

Supporting Information

of Alkaloids from the Flower of *Erythrina arborescens*

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Figure 1. Structures of New Alkaloids **1-8**

Figure 2. Structures of Known Alkaloids **9-25**

S1-S7: NMR and HRMS spectra of erythriarborine A (**1**)

S8-S14: NMR and HRMS spectra of erythriarborine B (**2**)

S15-S21: NMR and HRMS spectra of erythriarborine C (**3**)

S22-S27: NMR and HRMS spectra of erythriarborine D (**4**)

S28-S33: NMR and HRMS spectra of erythriarborine E (**5**)

S34-S39: NMR and HRMS spectra of erythriarborine F (**6**)

S40-S45: NMR and HRMS spectra of erythriarborine G (**7**)

S46-S51: NMR and HRMS spectra of erythriarborine H (**8**)

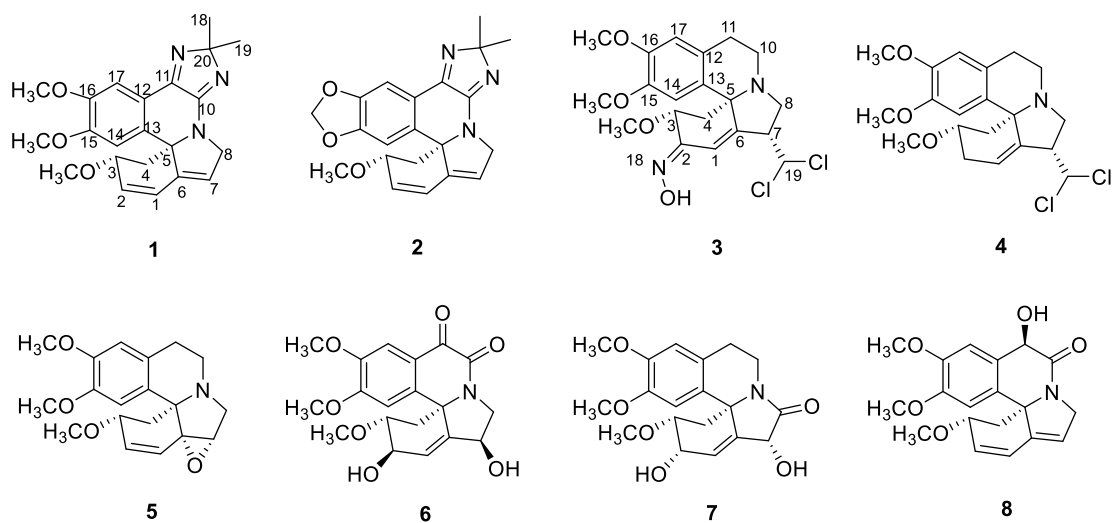


Figure 1. Structures of New Alkaloids **1-8**

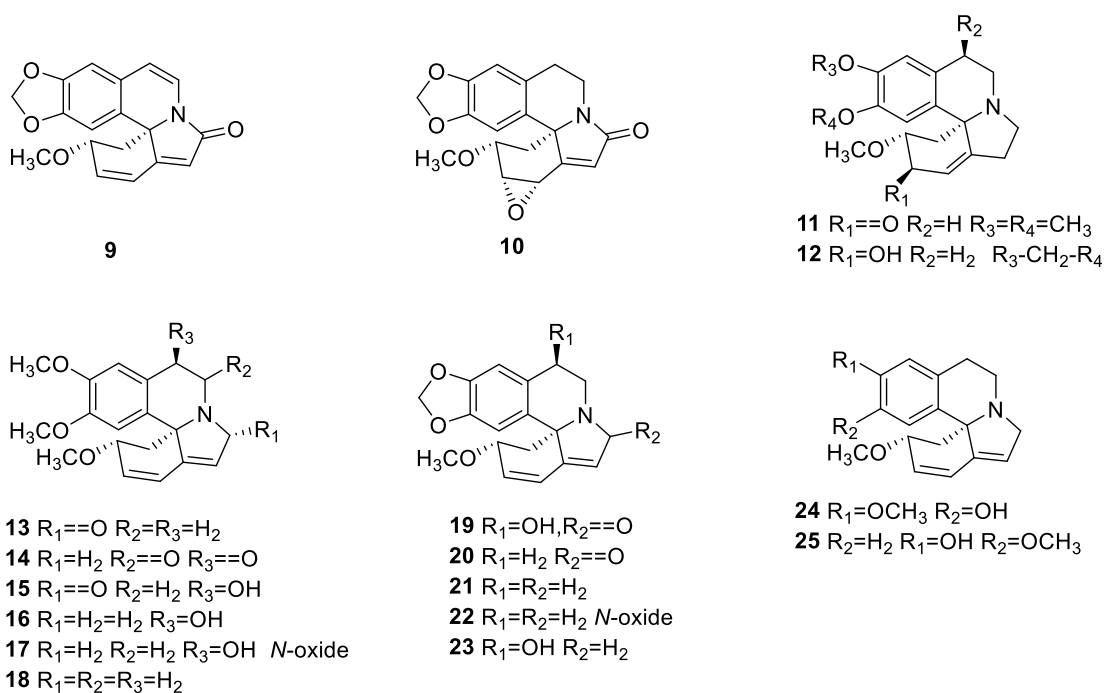
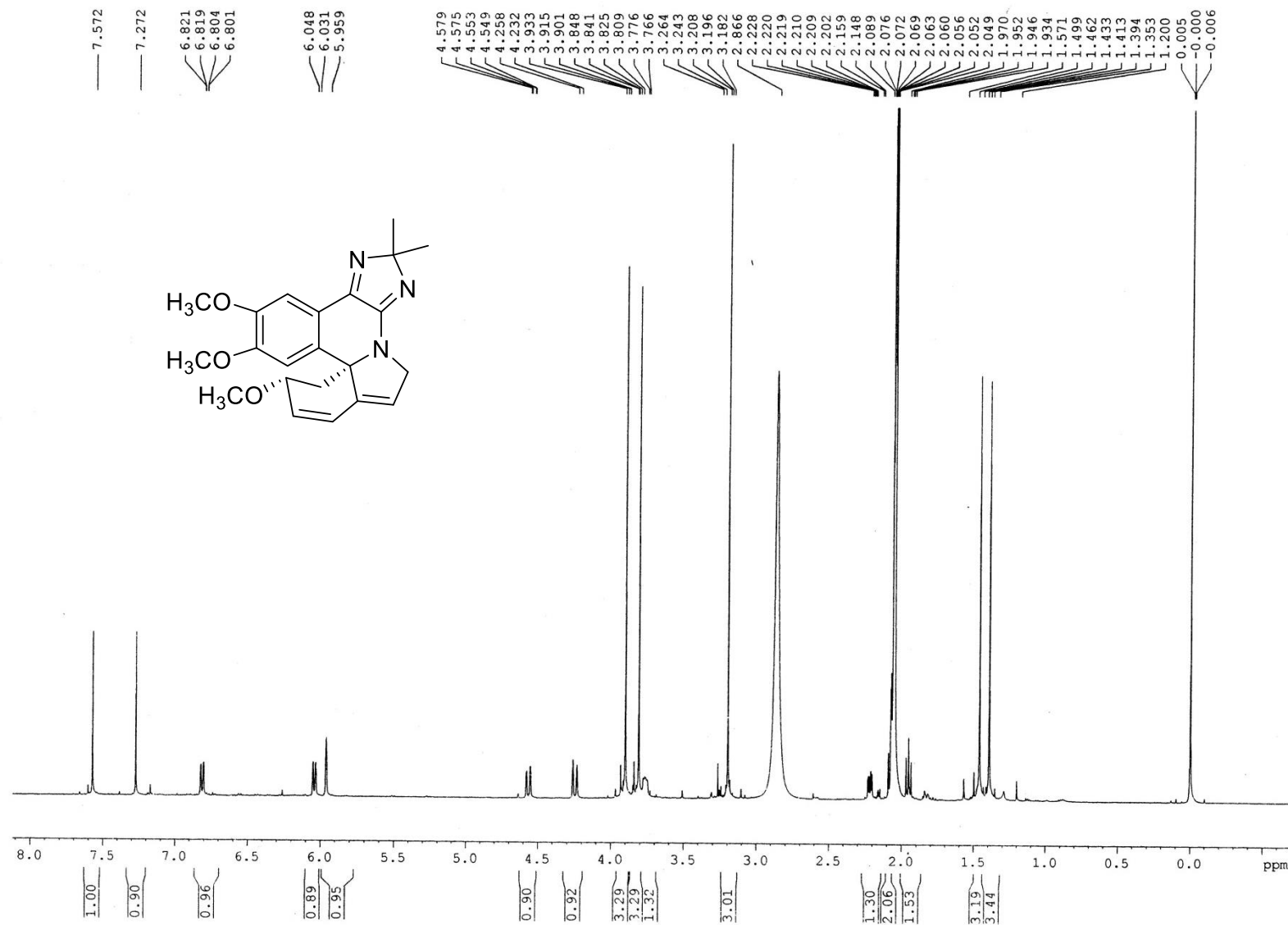


Figure 2. Structures of Known Alkaloids **9-25**

S1. ¹H NMR Spectrum of erytharborine A (1)

h Acetone av600



```

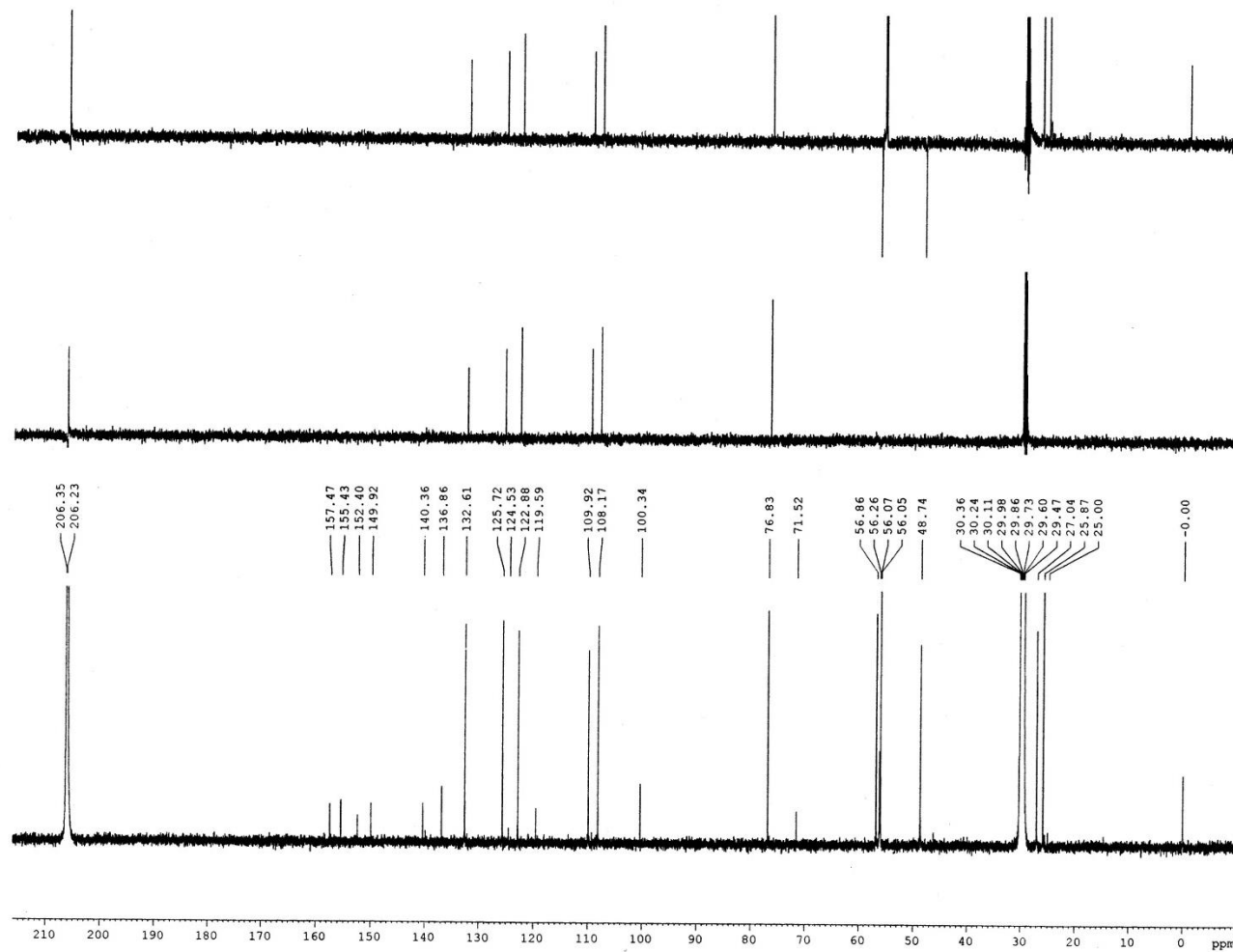
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EXPNO     41
PROCNO    1
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PULPROG    zg30
TD         65536
SOLVENT    Acetone
NS         4
DS         2
SWH         16741.072 Hz
FIDRES      0.255448 Hz
AQ          1.9573919 sec
RG          40.3
DW          29.867 usec
DE          20.00 usec
TE          298.0 K
D1          1.00000000 sec
TDO         1
  
```

```

===== CHANNEL f1 =====
NUC1       1H
P1         8.00 usec
PL1        6.40 dB
PL1W       3.73460507 W
SFO1       600.1337060 MHz
SI         32768
SF         600.1300153 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
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S2. ^{13}C NMR Spectrum of erytharborine A (1)

c13 Acetone av600



```

NAME          wea3
EXPNO         44
PROCNO        1
Date_         20150306
Time_         11.22
INSTRUM       spect
PROBHD        5 mm CPTCI 1H-
PULPROG       zgdc
TD            65536
SOLVENT       Acetone
NS            3200
DS            4
SWH           39062.500 Hz
FIDRES        0.596046 Hz
AQ            0.8389108 sec
RG            2050
DW            12.800 usec
DE            20.00 usec
TE            298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
  
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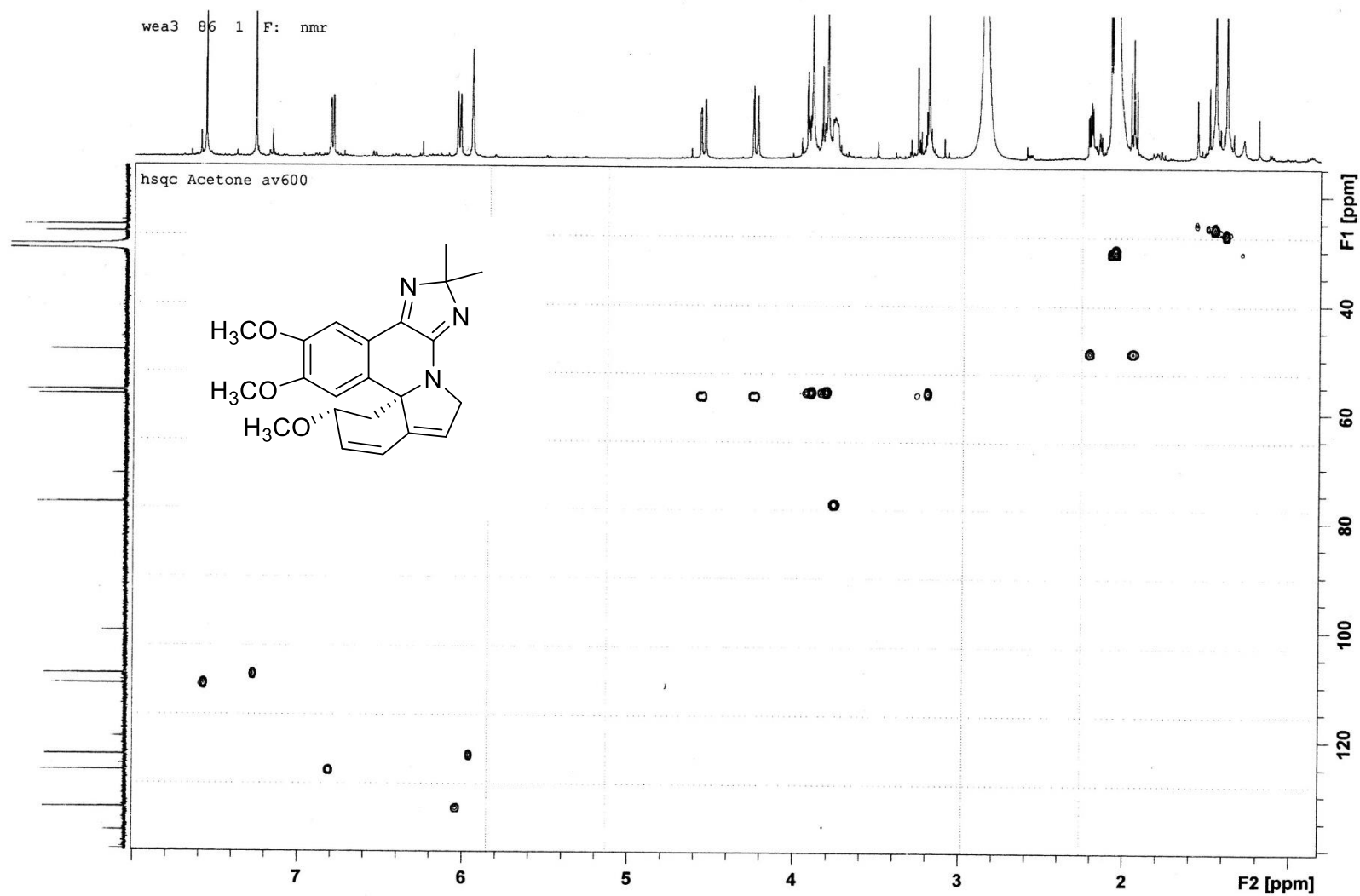
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===== CHANNEL f1 =====
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PL1           -0.60 dB
PL1W          93.44261932 W
SFO1          150.9194083 MHz
  
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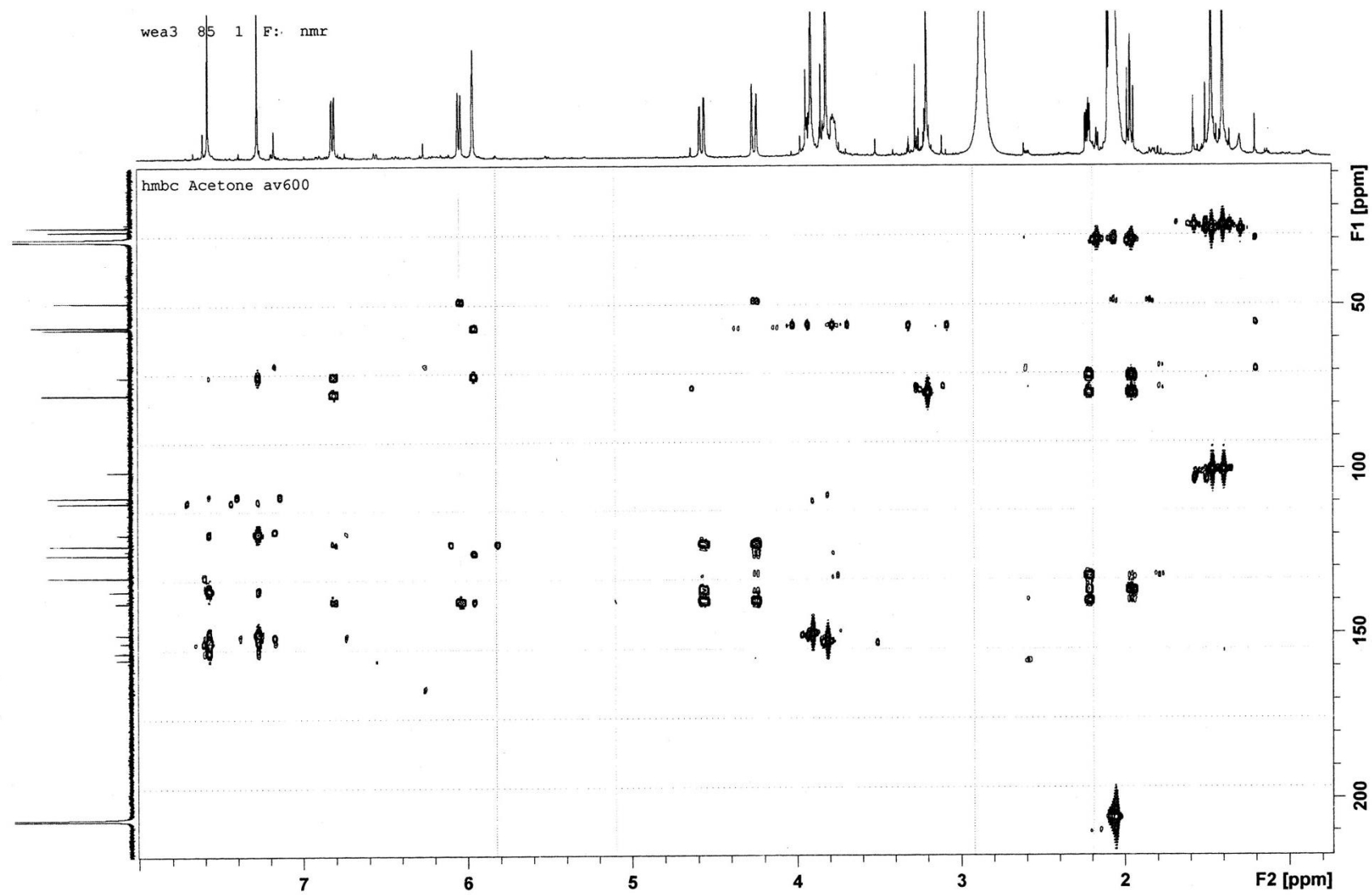
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NUC2          1H
PCPD2         80.00 usec
PL2           9.20 dB
PL12          25.68 dB
PL2W          1.95994878 W
PL12W         0.04408031 W
SFO2          600.1330006 MHz
SI            32768
SF            150.9026763 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
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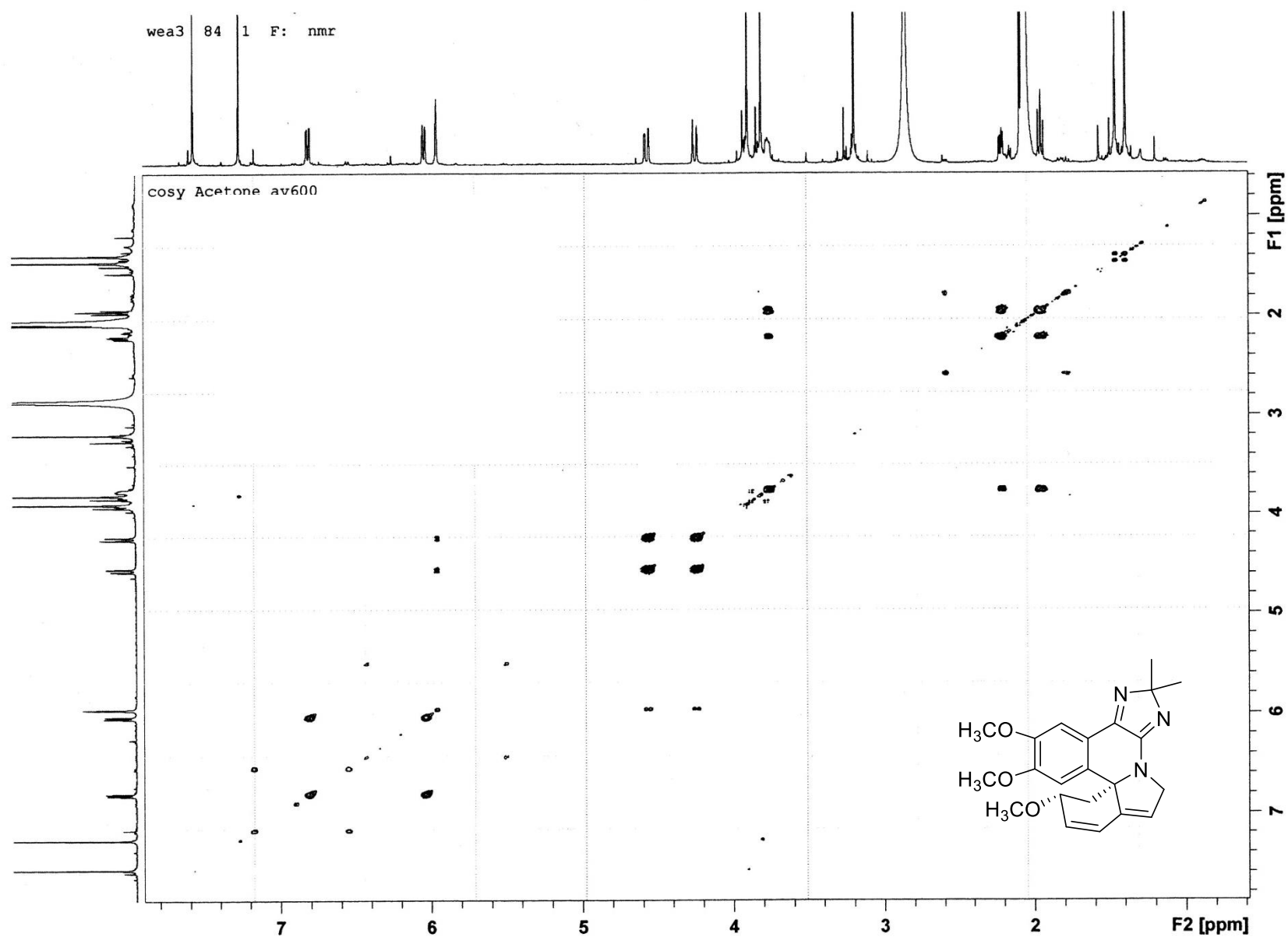
S3. HSQC Spectrum of erytharborine A (1)



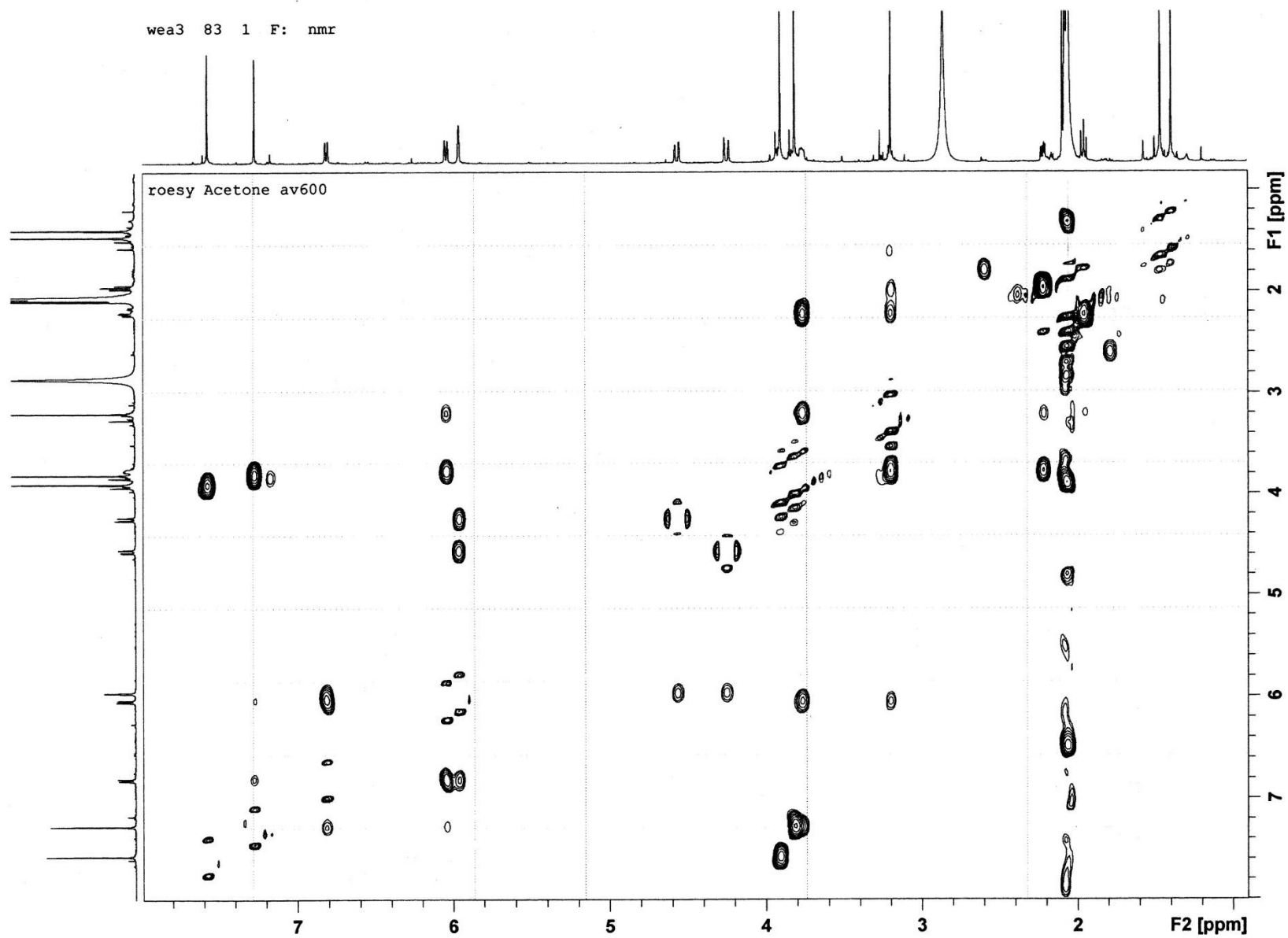
S4. HMBC Spectrum of erytharborine A



S5. ^1H - ^1H COSY Spectrum of erytharborine A (1)



