

Supporting Information

Title: Iridoids and Bis-iridoids from *Patrinia scabiosaefolia*

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Contents of Supporting Information

No.	Contents	Page
1.	Figure 1. ^1H NMR spectrum of Patriscabioin A (1) in CDCl_3	6
2.	Figure 2. ^{13}C NMR spectrum of Patriscabioin A (1) in CDCl_3	6
3.	Figure 3. HSQC spectrum of Patriscabioin A (1) in CDCl_3	7
4.	Figure 4. HMBC spectrum of Patriscabioin A (1) in CDCl_3	7
5.	Figure 5. ^1H - ^1H COSY spectrum of Patriscabioin A (1) in CDCl_3	8
6.	Figure 6. ROESY spectrum of Patriscabioin A (1) in CDCl_3	8
7.	Figure 7. HREIMS spectrum of Patriscabioin A (1)	9
8.	Figure 8. ^1H NMR spectrum of Patriscabioin B (2) in CDCl_3	10
9.	Figure 9. ^{13}C NMR spectrum of Patriscabioin B (2) in CDCl_3	10
10.	Figure 10. HSQC spectrum of Patriscabioin B (2) in CDCl_3	11
11.	Figure 11. HMBC spectrum of Patriscabioin B (2) in CDCl_3	11
12.	Figure 12. ^1H - ^1H COSY spectrum of Patriscabioin B (2) in CDCl_3	12
13.	Figure 13. ROESY spectrum of Patriscabioin B (2) in CDCl_3	12
14.	Figure 14. HREIMS spectrum of Patriscabioin B (2)	13
15.	Figure 15. ^1H NMR spectrum of Patriscabioin C (3) in CDCl_3	14
16.	Figure 16. ^{13}C NMR spectrum of Patriscabioin C (3) in CDCl_3	14
17.	Figure 17. HSQC spectrum of Patriscabioin C (3) in CDCl_3	15
18.	Figure 18. HMBC spectrum of Patriscabioin C (3) in CDCl_3	15
19.	Figure 19. ^1H - ^1H COSY spectrum of Patriscabioin C (3) in CDCl_3	16
20.	Figure 20. ROESY spectrum of Patriscabioin C (3) in CDCl_3	16
21.	Figure 21. HREIMS spectrum of Patriscabioin C (3)	17
22.	Figure 22. ^1H NMR spectrum of Patriscabioin D (4) in CDCl_3	18
23.	Figure 23. ^{13}C NMR spectrum of Patriscabioin D (4) in CDCl_3	18

24.	Figure 24. HSQC spectrum of Patriscabioin D (4) in CDCl ₃	19
25.	Figure 25. HMBC spectrum of Patriscabioin D (4) in CDCl ₃	19
26.	Figure 26. ¹ H- ¹ H COSY spectrum of Patriscabioin D (4) in CDCl ₃	20
27.	Figure 27. ROESY spectrum of Patriscabioin D (4) in CDCl ₃	20
28.	Figure 28. HREIMS spectrum of Patriscabioin D (4)	21
29.	Figure 29. ¹ H NMR spectrum of Patriscabioin E (5) in CDCl ₃	22
30.	Figure 30. ¹³ C NMR spectrum of Patriscabioin E (5) in CDCl ₃	22
31.	Figure 31. HSQC spectrum of Patriscabioin E (5) in CDCl ₃	23
32.	Figure 32. HMBC spectrum of Patriscabioin E (5) in CDCl ₃	23
33.	Figure 33. ¹ H- ¹ H COSY spectrum of Patriscabioin E (5) in CDCl ₃	24
34.	Figure 34. ROESY spectrum of Patriscabioin E (5) in CDCl ₃	24
35.	Figure 35. HREIMS spectrum of Patriscabioin E (5)	25
36.	Figure 36. ¹ H NMR spectrum of Patriscabioin F (6) in CDCl ₃	26
37.	Figure 37. ¹³ C NMR spectrum of Patriscabioin F (6) in CDCl ₃	26
38.	Figure 38. HSQC spectrum of Patriscabioin F (6) in CDCl ₃	27
39.	Figure 39. HMBC spectrum of Patriscabioin F (6) in CDCl ₃	27
40.	Figure 40. ¹ H- ¹ H COSY spectrum of Patriscabioin F (6) in CDCl ₃	28
41.	Figure 41. ROESY spectrum of Patriscabioin F (6) in CDCl ₃	28
42.	Figure 42. HREIMS spectrum of Patriscabioin F (6)	29
43.	Figure 43. ¹ H NMR spectrum of Patriscabioin G (7) in CDCl ₃	30
44.	Figure 44. ¹³ C NMR spectrum of Patriscabioin G (7) in CDCl ₃	30
45.	Figure 45. HSQC spectrum of Patriscabioin G (7) in CDCl ₃	31
46.	Figure 46. HMBC spectrum of Patriscabioin G (7) in CDCl ₃	31
47.	Figure 47. ¹ H- ¹ H COSY spectrum of Patriscabioin G (7) in CDCl ₃	32
48.	Figure 48. ROESY spectrum of Patriscabioin G (7) in CDCl ₃	32

49.	Figure 49. HREIMS spectrum of Patriscabioin G (7)	33
50.	Figure 50. ^1H NMR spectrum of Patriscabioin H (8) in CDCl_3	34
51.	Figure 51. ^{13}C NMR spectrum of Patriscabioin H (8) in CDCl_3	34
52.	Figure 52. HSQC spectrum of Patriscabioin H (8) in CDCl_3	35
53.	Figure 53. HMBC spectrum of Patriscabioin H (8) in CDCl_3	35
54.	Figure 54. ^1H - ^1H COSY spectrum of Patriscabioin H (8) in CDCl_3	36
55.	Figure 55. ROESY spectrum of Patriscabioin H (8) in CDCl_3	36
56.	Figure 56. HREIMS spectrum of Patriscabioin H (8)	37
57.	Figure 57. ^1H NMR spectrum of Patriscabioin I (9) in CDCl_3	38
58.	Figure 58. ^{13}C NMR spectrum of Patriscabioin I (9) in CDCl_3	38
59.	Figure 59. HSQC spectrum of Patriscabioin I (9) in CDCl_3	39
60.	Figure 60. HMBC spectrum of Patriscabioin I (9) in CDCl_3	39
61.	Figure 61. ^1H - ^1H COSY spectrum of Patriscabioin I (9) in CDCl_3	40
62.	Figure 62. ROESY spectrum of Patriscabioin I (9) in CDCl_3	40
63.	Figure 63. HREIMS spectrum of Patriscabioin I (9)	41
64.	Figure 64. ^1H NMR spectrum of Patriscabioin J (10) in CDCl_3	42
65.	Figure 65. ^{13}C NMR spectrum of Patriscabioin J (10) in CDCl_3	42
66.	Figure 66. HSQC spectrum of Patriscabioin J (10) in CDCl_3	43
67.	Figure 67. HMBC spectrum of Patriscabioin J (10) in CDCl_3	43
68.	Figure 68. ^1H - ^1H COSY spectrum of Patriscabioin J (10) in CDCl_3	44
69.	Figure 69. ROESY spectrum of Patriscabioin J (10) in CDCl_3	44
70.	Figure 70. HREIMS spectrum of Patriscabioin J (10)	45
71.	Figure 71. ^1H NMR spectrum of Patriscabiobisin A (11) in CDCl_3	46
72.	Figure 72. ^{13}C NMR spectrum of Patriscabiobisin A (11) in CDCl_3	46
73.	Figure 73. HSQC spectrum of Patriscabiobisin A (11) in CDCl_3	47

74.	Figure 74. HMBC spectrum of Patriscabiobisin A (11) in CDCl ₃	47
75.	Figure 75. ¹ H- ¹ H COSY spectrum of Patriscabiobisin A (11) in CDCl ₃	48
76.	Figure 76. ROESY spectrum of Patriscabiobisin A (11) in CDCl ₃	48
77.	Figure 77. HREIMS spectrum of Patriscabiobisin A (11)	49
78.	Figure 78. ECD spectrum of Patriscabiobisin A (11)	50
79.	Figure 79. ¹ H NMR spectrum of Patriscabiobisin B (12) in CDCl ₃	51
80.	Figure 80. ¹³ C NMR spectrum of Patriscabiobisin B (12) in CDCl ₃	51
81.	Figure 81. HSQC spectrum of Patriscabiobisin B (12) in CDCl ₃	52
82.	Figure 82. HMBC spectrum of Patriscabiobisin B (12) in CDCl ₃	52
83.	Figure 83. ¹ H- ¹ H COSY spectrum of Patriscabiobisin B (12) in CDCl ₃	53
84.	Figure 84. ROESY spectrum of Patriscabiobisin B (12) in CDCl ₃	53
85.	Figure 85. HREIMS spectrum of Patriscabiobisin B (12)	54
86.	Figure 86. ECD spectrum of Patriscabiobisin B (12)	55
87.	Figure 87. ¹ H NMR spectrum of Patriscabiobisin C (13) in MeOH	56
88.	Figure 88. ¹³ C NMR spectrum of Patriscabiobisin C (13) in MeOH	56
89.	Figure 89. HSQC spectrum of Patriscabiobisin C (13) in MeOH	57
90.	Figure 90. HMBC spectrum of Patriscabiobisin C (13) in MeOH	57
91.	Figure 91. ¹ H- ¹ H COSY spectrum of Patriscabiobisin C (13) in MeOH	58
92.	Figure 92. ROESY spectrum of Patriscabiobisin C (13) in MeOH	58
93.	Figure 93. HREIMS spectrum of Patriscabiobisin C (13)	59

Figure 1. ^1H NMR spectrum of Patriscabioin A (**1**) in CDCl_3 .

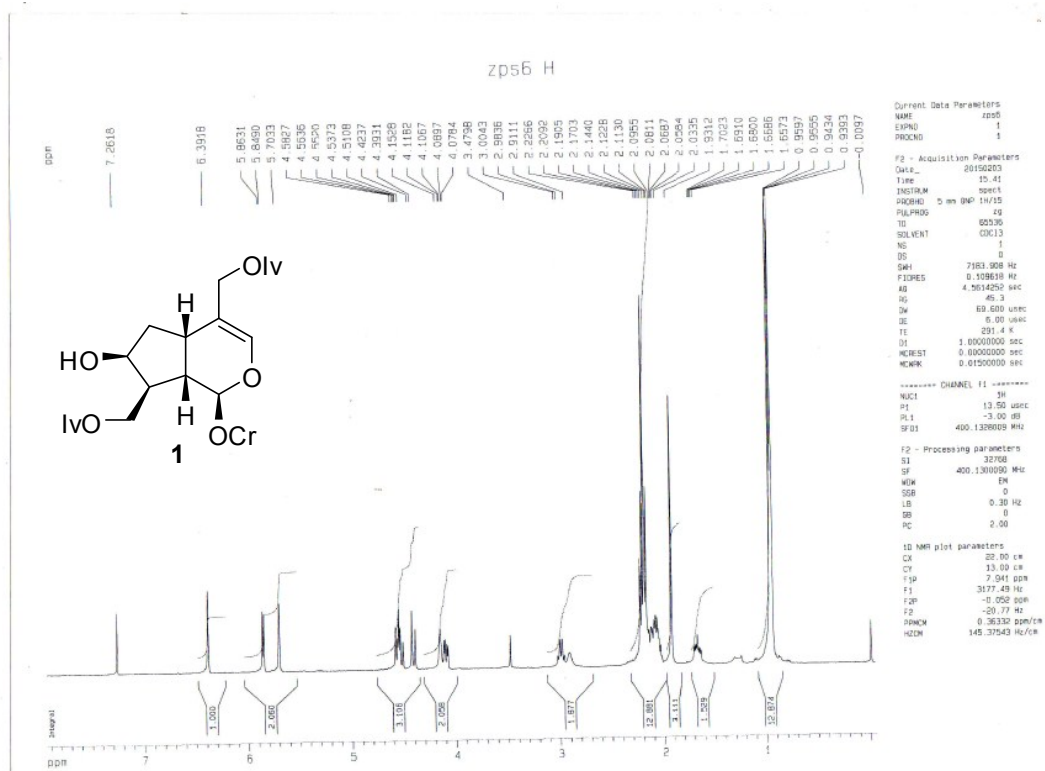
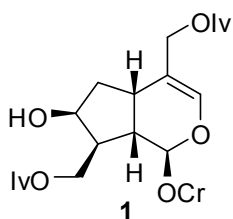


Figure 2. ^{13}C NMR spectrum of Patriscabioin A (**1**) in CDCl_3 .



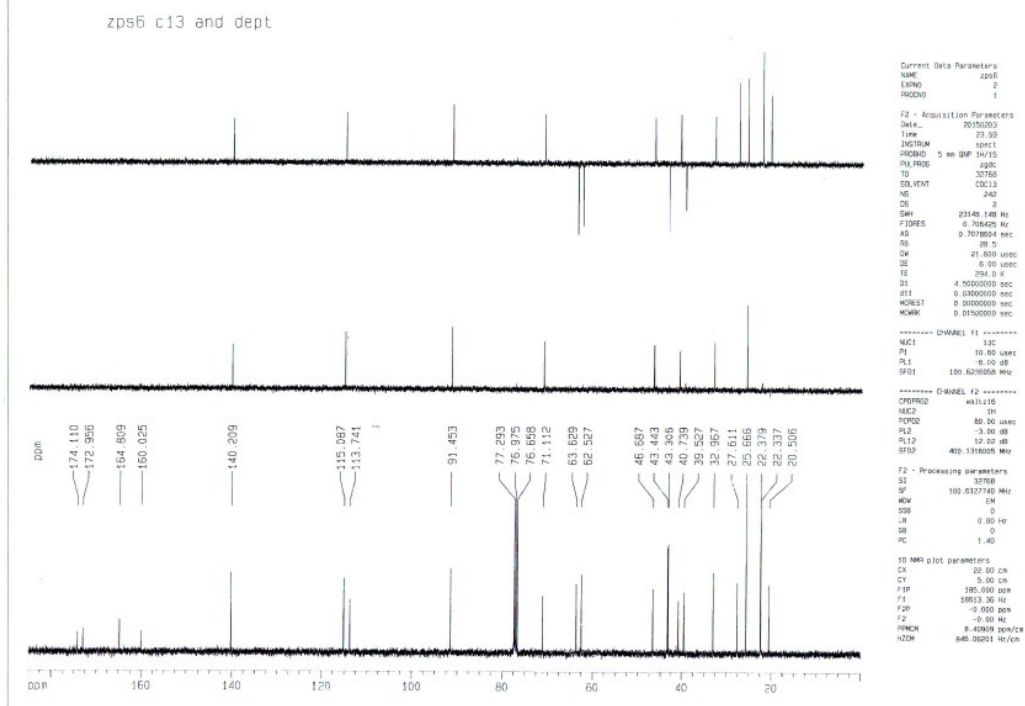


Figure 3. HSQC spectrum of Patriscabioin A (1) in CDCl₃.

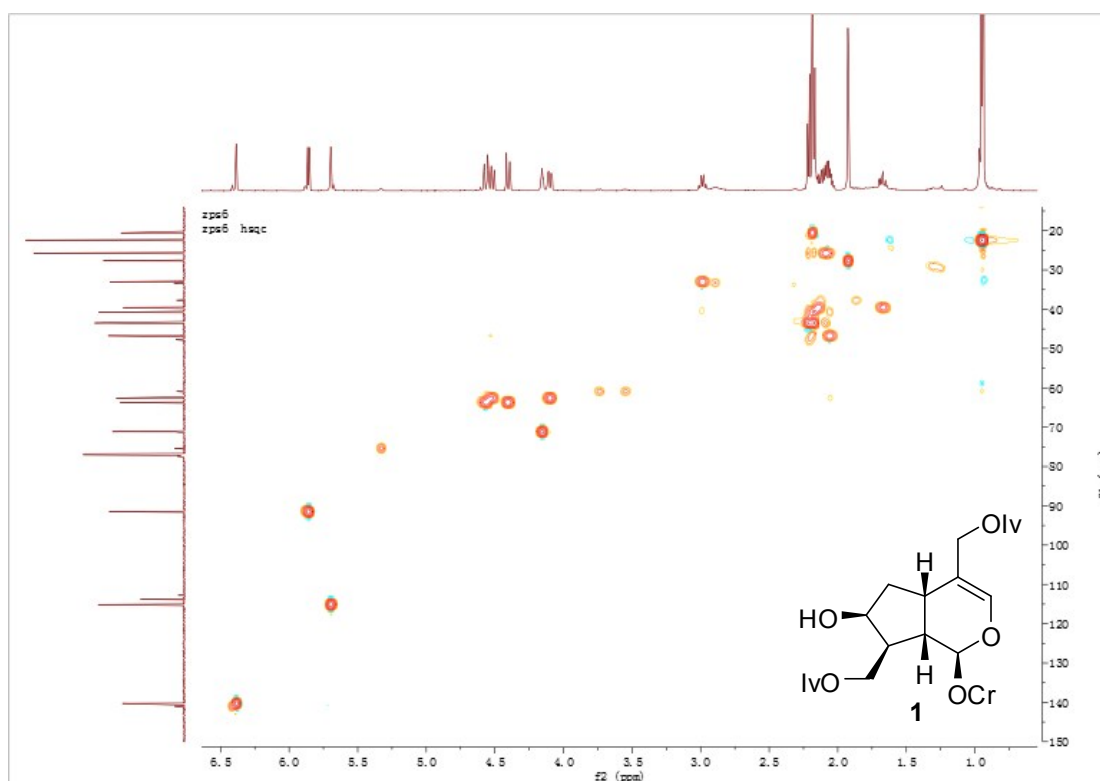


Figure 4. HMBC spectrum of Patriscabioin A (1) in CDCl₃.

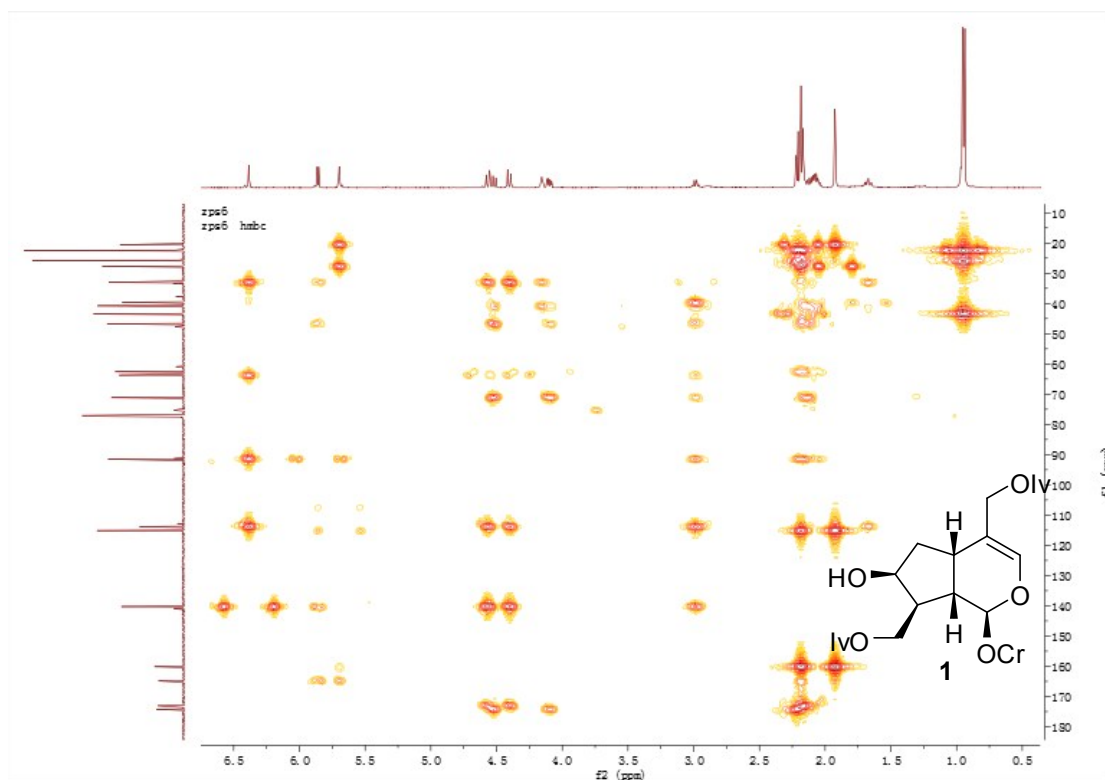


Figure 5. ^1H - ^1H COSY spectrum of Patriscabioin A (1) in CDCl_3 .

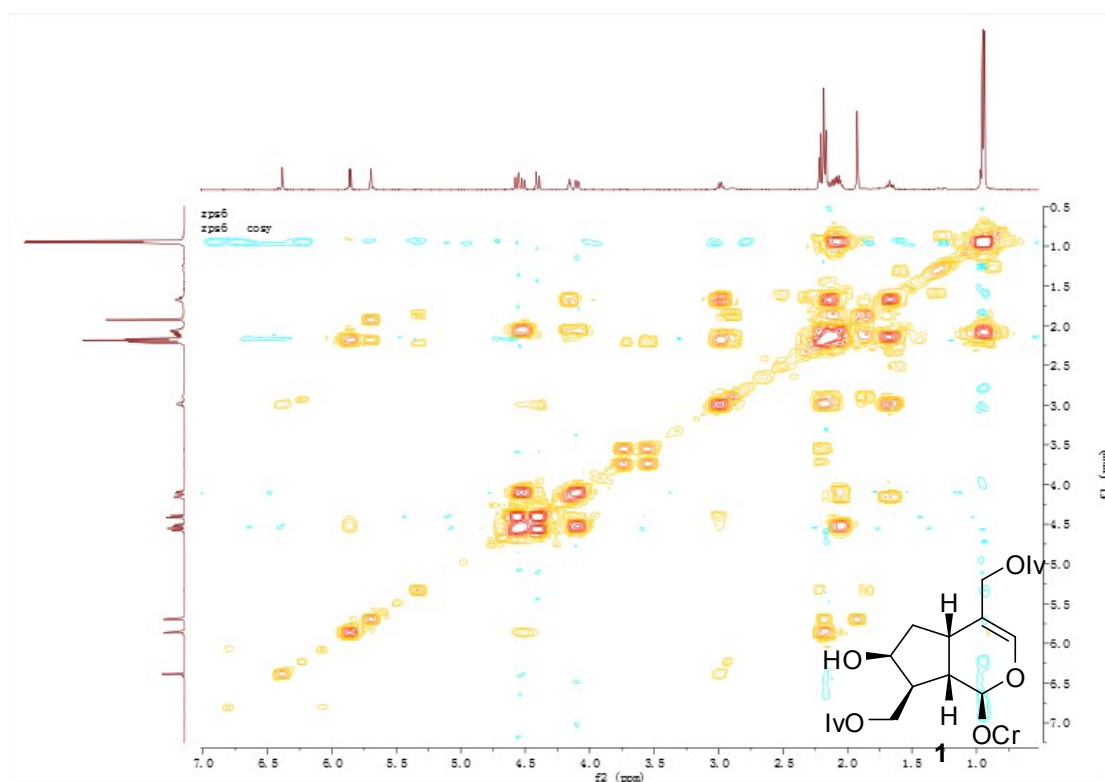


Figure 6. ROESY spectrum of Patriscabioin A (1) in CDCl_3 .

Data File: E:\DATA\20151105\zps-6-3.lcd

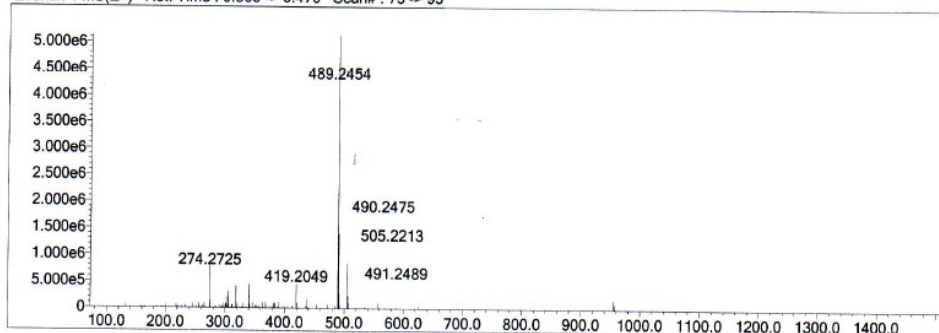
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C	4	0	50	Br	1	0	0	
N	3	0	10					

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 Max Isotopes: all
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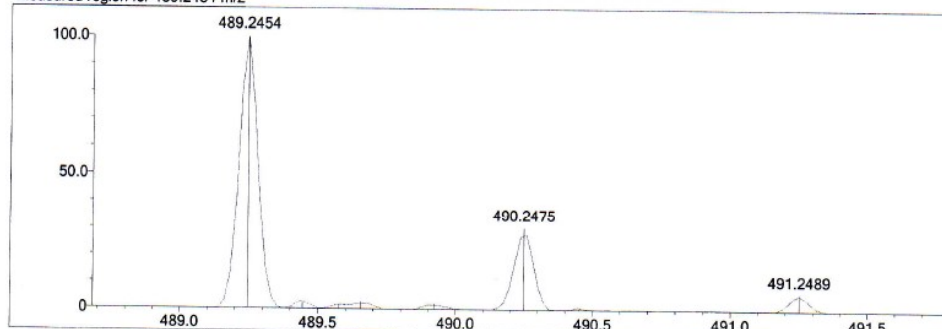
DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 10000
 Max Results: 100

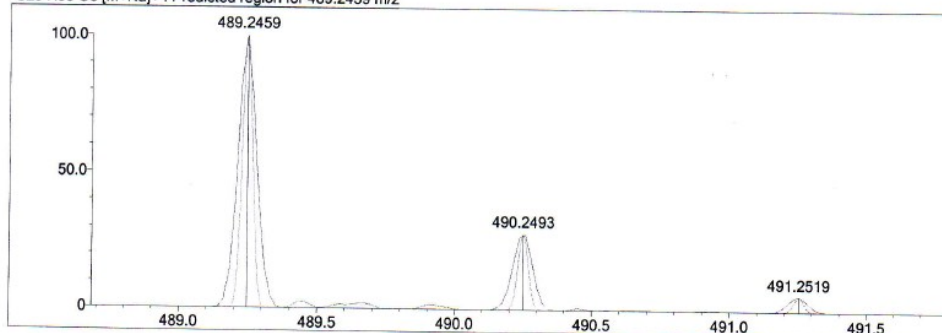
Event#: 1 MS(E+) Ret. Time : 0.360 -> 0.470 Scan#: 73 -> 95



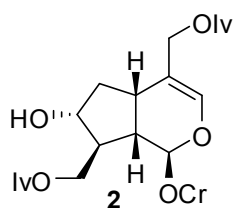
Measured region for 489.2454 m/z



C25 H38 O8 [M+Na]+ : Predicted region for 489.2459 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	99.95	C25 H38 O8	[M+Na]+	489.2454	489.2459	-0.5	-1.02	100.00	7.0

Figure 8. ^1H NMR spectrum of Patriscabioin B (2) in CDCl_3 .

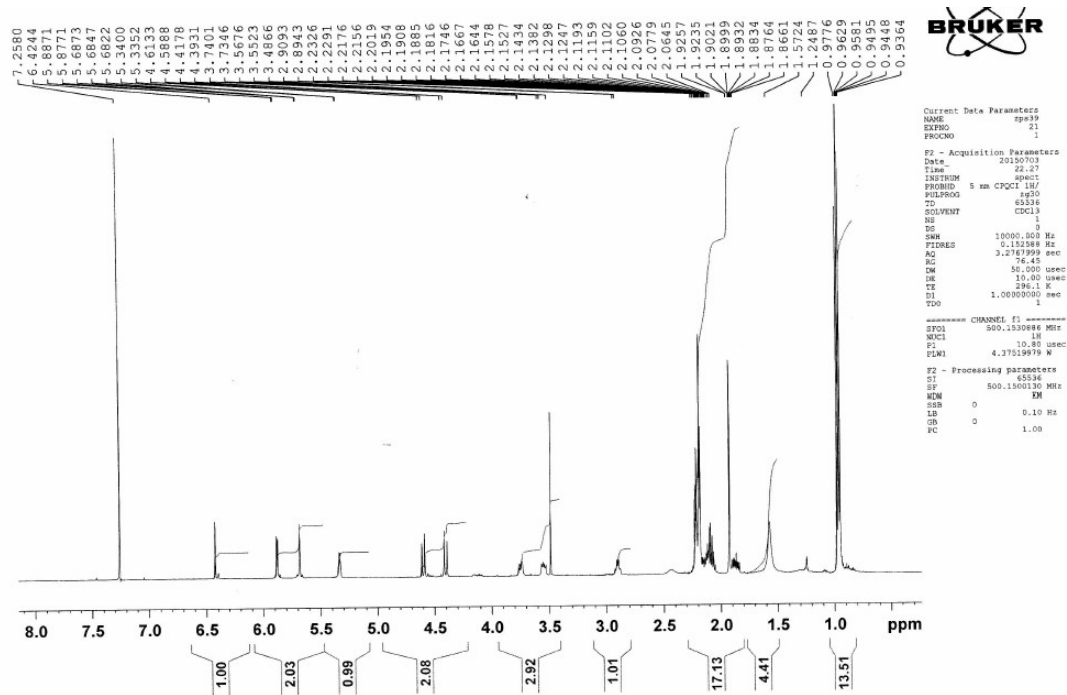


Figure 9. ^{13}C NMR spectrum of Patriscabioin B (2) in CDCl_3 .

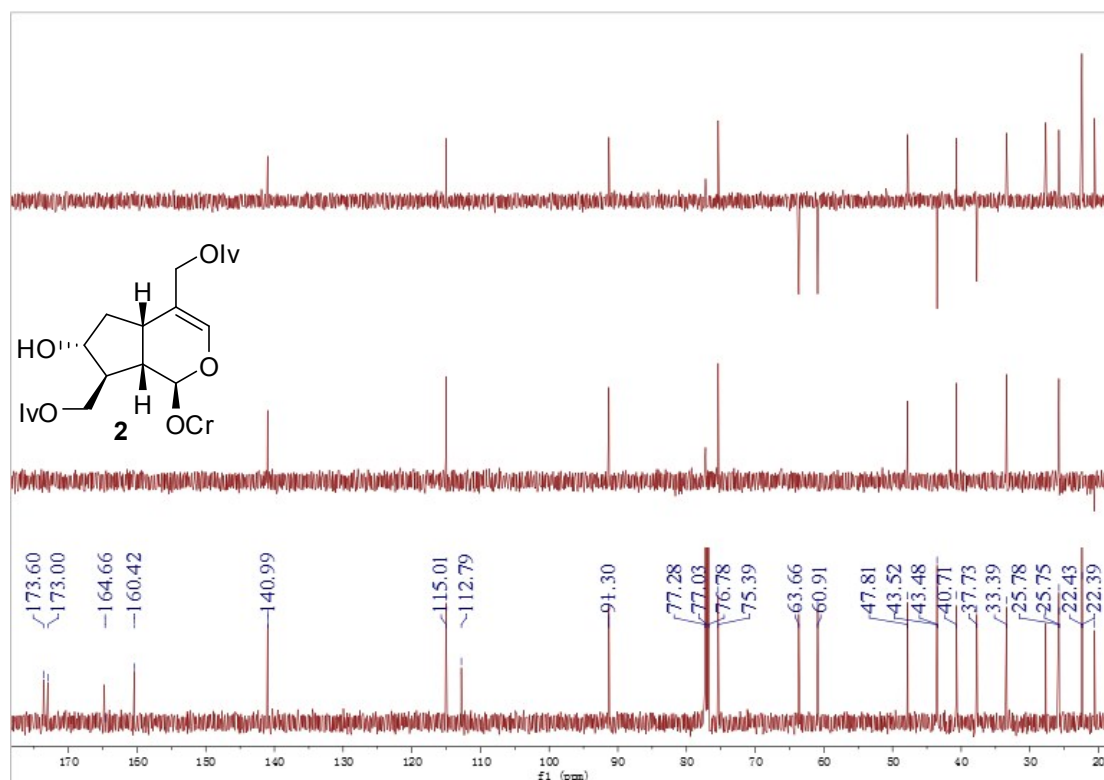


Figure 10. HSQC spectrum of Patriscabioin B (2) in CDCl_3 .

