Electronic Supplementary Information (ESI)

Ancistrolikokines E-H and Related 5,8'-Coupled Naphthylisoquinoline Alkaloids from the Congolese Liana *Ancistrocladus likoko* with Antiausterity Activities against PANC-1 Human Pancreatic Cancer Cells

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[b] *Faculté des Sciences, Université de Kinshasa, B.P. 202, Kinshasa XI, Democratic Republic of the Congo.*

[c] *Division of Natural Drug Discovery, Institute of Natural Medicine, University of Toyama, 2630 Sugitani, Toyama 930-0194, Japan.*

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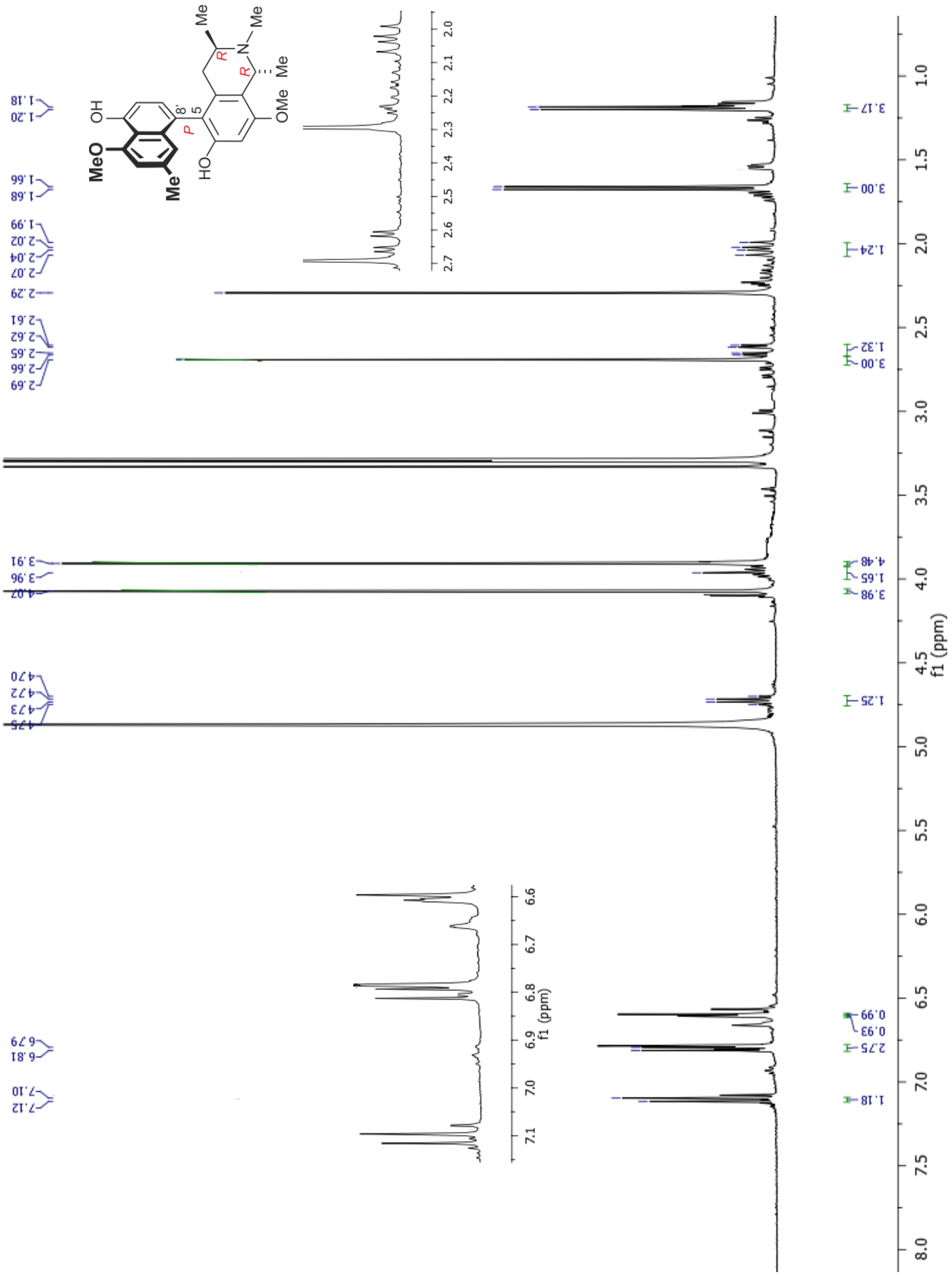


Figure S1. ^{1}H NMR spectrum of ancistrolikokine A_2 (**13**).

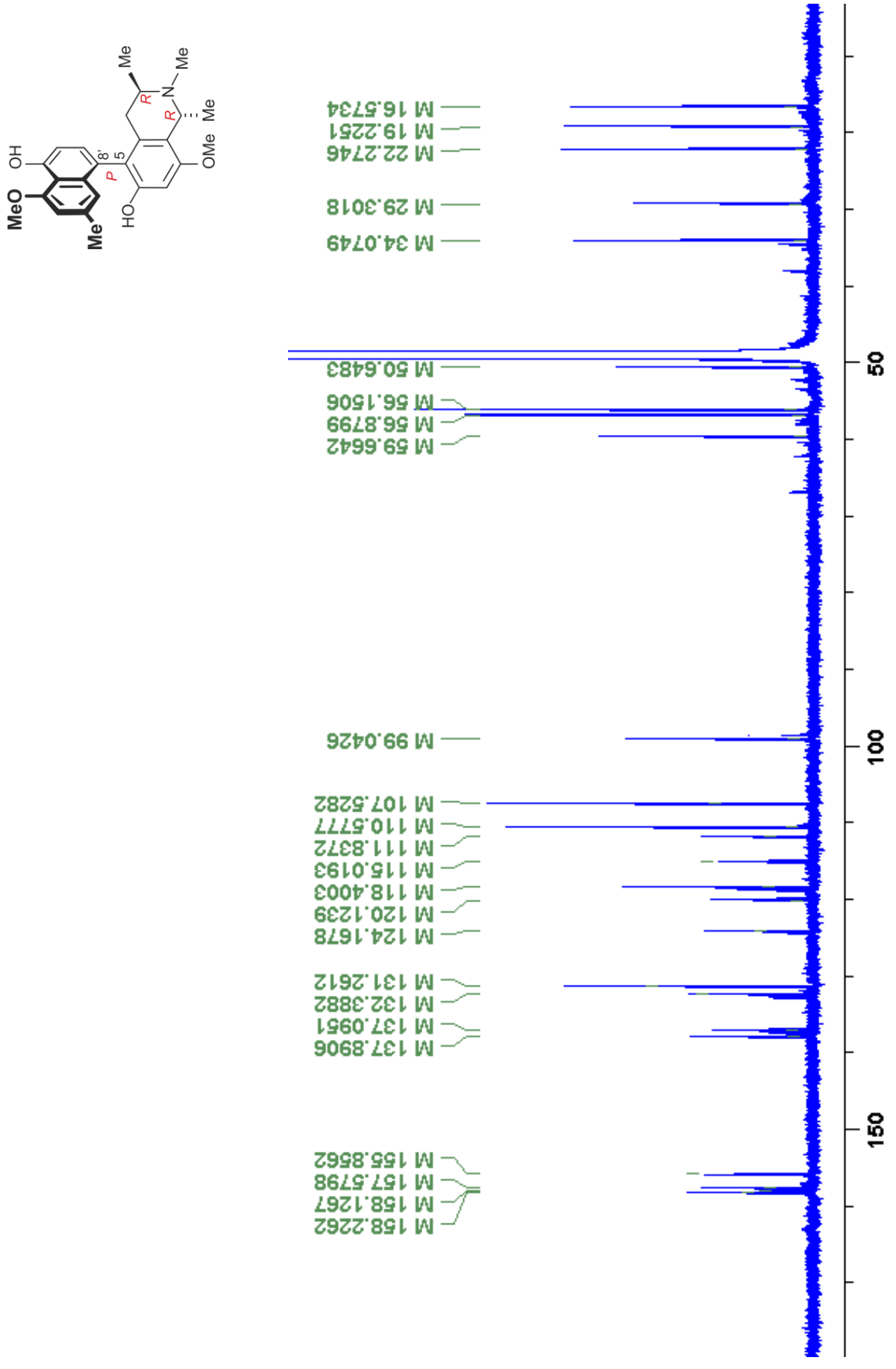


Figure S2. ^{13}C NMR spectrum of ancistrolikokine A_2 (**13**).

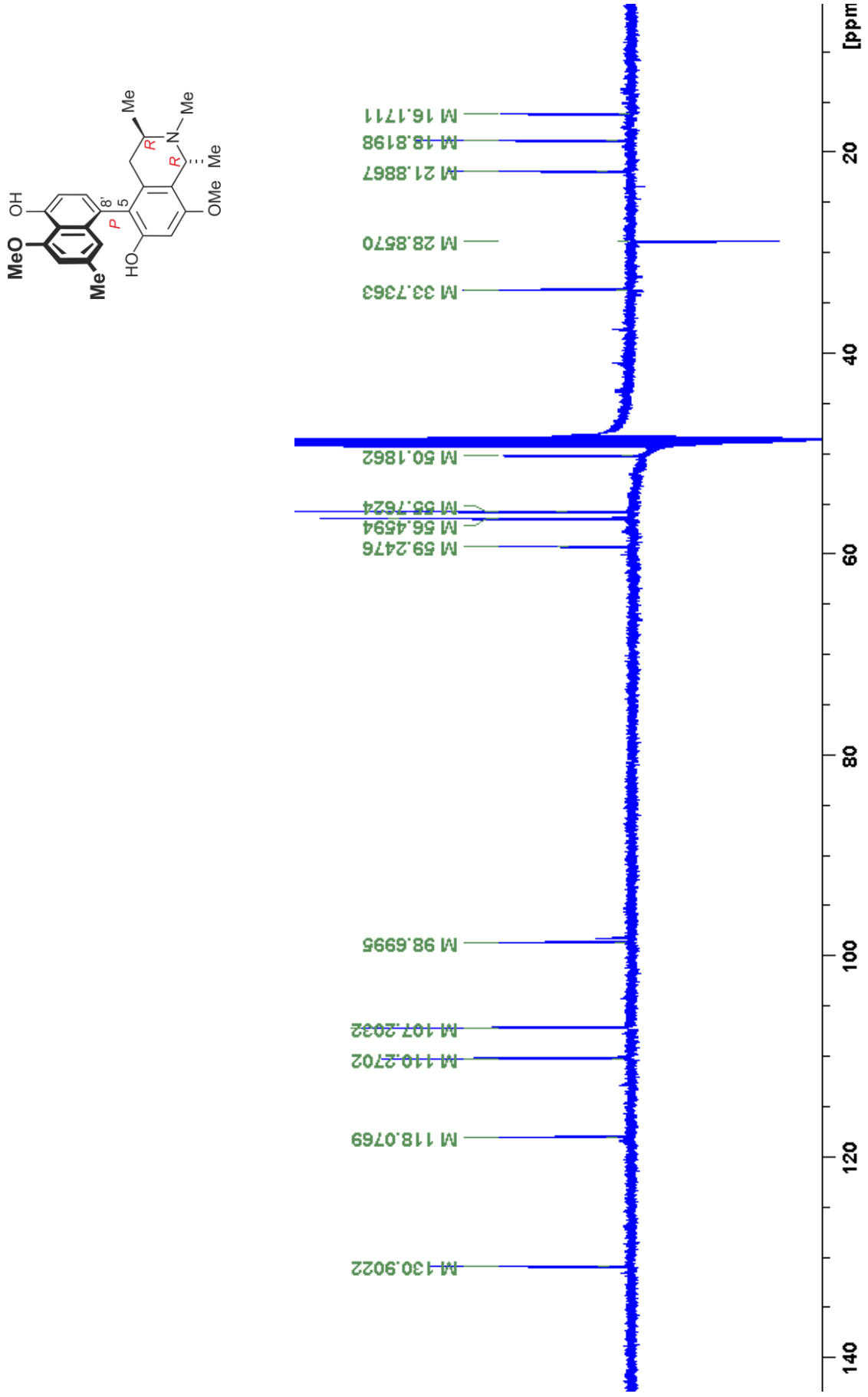


Figure S3. ^{13}C DEPT spectrum of ancistrolikokine A_2 (**13**).

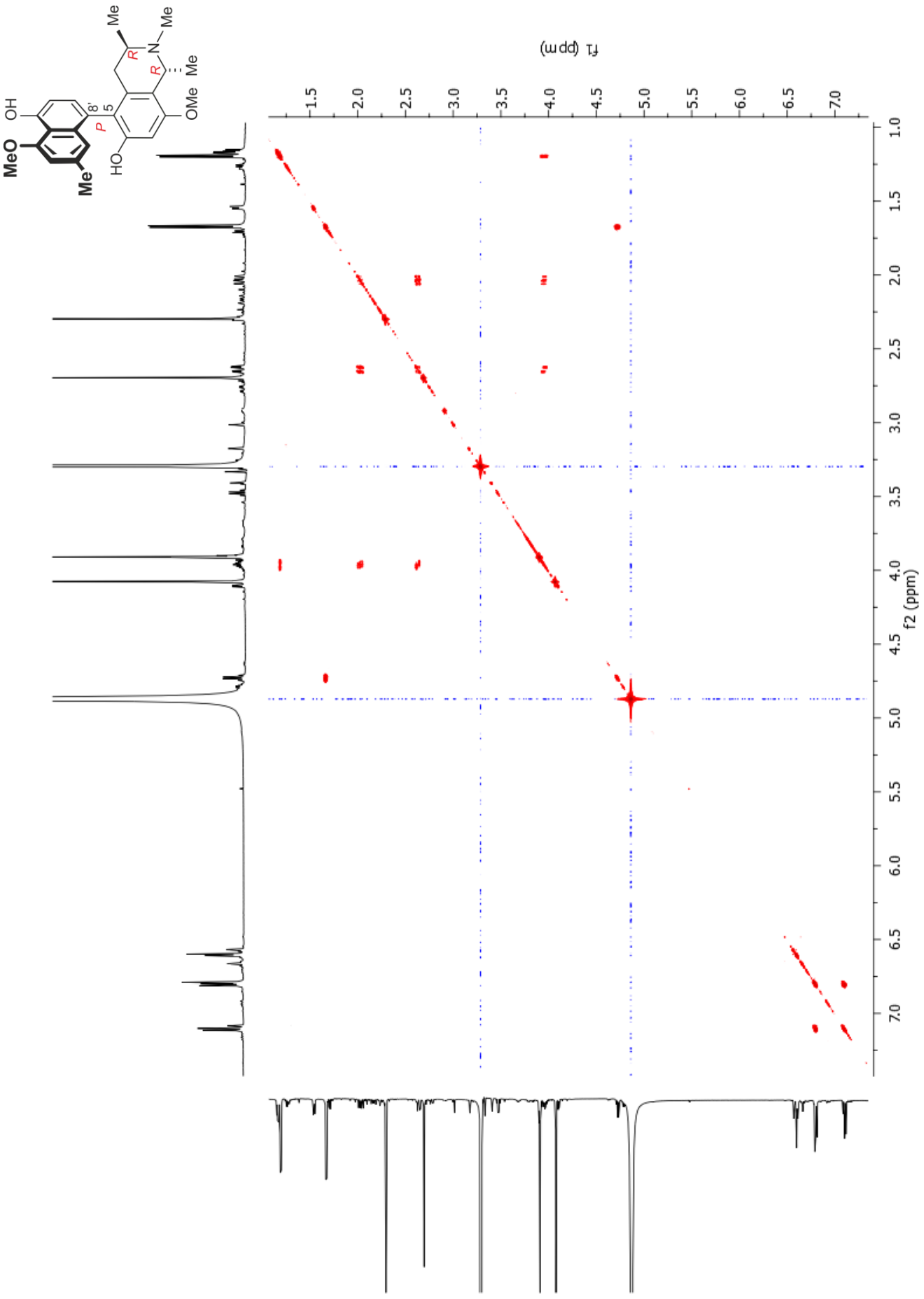


Figure S4. COSY spectrum of ancistrolikokine A_2 (**13**).

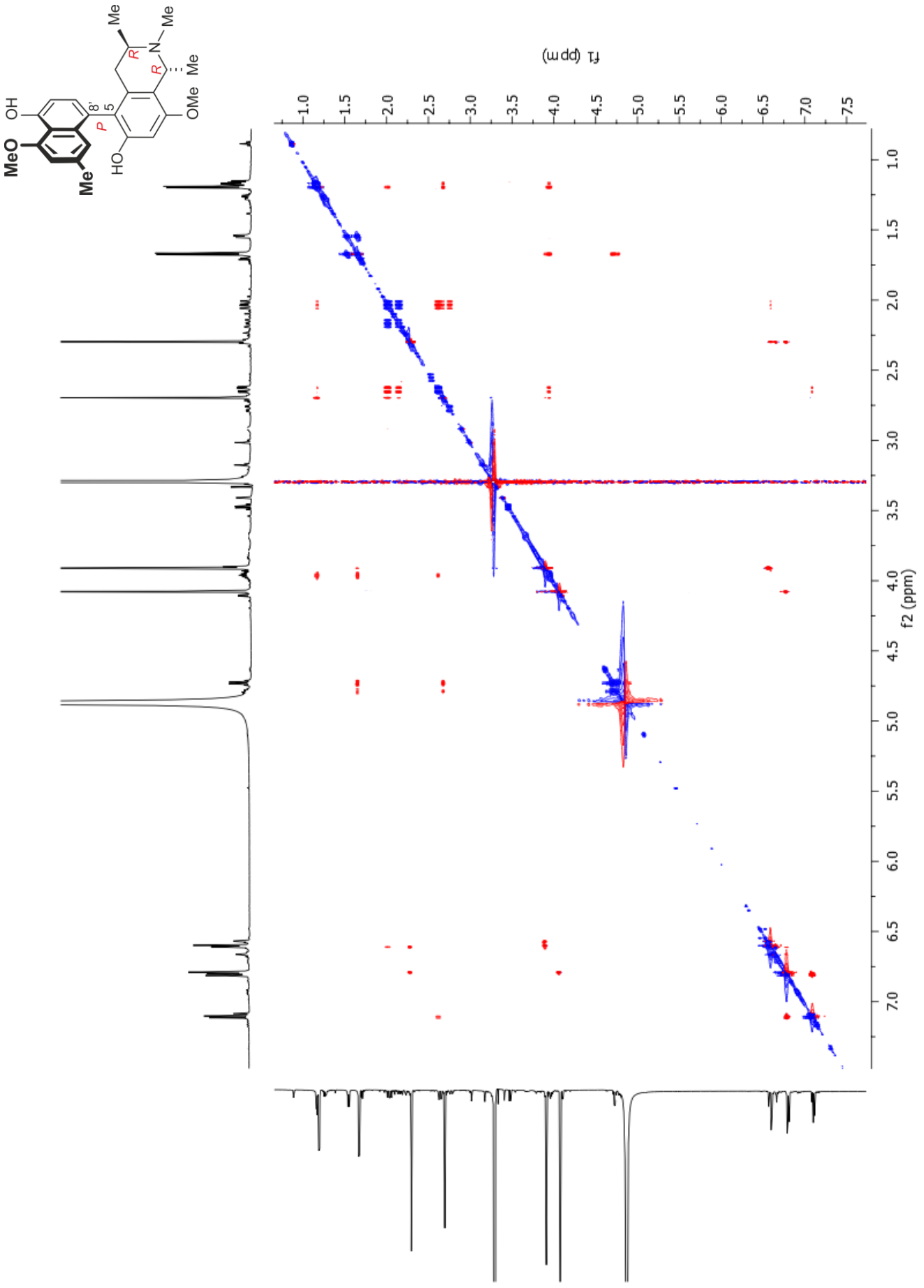


Figure S5. ^{1}H-^{1}H NOESY spectrum of ancistrolikokine A_2 (**13**).

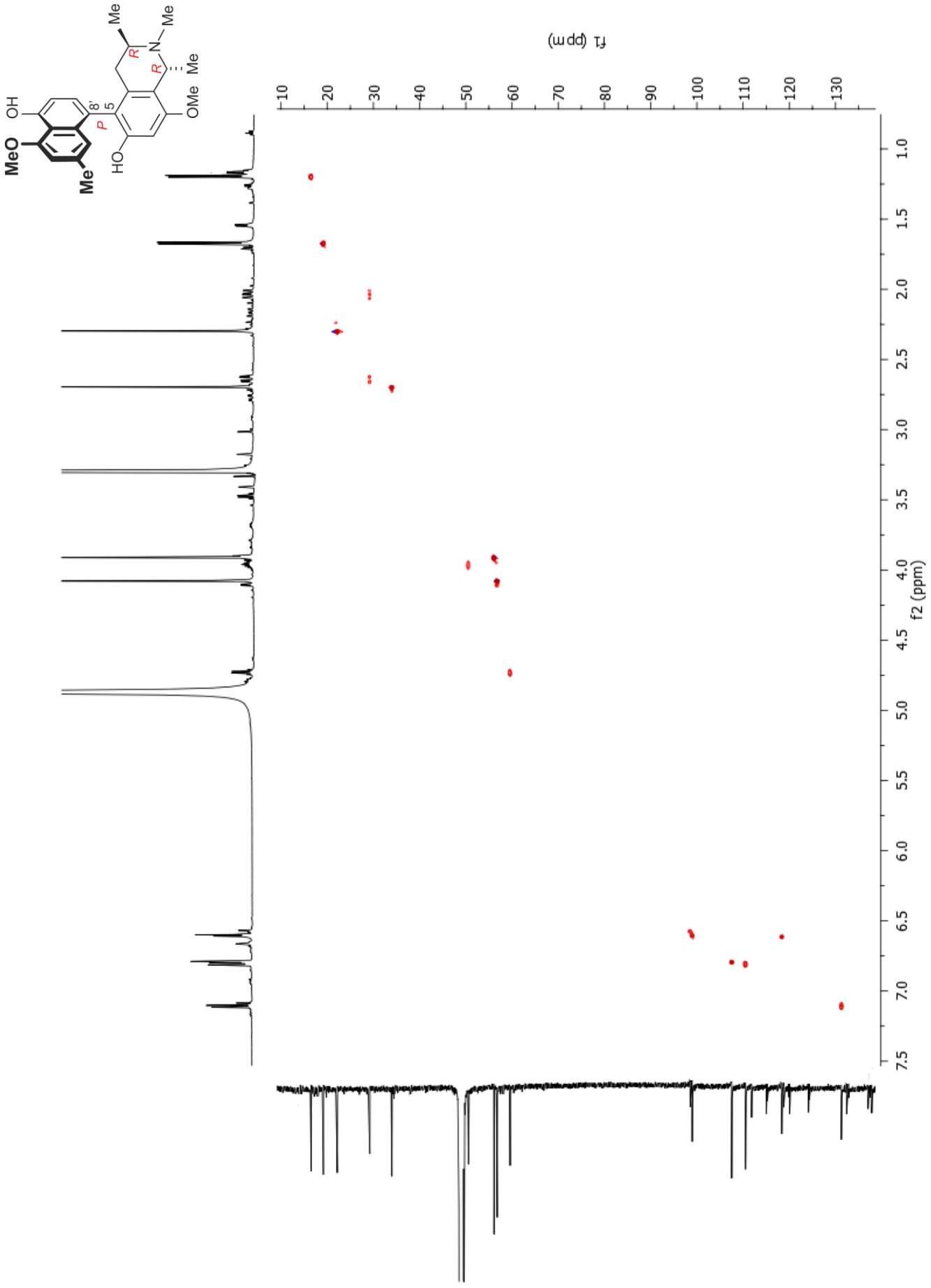


Figure S6. HSQC spectrum of ancistrolikokine A_2 (**13**).

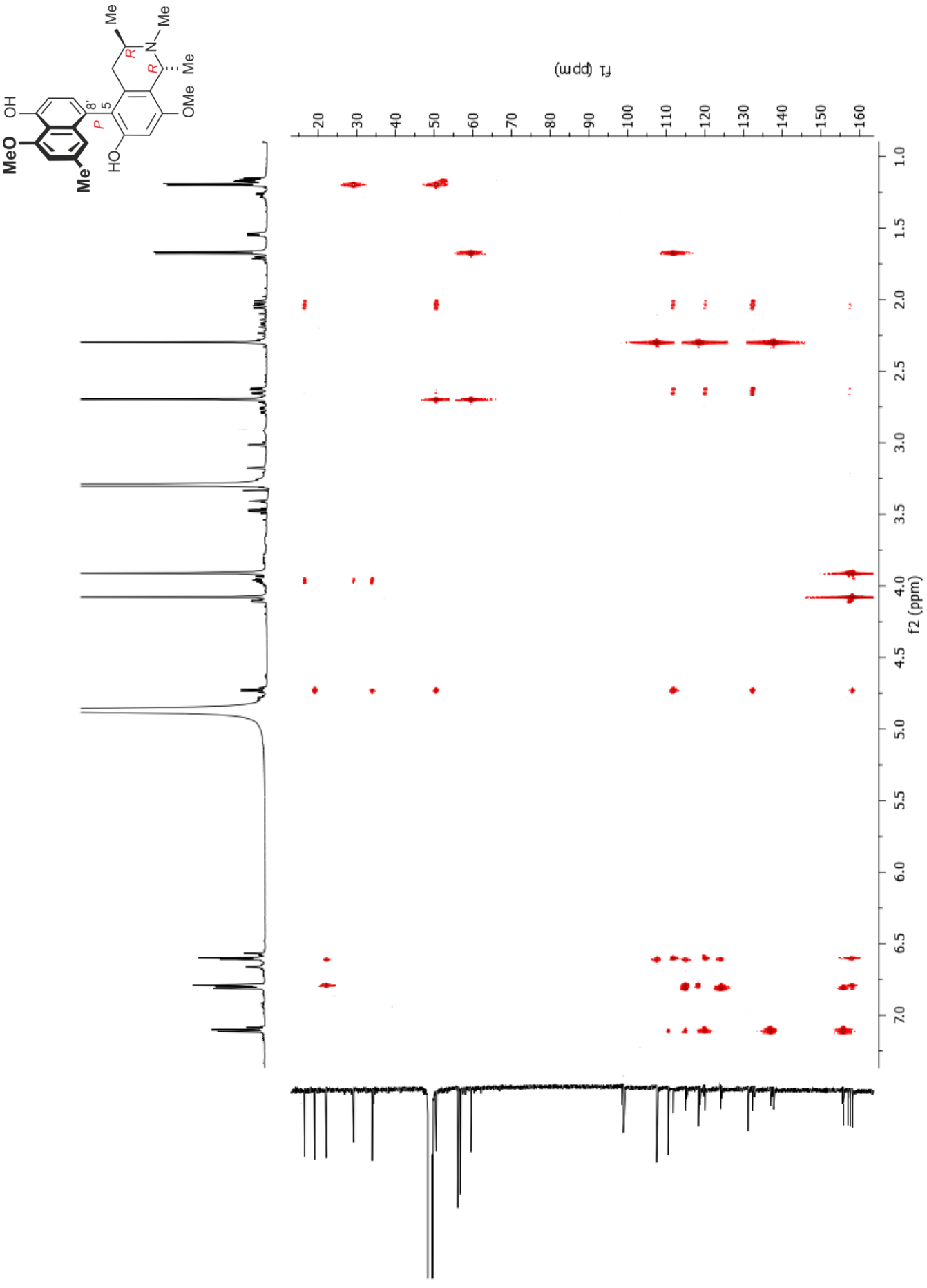
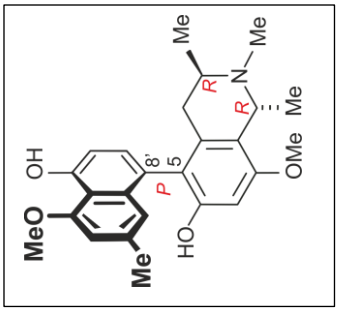


Figure S7. HMBC spectrum of ancistrolikokine A_2 (**13**).



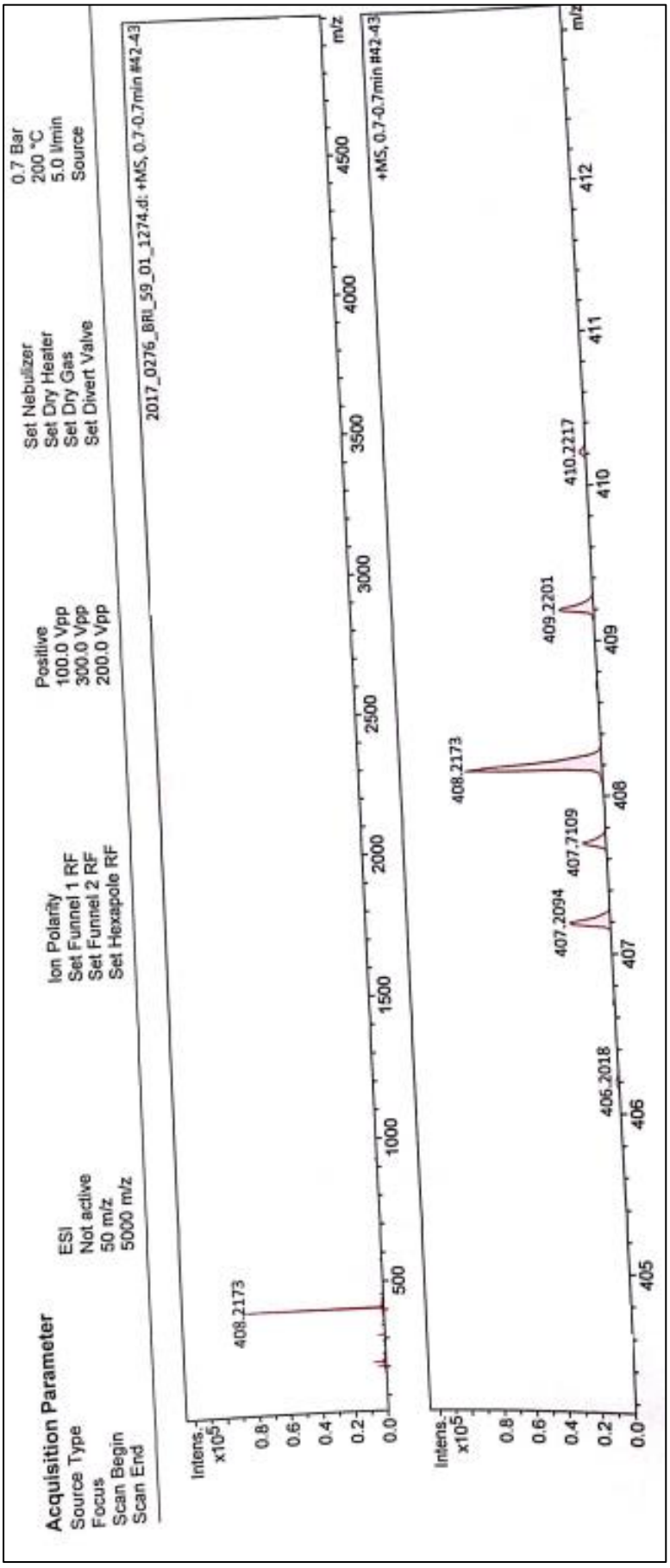
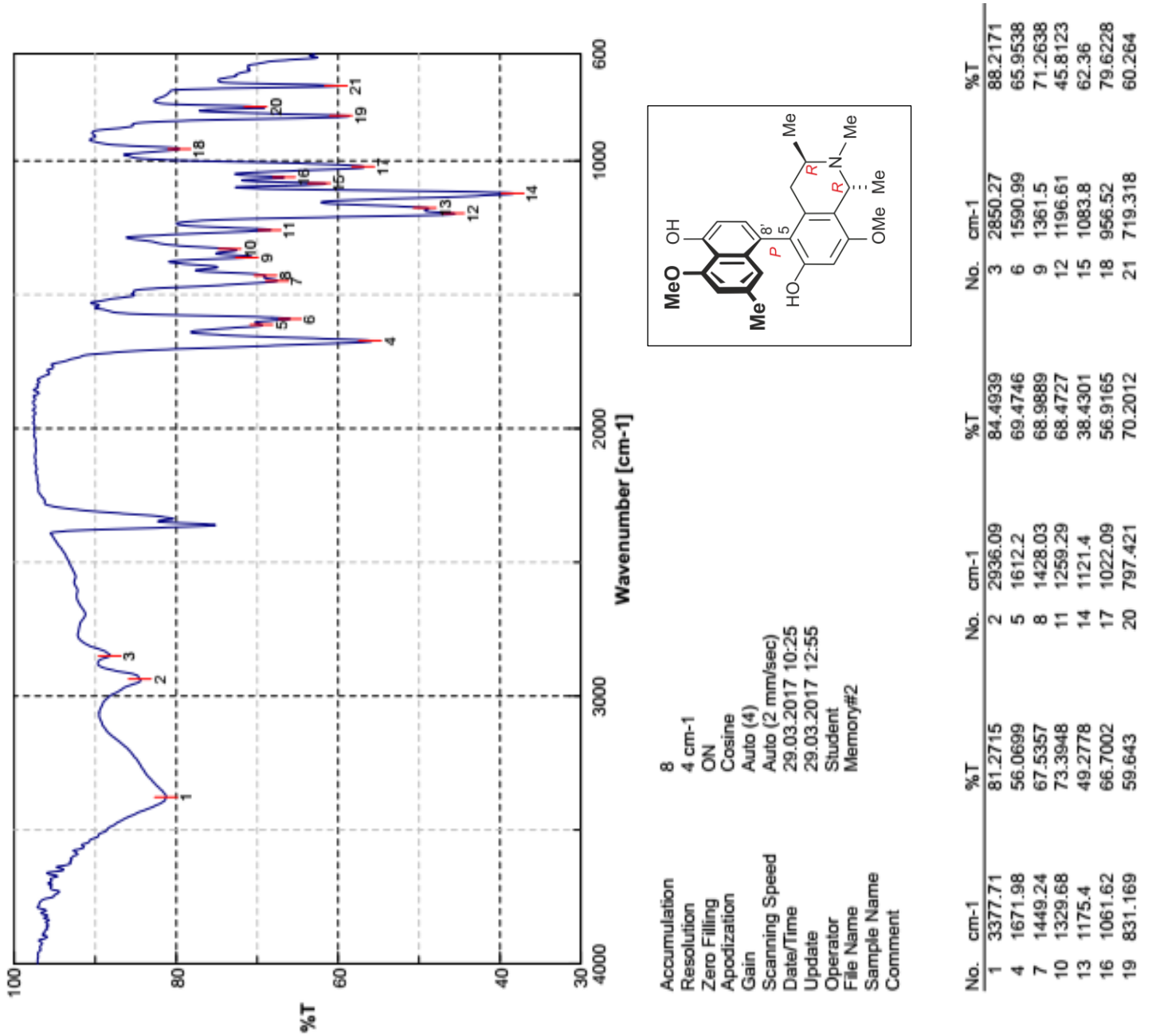


Figure S8. HRESIMS spectrum of ancistrolikokine A_2 (**13**).



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7	1449.24	67.5357	8	1428.03	68.9889	9	1361.5	71.2638
10	1329.68	73.3948	11	1259.29	68.4727	12	1196.61	45.8123
13	1175.4	49.2778	14	1121.4	38.4301	15	1083.8	62.36
16	1061.62	66.7002	17	1022.09	56.9165	18	956.52	79.6228
19	831.169	59.643	20	797.421	70.2012	21	719.318	60.264

Figure S9. IR spectrum of ancistrolikokine A_2 (**13**).