S6. ROESY Spectrum of erytharborine A (1)



S7. HRESIMS of erytharborine A (1)

Formula Predictor Report - wea-3.lcd

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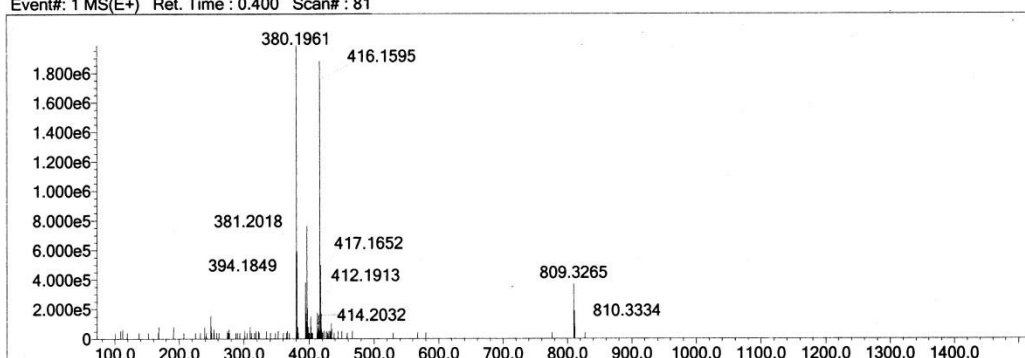
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B	3	0	0	O	2	0	40	S	2	0	0	Pt	2	0	0	
C	4	0	80	F	1	0	0	Cl	1	0	5					

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 Max Isotopes: all
 MSn Iso RI (%): 75.00

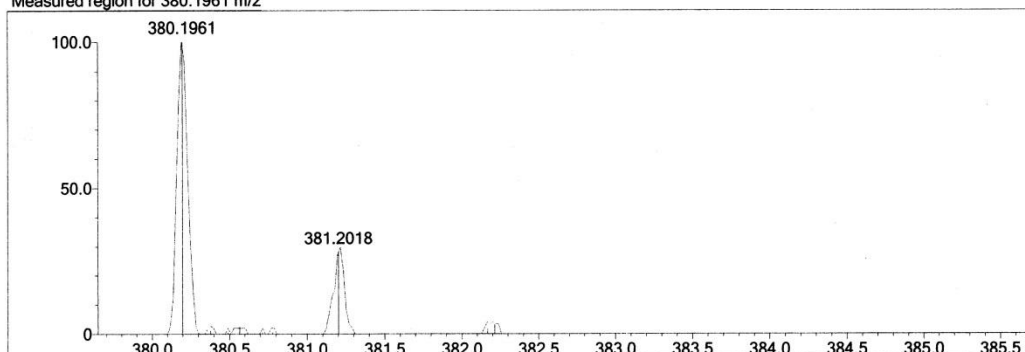
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 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 10000
 Max Results: 10

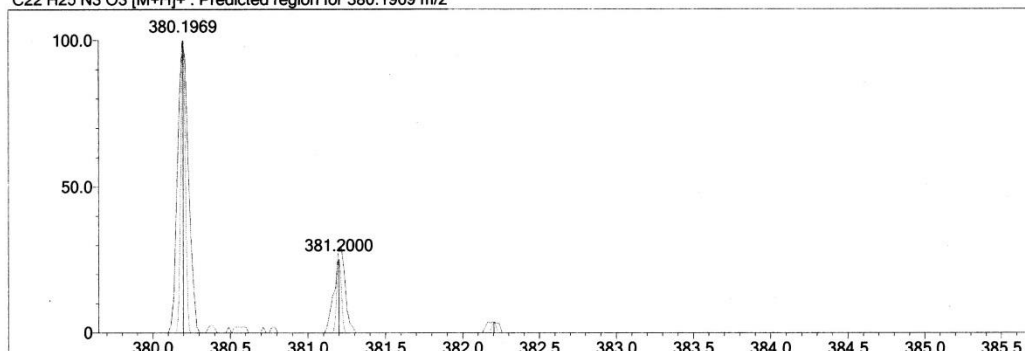
Event#: 1 MS(E+) Ret. Time : 0.400 Scan#: 81



Measured region for 380.1961 m/z



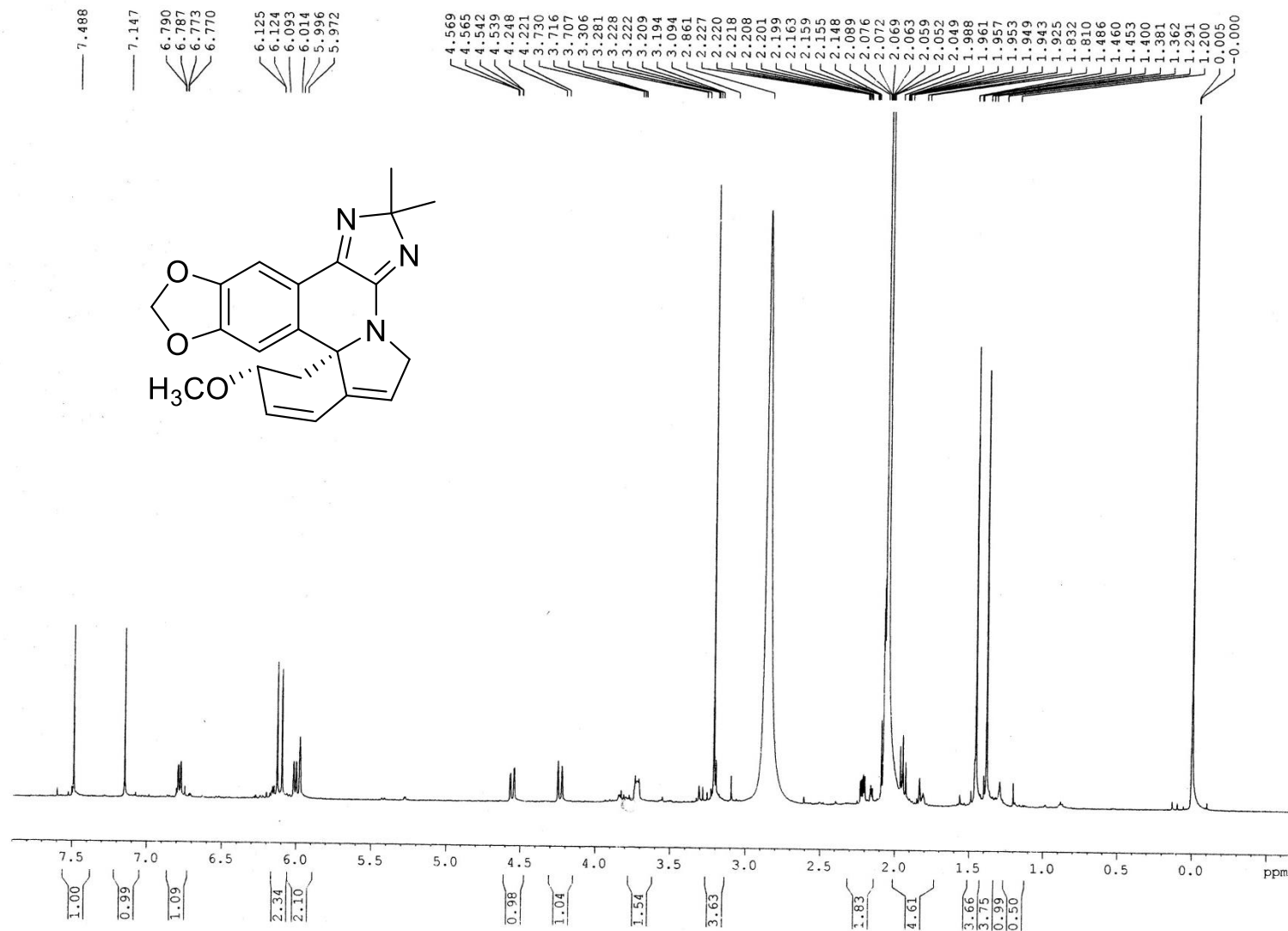
C22 H25 N3 O3 [M+H]⁺ : Predicted region for 380.1969 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	83.41	C22 H25 N3 O3	[M+H] ⁺	380.1961	380.1969	-0.8	-2.10	85.77	12.0

S8.¹H NMR Spectrum of erytharborine B (2)

h Acetone av600

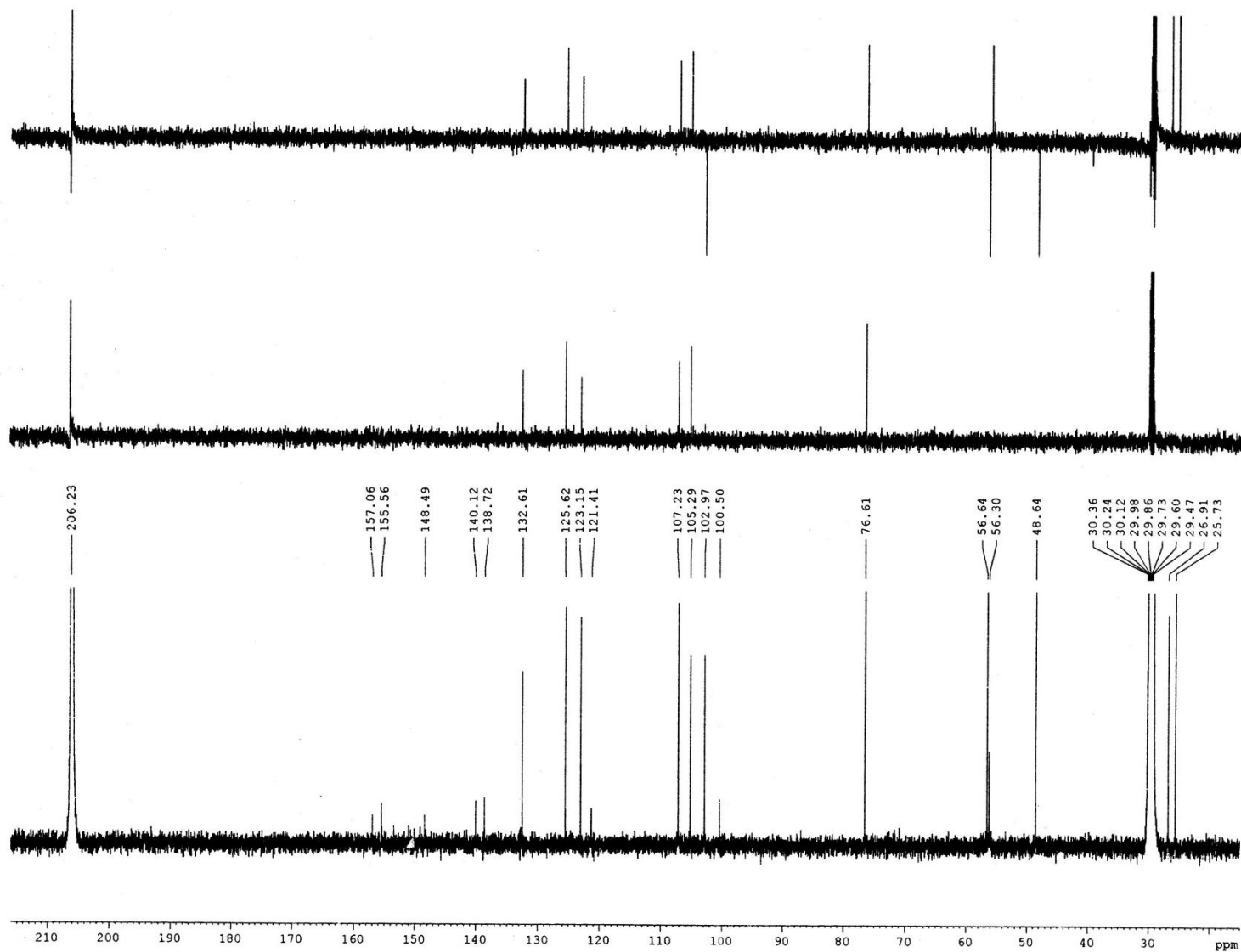


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PROCNO    1
Date_     20150305
Time      9.29
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PULPROG   zg30
TD        65536
SOLVENT   Acetone
NS        4
DS        2
SWH       16741.072 Hz
FIDRES    0.255448 Hz
AQ        1.9573919 sec
RG        45.2
DW        29.867 usec
DE        20.00 usec
TE        297.9 K
D1        1.00000000 sec
TDO       1