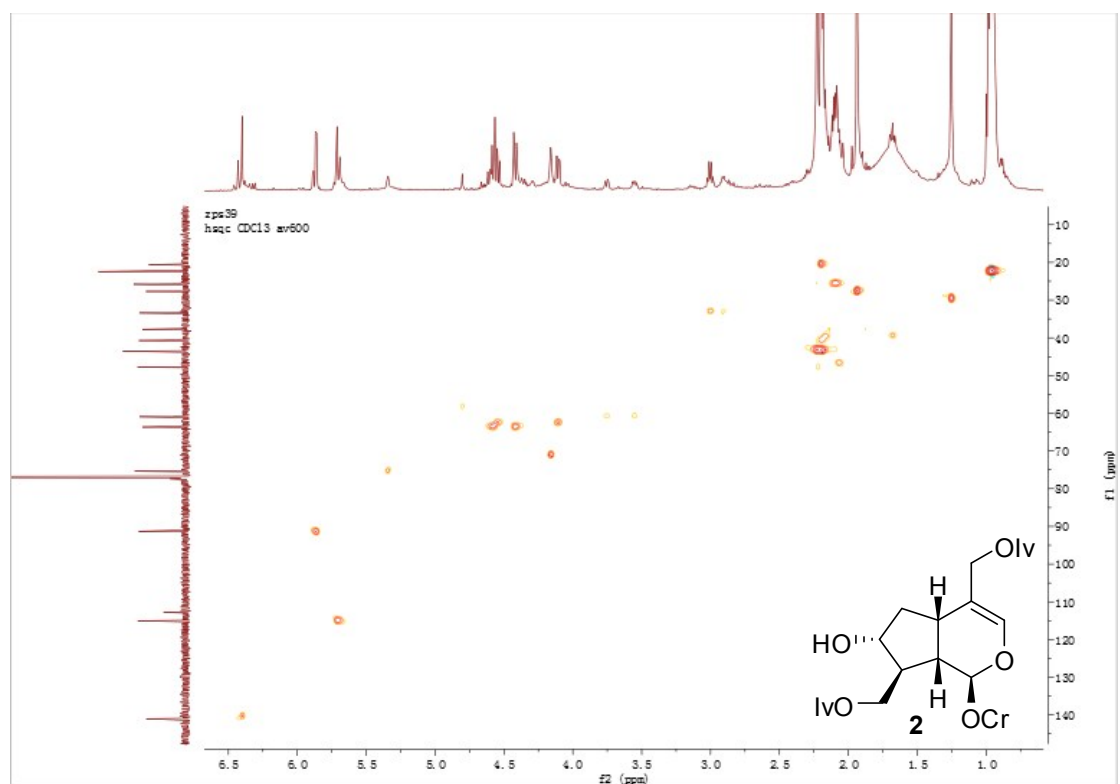


Figure 11. HMBC spectrum of Patriscabioin B (2) in CDCl₃.

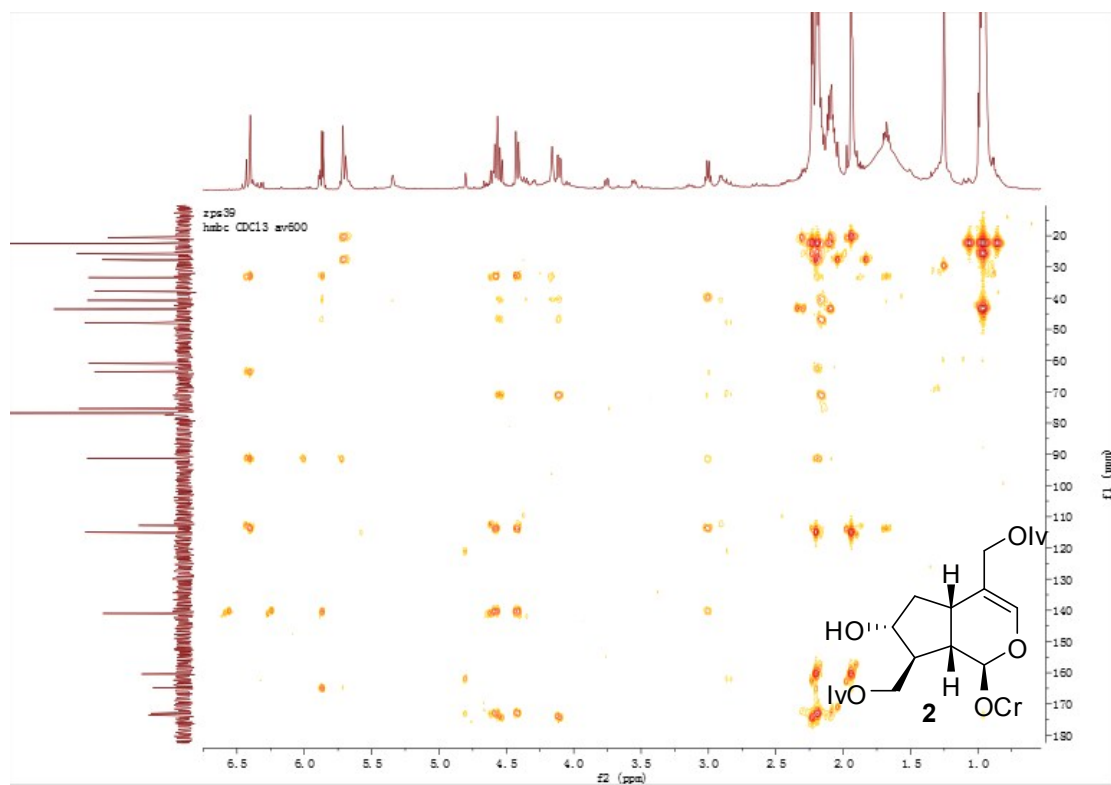


Figure 12. ¹H-¹H COSY spectrum of Patriscabioin B (2) in CDCl₃.

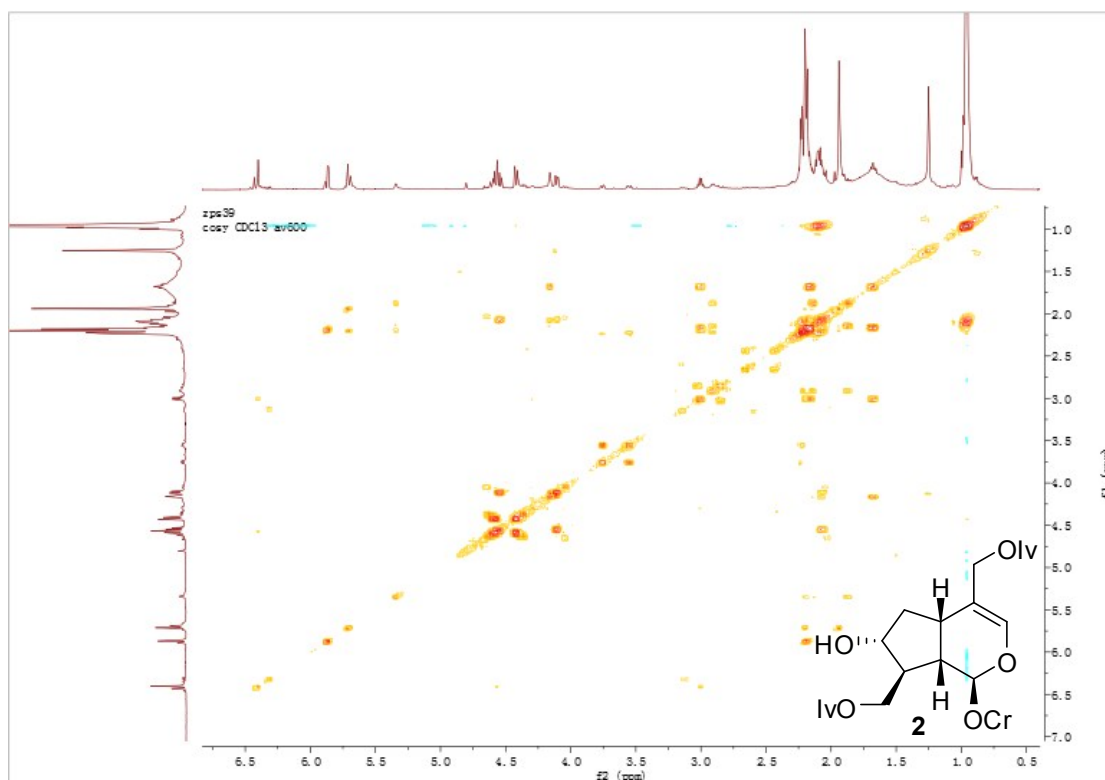


Figure 13. ROESY spectrum of Patriscabioin B (2) in CDCl_3 .

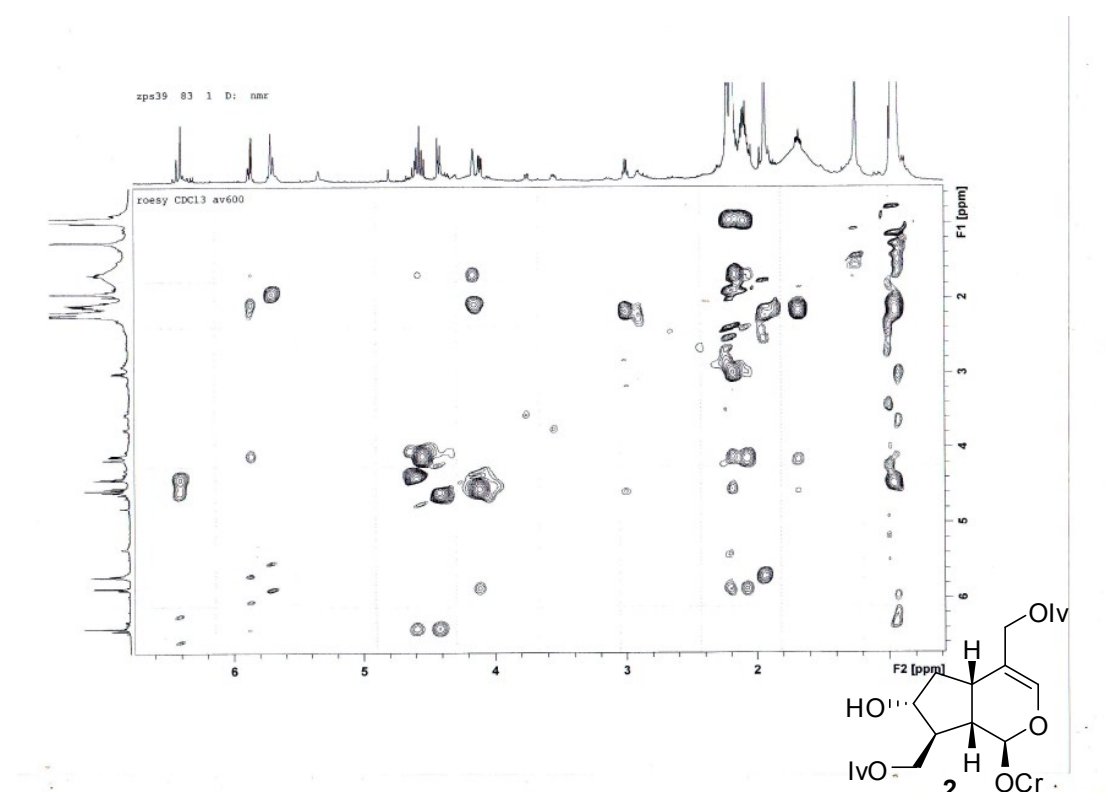


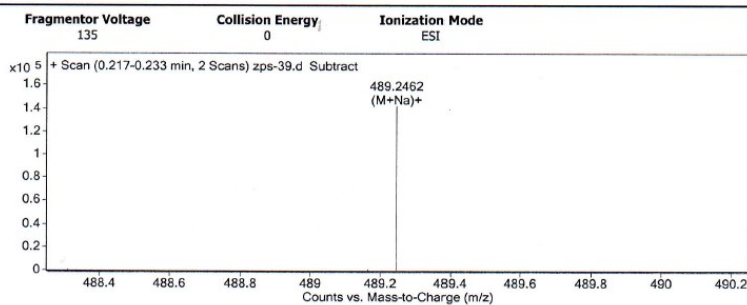
Figure 14. HREIMS spectrum of Patriscabioin B (2).

Qualitative Analysis Report

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Sample Type	Sample	Position	P1-C7
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	4/19/2016 3:38:19 PM
IRM Calibration Status	Success	DA Method	ESI+.m
Comment			

Sample Group	Info.
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.2)

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
274.2745	1	156038.95		
318.3008	1	195575.78		
319.3042	1	38183.13		
362.327	1	66658.2		
484.2908	1	70822.38		
489.2462	1	142474.86	C25 H38 O8	(M+Na)+
505.2202	1	137884		
955.5031	1	75508.64		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C25 H38 O8	466.2567	489.2459	489.2462	-0.7	-1.5	7.0000

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Figure 15. ¹H NMR spectrum of Patriscabioin C (3) in CDCl₃.

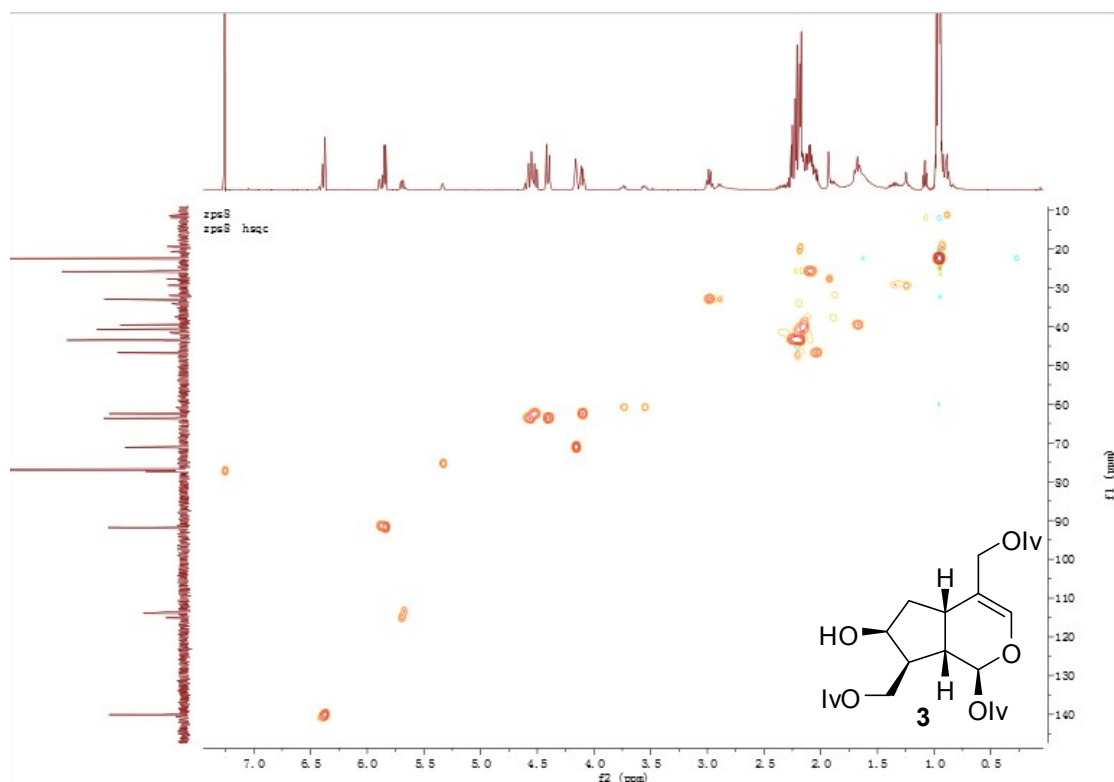


Figure 18. HMBC spectrum of Patriscabioin C (3) in CDCl₃

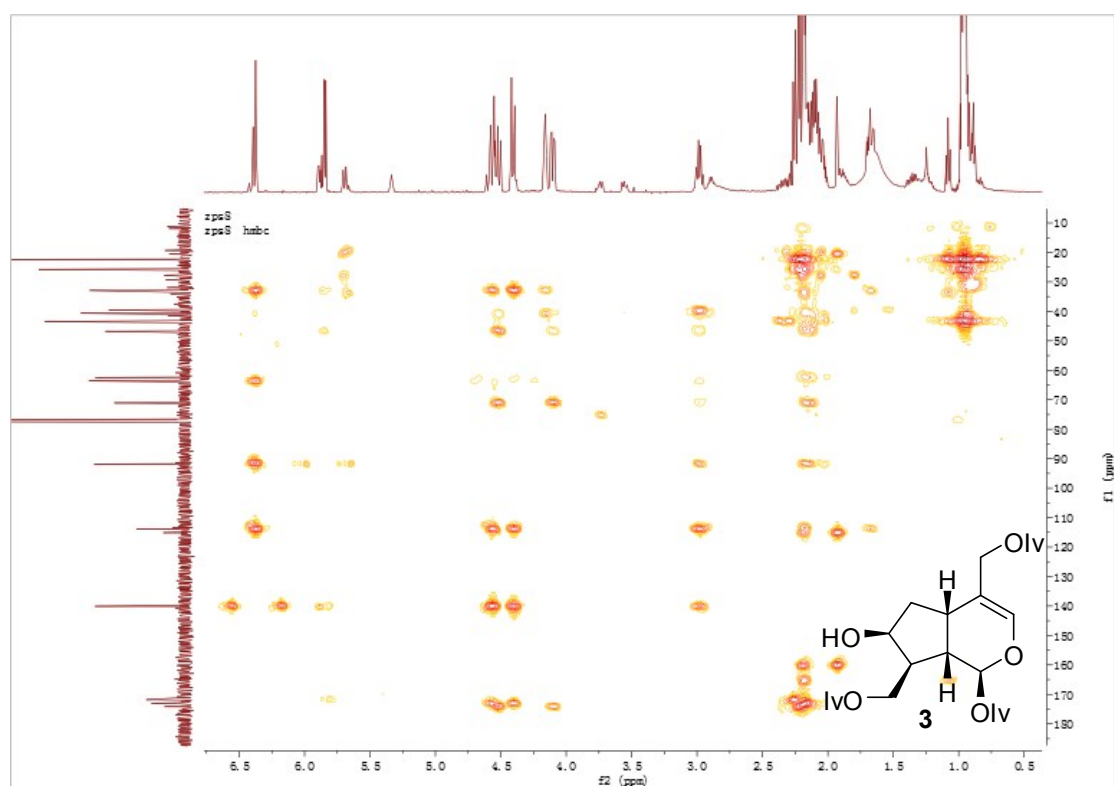


Figure 19. ¹H-¹H COSY spectrum of Patriscabioin C (3) in CDCl₃.

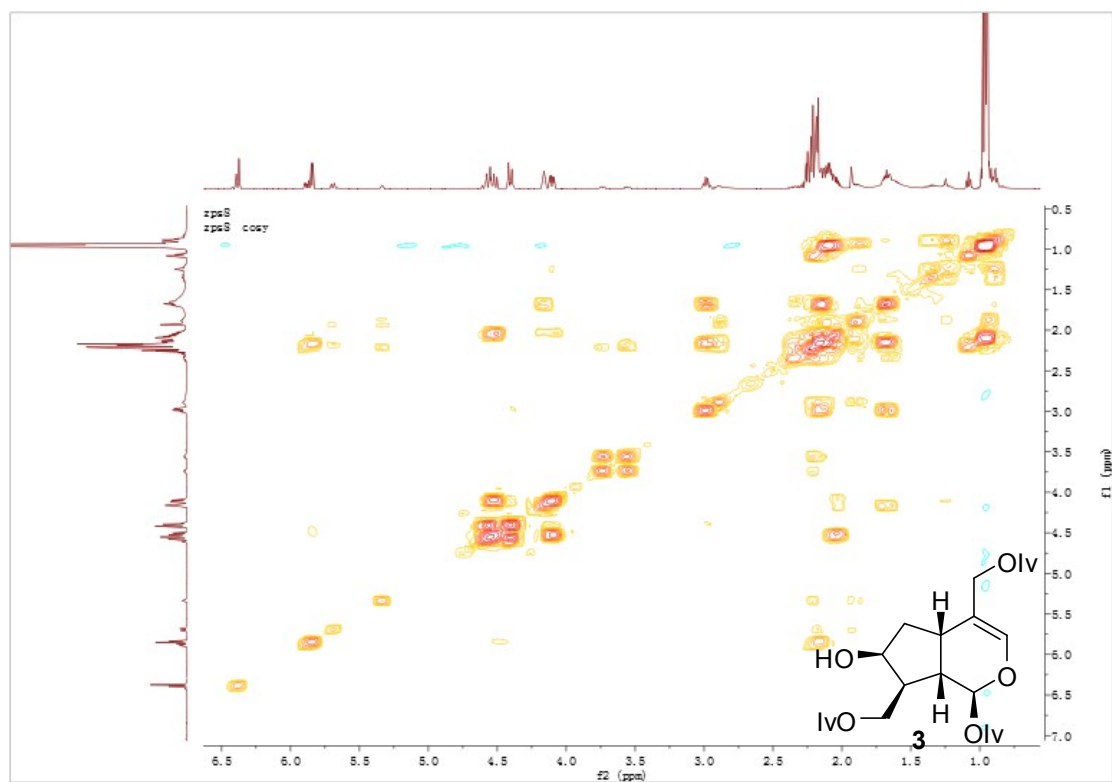


Figure 20. ROESY spectrum of Patriscabioin C (3) in CDCl_3 .

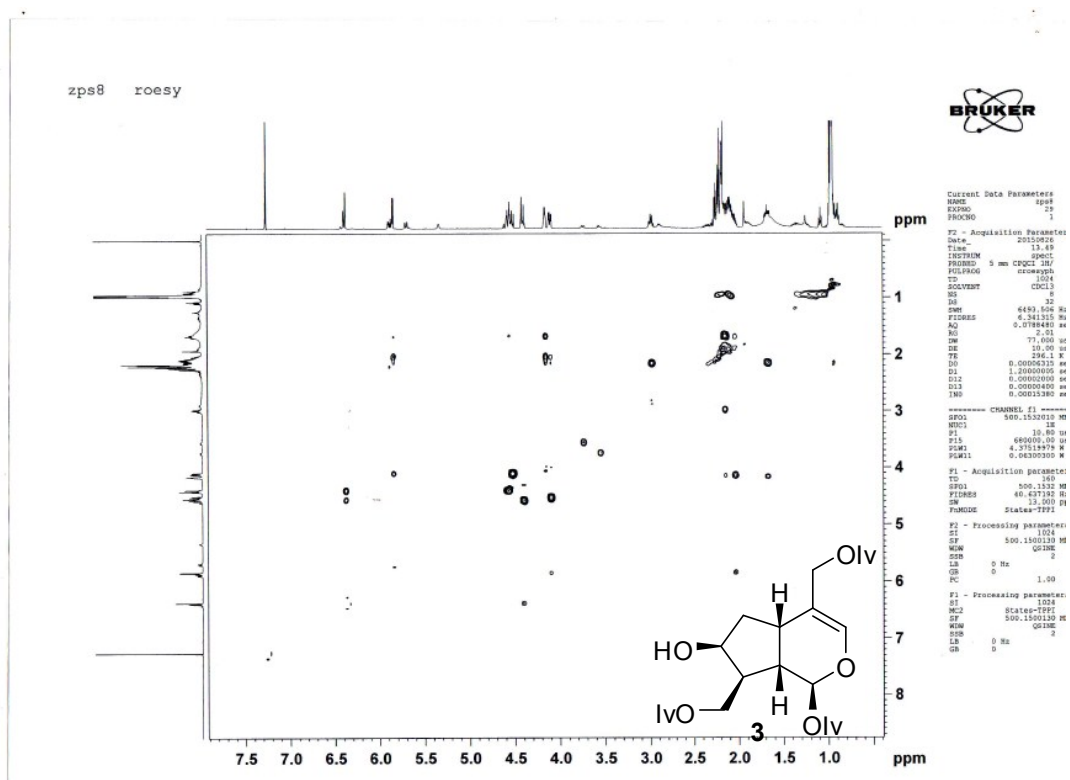


Figure 21. HREIMS spectrum of Patriscabioin C (3).

Data File: E:\DATA\20151106\zps-8.lcd

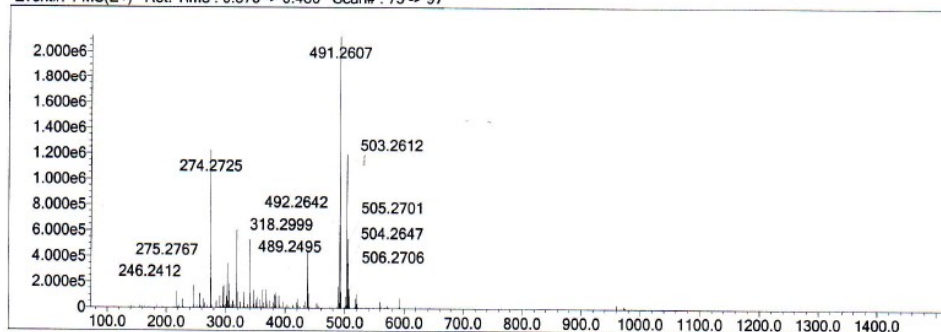
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	40	Na
C	4	0	50	Br	1	0	0	
N	3	0	10					

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

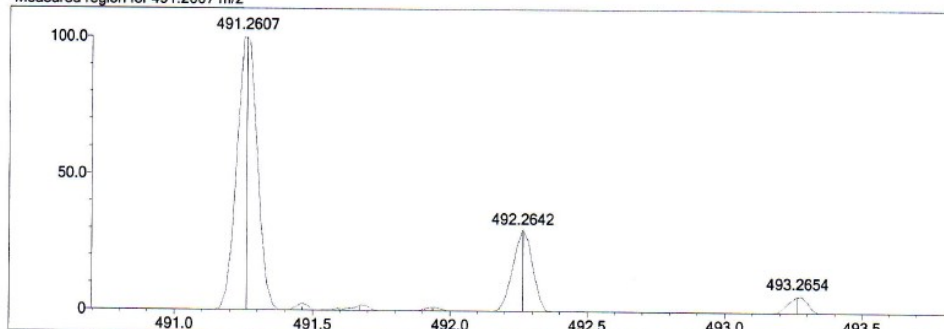
DBE Range: -2.0 - 1000.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 100

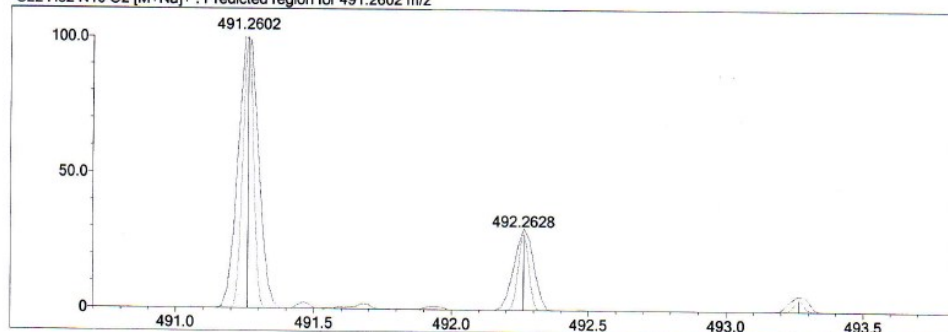
Event#: 1 MS(E+) Ret. Time : 0.370 -> 0.480 Scan#: 75 -> 97



Measured region for 491.2607 m/z



C22 H32 N10 O2 [M+Na]+ : Predicted region for 491.2602 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	99.95	C22 H32 N10 O2	[M+Na]+	491.2607	491.2602	0.5	1.02	100.00	12.0

Figure 22. ^1H NMR spectrum of Patriscabioin D (4) in CDCl_3 .