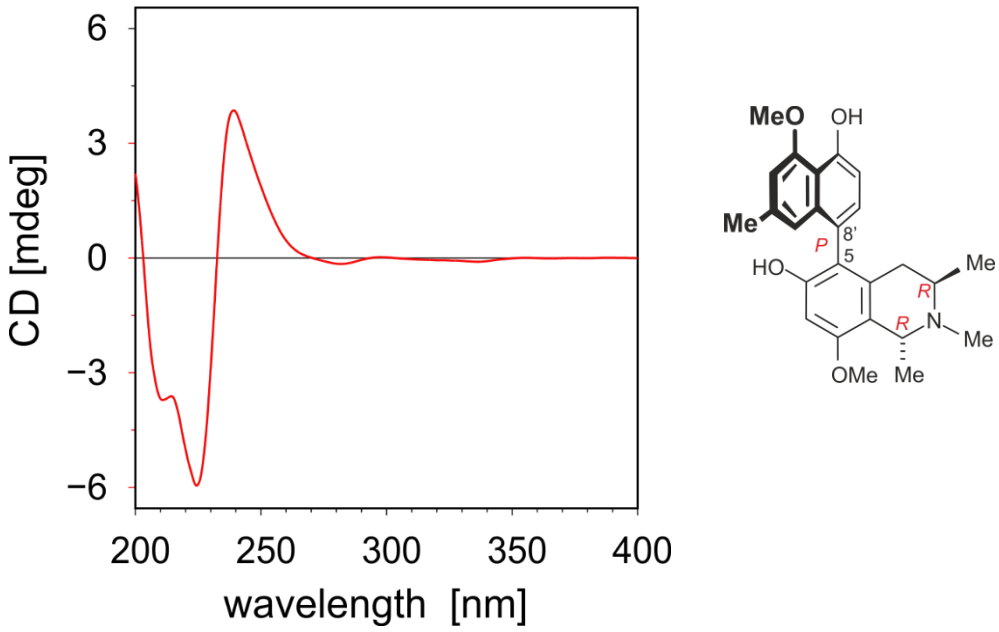
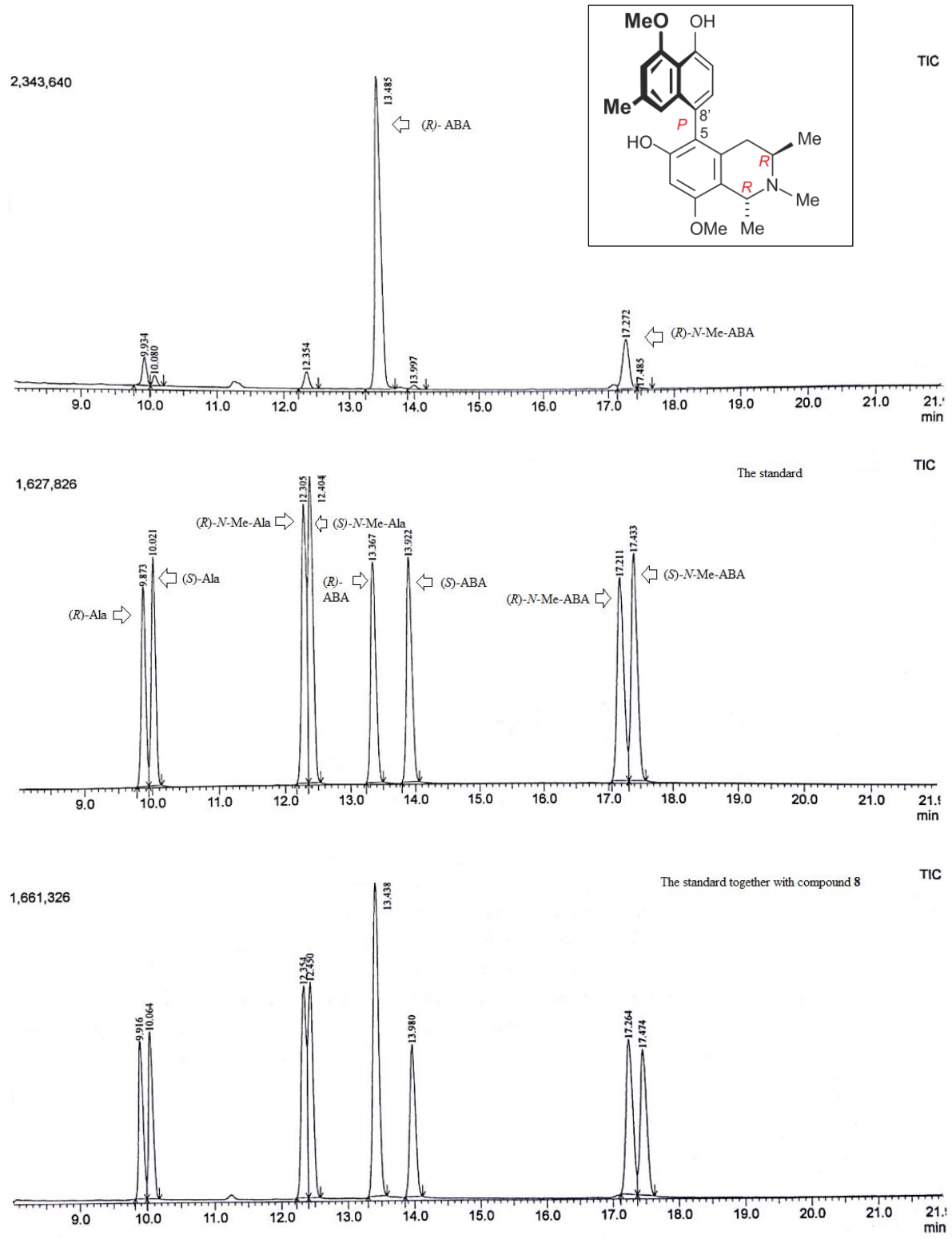


Figure S10. ECD spectrum of ancistrolikokine A_2 (**13**).



Ala = Alanine *N*-Me-Ala = *N*-Methylalanine

ABA = 3-Aminobutyric acid *N*-Me-ABA = *N*-Methyl-3-aminobutyric acid

Figure S11. Oxidative degradation products of ancistrolikokine A_2 (**13**).

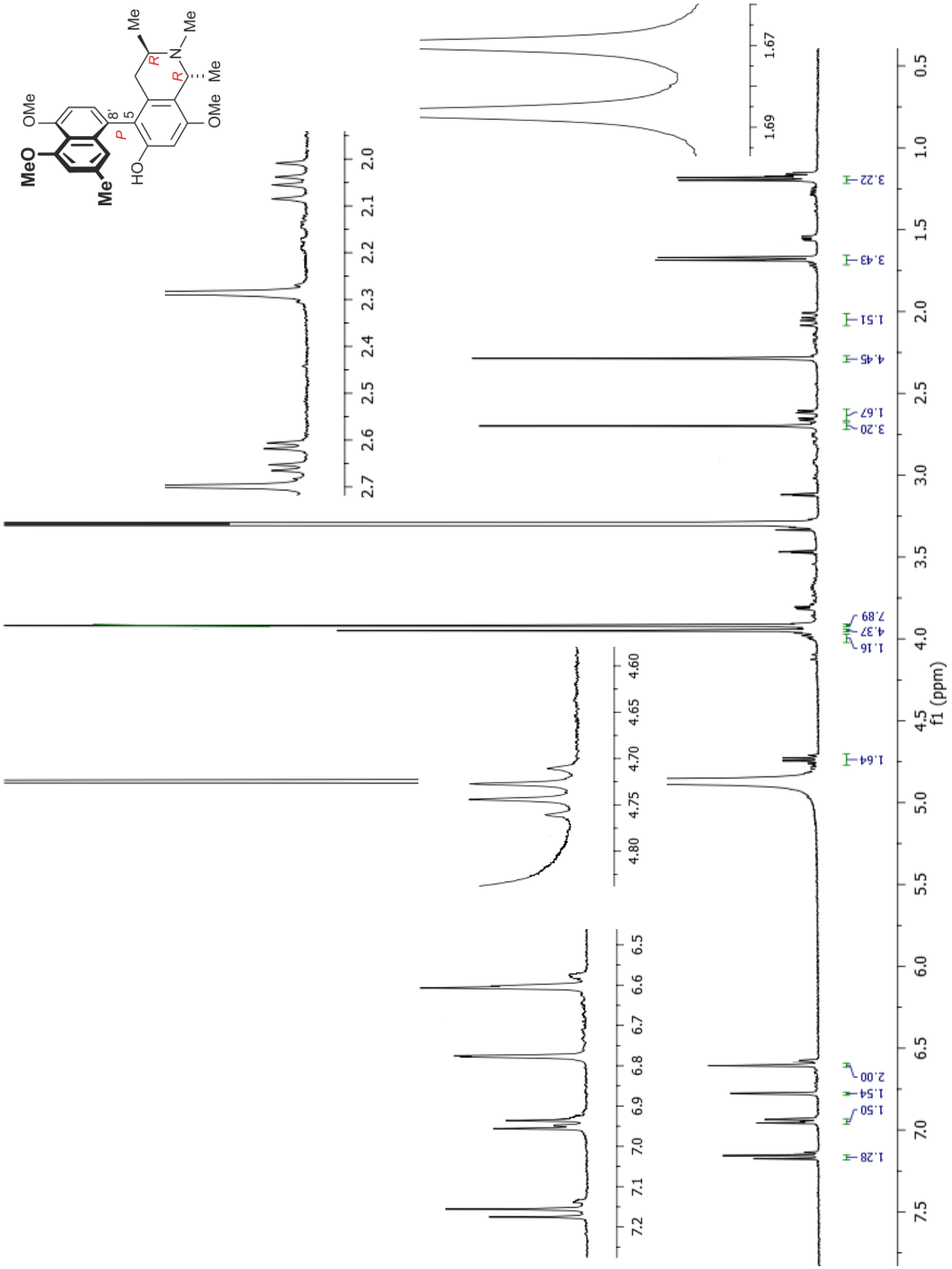


Figure S12. ^{1}H NMR spectrum of ancistrolikokine A_3 (**14**).

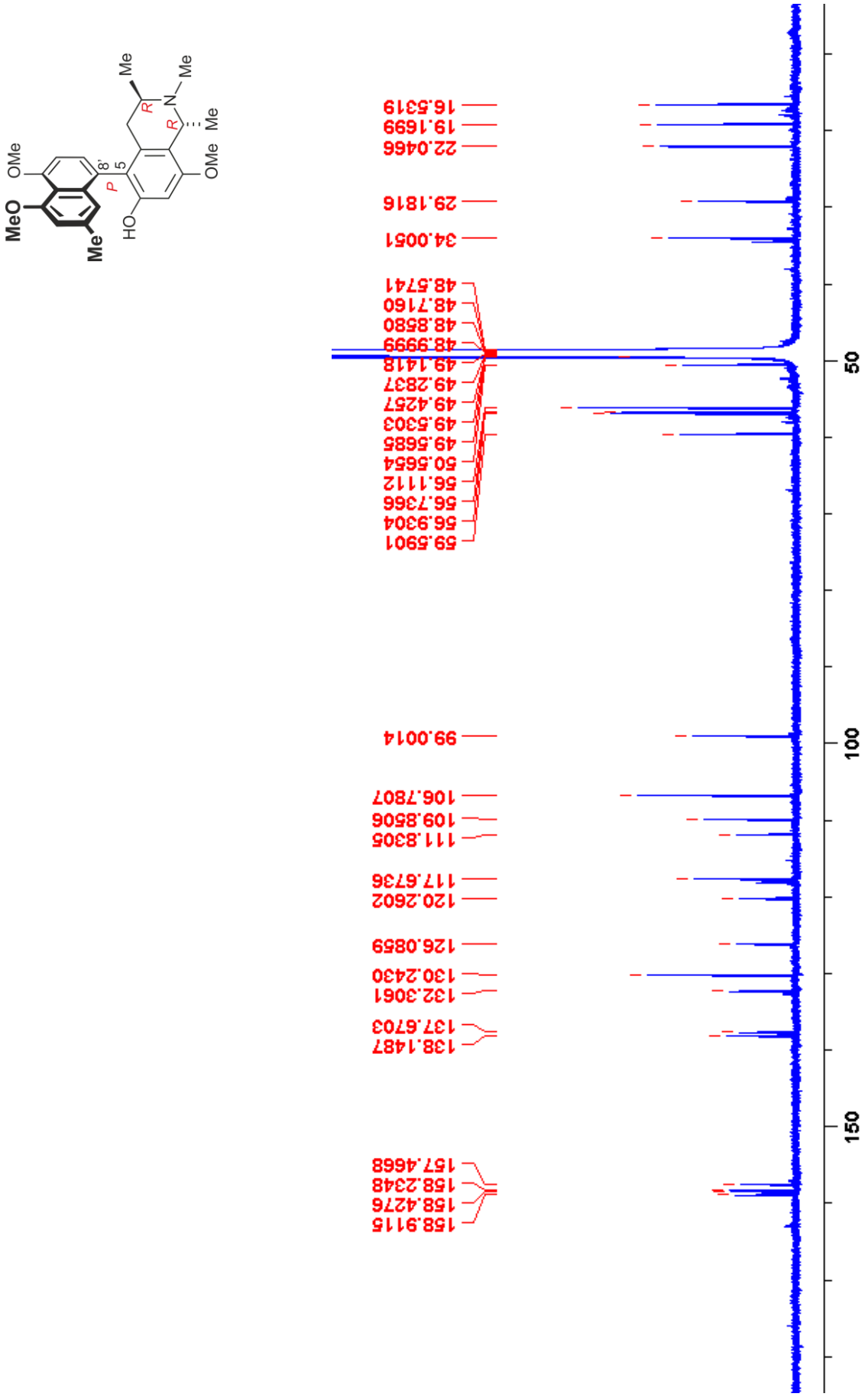


Figure S13. ^{13}C NMR spectrum of ancistrolikokine A_3 (**14**).

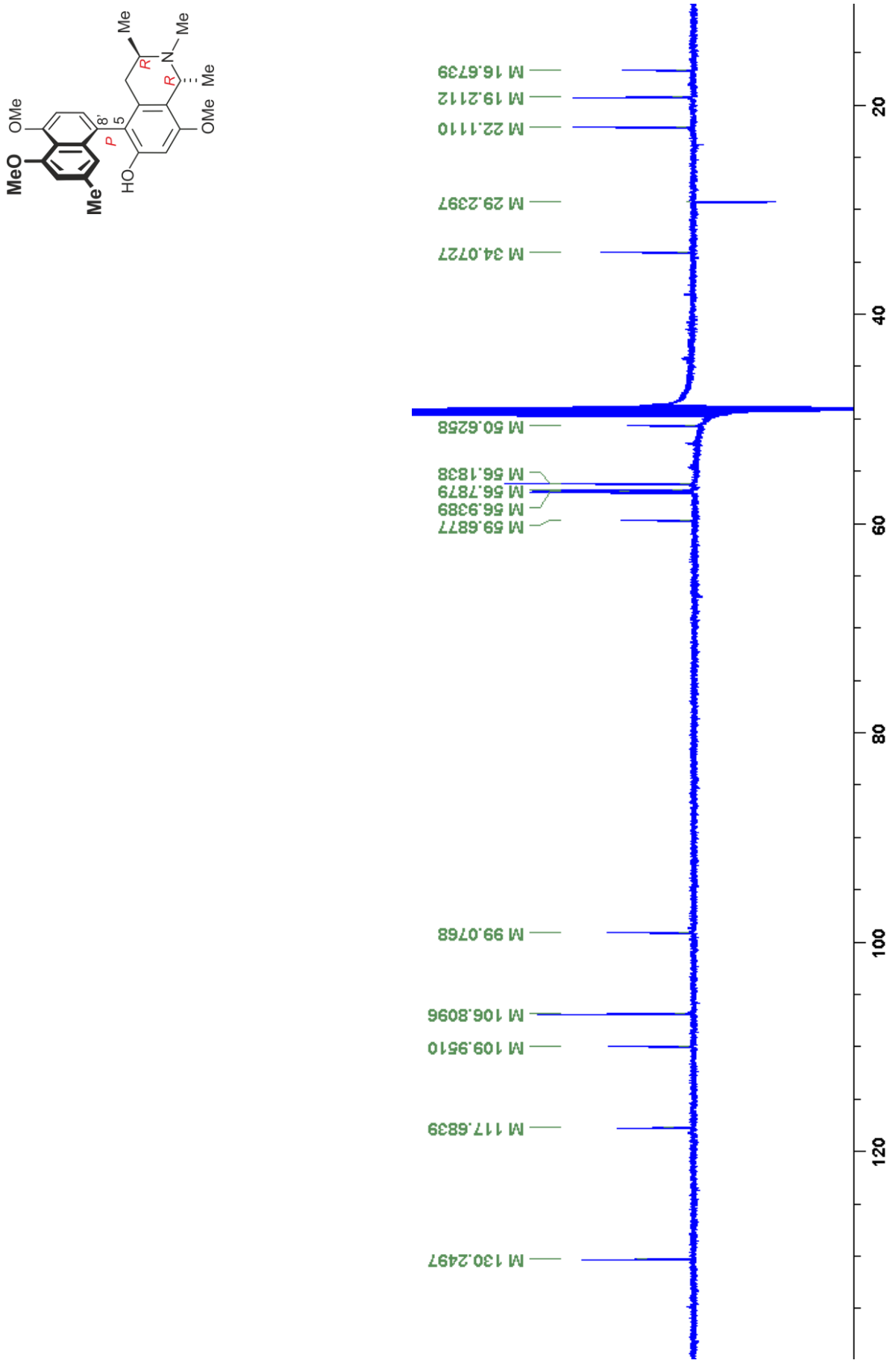


Figure S14. ^{13}C DEPT spectrum of ancistrolikokine A_3 (**14**).

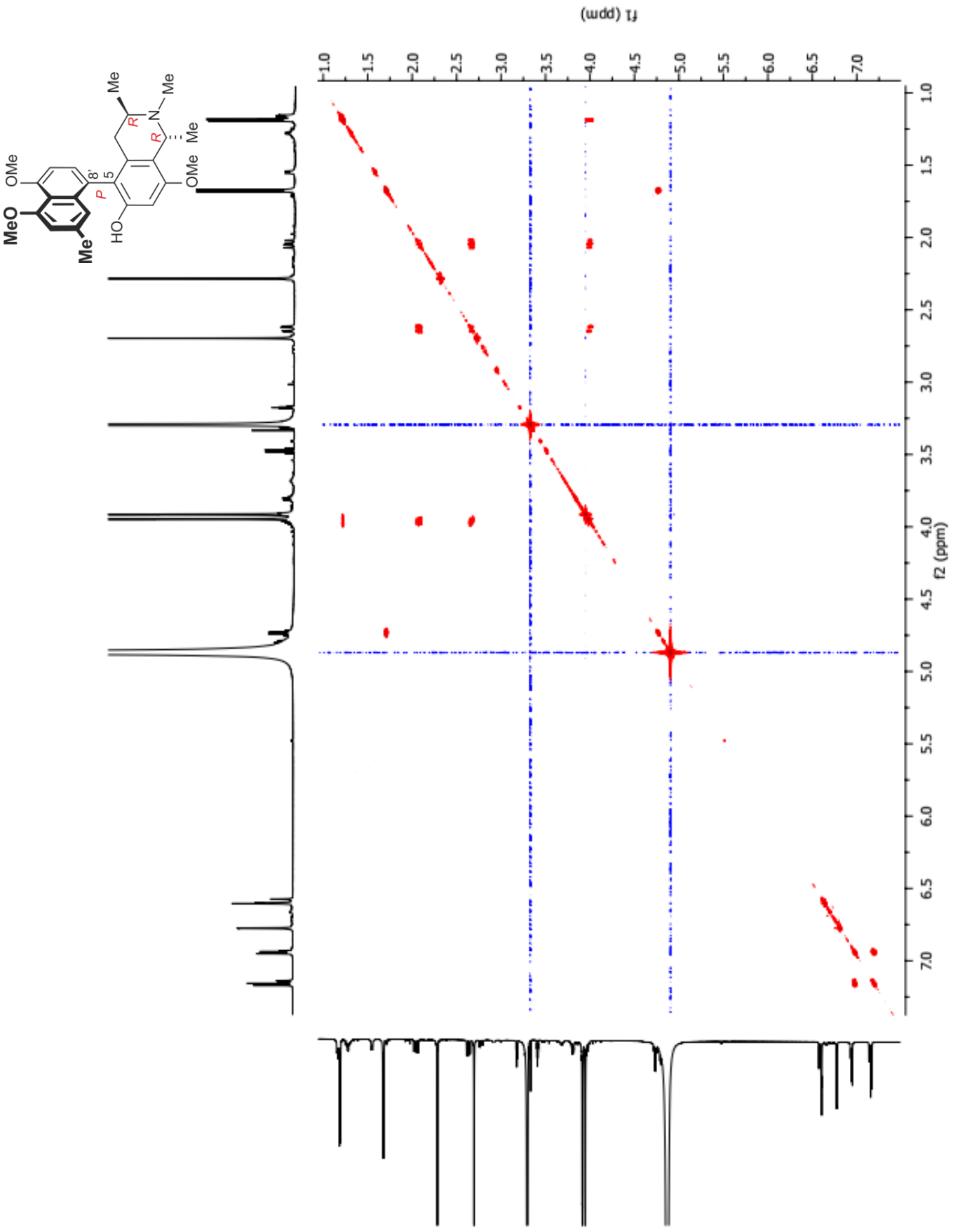


Figure S15. COSY spectrum of ancistrolikokine A_3 (**14**).

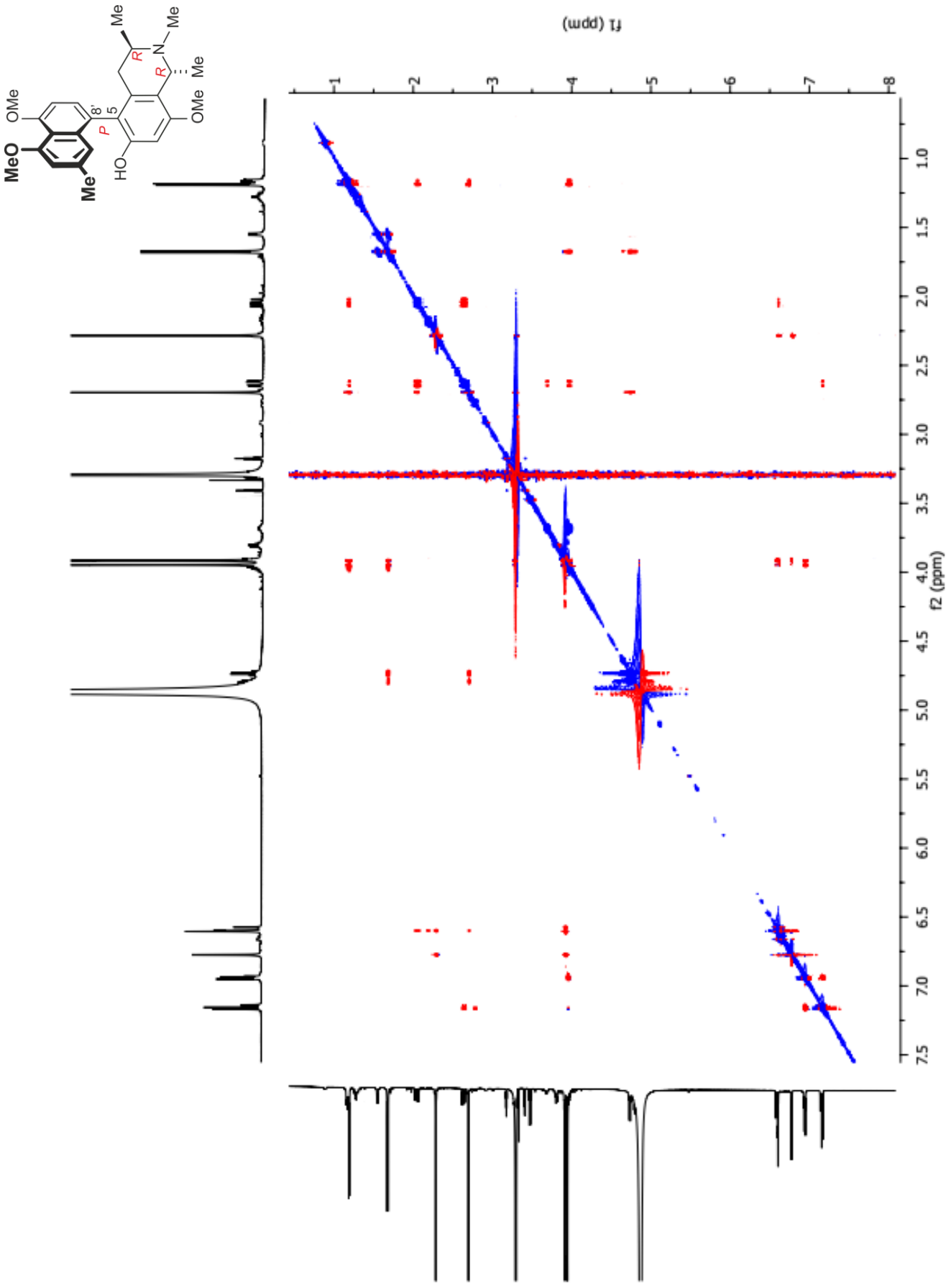


Figure S16. NOESY spectrum of ancistrolikokine A_3 (**14**).

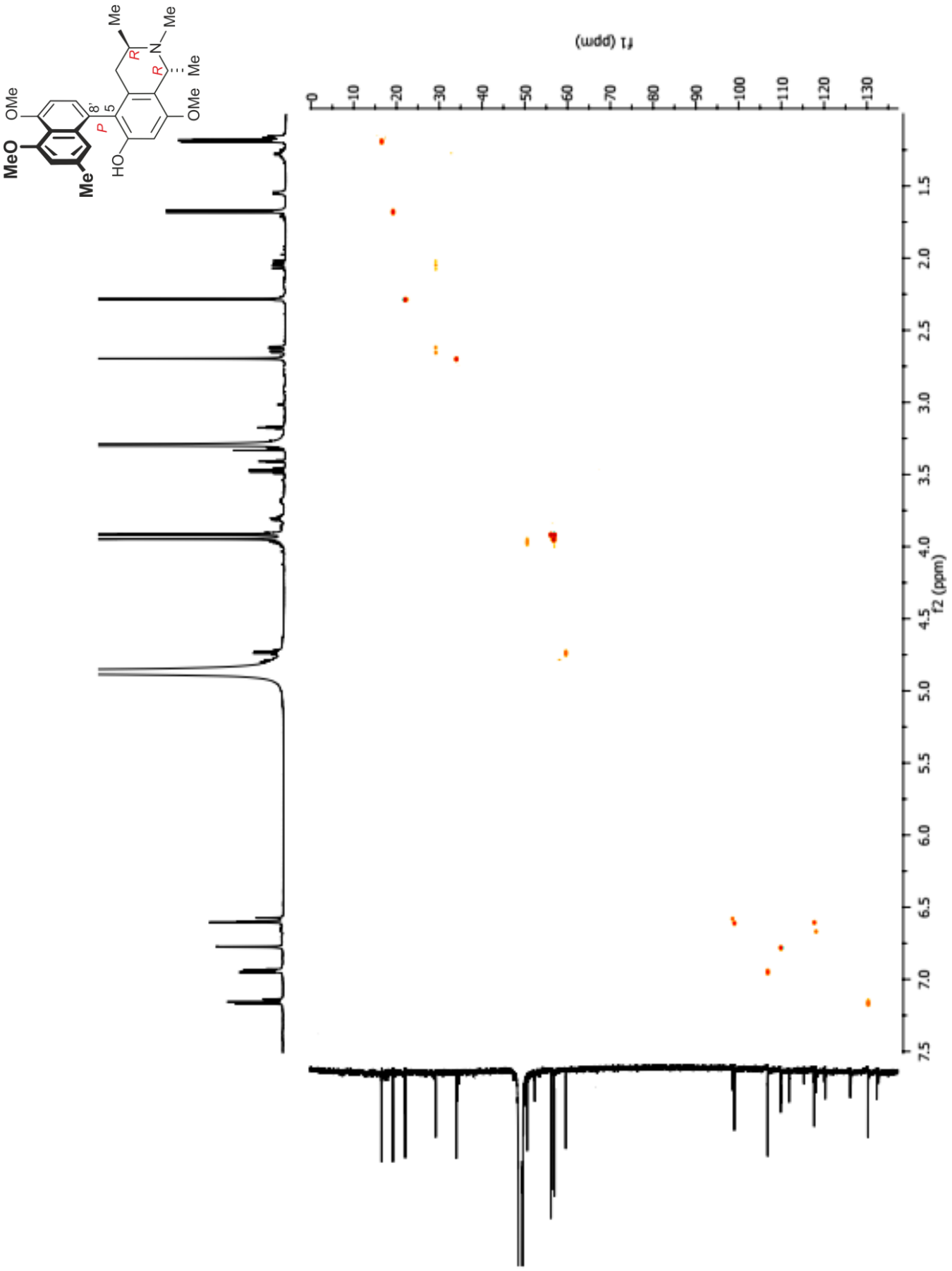


Figure S17. HSQC spectrum of ancistrolikokine A_3 (**14**).

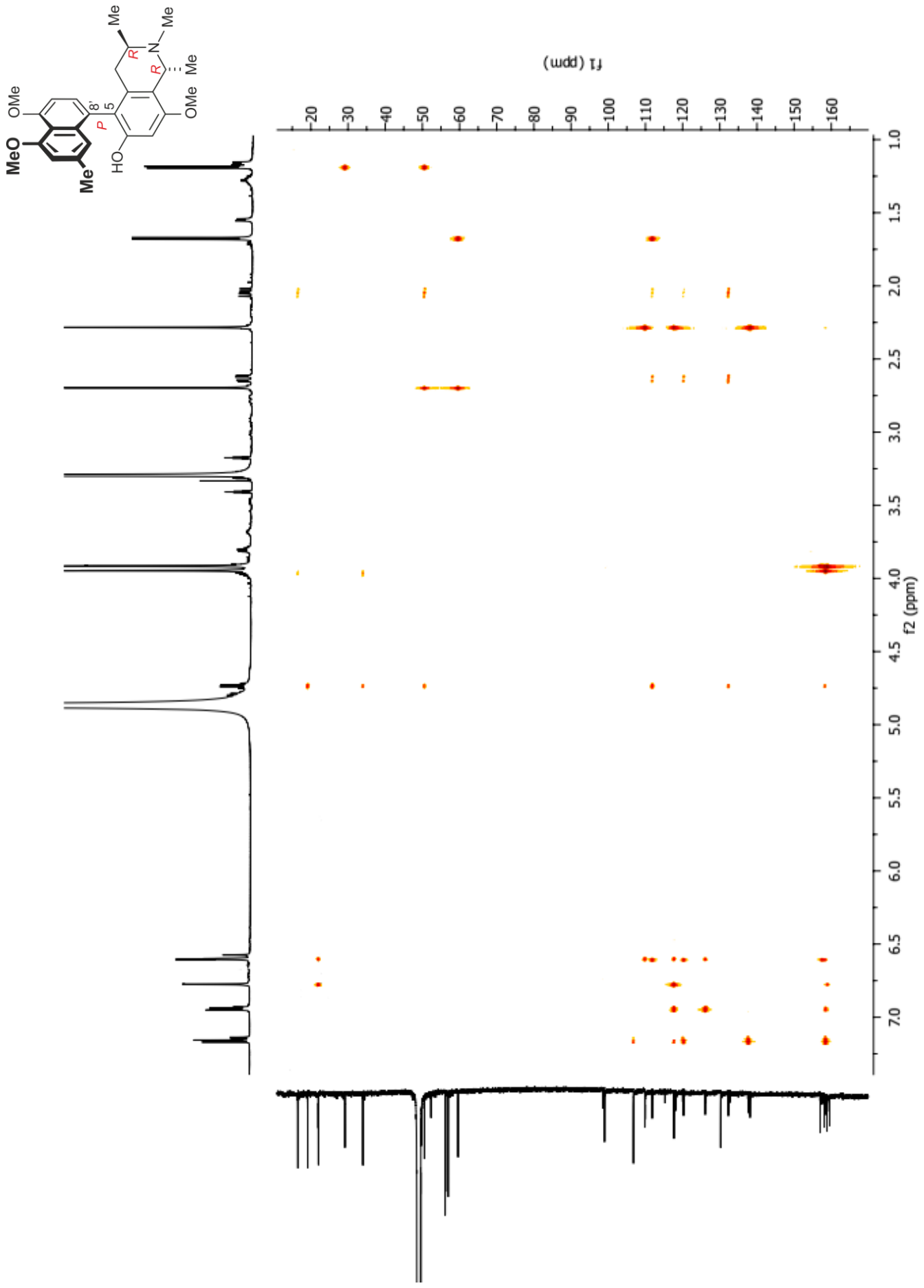
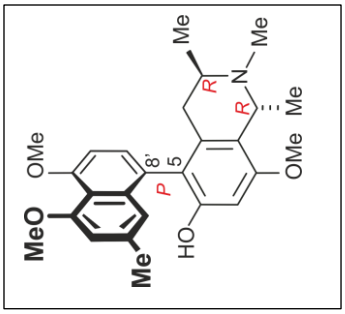


Figure S18. HMBC spectrum of ancistrolikokine A_3 (**14**).



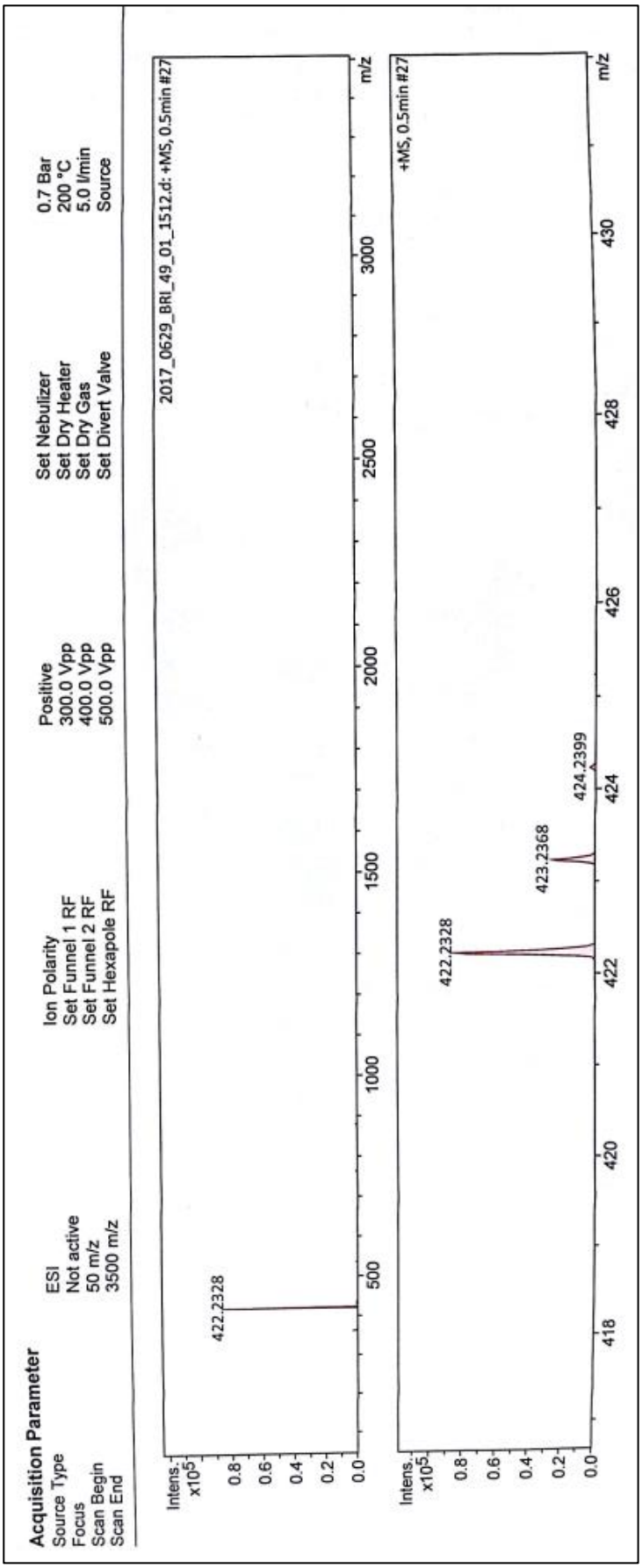
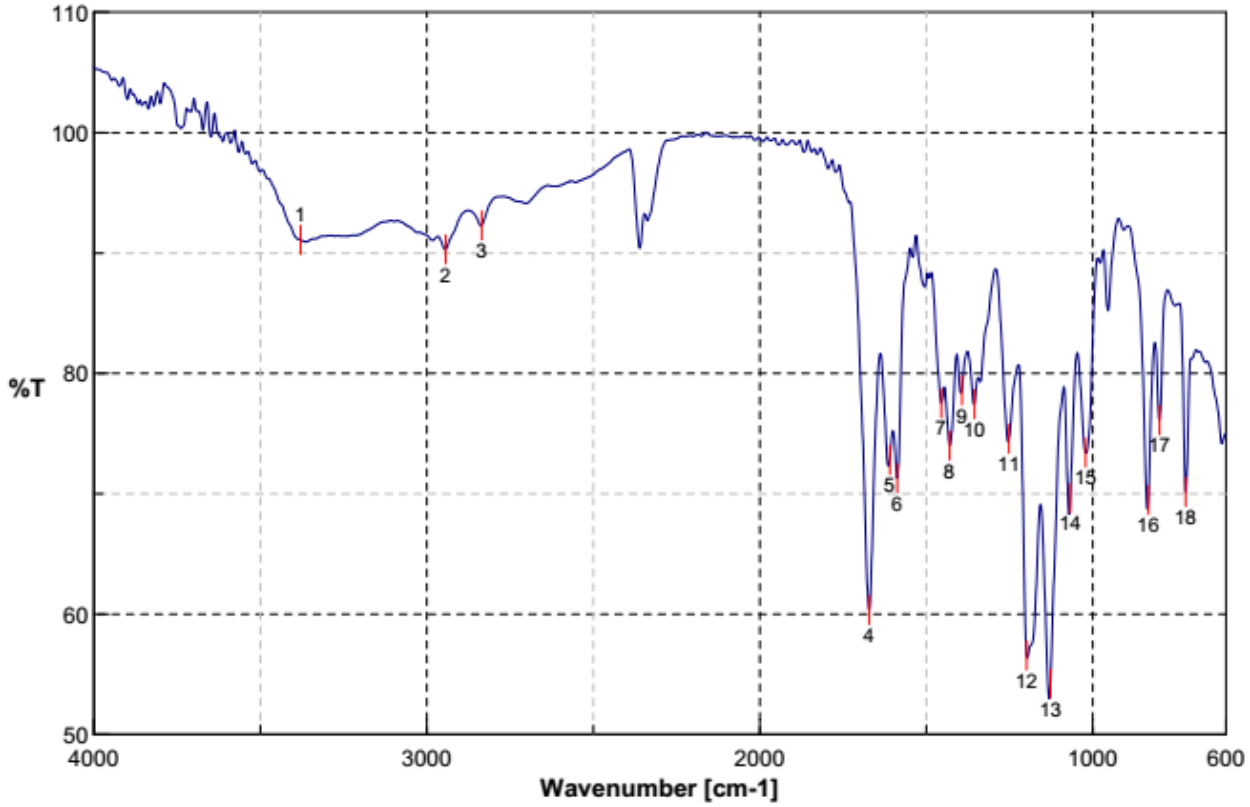


Figure S19. HRESI-MS spectrum of ancistrolikokine A_3 (**14**).



