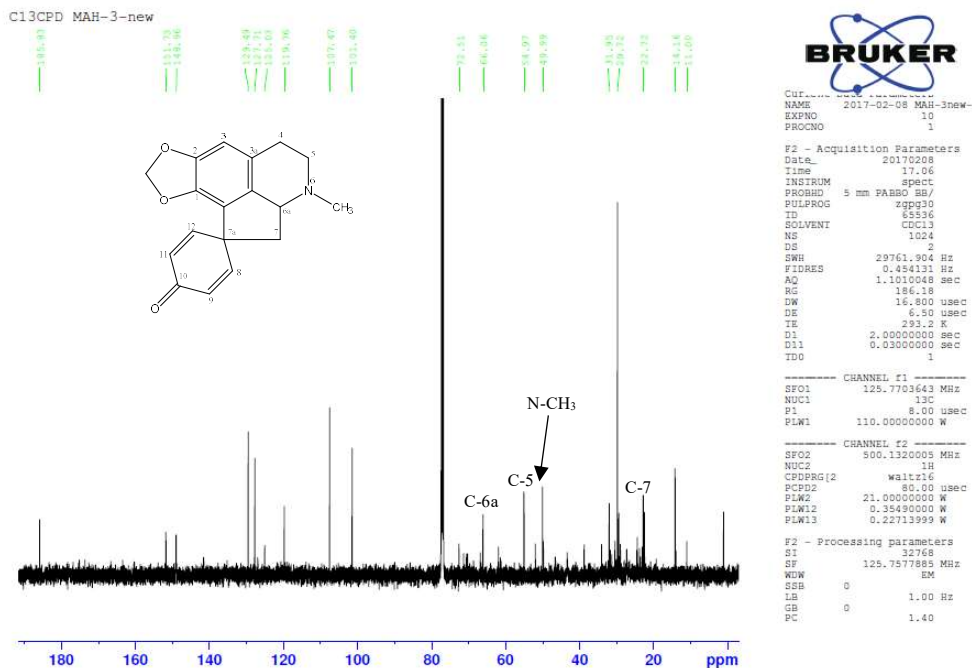
S96: Expansion of the $^1\text{H-NMR}$ (500 MHz) Spectrum of Compound 6 (mecambrine)



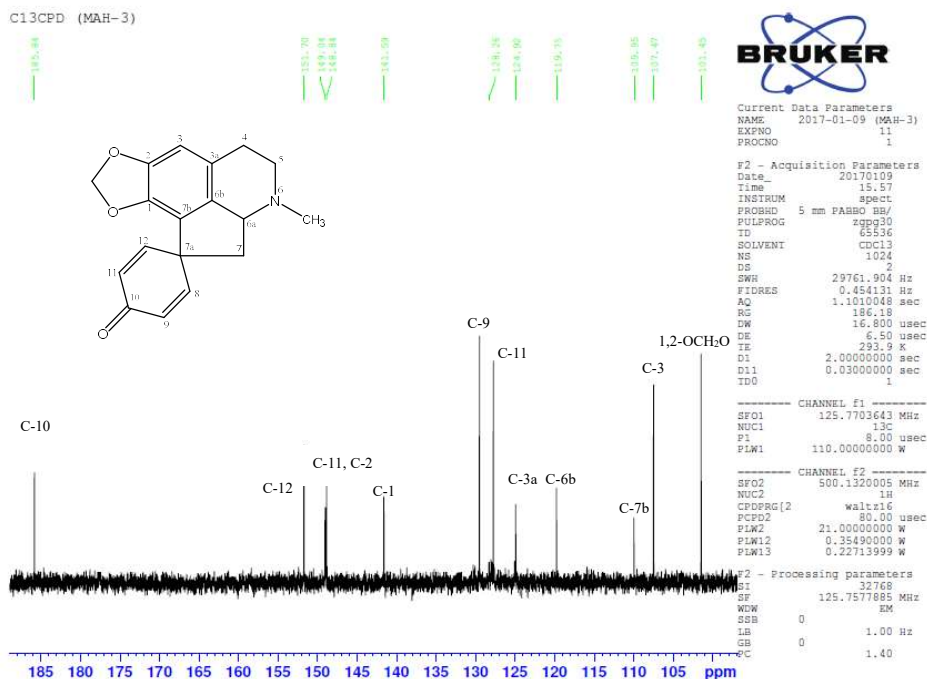
S97: Expansion of the ¹H-NMR (500 MHz) Spectrum of Compound 6 (mecambrine)