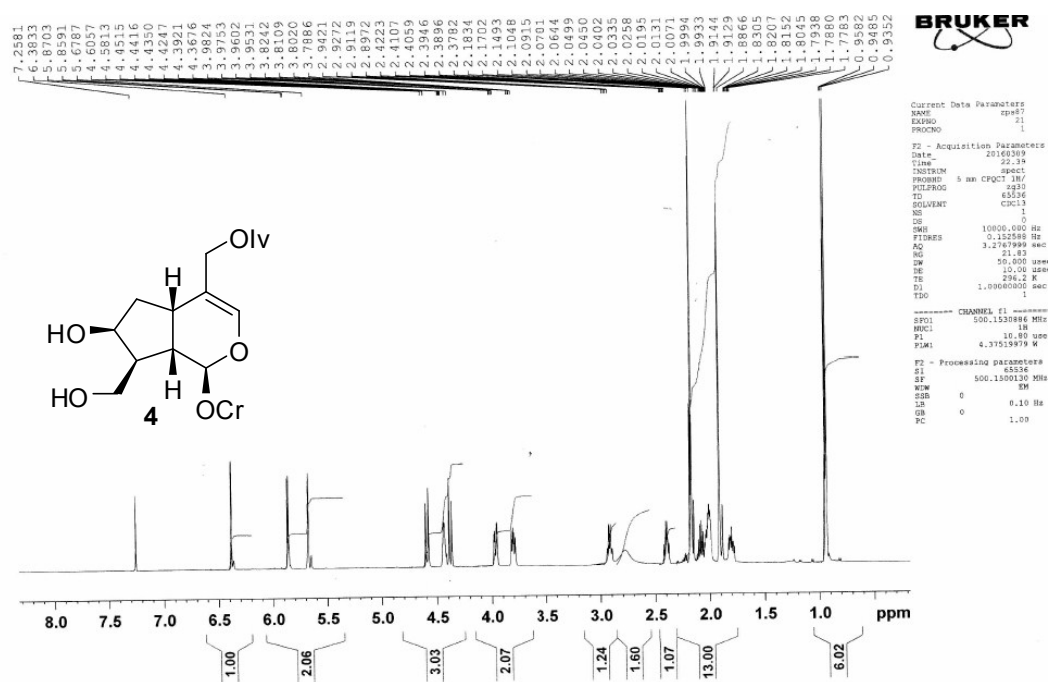


Figure 23. ^{13}C NMR spectrum of Patriscabioin D (4) in CDCl_3

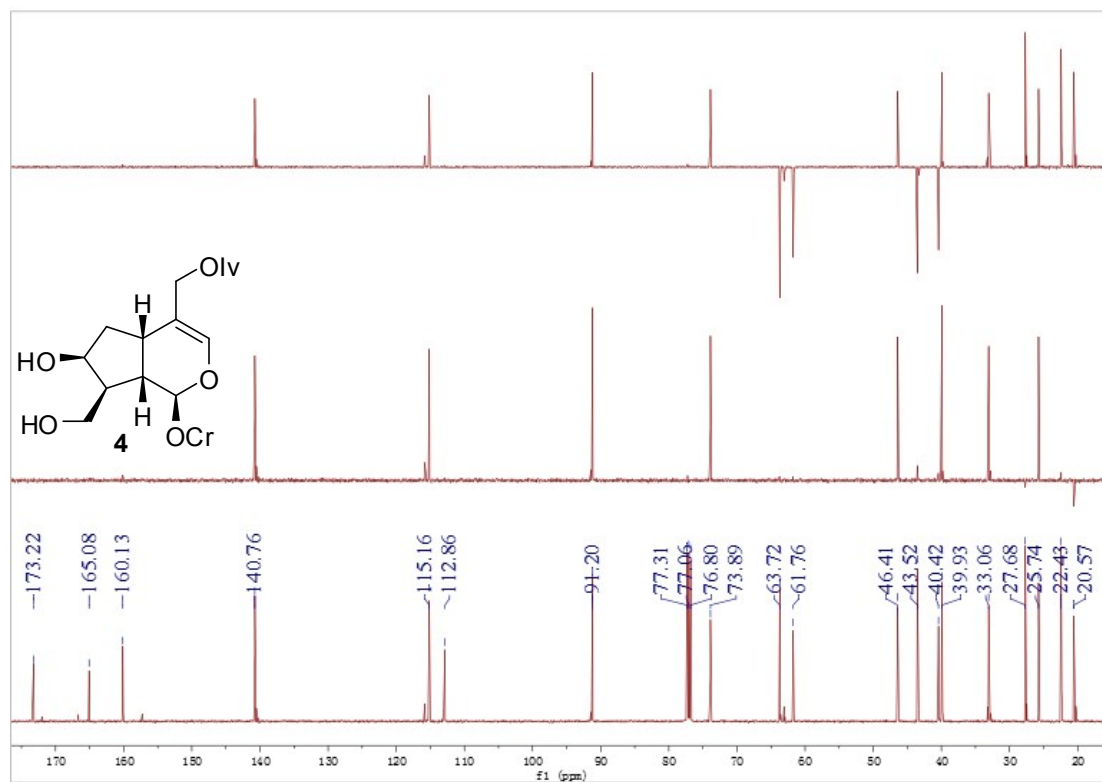


Figure 24. HSQC spectrum of Patriscabioin D (4) in CDCl_3 .

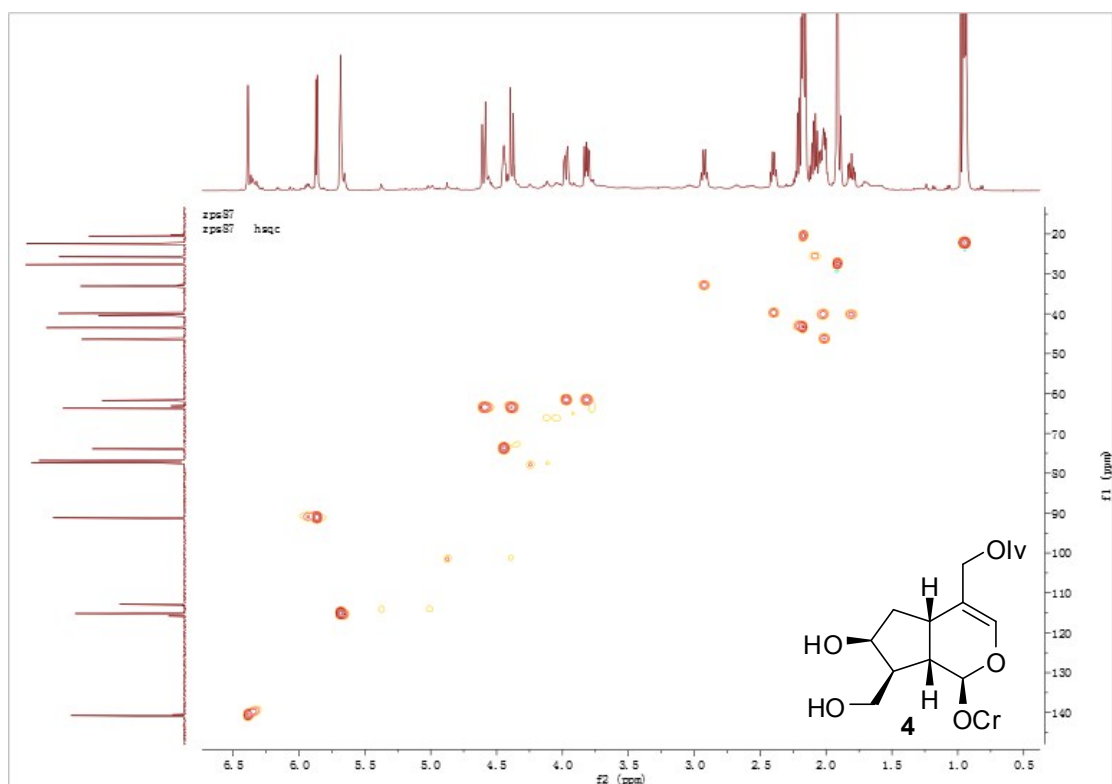


Figure 25. HMBC spectrum of Patriscabioin D (4) in CDCl₃.

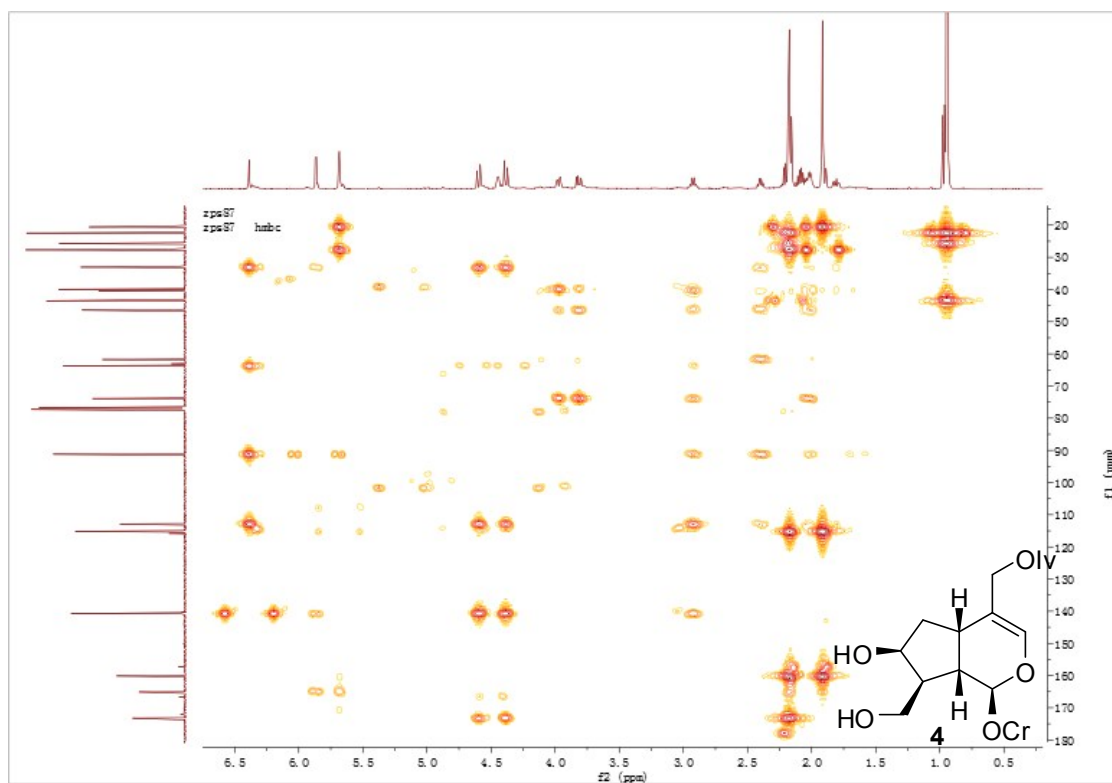


Figure 26. ¹H-¹H COSY spectrum of Patriscabioin D (4) in CDCl₃.

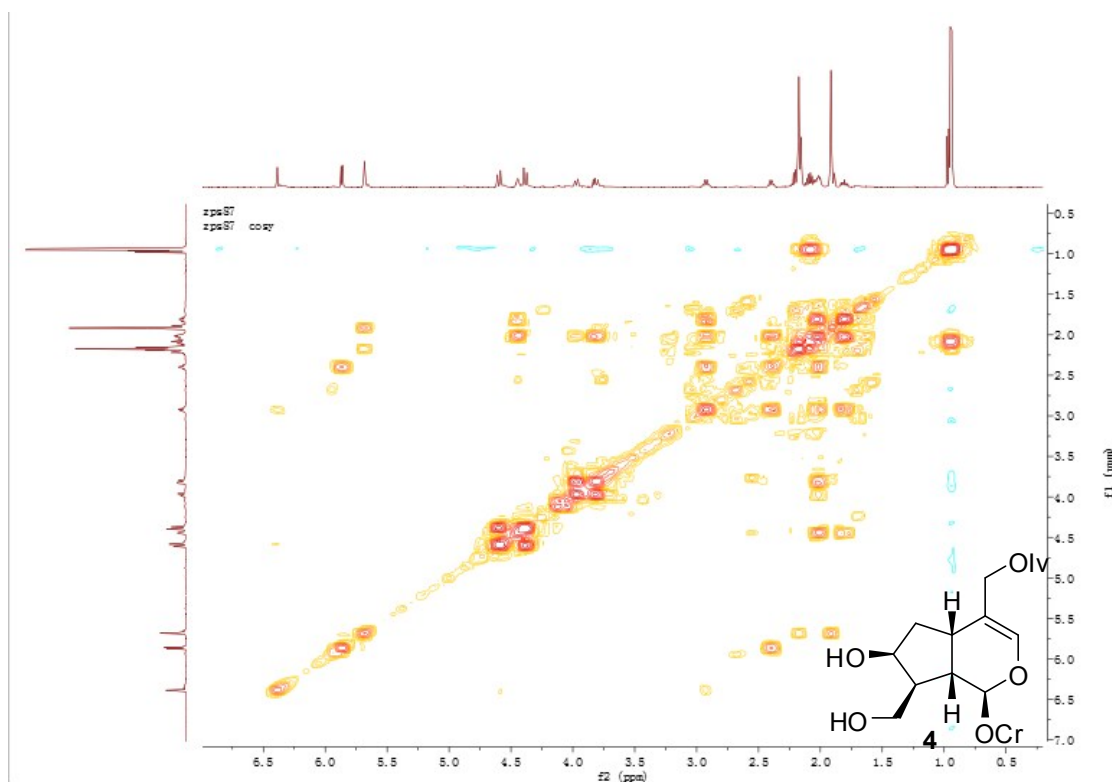


Figure 27. ROESY spectrum of Patriscabioin D (4) in CDCl_3 .

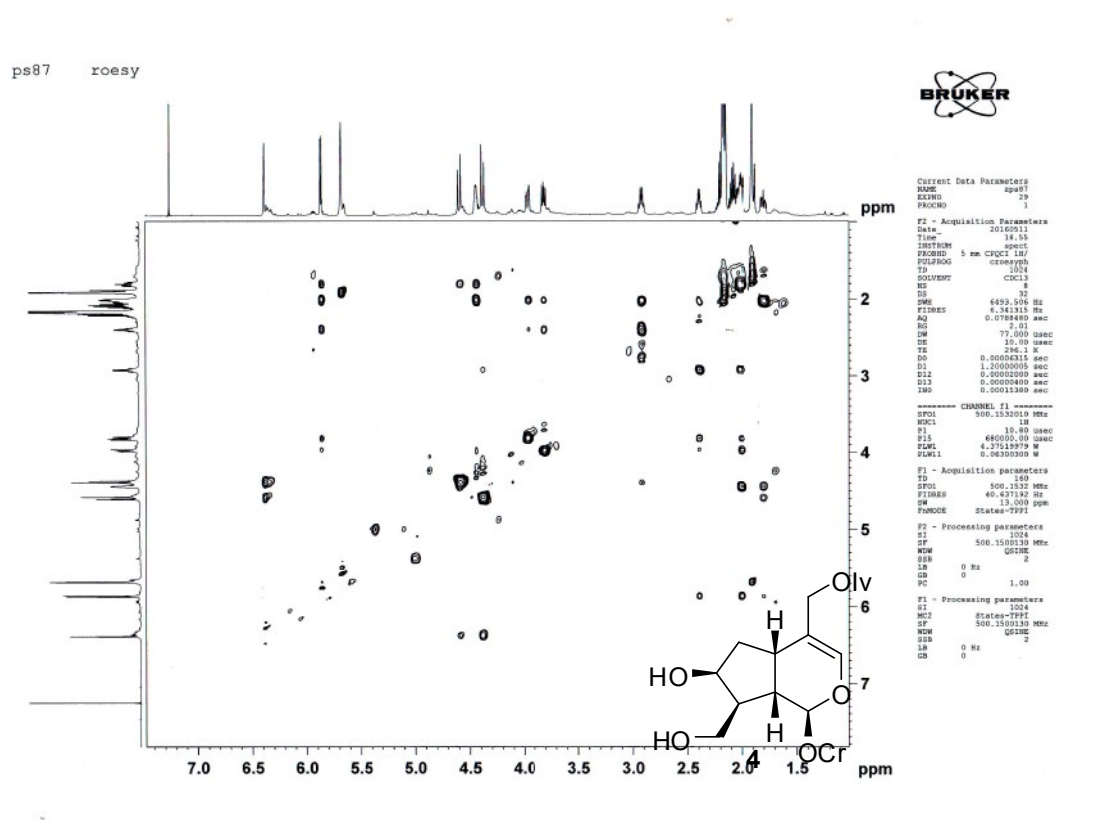


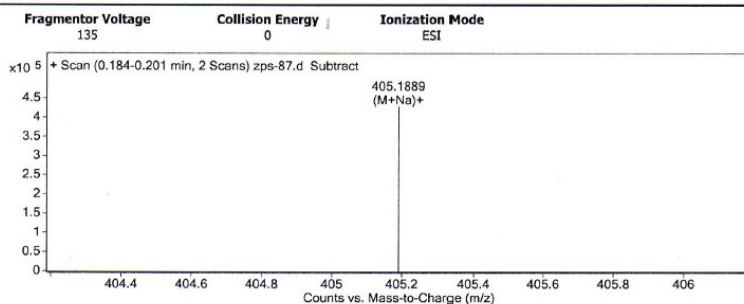
Figure 28. HREIMS spectrum of Patriscabioin D (4).

Qualitative Analysis Report

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Sample Type	Sample	Position	P1-C8
Instrument Name	Instrument 1	User Name	
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IRM Calibration Status	Success	DA Method	ESI+.m
Comment			

Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125.2)	

User Spectra



Peak List

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421.1626	1	286921.09		
785.373	1	215689		
786.3758	1	86365.39		
787.3884		824728		
788.3919	1	338700.53		
789.3978	1	126465.7		

Formula Calculator Element Limits

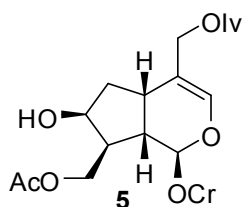
Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C ₂₀ H ₃₀ O ₇	382.1992	405.1884	405.1889	-0.8	-2.1	6.0000

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Figure 29. ¹H NMR spectrum of Patriscabioin E (**5**) in CDCl₃.



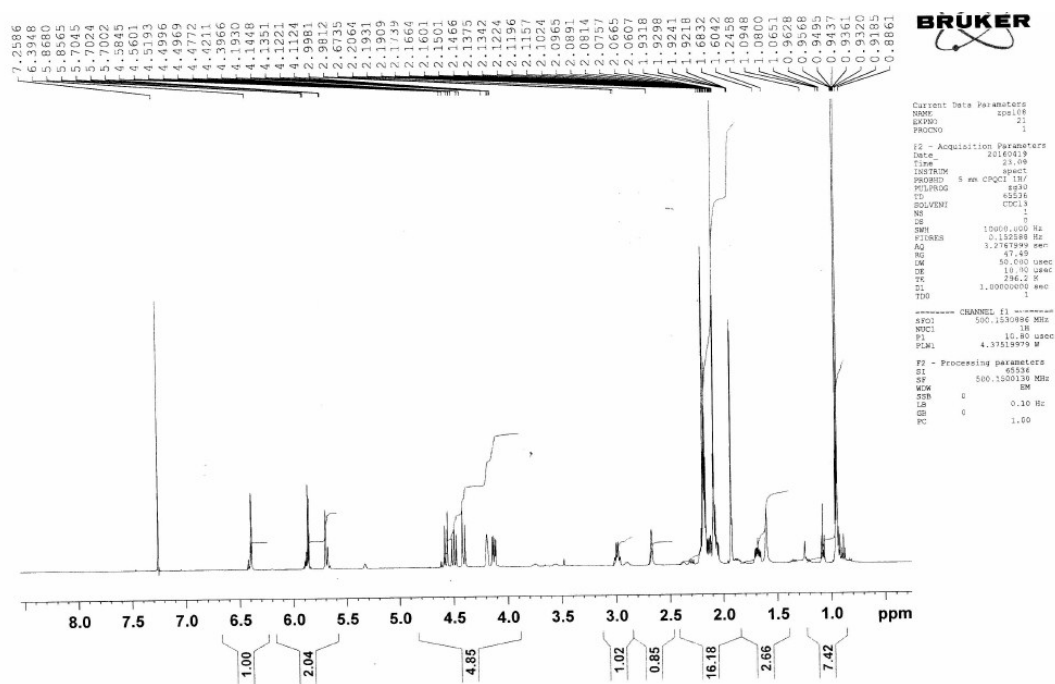


Figure 30. ^{13}C NMR spectrum of Patriscabioin E (**5**) in CDCl_3

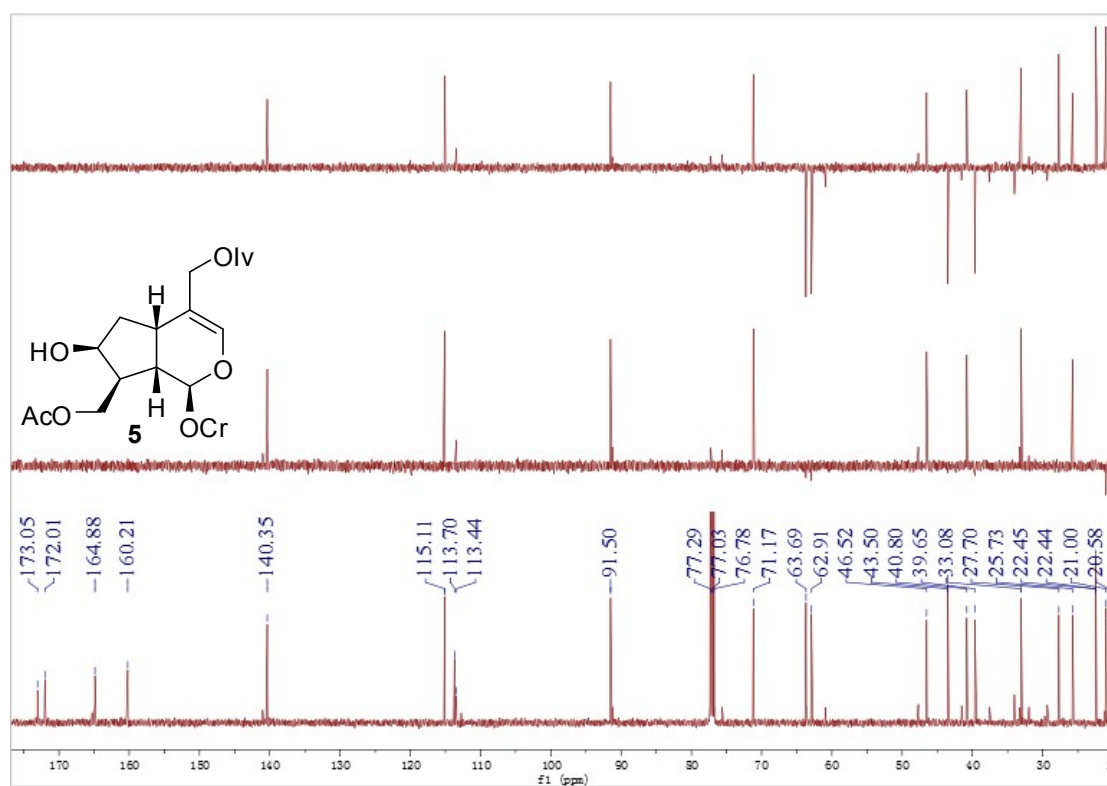


Figure 31. HSQC spectrum of Patriscabioin E (**5**) in CDCl_3 .

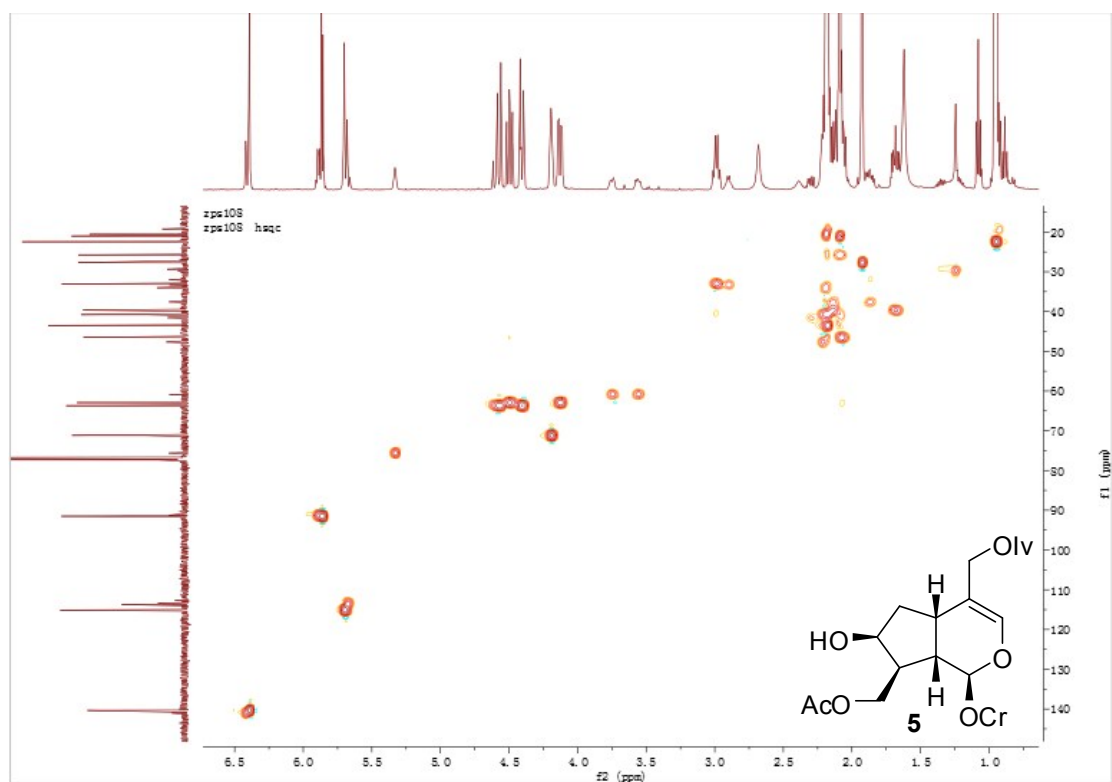


Figure 32. HMBC spectrum of Patriscabioin E (5) in CDCl_3 .

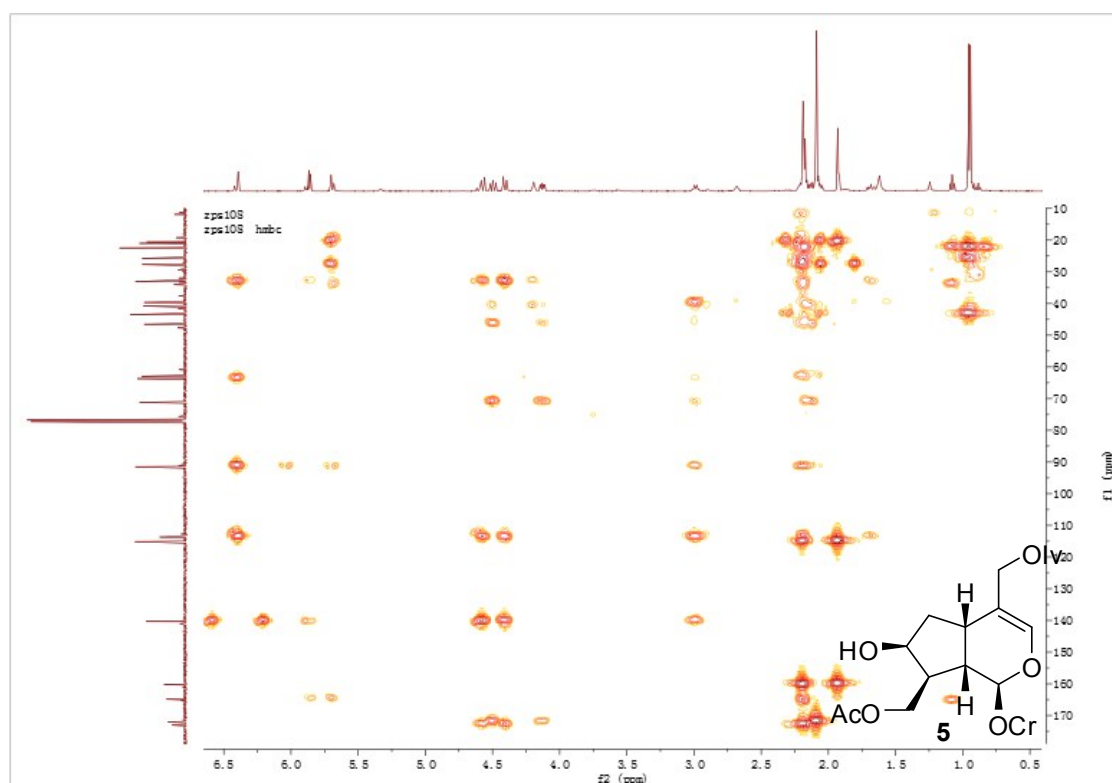


Figure 33. ^1H - ^1H COSY spectrum of Patriscabioin E (5) in CDCl_3 .

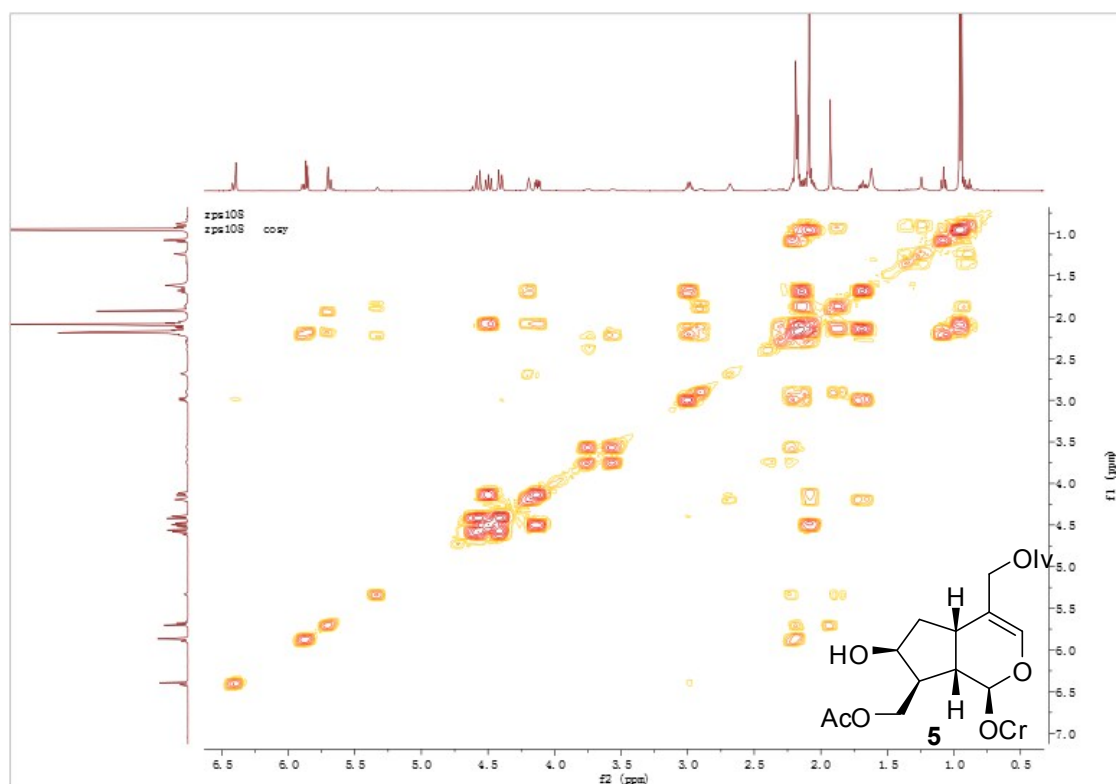


Figure 34. ROESY spectrum of Patriscabioin E (**5**) in CDCl₃.