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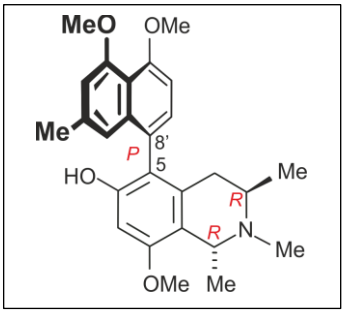

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7	1455.03	77.5322	8	1429.96	74.0047	9	1393.32	78.5954
10	1355.71	77.4521	11	1251.58	74.5724	12	1198.54	56.5815
13	1127.19	54.2445	14	1067.41	69.6287	15	1022.09	73.4356
16	833.098	69.4919	17	799.35	76.1202	18	721.247	70.1632

Figure S20. IR spectrum of ancistrolikokine A_3 (**14**).

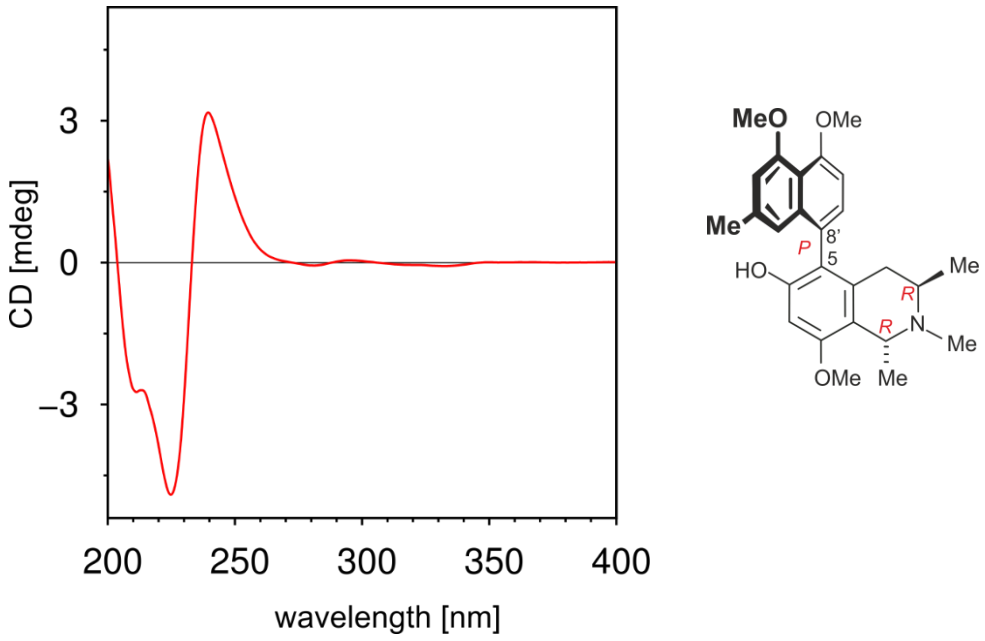
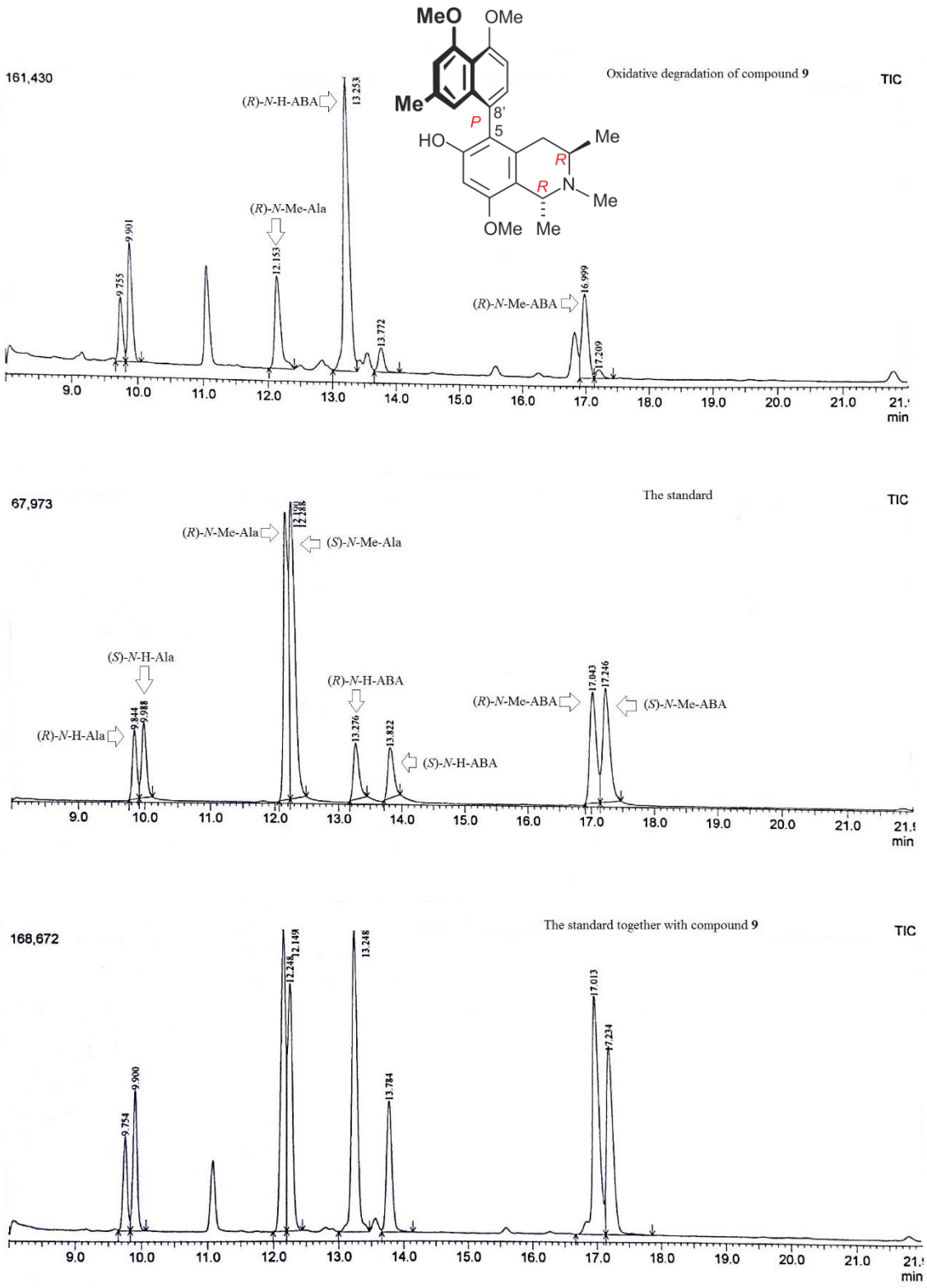


Figure S21. ECD spectrum of ancistrolikokine A_3 (**14**).



Ala = Alanine *N*-Me-Ala = *N*-Methylalanine

ABA = 3-Aminobutyric acid *N*-Me-ABA = *N*-Methyl-3-aminobutyric acid

Figure S22. Oxidative degradation products of ancistrolikokine A_3 (**14**).

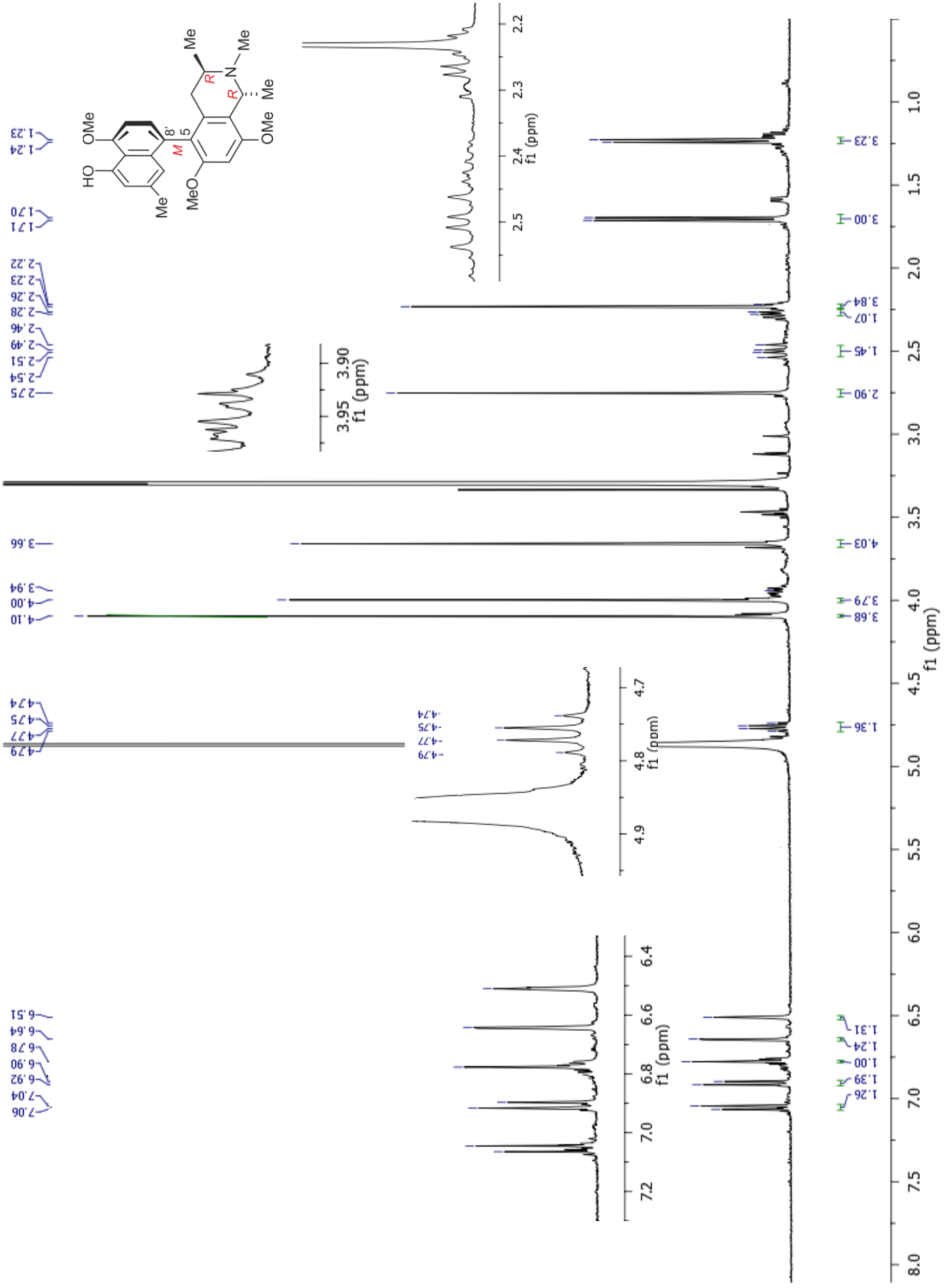


Figure S23. ^{1}H NMR spectrum of ancistrolikokine C_2 (**5**).

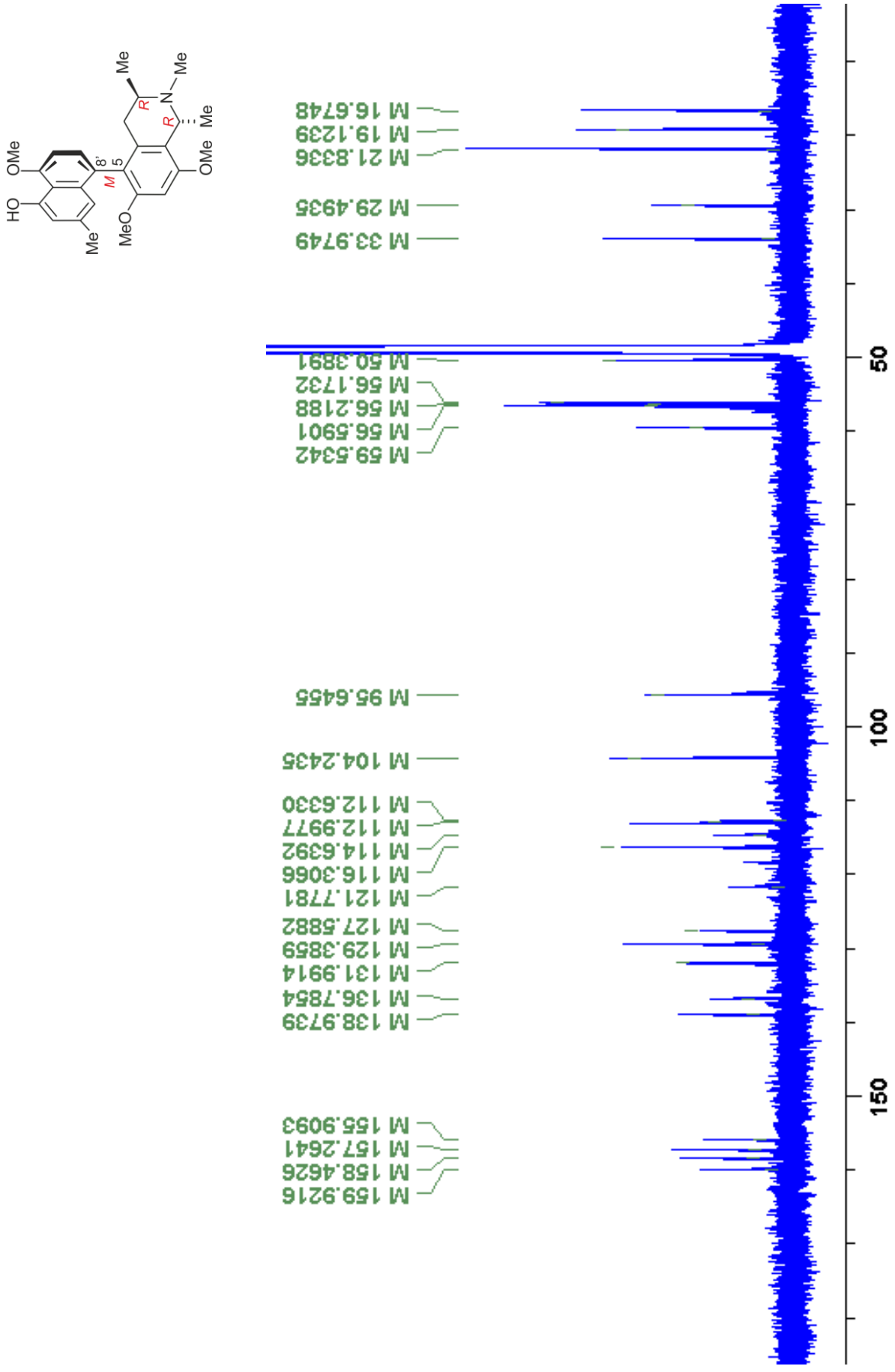


Figure S24. ^{13}C NMR spectrum of ancistrolikokine C_2 (**5**).

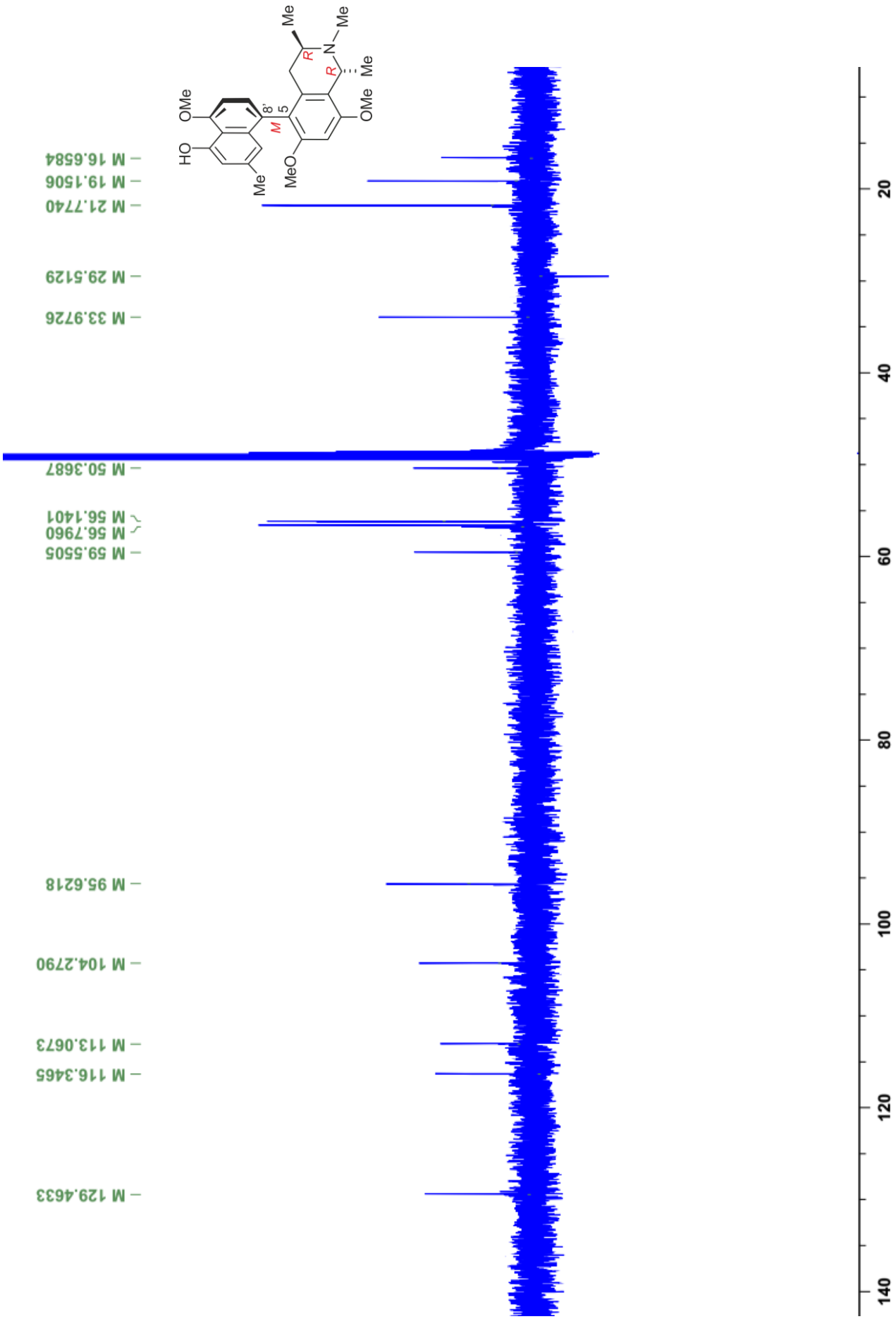


Figure S25. ^{13}C DEPT spectrum of ancistrolikokine C_2 (**5**).

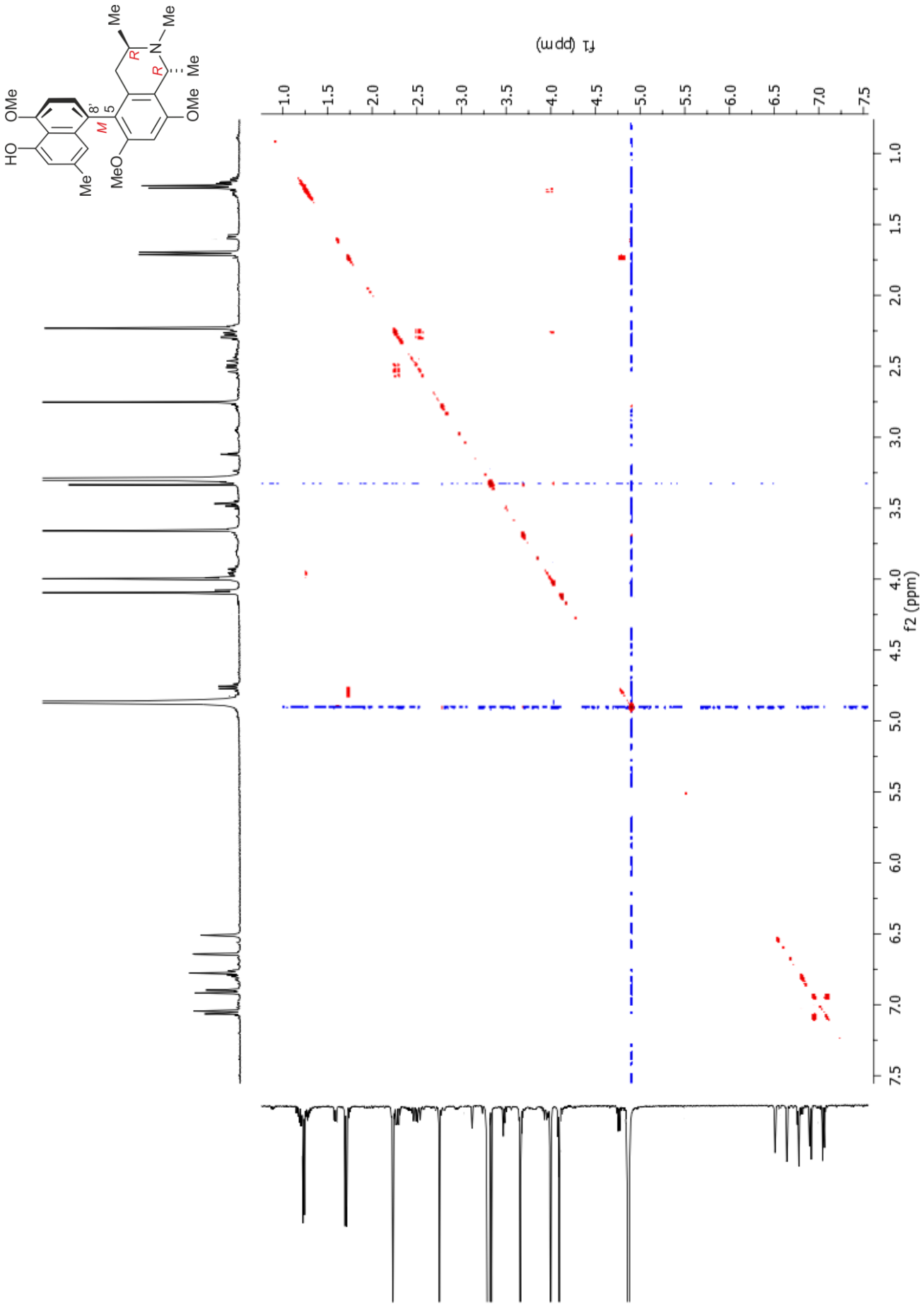


Figure S26. COSY spectrum of ancistrolikokine C_2 (**5**).

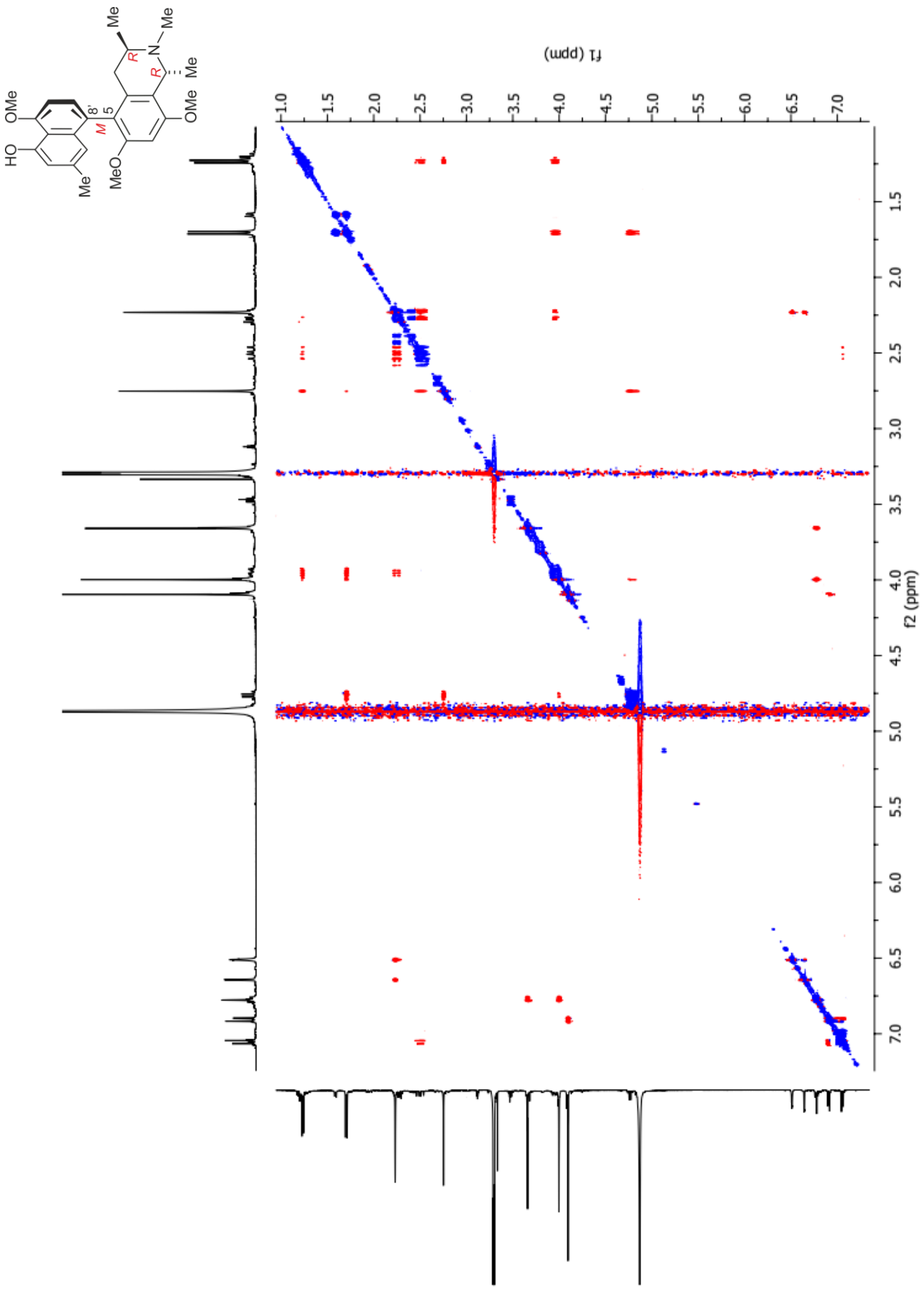


Figure S27. NOESY spectrum of ancistrolikokine C_2 (**5**).

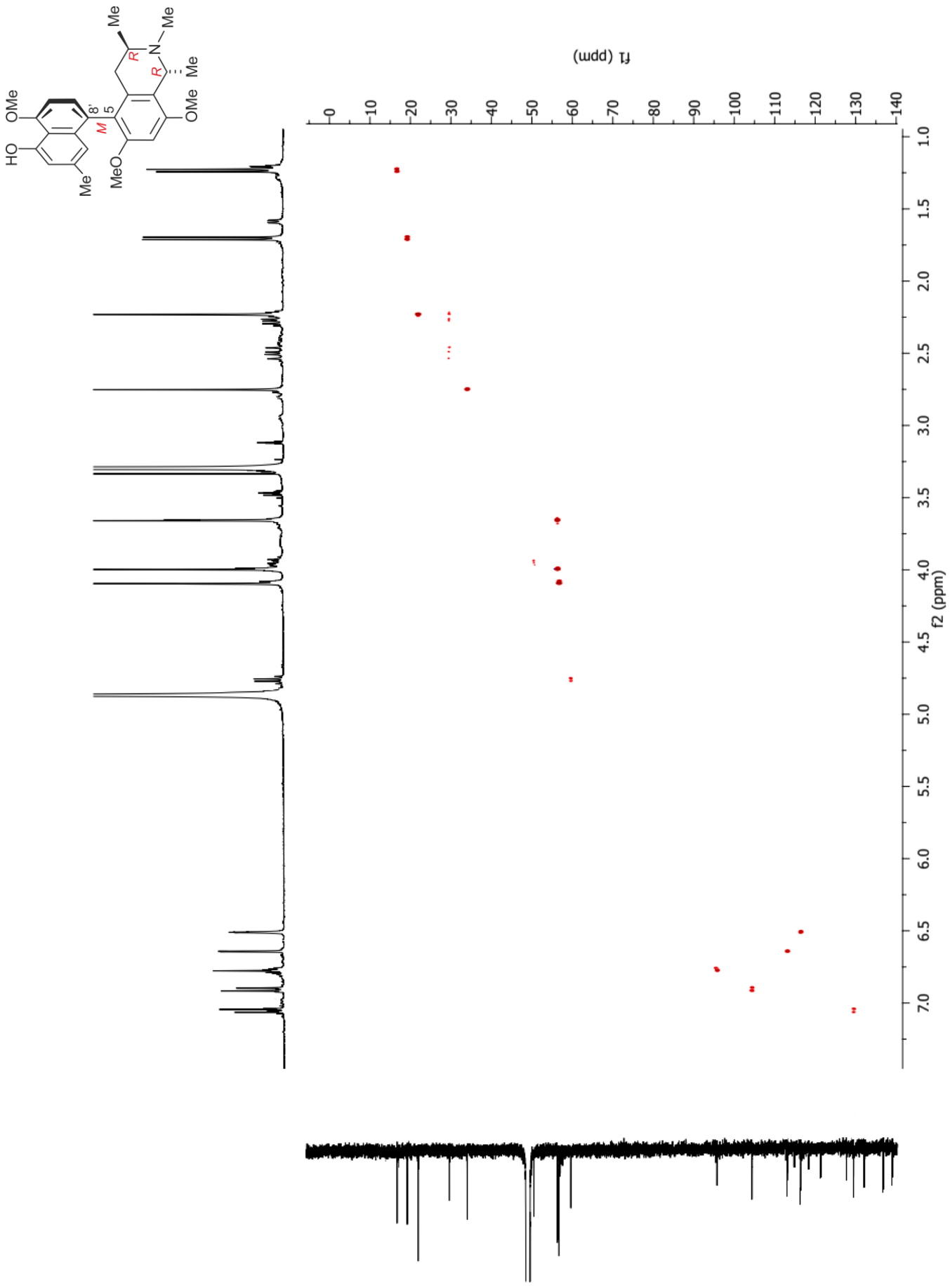


Figure S28. HSQC spectrum of ancistrolikokine C_2 (**5**).

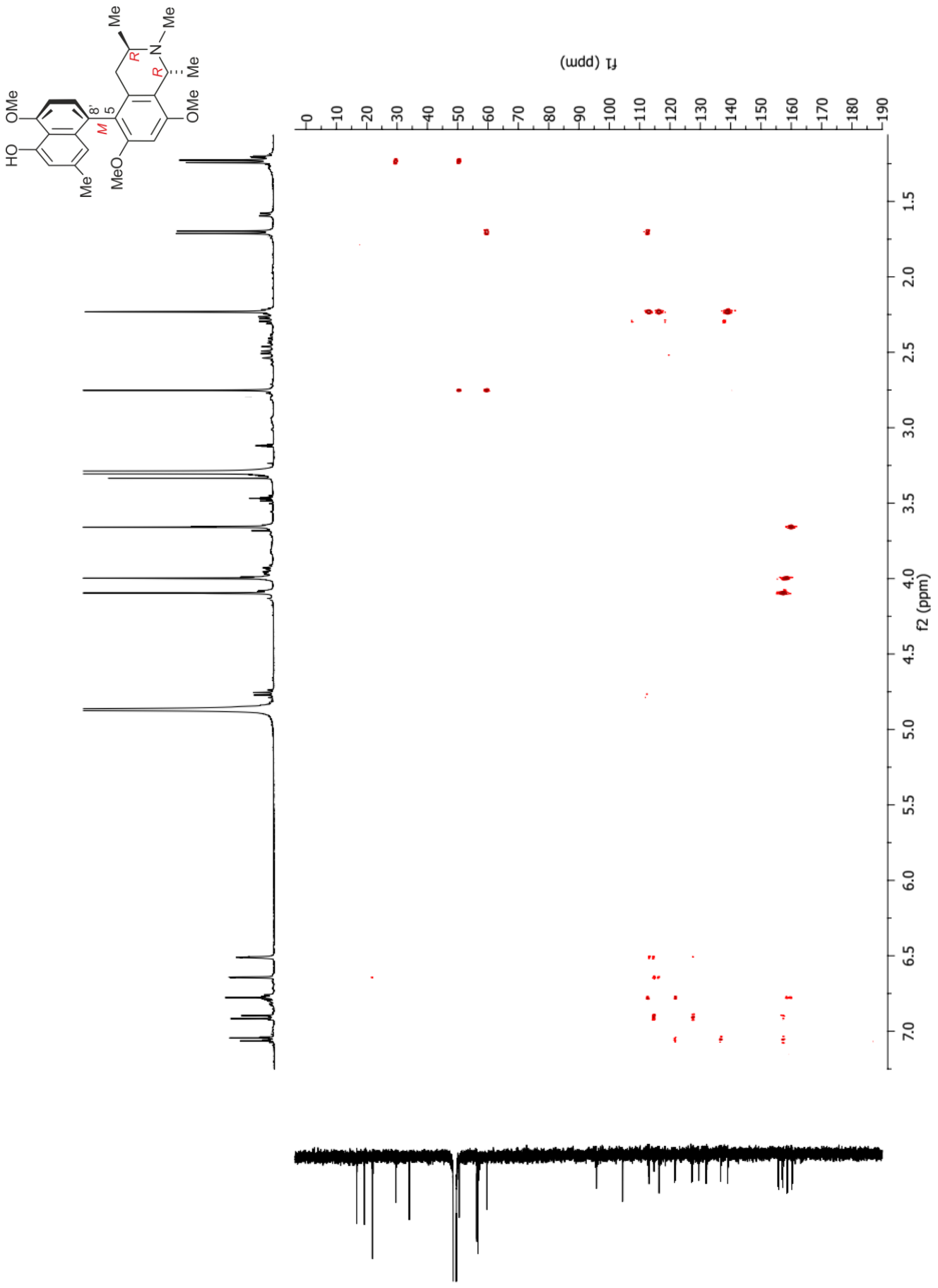
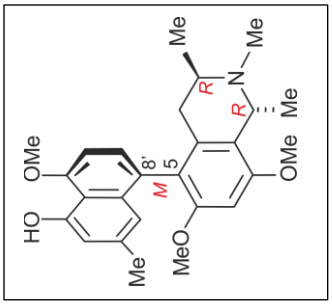


Figure S29. HMBC spectrum of ancistrolikokine C_2 (**5**).