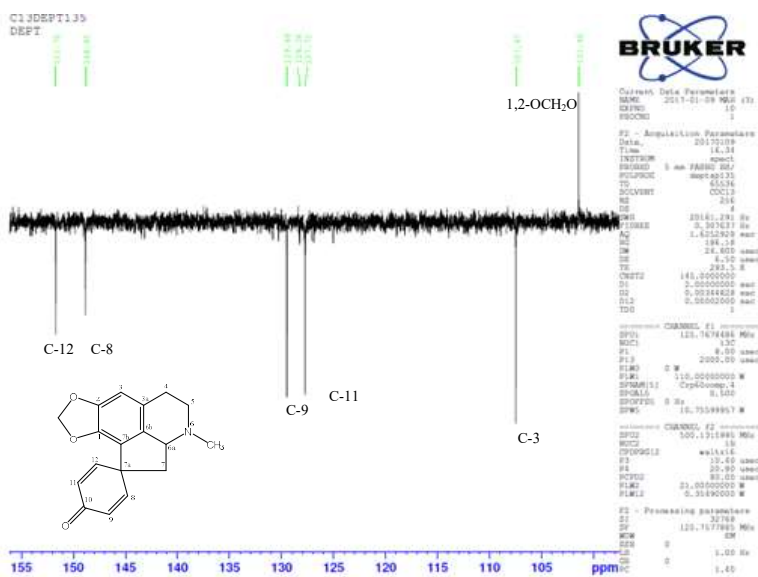
S98: Expansion of the ¹H-NMR (500 MHz) Spectrum of Compound 6 (mecambrine)



S99: ^{13}C -NMR (500 MHz) Spectrum of Compound **6** (mecambrine)