===== CHANNEL f1 =====
NUC1      1H
P1        8.00 usec
PL1       6.40 dB
PL1W      3.73460507 W
SFO1      600.1337060 MHz
SI        32768
SF        600.1300153 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
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S9. ^{13}C NMR Spectrum of erytharborine B (2)



```

NAME          wea5
EXPNO         44
PROCNO        1
Date_         20150307
Time_         1.05
INSTRUM       spect
PROBHD        5 mm CPTCI 1H-
PULPROG       zgdc
TD            65536
SOLVENT       Acetone
NS            3200
DS            4
SWH           39062.500 Hz
FIDRES        0.596046 Hz
AQ            0.8389108 sec
RG            2050
DW            12.800 usec
DE            20.00 usec
TE            298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
  
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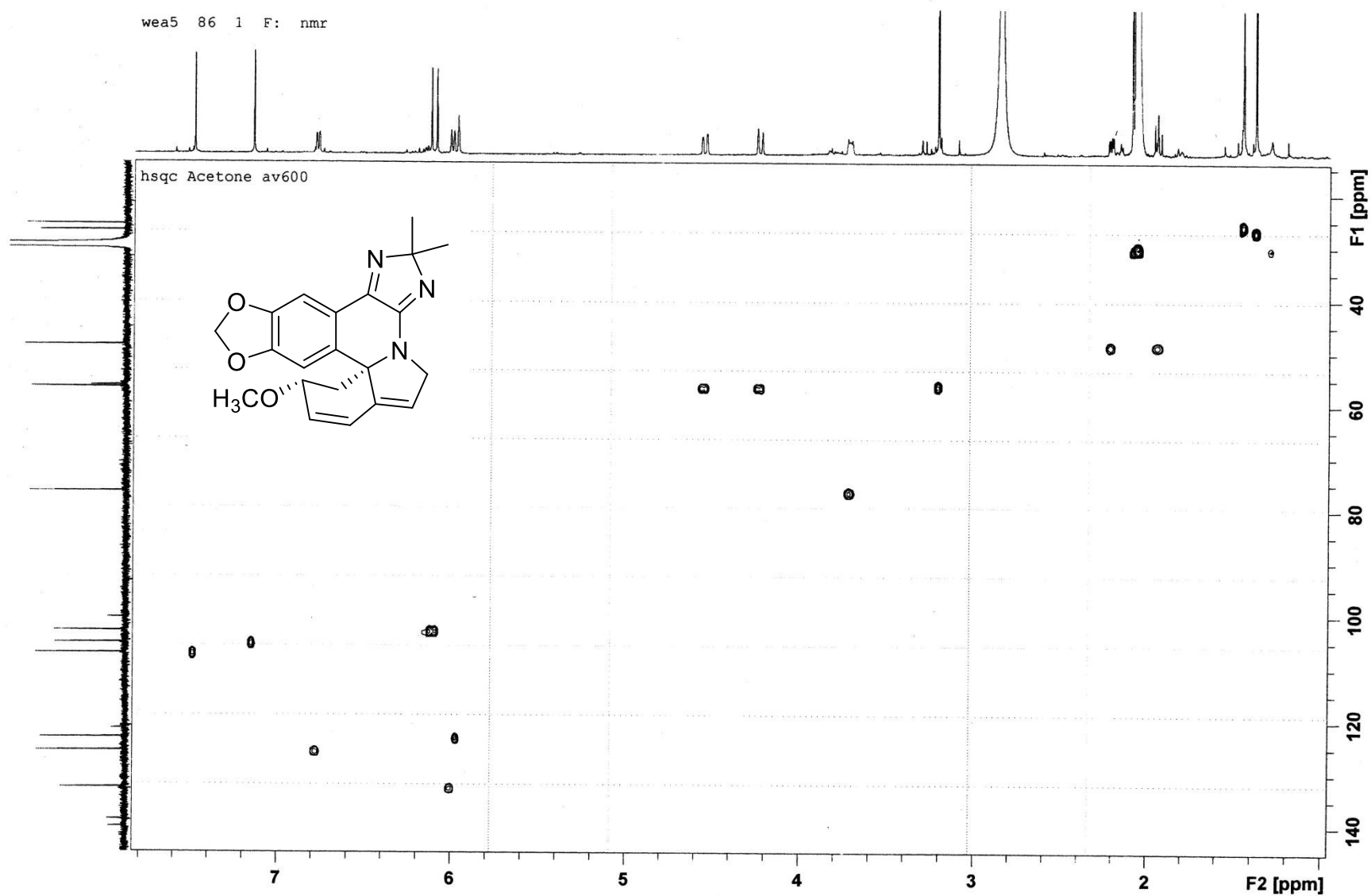
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===== CHANNEL f1 =====
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P1            12.00 usec
PL1           -0.60 dB
PL1W          93.44261932 W
SFO1          150.9194083 MHz
  
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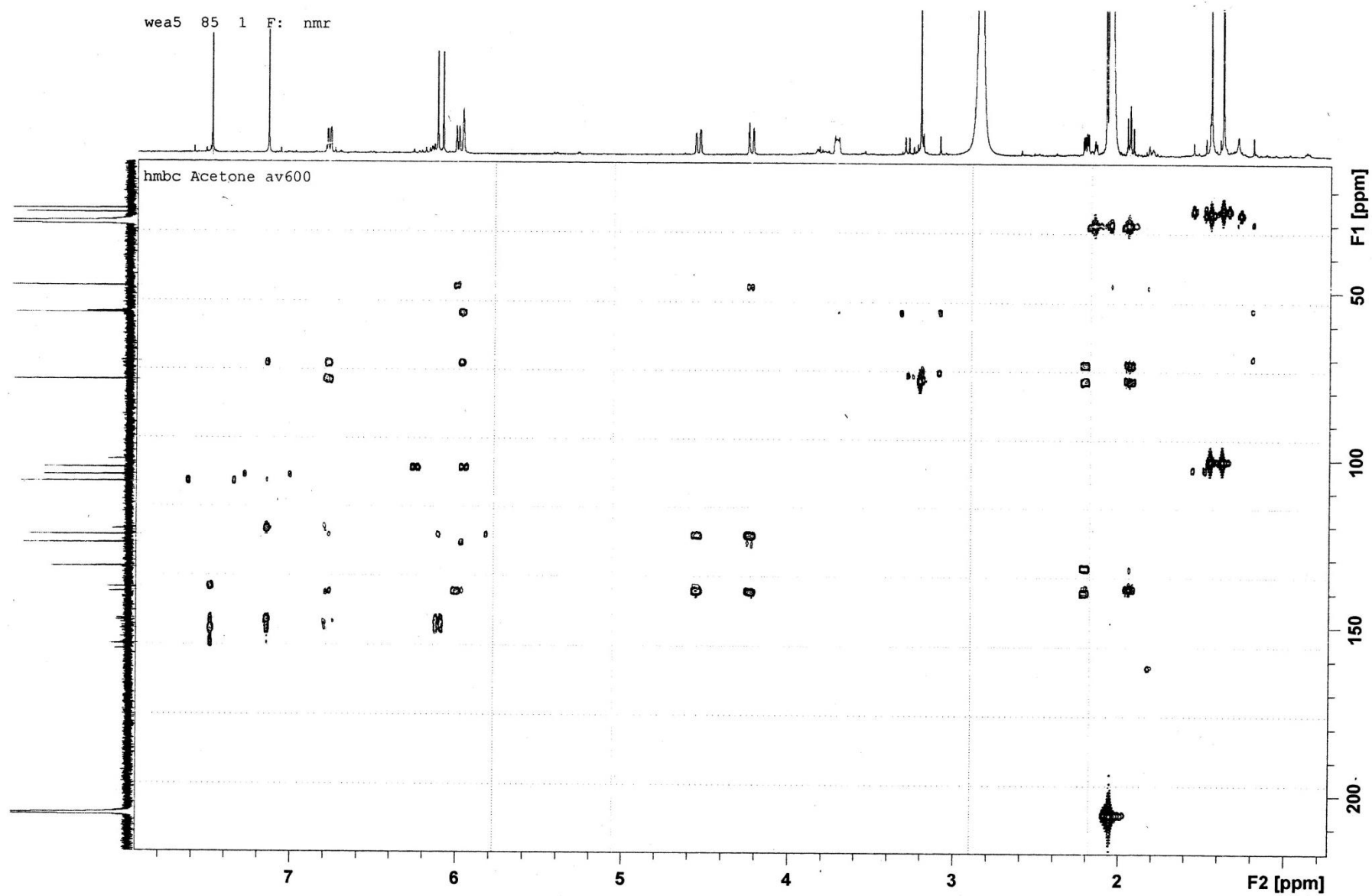
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===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           9.20 dB
PL12          25.68 dB
PL2W          1.95994878 W
PL12W         0.04408031 W
SFO2          600.1330006 MHz
SI            32768
SF            150.9026762 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
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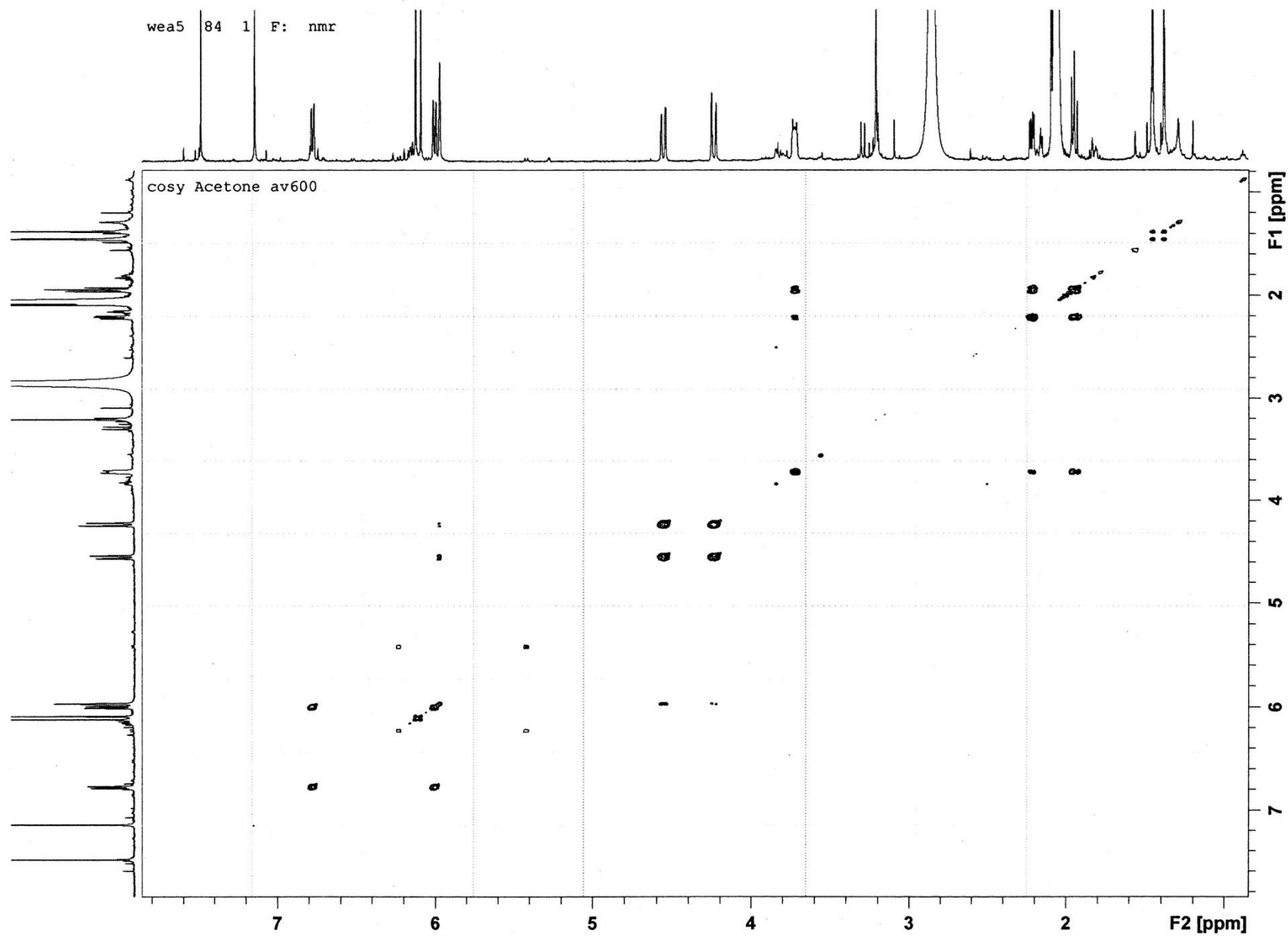
S10. HSQC Spectrum of erytharborine B (2)



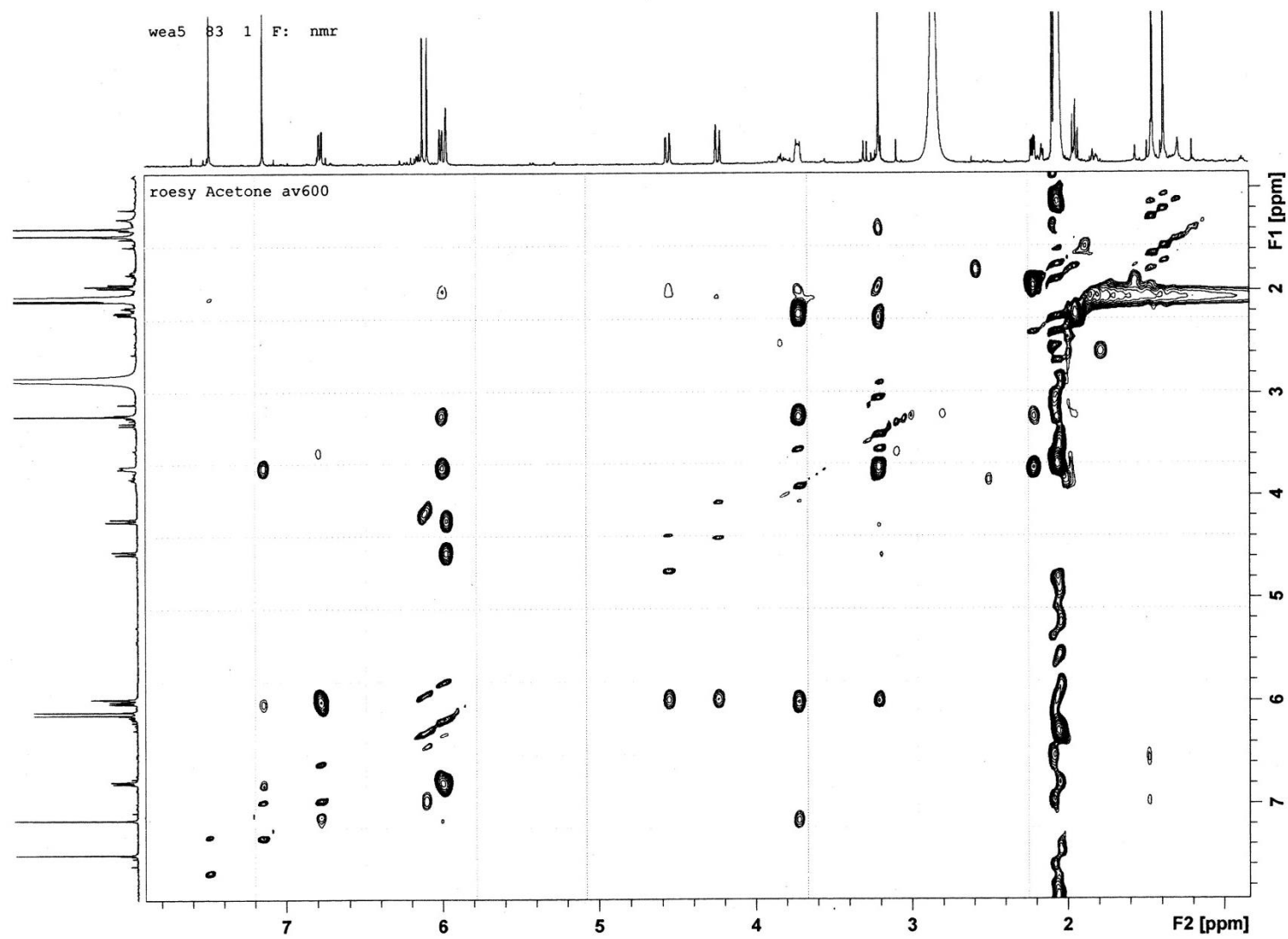
S11. HMBC Spectrum of erytharborine B (2)



S12. ^1H - ^1H COSY Spectrum of erytharborine B (2)



S13. ROESY Spectrum of erytharborine B (2)



S14. HRESIMS of erytharborine B (2)

Formula Predictor Report - wea-5.lcd

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Data File: E:\DATA\2016\0505\wea-5.lcd

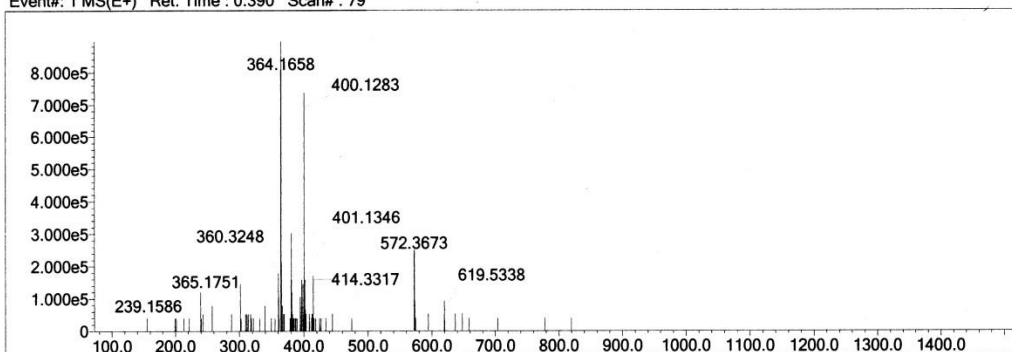
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B	3	0	0	O	2	0	40	S	2	0	0	Pt	2	0	0	
C	4	0	80	F	1	0	0	Cl	1	0	5					

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

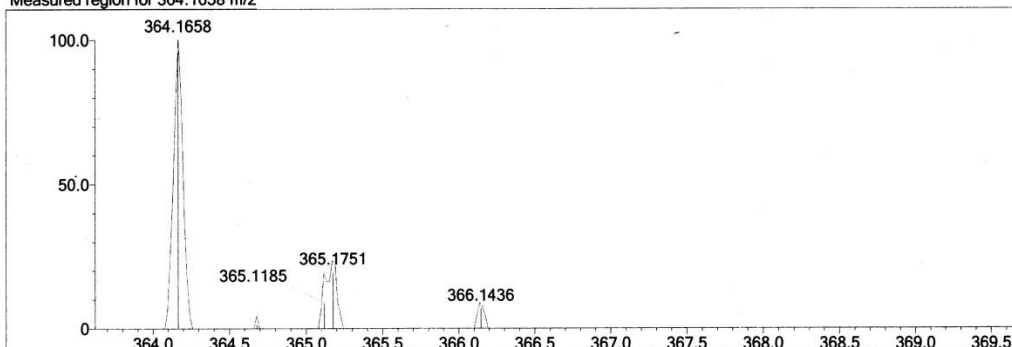
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 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 10000
 Max Results: 10

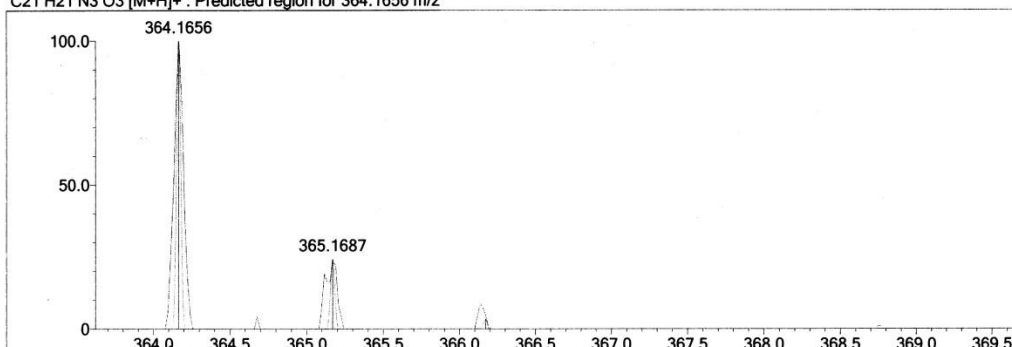
Event#: 1 MS(E+) Ret. Time : 0.390 Scan#: 79



Measured region for 364.1658 m/z

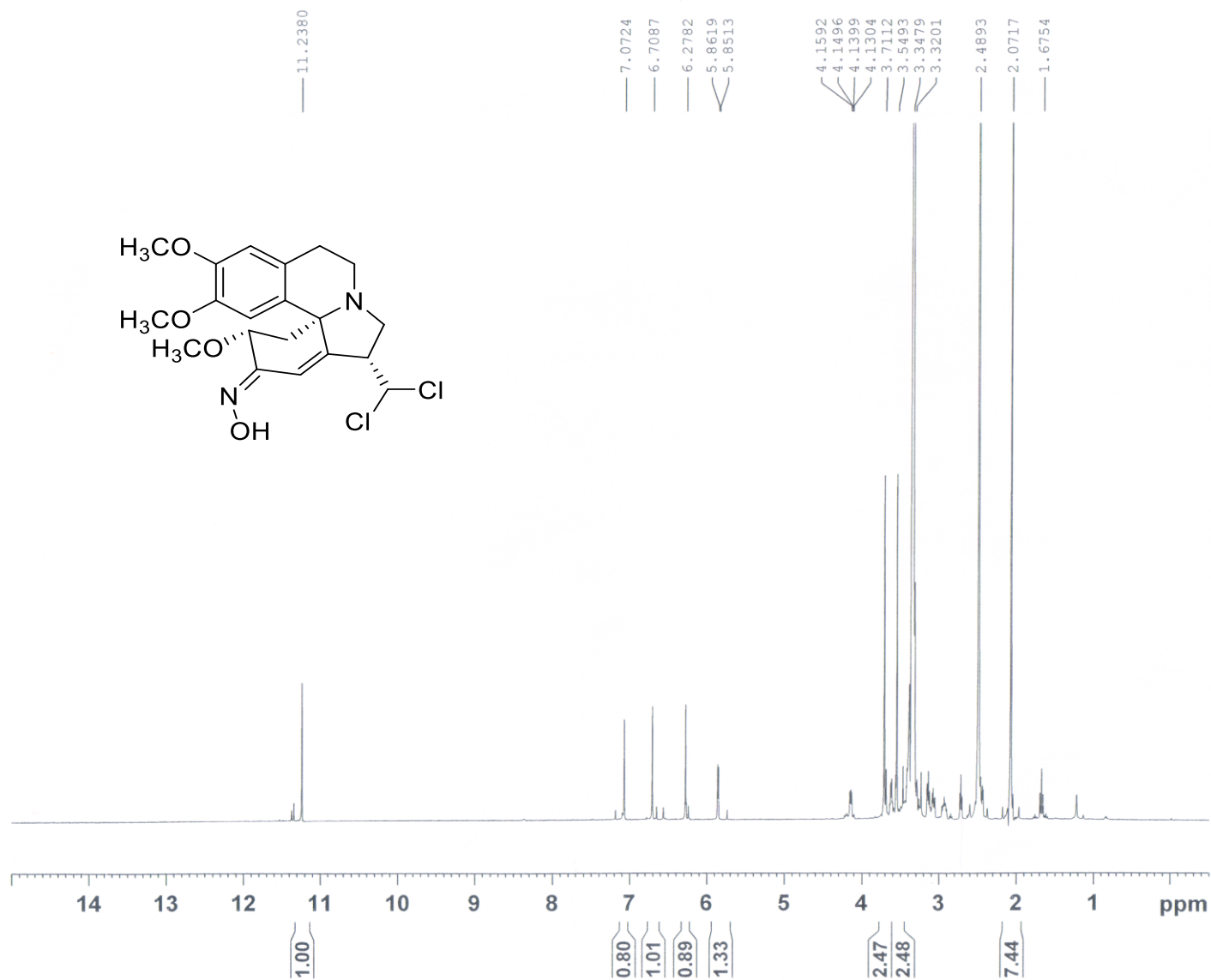


C21 H21 N3 O3 [M+H]⁺ : Predicted region for 364.1656 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	54.38	C21 H21 N3 O3	[M+H] ⁺	364.1658	364.1656	0.2	0.55	54.38	13.0

S15. ^1H -NMR spectrum of erythriarborine C (3)



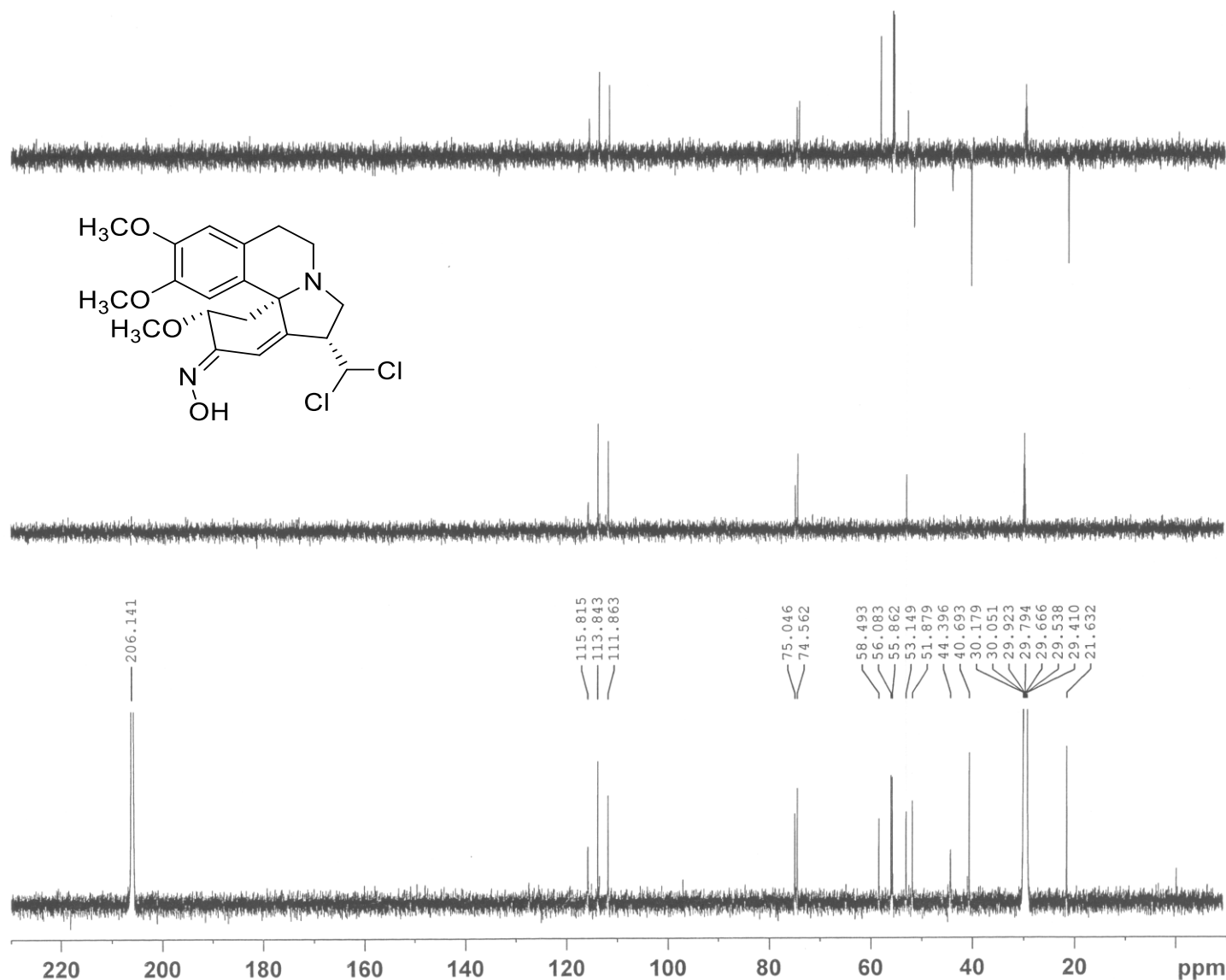
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 PROBHD 5 mm CPQCI 1H-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 4
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 15.82
 DW 41.600 usec
 DE 10.00 usec
 TE 298.0 K
 D1 10.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 600.2307066 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 2.89730000 W

F2 - Processing parameters
 SI 65536
 SF 600.2270156 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S16. ^{13}C -NMR spectrum(in acetone) of erythriarborine C (3)



Current Data Parameters
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EXPNO 4
PROCNO 1

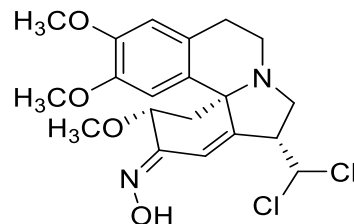
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Date_ 20160404
Time_ 21.51
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zgdc
TD 65536
SOLVENT Acetone
NS 512
DS 4
SWH 36231.883 Hz
FIDRES 0.552855 Hz
AQ 0.9043968 sec
RG 199.06
DW 13.800 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9438010 MHz
NUC1 ^{13}C
P1 11.20 usec
PLW1 94.00000000 W

===== CHANNEL f2 =====
SFO2 600.2294009 MHz
NUC2 ^1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 2.89730000 W
PLW12 0.06519000 W

F2 - Processing parameters
SI 131072
SF 150.9270732 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S17. ^{13}C -NMR spectrum (in DMSO) of erythriarborine C (3)



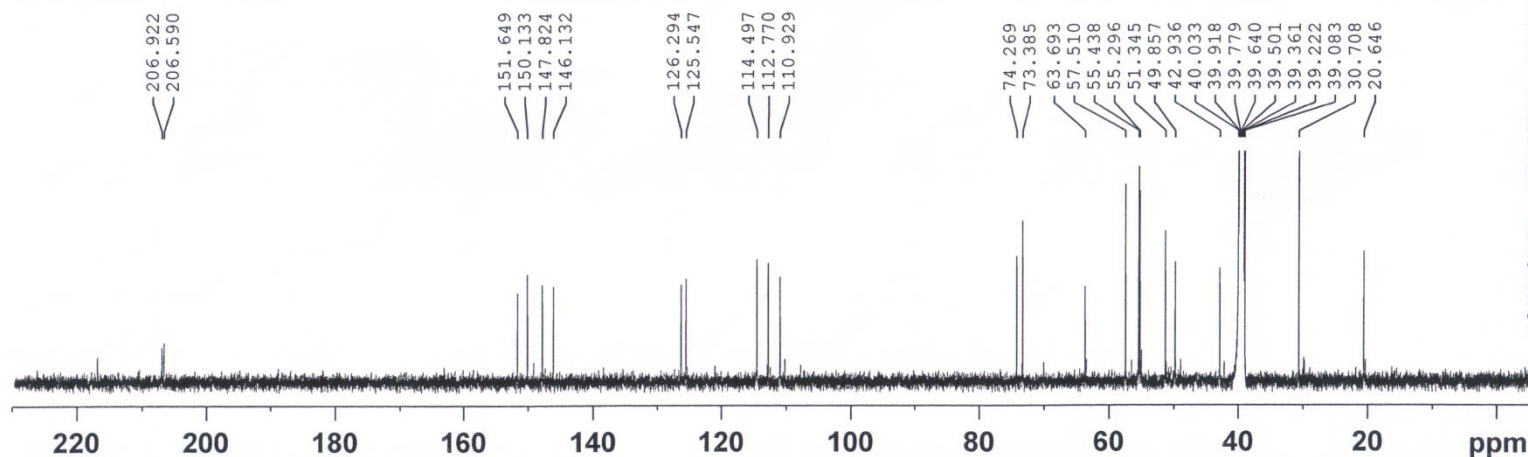
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EXPNO 62
PROCNO 1

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PULPROG zgdc
TD 65536
SOLVENT DMSO
NS 850
DS 4
SWH 36231.883 Hz
FIDRES 0.552855 Hz
AQ 0.9043968 sec
RG 199.06
DW 13.800 usec
DE 18.00 usec
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D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

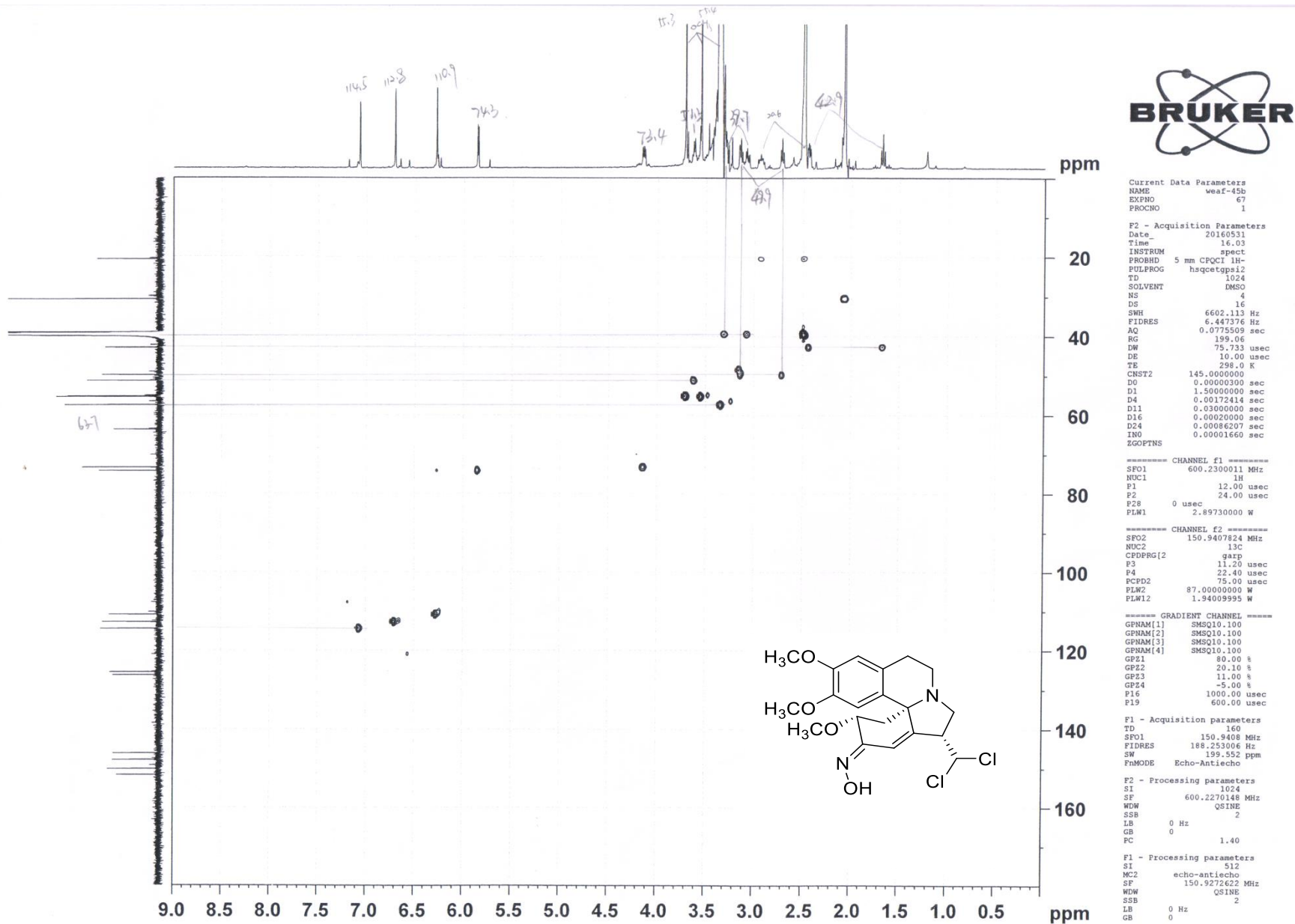
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NUC1 ^{13}C
P1 11.20 usec
PLW1 94.00000000 W

===== CHANNEL f2 =====
SFO2 600.2294009 MHz
NUC2 ^1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 2.89730000 W
PLW12 0.06519000 W

F2 - Processing parameters
SI 131072
SF 150.9272692 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



S17. HSQC spectrum of erythriarborine C (3)



S18. HMBC spectrum of erythriarborine C (3)



Current Data Parameters
NAME weaf-45b
EXPNO 68
PROCNO 1

F2 - Acquisition Parameters
Date 20160528
Time 5.51
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
FULPROG hmbcgp1pndgdf
TD 1024
SOLVENT DMSO
NS 12
DS 16
SWH 9014.423 Hz
FIDRES 8.803147 Hz
AQ 0.0567979 sec
RG 199.06
DW 55.467 usec
DE 10.00 usec
TE 298.0 K
CNST2 145.0000000
CNST13 8.0000000
DO 0.00000300 sec
D1 1.50000000 sec
D2 0.00344828 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001450 sec

===== CHANNEL f1 =====
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NUC1 1H
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P2 24.00 usec
PLW1 2.89730000 W

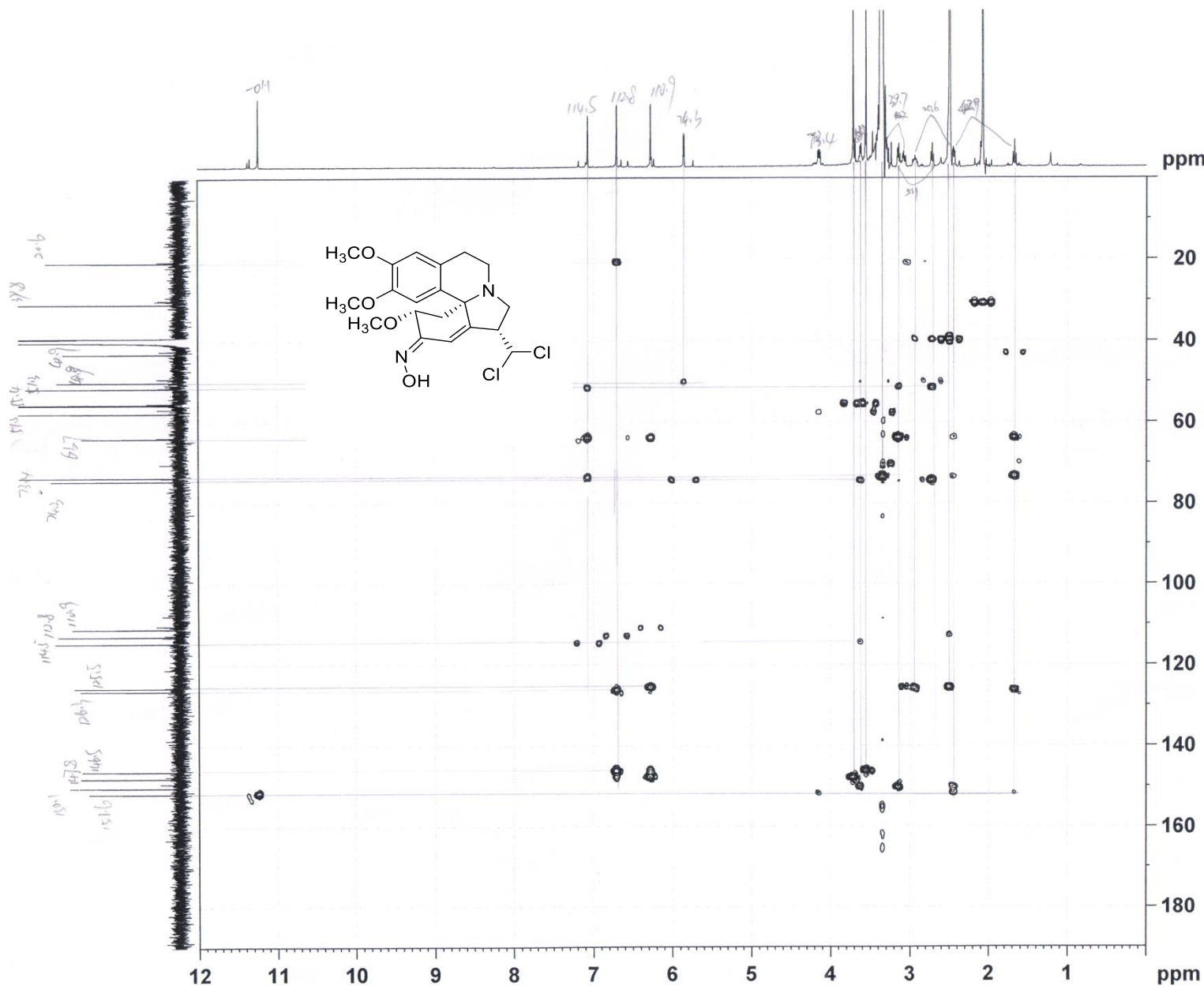
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SFO2 150.9442538 MHz
NUC2 13C
P3 11.20 usec
PLW2 87.00000000 W

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GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

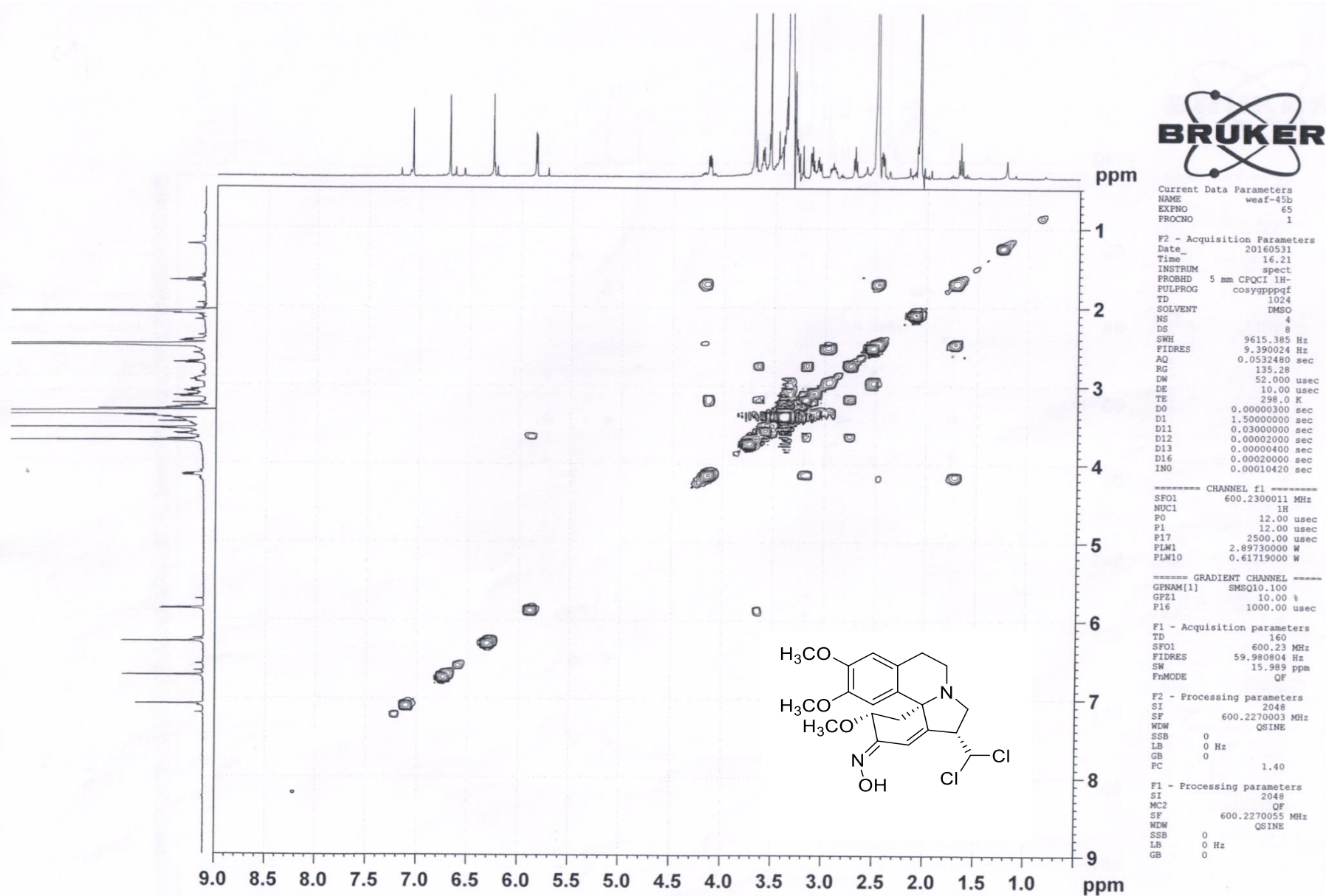