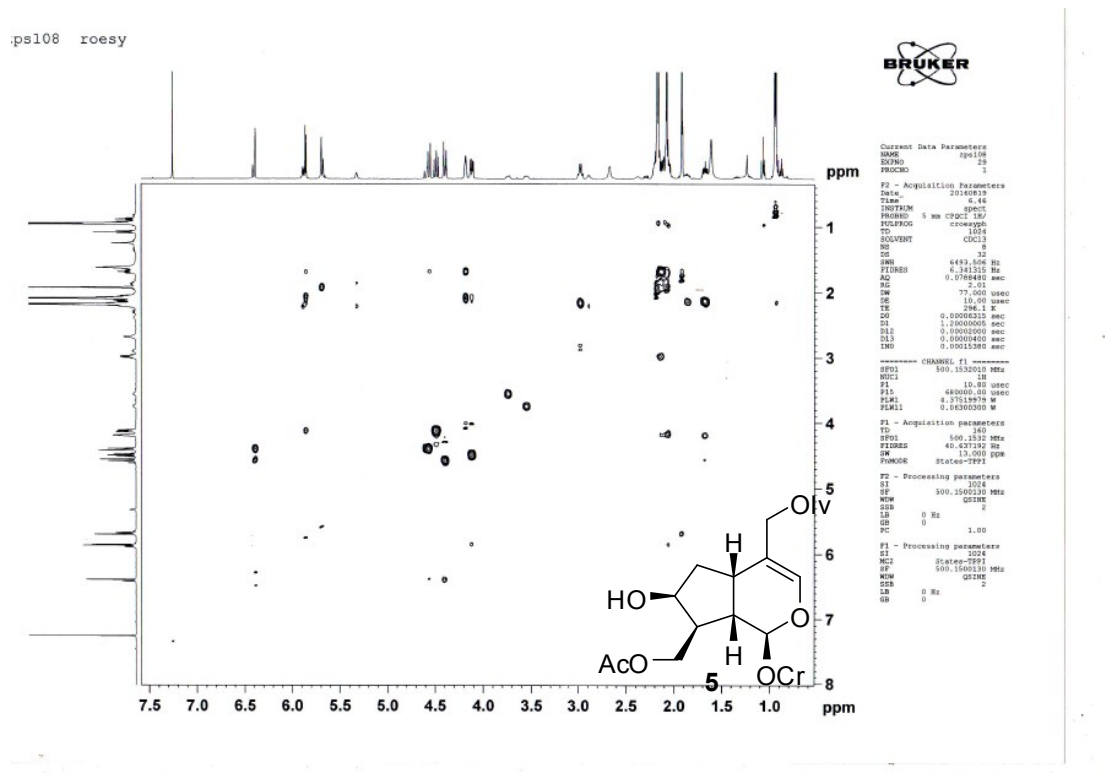


Figure 35. HREIMS spectrum of Patriscabioin E (**5**).

Data File: E:\DATA\2016\0525\zps-108.lcd

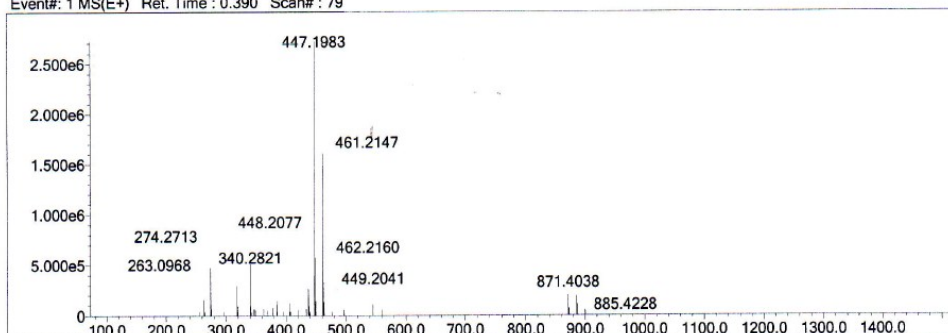
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	100	N	3	0	20	Na	1	0	0	Cl	1	0	0	Na
B	3	0	0	O	2	0	40	Si	4	0	0	Br	1	0	0	
C	4	0	80	F	1	0	0	S	2	0	0	Pt	2	0	0	

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

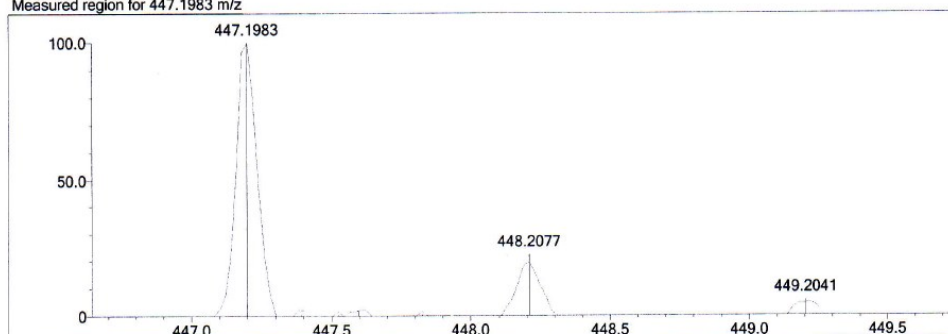
DBE Range: -2.0 - 100.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

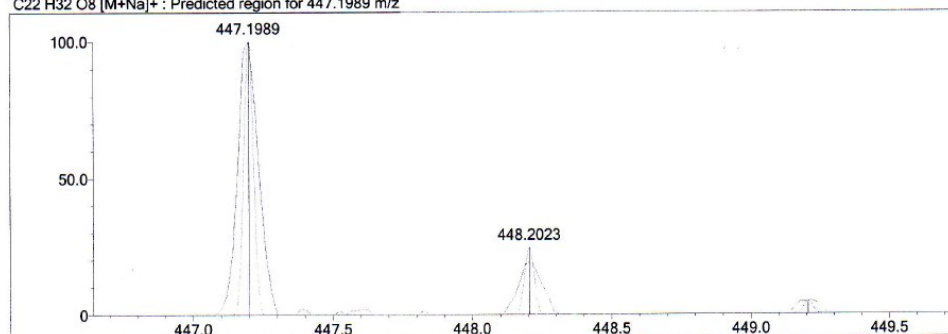
Event#: 1 MS(E+) Ret. Time : 0.390 Scan#: 79



Measured region for 447.1983 m/z



C22 H32 O8 [M+Na]+ : Predicted region for 447.1989 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	85.05	C22 H32 O8	[M+Na]+	447.1983	447.1989	-0.6	-1.34	85.78	7.0

Figure 36. ^1H NMR spectrum of Patriscabioin F (6) in CDCl_3 .

Figure 38. HSQC spectrum of Patriscabioin F (**6**) in CDCl₃.

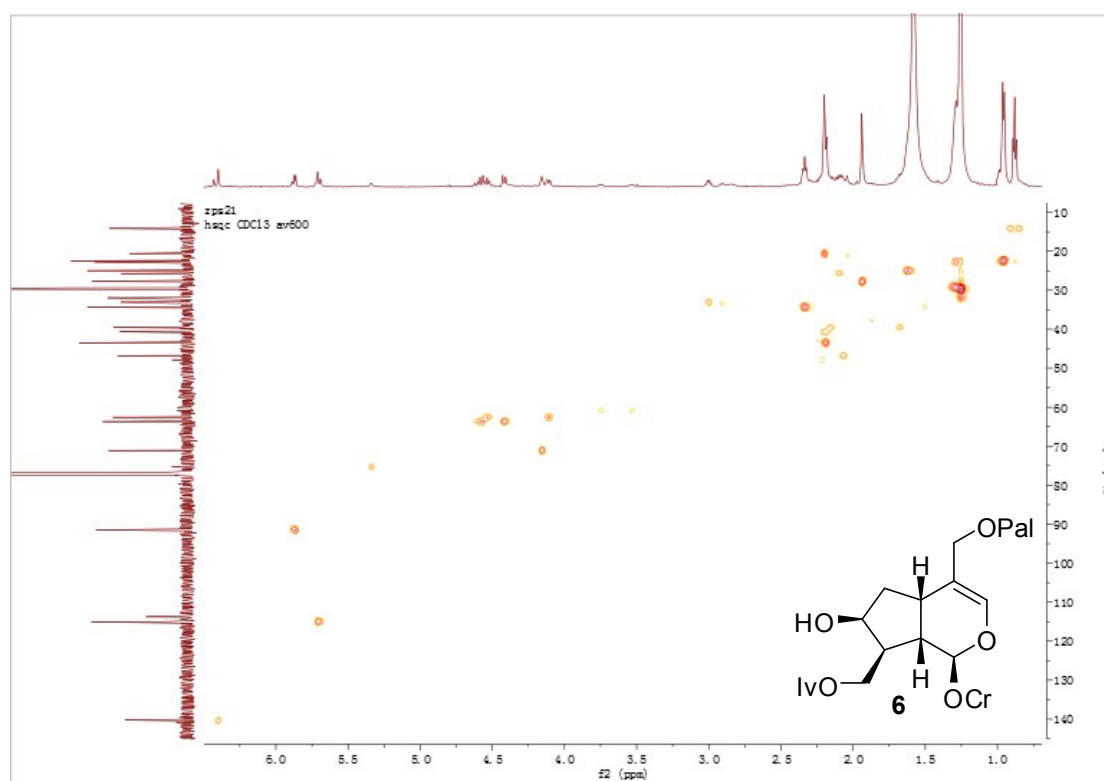


Figure 39. HMBC spectrum of Patriscabioin F (**6**) in CDCl₃.

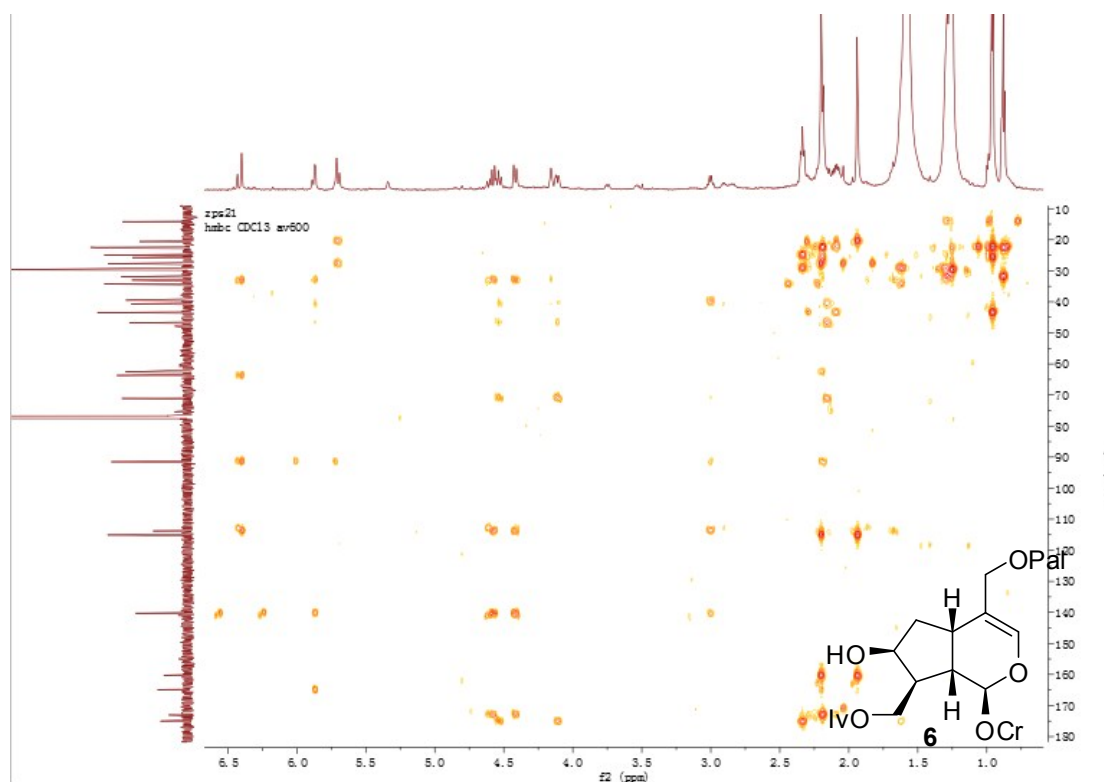


Figure 40. ^1H - ^1H COSY spectrum of Patriscabioin F (**6**) in CDCl_3 .

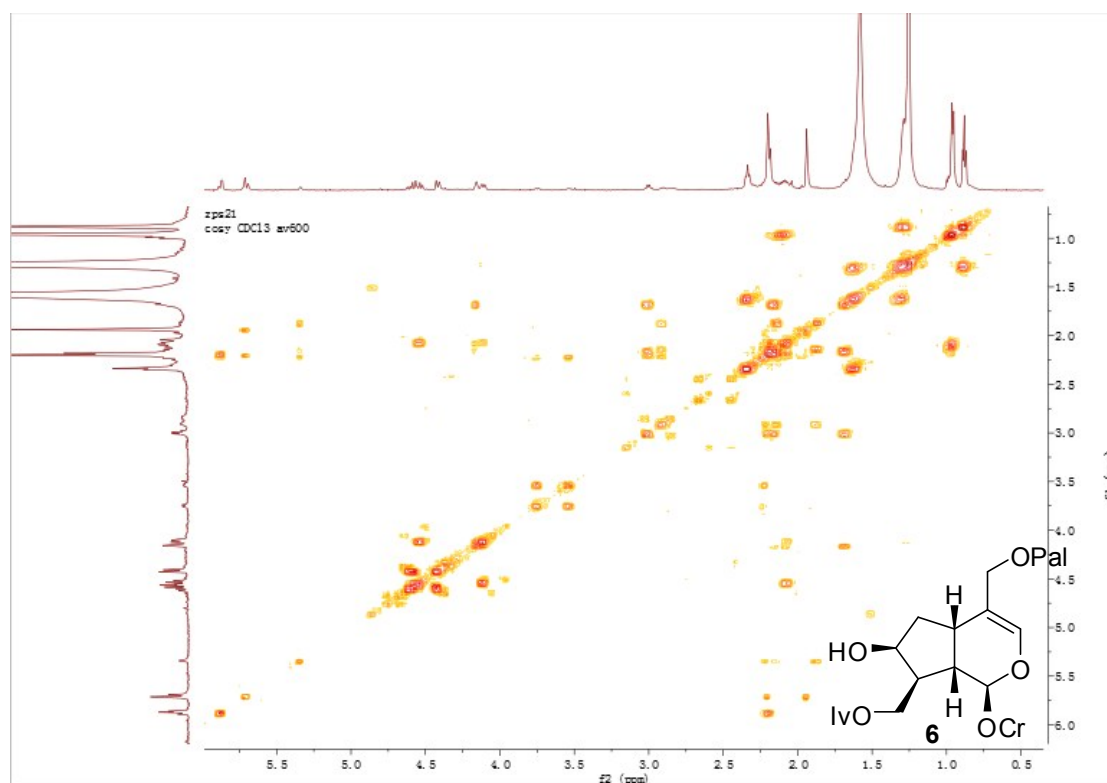


Figure 41. ROESY spectrum of Patriscabioin F (**6**) in CDCl_3 .

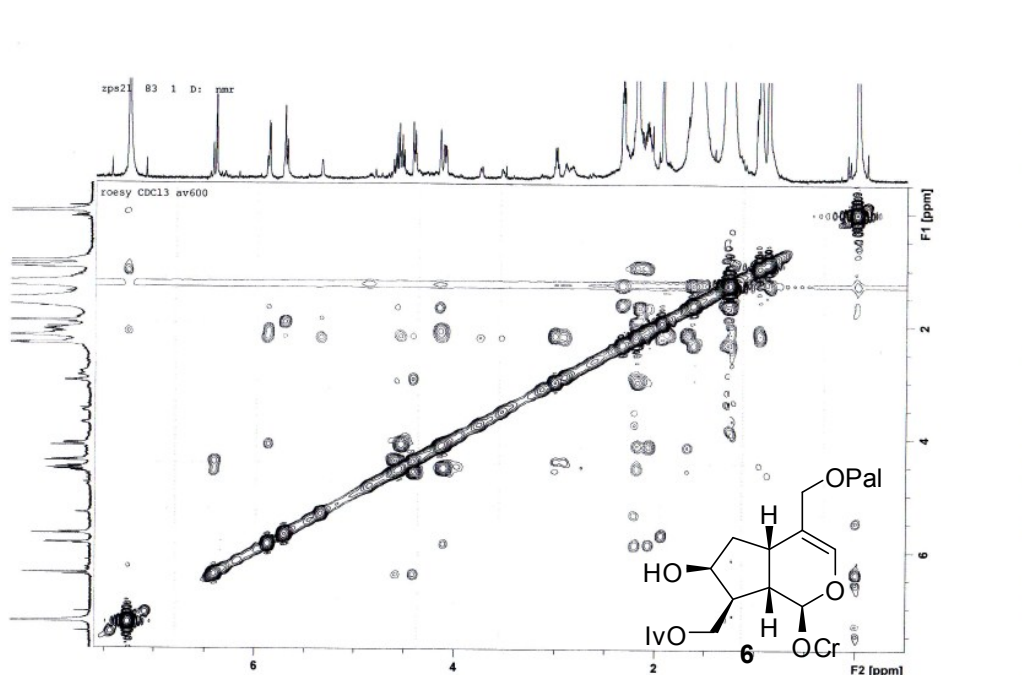


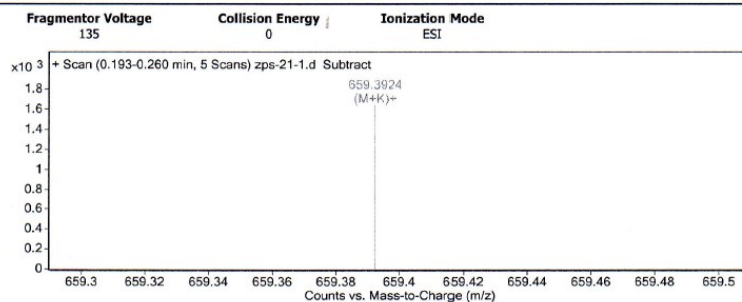
Figure 42. HREIMS spectrum of Patriscabioin F (6).

Qualitative Analysis Report

Data Filename	zps-21-1.d	Sample Name	zps-21
Sample Type	Sample	Position	P1-C6
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	4/19/2016 3:54:34 PM
IRM Calibration Status	Success	DA Method	ESI+.m
Comment			

Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125.2)	

User Spectra



Peak List

m/z	z	Abund
274.2746	1	216462.16
275.2775	1	38565.11
318.3009	1	265295.72
319.304	1	49325.3
362.3269	1	86683.3
363.3301	1	18486.81
453.1676	1	20150.49
473.265	1	17250.22

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C36 H60 O8	620.4288	659.3920	659.3924	-0.3	-0.5	7.0000

--- End Of Report ---

[illegible]

Chemical structure of compound **7** is shown. The structure is a bicyclic system with a hydroxyl group, a methoxy group, and a butoxy group.

¹³C NMR spectrum (CDCl₃) of compound **7** is shown. The spectrum displays peaks from 165 to 13 ppm, with major signals at 165.15, 159.91, 138.87, 115.24, 114.55, 91.35, 77.29, 77.04, 76.78, 74.18, 70.04, 69.21, 61.92, 46.42, 40.43, 40.08, 32.91, 31.77, 27.65, 20.54, 19.44, and 13.97 ppm.

Figure 45. HSQC spectrum of Patriscabioin G (7) in CDCl₃.

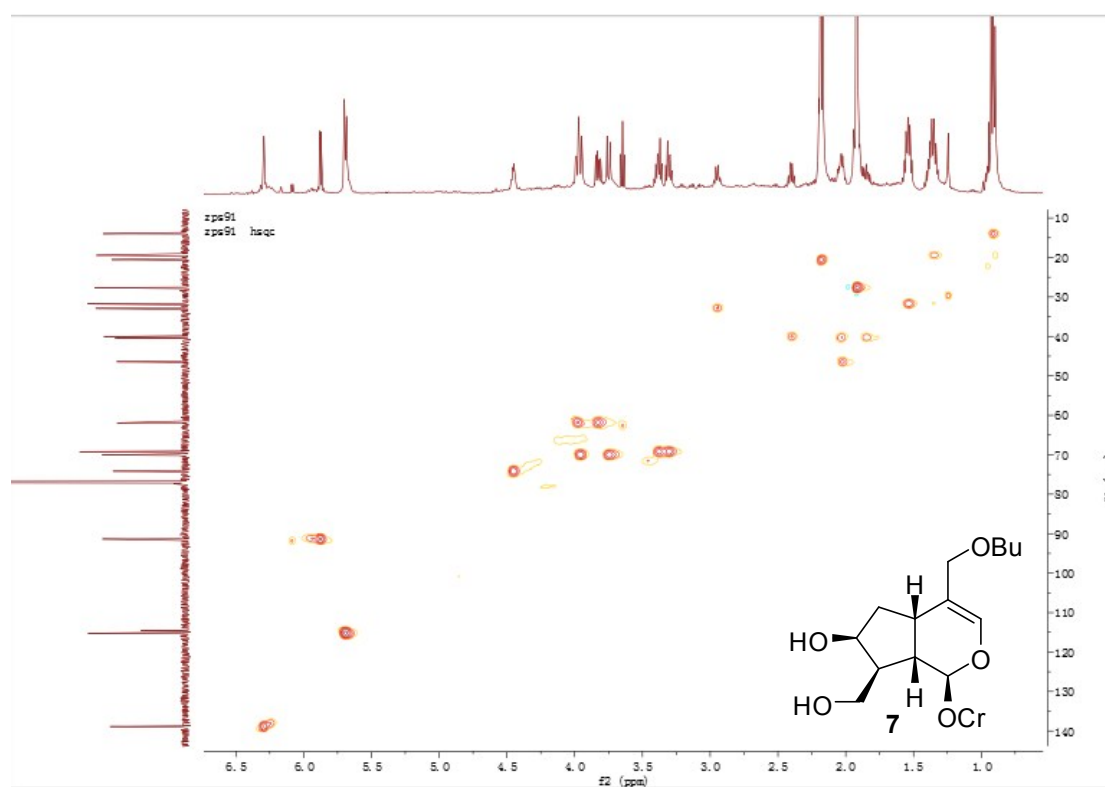


Figure 46. HMBC spectrum of Patriscabioin G (7) in CDCl₃.

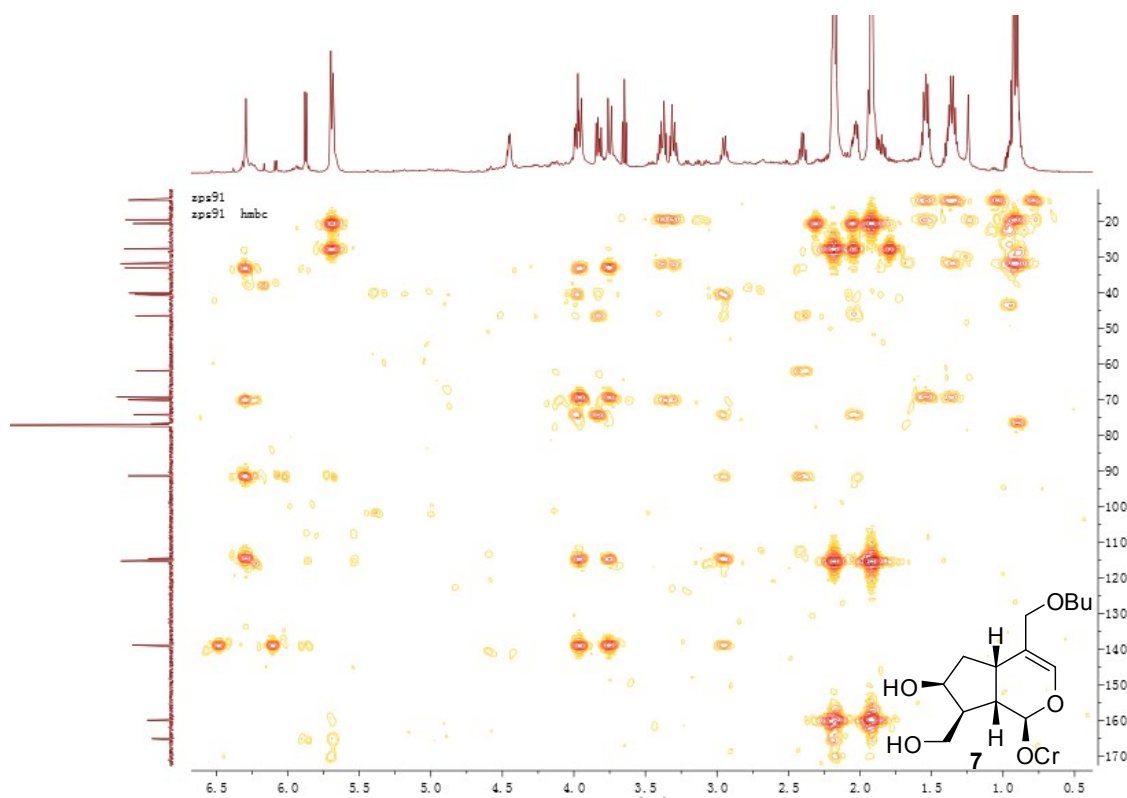


Figure 47. ^1H - ^1H COSY spectrum of Patriscabioin G (7) in CDCl_3 .

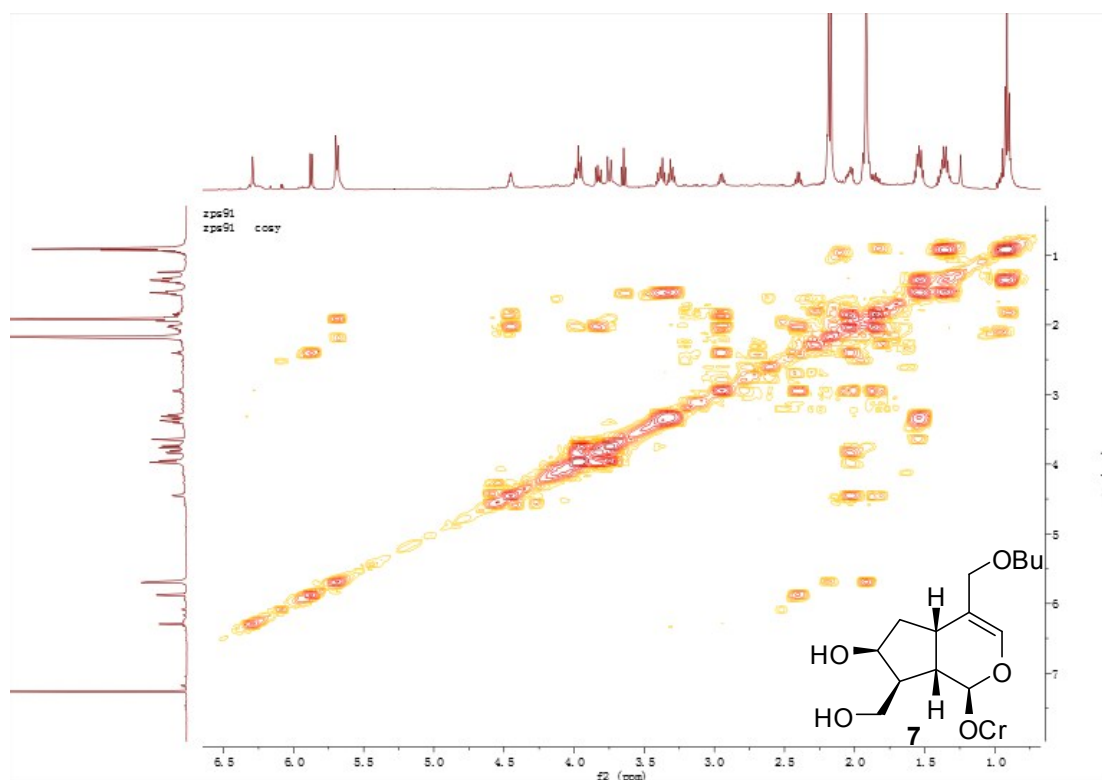


Figure 48. ROESY spectrum of Patriscabioin G (7) in CDCl_3 .

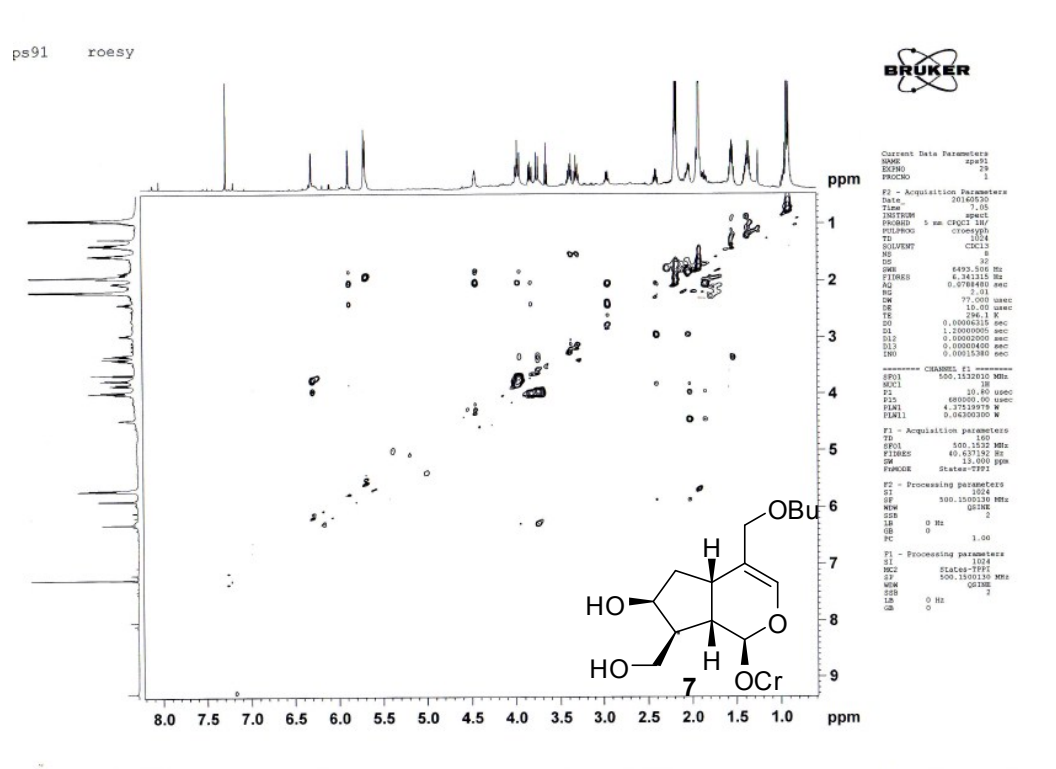


Figure 49. HREIMS spectrum of Patriscabioin G (7).