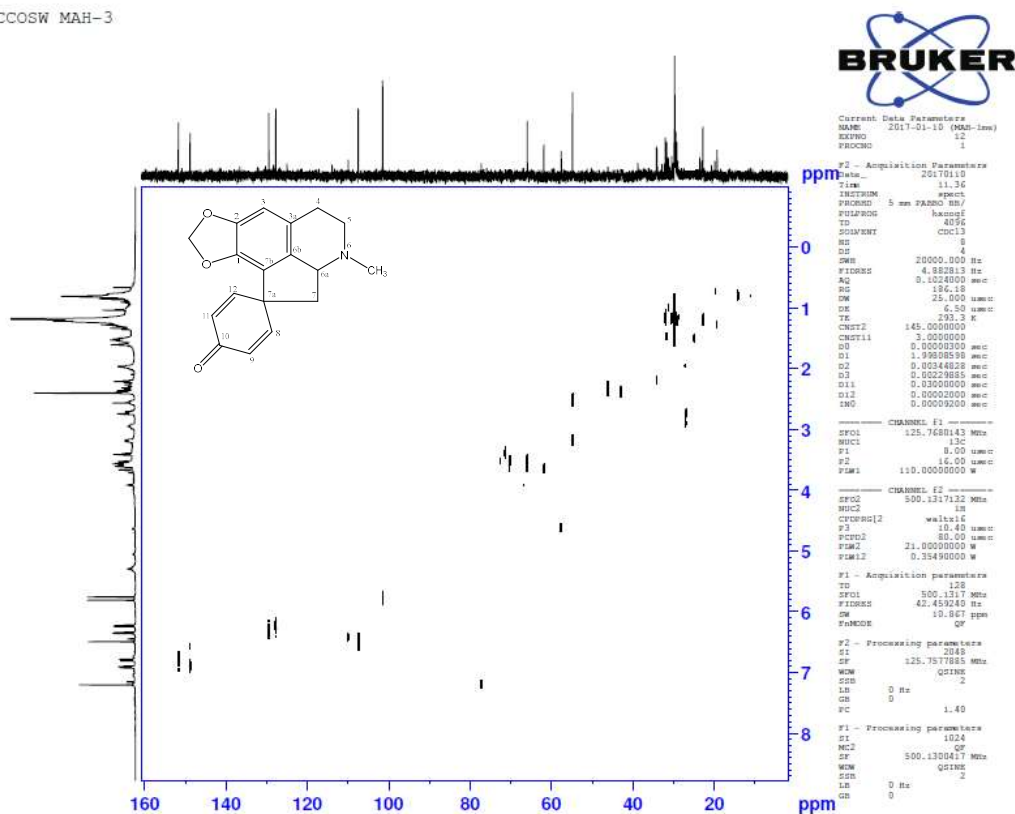


S100: Expansion of the ^{13}C -NMR (500 MHz) Spectrum of Compound **6** (mecambrine)

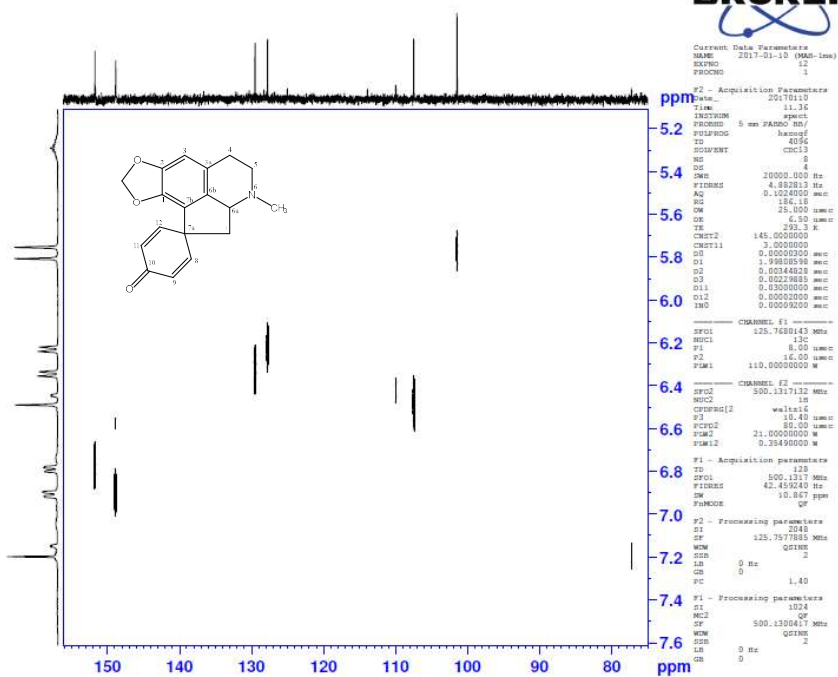


S101: DEPT (500 MHz) Spectrum of Compound 6 (mecambrine)