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FIDRES 172.413788 Hz
SW 228.447 ppm
FhMODE QF

F2 - Processing parameters
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SF 600.2270210 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

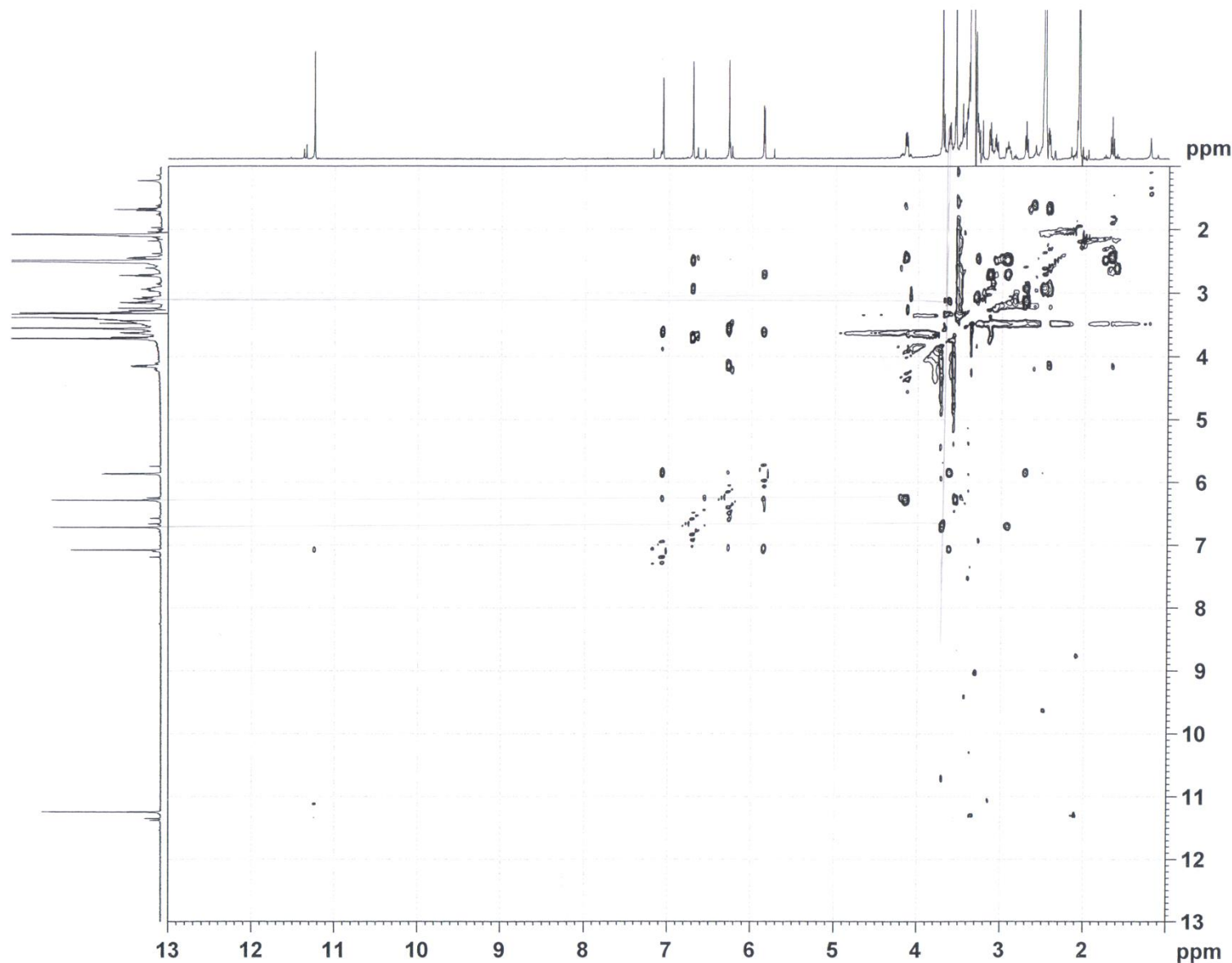
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SI 512
MC2 QF
SF 150.9272322 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



S19. ^1H - ^1H COSY spectrum of erythriarborine C (3)



S20. ROESY spectrum of erythriarborine C (3)



Current Data Parameters
NAME weaf-45b
EXPNO 69
PROCNO 1

F2 - Acquisition Parameters
Date 20160602
Time 5.22
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG roesyphpr.2
TD 1024
SOLVENT DMSO
NS 8
DS 16
SWH 9615.385 Hz
FIDRES 9.390024 Hz
AQ 0.0532480 sec
RG 177.86
DW 52.000 usec
DE 10.00 usec
TE 298.0 K
DO 0.00004046 sec
D1 1.50000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
IN0 0.00010420 sec
L4 1786
P15 300000.00 usec

===== CHANNEL f1 =====
SFO1 600.2290252 MHz
NUC1 1H
P1 12.00 usec
P25 84.00 usec
PLW1 2.89730000 W
PLW9 0.00001669 W
PLW27 0.23652001 W

F1 - Acquisition parameters
TD 160
SFO1 600.229 MHz
FIDRES 59.980804 Hz
SW 15.989 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 2048
SF 600.2270160 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 2048
MC2 States-TPPI
SF 600.2270143 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

S21. HRESIMS spectrum of erythriarborine C (3)

Formula Predictor Report - weaf-45b.lcd

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Data File: E:\DATA\2016\0520\weaf-45b.lcd

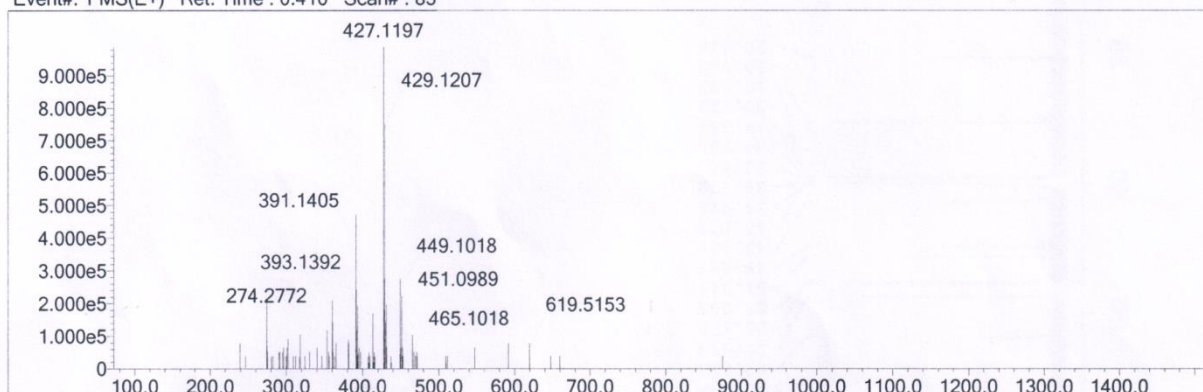
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H	1	0	100	N	3	0	20	Si	4	0	0	Br	1	0	0	H
B	3	0	0	O	2	0	40	S	2	0	0	Pt	2	0	0	
C	4	0	80	F	1	0	0	Cl	1	0	5					

Error Margin (ppm): 100
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

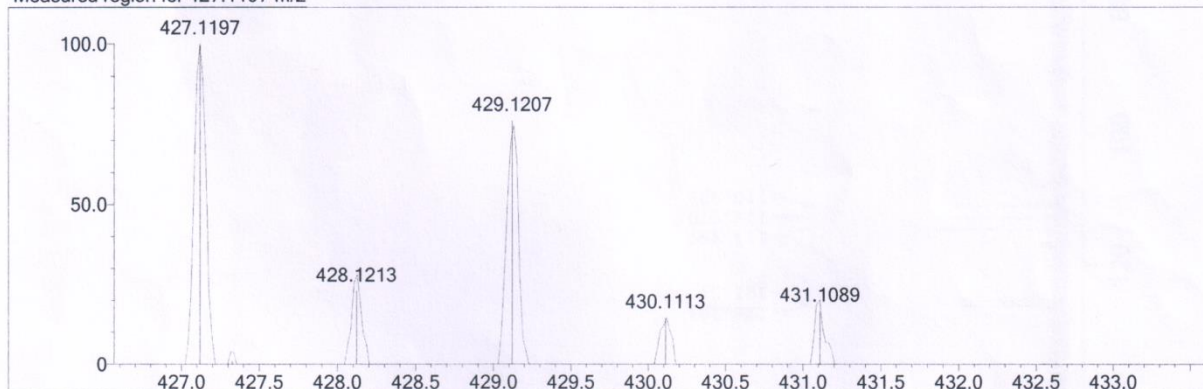
DBE Range: -2.0 - 100.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 10000
 Max Results: 10

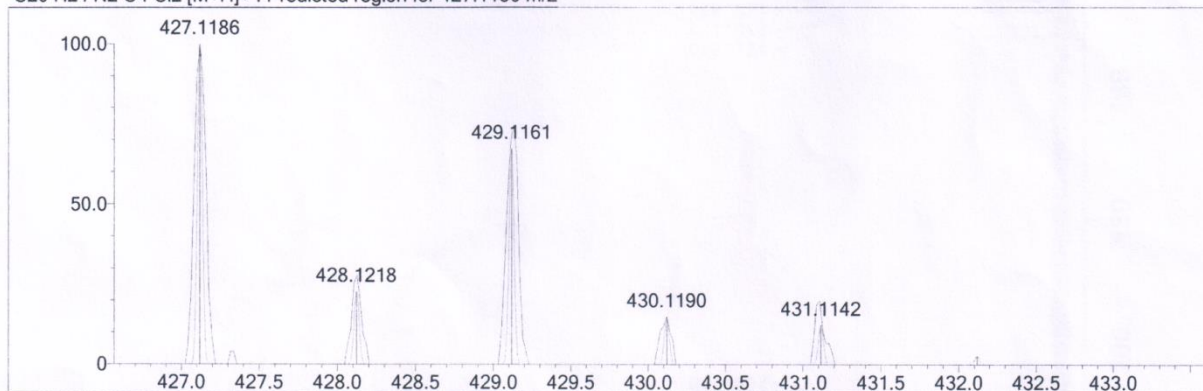
Event#: 1 MS(E+) Ret. Time : 0.410 Scan# : 83



Measured region for 427.1197 m/z

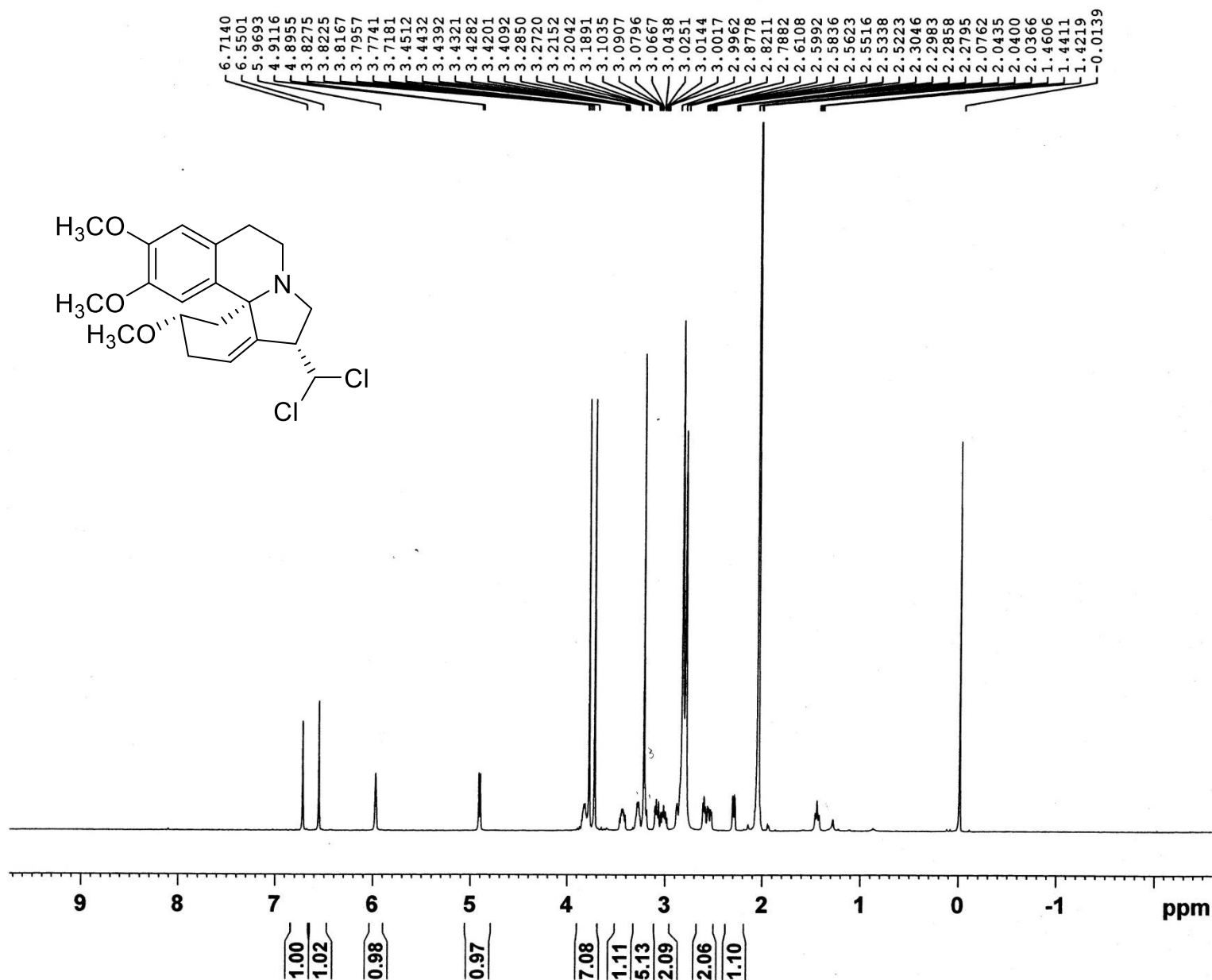


C20 H24 N2 O4 Cl2 [M+H]⁺ : Predicted region for 427.1186 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	92.02	C21 H20 N6 Cl2	[M+H] ⁺	427.1197	427.1199	-0.2	-0.47	92.02	14.0
> 2	90.46	C20 H24 N2 O4 Cl2	[M+H] ⁺	427.1197	427.1186	1.1	2.58	94.18	9.0
3	86.22	C5 H20 N14 O5 Cl2	[M+H] ⁺	427.1197	427.1191	0.6	1.40	87.09	2.0
4	83.54	C6 H16 N18 O Cl2	[M+H] ⁺	427.1197	427.1204	-0.7	-1.64	84.90	7.0

S22. ¹H NMR Spectrum of erytharborine D (4)



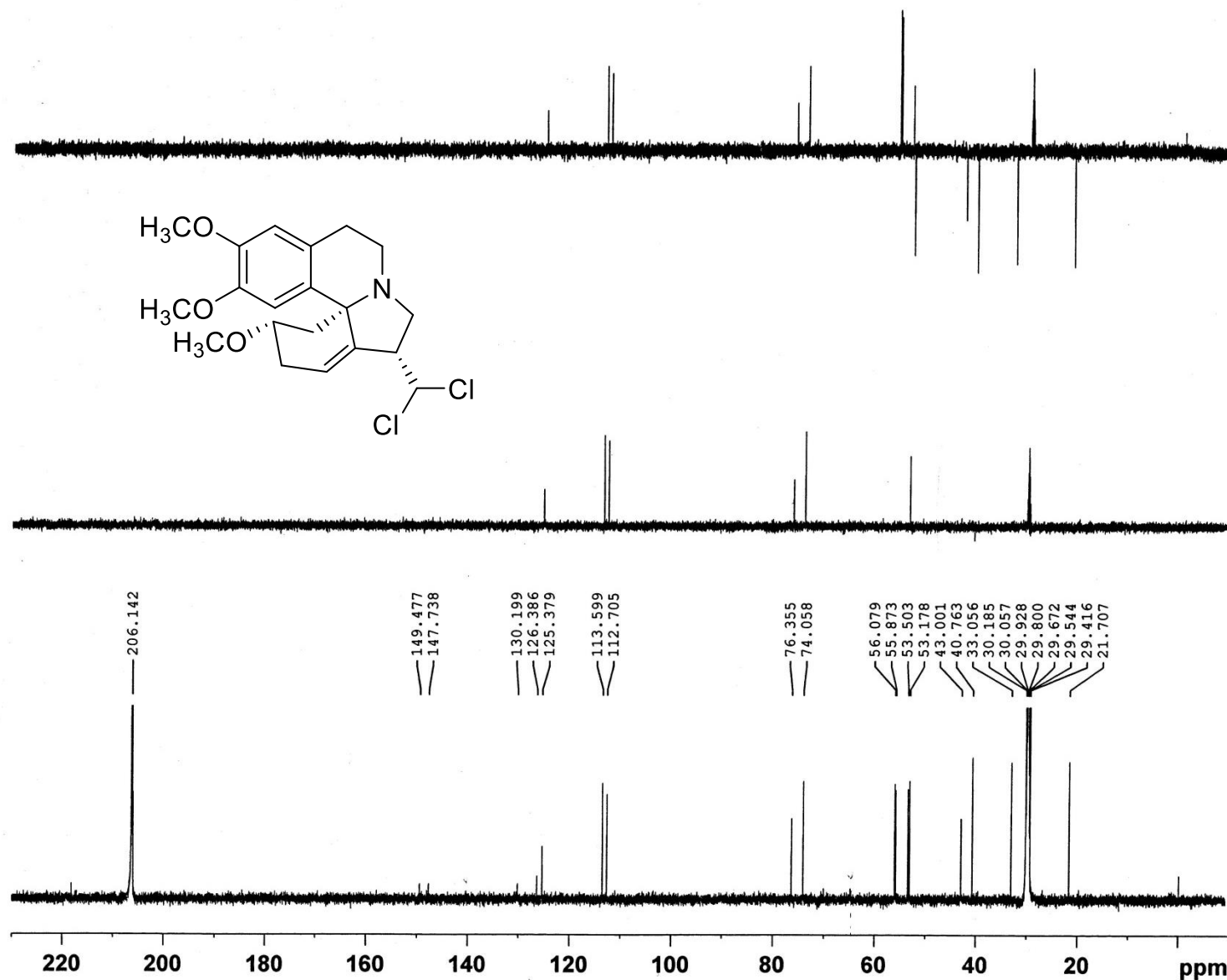
Current Data Parameters
NAME weaf-50
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160322
Time 1.03
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 4
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 15.82
DW 41.600 usec
DE 10.00 usec
TE 298.0 K
D1 10.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 600.2307066 MHz
NUC1 1H
P1 12.00 usec
PLW1 2.89730000 W

F2 - Processing parameters
SI 65536
SF 600.2270184 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S23. ^{13}C NMR Spectrum of erytharborine D (4)



Current Data Parameters
 NAME weaf-50
 EXPNO 4
 PROCNO 1

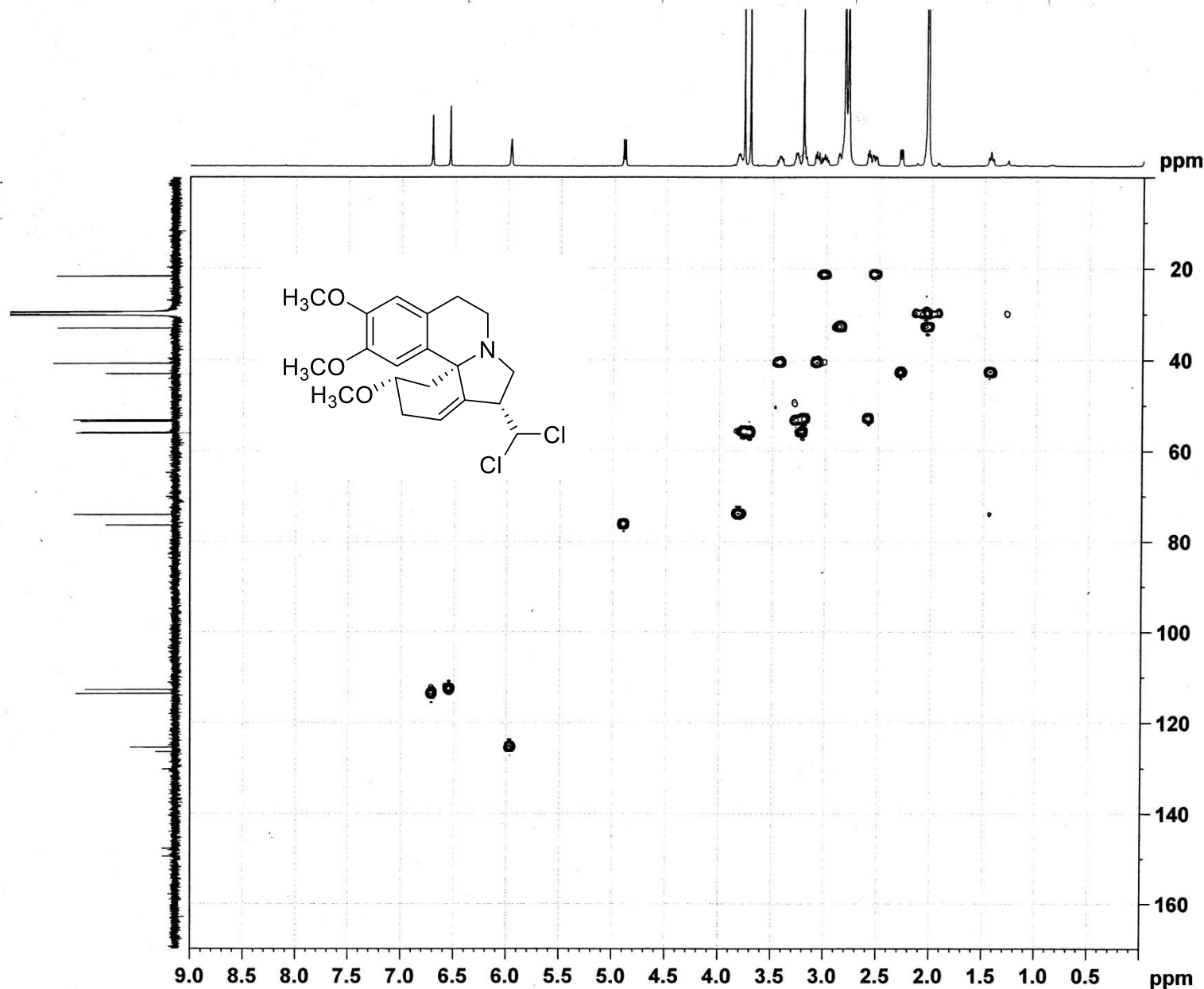
F2 - Acquisition Parameters
 Date_ 20160325
 Time 11.46
 INSTRUM spect
 PROBHD 5 mm CPQCI 1H-
 PULPROG zgdc
 TD 65536
 SOLVENT Acetone
 NS 600
 DS 4
 SWH 36231.883 Hz
 FIDRES 0.552855 Hz
 AQ 0.9043968 sec
 RG 199.06
 DW 13.800 usec
 DE 18.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9438010 MHz
 NUC1 ^{13}C
 P1 11.20 usec
 PLW1 94.00000000 W

===== CHANNEL f2 =====
 SFO2 600.2294009 MHz
 NUC2 ^1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 2.89730000 W
 PLW12 0.06519000 W

F2 - Processing parameters
 SI 131072
 SF 150.9270711 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

S24. HSQC Spectrum of erytharborine D (4)



Current Data Parameters
NAME weaf-50
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160412
Time 20.23
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG haqcetgps12
TD 1024
SOLVENT Acetone
NS 4
DS 16
SWH 8417.509 Hz
FIDRES 8.220223 Hz
AQ 0.0608256 sec
RG 199.06
DW 59.400 usec
DE 10.00 usec
TE 298.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086207 sec
INO 0.0001660 sec
ZGPTNS

===== CHANNEL f1 =====
SFO1 600.2300011 MHz
NUC1 1H
P1 12.00 usec
F2 24.00 usec
P28 0 usec
PLW1 2.89730000 W

===== CHANNEL f2 =====
SFO2 150.9407824 MHz
NUC2 13C
CPDPRG2 garp
P3 11.20 usec
P4 22.40 usec
PCPD2 75.00 usec
PLW2 87.00000000 W
PLW12 1.94009995 W

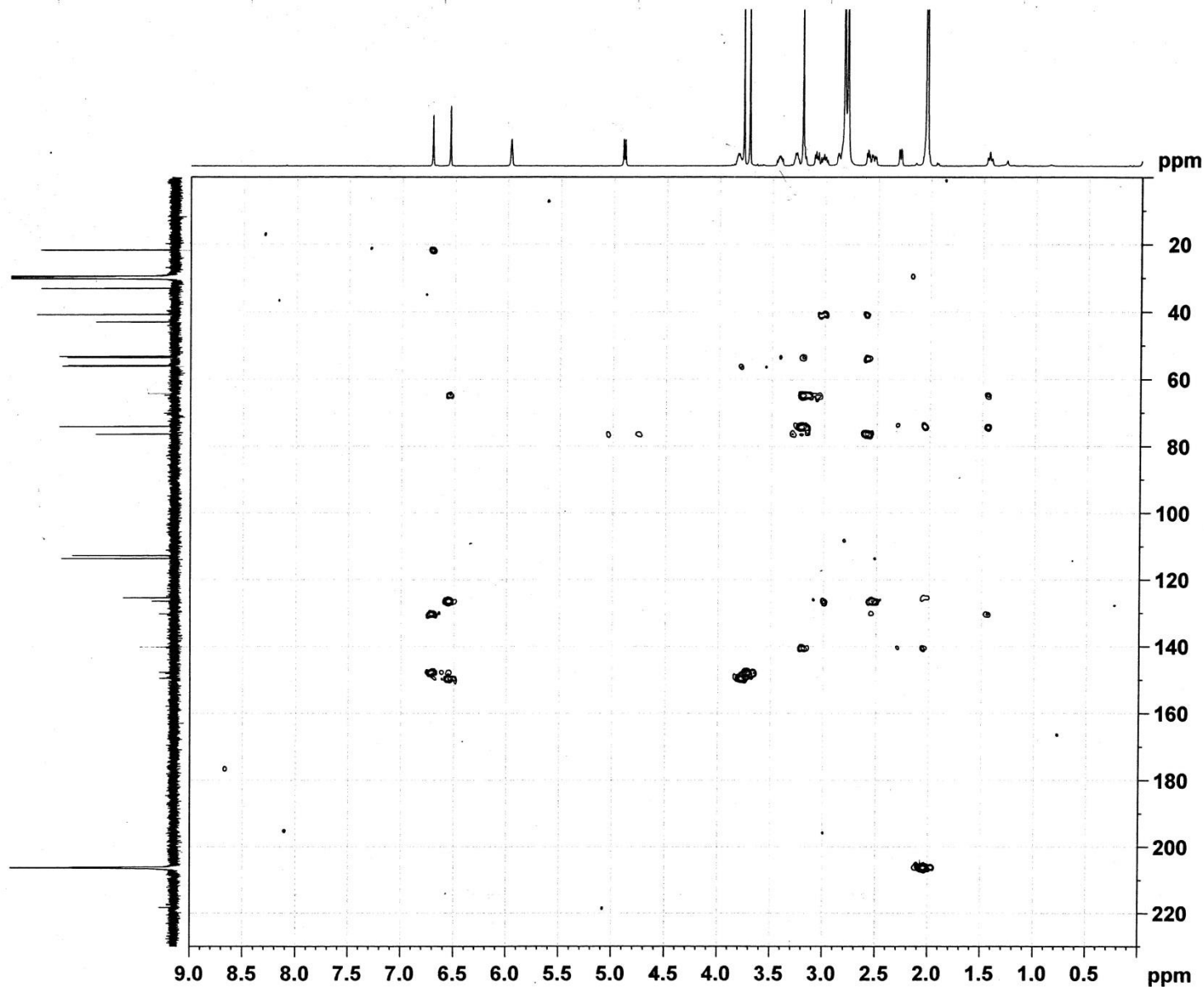
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GP21 80.00 %
GP22 20.10 %
GP23 11.00 %
GP24 -5.00 %
P16 1000.00 usec
P18 600.00 usec

F1 - Acquisition parameters
TD 160
SFO1 150.9408 MHz
FIDRES 188.253006 Hz
SW 199.552 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.2270335 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 512
MC2 echo-antiecho
SF 150.9270882 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

S25. HMBC Spectrum of erytharborine D (4)



Current Data Parameters
NAME weaf-50
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160412
Time 20.41
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG hmbcpglpndqf
TD 1024
SOLVENT Acetone
NS 8
DS 16
SWH 8417.509 Hz
FIDRES 8.220223 Hz
AQ 0.0608256 sec
RG 199.06
DW 59.400 usec
DE 10.00 usec
TE 298.0 K
CNST2 145.0000000
CNST13 8.0000000
DO 0.00000300 sec
D1 1.50000000 sec
D2 0.00344828 sec
D6 0.06250000 sec
D16 0.00020000 sec
INO 0.0001450 sec

===== CHANNEL f1 =====
SFO1 600.2300011 MHz
NUC1 1H
P1 12.00 usec
P2 24.00 usec
PLW1 2.89730000 W

===== CHANNEL f2 =====
SFO2 150.9442538 MHz
NUC2 13C
P3 11.20 usec
PLW2 87.00000000 W

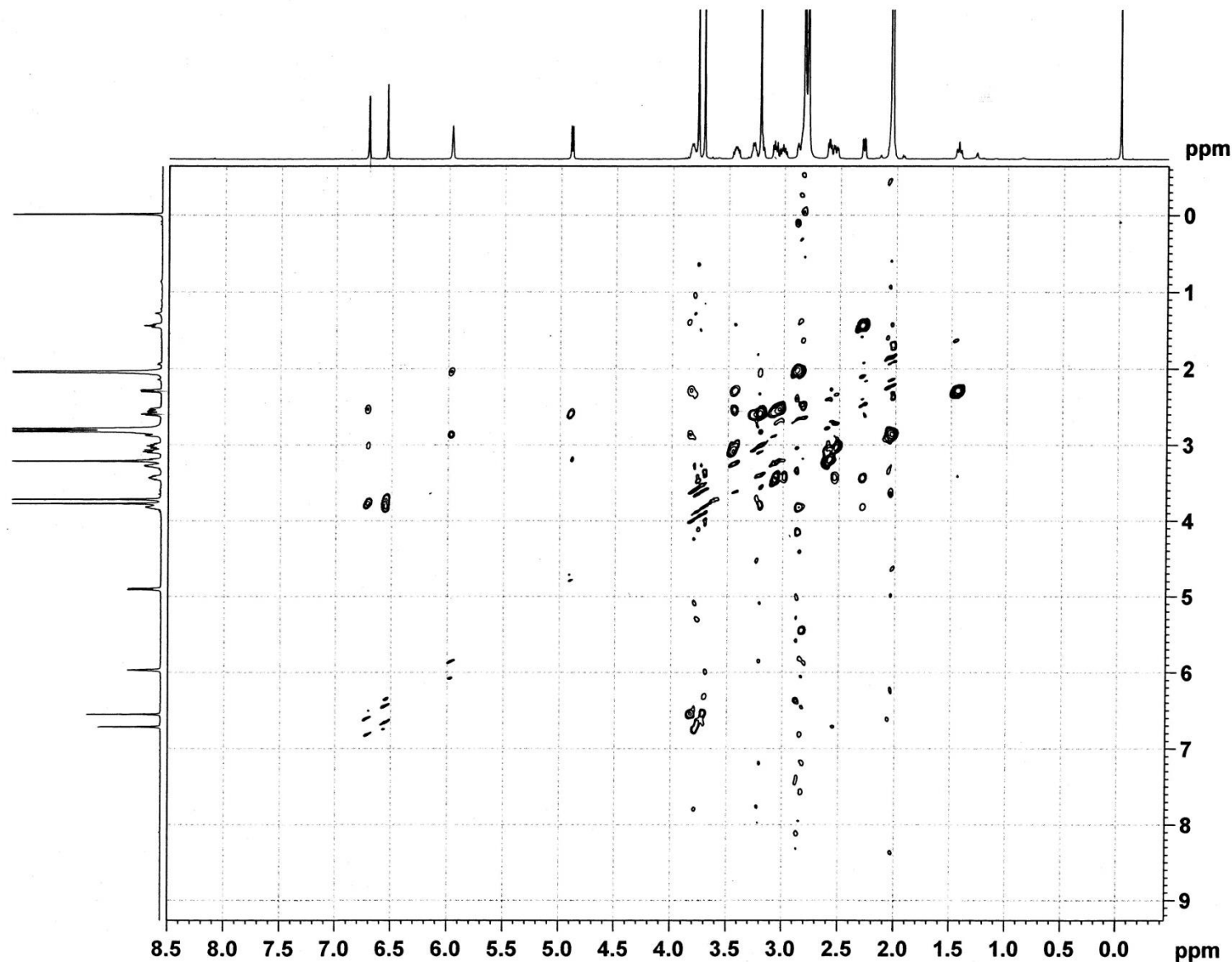
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
F16 1000.00 usec

F1 - Acquisition parameters
TD 148
SFO1 150.9443 MHz
FIDRES 232.991608 Hz
SW 228.447 ppm
FMODE QF

F2 - Processing parameters
SI 2048