Formula Predictor Report - ZPS-91.lcd

Page 1 of 1

Data File: E:\DATA\2016\0511\ZPS-91.lcd

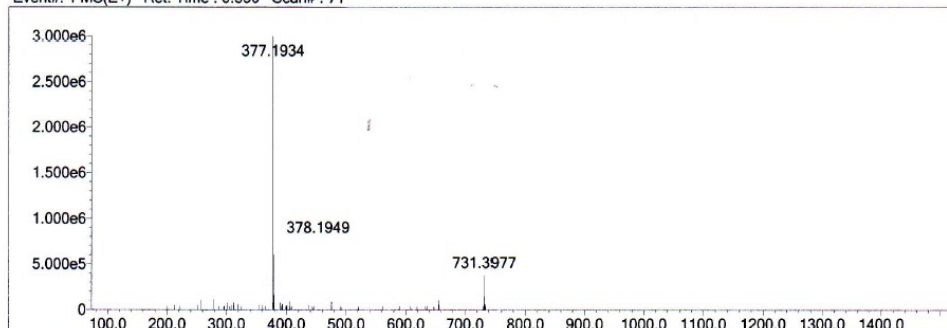
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	100	N	3	0	10	Si	4	0	0	Br	1	0	0	Na
B	3	0	0	O	2	0	40	S	2	0	0	Pt	2	0	0	
C	4	0	80	F	1	0	0	Cl	1	0	0					

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

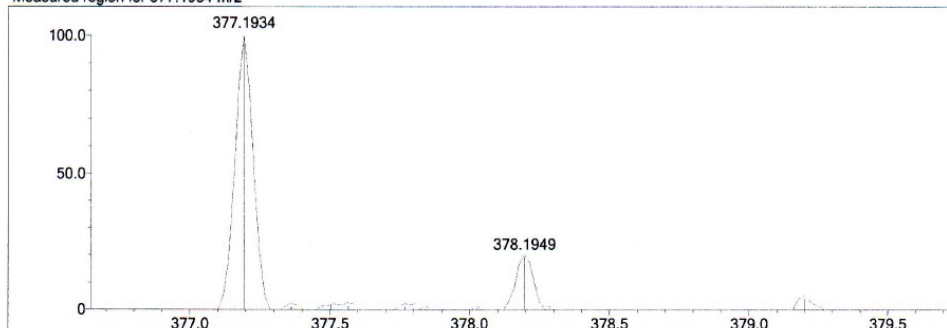
DBE Range: -2.0 - 100.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

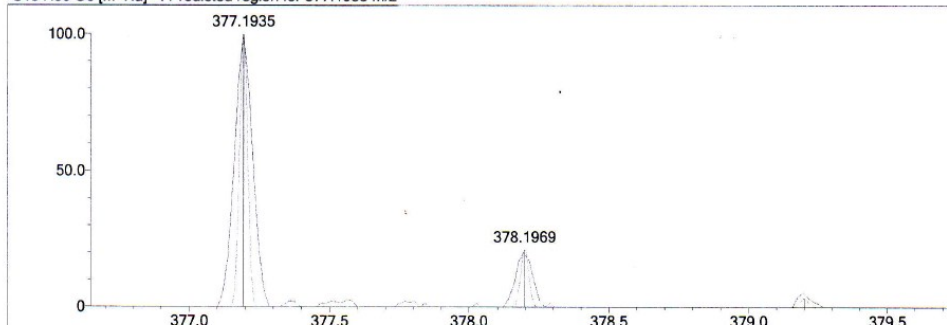
Event#: 1 MS(E+) Ret. Time : 0.350 Scan#: 71



Measured region for 377.1934 m/z



C19 H30 O6 [M+Na]+ : Predicted region for 377.1935 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	88.97	C19 H30 O6	[M+Na]+	377.1934	377.1935	-0.1	-0.27	88.97	5.0

Figure 50. ^1H NMR spectrum of Patriscabioin H (**8**) in CDCl_3 .

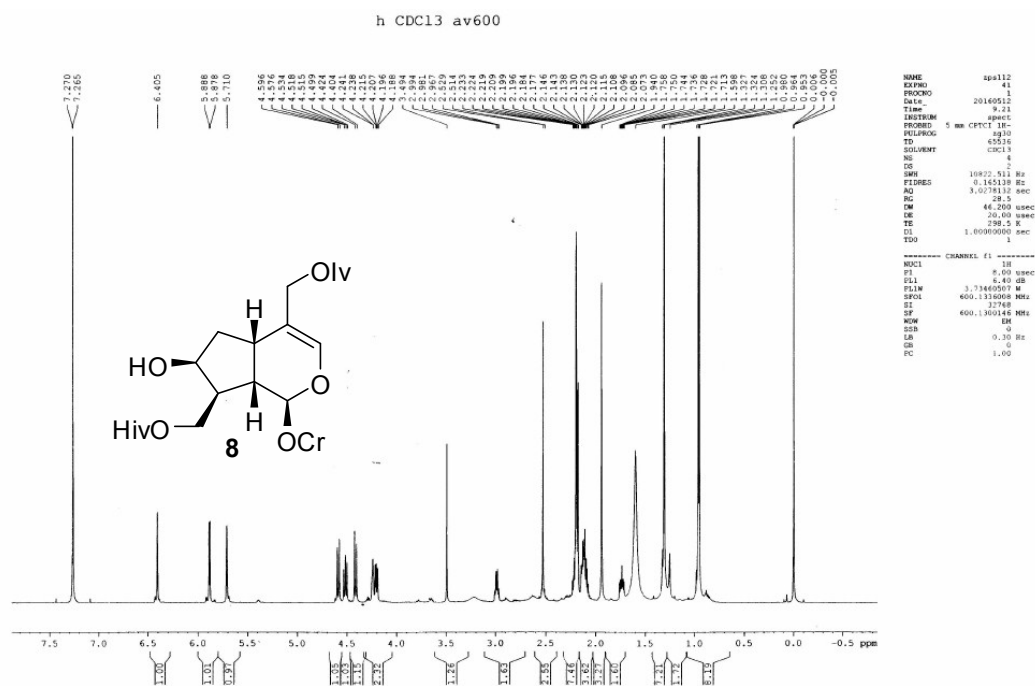


Figure 51. ^{13}C NMR spectrum of Patriscabioin H (**8**) in CDCl_3 .

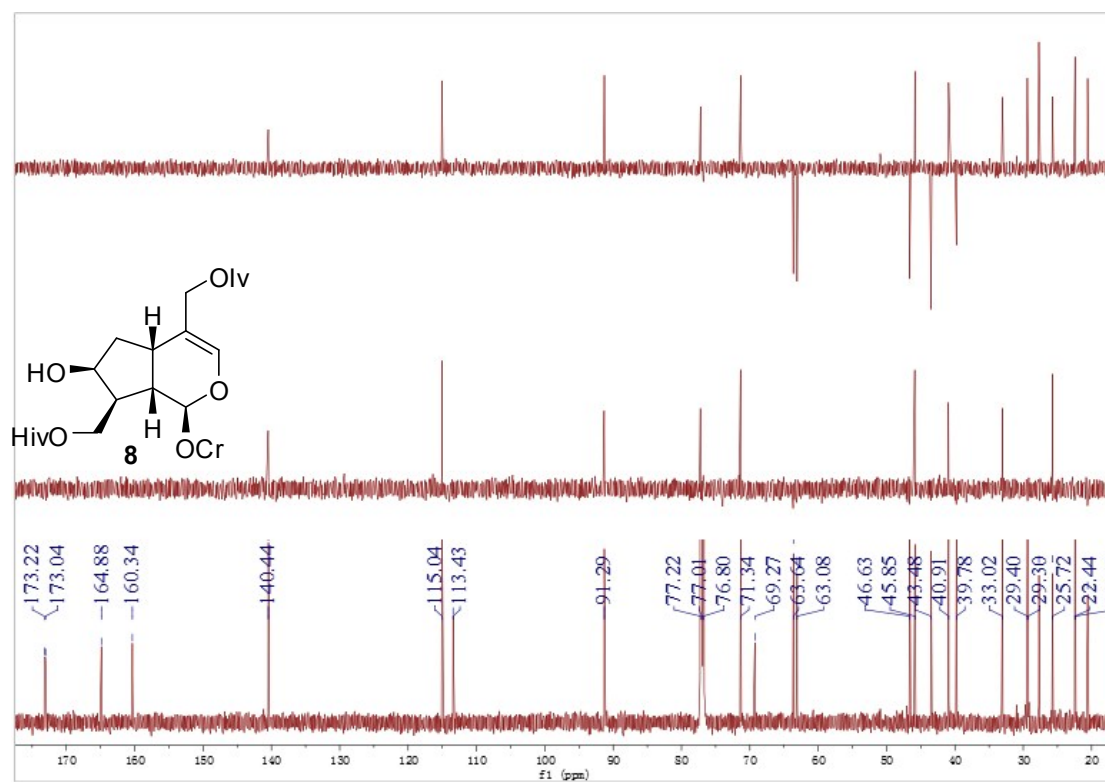


Figure 52. HSQC spectrum of Patriscabioin H (**8**) in CDCl₃.

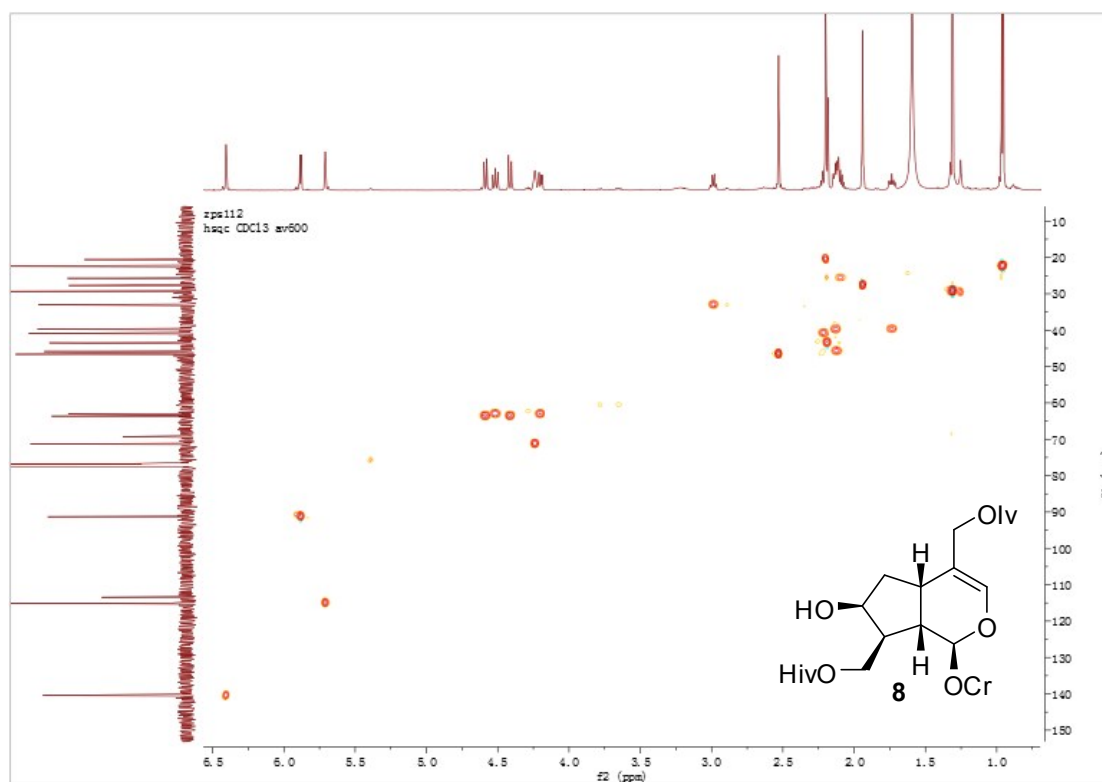


Figure 53. HMBC spectrum of Patriscabioin H (**8**) in CDCl₃.

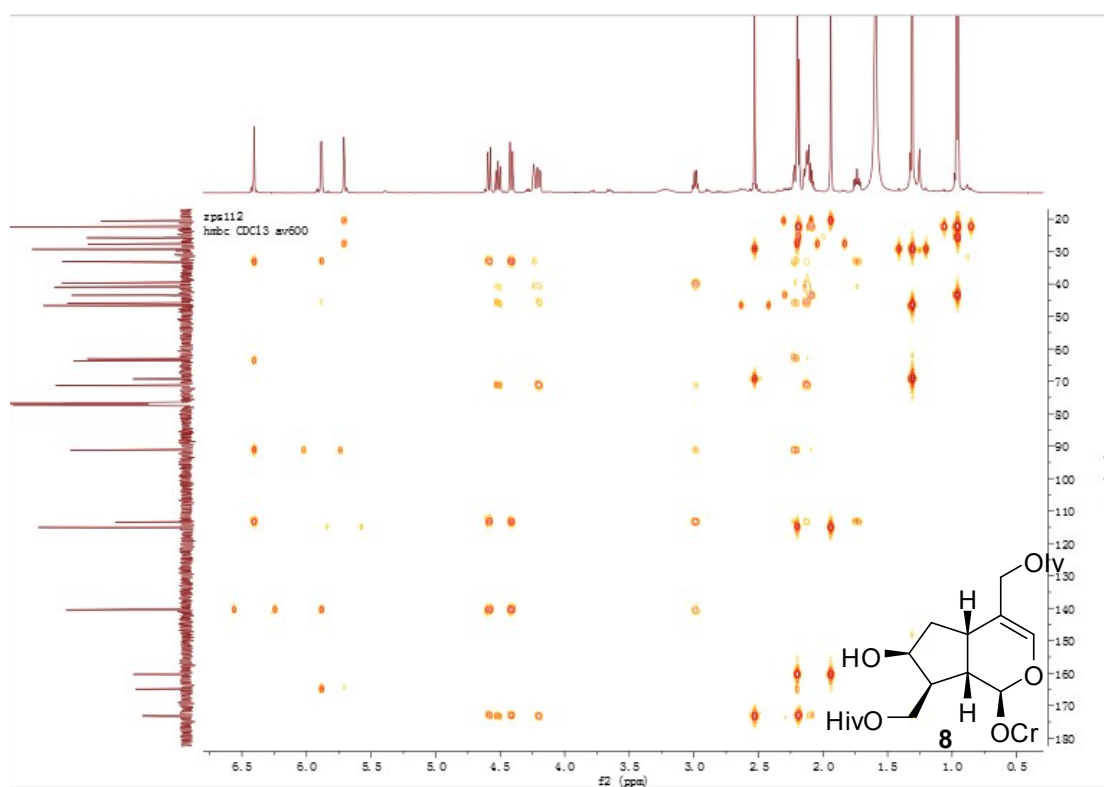


Figure 54. ^1H - ^1H COSY spectrum of Patriscabioin H (**8**) in CDCl_3 .

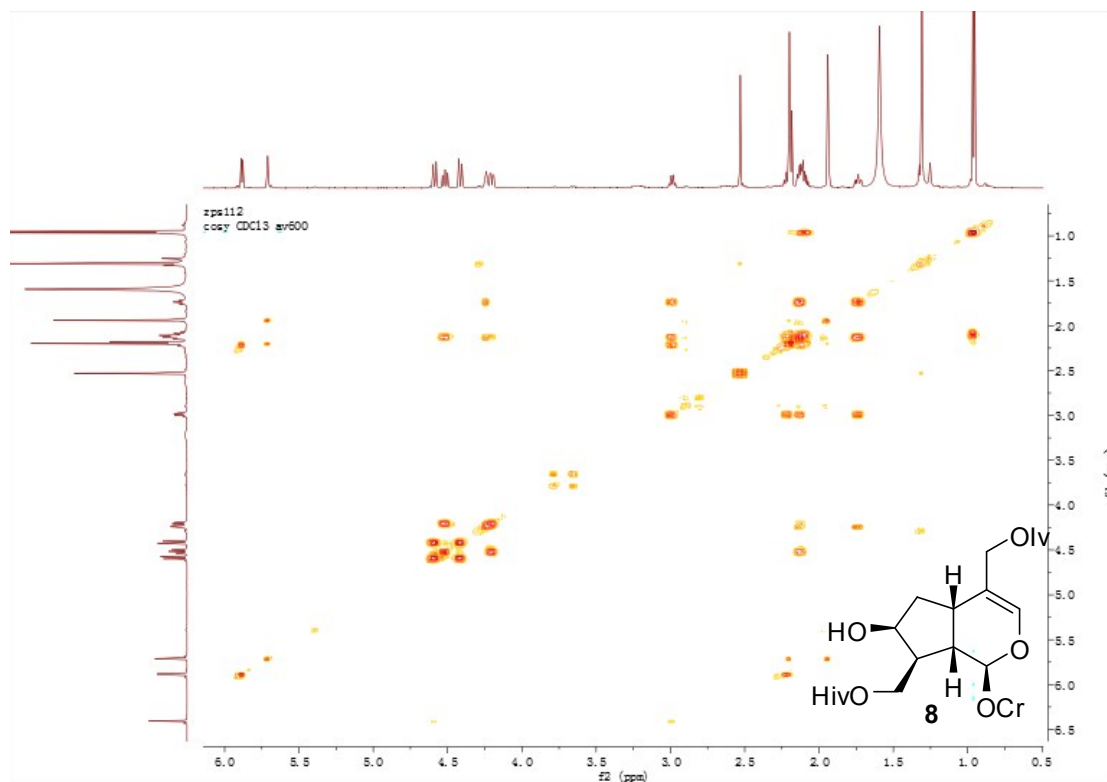


Figure 55. ROESY spectrum of Patriscabioin H (**8**) in CDCl_3 .

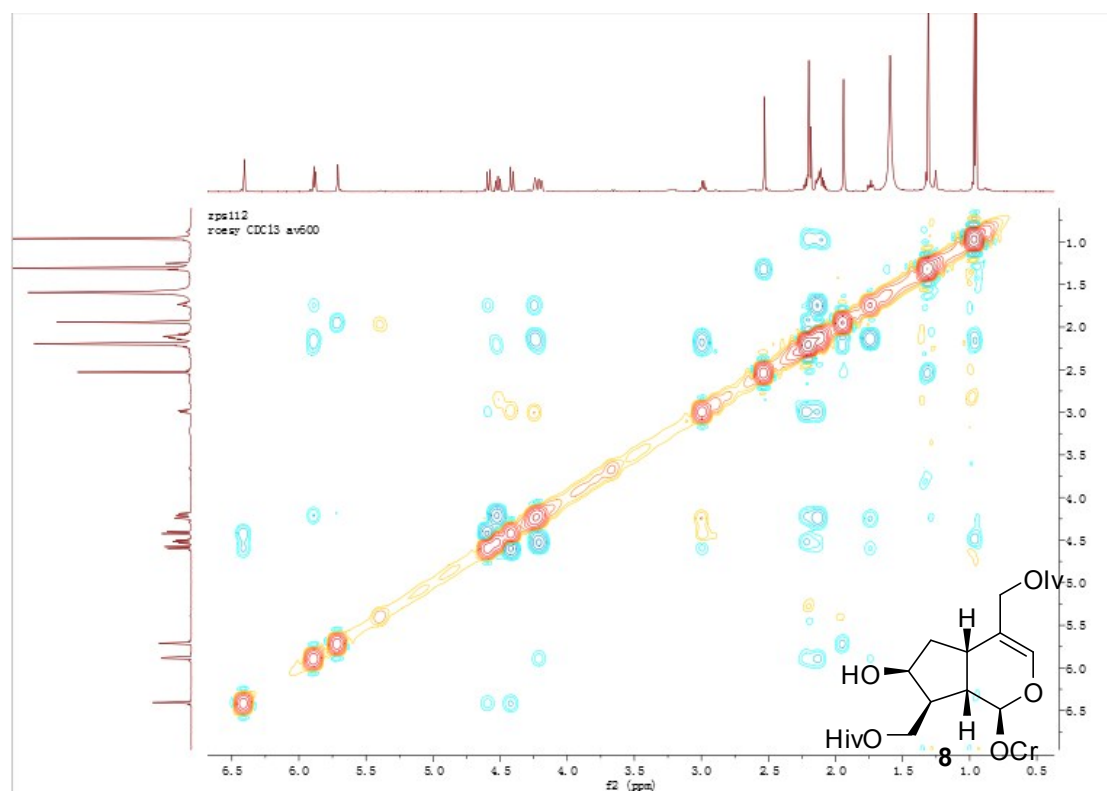


Figure S6. HREIMS spectrum of Patriscabioin H (8).

Formula Predictor Report - zps-112.lcd

Page 1 of 1

Data File: E:\DATA\2016\1020\zps-112.lcd

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

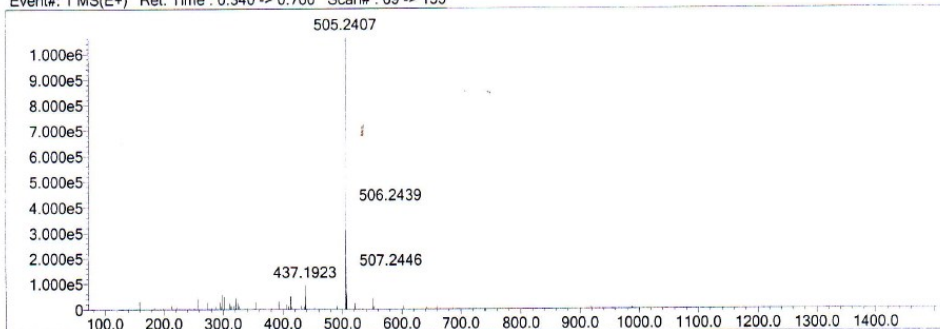
Electron Ions: both

Use MSn Info: yes

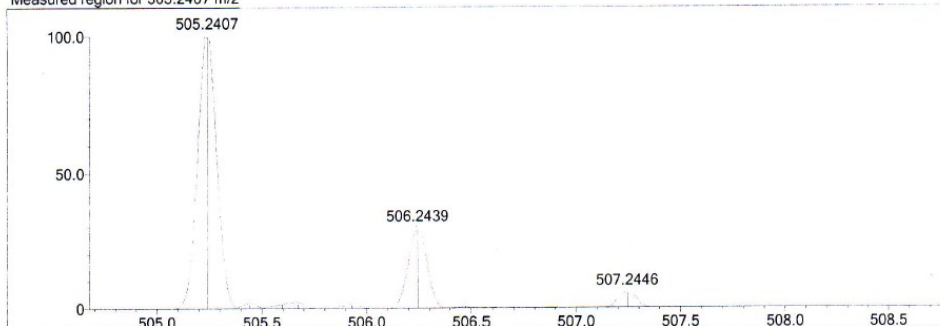
Isotope Res: 10000

Max Results: 10

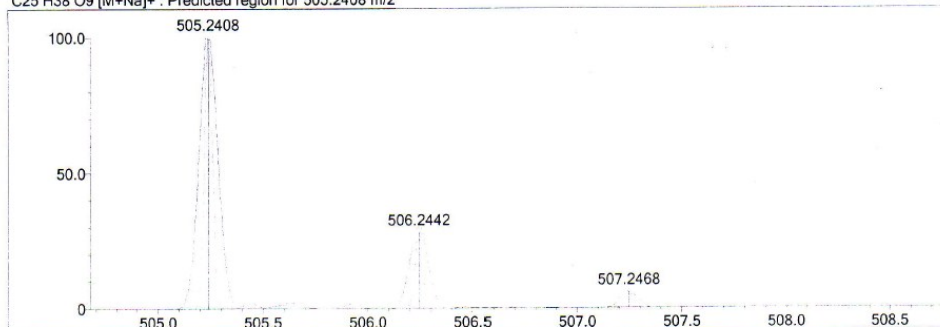
Event#: 1 MS(E+) Ret. Time : 0.340 -> 0.760 Scan#: 69 -> 153



Measured region for 505.2407 m/z



C25 H38 O9 [M+Na]+ : Predicted region for 505.2408 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	94.10	C25 H38 O9	[M+Na]+	505.2407	505.2408	-0.1	-0.20	94.10	7.0

Figure 57. ^1H NMR spectrum of Patriscabioin I (**9**) in CDCl_3 .

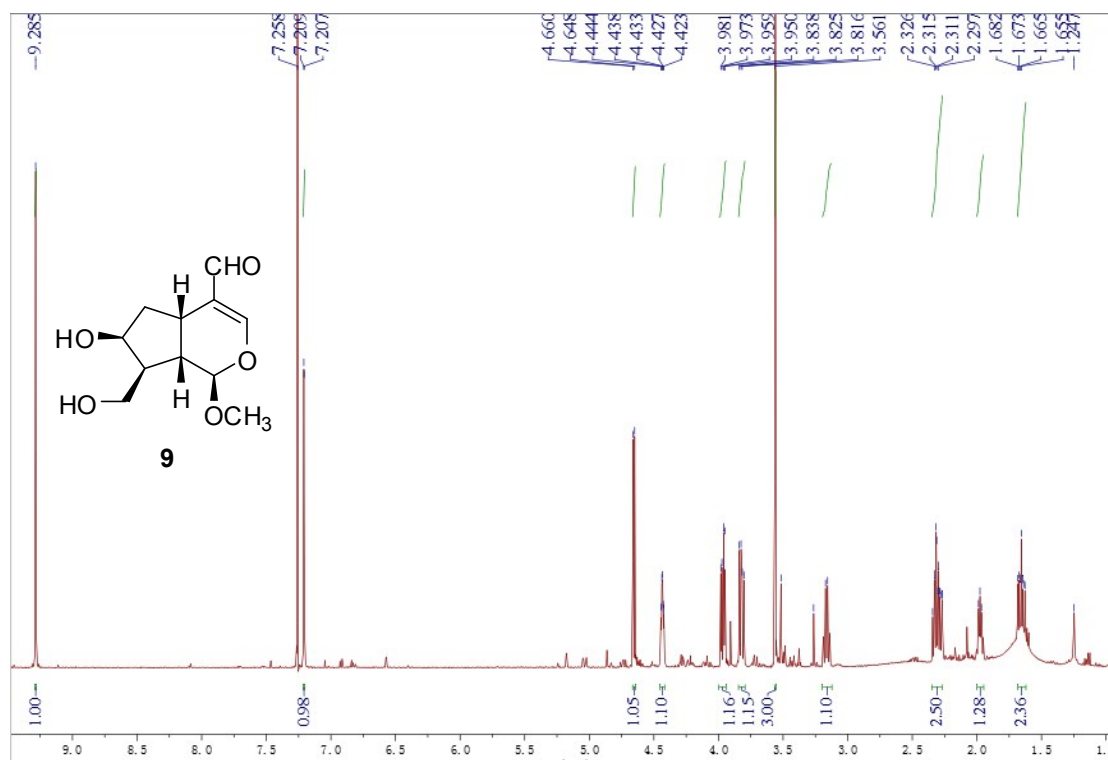


Figure 58. ^{13}C NMR spectrum of Patriscabioin I (**9**) in CDCl_3 .

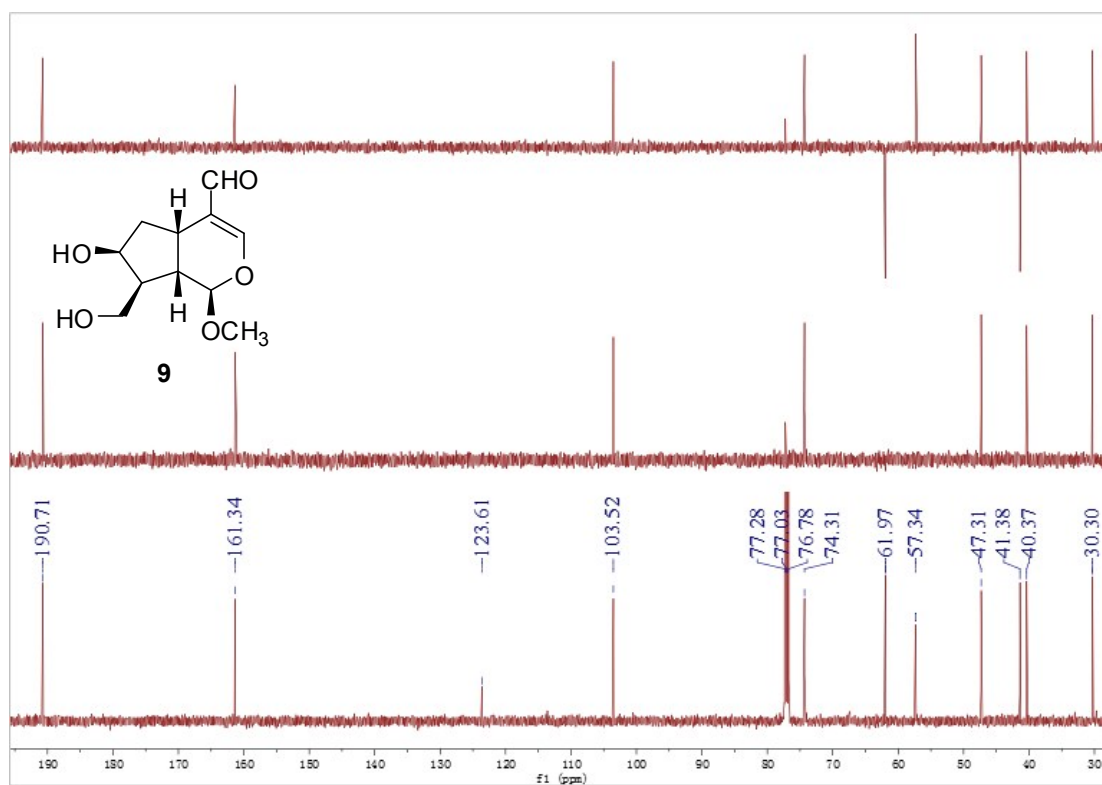


Figure 59. HSQC spectrum of Patriscabioin I (**9**) in CDCl₃.

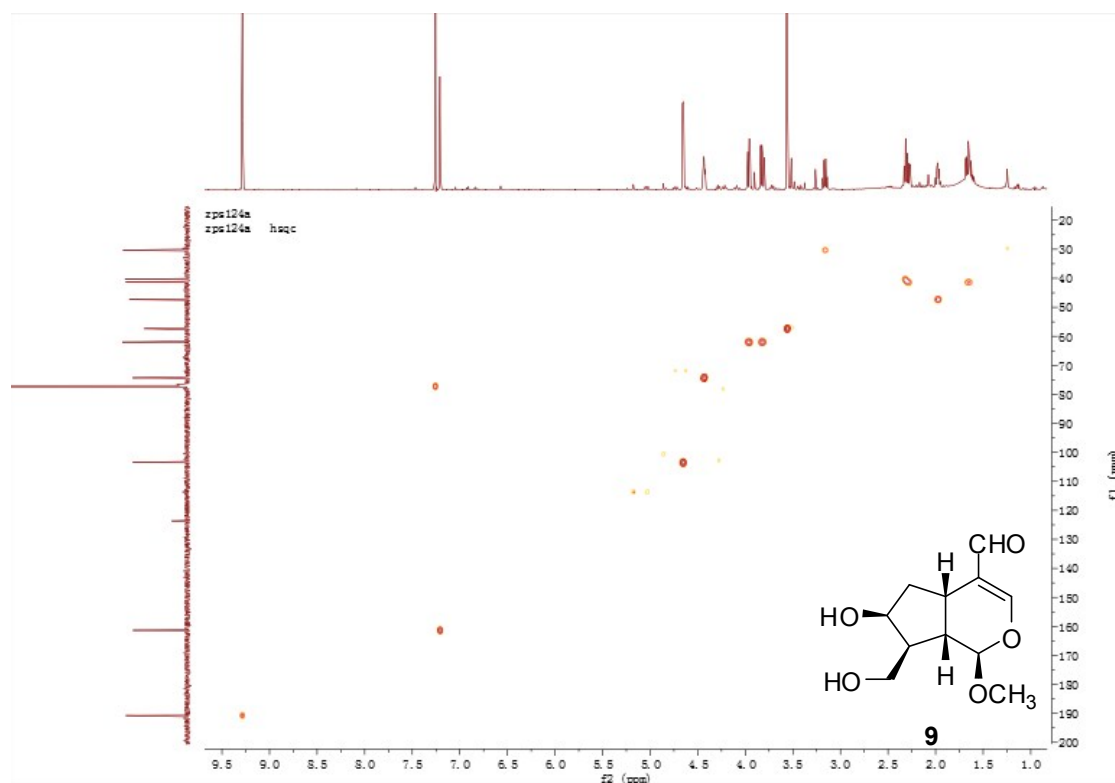


Figure 60. HMBC spectrum of Patriscabioin I (**9**) in CDCl₃.