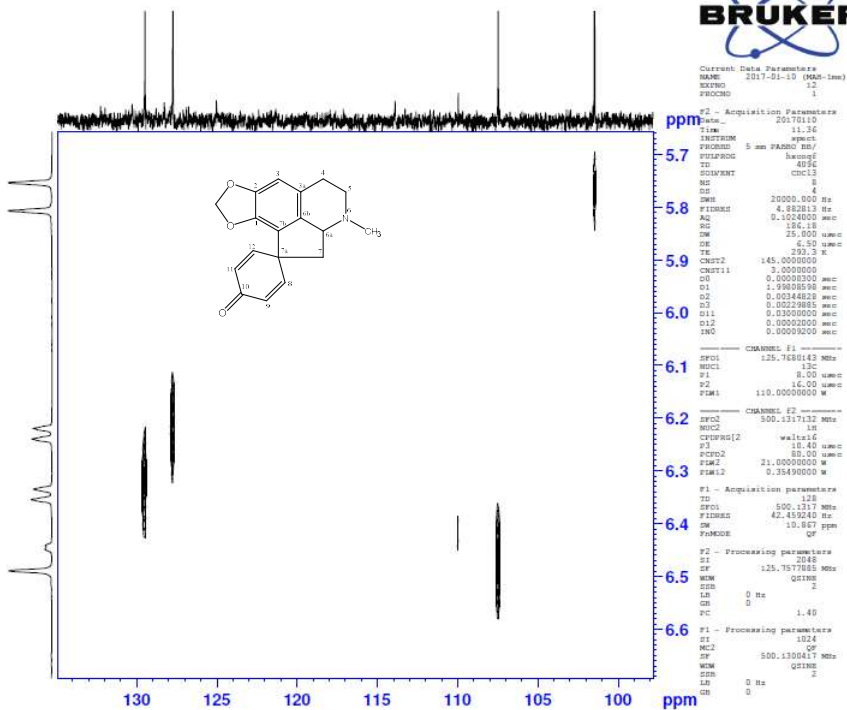
HCCOSW MAH-3



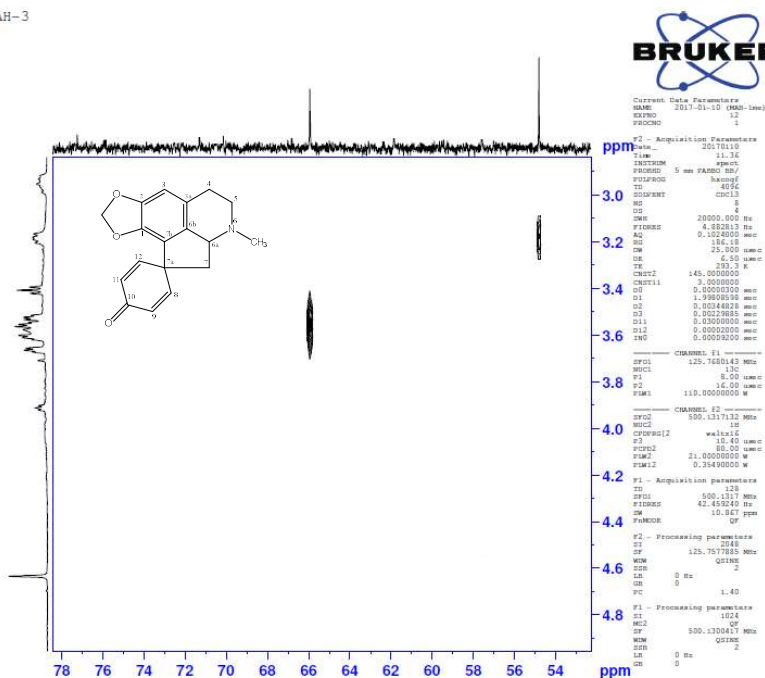
S102: HCCOSY Spectrum of Compound 6 (mecambrine)