SF 600.2270396 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 512
MC2 QF
SF 150.9270305 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

S26. ROESY Spectrum of erytharborine D (4)



Current Data Parameters
NAME weaf-50
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160412
Time 19.41
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG roesyphpp.2
TD 1024
SOLVENT Acetone
NS 8
DS 16
SWH 8417.509 Hz
FIDRES 8.220223 Hz
AQ 0.0608256 sec
RG 199.06
DW 59.400 usec
DE 10.00 usec
TE 298.0 K
D0 0.00004786 sec
D1 1.50000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
IN0 0.00011900 sec
L4 1786
P15 300000.00 usec

----- CHANNEL f1 -----
SFO1 600.2300011 MHz
NUC1 1H
P1 12.00 usec
P17 2500.00 usec
P25 84.00 usec
PLW1 2.89730000 W
PLW10 0.61719000 W
PLW27 0.23652001 W

F1 - Acquisition parameters
TD 160
SFO1 600.23 MHz
FIDRES 52.521008 Hz
SW 14.000 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 2048
SF 600.2270345 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 2048
MC2 States-TPPI
SF 600.2270375 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

S27. HRESIMS spectrum of erythriarborine D (4)

Formula Predictor Report - weaf-50.lcd

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Data File: E:\DATA\2016\0415\weaf-50.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	100	N	3	0	20	Si	4	0	0	Br	1	0	0	H
B	3	0	0	O	2	0	40	S	2	0	0	Pt	2	0	0	
C	4	0	80	F	1	0	0	Cl	1	0	2					

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: -2.0 - 100.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

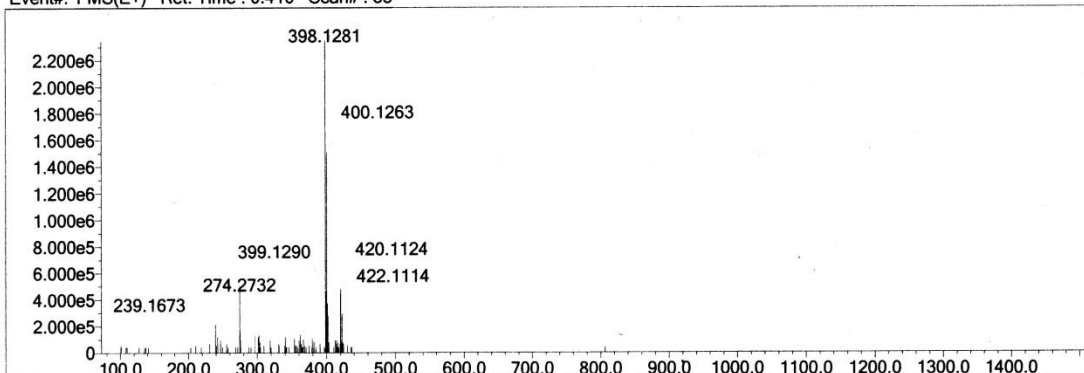
Electron Ions: both

Use MSn Info: yes

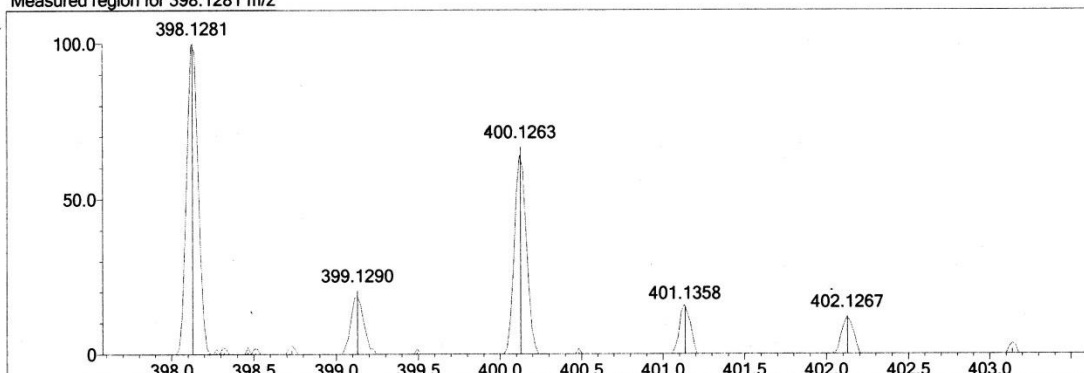
Isotope Res: 10000

Max Results: 10

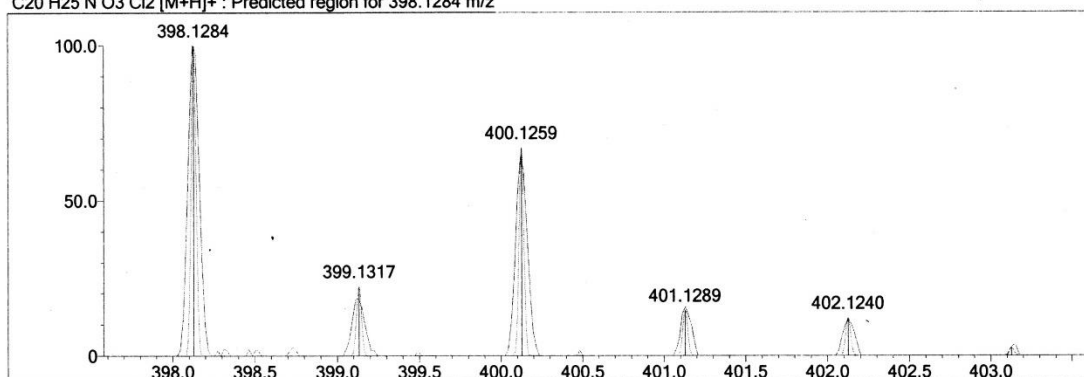
Event#: 1 MS(E+) Ret. Time : 0.410 Scan#: 83



Measured region for 398.1281 m/z



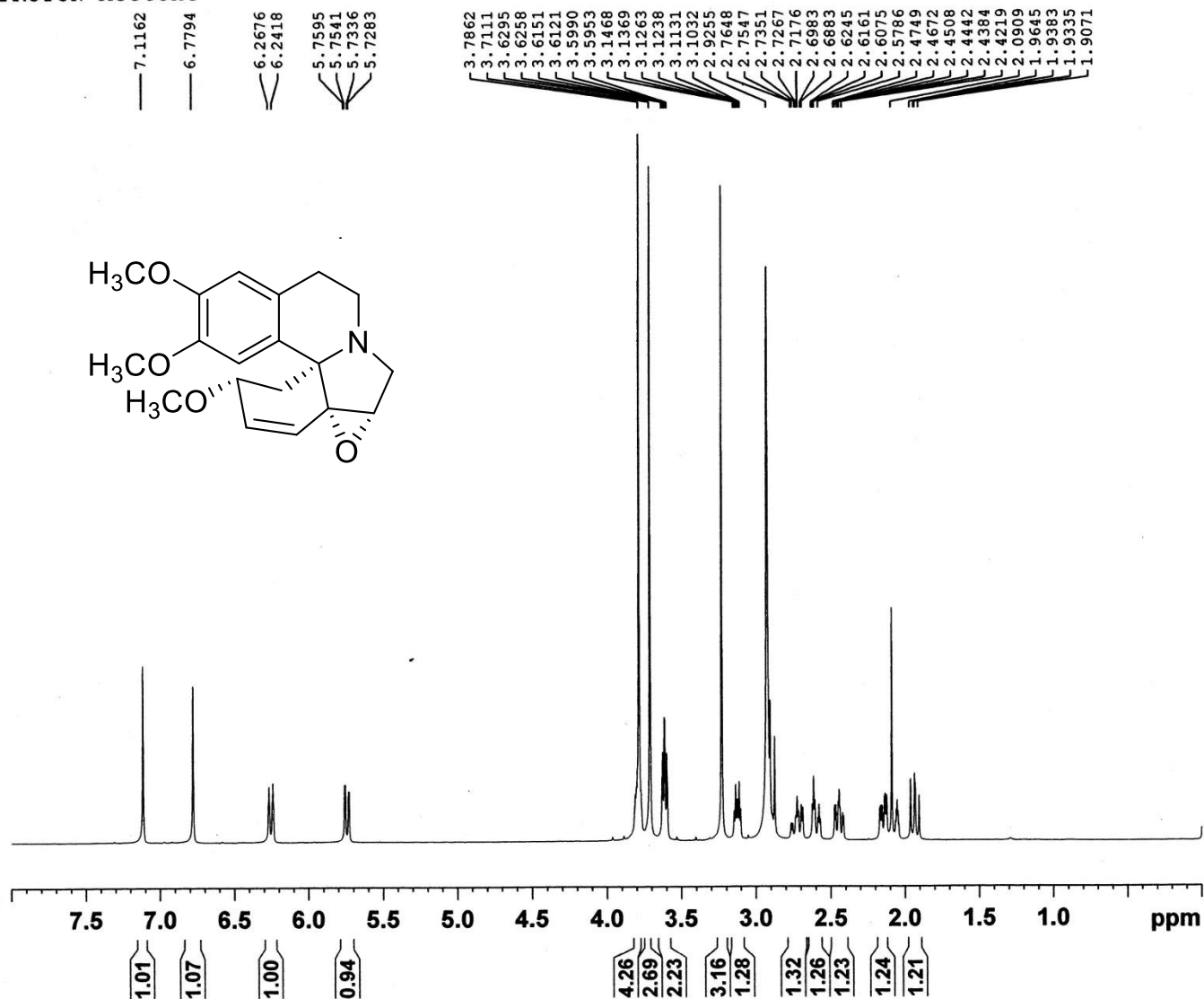
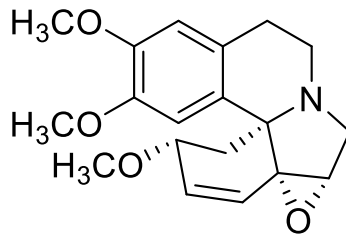
C20 H25 N O3 Cl2 [M+H]⁺ : Predicted region for 398.1284 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	100.00	C20 H25 N O3 Cl2	[M+H] ⁺	398.1281	398.1284	-0.3	-0.75	100.00	8.0

S28. ^1H NMR Spectrum of erythriarborine E (5)

weaf-12
PROTON Acetone



Current Data Parameters
NAME weaf-12
EXPNO 1
PROCNO 1

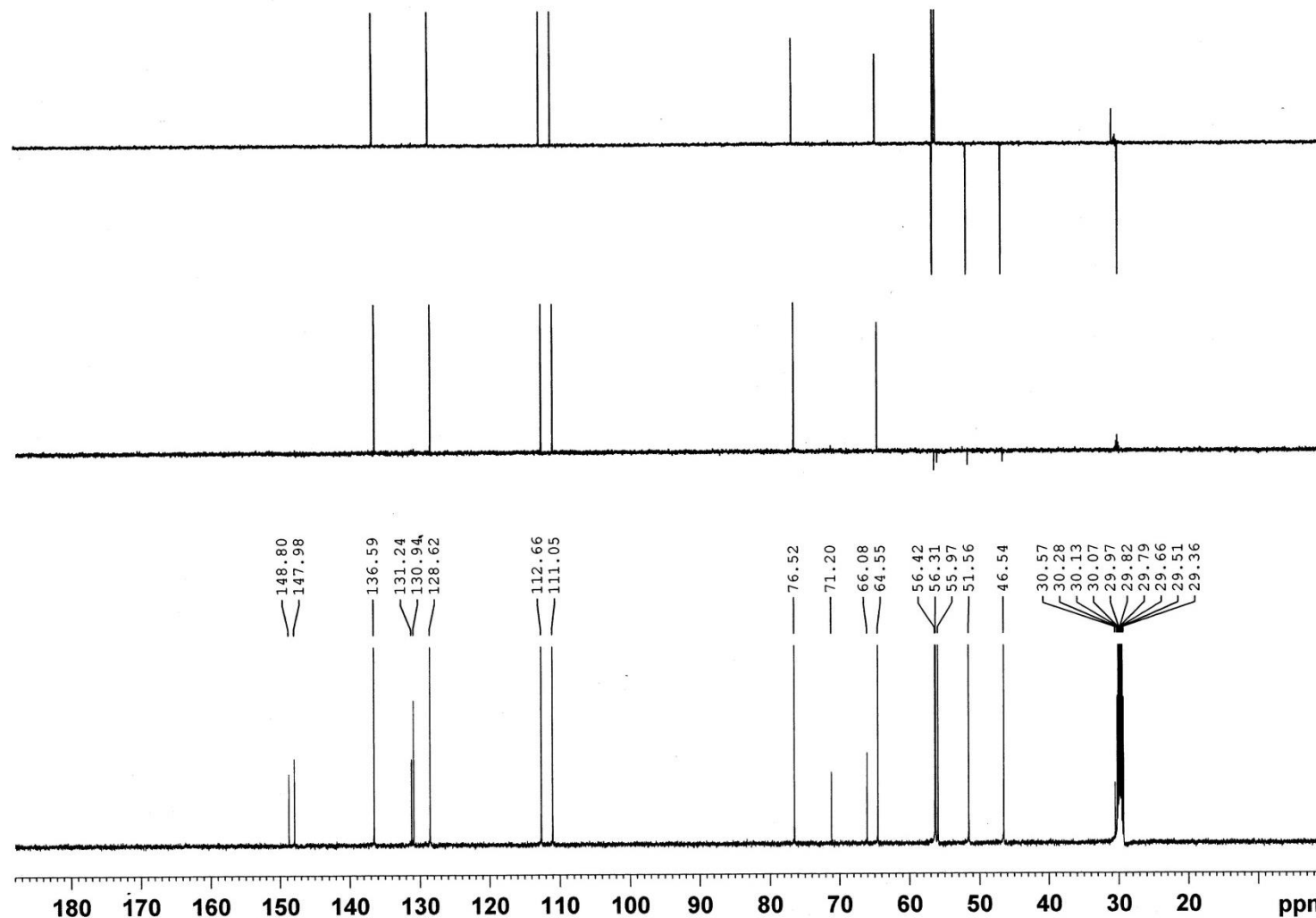
F2 - Acquisition Parameters
Date_ 20160103
Time_ 21.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 14.09
DW 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1318812 MHz
NUC1 1H
P1 12.00 usec
PLW1 11.69999981 W

F2 - Processing parameters
SI 65536
SF 400.1300050 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

S29. ¹³CNMR Spectrum of erythriarborine E (5)

weaf12 c13 and dept



Current Data Parameters
 NAME weaf12
 EXPNO 22
 PROCNO 1

F2 - Acquisition Parameters
 Date 20160106
 Time 6.18
 INSTRUM spect
 PROBHD 5 mm CPQCI 1H/
 FULPROG zgpg
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 187.72
 DW 16.800 usec
 DE 18.00 usec
 TE 296.2 K
 D1 3.00000000 sec
 D11 0.03000000 sec
 TDO 1

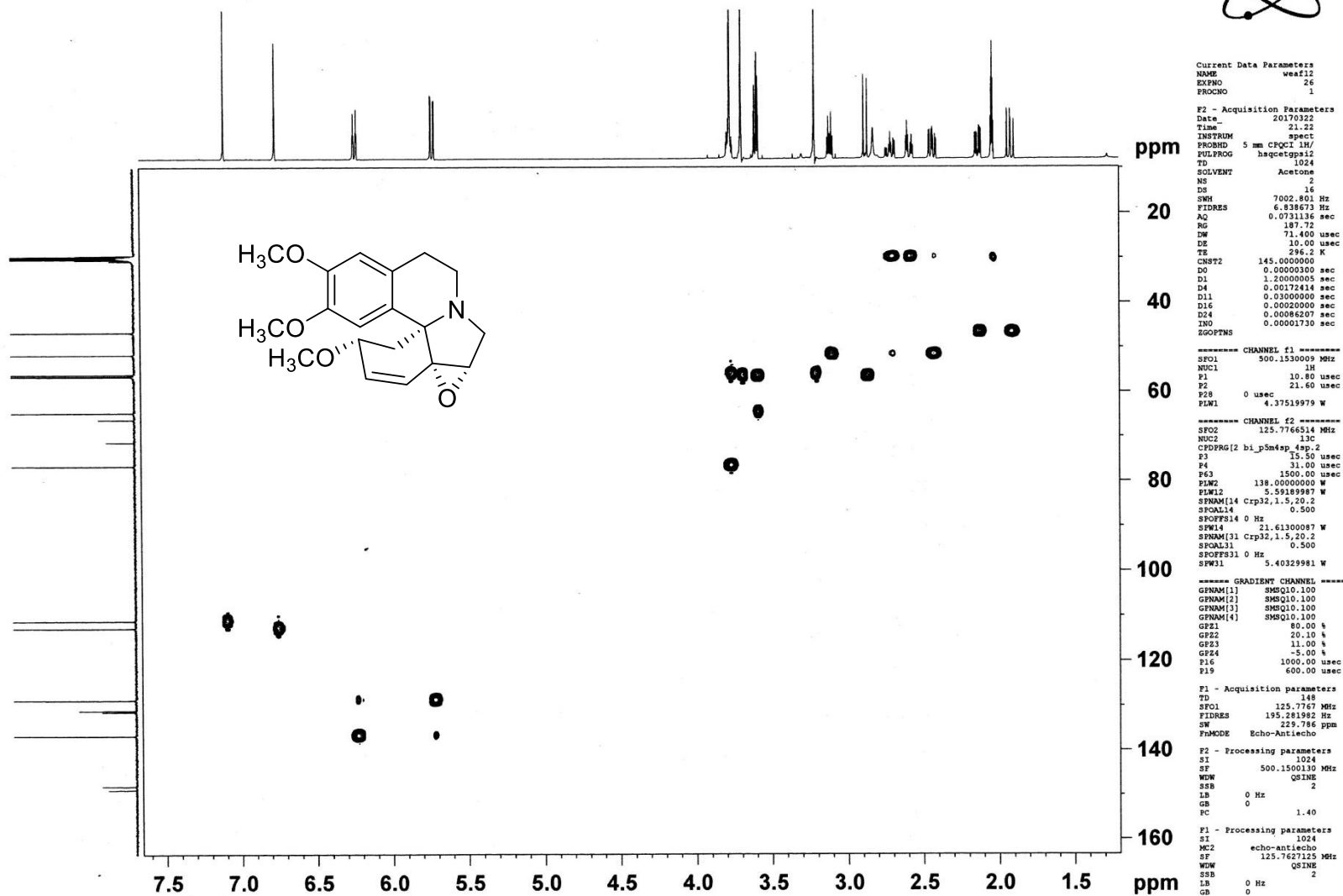
===== CHANNEL f1 =====
 SFO1 125.7769030 MHz
 NUC1 13C
 P1 11.70 usec
 PLW1 160.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1527508 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 100.00 usec
 FIM2 4.37519979 W
 PLW2 0.05390700 W

F2 - Processing parameters
 SI 32768
 SF 125.7627125 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

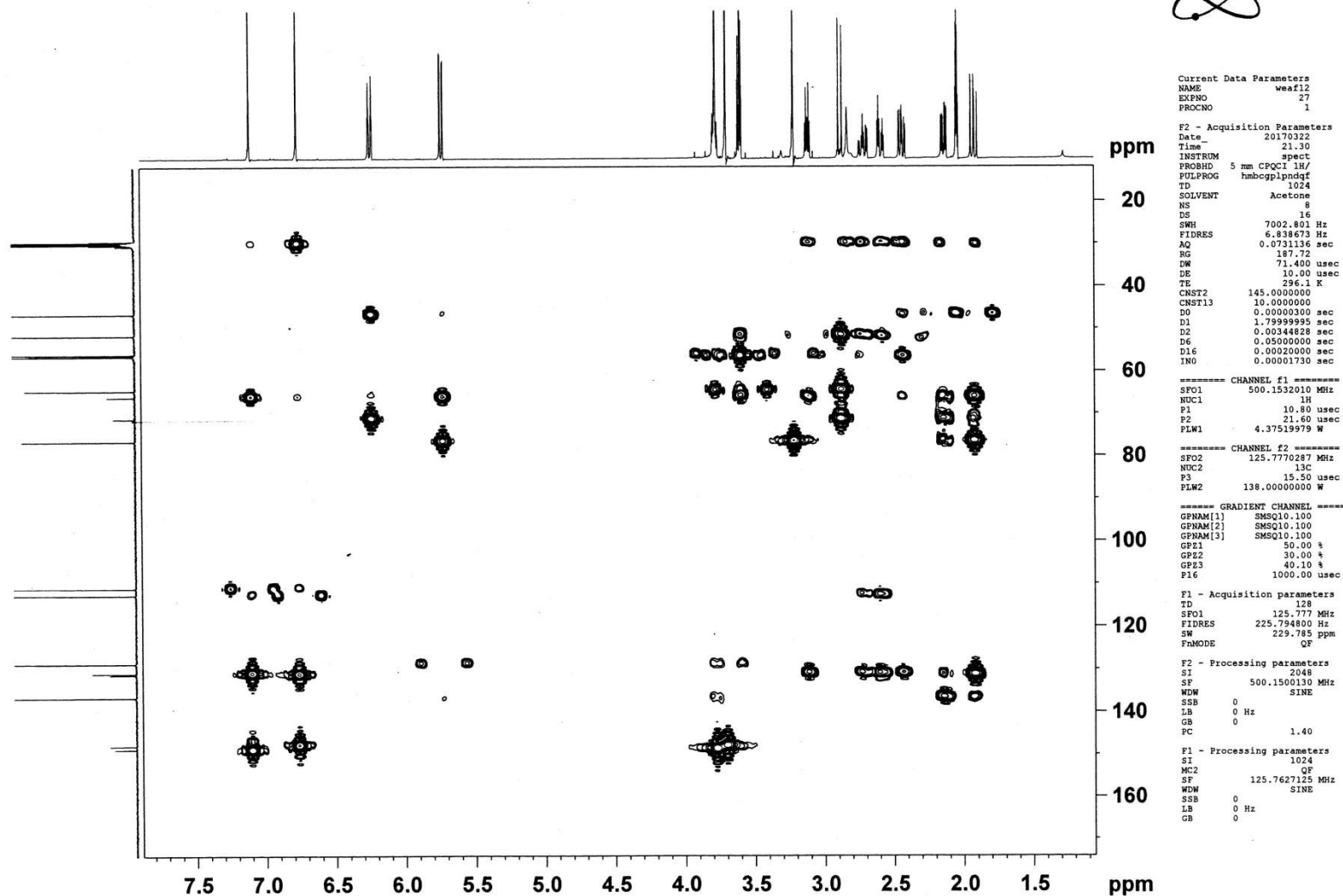
S30. HSQC Spectrum of erythriarborine E (5)

weaf12 hsqc



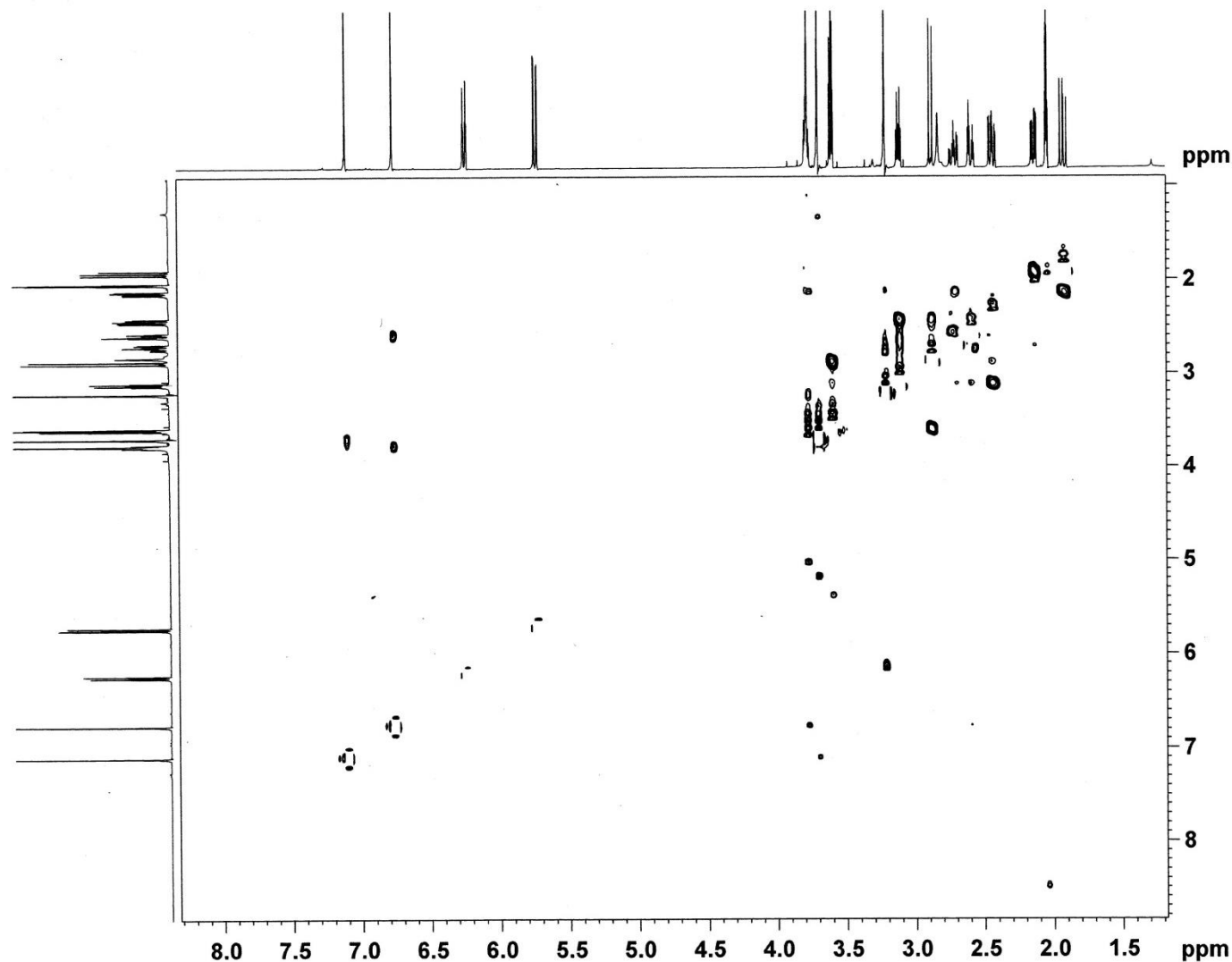
S31. HMBC Spectrum of erythriarborine E (5)

weaf12 hmbc



S32. ROESY Spectrum of erythriarborine E (5)

weaf12 roesy



Current Data Parameters
NAME weaf12
EXPNO 28
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170322
Time 22.04
INSTRUM spect
PROBHD 5 mm CPQCI 1H/
PULPROG croesyph
TD 1024
SOLVENT Acetone
NS 8
DS 32
SWH 6493.506 Hz
FIDRES 6.341315 Hz
AQ 0.0788480 sec
RG 2.01
DW 77.000 usec
DE 10.00 usec
TE 296.2 K
DO 0.00006315 sec
D1 1.20000005 sec
D12 0.00002000 sec
D13 0.00004000 sec
INO 0.00015380 sec

----- CHANNEL f1 -----
SFO1 500.1532010 MHz
NUC1 1H
P1 10.80 usec
P15 680000.00 usec
PLW1 4.3751979 W
PLW11 0.06300300 W

F1 - Acquisition parameters
TD 160
SFO1 500.1532 MHz
FIDRES 40.637192 Hz
SW 13.000 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 500.1500130 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 500.1500130 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

S33. HRESIMS Spectrum of erythriarborine E (5)

Formula Predictor Report - weaf-12.lcd

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Data File: E:\DATA\2017\0221\weaf-12.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	150	O	2	0	50	S	2	0	0	Pt	2	0	0	H
B	3	0	0	F	1	0	0	Cl	1	0	0					Na
C	4	0	100	Na	1	0	0	Br	1	0	0					
N	3	0	20	Si	4	0	0	I	3	0	0					

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: -2.0 - 100.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

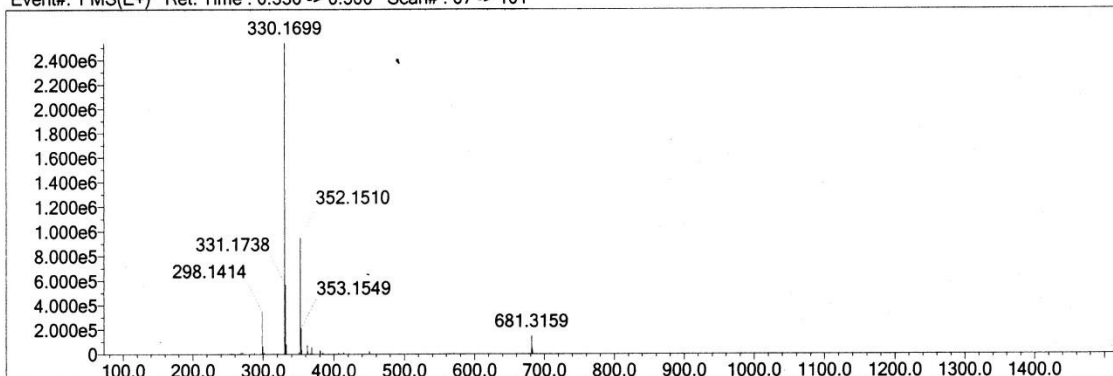
Electron Ions: both

Use MSn Info: yes

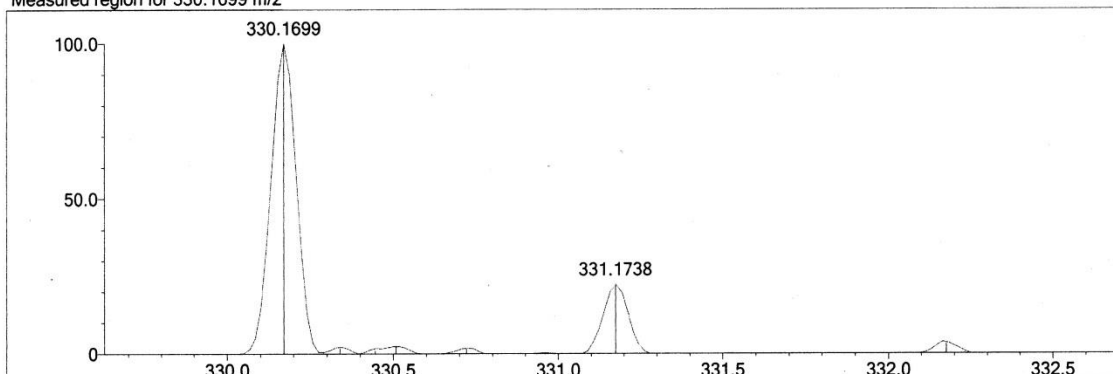
Isotope Res: 10000

Max Results: 10

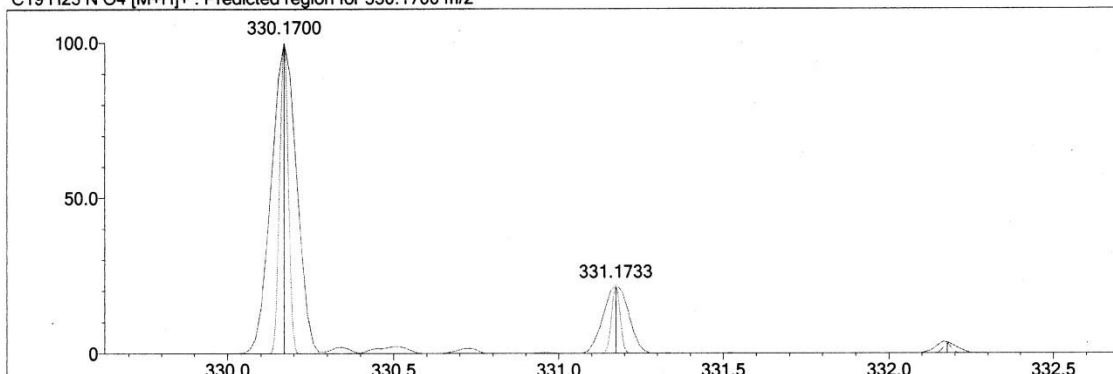
Event#: 1 MS(E+) Ret. Time : 0.330 -> 0.500 Scan#: 67 -> 101



Measured region for 330.1699 m/z

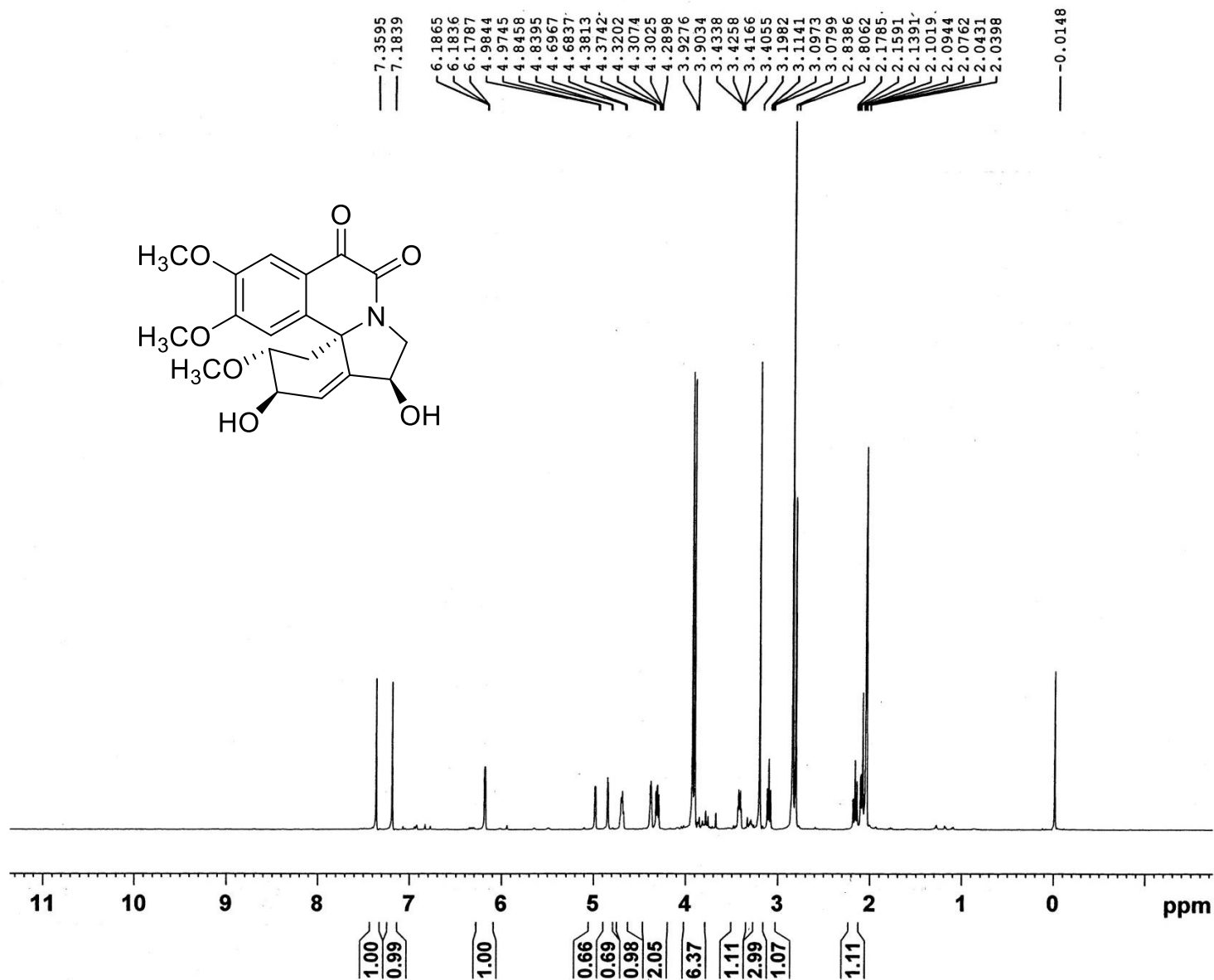


C19 H23 N O4 [M+H]⁺ : Predicted region for 330.1700 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C19 H23 N O4	[M+H] ⁺	330.1699	330.1700	-0.1	-0.30	9.0

S34. ^1H NMR Spectrum of erythriarborine F (6)



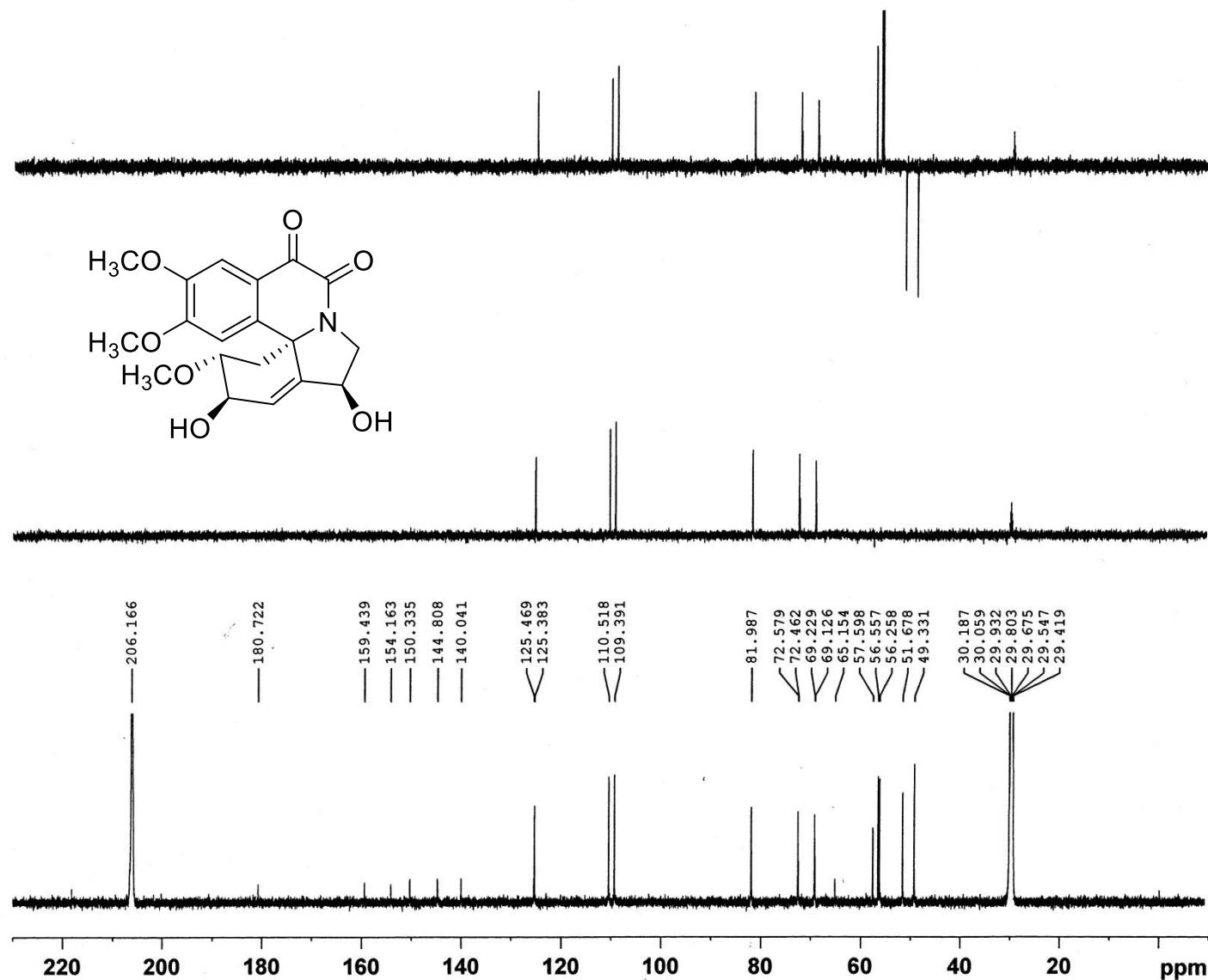
Current Data Parameters
NAME weaf-58
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160331
Time_ 8.02
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 4
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 15.82
DW 41.600 usec
DE 10.00 usec
TE 298.0 K
D1 10.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 600.2307066 MHz
NUC1 1H
P1 12.00 usec
PLW1 2.89730000 W

F2 - Processing parameters
SI 65536
SF 600.2270183 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S35. ^{13}C NMR Spectrum of erythriarborine F (6)



Current Data Parameters
NAME weaf-58