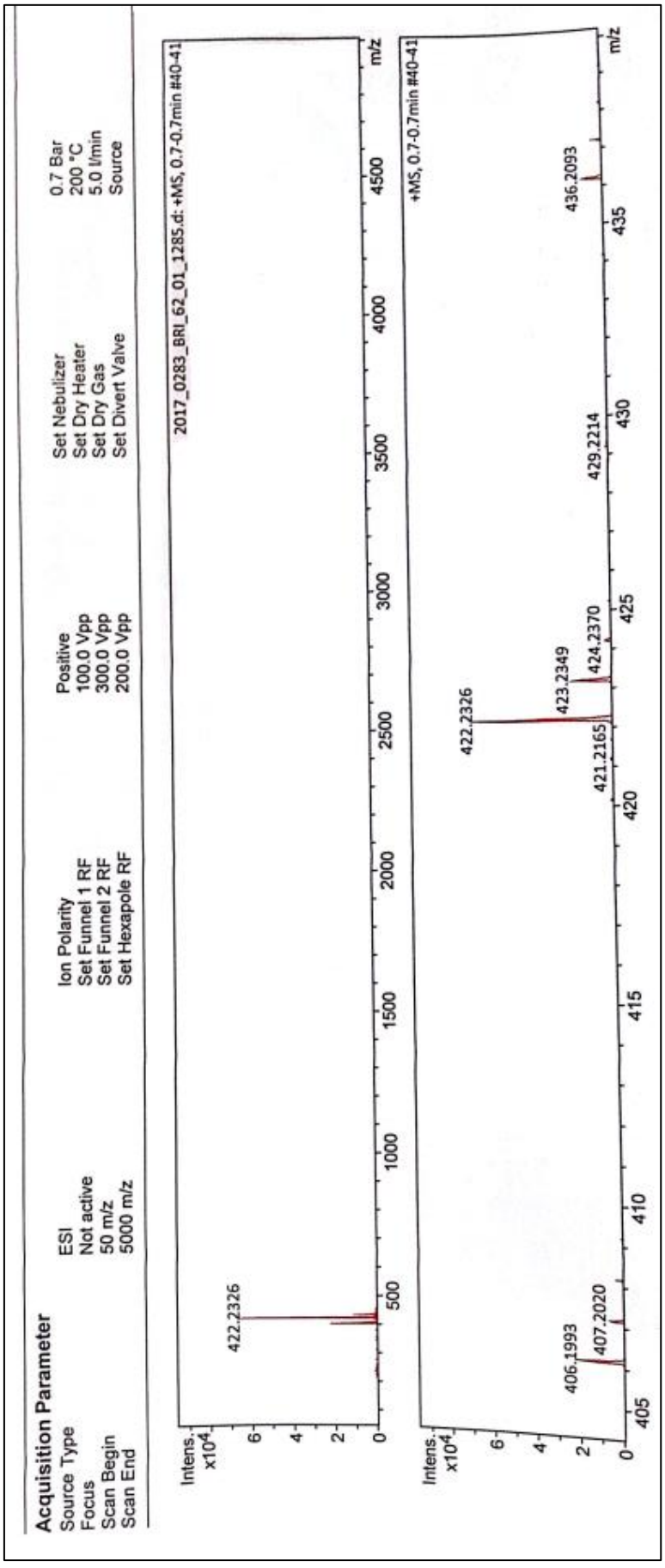
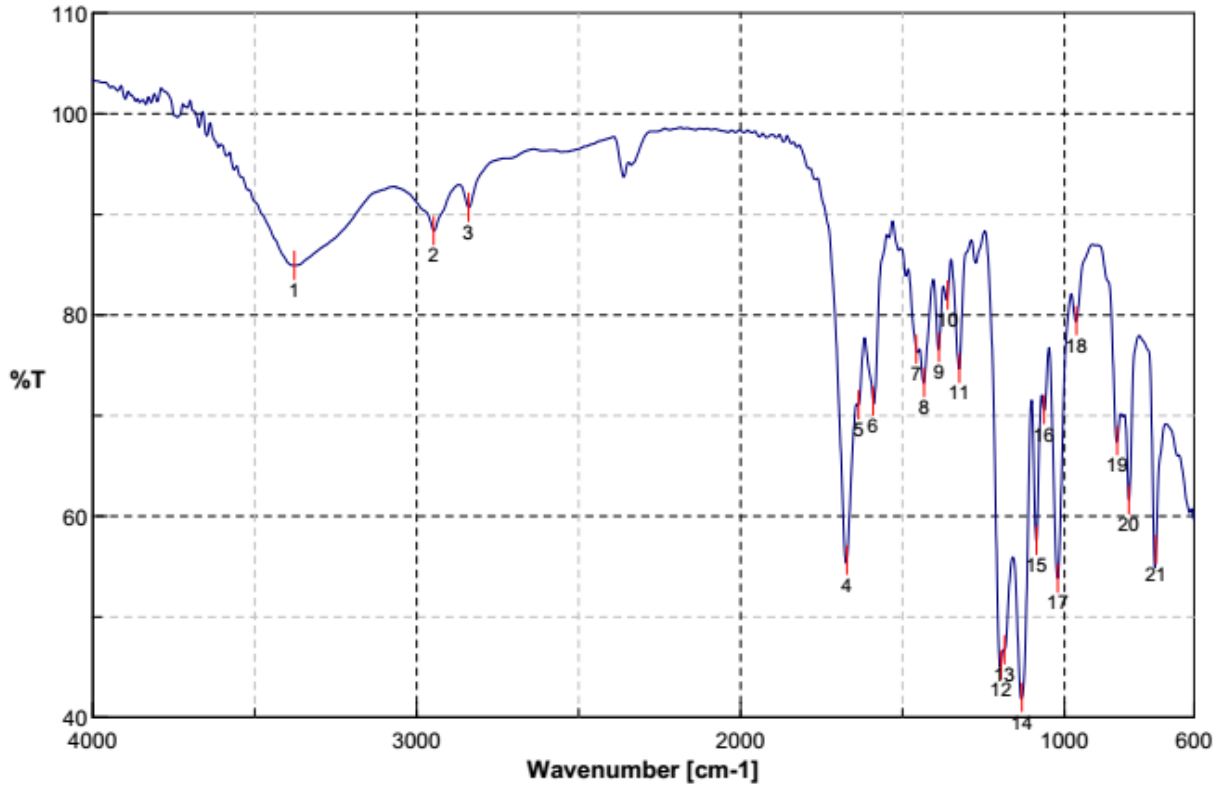


Figure S30. HRESI-MS spectrum of ancistrolikokine C_2 (**5**).



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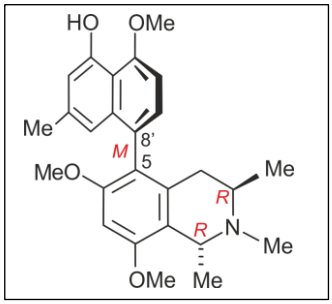

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7	1457.92	76.6202	8	1433.82	73.2977	9	1387.53	76.782
10	1360.53	81.9906	11	1324.86	74.6841	12	1196.61	45.2105
13	1185.04	46.7206	14	1131.05	42.005	15	1086.69	57.6038
16	1063.55	70.6183	17	1021.12	53.8294	18	963.269	79.4352
19	836.955	67.5177	20	801.278	61.6416	21	717.39	56.691

Figure S31. IR spectrum of ancistrolikokine C_2 (**5**).

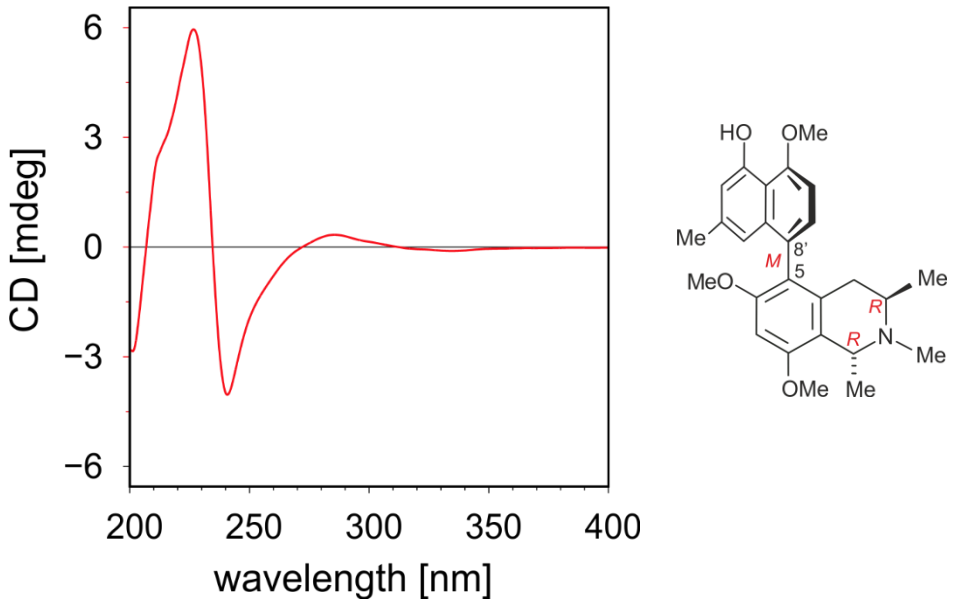
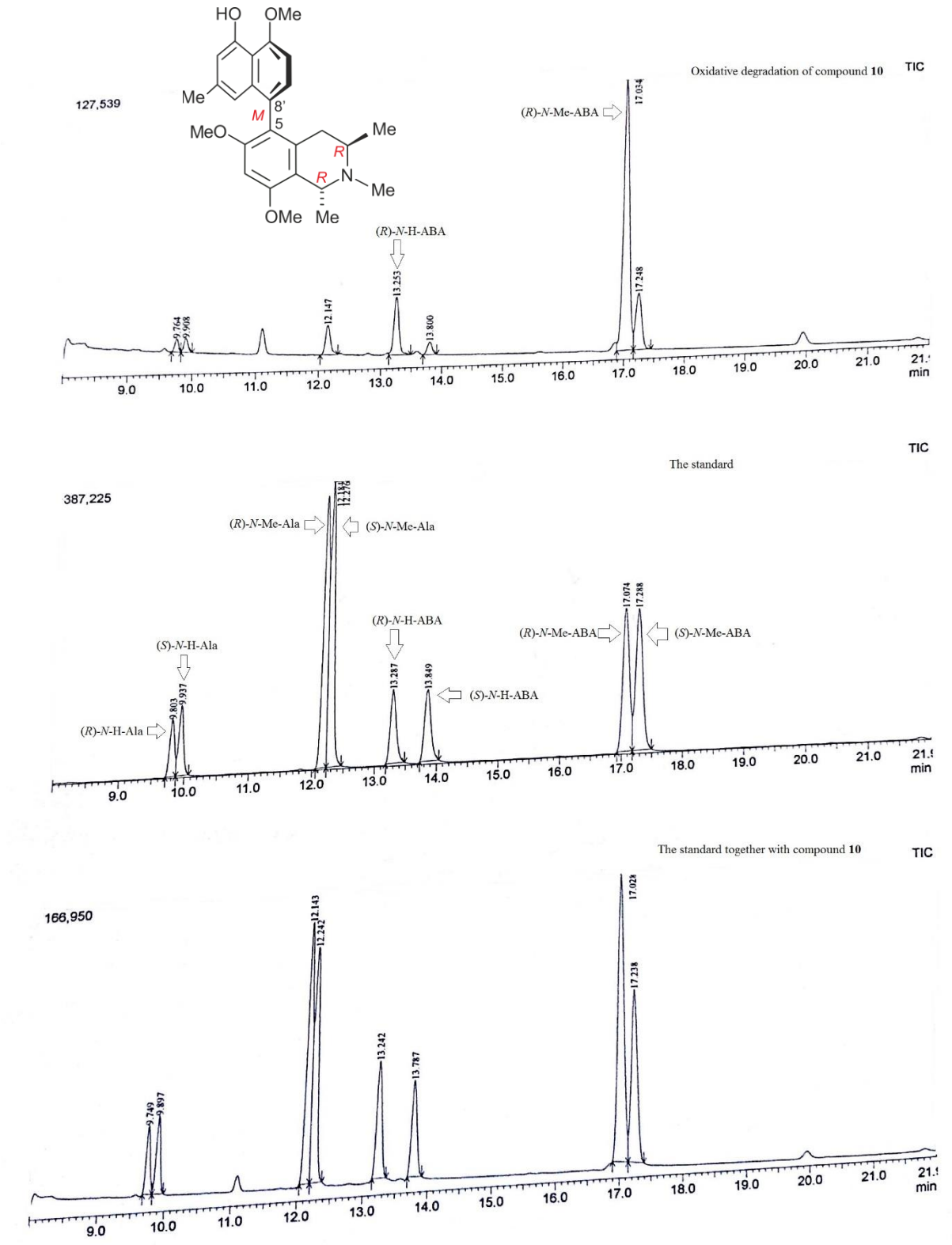


Figure S32. ECD spectrum of ancistrolikokine C_2 (**5**).



Ala = Alanine *N*-Me-Ala = *N*-Methylalanine

ABA = 3-Aminobutyric acid *N*-Me-ABA = *N*-Methyl-3-aminobutyric acid

Figure S33. Oxidative degradation products of ancistrolikokine C_2 (**5**).

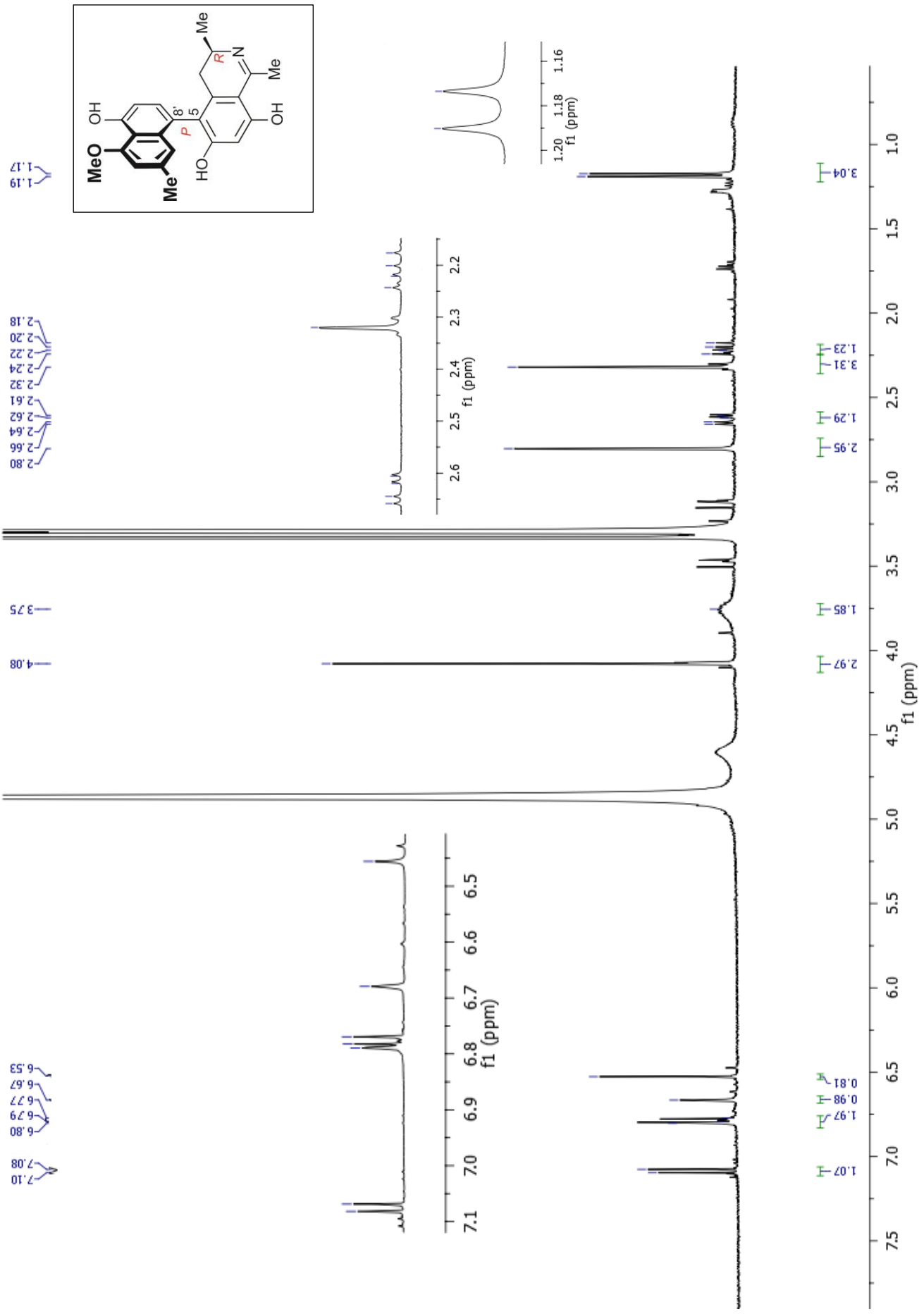


Figure S34. ^{1}H NMR spectrum of ancistrolikokine E (**9**).

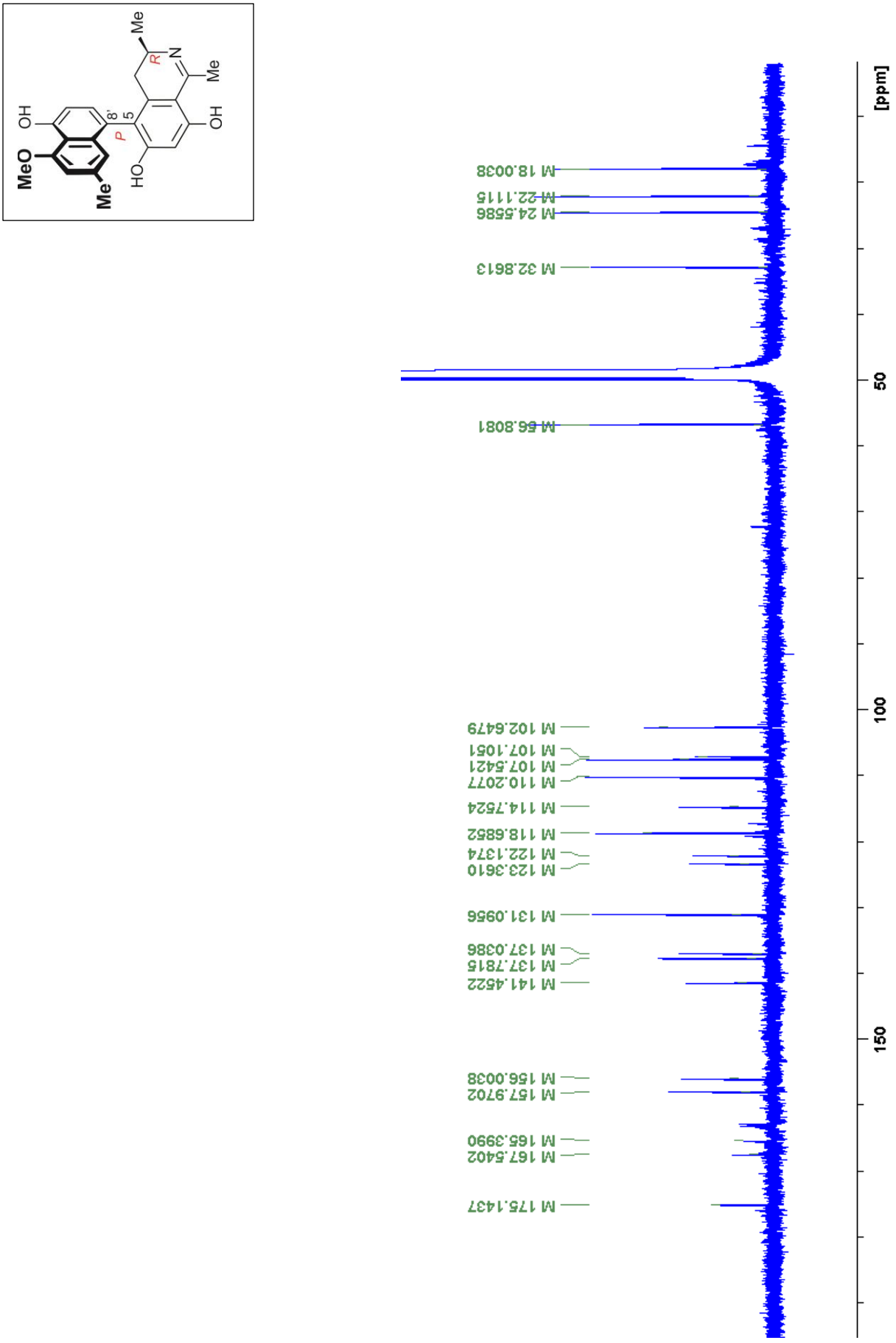


Figure S35. ^{13}C NMR spectrum of ancistrolikokine E (**9**).

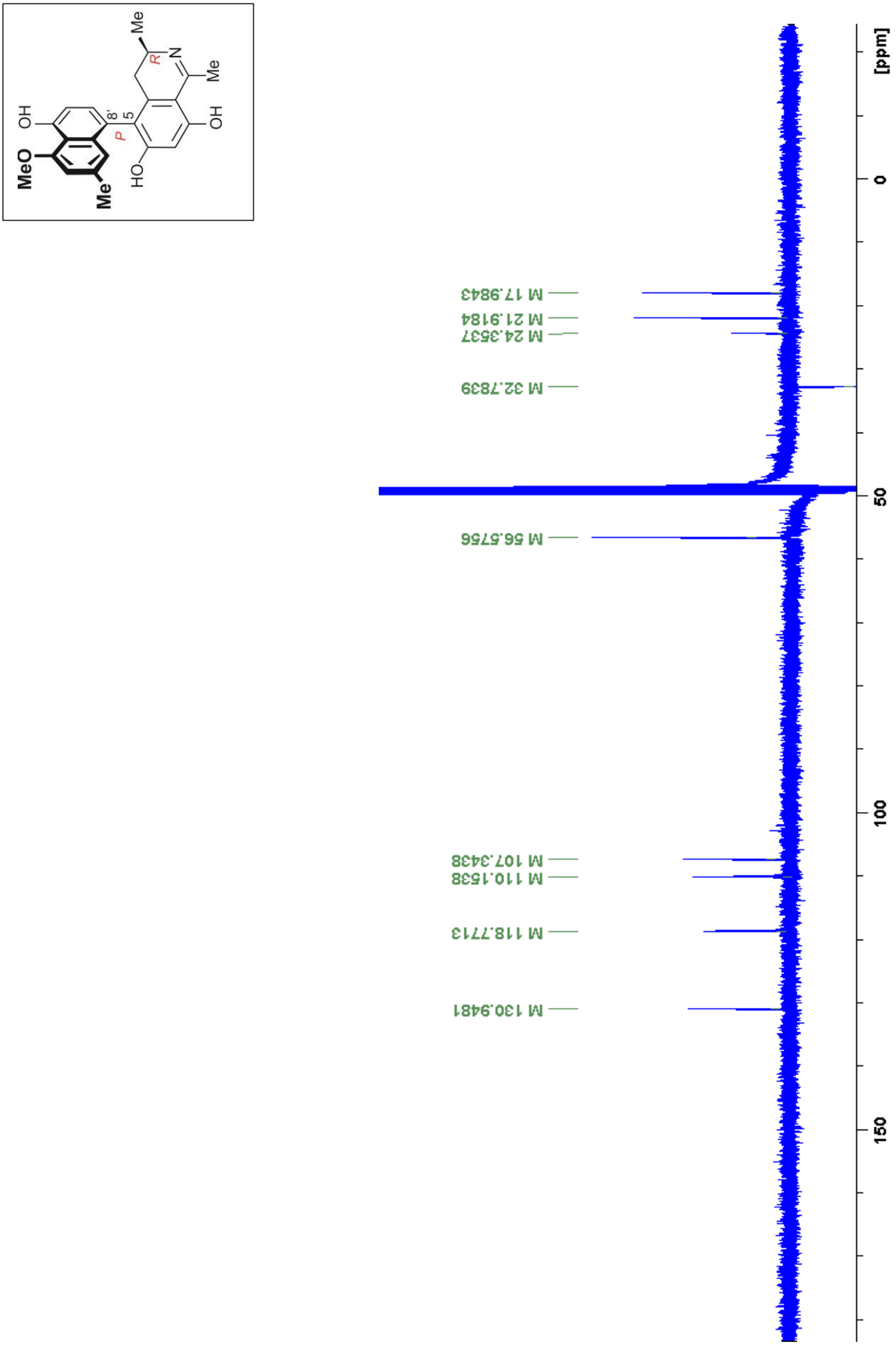


Figure S36. ^{13}C DEPT NMR spectrum of ancistrolikokine E (**9**).

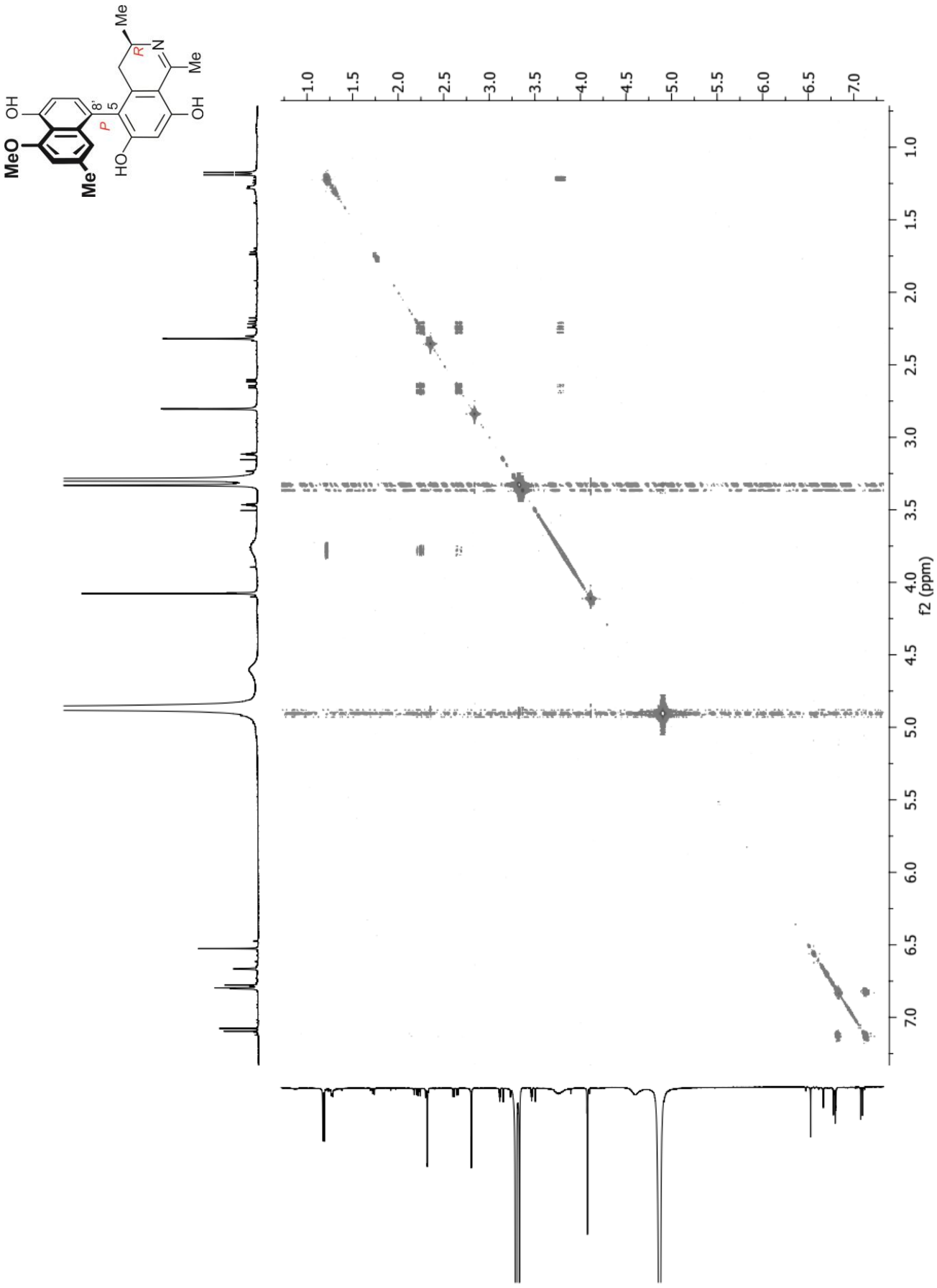


Figure S37. COSY spectrum of ancistrolikokine E (**9**).

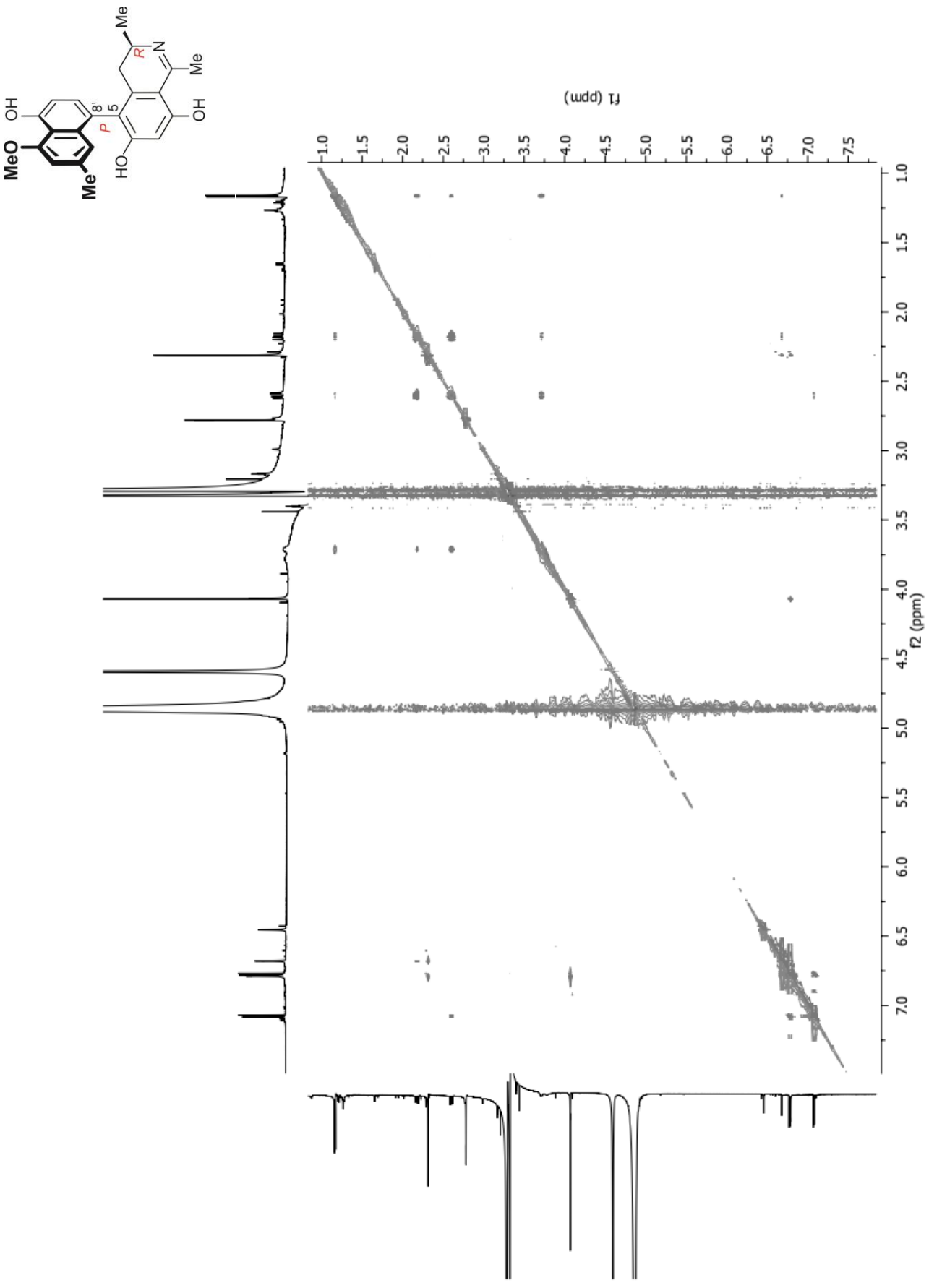


Figure S38. NOESY spectrum of ancistrolikokine E (**9**).

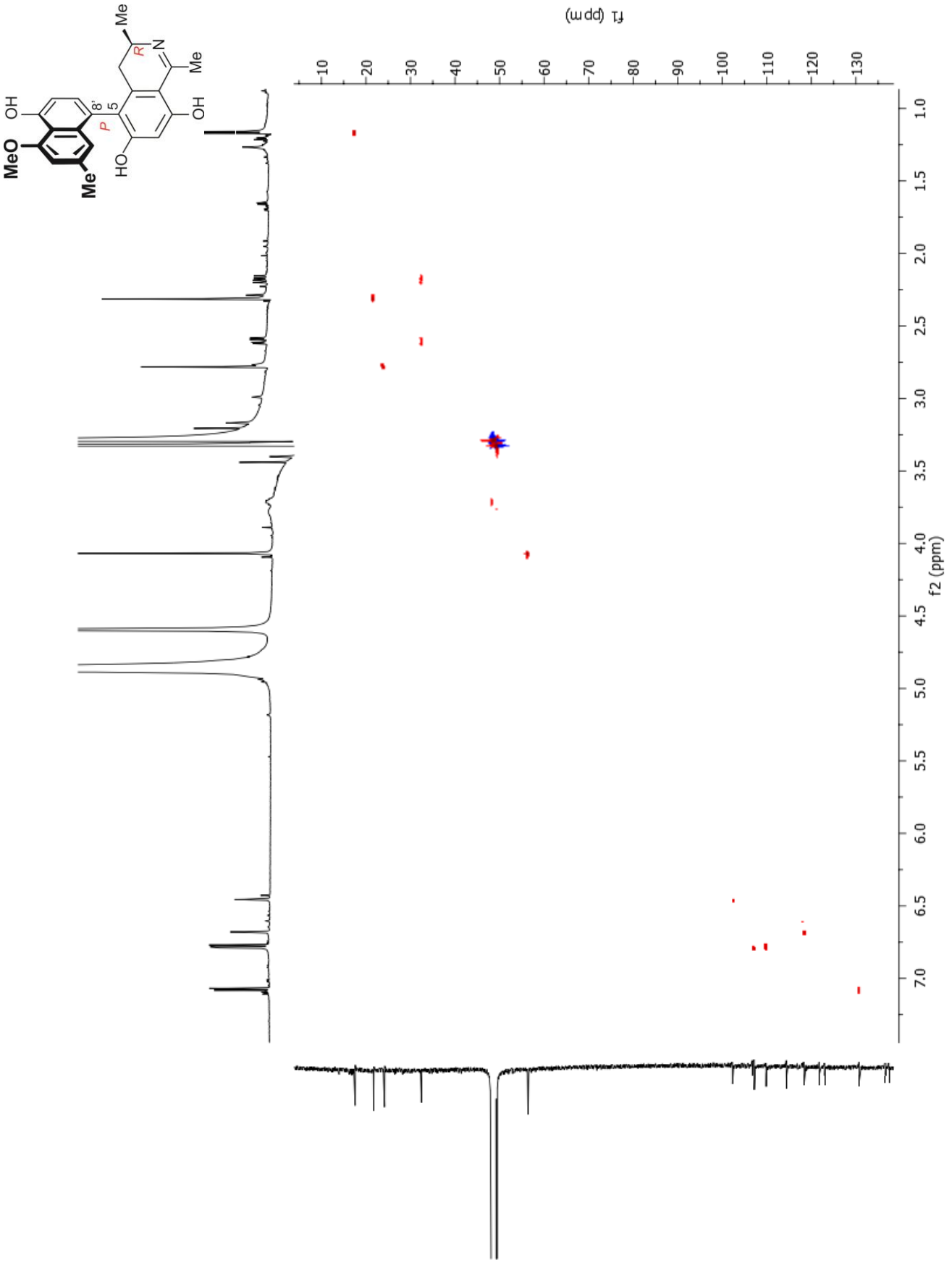


Figure S39. HSQC spectrum of ancistrolikokine E (**9**).