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

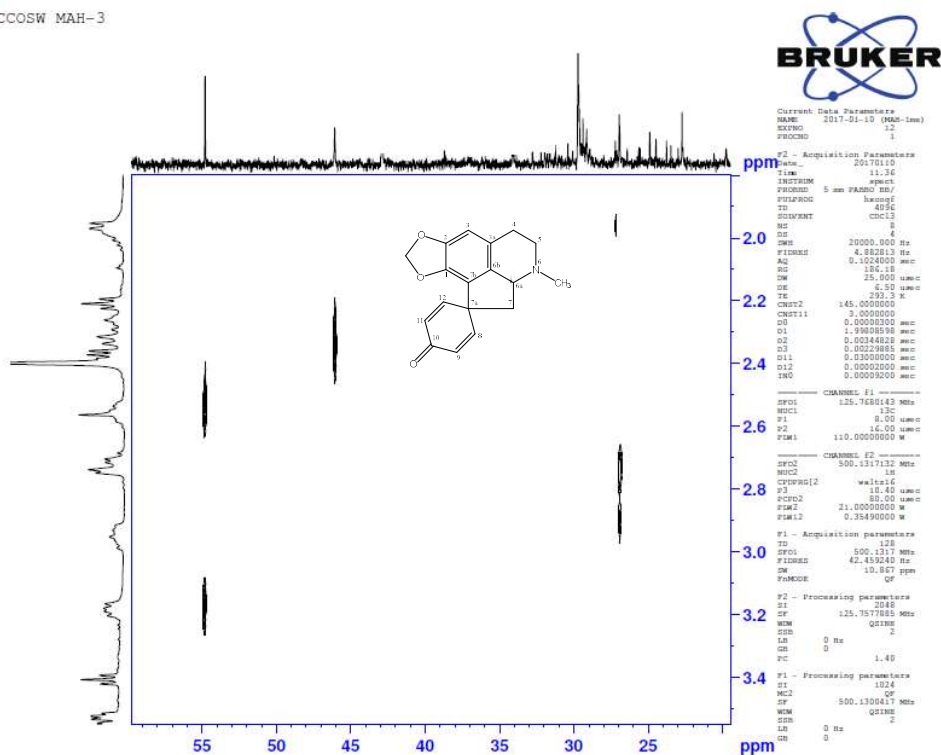


S104: Expansion of the HCCOW Spectrum of Compound 6 (mecambrine)



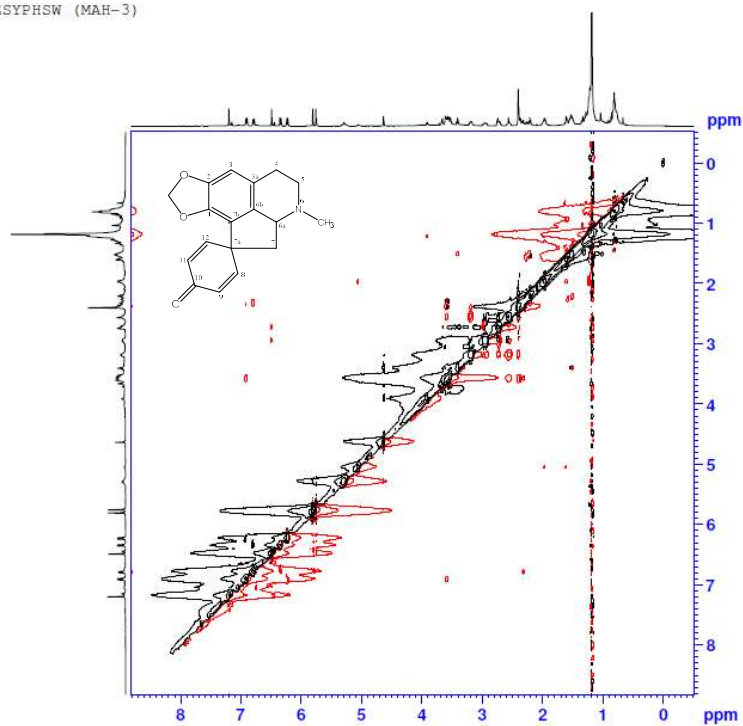
S105: Expansion of the HCCOW Spectrum of Compound 6 (mecambrine)

HCCOSW MAH-3



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

NOESYPSHW (MAH-3)