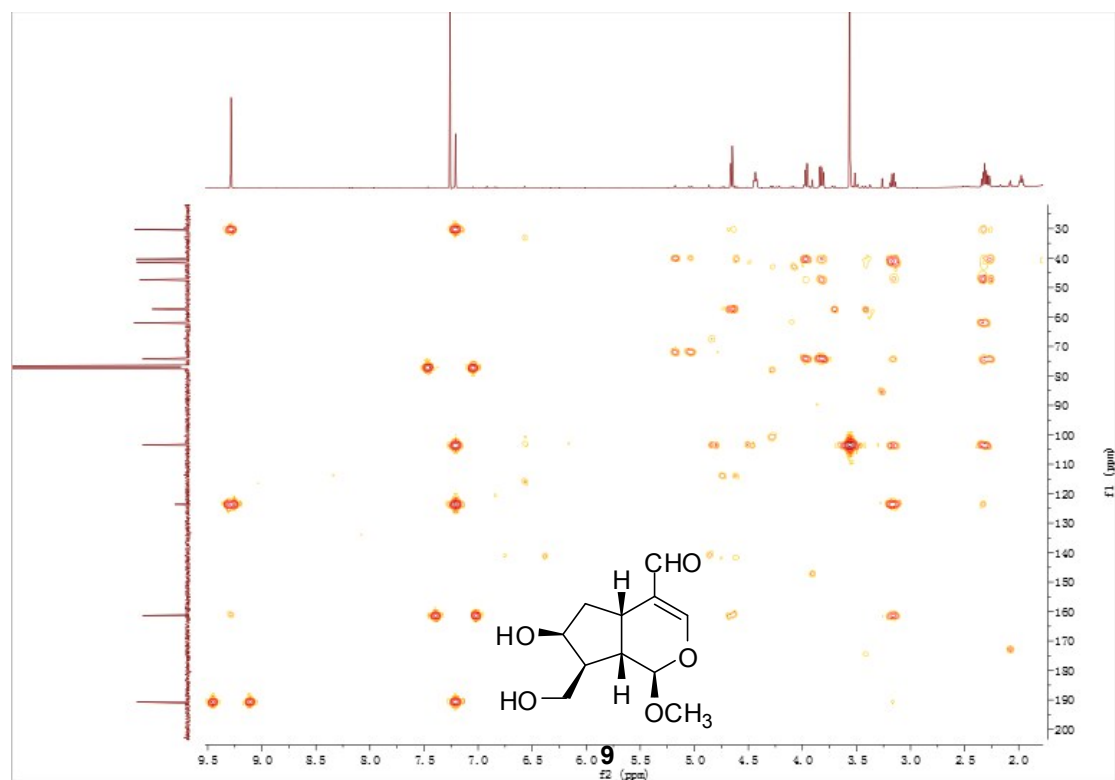


Figure 61. ^1H - ^1H COSY spectrum of Patriscabioin I (**9**) in CDCl_3 .

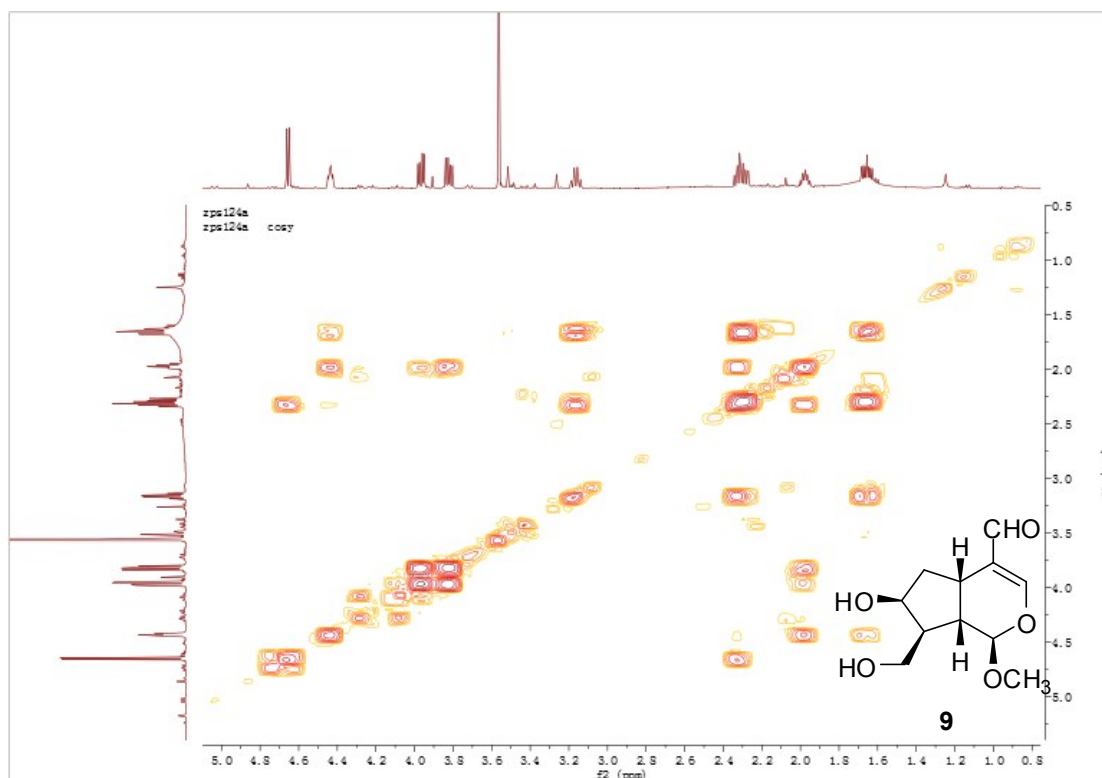


Figure 62. ROESY spectrum of Patriscabioin I (**9**) in CDCl_3 .

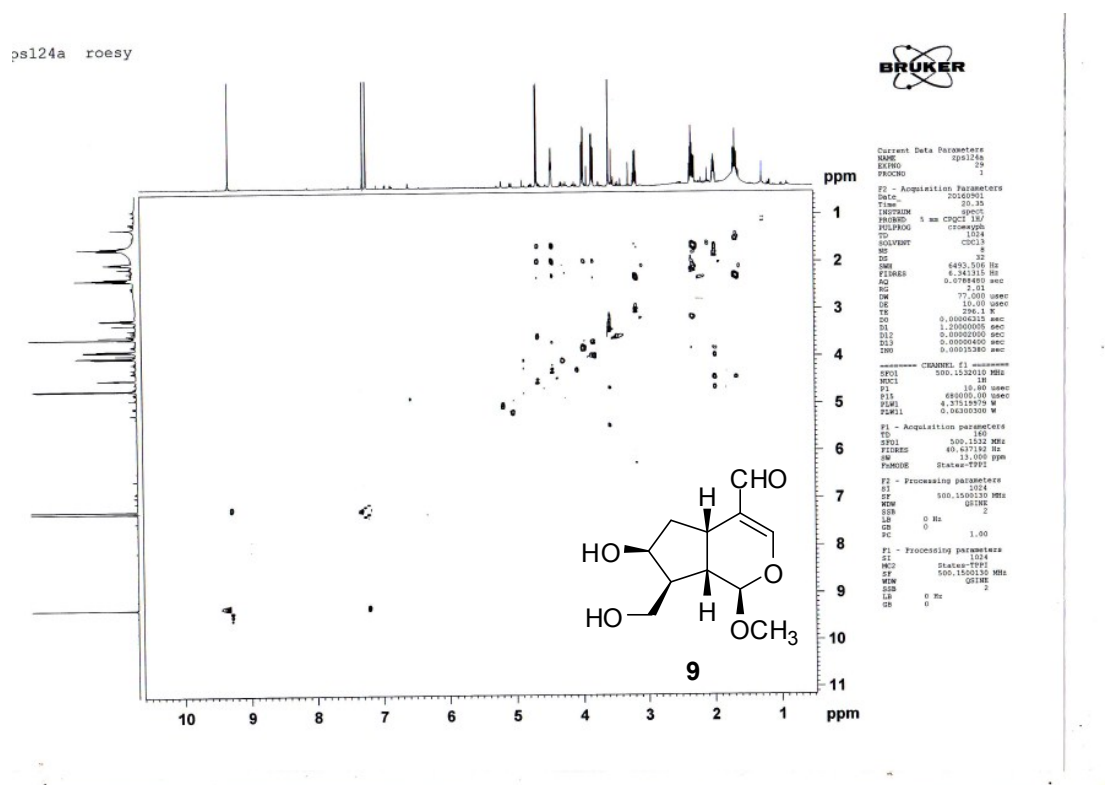


Figure 63. HREIMS spectrum of Patriscabioin I (9).

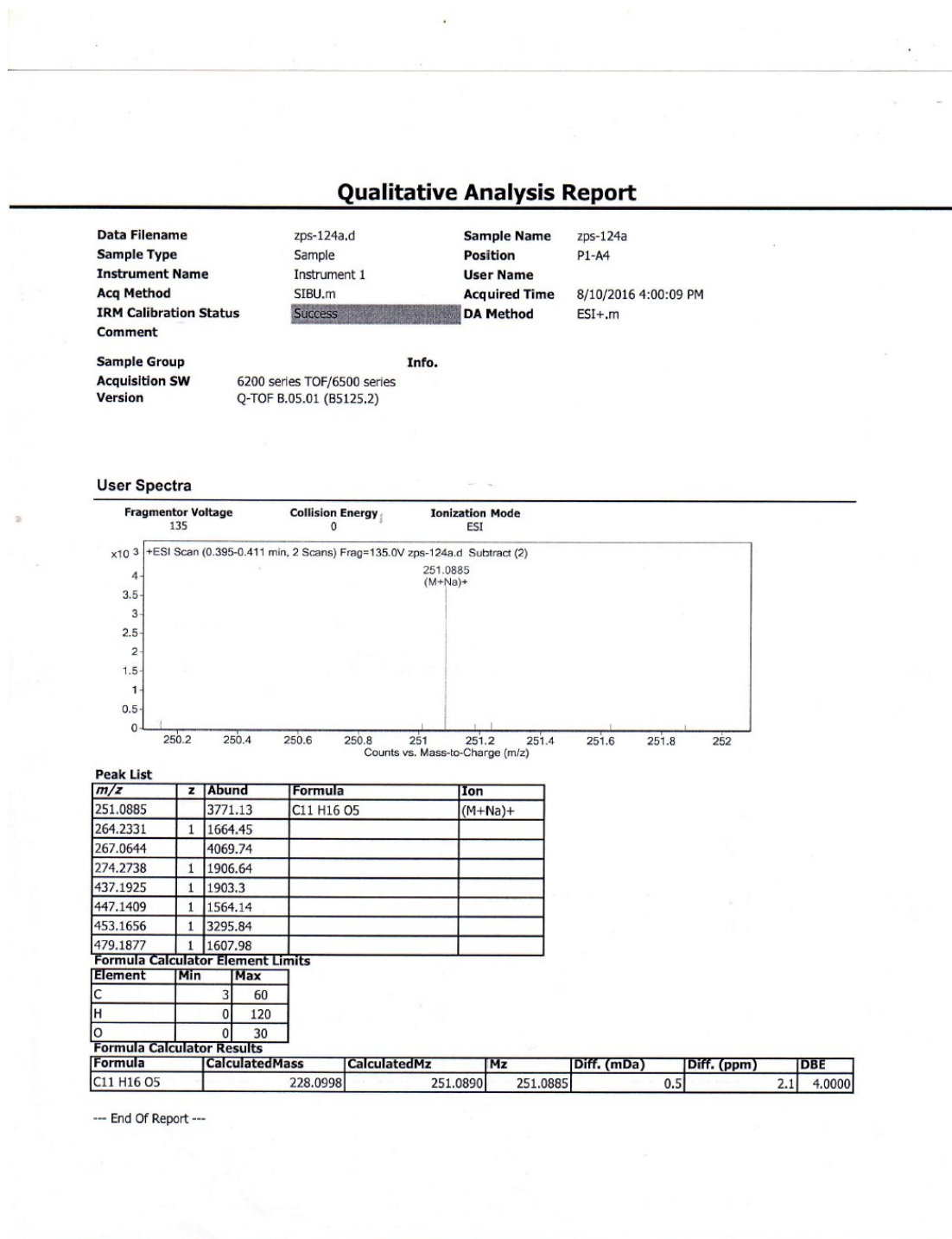


Figure 64. ^1H NMR spectrum of Patriscabioin J (10) in CDCl_3 .

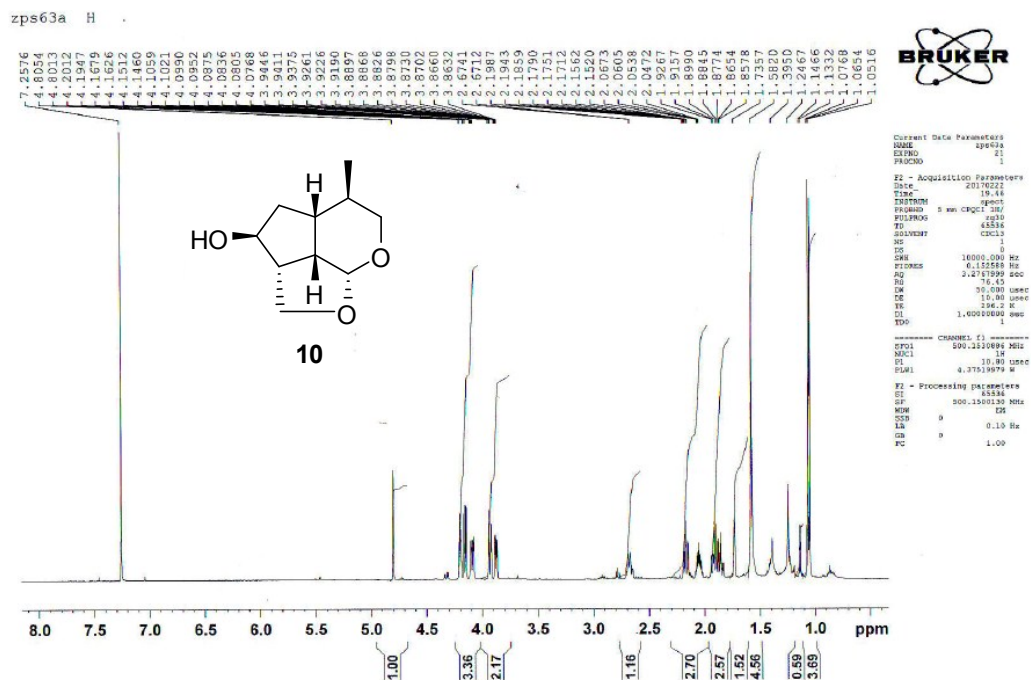


Figure 66. HSQC spectrum of Patriscabioin J (**10**) in CDCl₃.

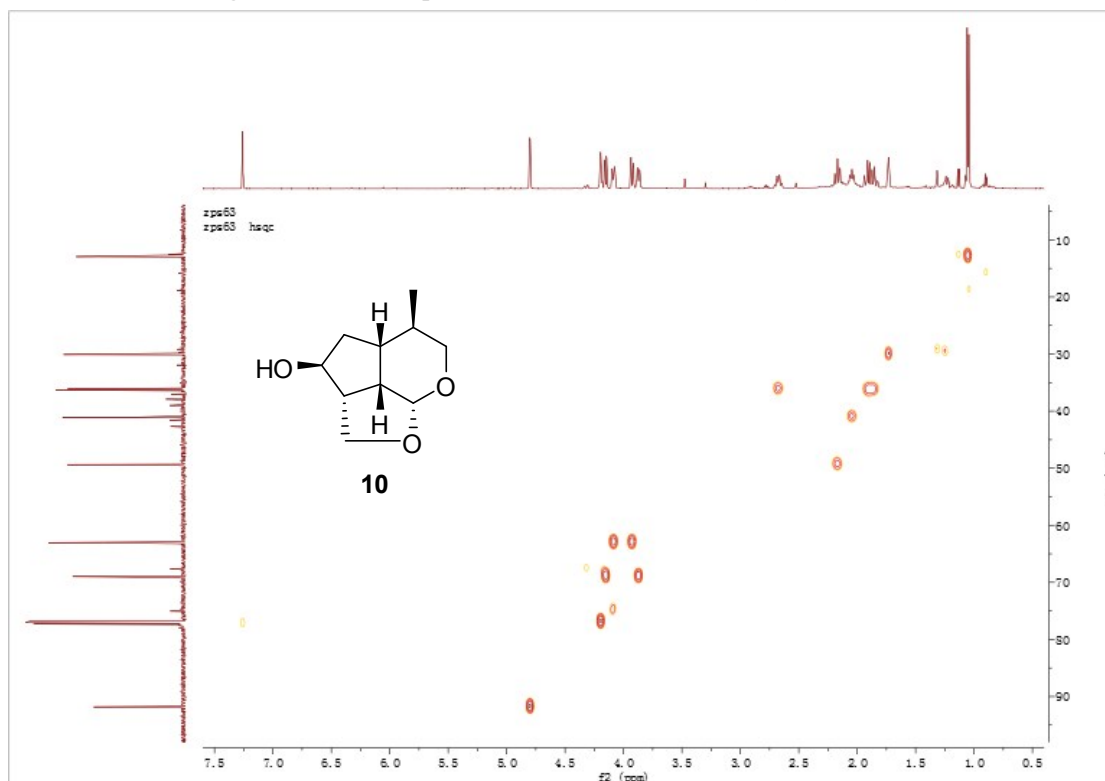


Figure 67. HMBC spectrum of Patriscabioin J (**10**) in CDCl₃.

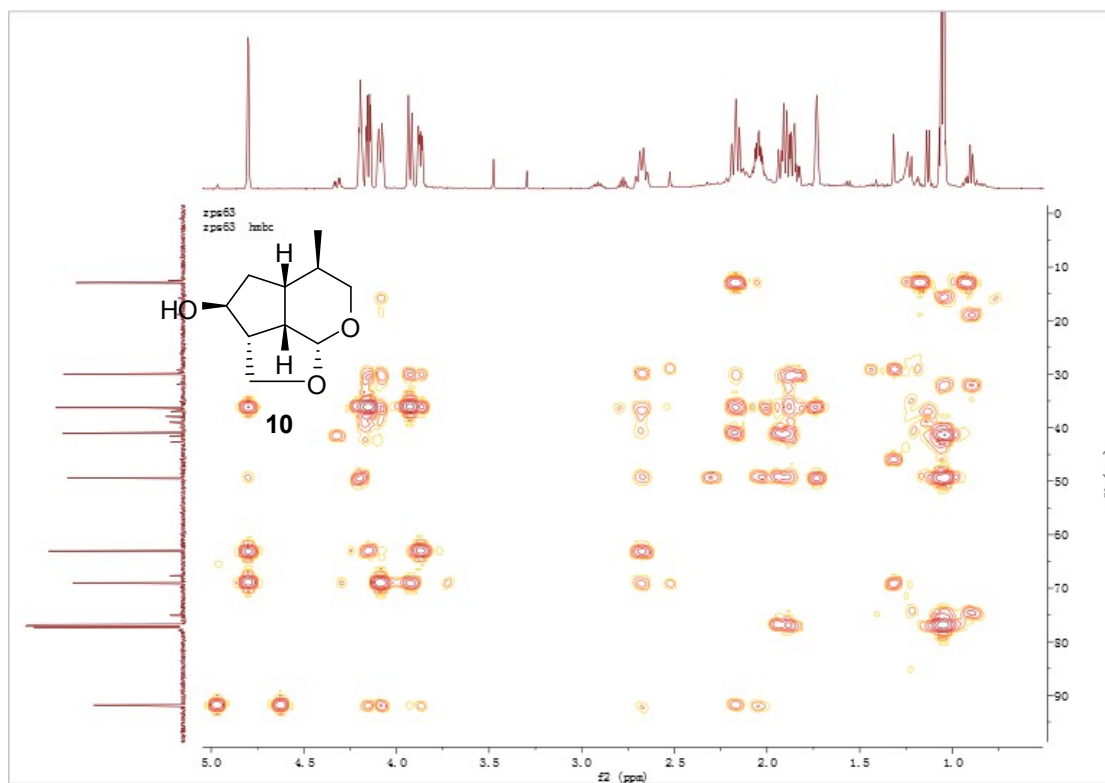


Figure 68. ^1H - ^1H COSY spectrum of Patriscabioin J (**10**) in CDCl_3 .

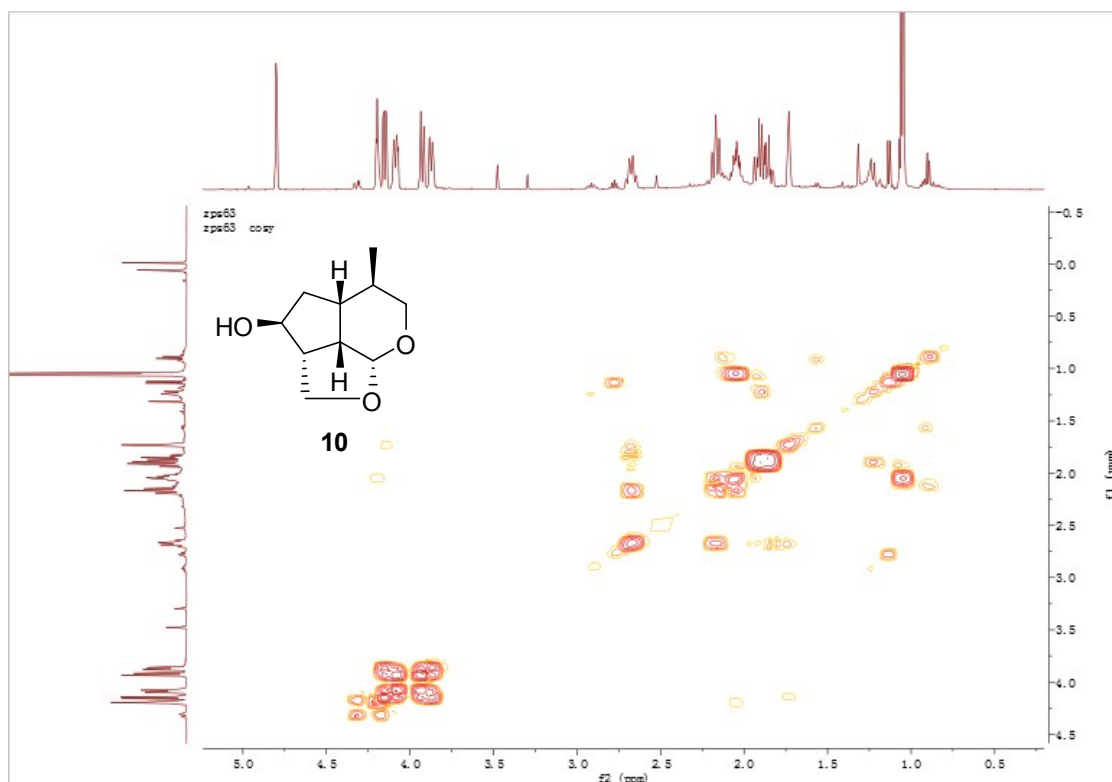


Figure 69. ROESY spectrum of Patriscabioin J (**10**) in CDCl_3 .

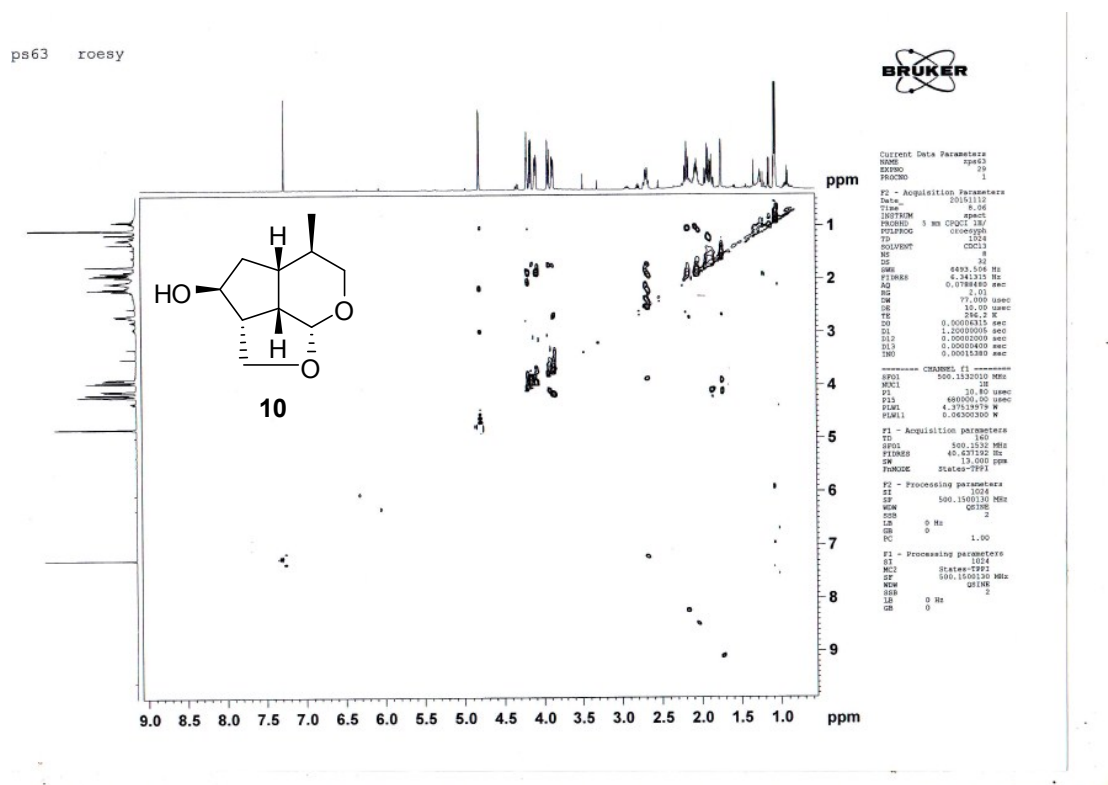


Figure 70. HREIMS spectrum of Patriscabioin J (10).

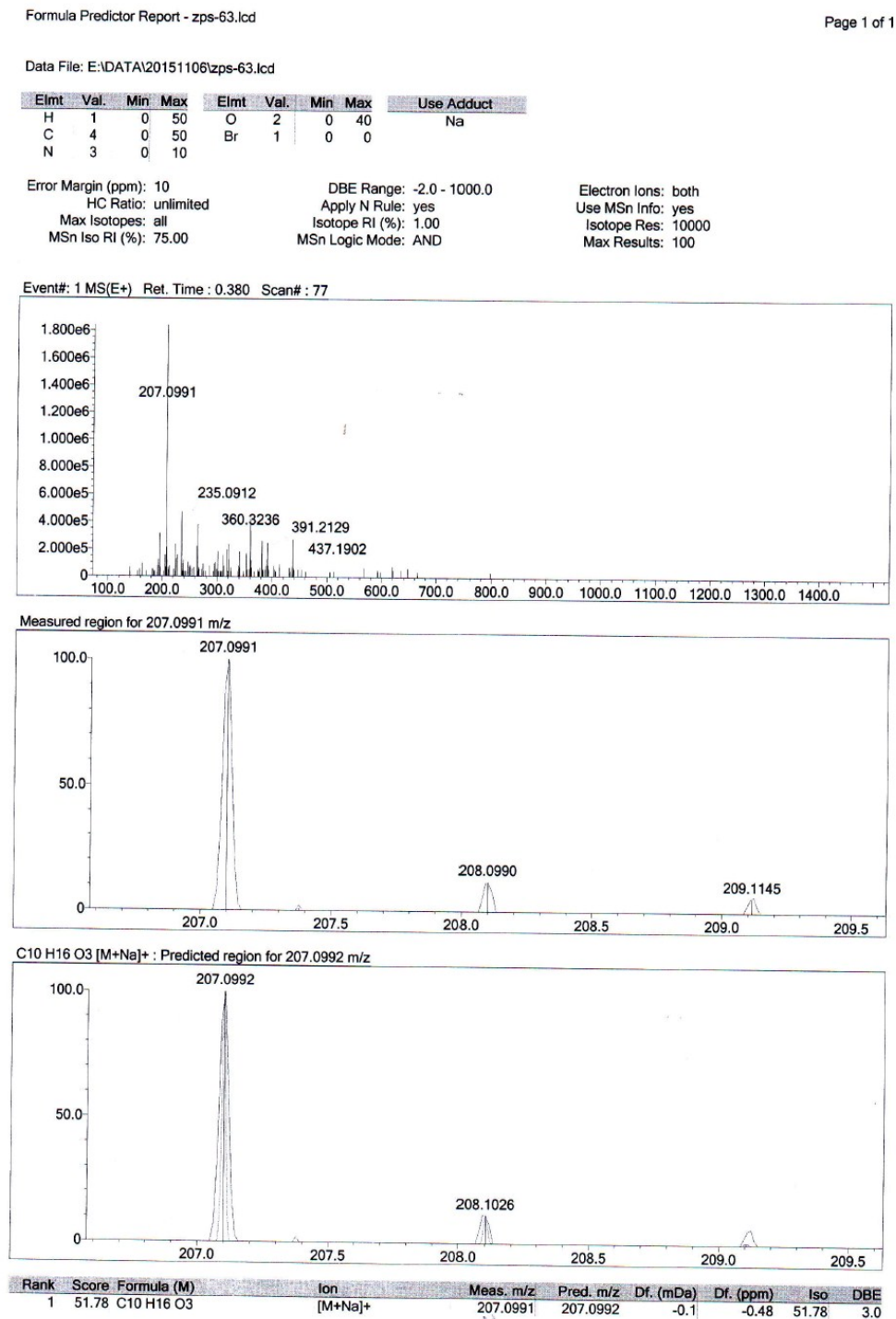


Figure 71. ^1H NMR spectrum of Patriscabiobisin A (**11**) in CDCl_3 .