EXPNO 4
PROCNO 1

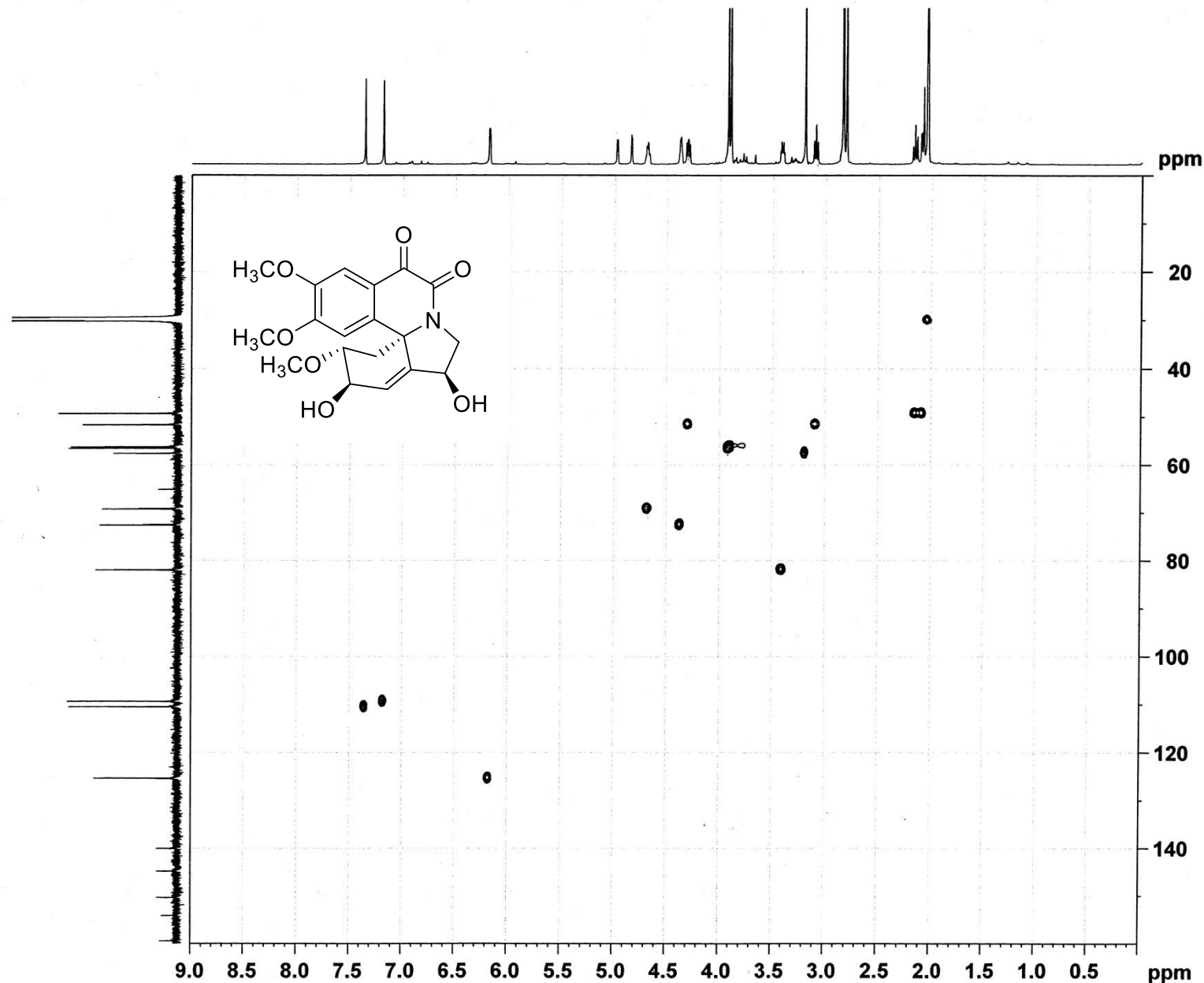
F2 - Acquisition Parameters
Date_ 20160405
Time_ 10.41
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zgdc
TD 65536
SOLVENT Acetone
NS 512
DS 4
SWH 36231.883 Hz
FIDRES 0.552855 Hz
AQ 0.9043968 sec
RG 199.06
DW 13.800 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 150.9438010 MHz
NUC1 ^{13}C
P1 11.20 usec
PLW1 94.00000000 W

----- CHANNEL f2 -----
SFO2 600.2294009 MHz
NUC2 ^1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 2.89730000 W
PLW12 0.06519000 W

F2 - Processing parameters
SI 131072
SF 150.9270744 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S36. HSQC Spectrum of erythriarborine F (6)



Current Data Parameters
NAME weaf-58
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160414
Time 5.47
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG hsqcetgps12
TD 1024
SOLVENT Acetone
NS 4
DS 16
SWH 8417.509 Hz
FIDRES 8.220223 Hz
AQ 0.0608256 sec
RG 199.06
DW 59.400 usec
DE 10.00 usec
TE 298.0 K
CNST2 145.0000000
DO 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086207 sec
IN0 0.00001660 sec
ZGPTNS

===== CHANNEL f1 =====
SFO1 600.2300011 MHz
NUC1 1H
P1 12.00 usec
P2 24.00 usec
P28 0 usec
PLW1 2.89730000 W

===== CHANNEL f2 =====
SFO2 150.9407824 MHz
NUC2 13C
CPDPRG2 garp
P3 11.20 usec
P4 22.40 usec
PCPD2 75.00 usec
PLW2 87.0000000 W
PLW12 1.94009995 W

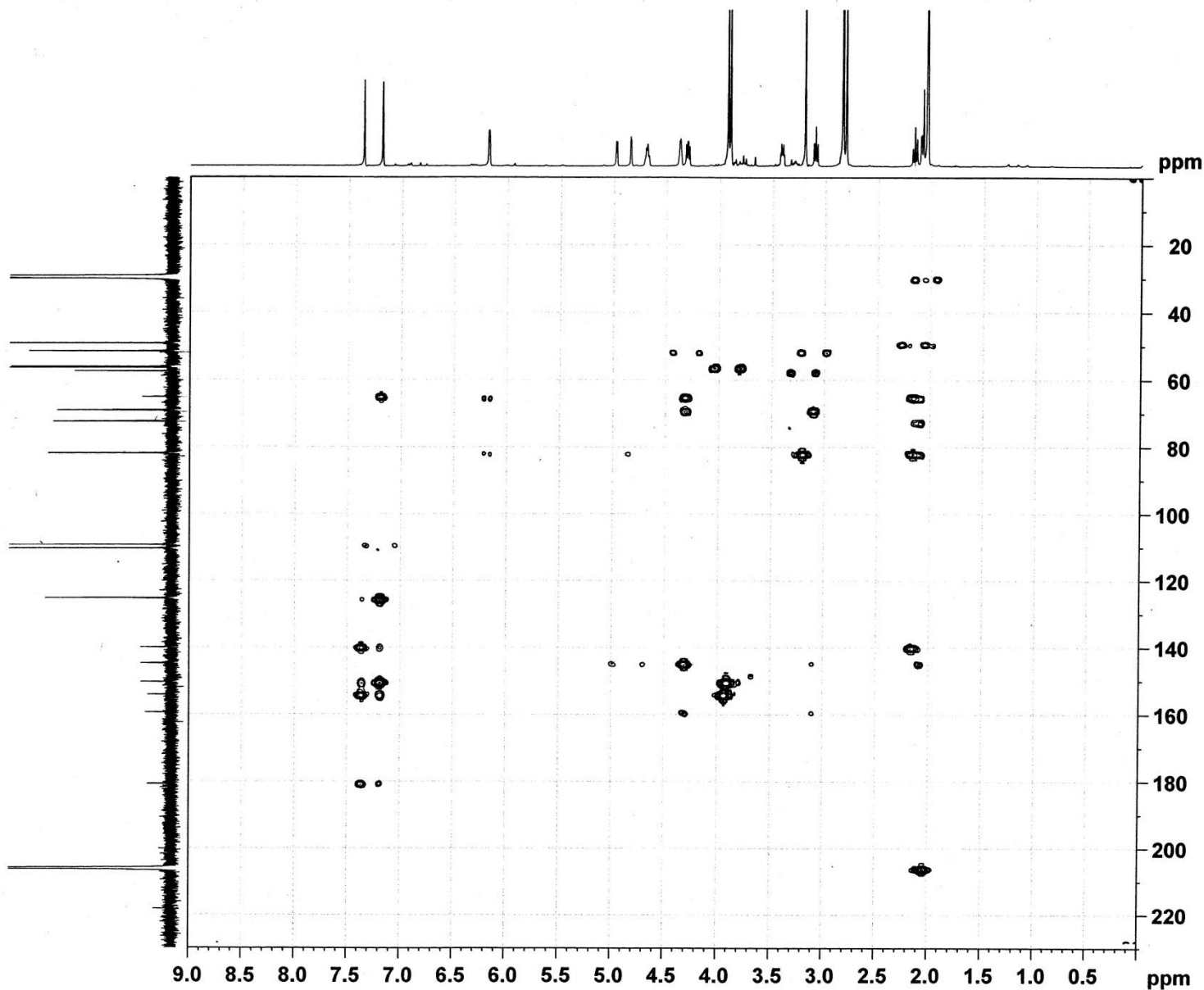
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 160
SFO1 150.9408 MHz
FIDRES 188.253006 Hz
SW 199.552 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.2270199 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 512
MC2 echo-antiecho
SF 150.9270764 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

S37. HMBC Spectrum of taberdivarine E



Current Data Parameters
NAME wesf-58
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160414
Time 6.05
INSTRUM spect
PROBHD 5 mm CPOCT 1H-
PULPROG hmbcpglpndqf
TD 1024
SOLVENT Acetone
NS 8
DS 16
SWH 8417.509 Hz
FIDRES 8.220223 Hz
AQ 0.0608256 sec
RG 199.06
DW 59.400 usec
DE 10.00 usec
TE 298.0 K
CNST2 145.0000000
CNST13 8.0000000
D0 0.0000300 sec
D1 1.50000000 sec
D2 0.00344828 sec
D6 0.06250000 sec
D14 0.00020000 sec
INO 0.00001450 sec

===== CHANNEL f1 =====
SFO1 600.2300011 MHz
NUC1 1H
P1 12.00 usec
P2 24.00 usec
PLW1 2.89730000 W

===== CHANNEL f2 =====
SFO2 150.9442538 MHz
WUC2 13C
P3 11.20 usec
PLW2 87.00000000 W

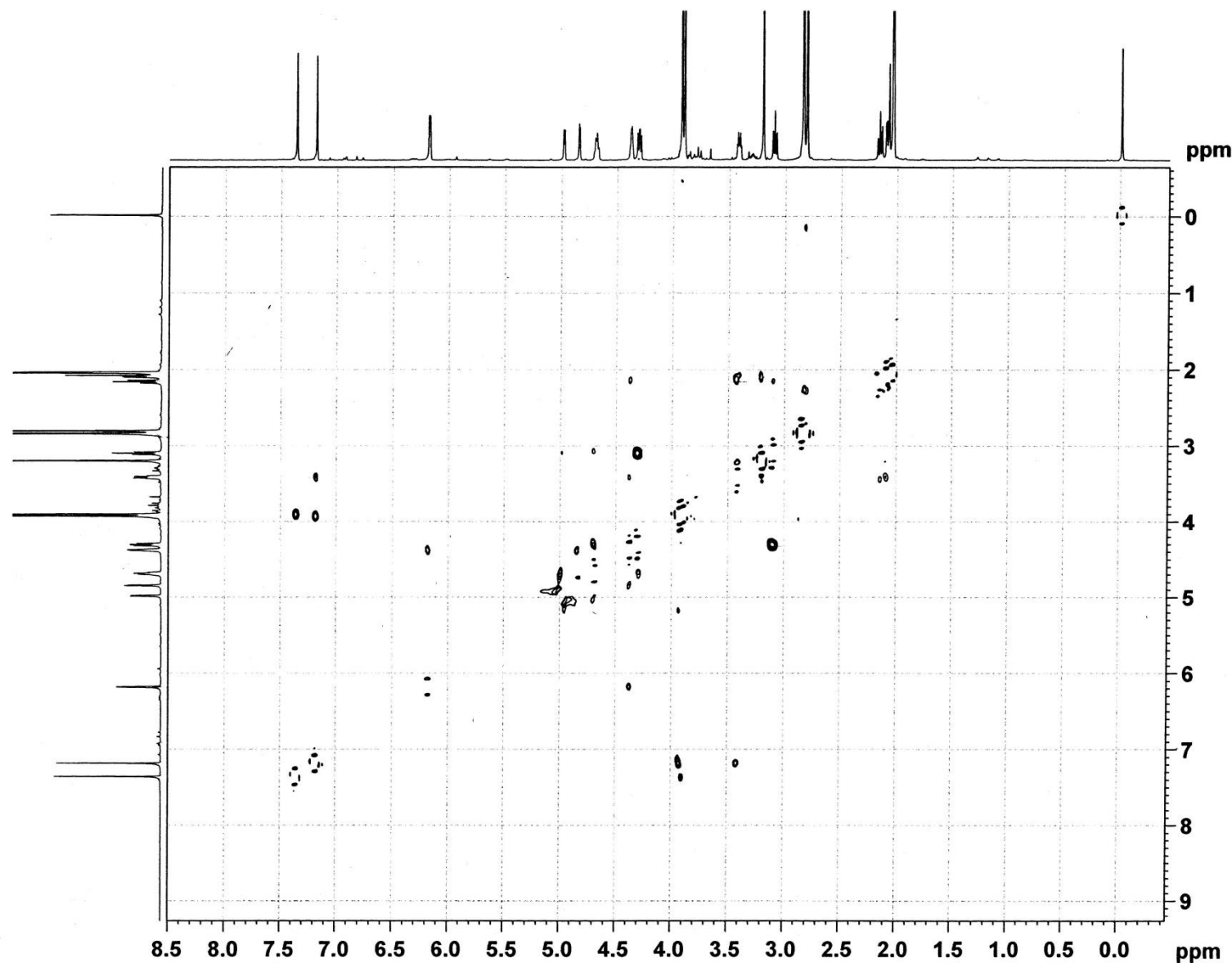
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GP21 50.00 %
GP22 30.00 %
GP23 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 148
SFO1 150.9443 MHz
FIDRES 232.991608 Hz
SW 228.447 ppm
FMODE QF

F2 - Processing parameters
SI 2048
SF 600.2270195 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 512
WC2 QF
SF 150.9270127 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

S38. ROESY Spectrum of erythriarborine F (6)



Current Data Parameters
NAME weaf-58
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160414
Time 5.05
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG roesyphpp2
TD 1024
SOLVENT Acetone
NS 8
DS 16
SWH 8417.509 Hz
FIDRES 8.220223 Hz
AQ 0.0608256 sec
RG 199.06
DW 59.400 usec
DE 10.00 usec
TE 298.0 K
DO 0.00004786 sec
D1 1.50000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
INO 0.00011900 sec
L4 1786
P15 300000.00 usec

===== CHANNEL f1 =====
SFO1 600.2300011 MHz
NUC1 1H
P1 12.00 usec
P17 2500.00 usec
P25 84.00 usec
PLW1 2.89730000 W
PLW10 0.61719000 W
PLW27 0.23652001 W

F1 - Acquisition parameters
TD 160
SFO1 600.23 MHz
FIDRES 52.521008 Hz
SW 14.000 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 2048
SF 600.2270197 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 2048
MC2 States-TPPI
SF 600.2270191 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

S39. HRESIMS Spectrum of erythriarborine F (6)

Formula Predictor Report - weaf-58.lcd

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Data File: E:\DATA\2017\0221\weaf-58.lcd

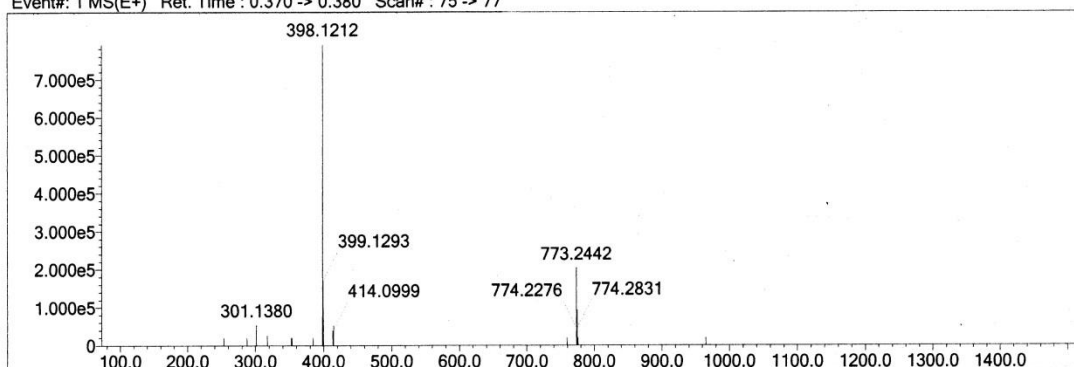
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	150	O	2	0	50	S	2	0	0	Pt	2	0	0	H
B	3	0	0	F	1	0	0	Cl	1	0	0					Na
C	4	0	100	Na	1	0	0	Br	1	0	0					
N	3	0	20	Si	4	0	0	I	3	0	0					

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

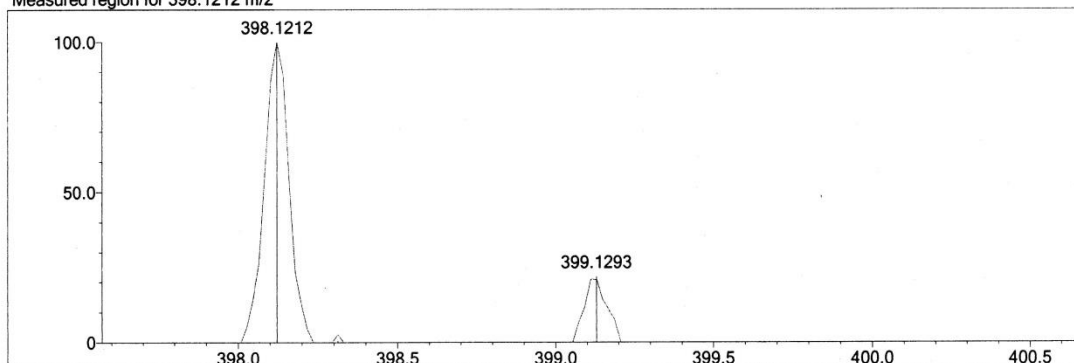
DBE Range: -2.0 - 100.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 10000
 Max Results: 10

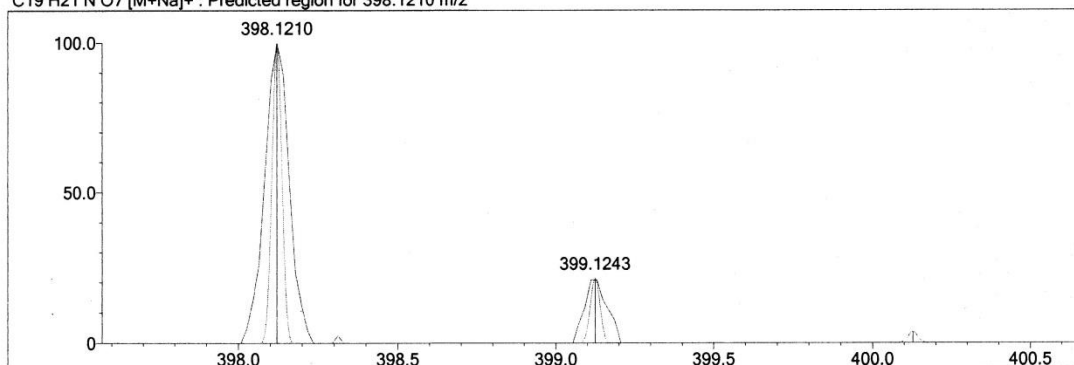
Event#: 1 MS(E+) Ret. Time : 0.370 -> 0.380 Scan#: 75 -> 77



Measured region for 398.1212 m/z

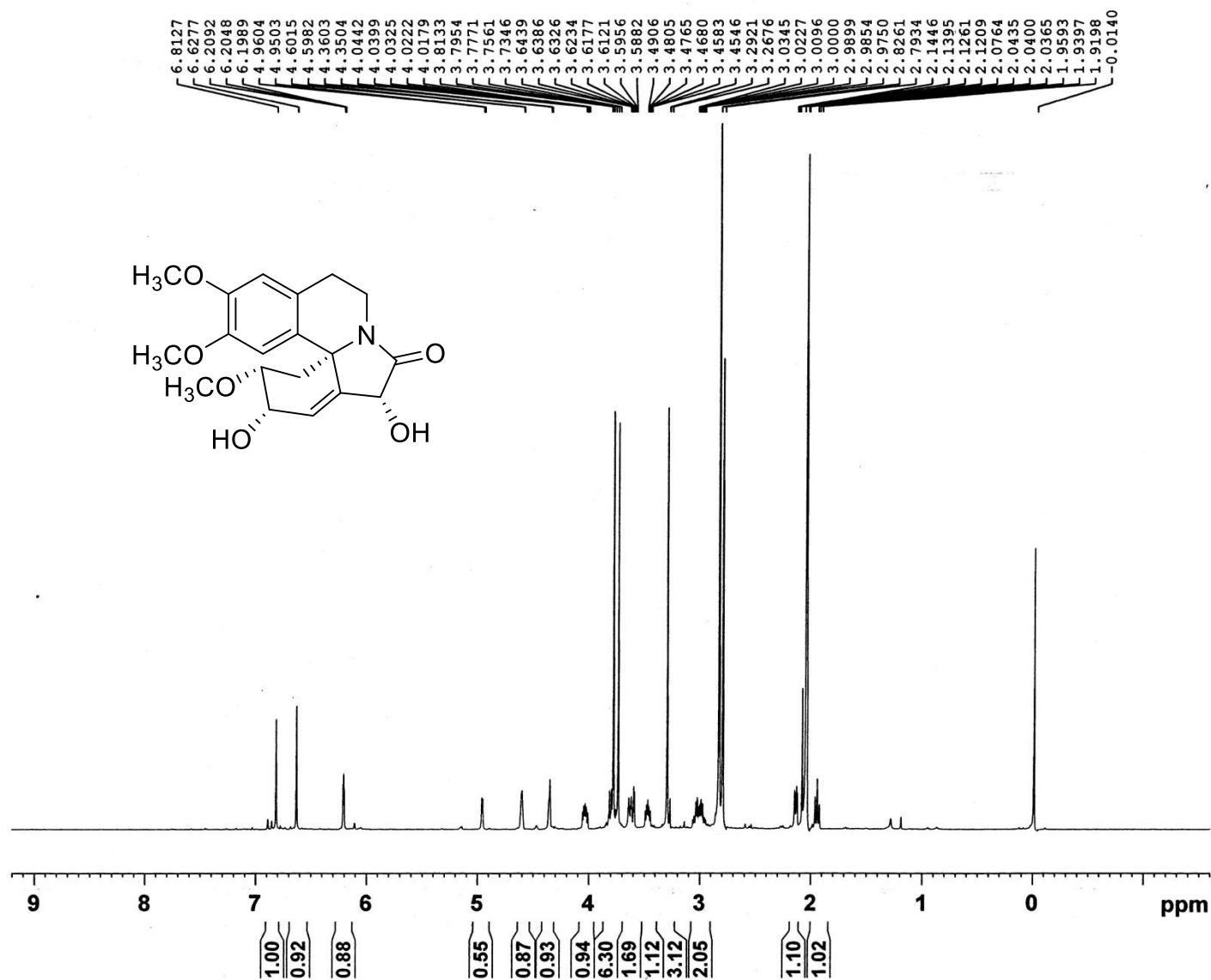


C19 H21 N O7 [M+Na]+ : Predicted region for 398.1210 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C19 H21 N O7	[M+Na]+	398.1212	398.1210	0.2	0.50	10.0

S40. ^1H NMR Spectrum of erythriarborine G (7)



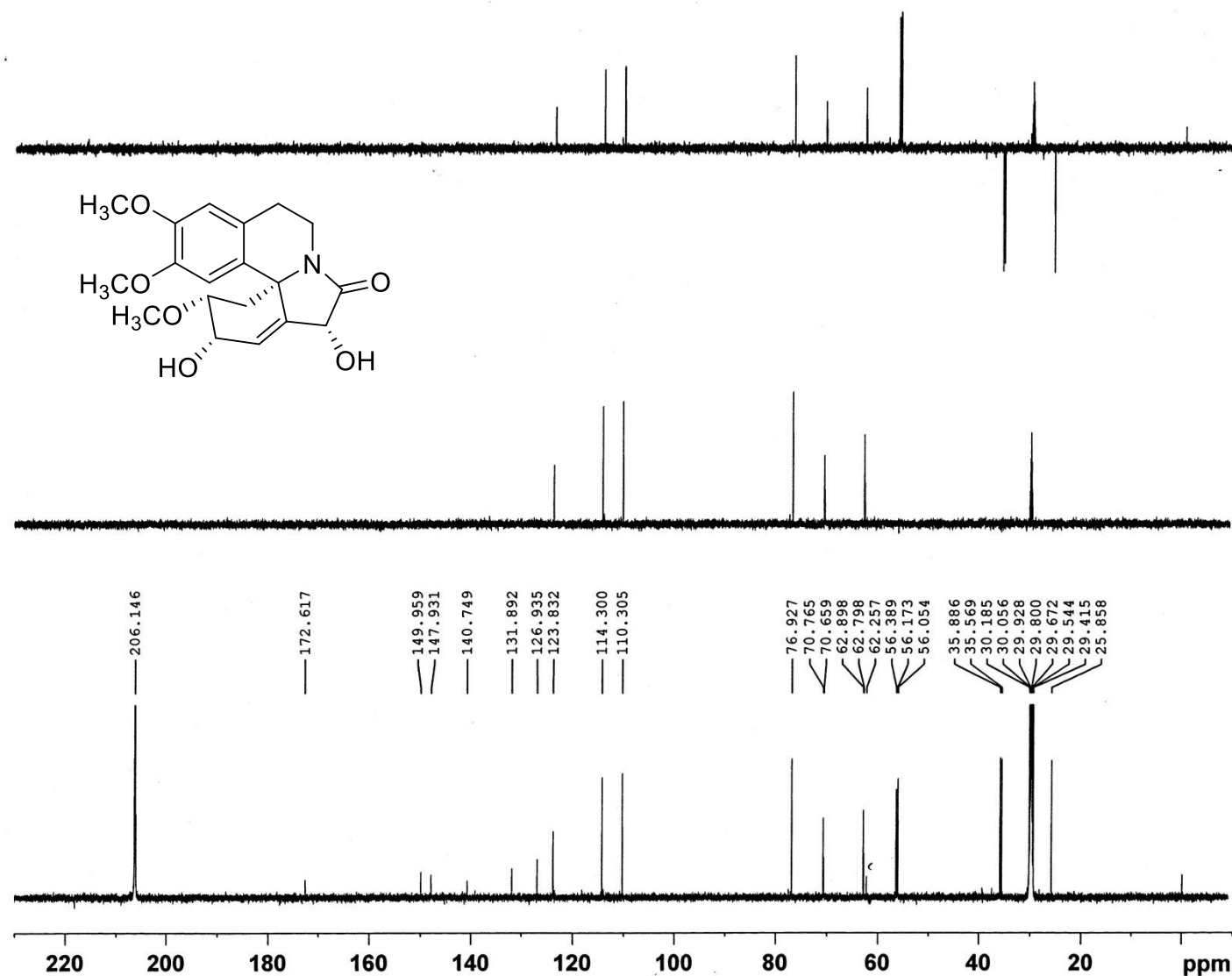
Current Data Parameters
NAME weaf-59
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160331
Time 13.22
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 4
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 15.82
DW 41.600 usec
DE 10.00 usec
TE 298.0 K
D1 10.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 600.2307066 MHz
NUC1 1H
P1 12.00 usec
PLW1 2.89730000 W

F2 - Processing parameters
SI 65536
SF 600.2270179 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S41. ^{13}C NMR Spectrum of erythriarborine G (7)



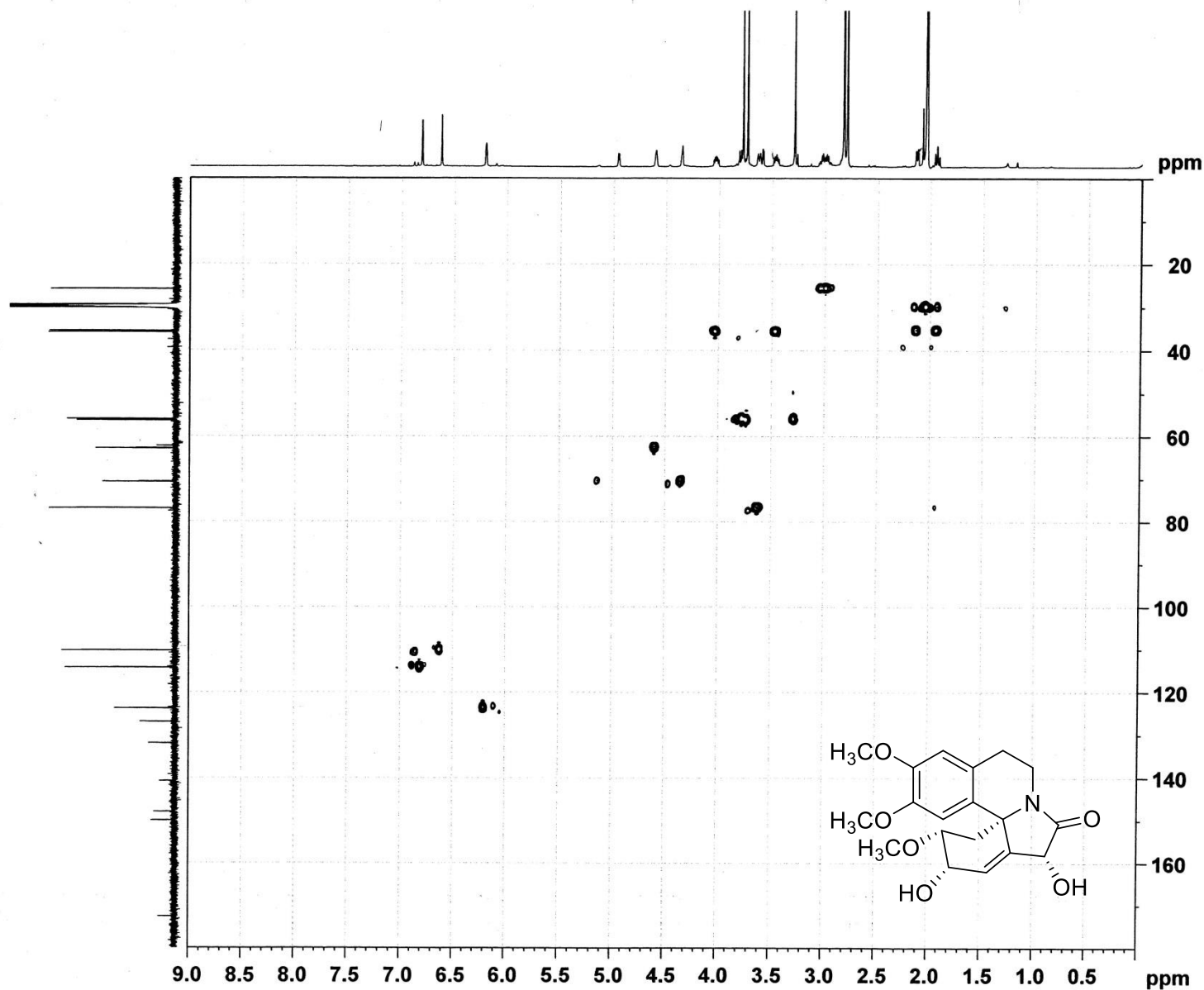
Current Data Parameters
 NAME weaf-59
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160404
 Time_ 4.02
 INSTRUM spect
 PROBHD 5 mm CPQCI 1H-
 PULPROG zgdc
 TD 65536
 SOLVENT Acetone
 NS 512
 DS 4
 SWH 36231.883 Hz
 FIDRES 0.552855 Hz
 AQ 0.9043968 sec
 RG 199.06
 DW 13.800 usec
 DE 18.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 150.9438010 MHz
 NUC1 ^{13}C
 P1 11.20 usec
 PLW1 94.00000000 W

----- CHANNEL f2 -----
 SFO2 600.2294009 MHz
 NUC2 ^1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 2.89730000 W
 PLW12 0.06519000 W

F2 - Processing parameters
 SI 131072
 SF 150.9270714 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