BRUKER

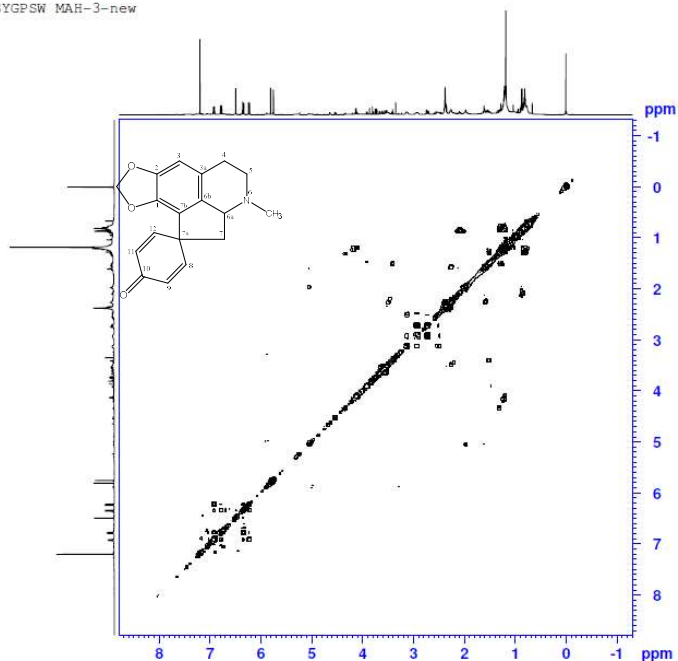
```

C:\
NAME      XXXMO
PROCNO    1
-----
F2 - Acquisition Parameters
Date_     20170111
Time      12.45
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   noesypprog
TD         2048
SOLVENT   CDCl3
NS         4
DS         2
SWH        5555.556 Hz
FIDRES    2.712674 Hz
AQ         0.1843200 sec
RG         31.47
DM         90.000 usec
DE         6.50 usec
TE         292.2 K
DO         0.0007676 sec
D1         2.02047992 sec
d11       0.30000000 sec
D12       0.00000000 sec
D15       0.00020000 sec
IND       0.00010000 sec
-----
CHANNEL f1 -----
SFO1      500.1316775 MHz
NUC1      1H
P1        19.40 usec
P2        20.80 usec
P17       2800.00 usec
P181      21.00000000 W
P1810     3.359999990 W
-----
GRABUNT CHANNEL -----
GRABUNT1  SMOQ10.100
CP11      15.00 %
P16       1000.00 usec
-----
F1 - Acquisition parameters
TD         2048
SFO1      500.1317 MHz
FIDRES    21.701389 Hz
SW         11.103 PPM
FREQCXC   States-TYPE
-----
F2 - Processing parameters
SI         1024
SF         500.1300424 MHz
WWM       Q2INK
SSB        0
LA         0 Hz
GB         0
PC         1.00
-----
F1 - Processing parameters
SI         1024
MC2       States-TYPE
SF         500.1300424 MHz
WWM       Q2INK
SSB        0
LA         0 Hz
GB         0