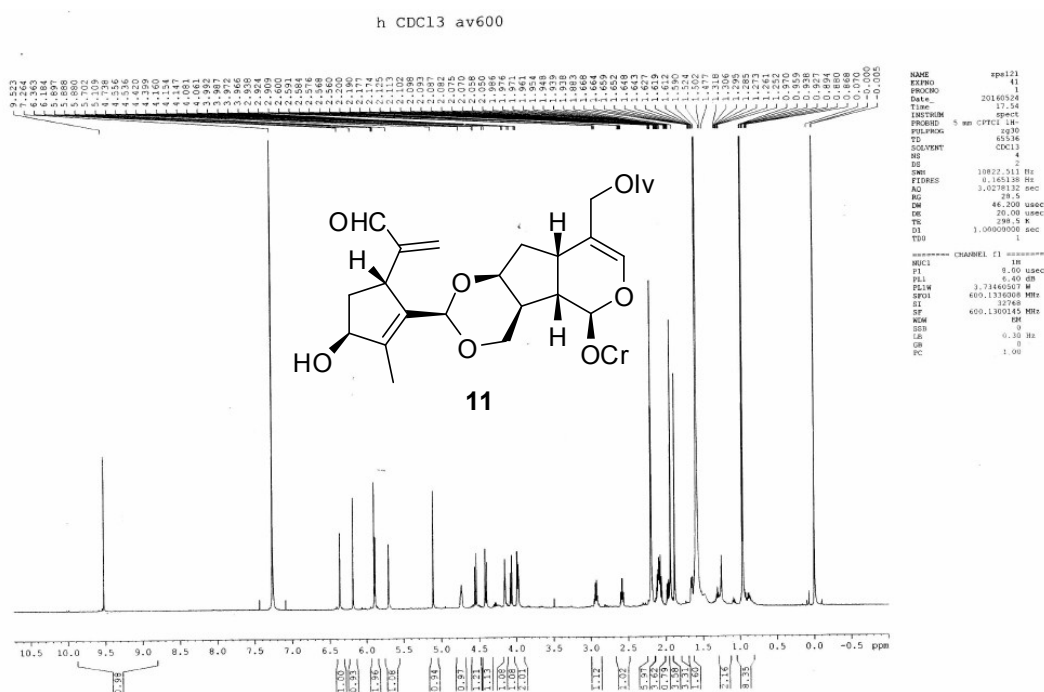


Figure 72. ^{13}C NMR spectrum of Patriscabiobisin A (**11**) in CDCl_3 .

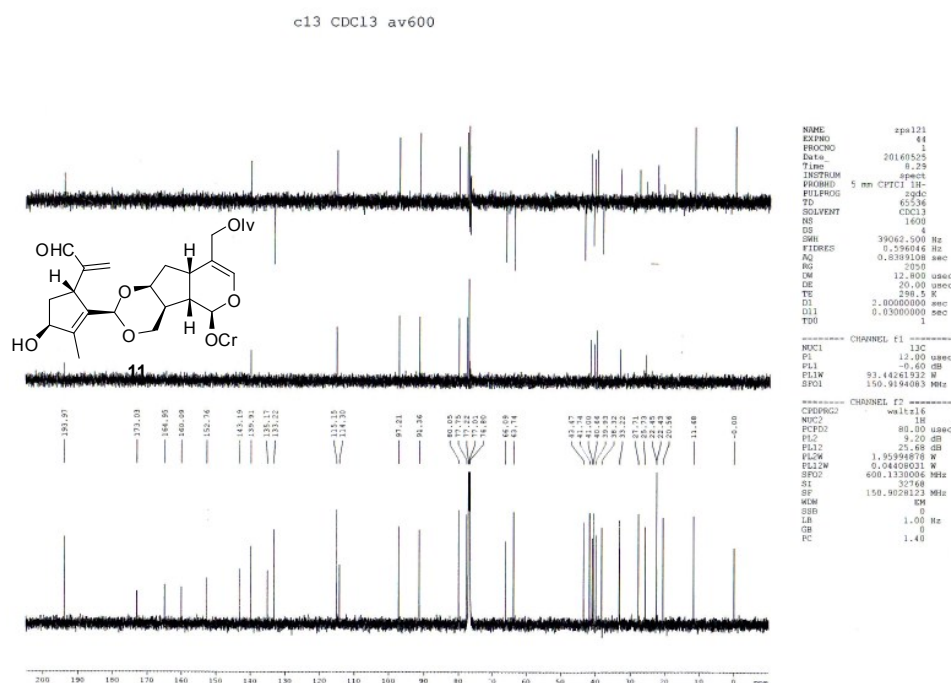


Figure 73. HSQC spectrum of Patriscabiobisin A (**11**) in CDCl₃.

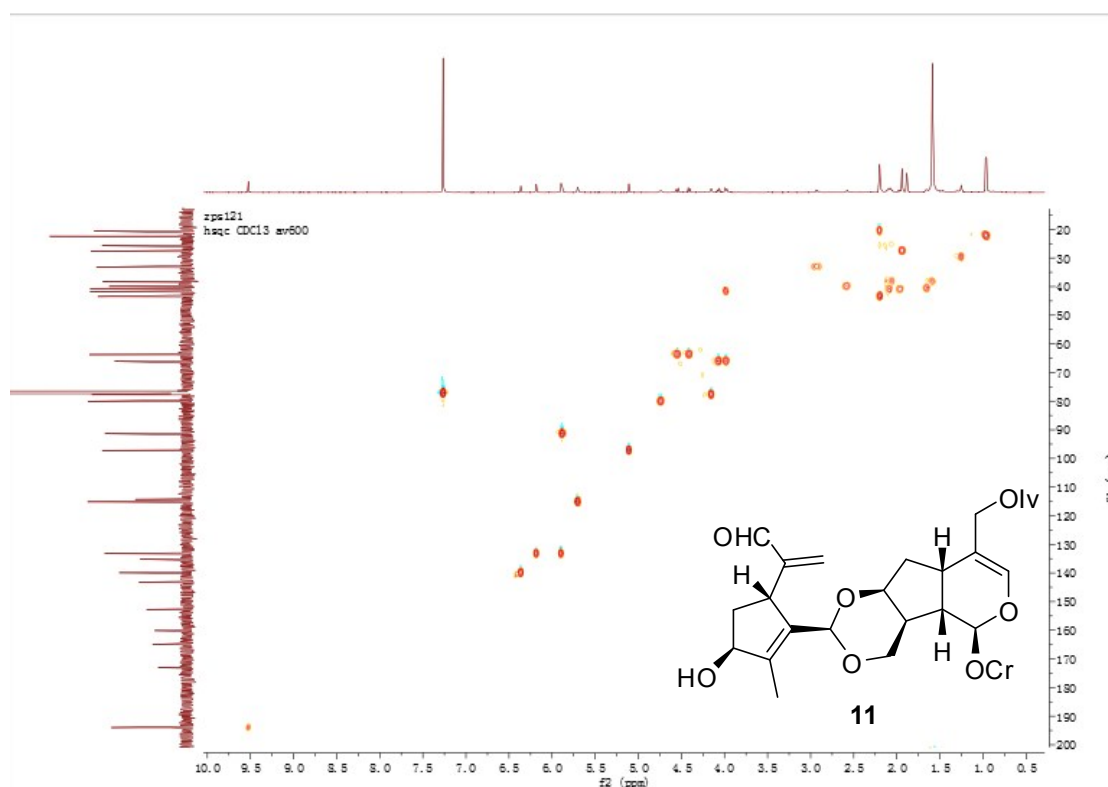


Figure 74. HMBC spectrum of Patriscabiobisin A (**11**) in CDCl₃.

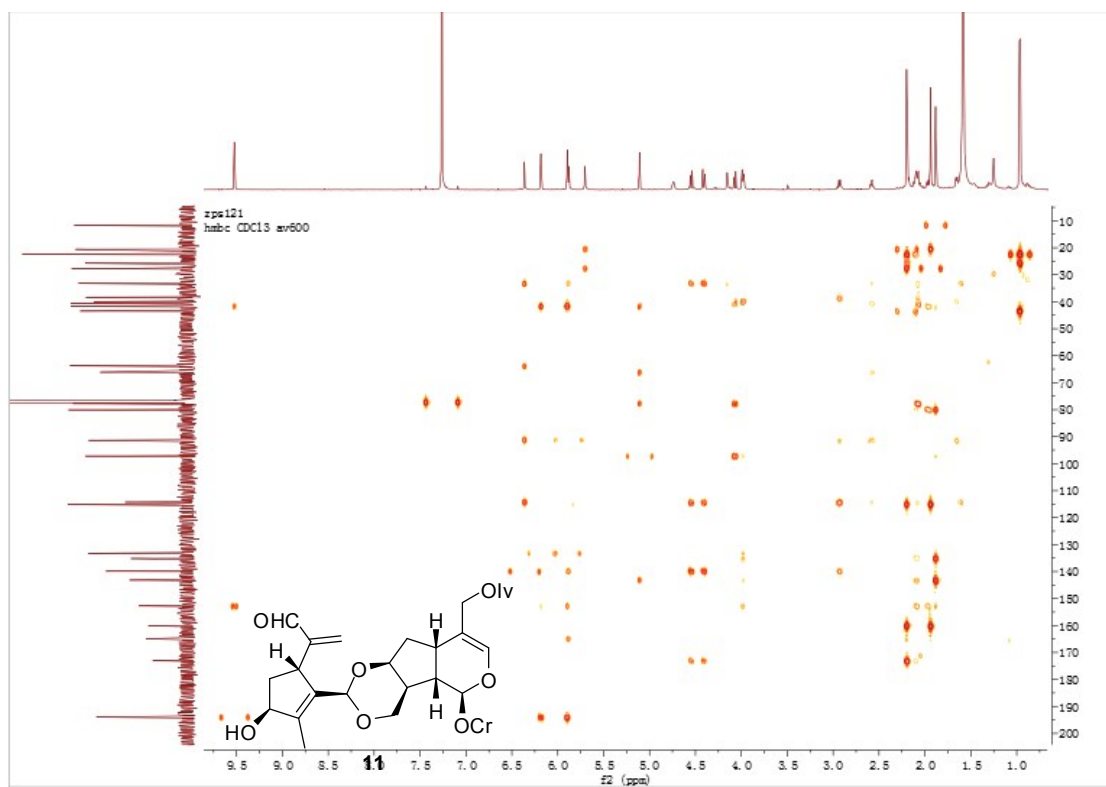


Figure 75. ^1H - ^1H COSY spectrum of Patriscabiobisin A (**11**) in CDCl_3 .

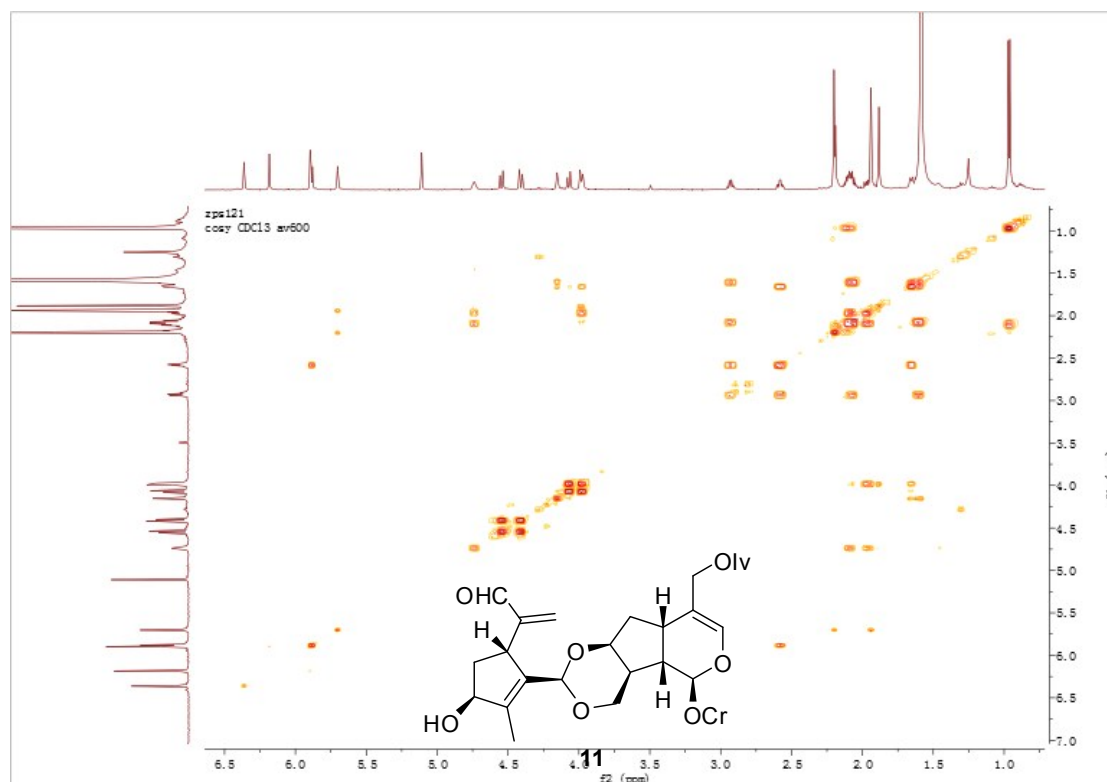


Figure 76. ROESY spectrum of Patriscabiobisin A (**11**) in CDCl_3 .

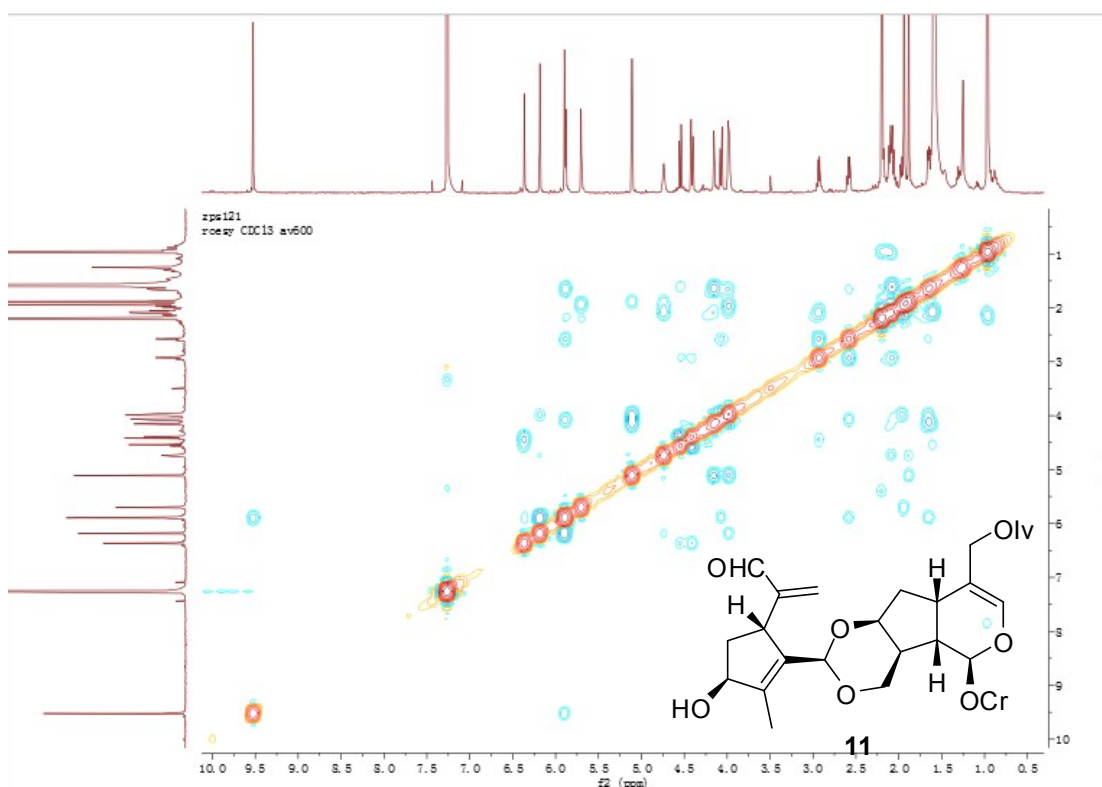


Figure 77. HREIMS spectrum of Patriscabiobisin A (11).

Formula Predictor Report - zps-121.lcd

Page 1 of 1

Data File: E:\DATA\2016\0921\zps-121.lcd

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

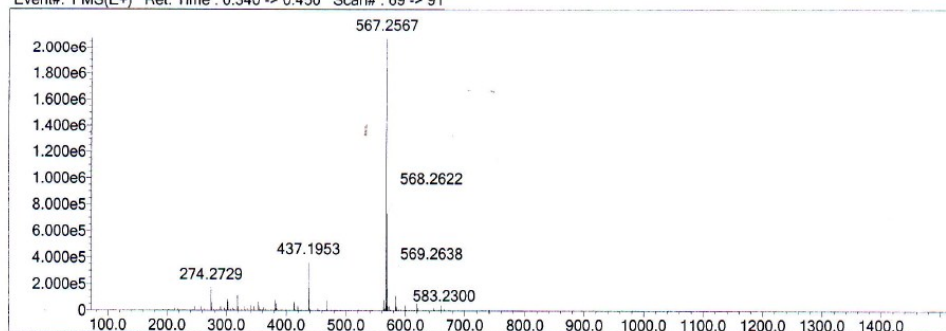
Electron Ions: both

Use MSn Info: yes

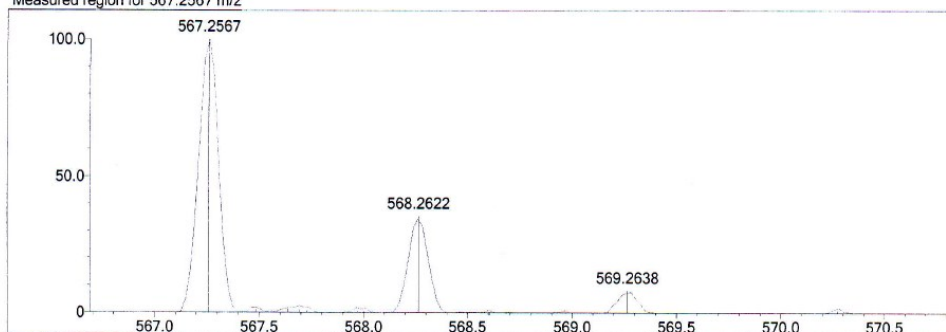
Isotope Res: 10000

Max Results: 10

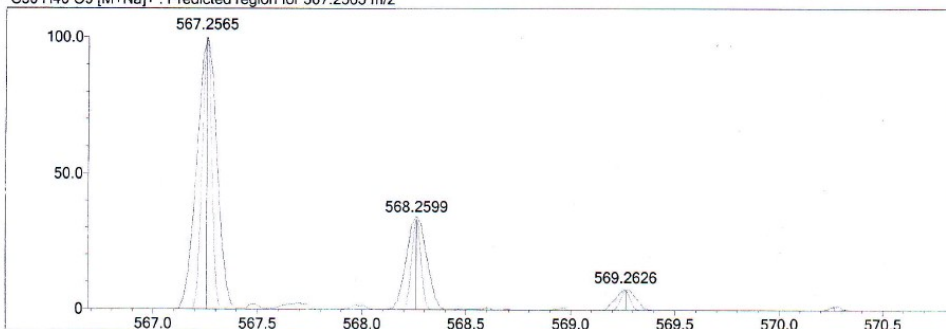
Event#: 1 MS(E+) Ret. Time : 0.340 -> 0.450 Scan#: 69 -> 91



Measured region for 567.2567 m/z



C30 H40 O9 [M+Na]⁺ : Predicted region for 567.2565 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	86.39	C30 H40 O9	[M+Na] ⁺	567.2567	567.2565	0.2	0.35	86.39	11.0

Figure 78. ECD spectrum of Patriscabiobisin A (11).

ZPS-121

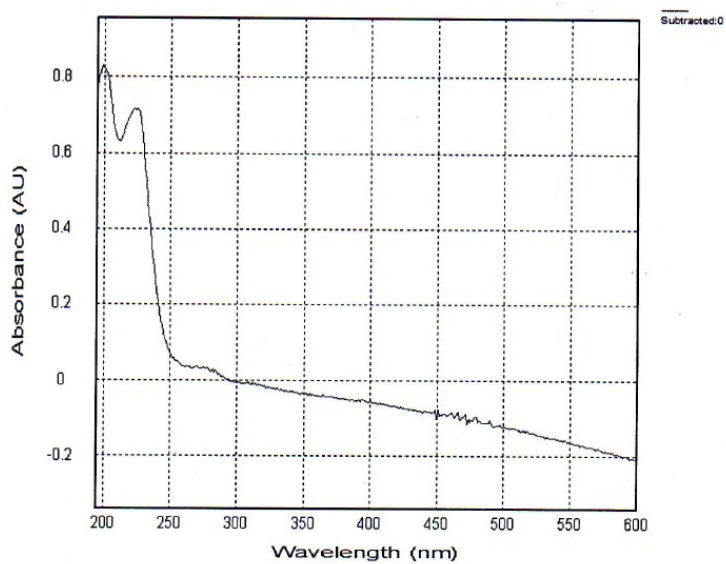
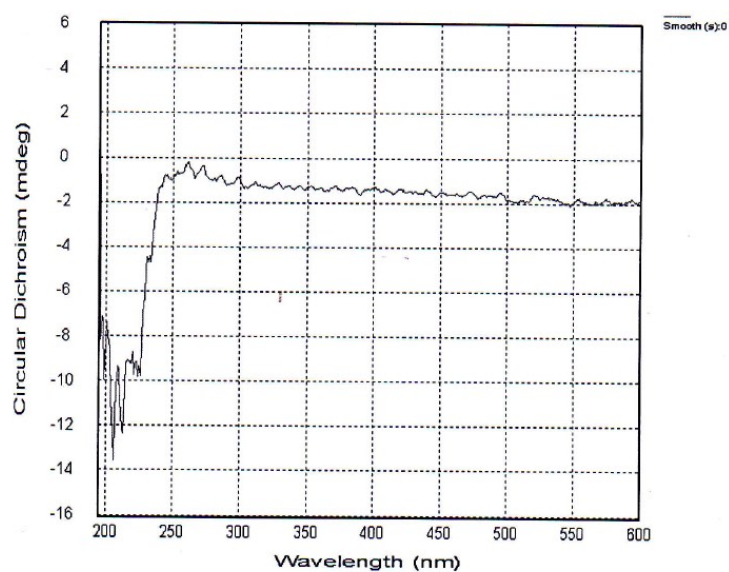


Figure 79. ^1H NMR spectrum of Patriscabiobisin B (**12**) in CDCl_3 .

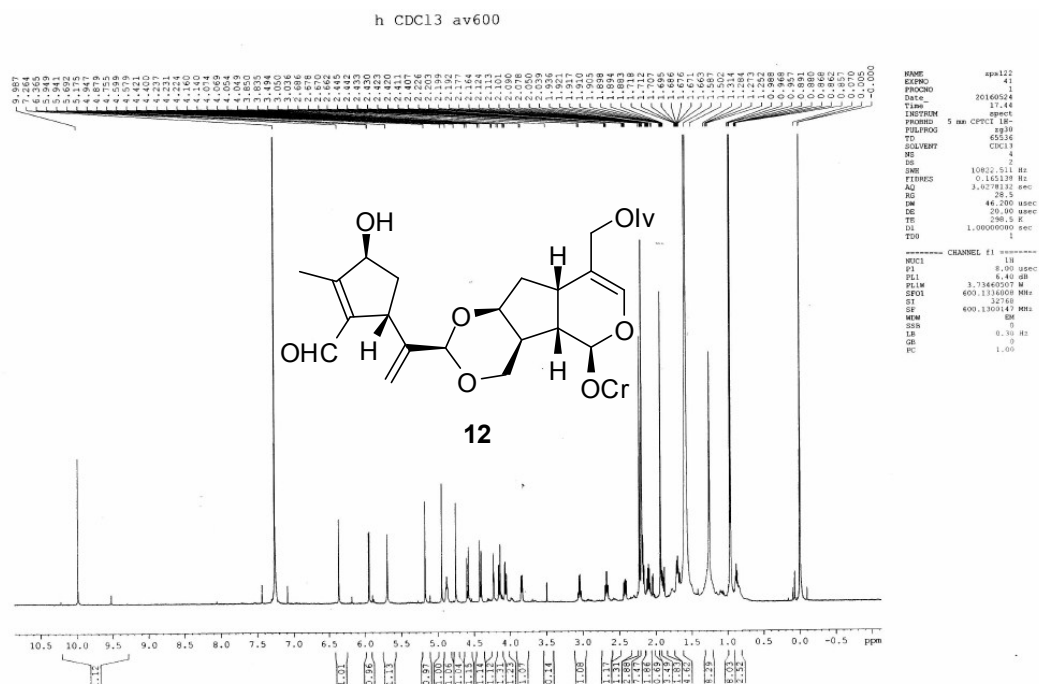


Figure 80. ^{13}C NMR spectrum of Patriscabiobisin B (**12**) in CDCl_3 .

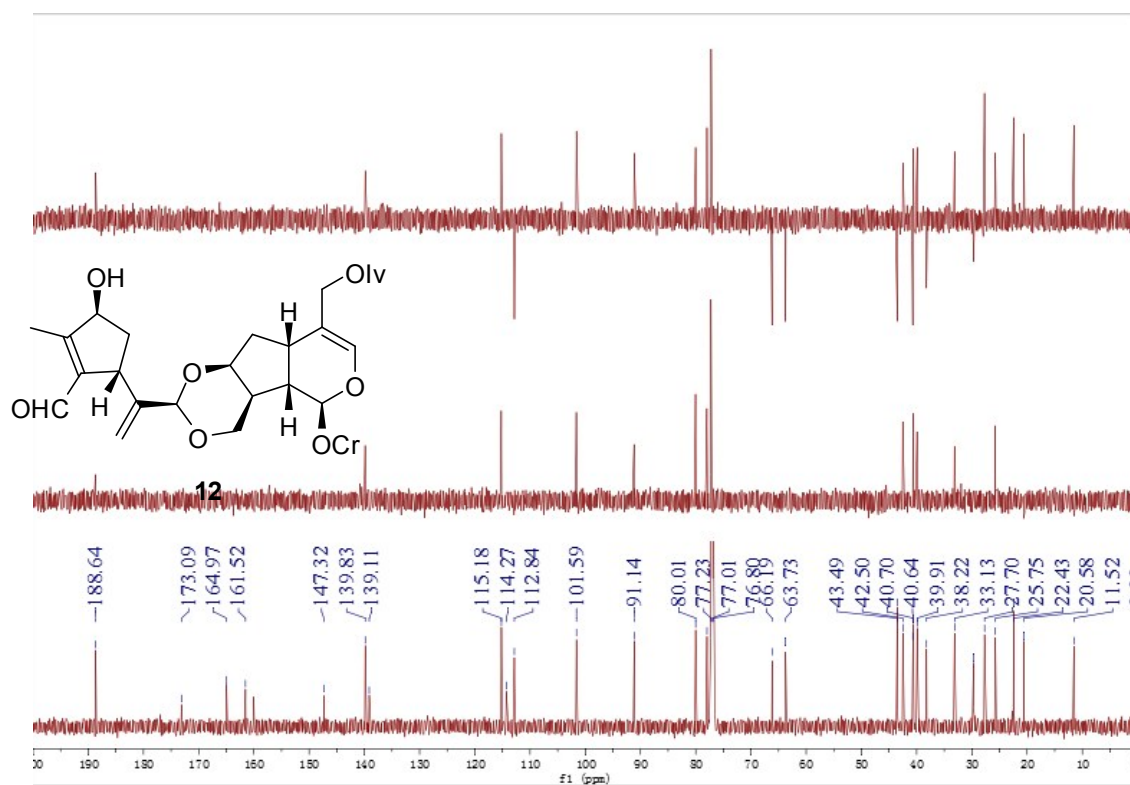


Figure 81. HSQC spectrum of Patriscabiobisin B (**12**) in CDCl₃.

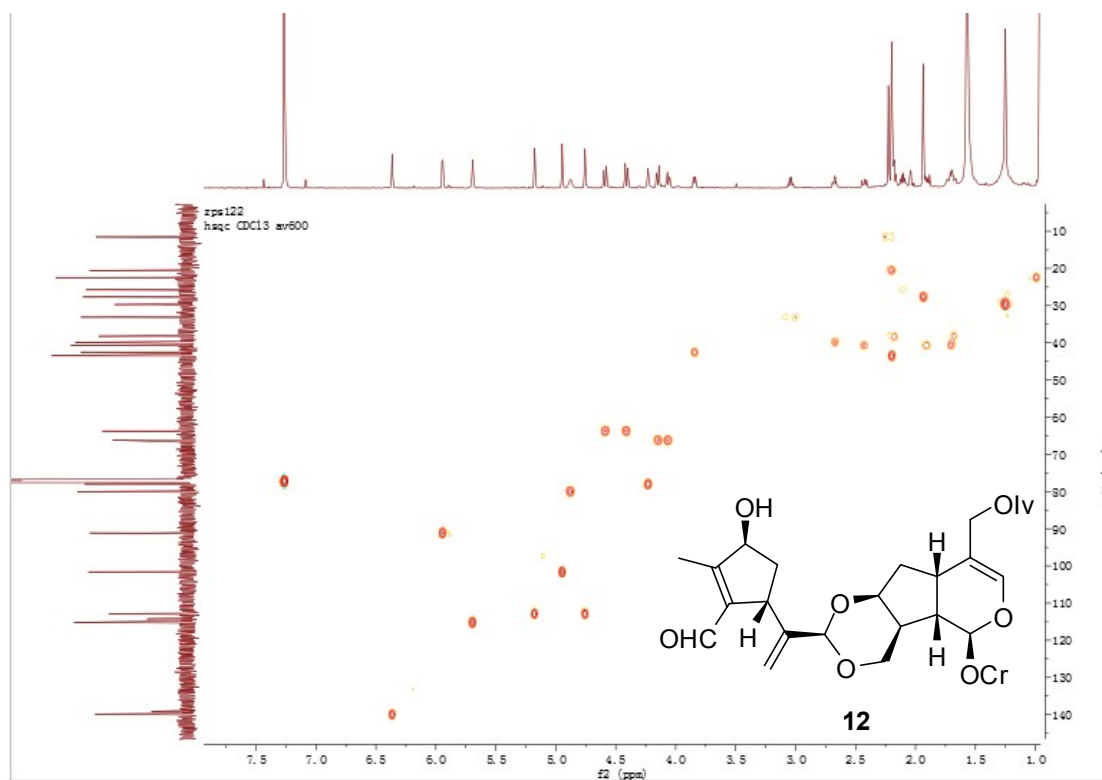


Figure 82. HMBC spectrum of Patriscabiobisin B (**12**) in CDCl₃.