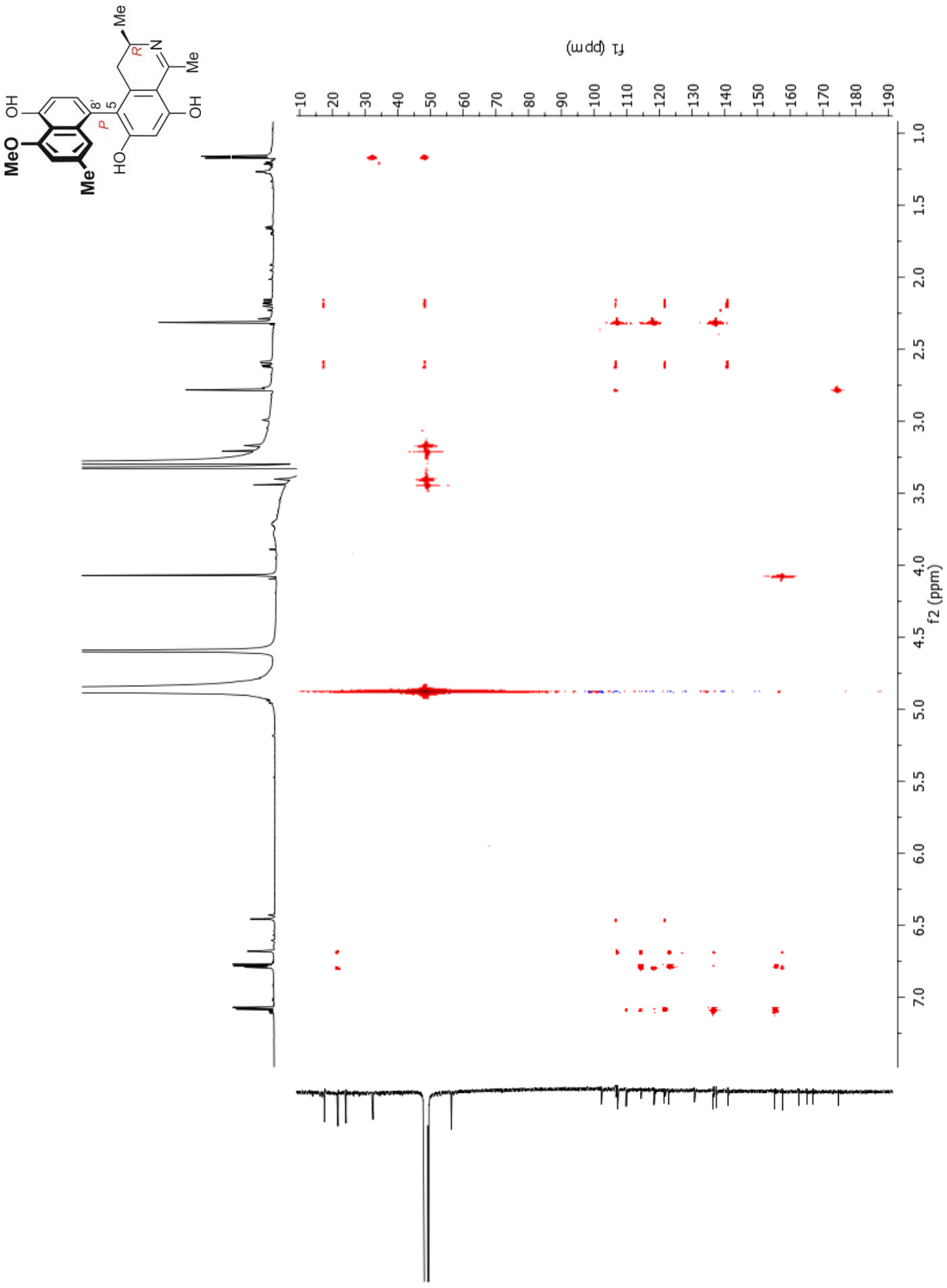
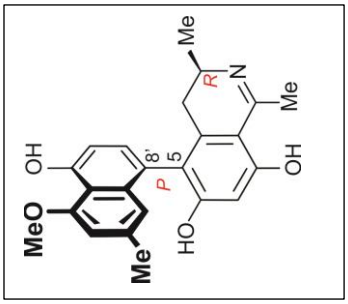


Figure S40. HMBC spectrum of ancistrolikokine E (**9**).



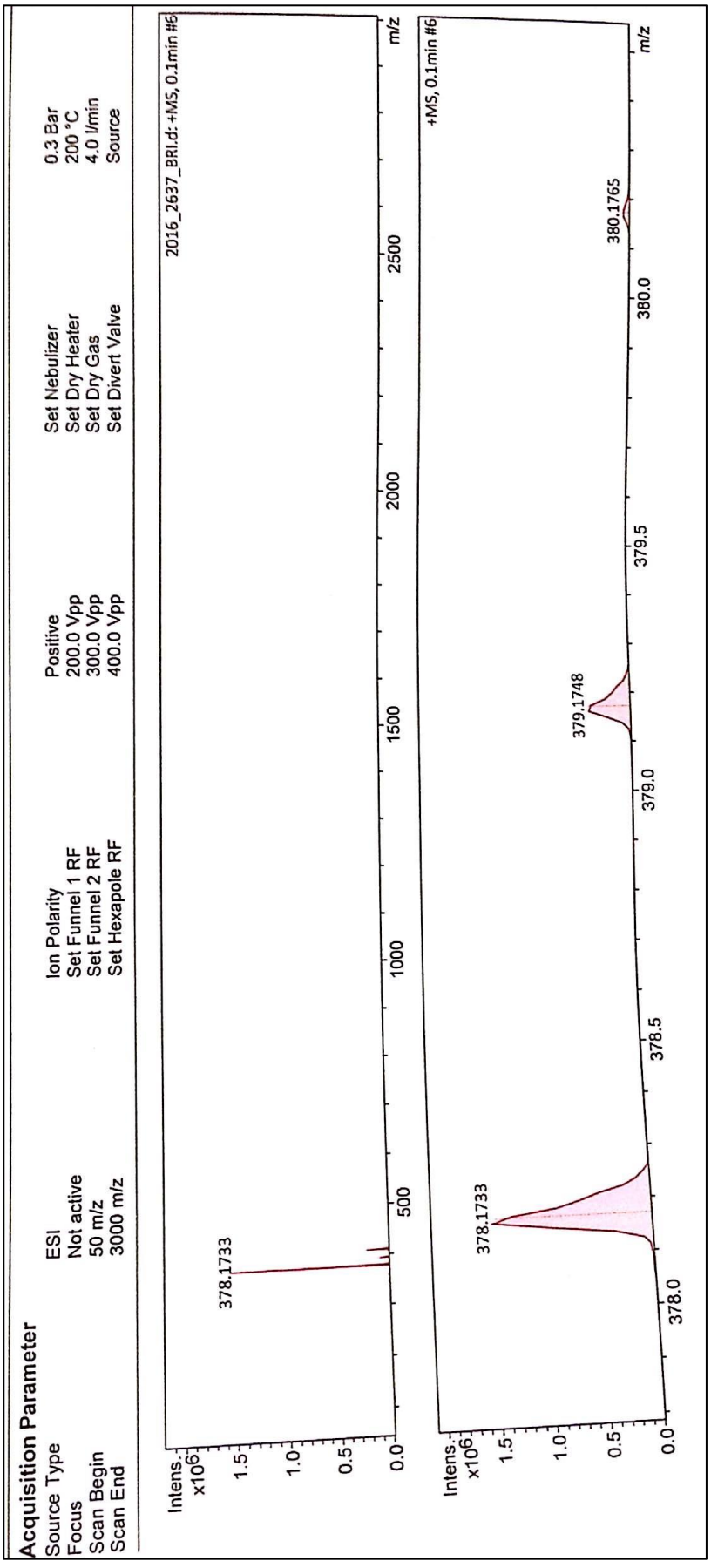


Figure S41. HRESI-MS spectrum of ancistrolikokine E (**9**).

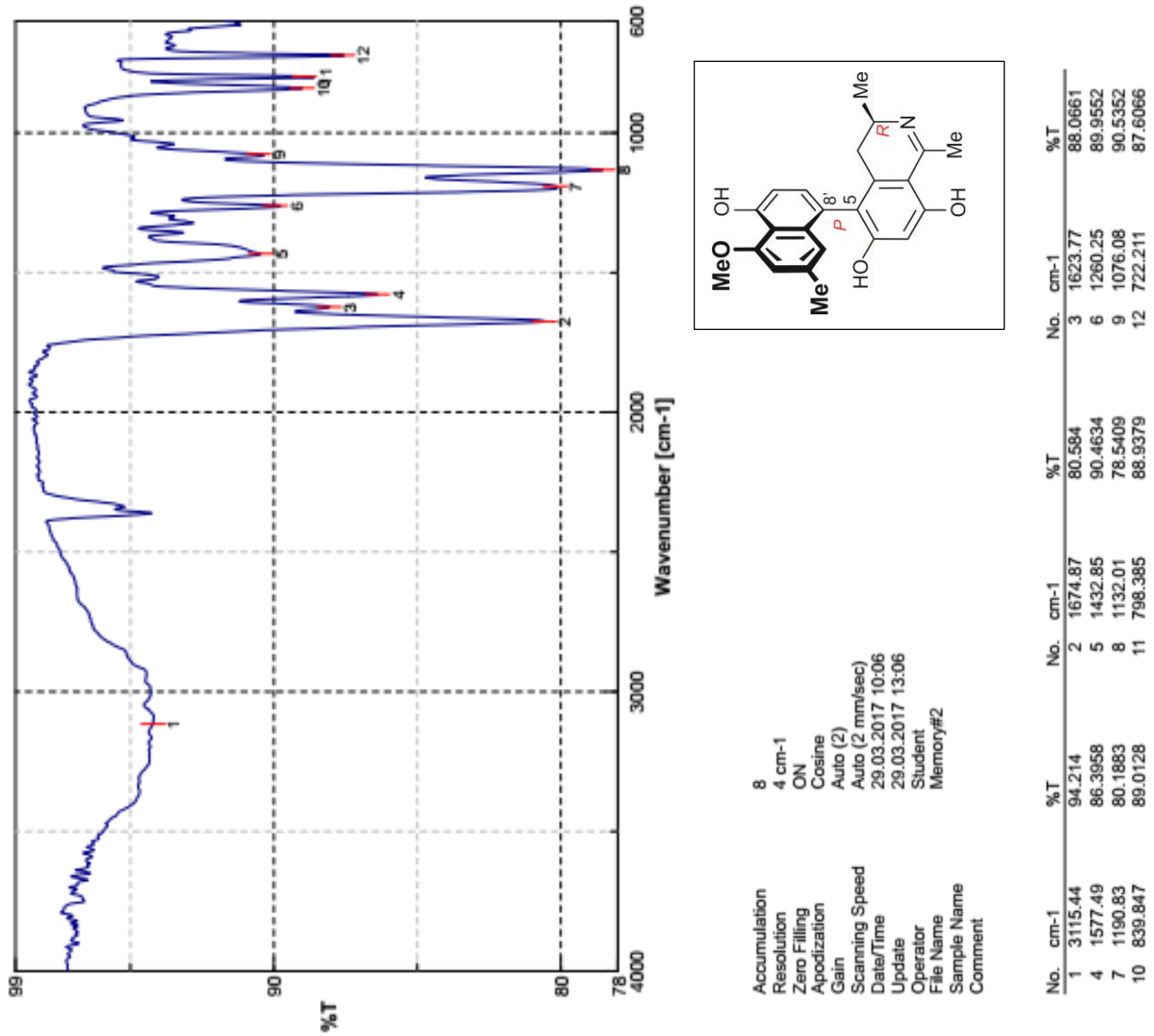


Figure S42. IR spectrum of ancistrolikokine E (**9**).

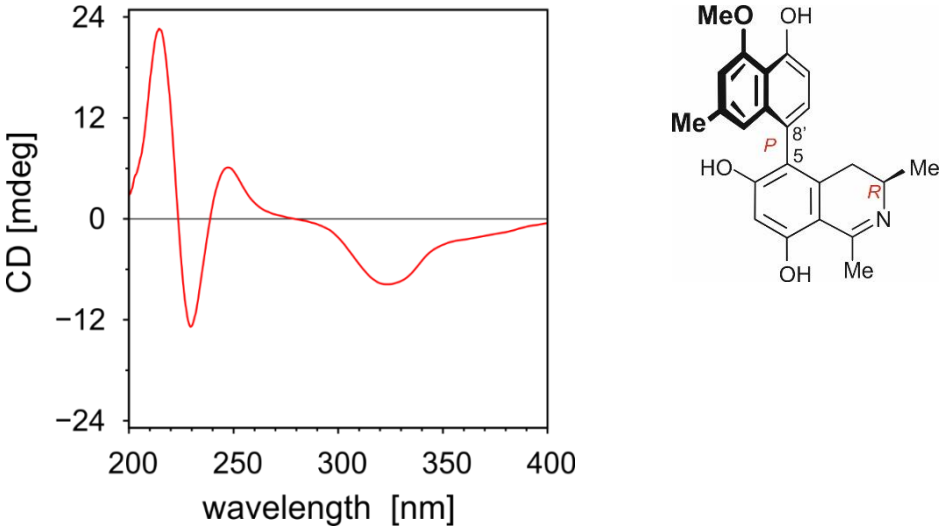
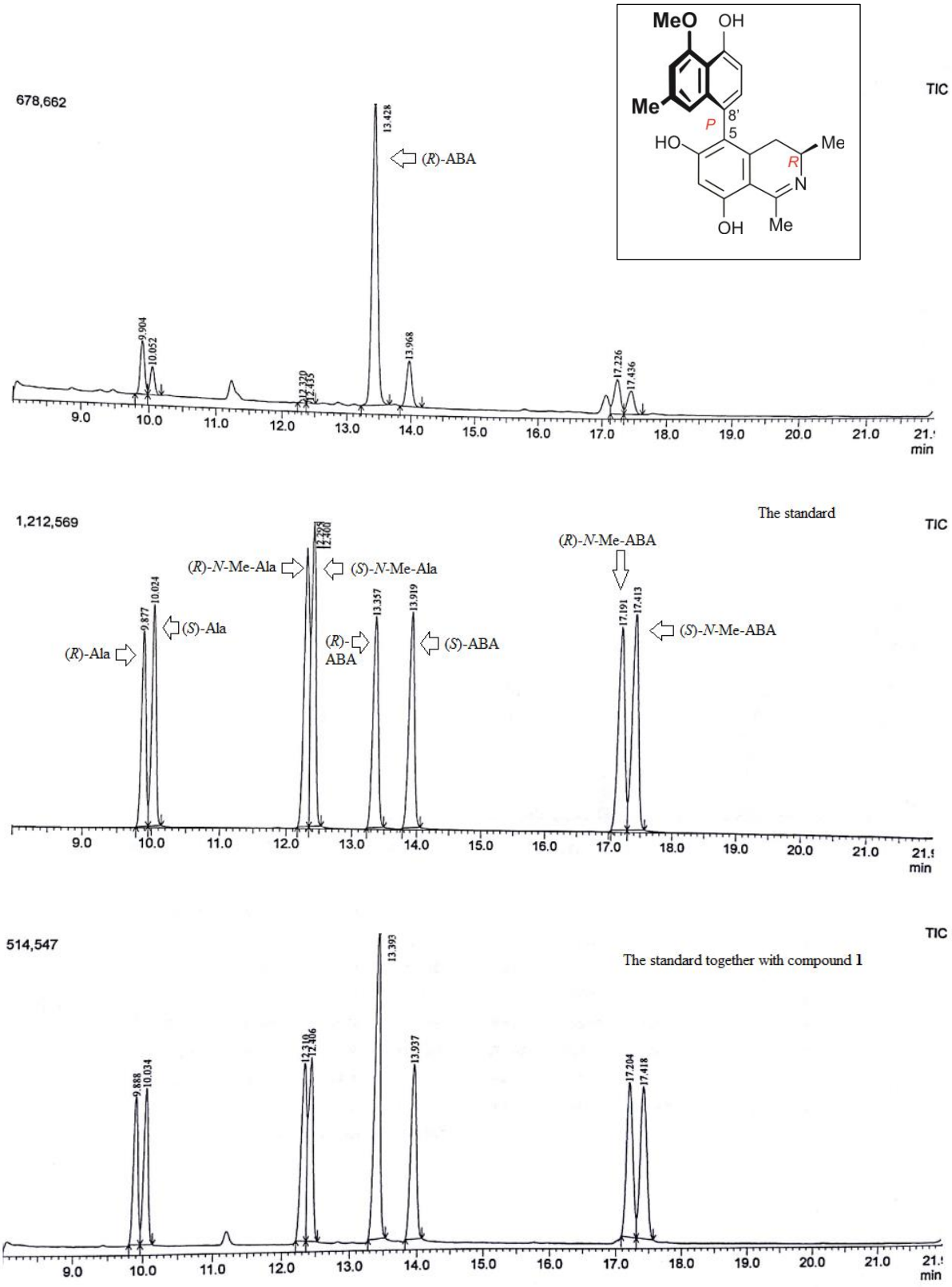


Figure S43. ECD spectrum of ancistrolikokine E (**9**).



Ala = Alanine *N*-Me-Ala = *N*-Methylalanine

ABA = 3-Aminobutyric acid *N*-Me-ABA = *N*-Methyl-3-aminobutyric acid

Figure S44. Oxidative degradation products of ancistrolikokine E (**9**).

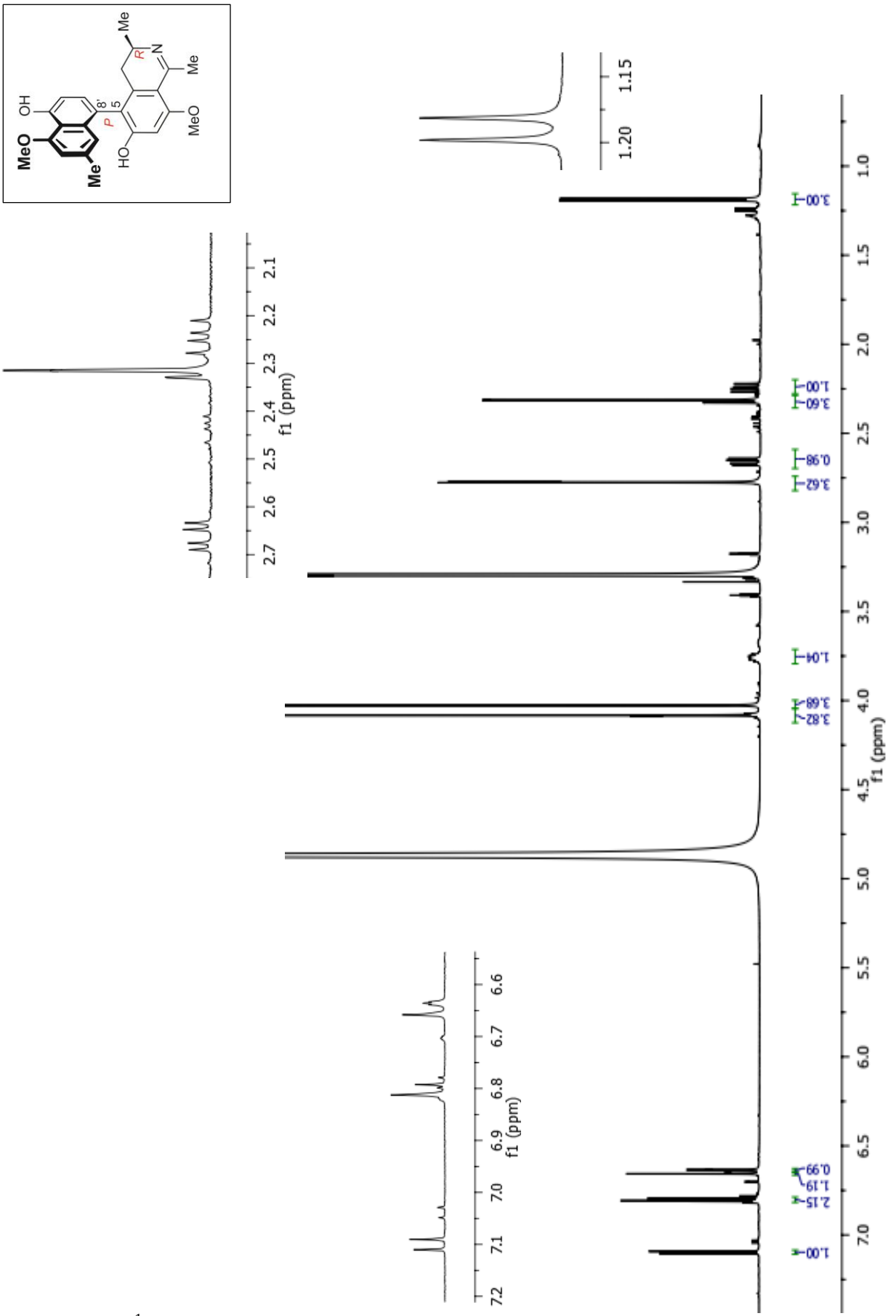
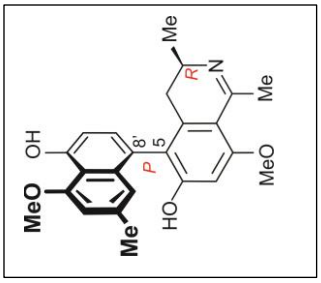


Figure S45. ^{1}H NMR spectrum of ancistrolikokine E_2 (**10**).



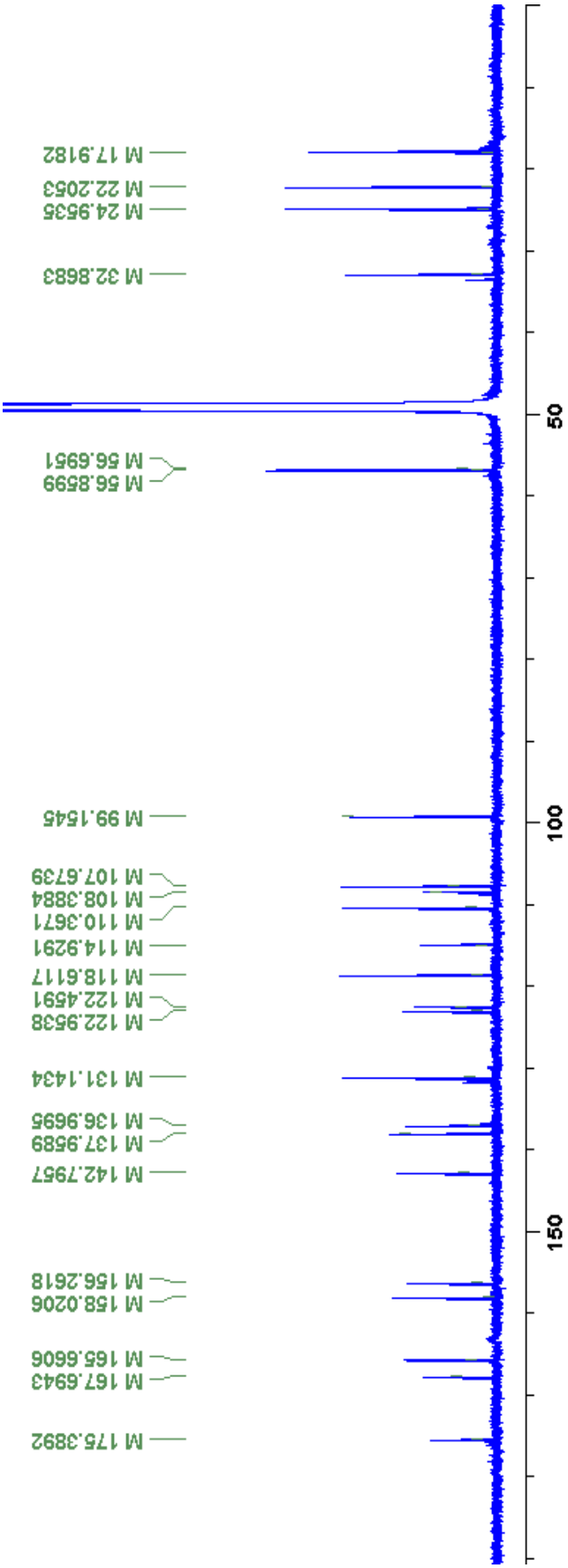


Figure S46. ^{13}C NMR spectrum of ancistrolikokine E_2 (**10**).

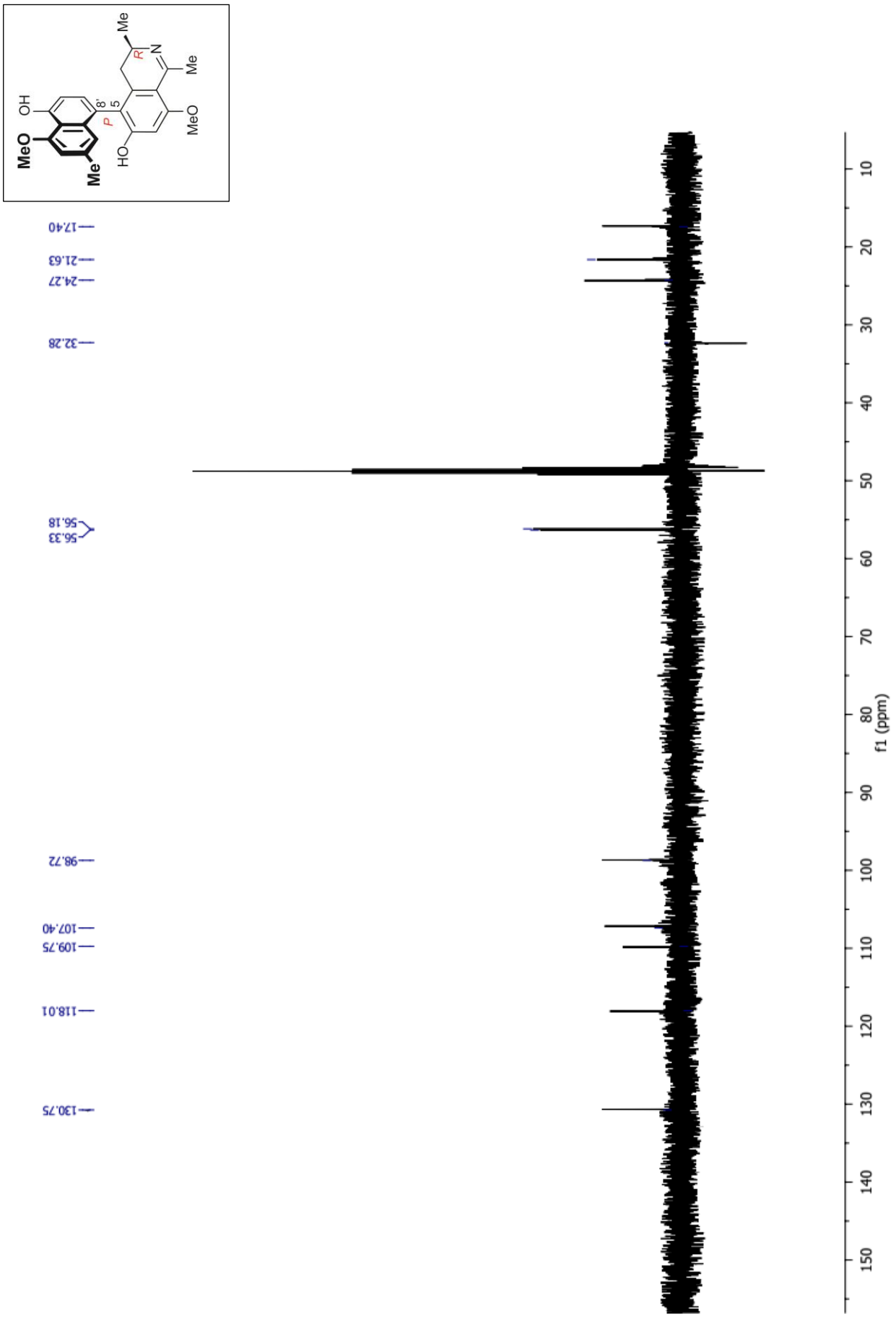


Figure S47. ^{13}C DEPT spectrum of ancistrolikokine E_2 (**10**).

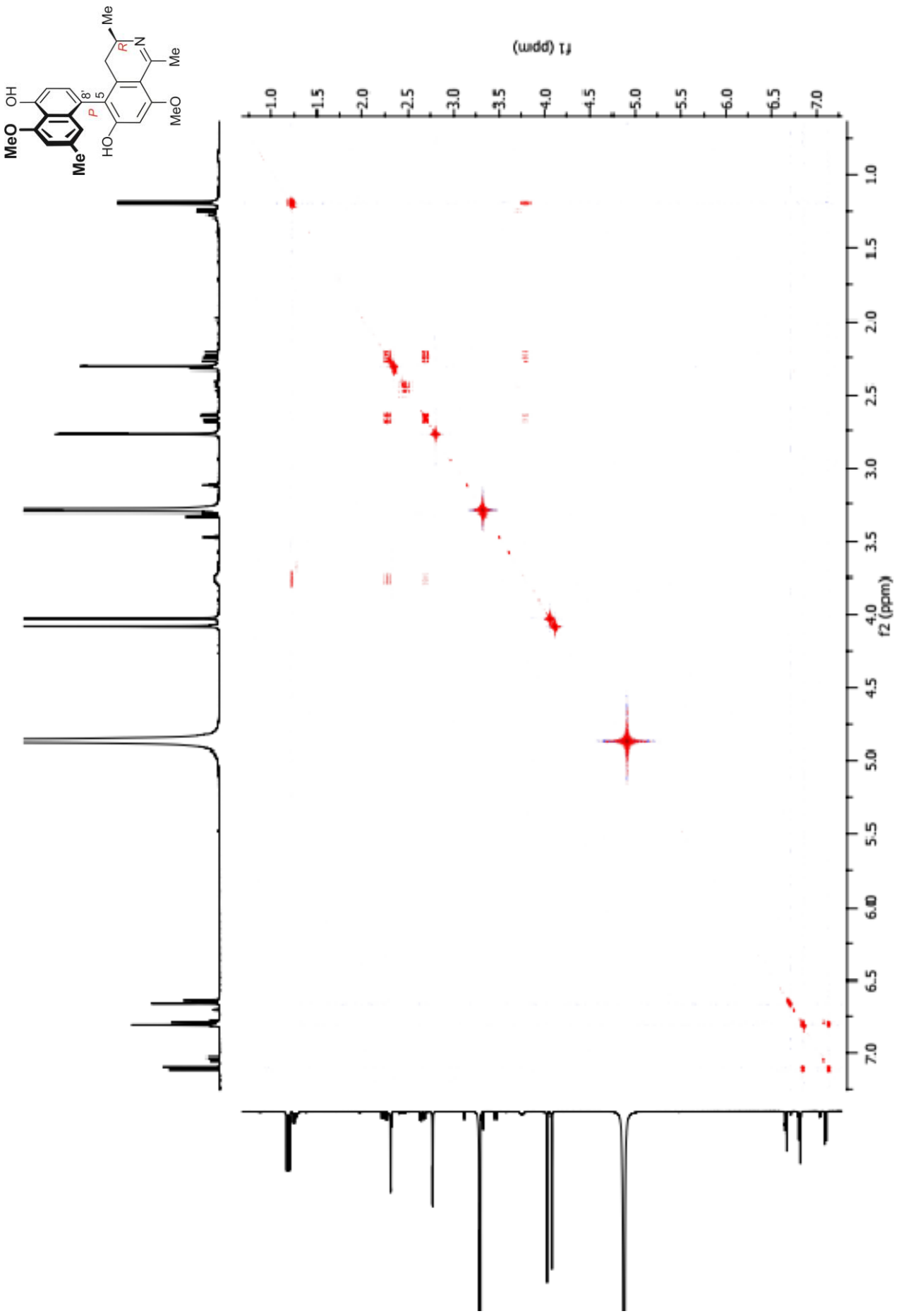


Figure S48. COSY spectrum of ancistrolikokine E_2 (**10**).

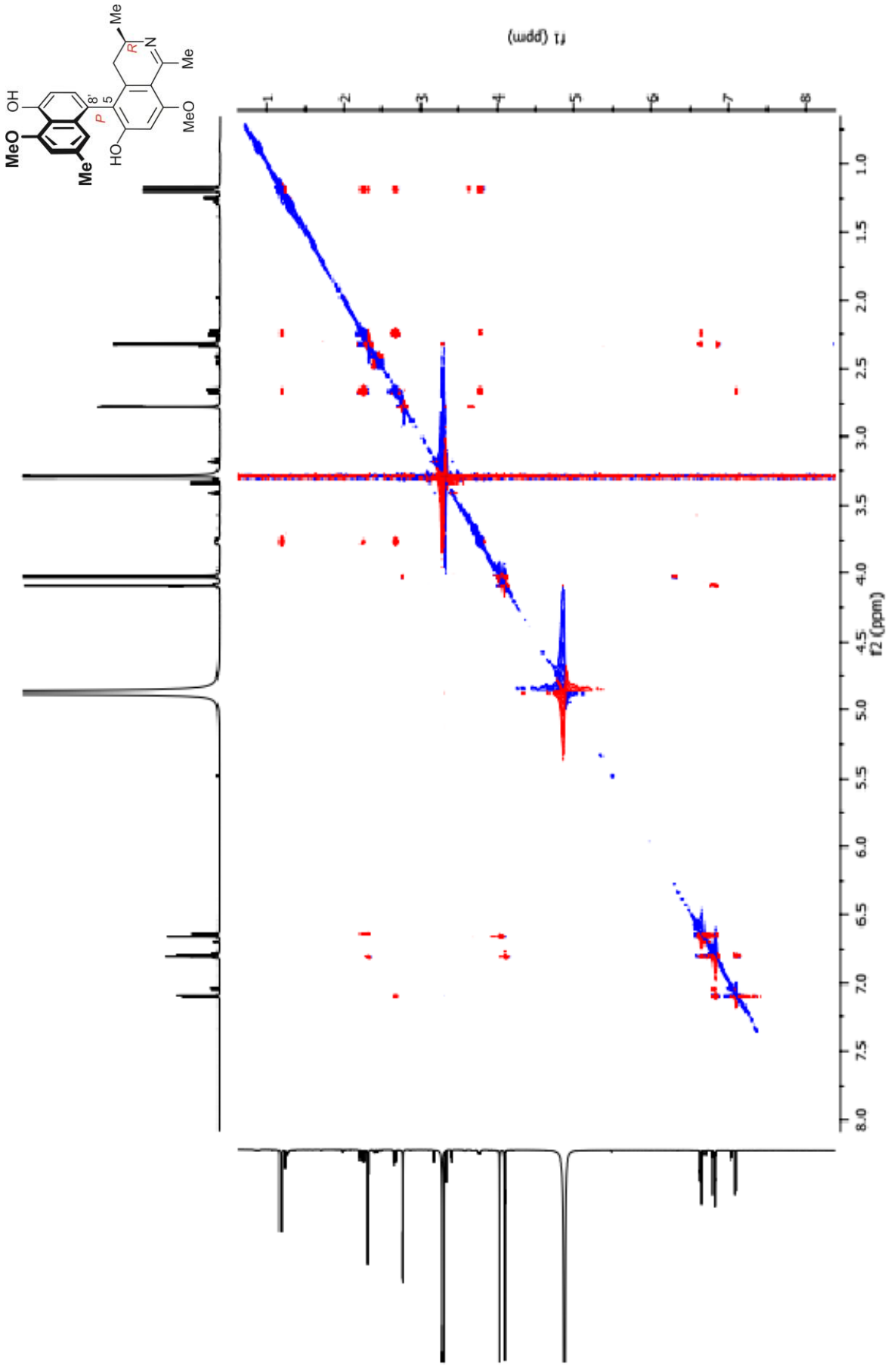


Figure S49. NOESY spectrum of ancistrolikokine E_2 (**10**).