```

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

1SYGPSW MAH-3-new



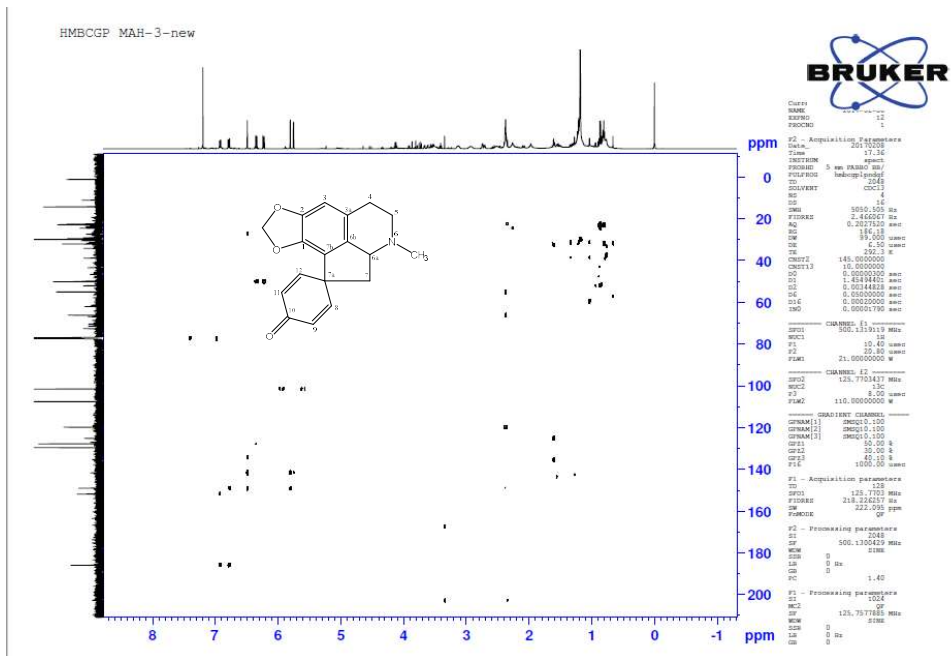
BRUKER

```

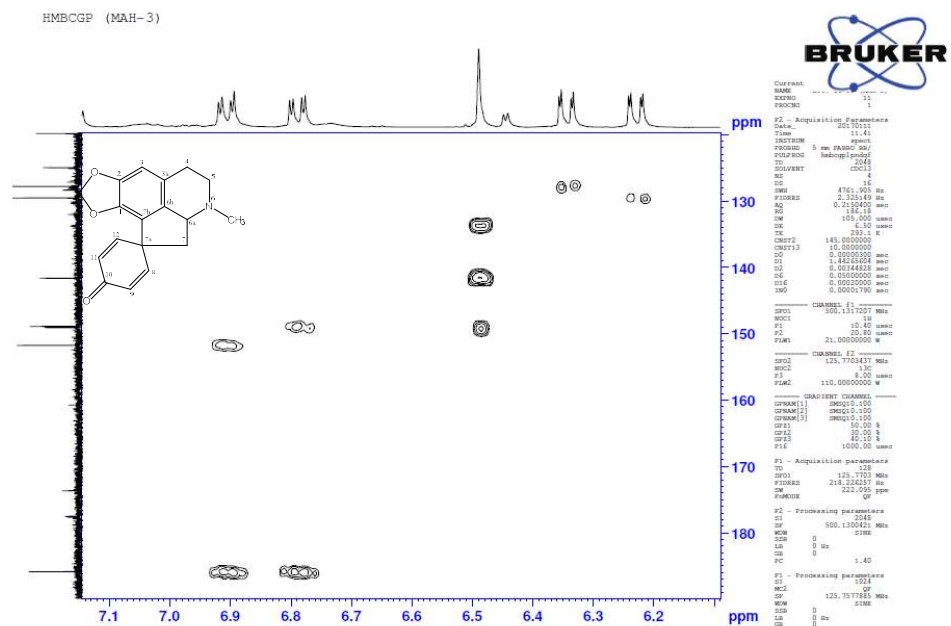
C:\
NAME      XXXMO
PROCNO    1
-----
F2 - Acquisition Parameters
Date_     20170111
Time      18.37
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   cosypprog
TD         2048
SOLVENT   CDCl3
NS         1
DS         2
SWH        5050.555 Hz
FIDRES    21.445057 Hz
AQ         0.2027620 sec
RG         48.3
DM         99.000 usec
DE         6.50 usec
TE         292.2 K
DO         0.00003000 sec
D1         1.90043602 sec
D11       0.03000000 sec
D12       0.00000000 sec
D13       0.00000400 sec
D15       0.00000000 sec
IND       0.00019800 sec
-----
CHANNEL f1 -----
SFO1      500.1319119 MHz
NUC1      1H
P1        19.40 usec
P2        19.40 usec
P17       2800.00 usec
P181      21.00000000 W
P1810     3.359999990 W
-----
GRABUNT CHANNEL -----
GRABUNT1  SMOQ10.100
CP11      15.00 %
P16       1000.00 usec
-----
F1 - Acquisition parameters
TD         128
SFO1      500.1319 MHz
FIDRES    39.457049 Hz
SW         10.000 PPM
FREQCXC   QF
-----
F2 - Processing parameters
SI         1024
SF         500.1300429 MHz
WWM       Q2INK
SSB        0
LA         0 Hz
GB         0
PC         1.40
-----
F1 - Processing parameters
SI         1024
MC2       QF
SF         500.1300429 MHz
WWM       Q2INK
SSB        0
LA         0 Hz
GB         0