```

Current Data Parameters
NAME          wear-59
EXPNO         20
PROCNO        1

F2 - Acquisition Parameters
Date_         20160414
Time          7.25
INSTRUM       spect
PROBHD        5 mm CPCL1 1H-
PULPROG       hsqcpgpsp12
TD            1024
SOLVENT       Acetone
NS            4
DS            16
SWH           8417.500 Hz
FIDRES        8.220223 Hz
AQ            0.0608256 sec
RG            199.06
DW            59.400 usec
DE            10.00 usec
TE            298.0 K
CNS2?        145.0000000 sec
D0            0.00000300 sec
D1            1.500000000 sec
D2            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
INO           0.00001560 sec
ZGPPRMS

===== CHANNEL F1 =====
SFO1         600.2300011 MHz
NUC1          1H
P1            12.00 usec
F2            60.2400000 MHz
P28           0 usec
PLW1         2.89730000 W

===== CHANNEL F2 =====
SFO2         150.9407824 MHz
NUC2          13C
PCPDPRG[2]   CPDPRG2
P3            11.20 usec
P4            22.40 usec
PCPD2?        75.00 usec
PLW2         87.0000000 W
PLW12        1.94009995 W

===== GRADIENT CHANNEL =====
GFMAG[1]     SMSQ10.100
GFMAG[2]     SMSQ10.100
GFMAG[3]     SMSQ10.100
GFMAG[4]     SMSQ10.100
GPZ1         80.00 %
GPZ2         20.10 %
GPZ3         10.00 %
GPZ4         -5.00 %
P16          1000.00 usec
P19          600.00 usec

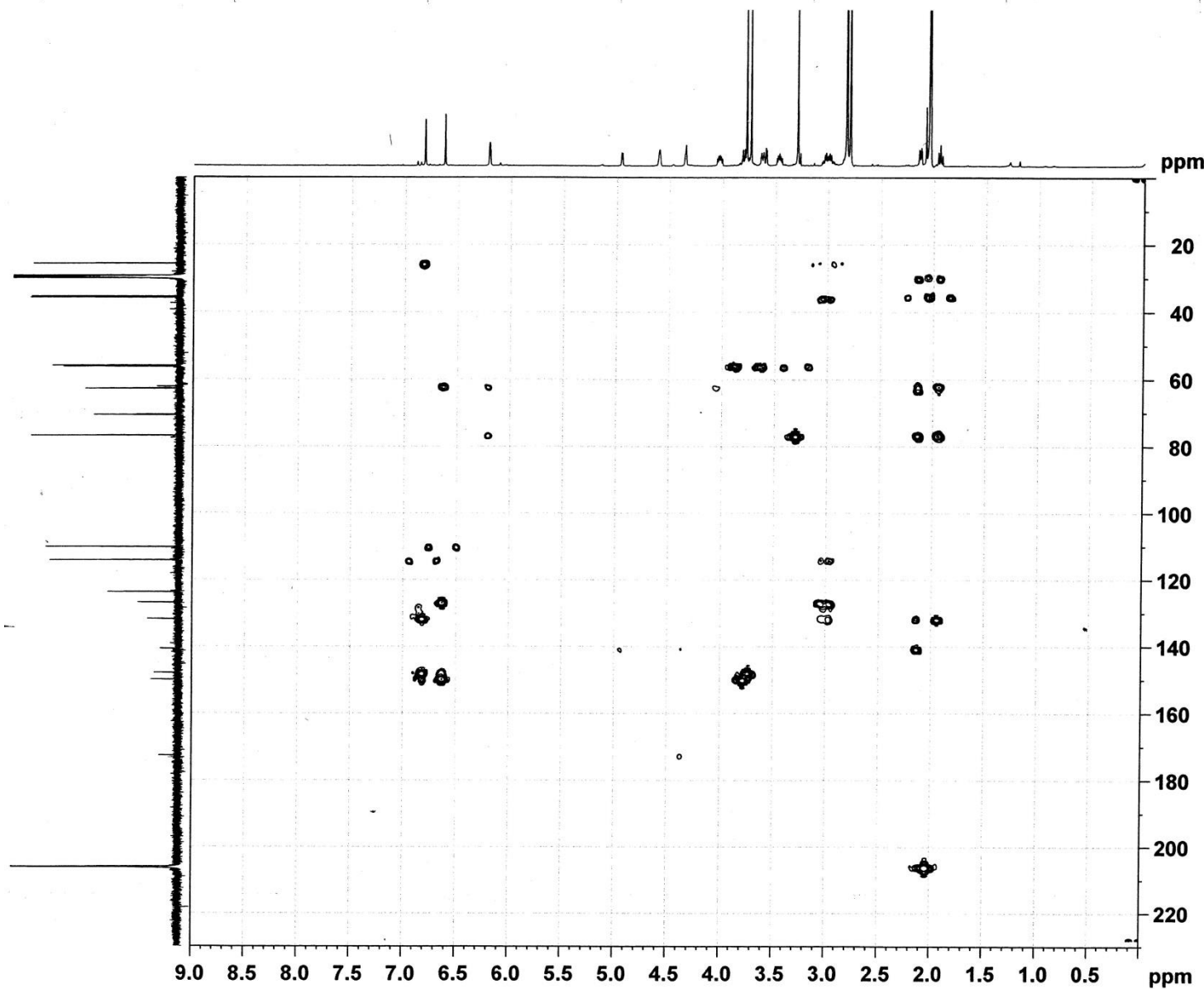
F1 - Acquisition parameters
SFO1         150.9408 MHz
FIDRES       188.253006 Hz
SW           199.552 ppm
FNAME0       Echo-AntiEcho

F2 - Processing parameters
SI           1024
SF           600.2270176 MHz
WDW          QSINE
SSB          2
LB           0 Hz
GB           0
PC           1.40