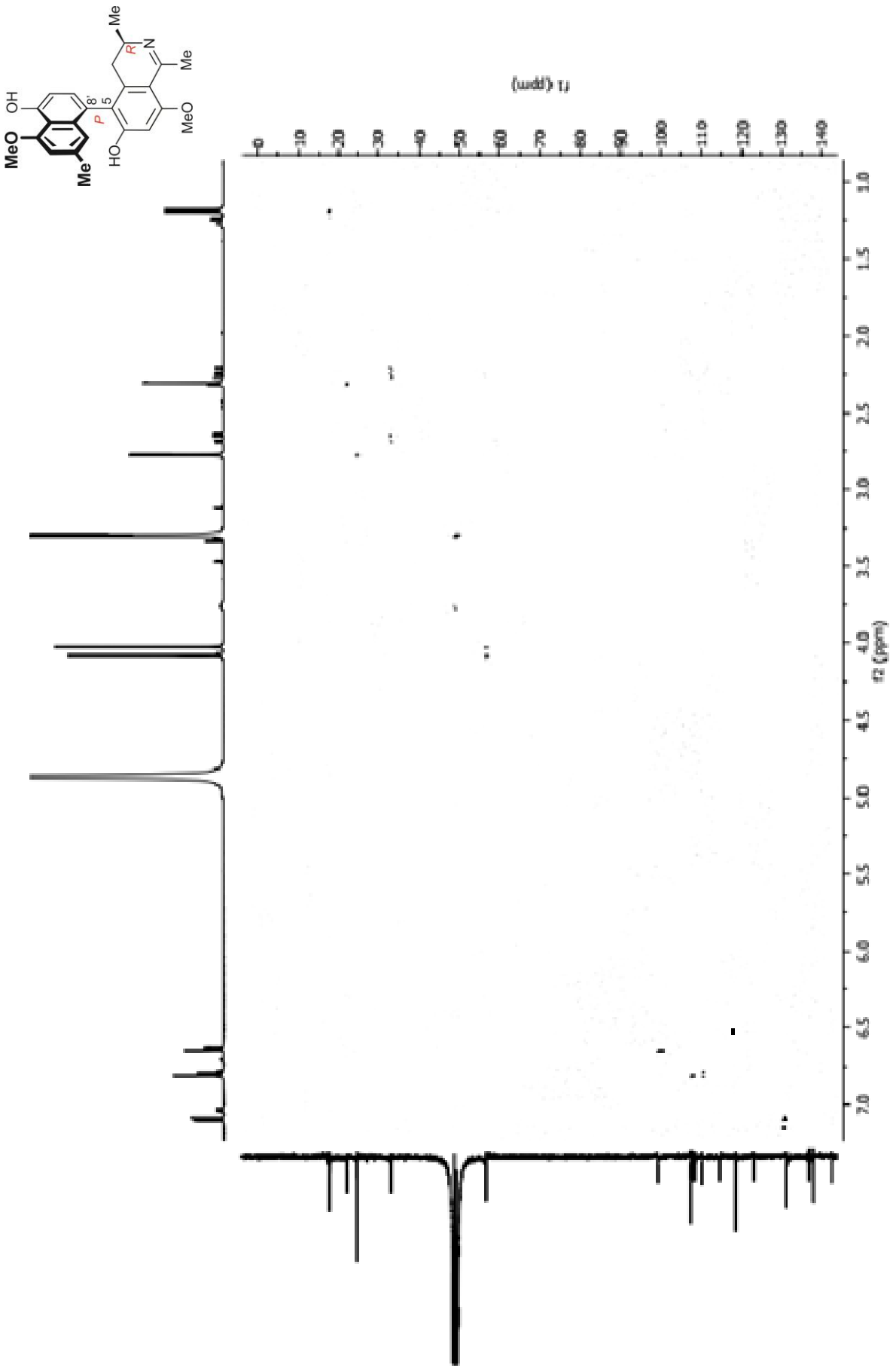


Figure S50. HSQC spectrum of ancistrolikokine E_2 (**10**).

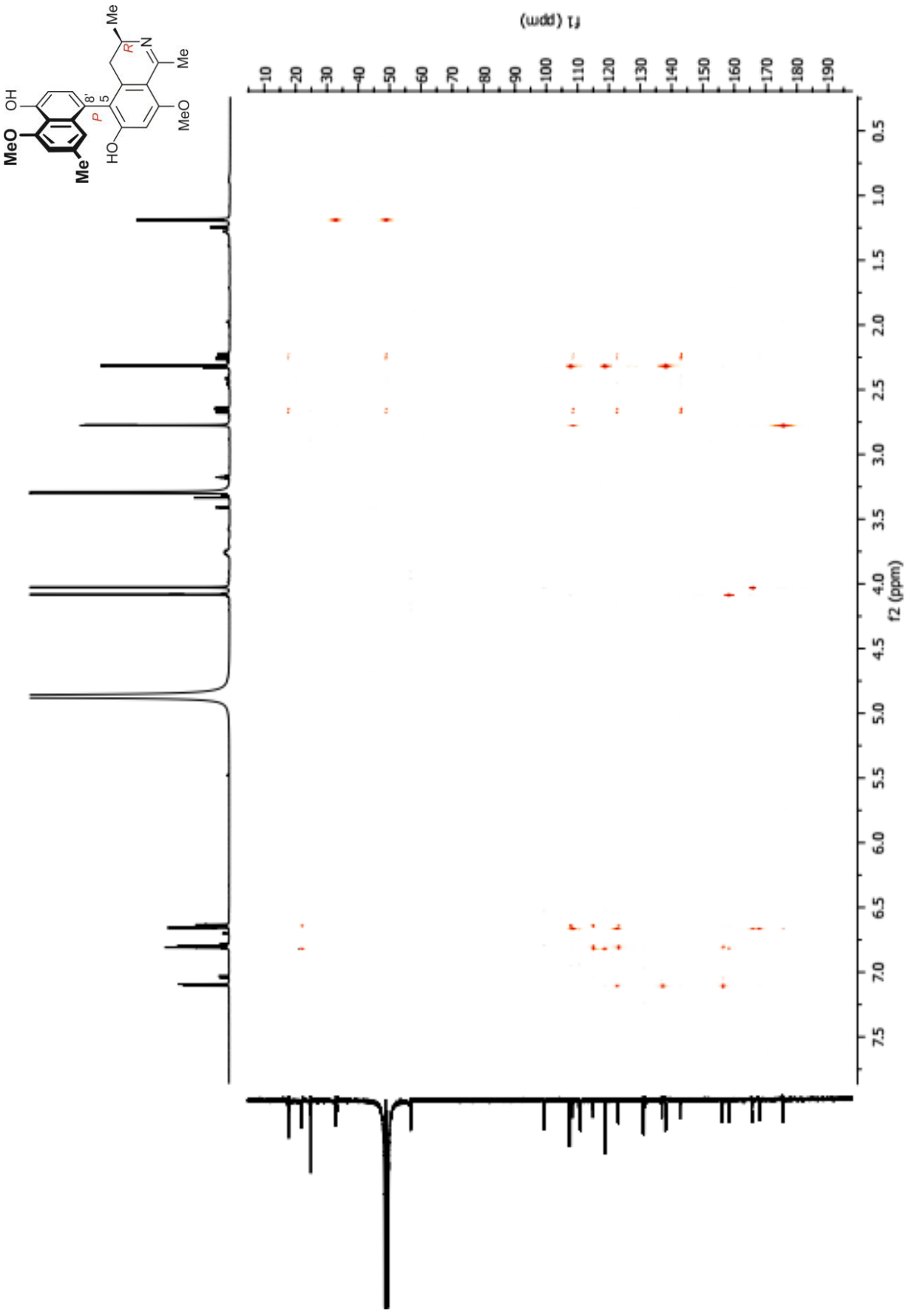


Figure S51. HMBC spectrum of ancistrolikokine E_2 (**10**).

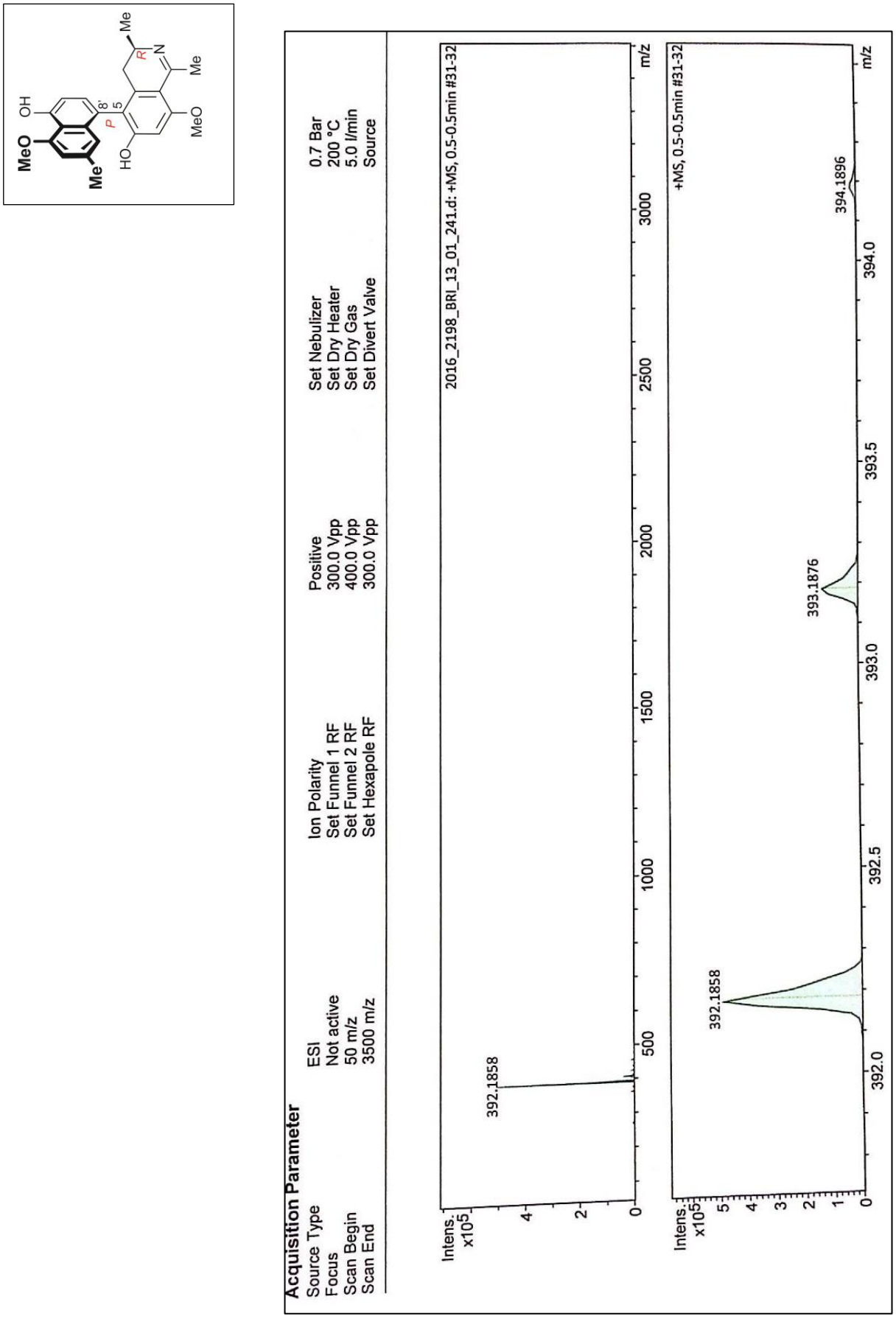


Figure S52. HRESI-MS spectrum of ancistrolikokine E_2 (**10**).

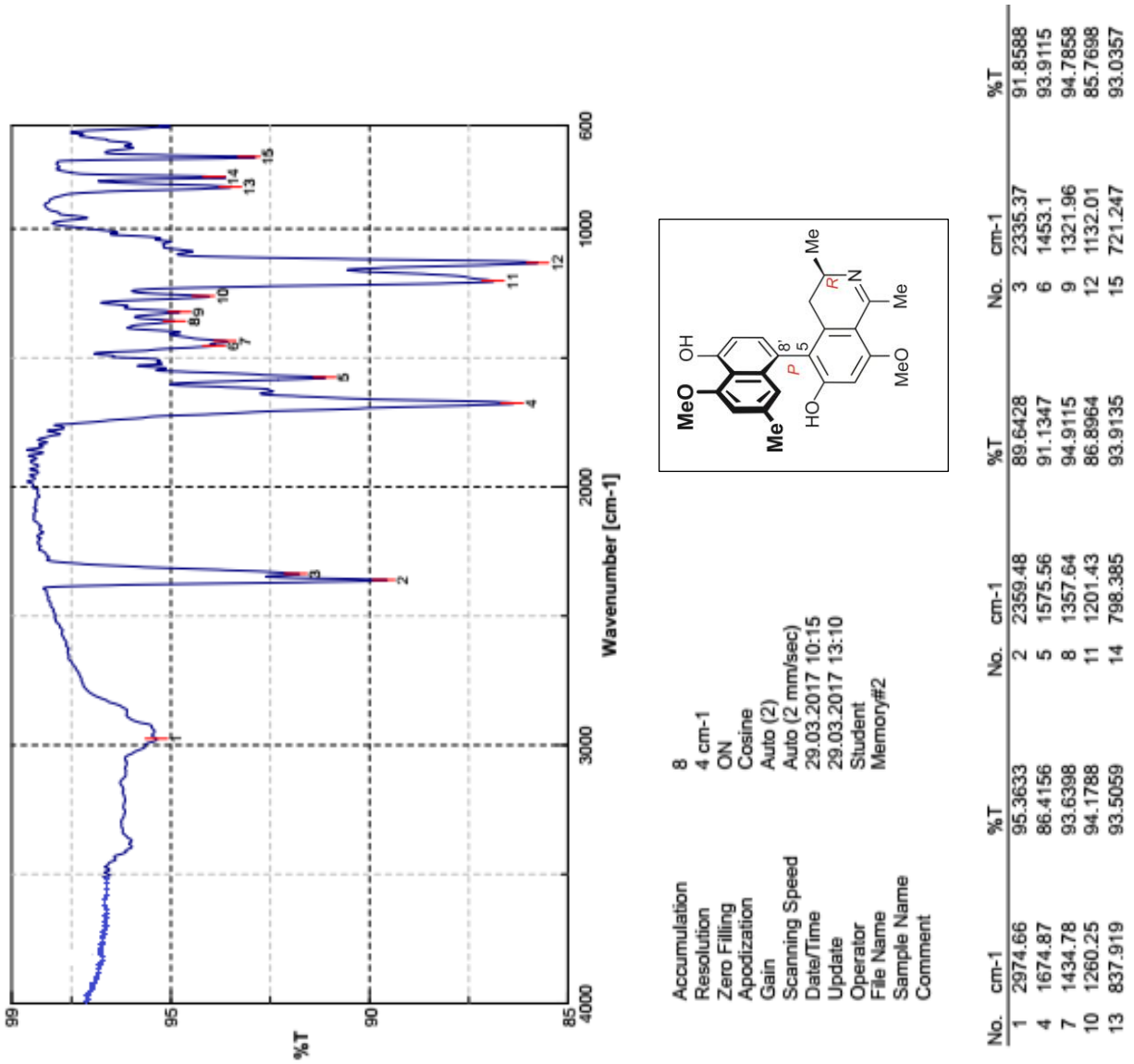


Figure S53. IR spectrum of ancistrolikokine E_2 (**10**).

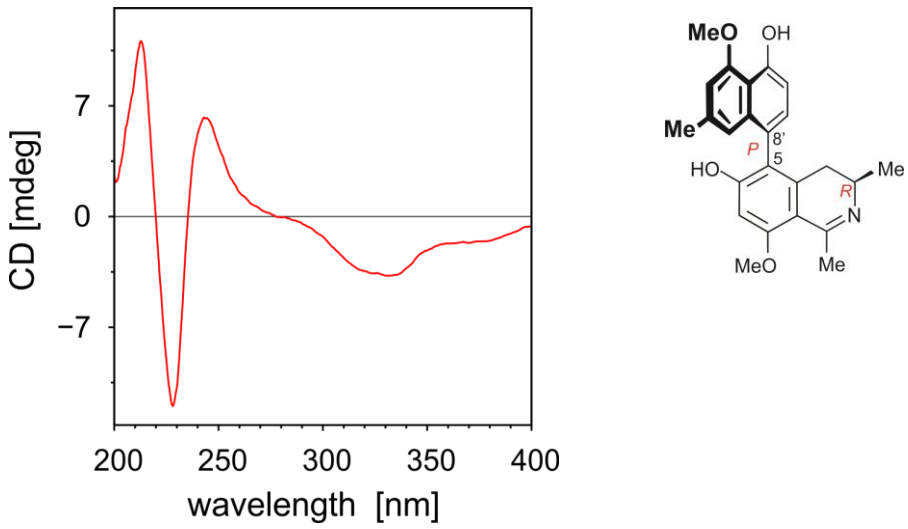
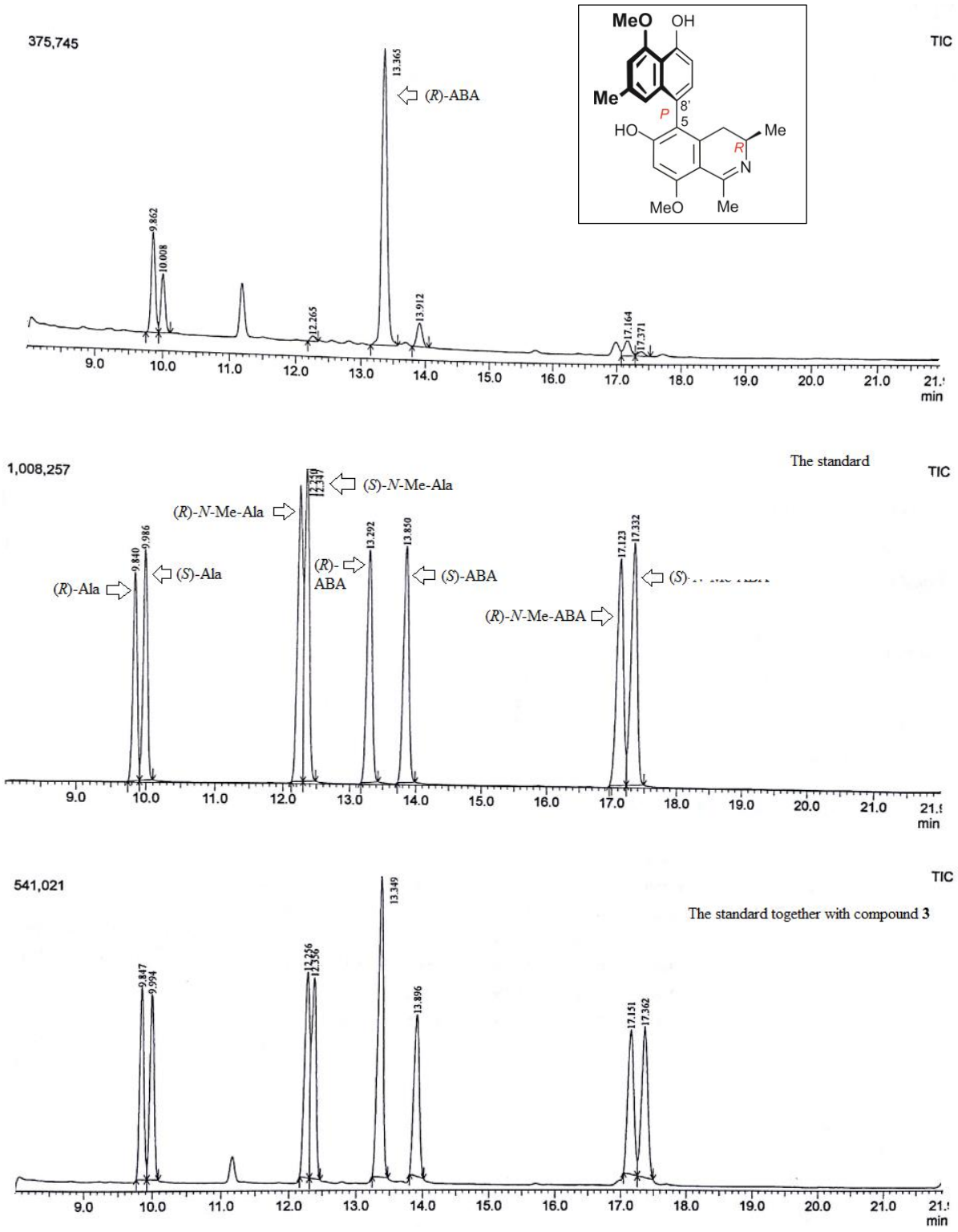


Figure S54. ECD spectrum of ancistrolikokine E_2 (**10**).



Ala = Alanine *N*-Me-Ala = *N*-Methylalanine

ABA = 3-Aminobutyric acid *N*-Me-ABA = *N*-Methyl-3-aminobutyric acid

Figure S55. Oxidative degradation products of ancistrolikokine E_2 (**10**).

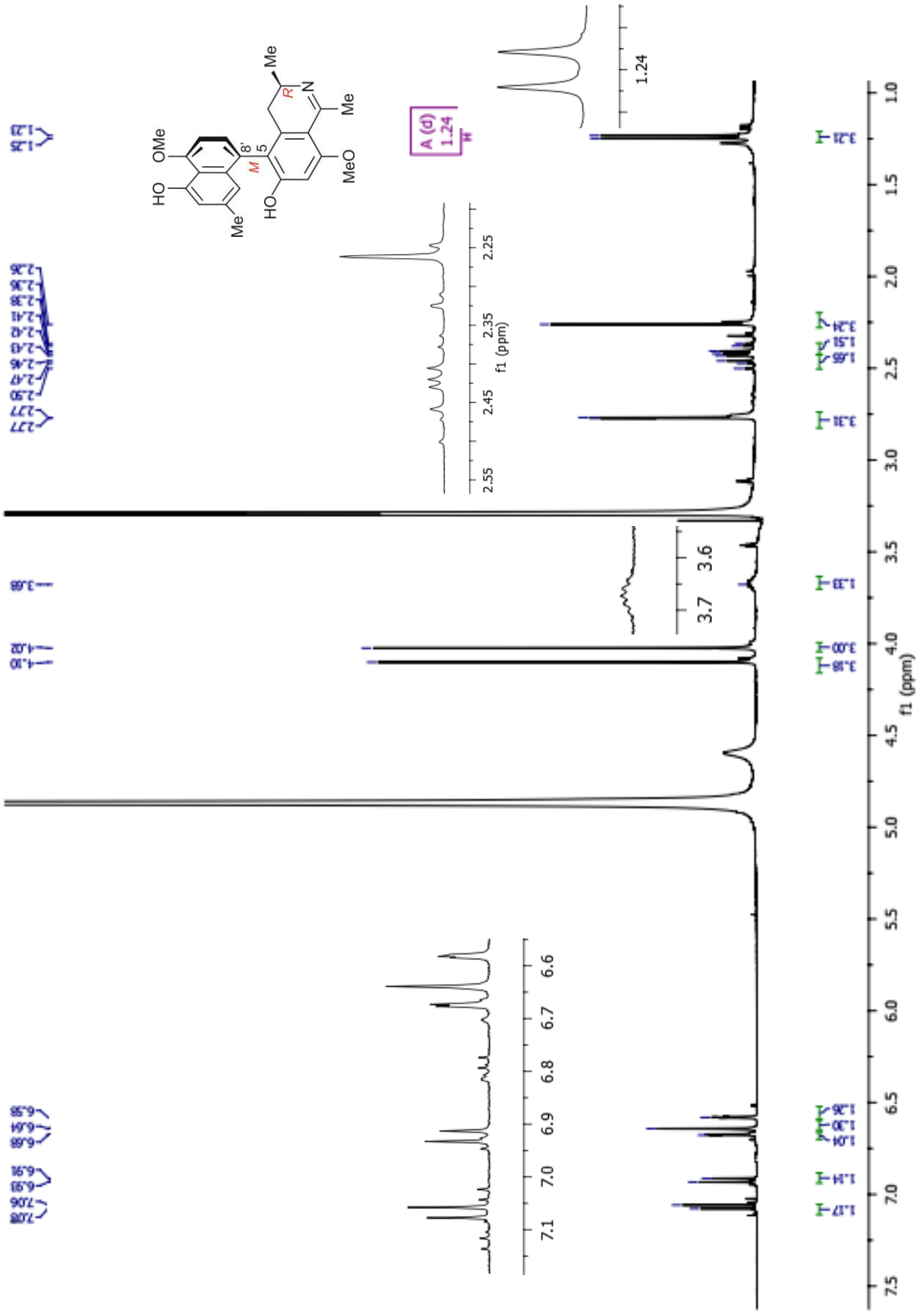


Figure S56. [1]H NMR spectrum of ancistrolikokine F (**11**).

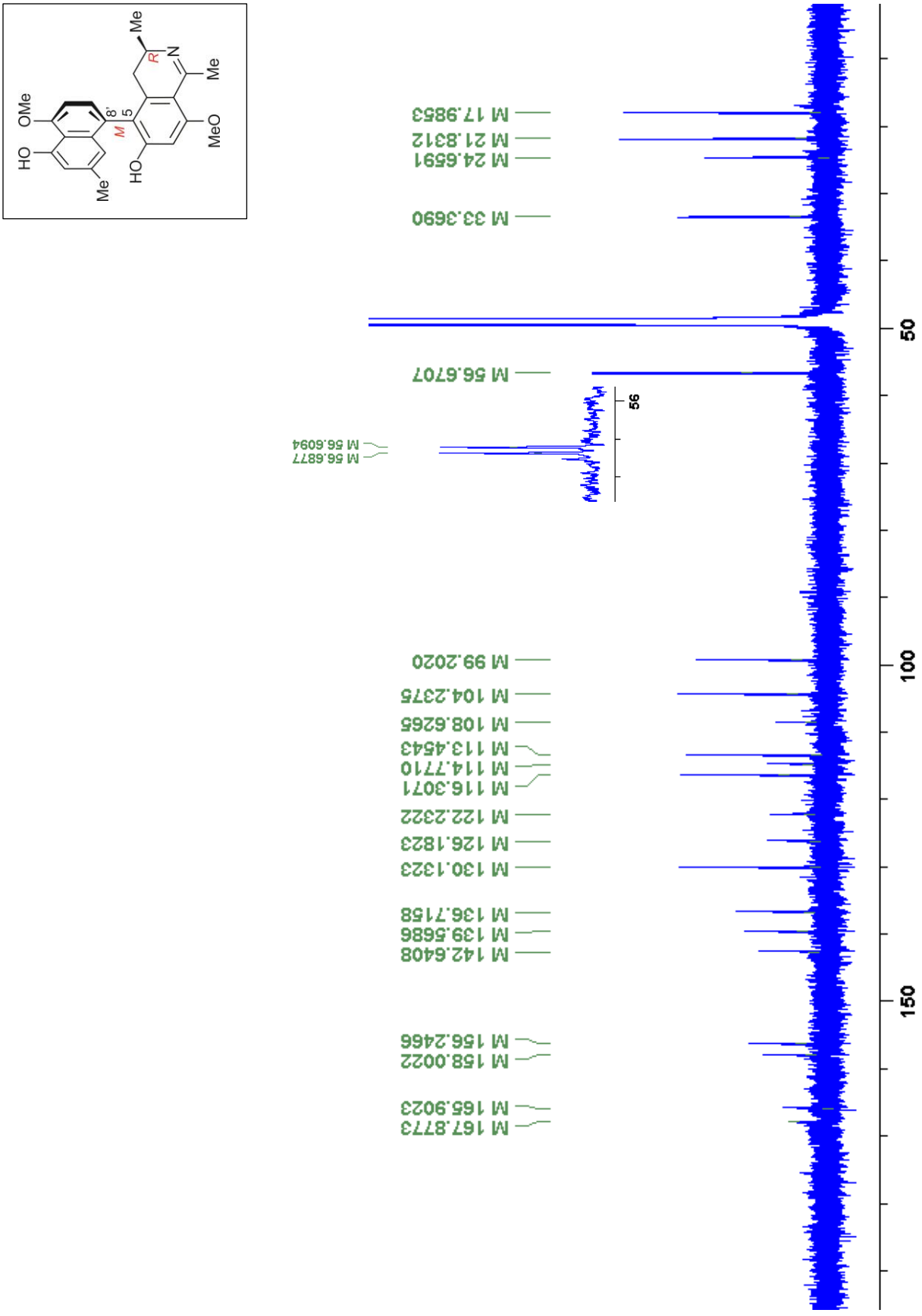


Figure S57. ^{13}C NMR spectrum of ancistrolikokine F (**11**).

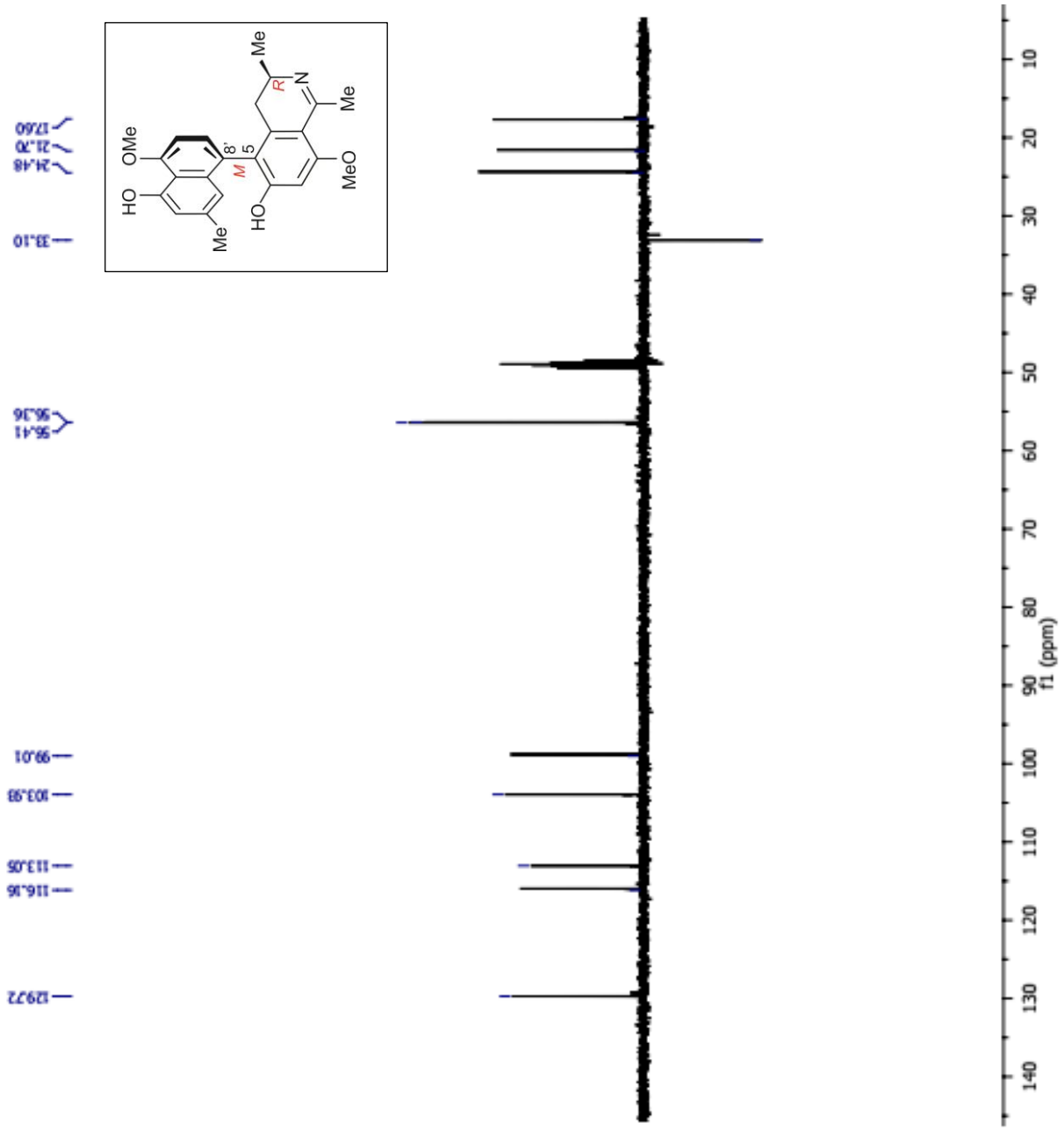


Figure S58. ^{13}C DEPT spectrum of ancistrolikokine F (**11**).

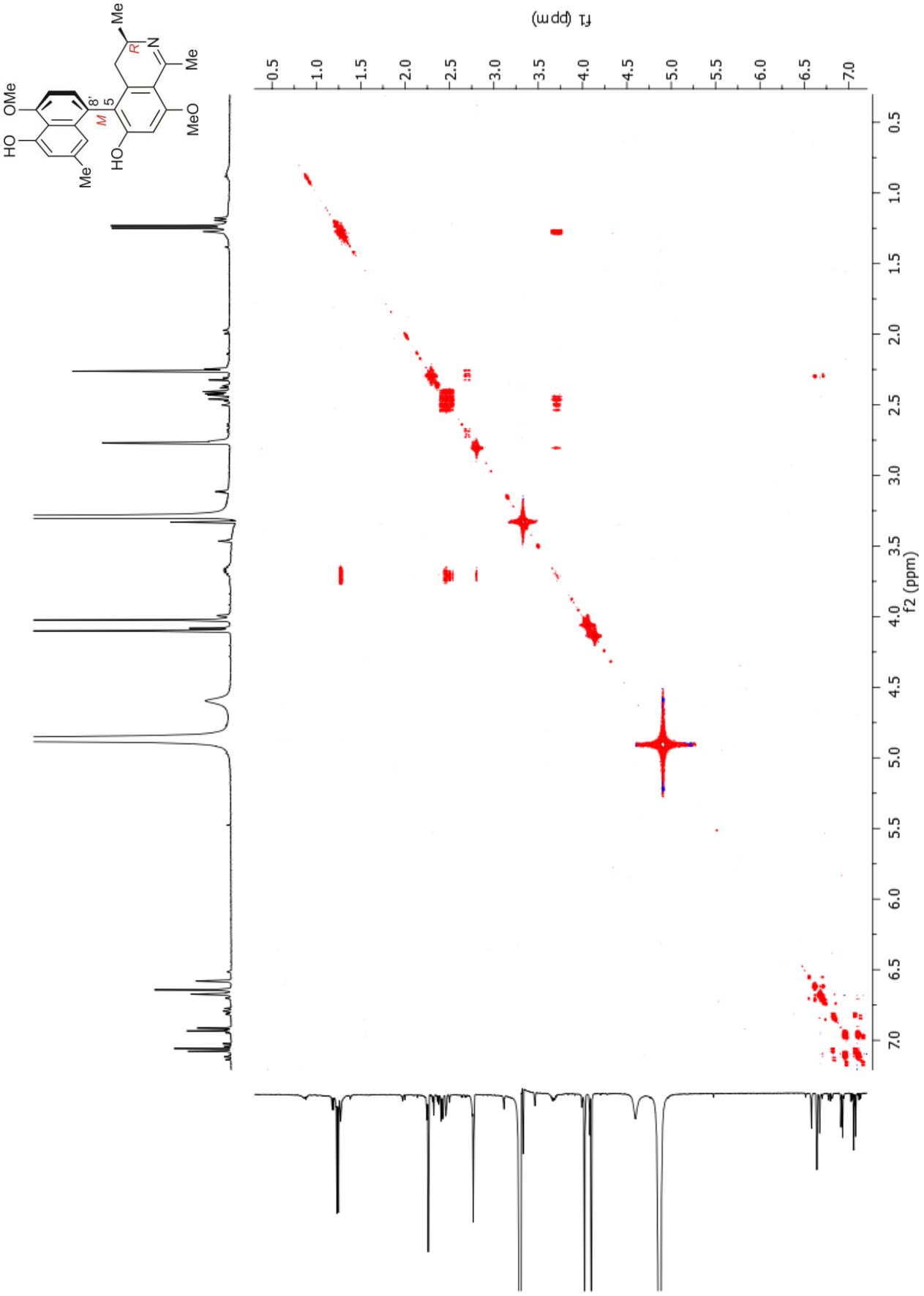


Figure S59. COSY spectrum of ancistrolikokine F (**11**).