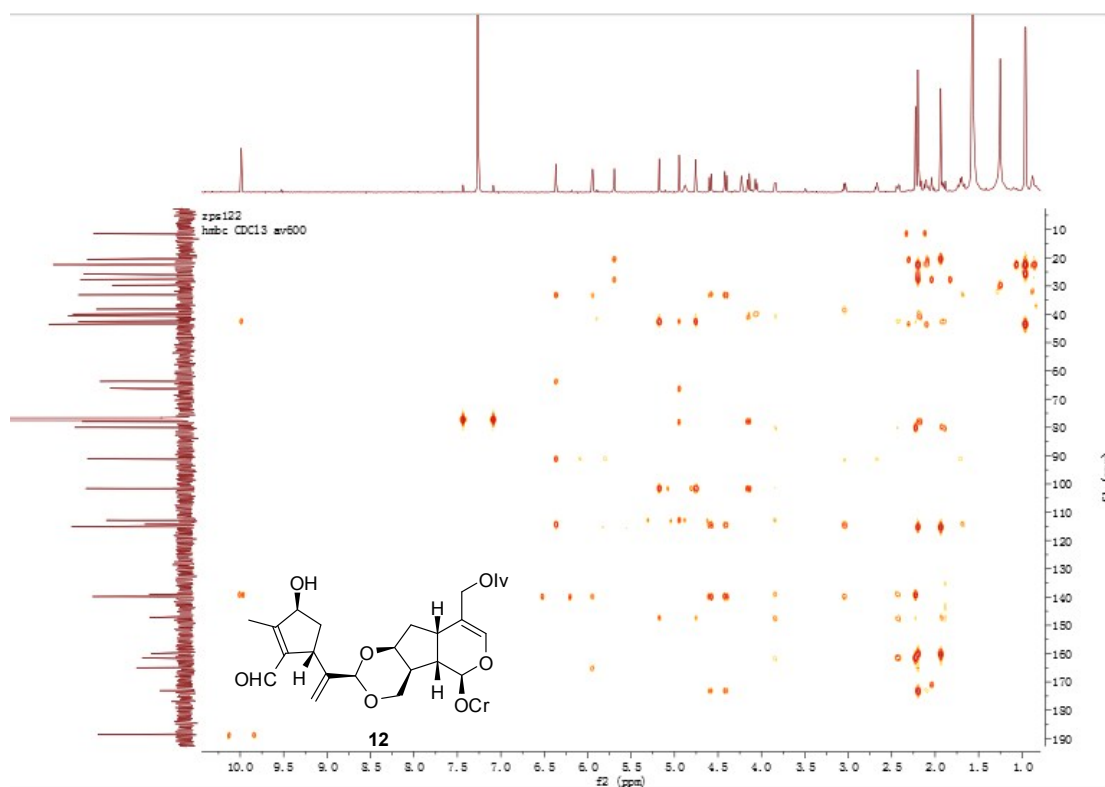


Figure 83. ^1H - ^1H COSY spectrum of Patriscabiobisin B (**12**) in CDCl_3 .

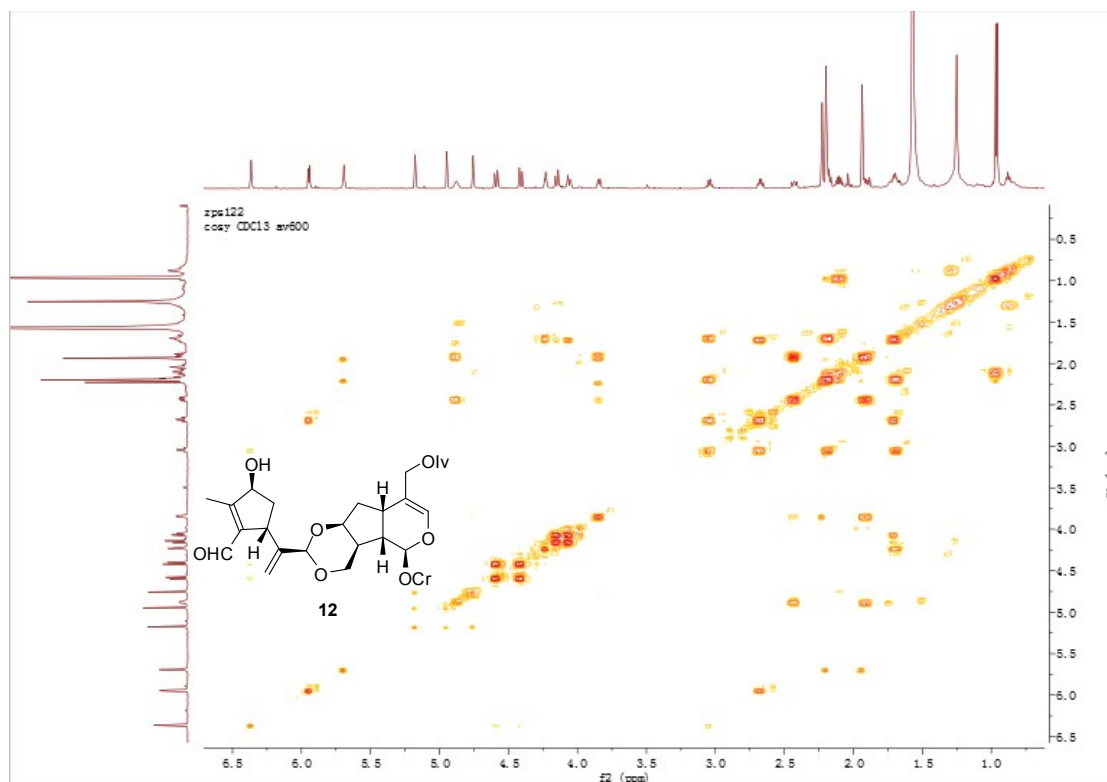


Figure 84. ROESY spectrum of Patriscabiobisin B (**12**) in CDCl_3 .

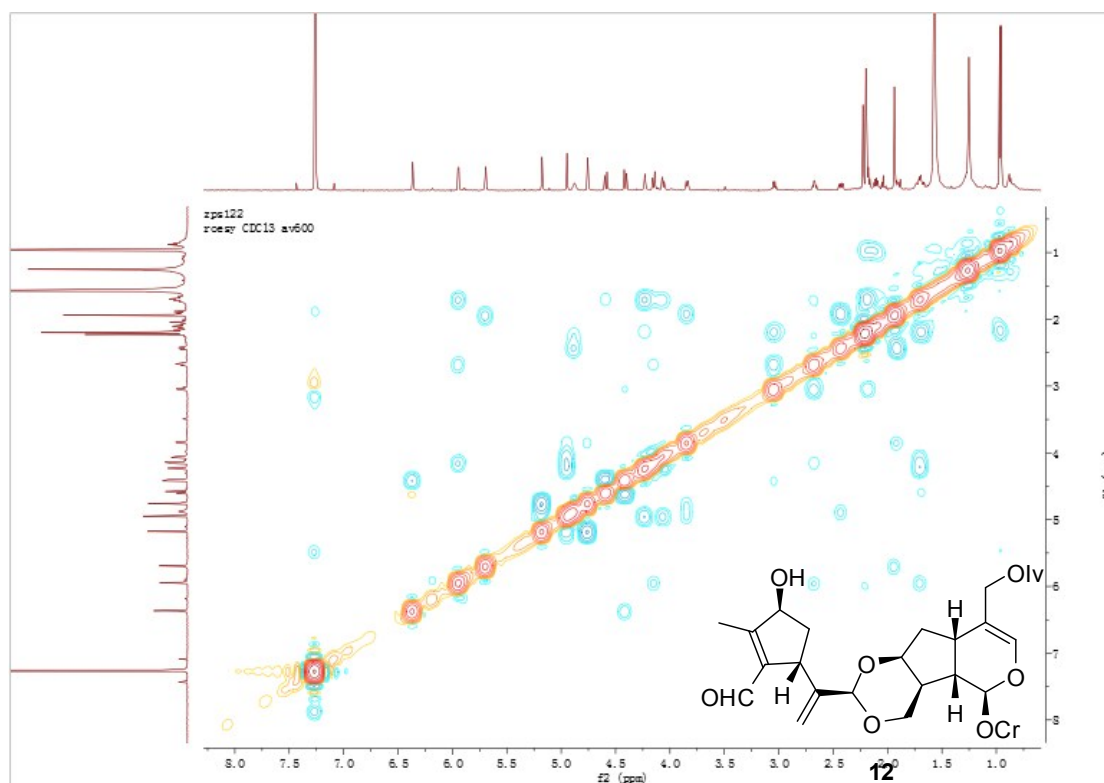


Figure 85. HREIMS spectrum of Patriscabiobisin B (12).

Formula Predictor Report - zps-122.lcd

Page 1 of 1

Data File: E:\DATA\2016\0921\zps-122.lcd

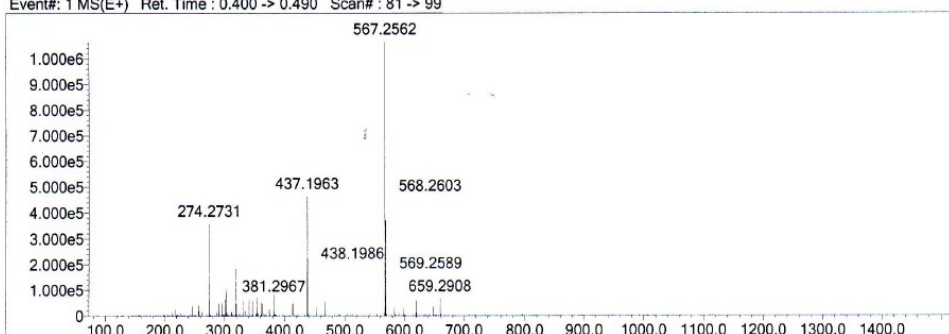
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	100	N	3	0	0	Na	1	0	0	Cl	1	0	0	Na
B	3	0	0	O	2	0	40	Si	4	0	0	Br	1	0	0	
C	4	0	80	F	1	0	0	S	2	0	0	Pt	2	0	0	

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

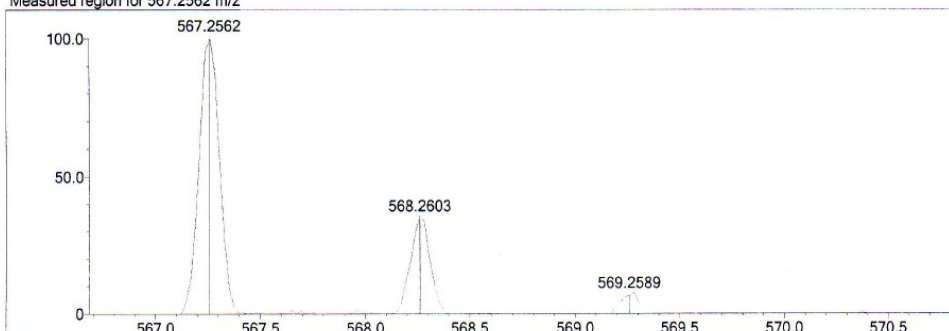
DBE Range: -2.0 - 100.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

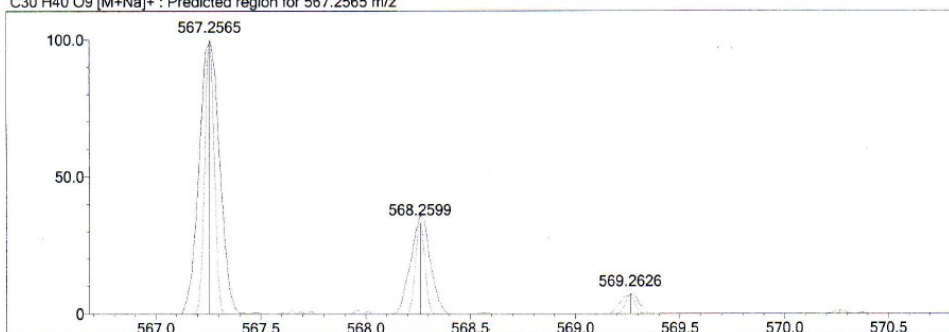
Event#: 1 MS(E+) Ret. Time : 0.400 -> 0.490 Scan#: 81 -> 99



Measured region for 567.2562 m/z



C30 H40 O9 [M+Na]⁺ : Predicted region for 567.2562 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	92.56	C30 H40 O9	[M+Na] ⁺	567.2562	567.2565	-0.3	-0.53	92.56	11.0

Figure 86. ECD spectrum of Patriscabiobisin B (12).

ZPS-122

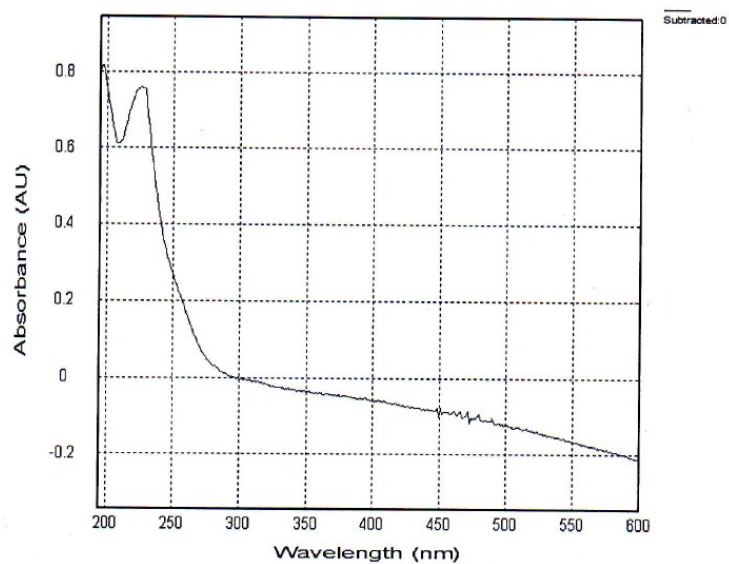
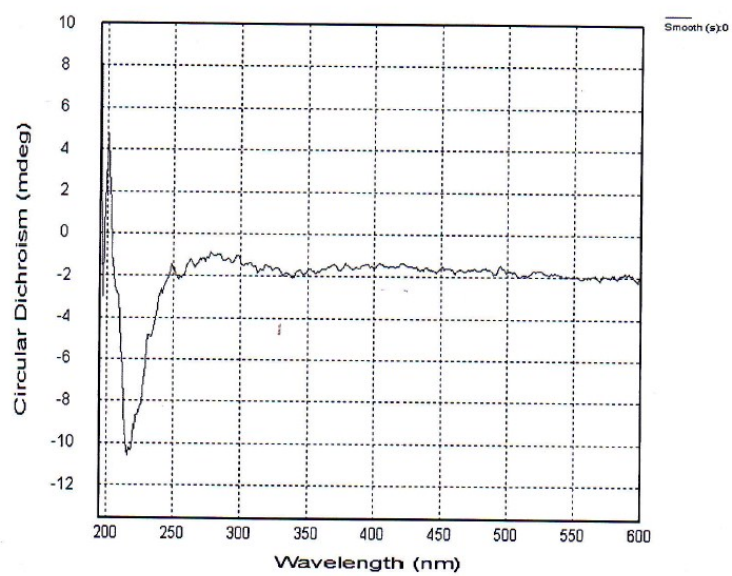


Figure 87. ^1H NMR spectrum of Patriscabiobisin C (**13**) in MeOH.

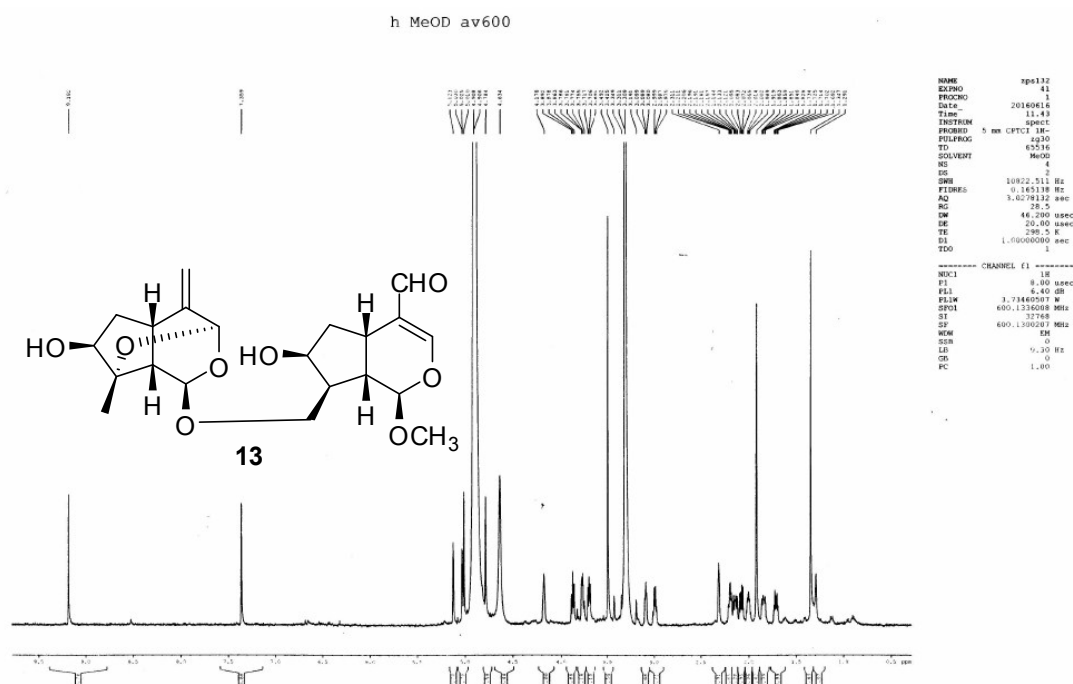


Figure 88. ^{13}C NMR spectrum of Patriscabiobisin C (**13**) in MeOH.

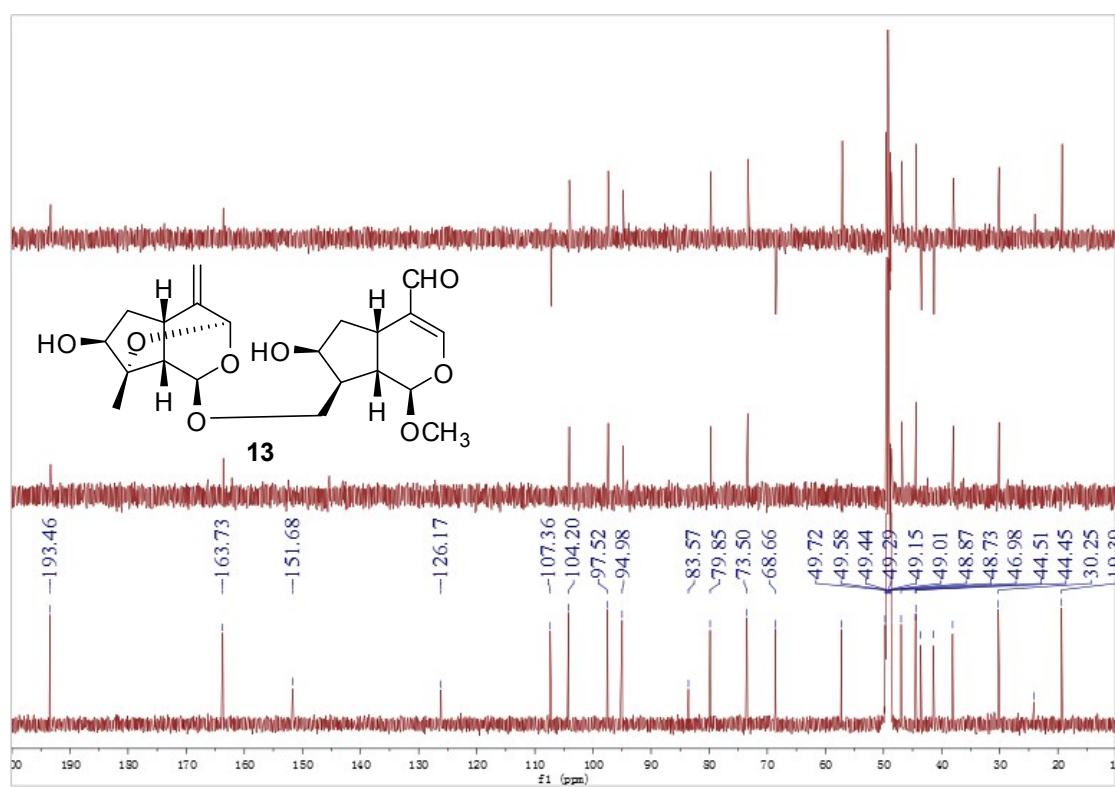


Figure 89. HSQC spectrum of Patriscabiobisin C (**13**) in MeOH.

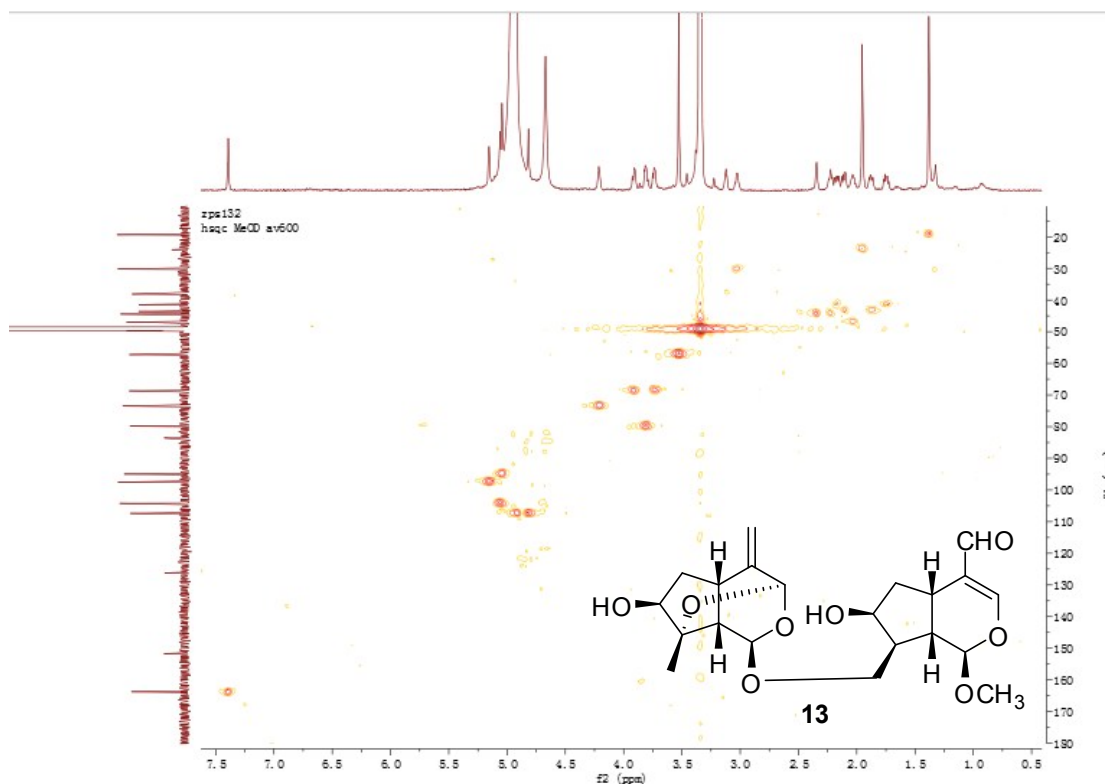


Figure 90. HMBC spectrum of Patriscabiobisin C (**13**) in MeOH.

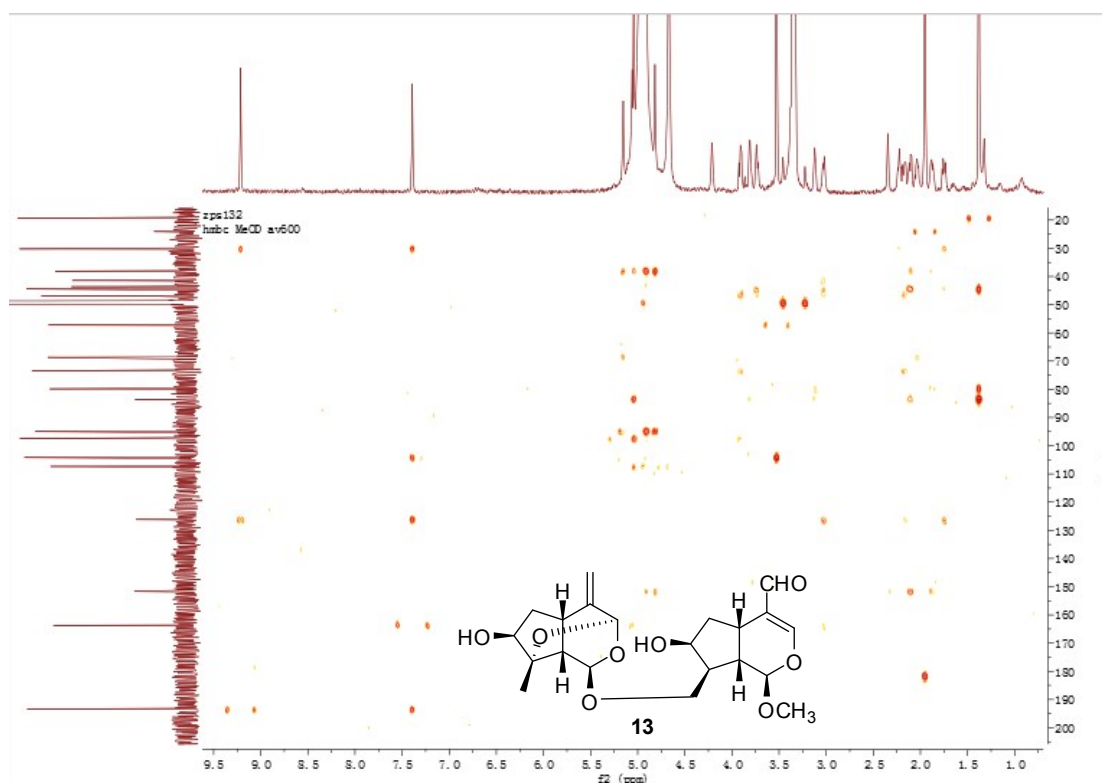


Figure 91. ^1H - ^1H COSY spectrum of Patriscabiobisin C (**13**) in MeOH.

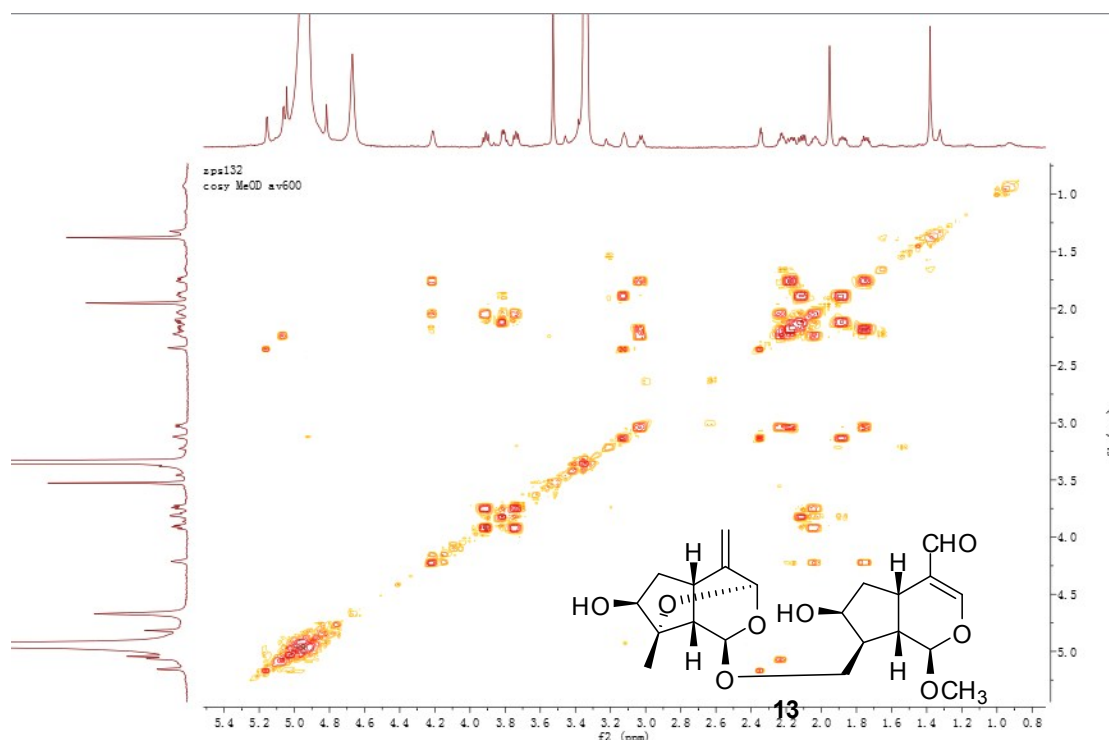


Figure 92. ROESY spectrum of Patriscabiobisin C (**13**) in MeOH

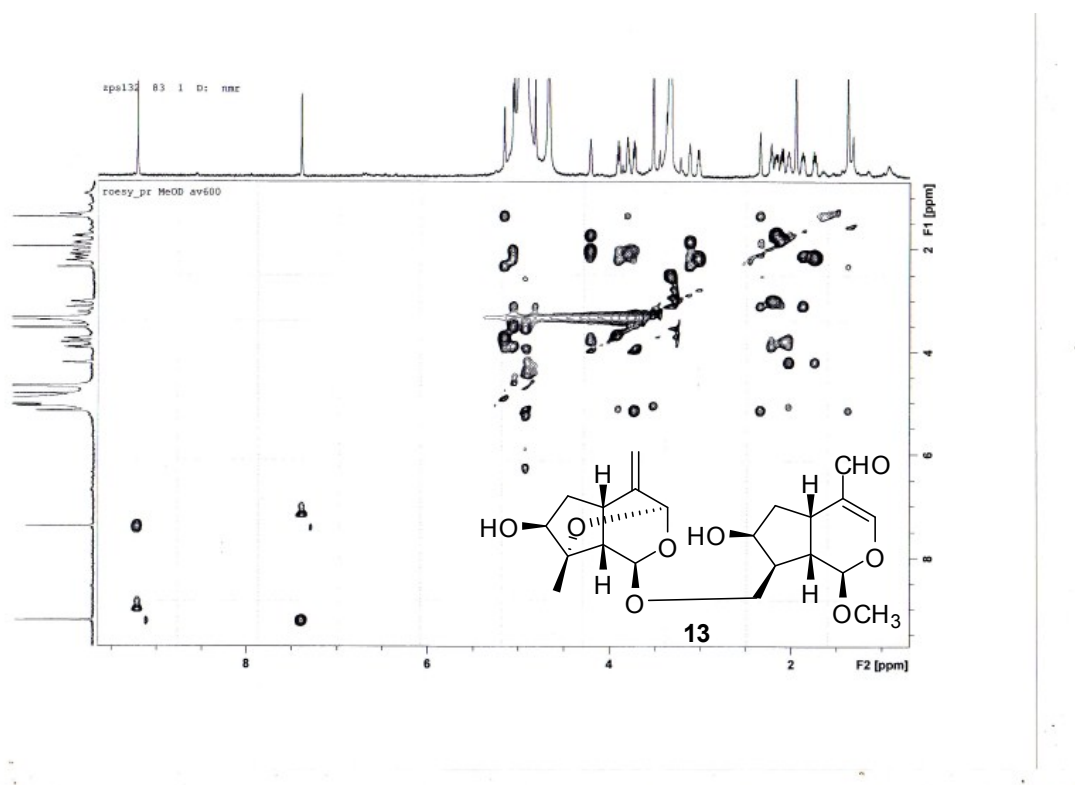


Figure 93. HREIMS spectrum of Patriscabiobisin C (13).