F1 - Processing parameters
SI           512
HC2          echo-antecho
SF           150.927018 MHz
WDW          QSINE
SSB          2
LB           0 Hz
GB           0
PC           0

```

S43. HMBC Spectrum of erythriarborine G (7)



Current Data Parameters
NAME wear-59
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160414
Time 7.43
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG hmbcgp1pndgf
TD 1024
SOLVENT Acetone
NS 8
DS 16
SWH 8417.509 Hz
FIDRES 8.220223 Hz
AQ 0.0608256 sec
RG 199.06
DW 59.400 usec
DE 10.00 usec
TE 298.0 K
CNST2 145.0000000
CNST13 9.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00344828 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001450 sec

----- CHANNEL f1 -----
SFO1 600.2300011 MHz
NUC1 1H
P1 12.00 usec
P2 24.00 usec
PLW1 2.89730000 W

----- CHANNEL f2 -----
SFO2 150.9442538 MHz
NUC2 13C
P3 11.20 usec
PLW2 87.00000000 W

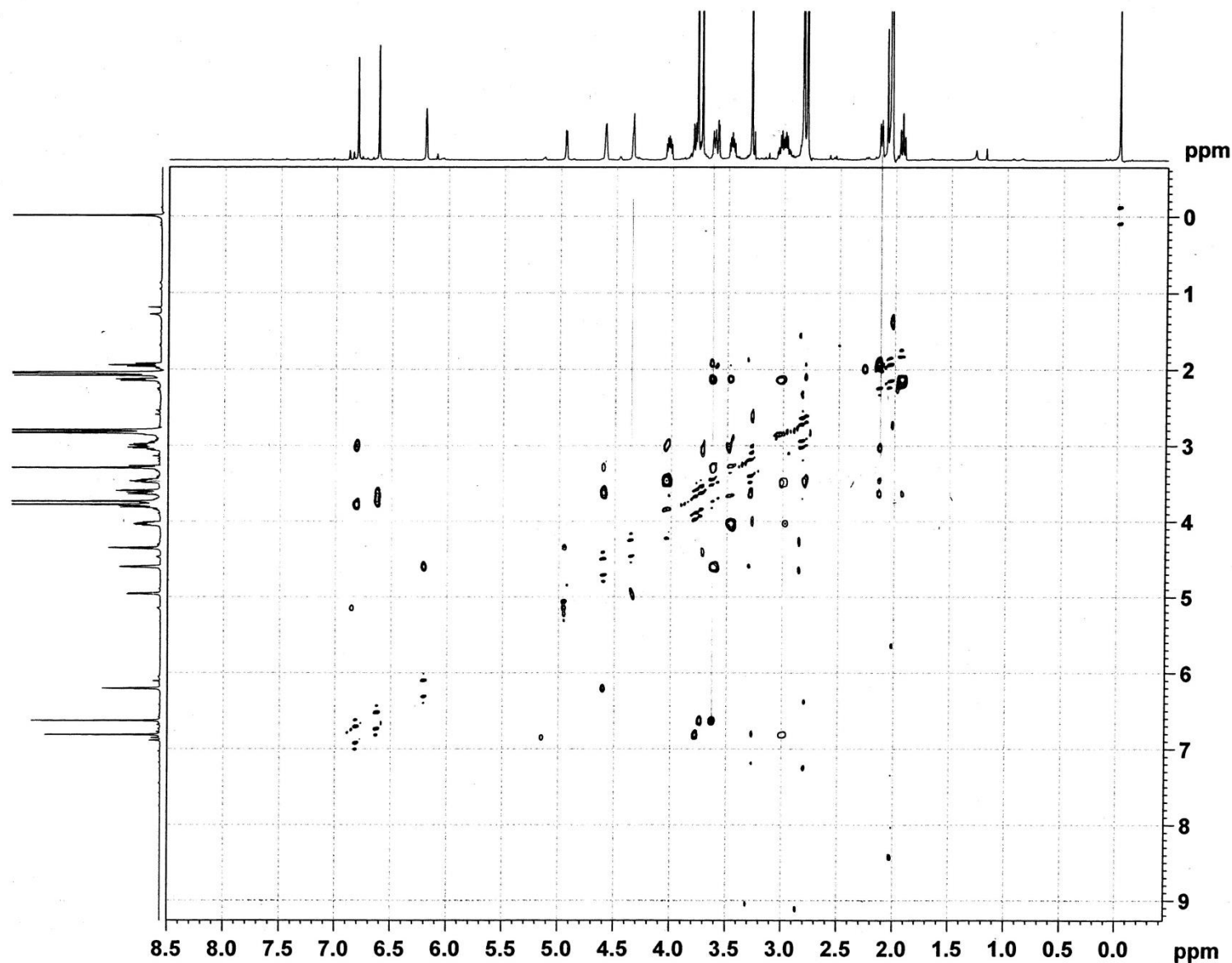
----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GP21 50.00 %
GP22 30.00 %
GP23 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 148
SFO1 150.9443 MHz
FIDRES 232.991608 Hz
SW 228.447 ppm
FMODE QF

F2 - Processing parameters
SI 2048
SF 600.2270186 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 512
MC2 QF
SF 150.9270249 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

S44. ROESY Spectrum of erythriarborine G (7)



Current Data Parameters
 NAME weaf-59
 EXPNO 14
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160414
 Time 6.43
 INSTRUM spect
 PROBHD 5 mm CPQCI 1H-
 PULPROG roesyphpp.2
 TD 1024
 SOLVENT Acetone
 NS 8
 DS 16
 SWH 8417.509 Hz
 FIDRES 8.220223 Hz
 AQ 0.0608256 sec
 RG 199.06
 DW 59.400 usec
 DE 10.00 usec
 TE 298.0 K
 D0 0.00004786 sec
 D1 1.50000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 IN0 0.00011900 sec
 L4 1786
 P15 300000.00 usec

===== CHANNEL f1 =====
 SF01 600.2300011 MHz
 NUC1 1H
 P1 12.00 usec
 P17 2500.00 usec
 P25 84.00 usec
 PLW1 2.89730000 W
 PLW10 0.61719000 W
 PLW27 0.23652001 W

F1 - Acquisition parameters
 TD 160
 SF01 600.23 MHz
 FIDRES 52.521008 Hz
 SW 14.000 ppm
 FMODE States-TPPI

F2 - Processing parameters
 SI 2048
 SF 600.2270191 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 2048
 MC2 States-TPPI
 SF 600.2270189 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0

S45. HRESIMS Spectrum of erythriarborine G (7)

Formula Predictor Report - weaf-59.lcd

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Data File: E:\DATA\2017\0221\weaf-59.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	150	O	2	0	50	S	2	0	0	Pt	2	0	0	H
B	3	0	0	F	1	0	0	Cl	1	0	0					Na
C	4	0	100	Na	1	0	0	Br	1	0	0					
N	3	0	20	Si	4	0	0	I	3	0	0					

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: -2.0 - 100.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

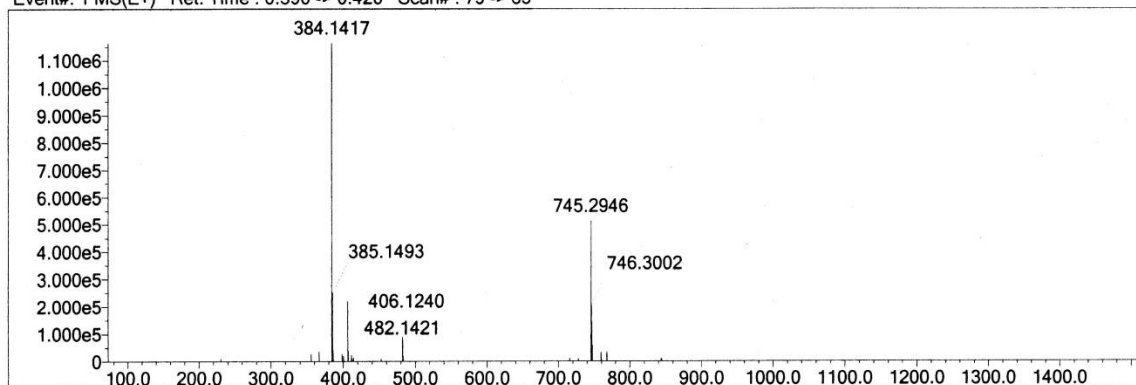
Electron Ions: both

Use MSn Info: yes

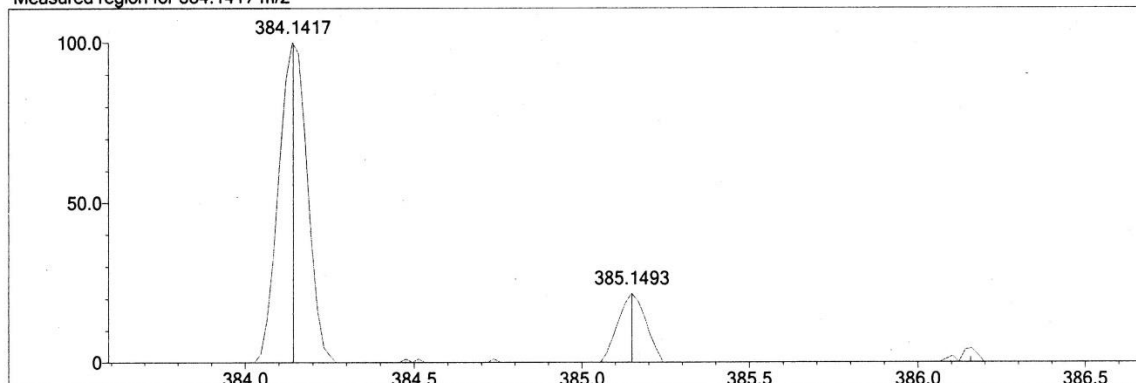
Isotope Res: 10000

Max Results: 10

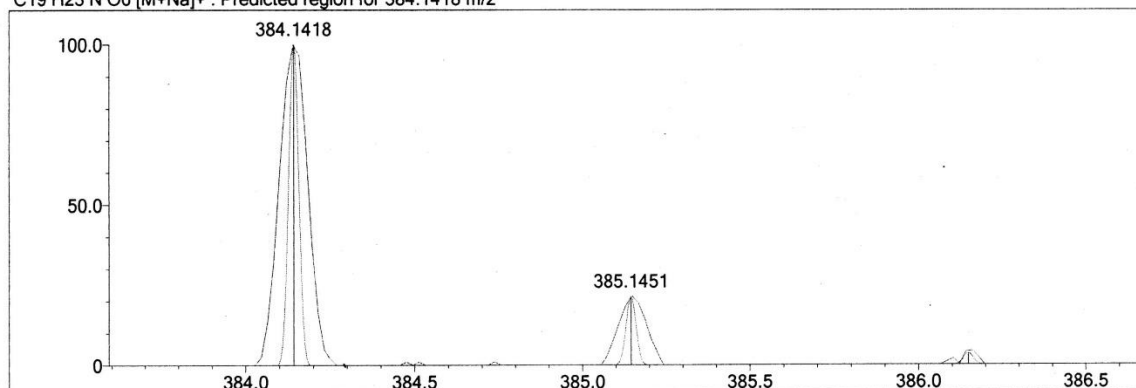
Event#: 1 MS(E+) Ret. Time : 0.390 -> 0.420 Scan#: 79 -> 85



Measured region for 384.1417 m/z



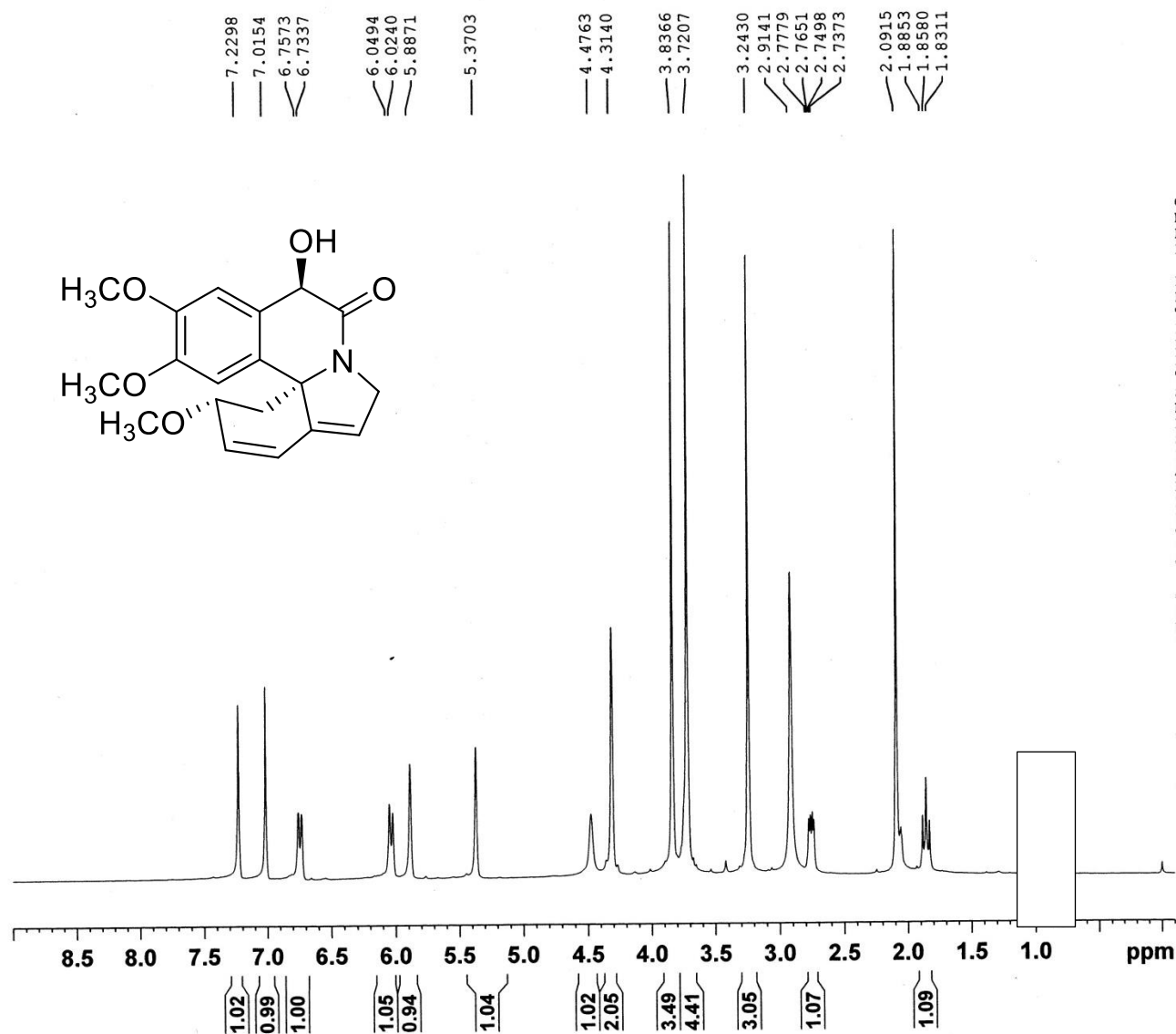
C19 H23 N O6 [M+Na]+ : Predicted region for 384.1418 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C19 H23 N O6	[M+Na]+	384.1417	384.1418	-0.1	-0.26	9.0

S46. ^1H NMR Spectrum of erythriarborine H (8)

H weaf-10



Current Data Parameters
NAME weaf-10
EXPNO 1
PROCNO 1

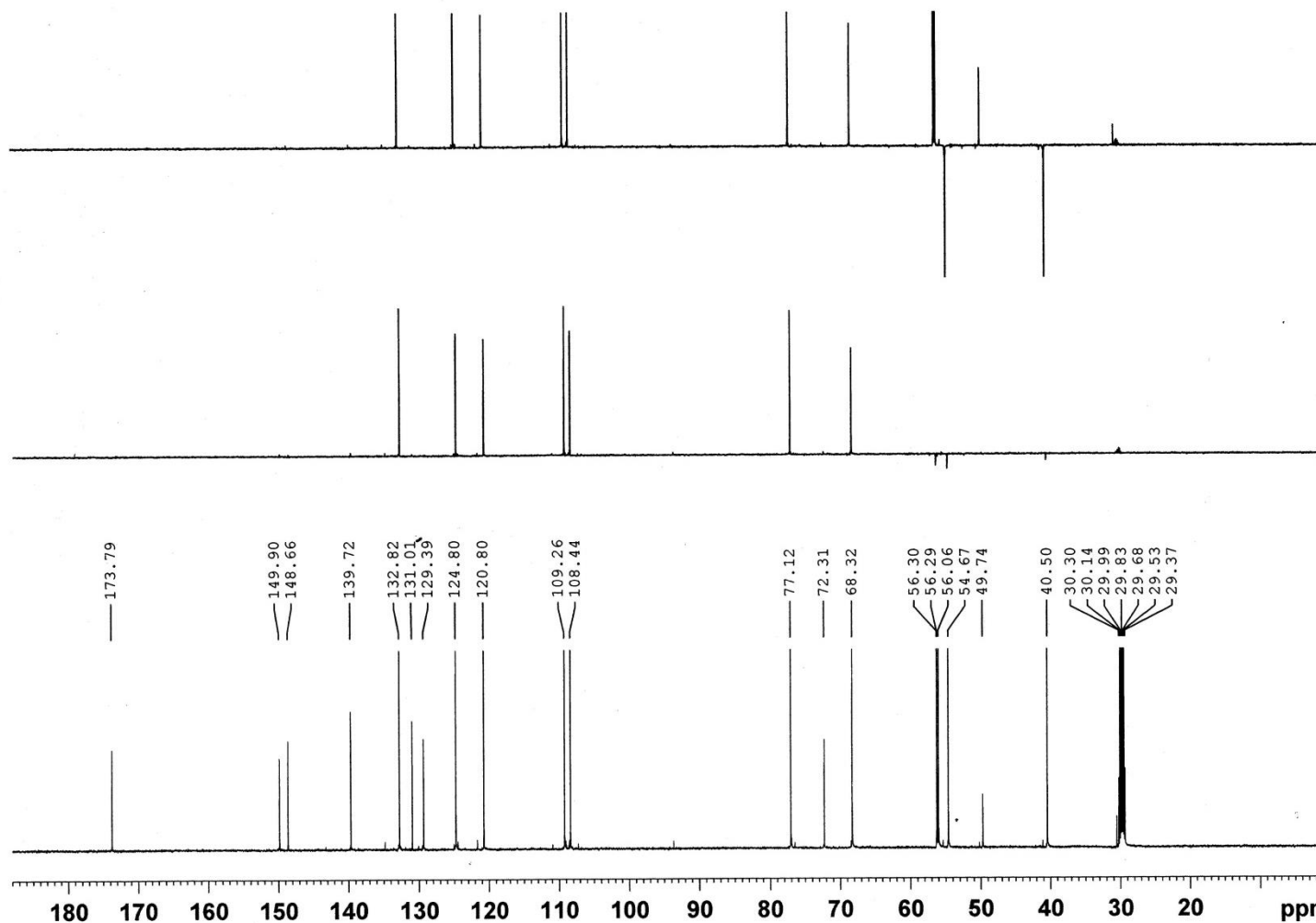
F2 - Acquisition Parameters
Date_ 20151229
Time_ 12.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 14.09
DW 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 400.1318812 MHz
NUC1 ^1H
P1 12.00 usec
PLW1 11.69999981 W

F2 - Processing parameters
SI 65536
SF 400.1300047 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

S47. ^{13}C -NMR Spectrum of erythriarborine H (8)

weaf10 c13 and dept



Current Data Parameters
NAME weaf10
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date 20160106
Time 5.57
INSTRUM spect
PROBHD 5 mm CPQCI 1H/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 187.72
DW 16.800 usec
DE 18.00 usec
TE 296.2 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1

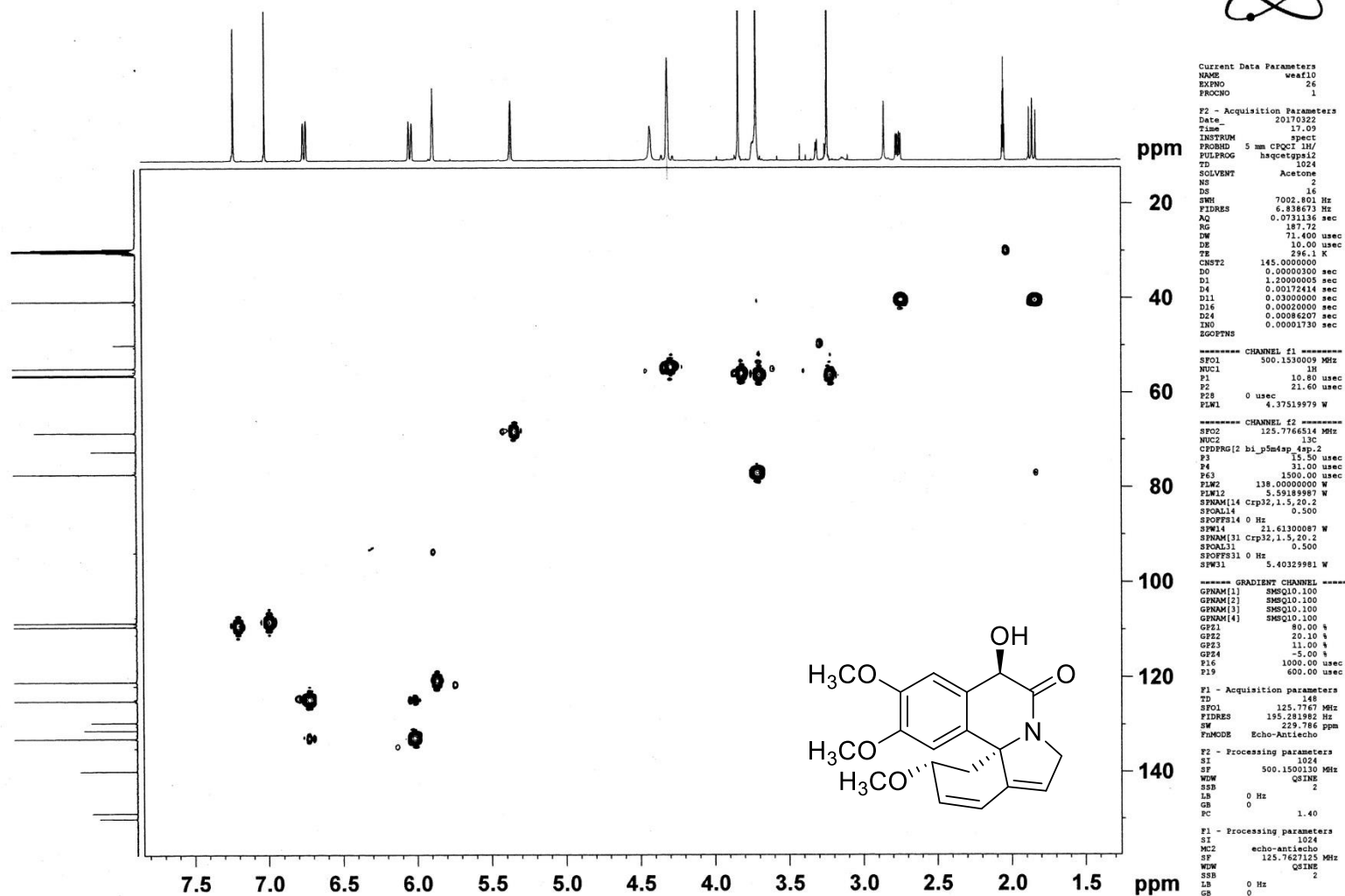
===== CHANNEL f1 =====
SFO1 125.7769030 MHz
NUC1 13C
P1 11.70 usec
PLW1 160.00000000 W

===== CHANNEL f2 =====
SFO2 500.1527508 MHz
NUC2 1H
PCPDPRG2 waltz16
PCPD2 100.00 usec
PLW2 4.37519979 W
PLW12 0.05390700 W

F2 - Processing parameters
SI 32768
SF 125.7627125 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

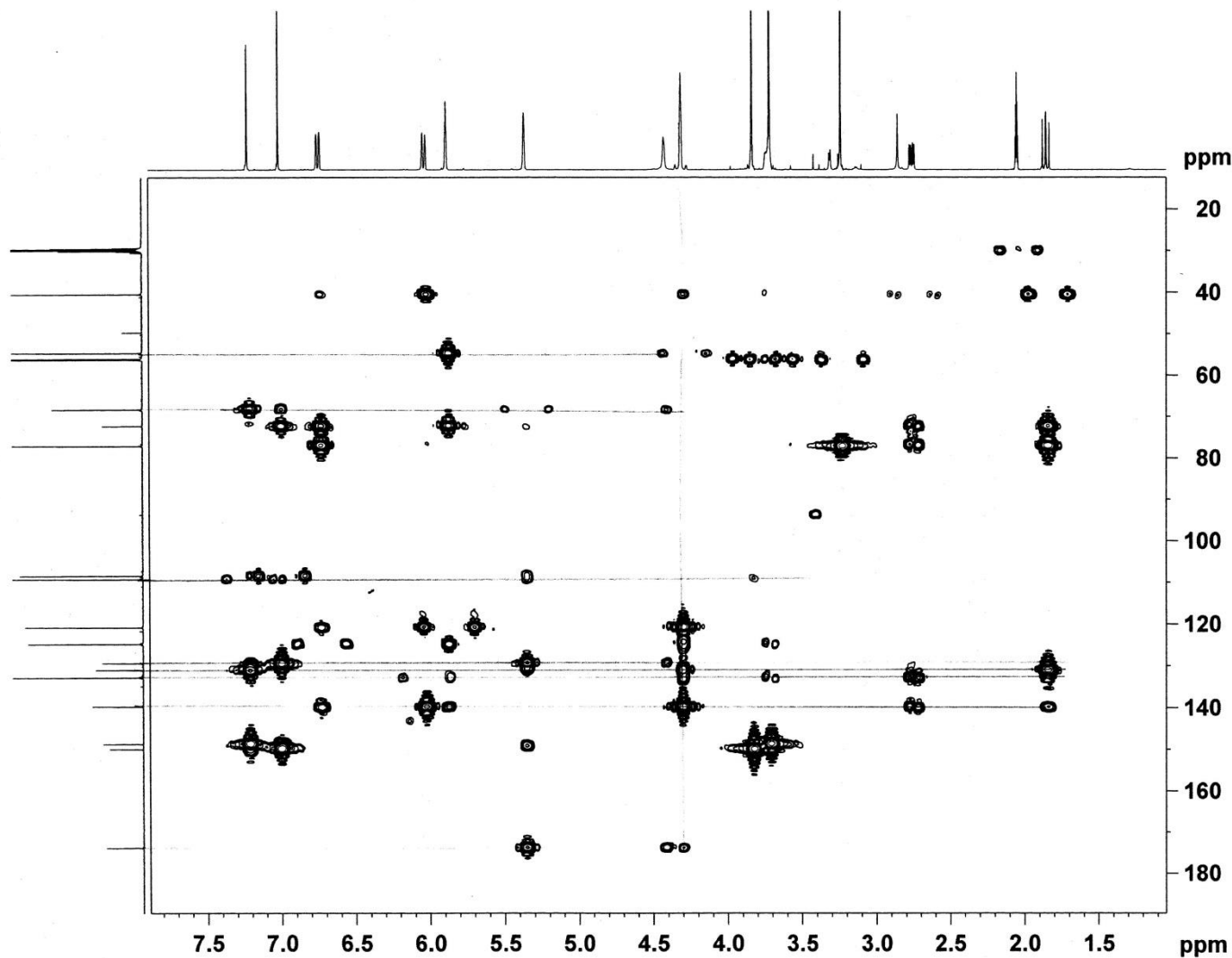
S48. HSQC Spectrum of erythriarborine H (8)

weaf10 hsqc



S49. HMBC Spectrum of erythriarborine H (8)

weaf10 hmhc



Current Data Parameters
NAME weaf10
EXPNO 27
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170322
Time 17.16
INSTRUM spect
PROBHD 5 mm CPQCI 1H/
PULPROG hmbcgp1pndqf
TD 1024
SOLVENT Acetone
NS 8
DS 16
SWH 7002.801 Hz
FIDRES 6.838673 Hz
AQ 0.0731136 sec
RG 187.72
DW 71.400 usec
DE 10.00 usec
TE 296.2 K
CNST2 145.0000000
CNST13 10.0000000
D0 0.00000300 sec
D1 1.79999995 sec
D2 0.00344828 sec
D6 0.05000000 sec
D16 0.00020000 sec
IN0 0.00001730 sec

===== CHANNEL f1 =====
SFO1 500.1532010 MHz
NUC1 1H
P1 10.80 usec
P2 21.60 usec
PLW1 4.37519979 W

===== CHANNEL f2 =====
SFO2 125.7770287 MHz
NUC2 13C
P3 15.50 usec
PLW2 138.00000000 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

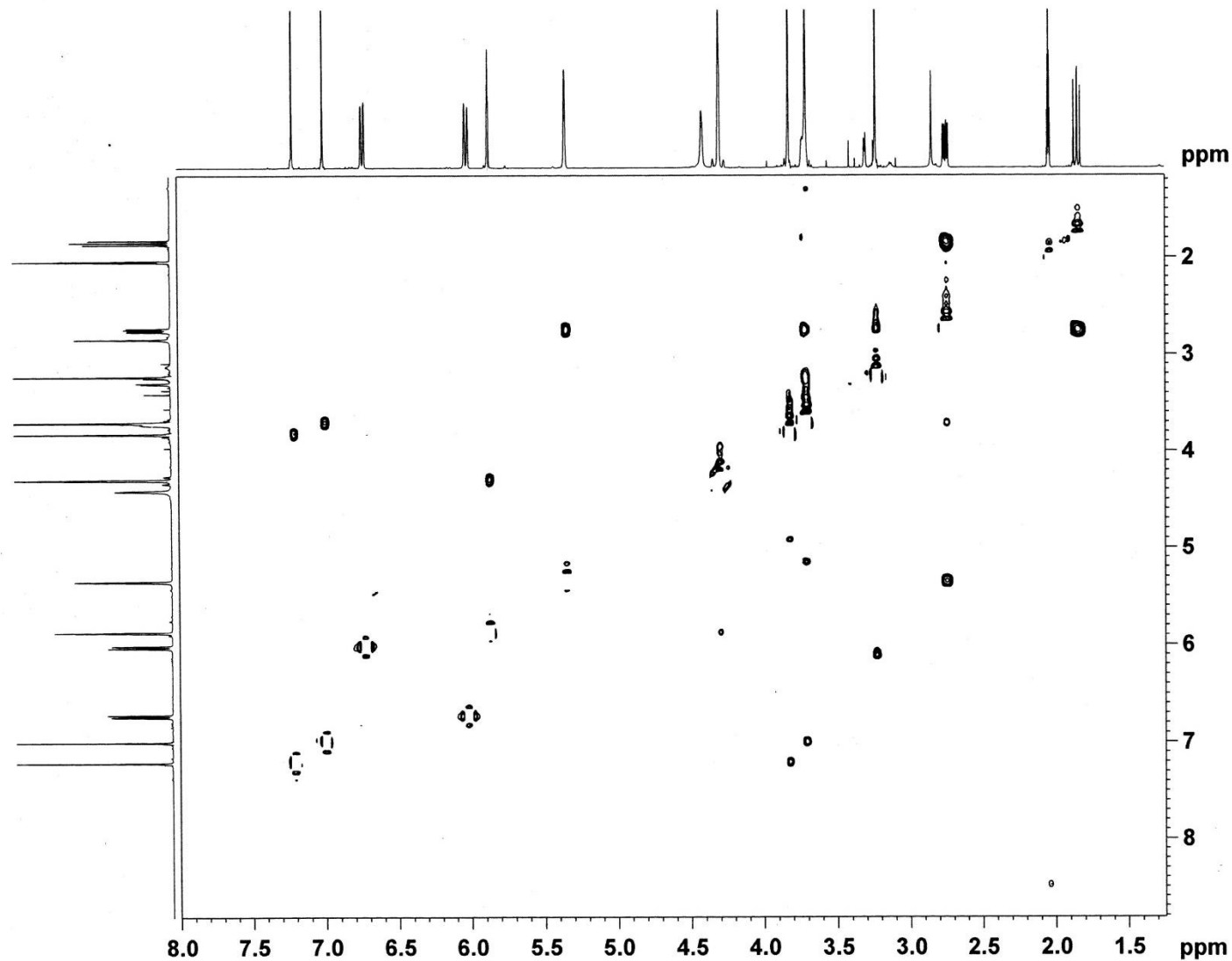
F1 - Acquisition parameters
TD 128
SFO1 125.777 MHz
FIDRES 225.794800 Hz
SW 229.785 ppm
FIRMODE QF

F2 - Processing parameters
SI 2048
SF 500.1500130 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 125.7627125 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

S50. ROESY Spectrum of erythriarborine H (8)

weaf10 roesy



Current Data Parameters
NAME weaf10
EXPNO 28
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170322
Time 17.50
INSTRUM spect
PROBHD 5 mm CPQCI 1H/
PULPROG croesyph
TD 1024
SOLVENT Acetone
NS 8
DS 32
SWH 6493.506 Hz
FIDRES 6.341315 Hz
AQ 0.0788480 sec
RG 2.01
DW 77.000 usec
DE 10.00 usec
TE 296.1 K
DO 0.00006315 sec
D1 1.20000005 sec
D12 0.00002000 sec
D13 0.00000400 sec
INO 0.00015380 sec

----- CHANNEL f1 -----
SFO1 500.1532010 MHz
NUC1 1H
P1 10.80 usec
P15 680000.00 usec
PLW1 4.37519979 W
PLW11 0.06300300 W

F1 - Acquisition parameters
TD 160
SFO1 500.1532 MHz
FIDRES 40.637192 Hz
SW 13.000 ppm
FMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 500.1500130 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 500.1500130 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

S51. HRESIMS Spectrum of erythriarborine H (8)

Formula Predictor Report - weaf-10.lcd

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Data File: E:\DATA\2017\0412\weaf-10.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	150	O	2	0	50	S	2	0	0	Pt	2	0	0	Na
B	3	0	0	F	1	0	0	Cl	1	0	0					
C	4	0	100	Na	1	0	0	Br	1	0	0					
N	3	0	10	Si	4	0	0	I	3	0	0					

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: -2.0 - 100.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

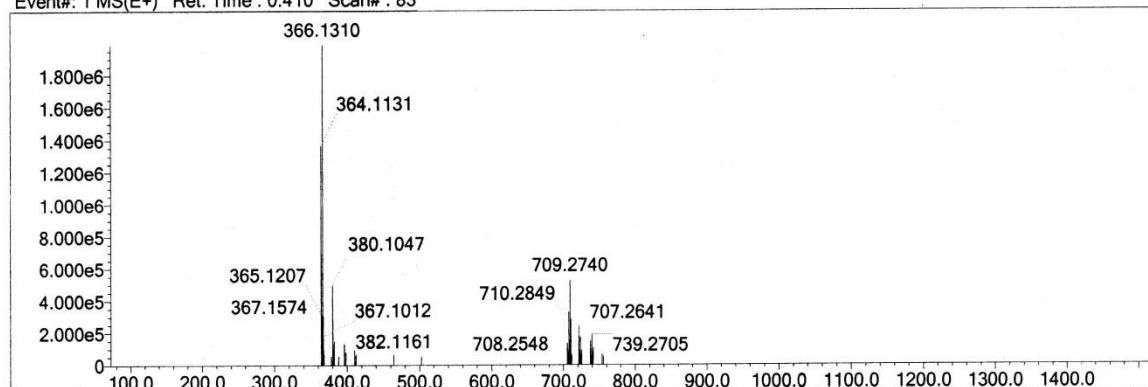
Electron Ions: both

Use MSn Info: yes

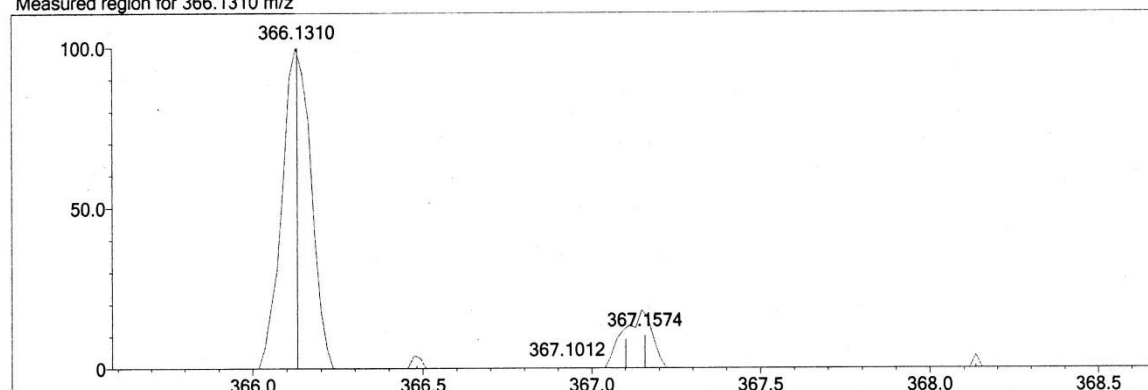
Isotope Res: 10000

Max Results: 10

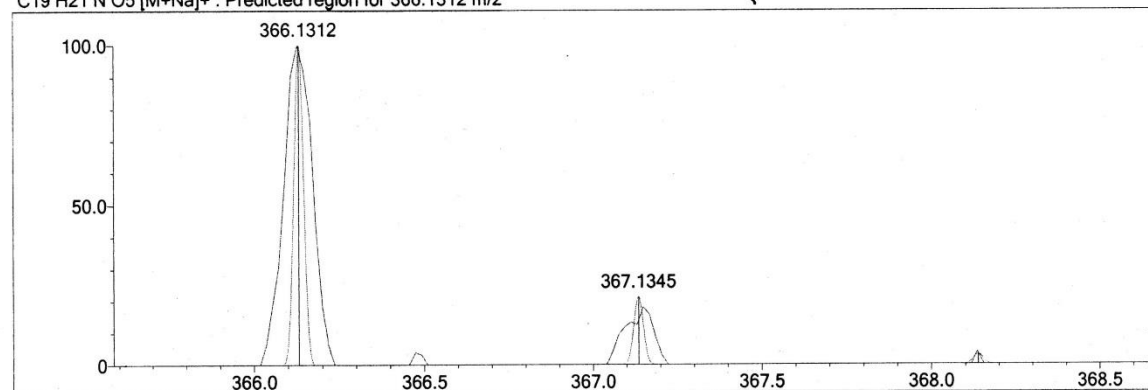
Event#: 1 MS(E+) Ret. Time: 0.410 Scan#: 83



Measured region for 366.1310 m/z



C19 H21 N O5 [M+Na]+ : Predicted region for 366.1312 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C19 H21 N O5	[M+Na]+	366.1310	366.1312	-0.2	-0.55	10.0