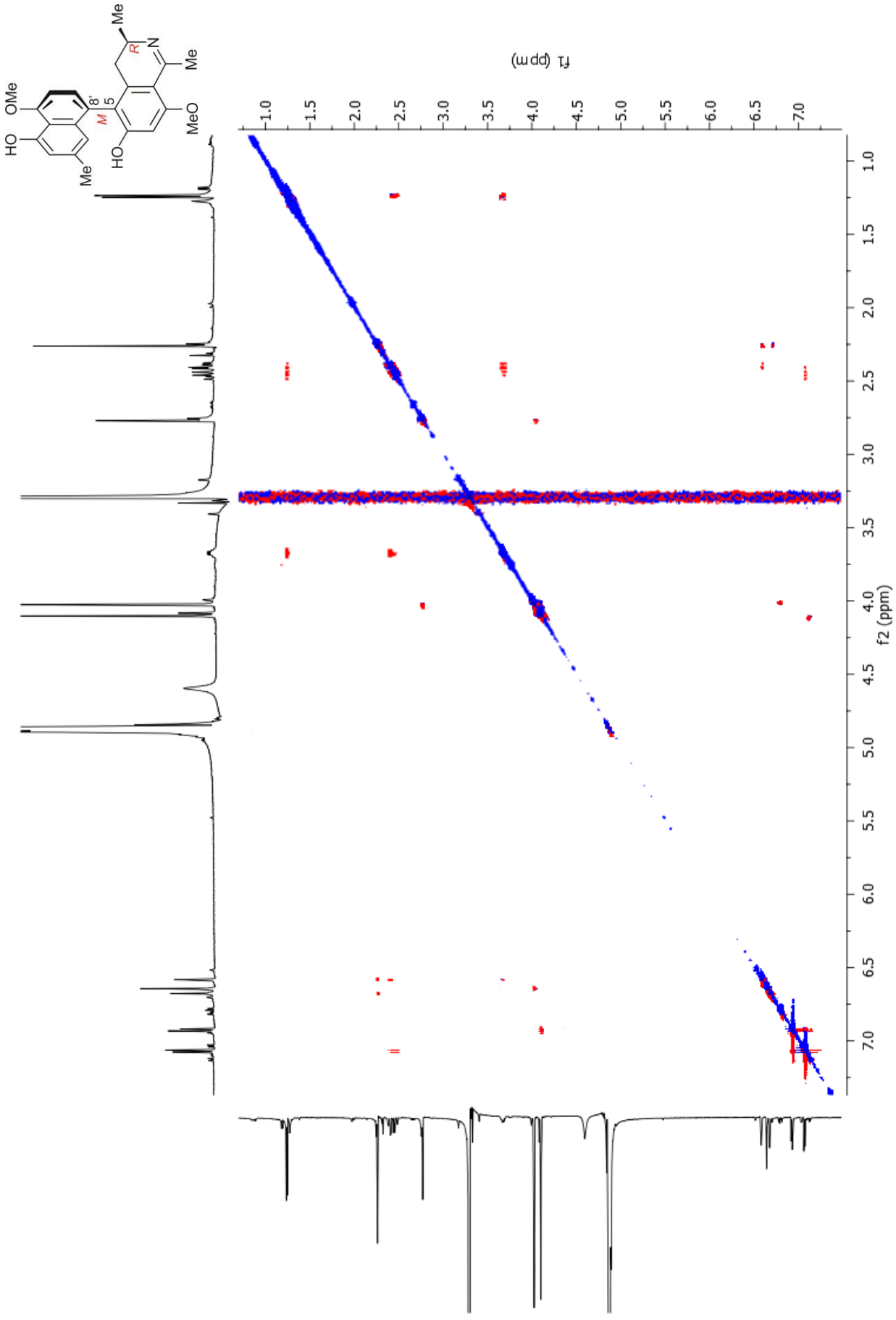


Figure S60. NOESY spectrum of ancistrolikokine F (**11**).

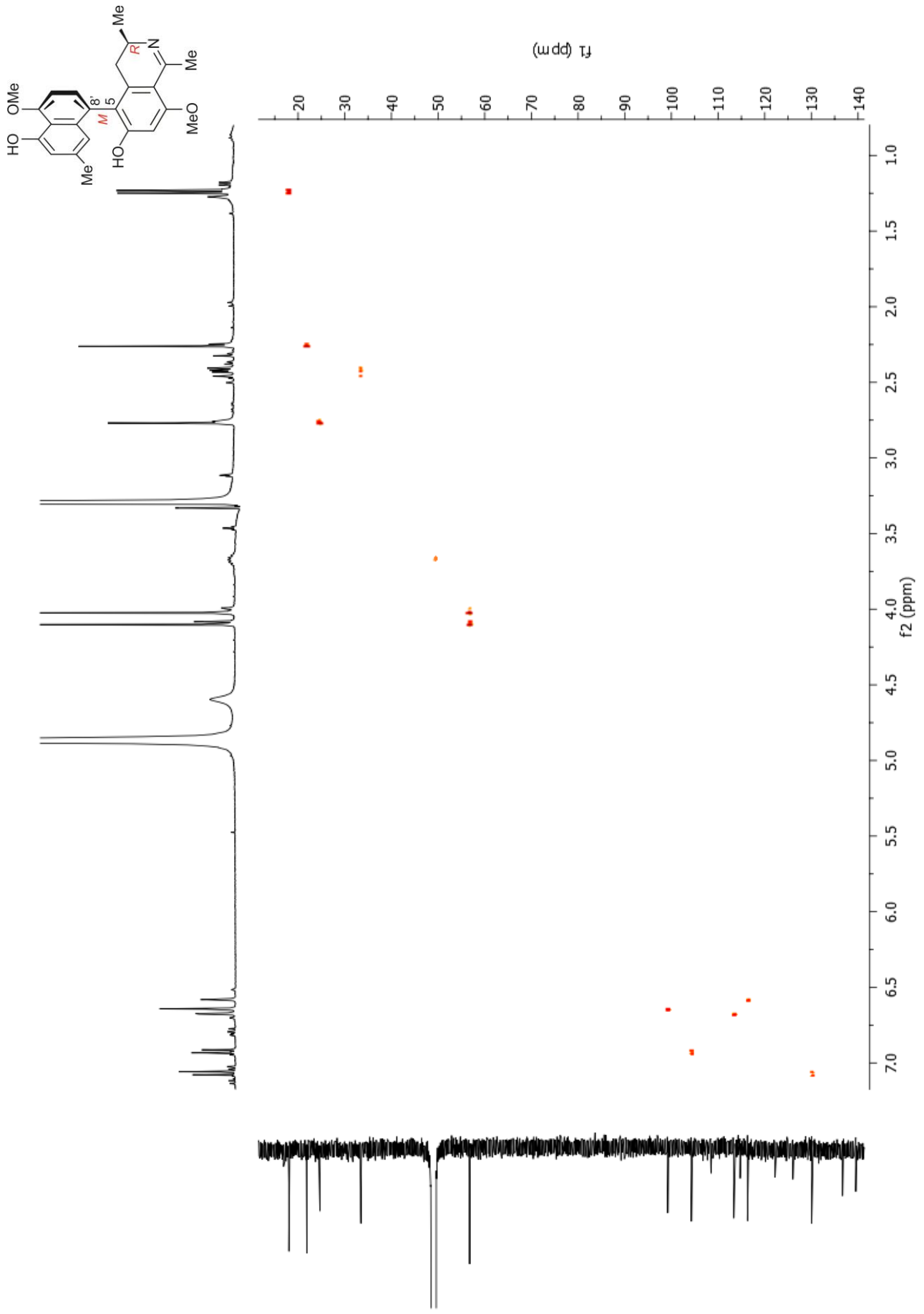


Figure S61. HSQC spectrum of ancistrolikokine F (**11**).

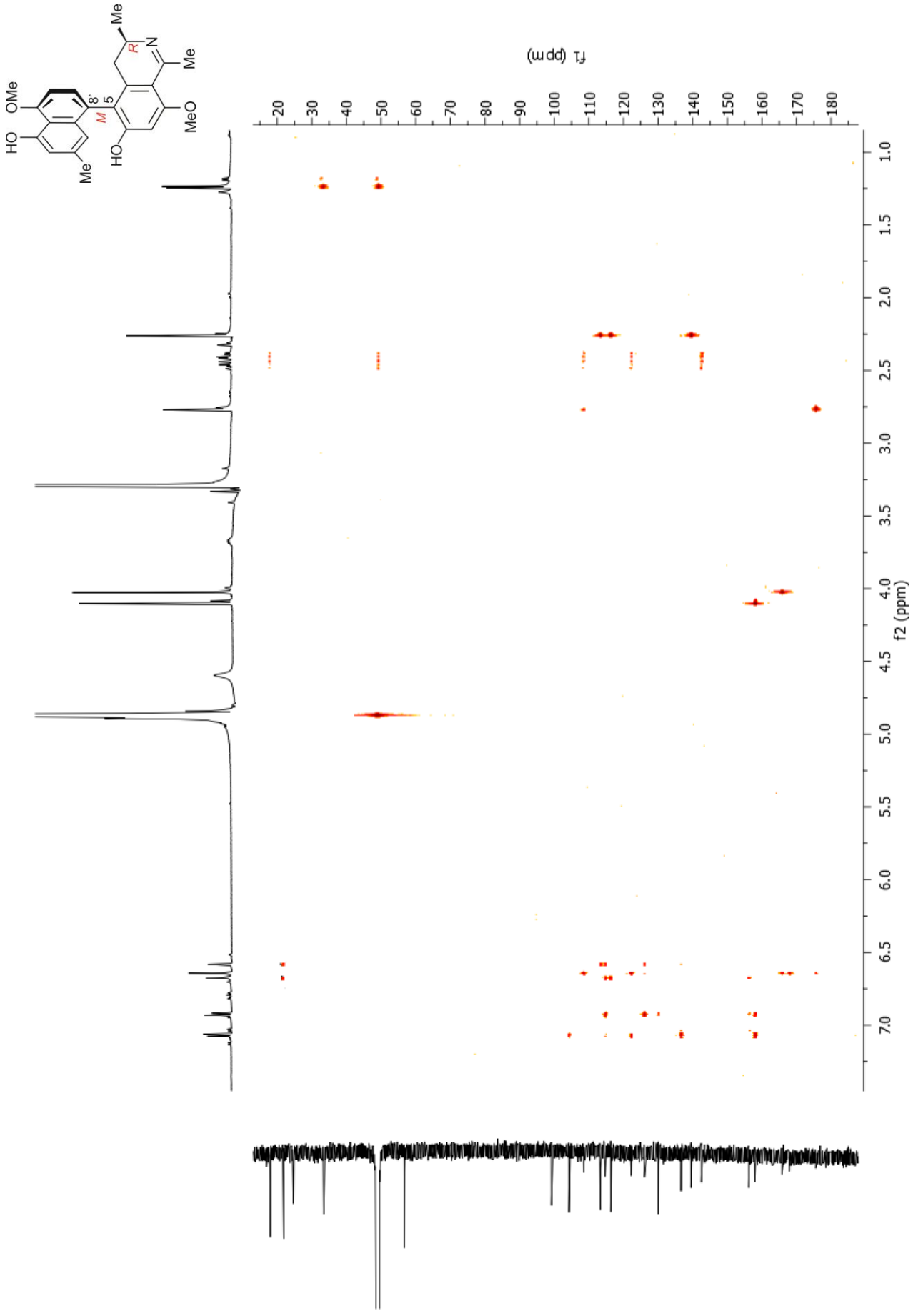


Figure S62. HMBC spectrum of ancistrolikokine F (**11**).

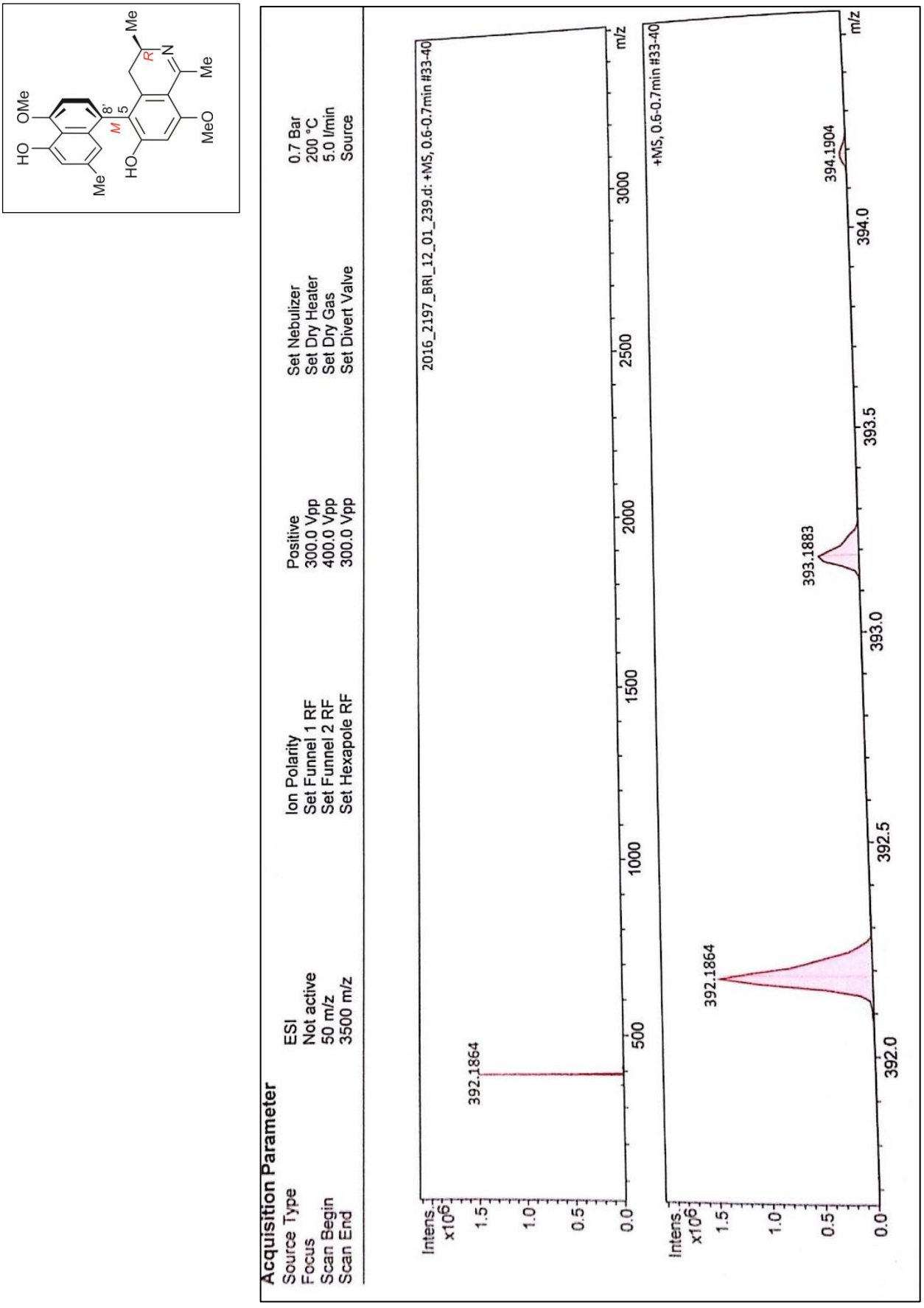


Figure S63. HRESI-MS spectrum of ancistrolikokine F (**11**).

Accumulation	8
Resolution	4 cm-1
Zero Filling	ON
Apodization	Cosine
Gain	Auto (4)
Scanning Speed	Auto (2 mm/sec)
Date/Time	29.03.2017 10:11
Update	29.03.2017 13:13
Operator	Student
File Name	Memory#2
Sample Name	
Comment	

No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3387.35	83.8859	2	2936.09	80.5335	3	2842.56	82.9225
4	1671.98	49.1887	5	1630.52	61.5658	6	1574.59	48.102
7	1433.82	69.5095	8	1385.6	67.566	9	1353.78	65.653
10	1327.75	62.958	11	1292.07	64.9747	12	1268.93	61.8003
13	1194.69	37.2577	14	1181.19	36.8184	15	1127.19	29.1127
16	1089.58	49.9883	17	1025.94	50.492	18	964.233	73.429
19	836.955	55.7794	20	798.385	59.0572	21	717.39	52.6294

Figure S64. IR spectrum of ancistrolikokine F (**11**).

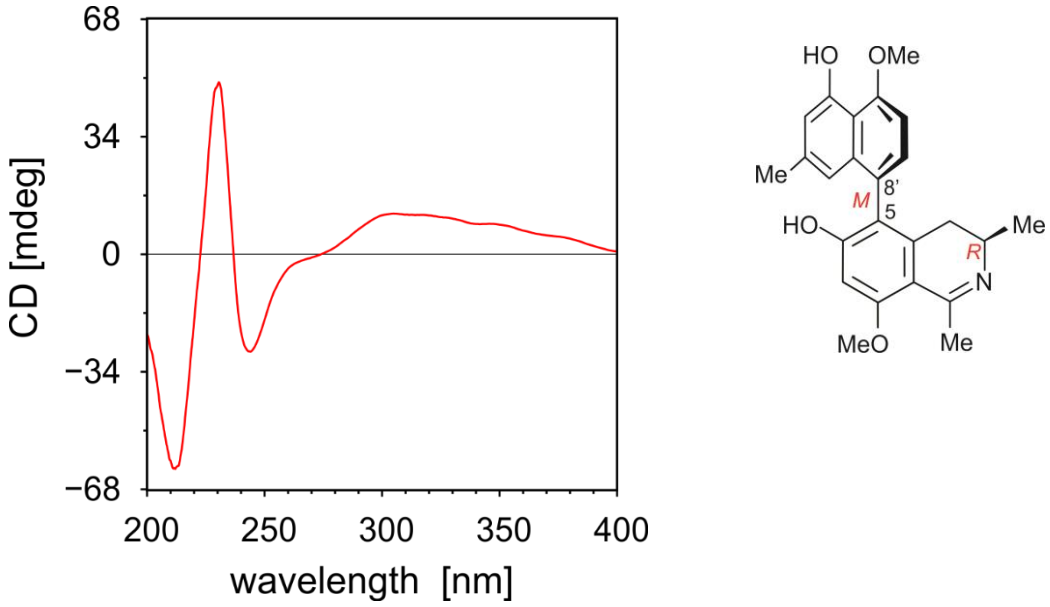
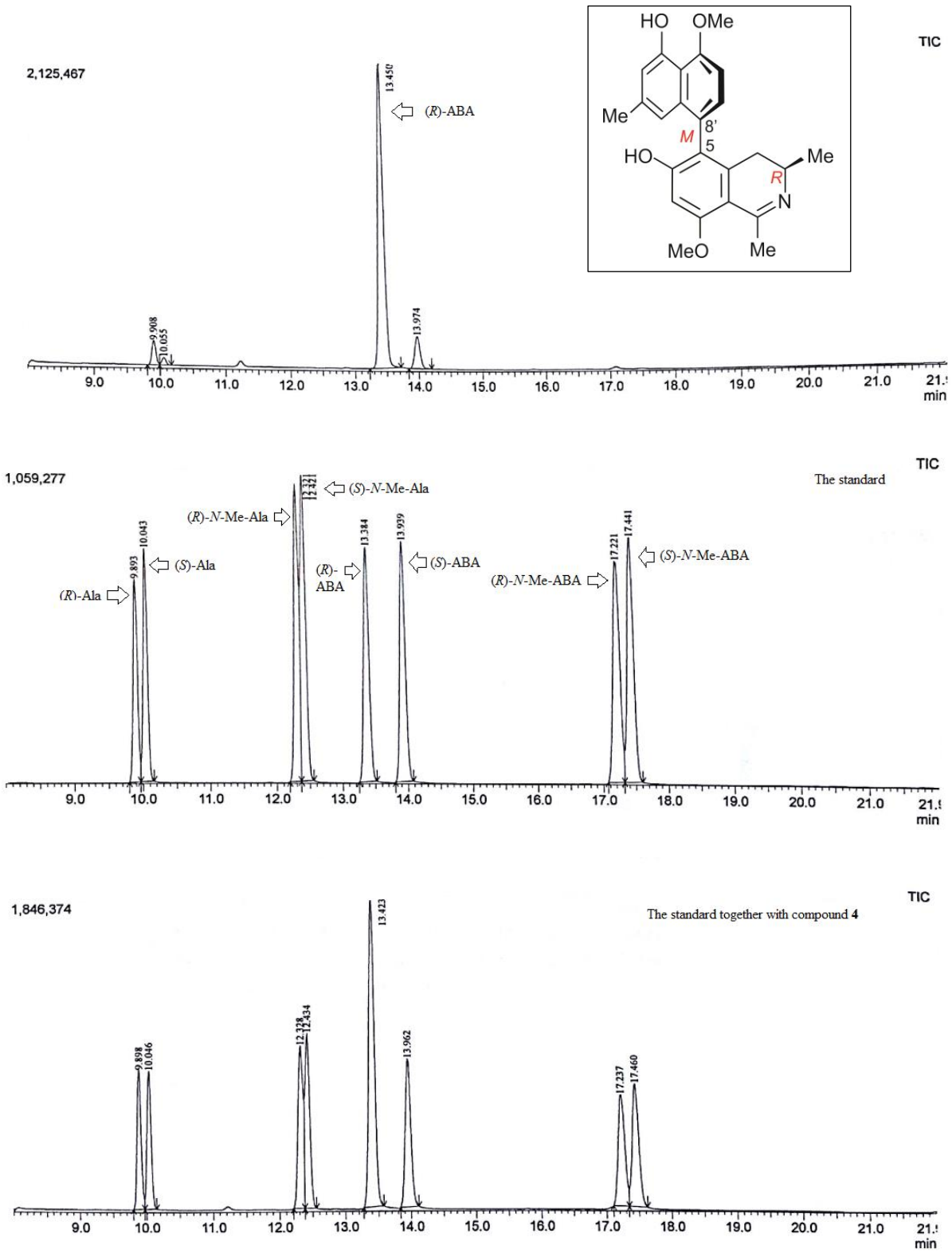


Figure S65. ECD spectrum of ancistrolikokine F (**11**).



Ala = Alanine *N*-Me-Ala = *N*-Methylalanine

ABA = 3-Aminobutyric acid *N*-Me-ABA = *N*-Methyl-3-aminobutyric acid

Figure S66. Oxidative degradation products of ancistrolikokine F (**11**).

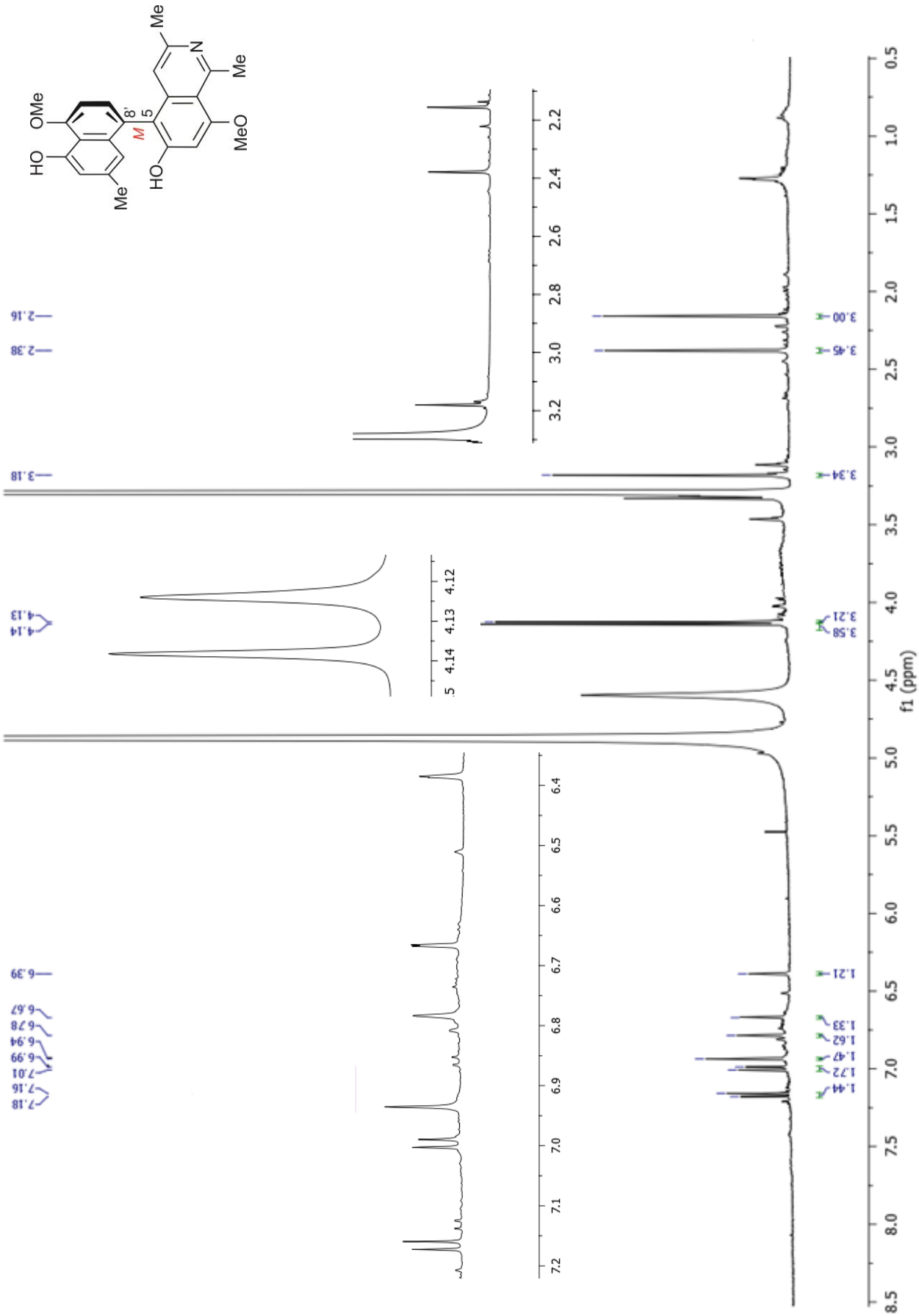
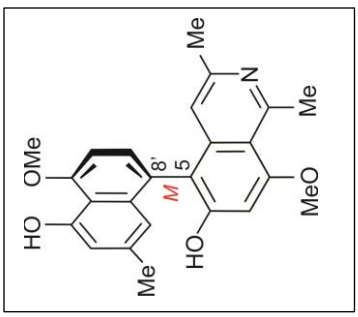


Figure S67. ^{1}H NMR spectrum of ancistrolikokine G (**12**).



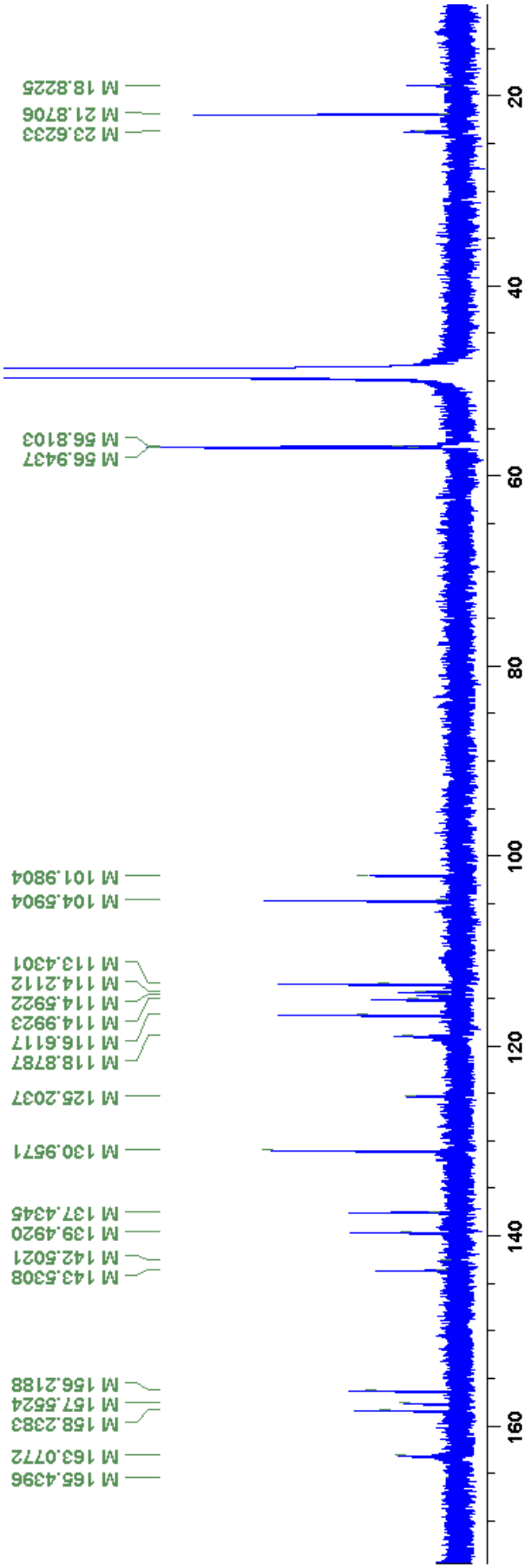


Figure S68. ^{13}C NMR spectrum of ancistrolikokine G (**12**).

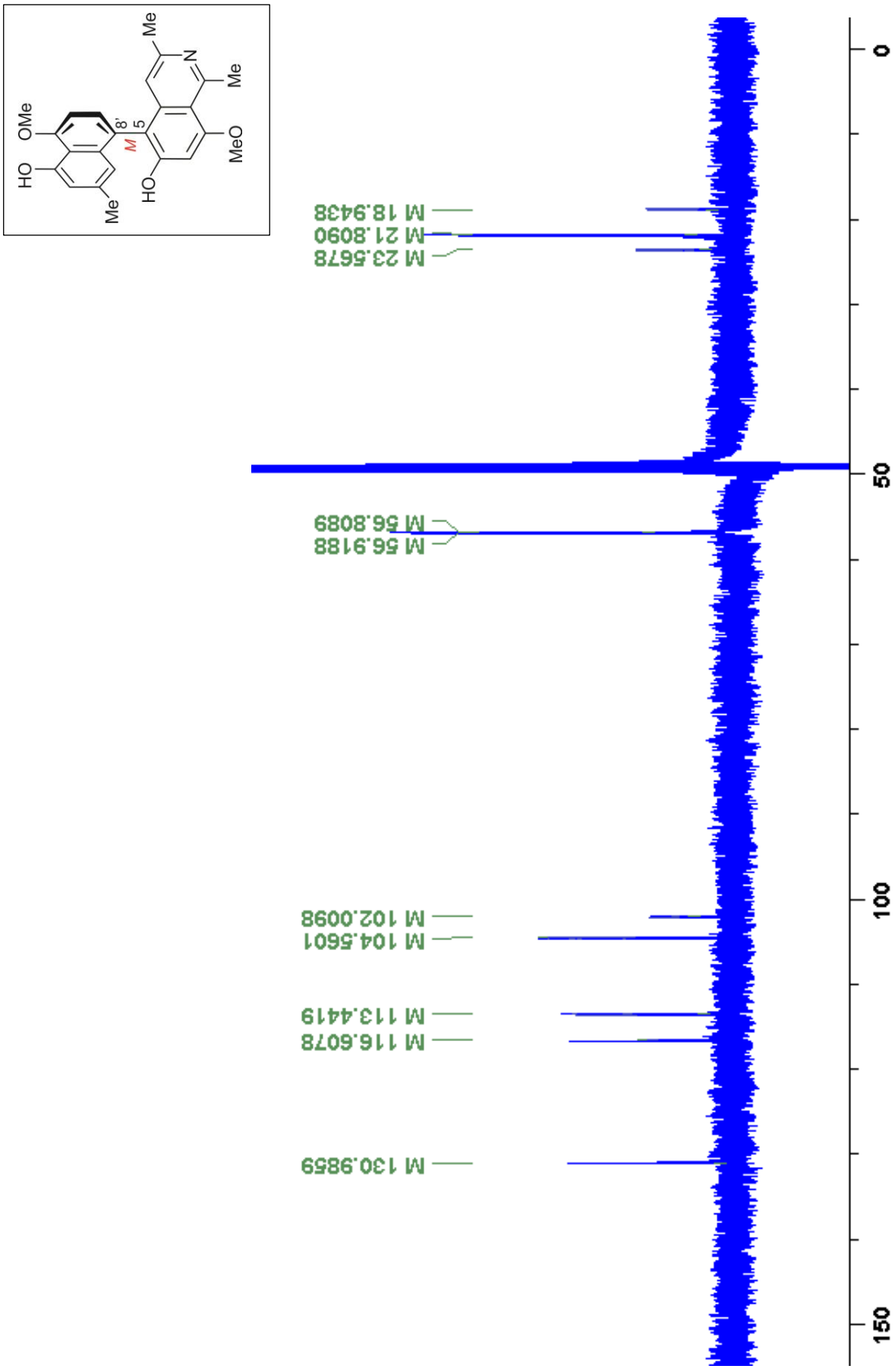
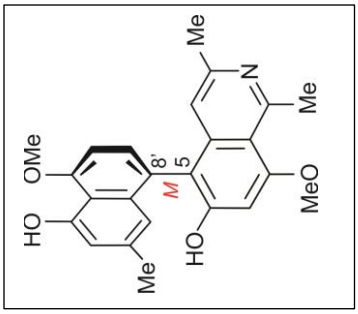


Figure S69. ^{13}C DEPT spectrum of ancistrolikokine G (**12**).



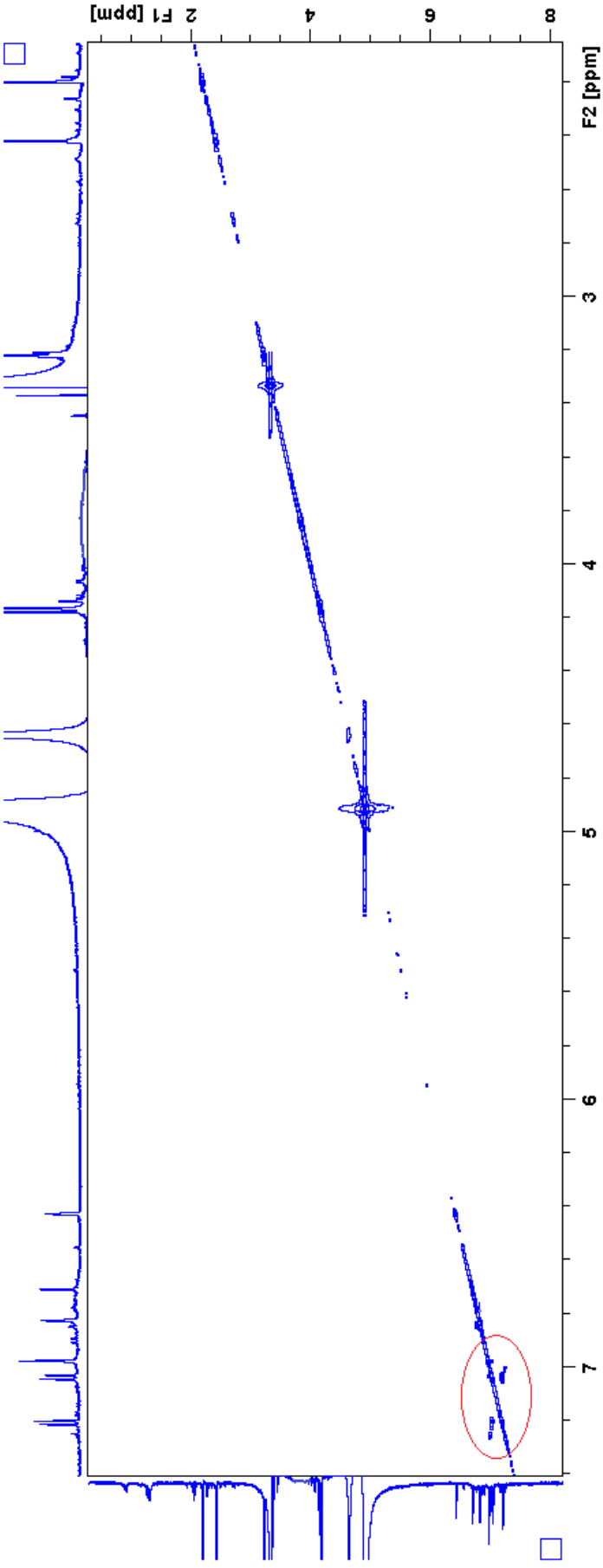


Figure S70. COSY spectrum of ancistrolikokine G (**12**).