```

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

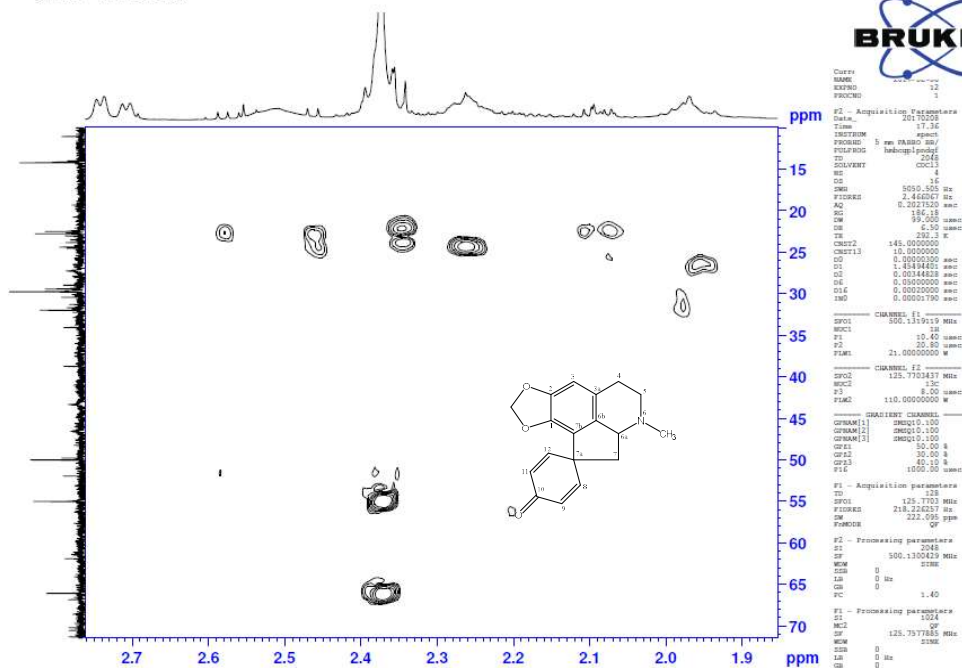


S109: HMBC (500 MHz, CDCl₃) Spectrum of Compound 6 (mecambrine)



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

HMBCGP MAH-3-new



```

Conv
NAME
KEYID
PROCNO
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P2 - Acquisition Parameters
Date_ 20170508
Time 17.36
INSTRUM spect
PROBHD 5 mm HAMBQ 5M/
PULPROG hzgpg130qdet
TD 2048
SOLVENT CDCl3
NS 4
DS 2
SWH 5059.505 Hz
F2REQ2 2.446007 Hz
AQ 0.2027020 sec
RG 186.18
CW 99.000 usec
DE 5.30 usec
TE 300.2 K
CHST2 149.000000
CHST13 19.000000
D0 1.800000 sec
D1 1.400000 sec
D2 0.000000 sec
D3 0.000000 sec
D4 0.000000 sec
D5 0.000000 sec
RG 0.00001790 sec
-----
CHANNEL F1
NUC1 506.1319119 MHz
P1 10.40 usec
P2 20.50 usec
PLM1 21.00000000 W
-----
CHANNEL F2
NUC2 125.770437 MHz
P3 8.00 usec
PLM2 110.00000000 W
-----
GRADIENT CHANNEL
GRAM11 ZMG10.100
GRAM12 ZMG10.100
GRAM13 ZMG10.100
GPF1 50.00 s
GPF2 20.00 s
GPF3 40.10 s
GFL 1000.00 usec
F1 - Acquisition Parameters
TD 208
SFO1 125.7703 MHz
PULPROG 218.224237 Hz
SW 202.000 ppm
FWDCCA OF
P2 - Processing parameters
SI 2048
SF 506.1300419 MHz
WDW EM
SSB 0
LA 0 Hz
GB 0
PC 1.40
F1 - Processing parameters
SI 2048
SF 125.7577035 MHz
WDW EM
SSB 0
LA 0 Hz
GB 0

```

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