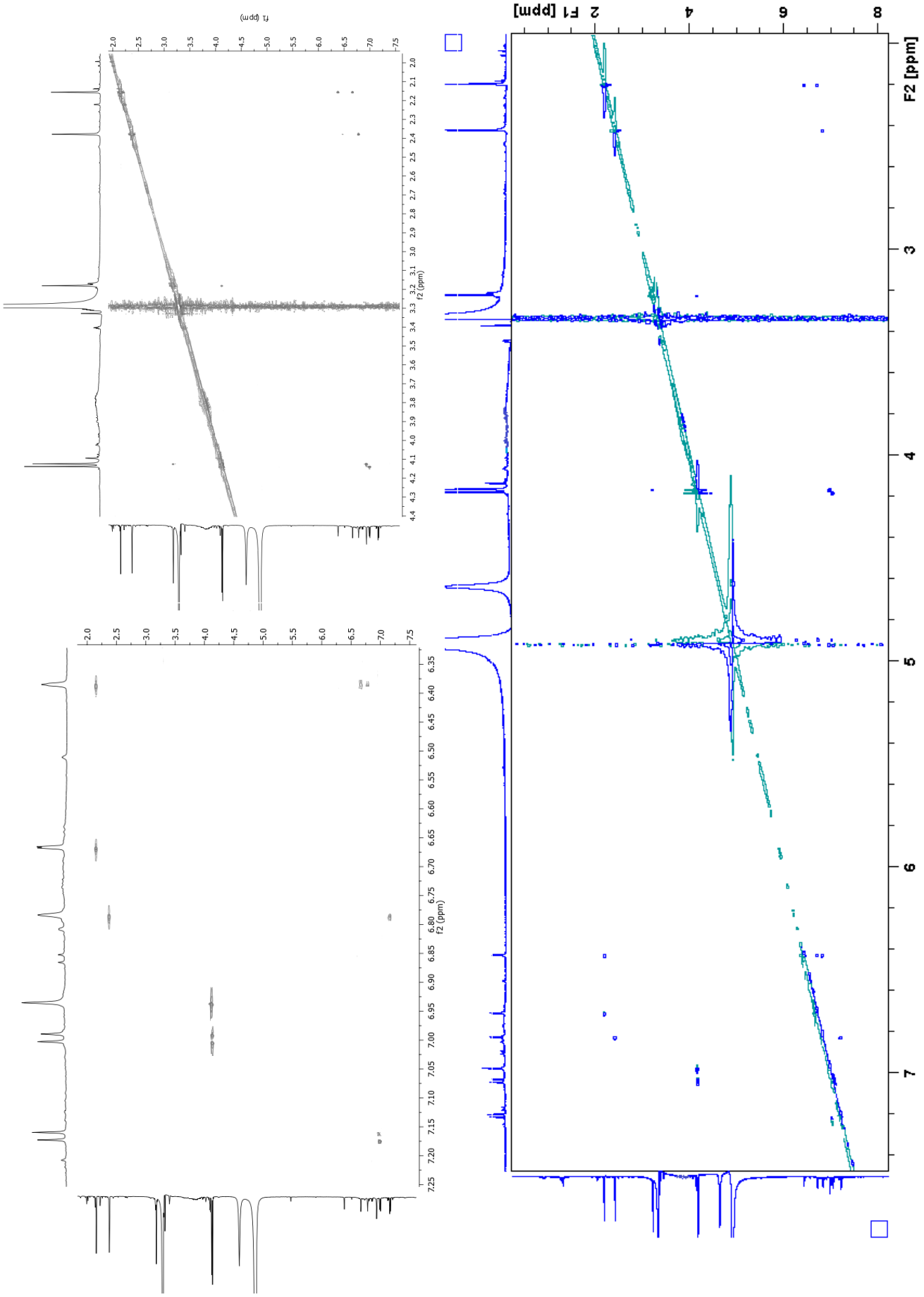


Figure S71. NOESY spectrum of ancistrolikokine G (**12**).

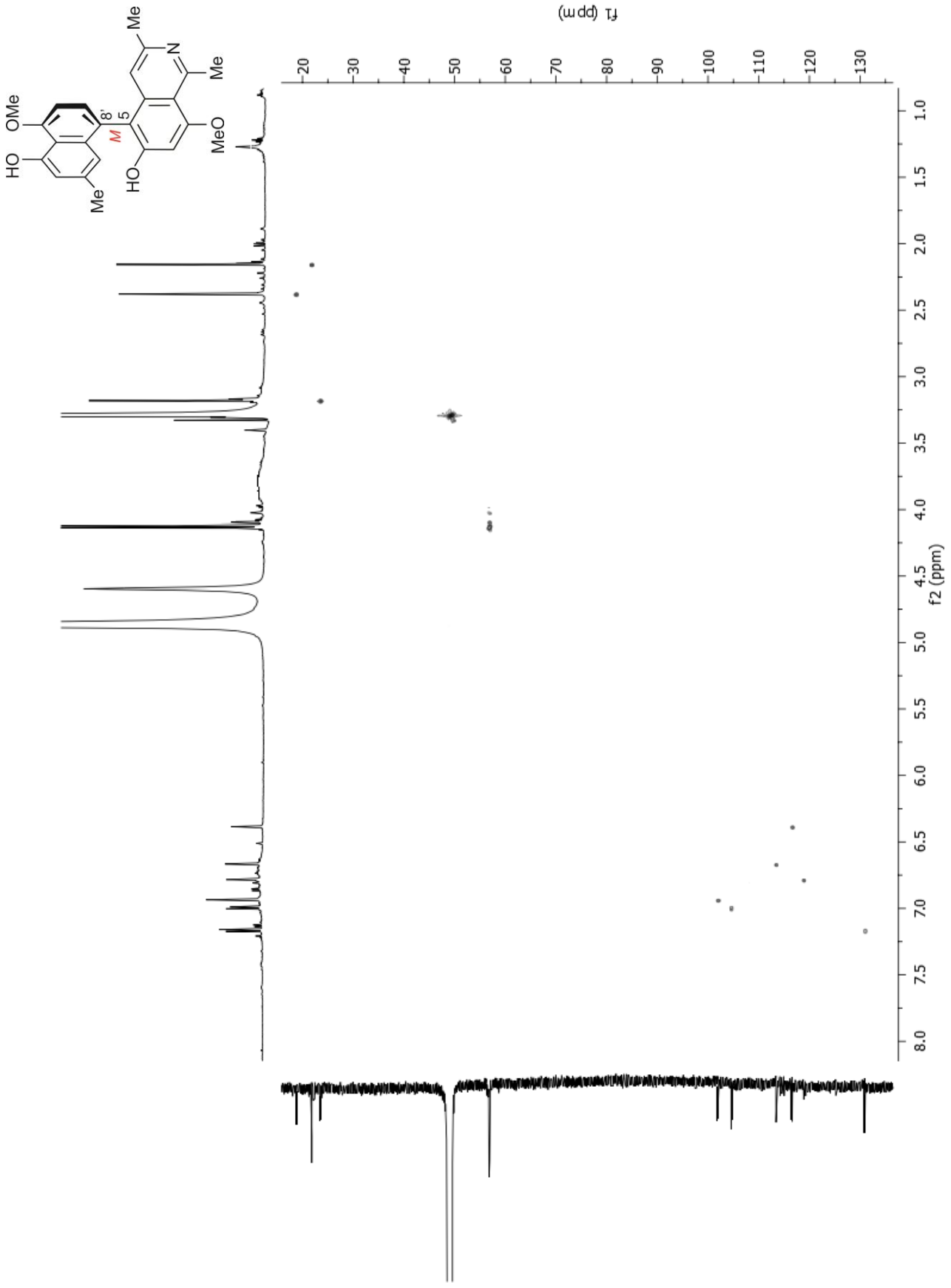


Figure S72. HSQC spectrum of ancistrolikokine G (**12**).

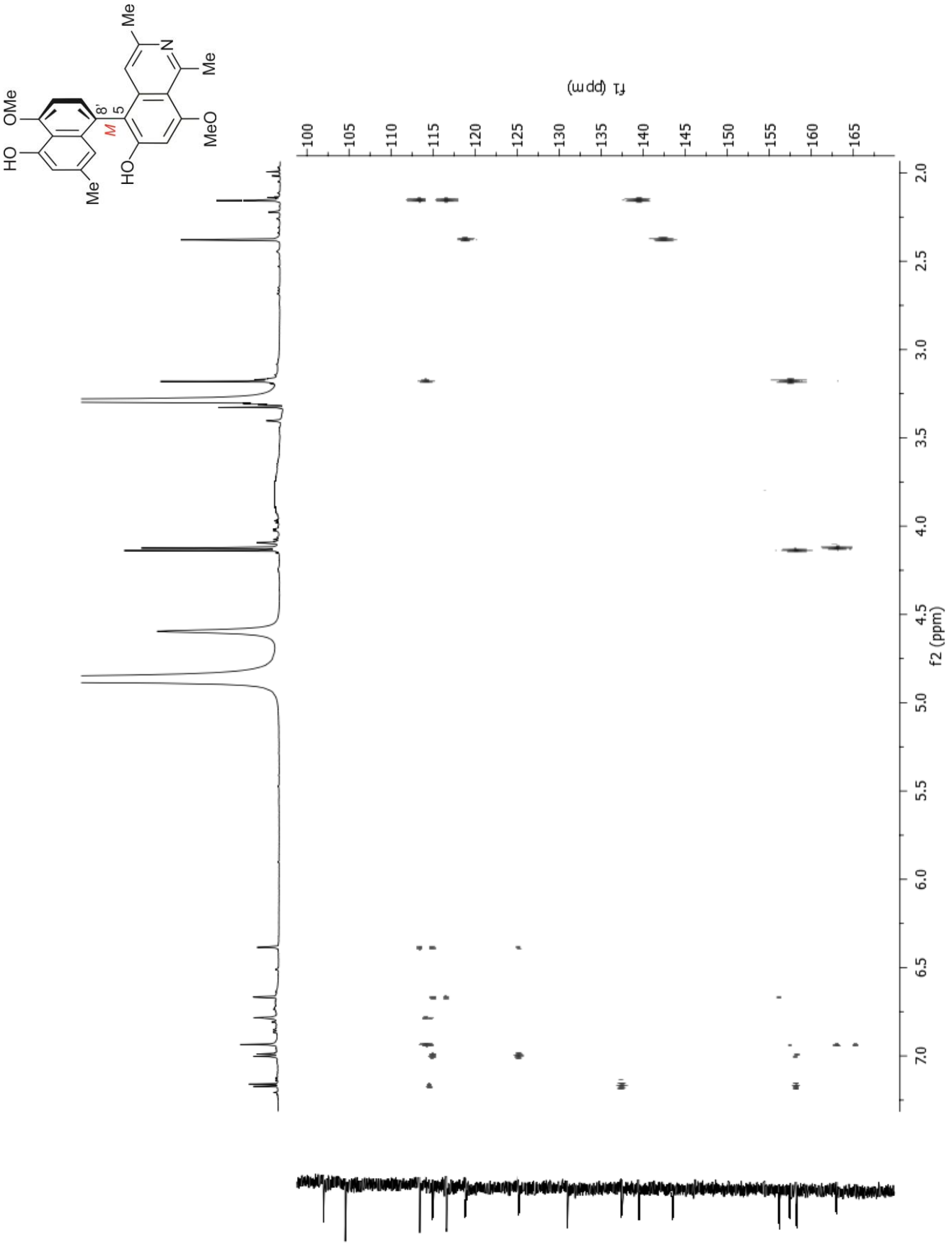


Figure S73. HMBC spectrum of ancistrolikokine G (**12**).

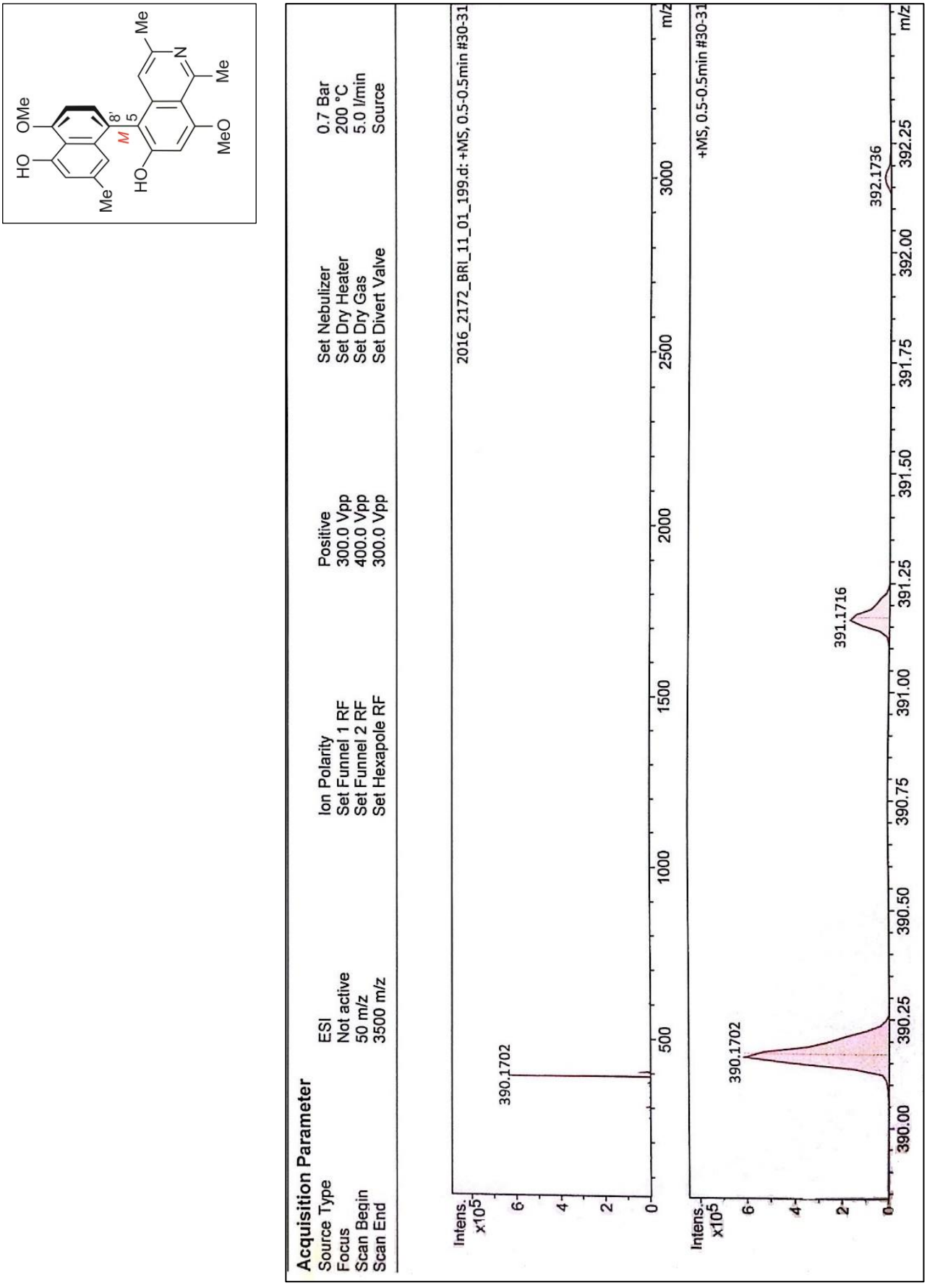
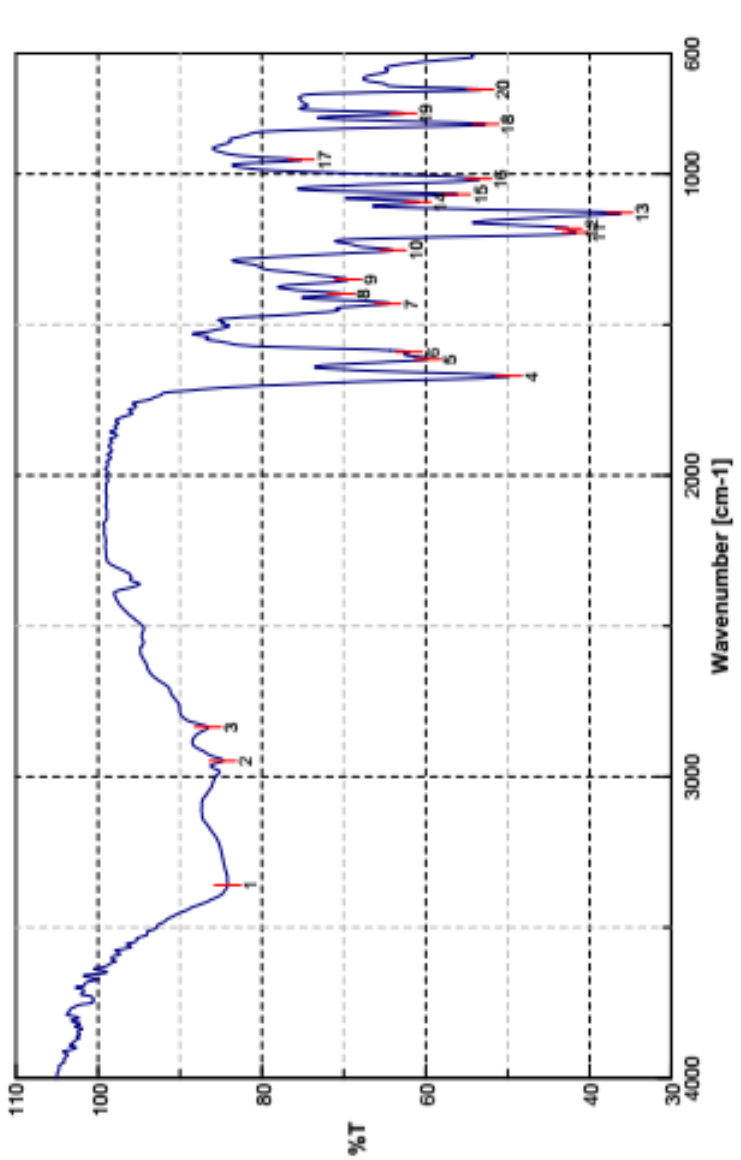


Figure S74. HRESI-MS spectrum of ancistrolikokine G (**12**).



Accumulation	8
Resolution	4 cm-1
Zero Filling	ON
Apodization	Cosine
Gain	Auto (4)
Scanning Speed	Auto (2 mm/sec)
Date/Time	29.03.2017 10:54
Update	29.03.2017 13:16
Operator	Student
File Name	Memory#2
Sample Name	
Comment	

No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3359.39	84.1728	2	2947.66	84.8073	3	2835.81	86.5895
4	1670.05	49.8611	5	1615.09	59.7726	6	1590.99	62.0302
7	1430.92	64.6073	8	1397.17	70.3158	9	1349.93	69.4847
10	1252.54	64.0325	11	1194.69	41.6542	12	1181.19	42.5702
13	1129.12	36.3551	14	1092.48	60.9829	15	1067.41	56.1412
16	1016.3	53.5658	17	952.663	75.2334	18	835.026	52.7181
19	798.385	62.7362	20	719.318	53.329			

Figure S75. IR spectrum of ancistrolikokine G (**12**).

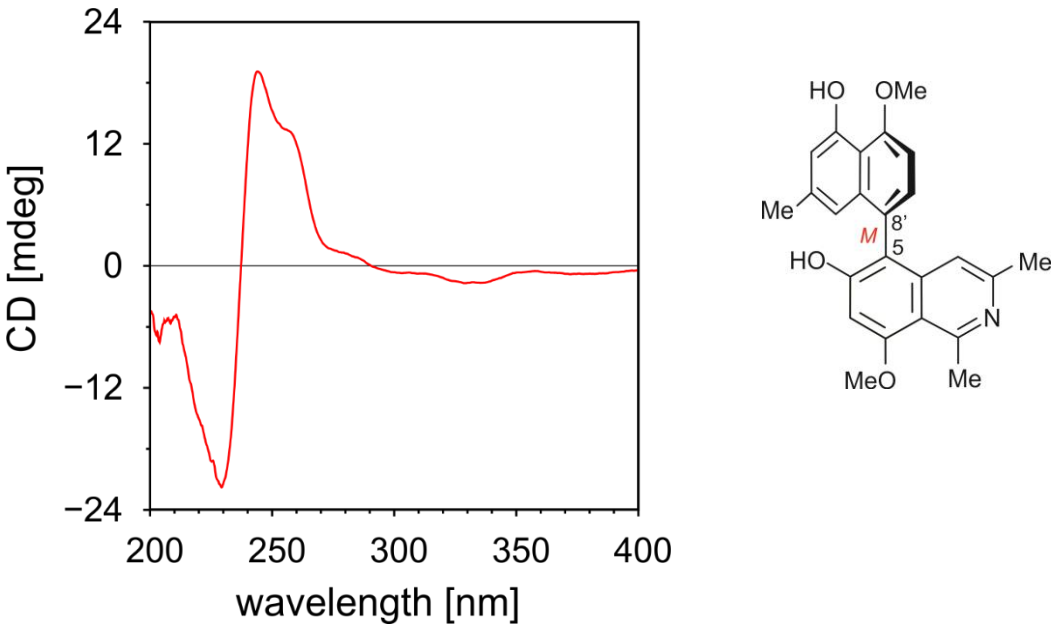


Figure S76. ECD spectrum of ancistrolikokine G (**12**).

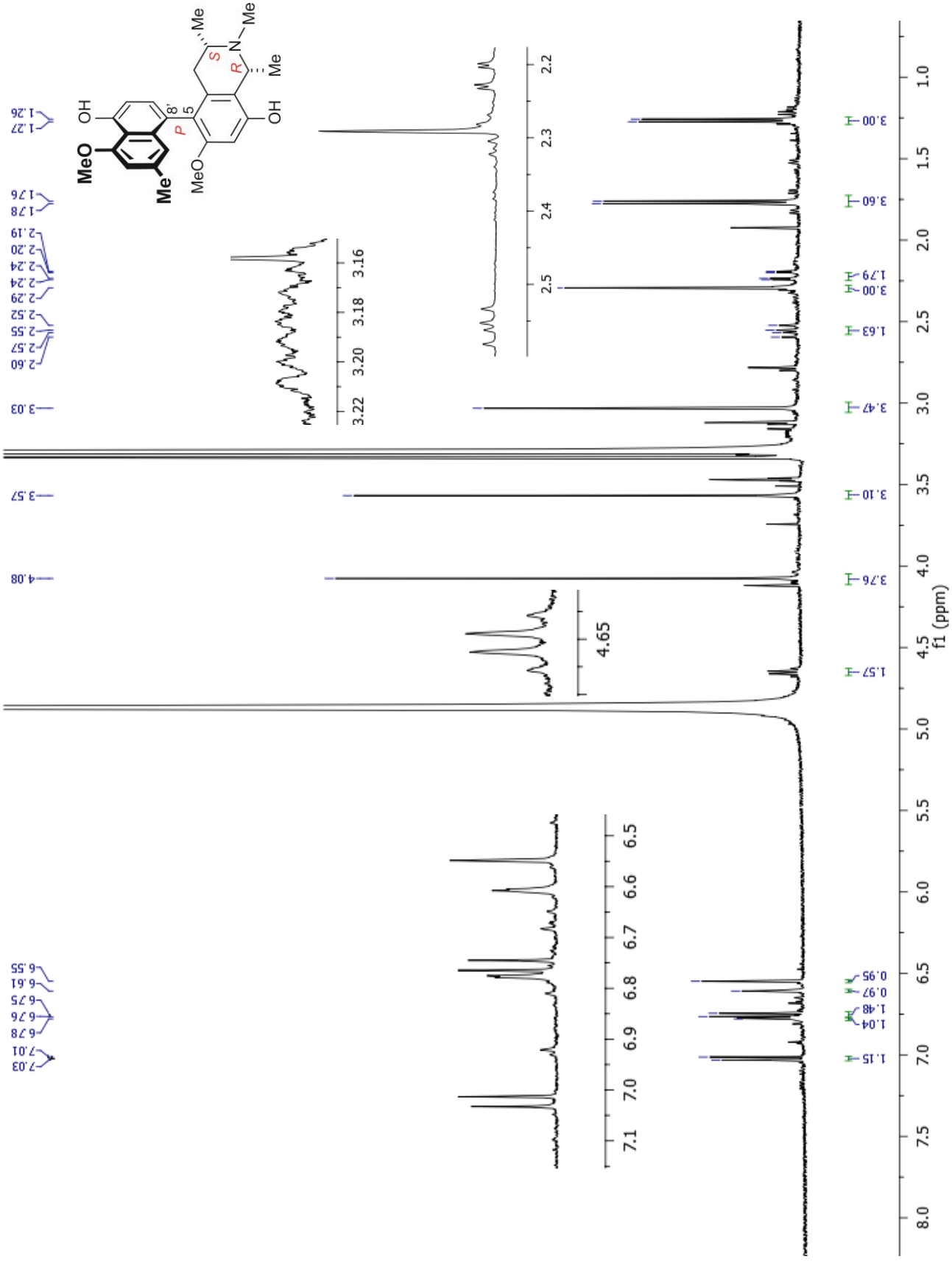
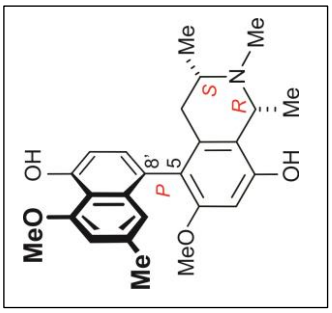


Figure S77. ^{1}H NMR spectrum of ancistrolikokine H (**15**).



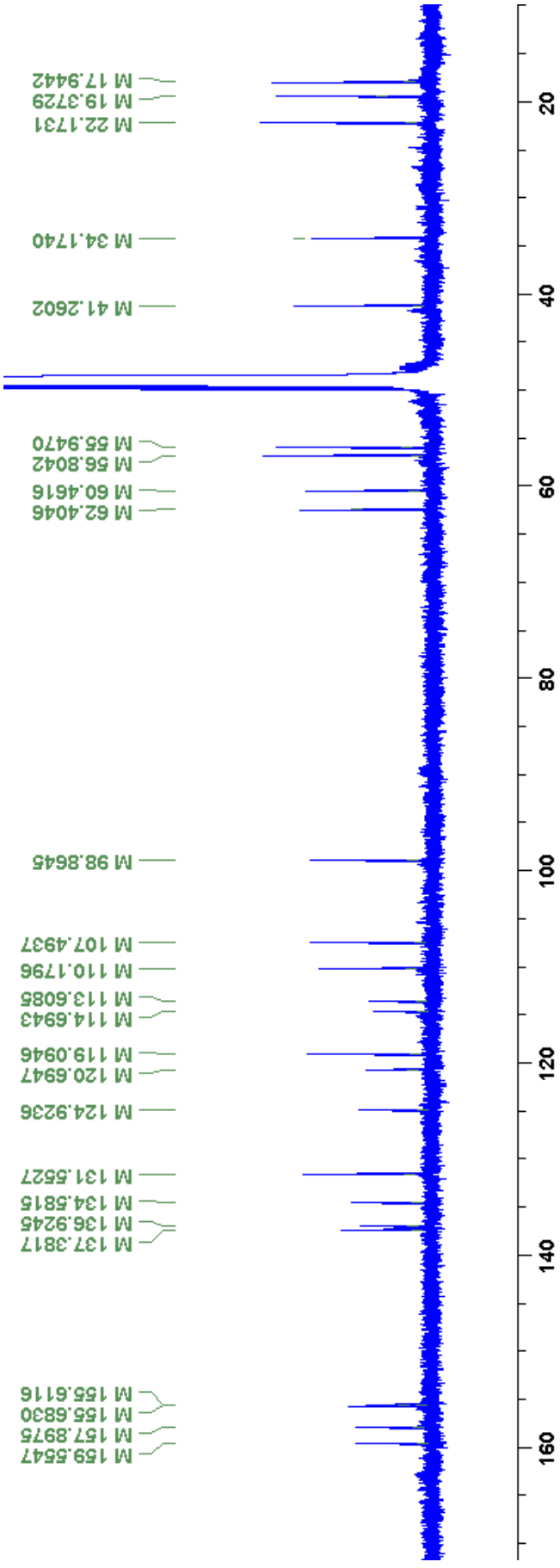


Figure S78. ^{13}C NMR spectrum of ancistrolikokine H (**15**).

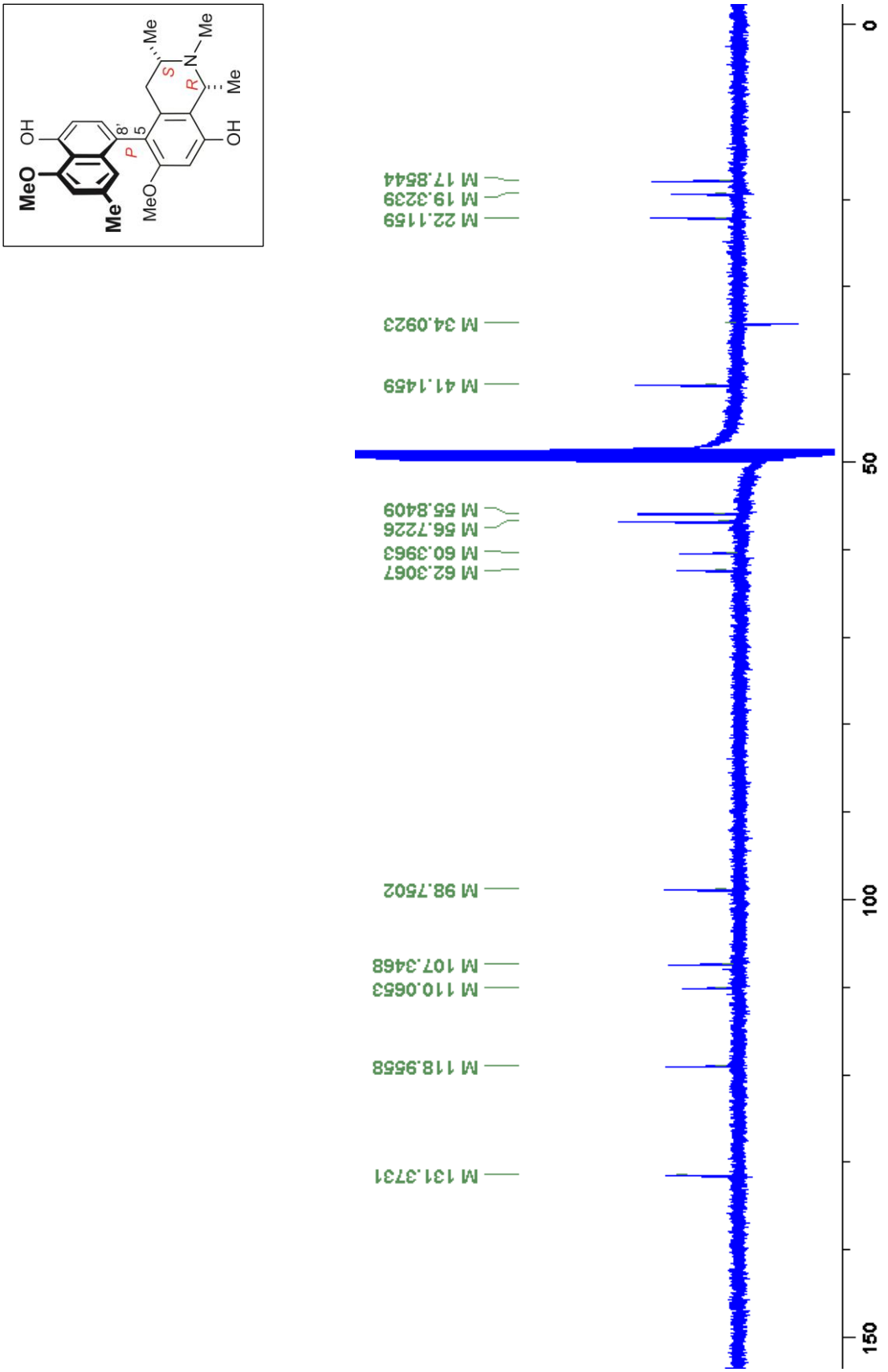


Figure S79. ^{13}C DEPT spectrum of ancistrolikokine H (**15**).

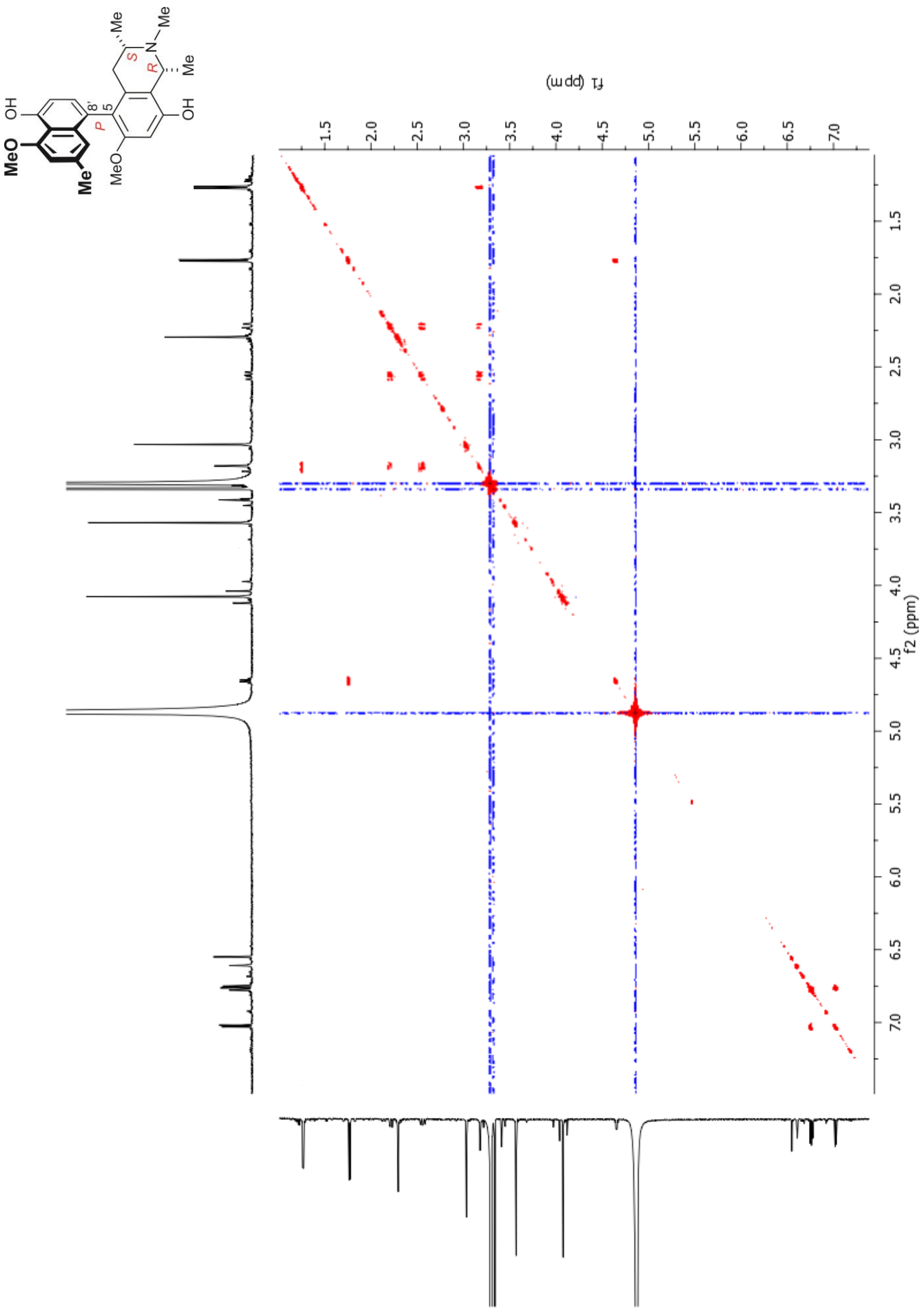


Figure S80. COSY spectrum of ancistrolikokine H (**15**).

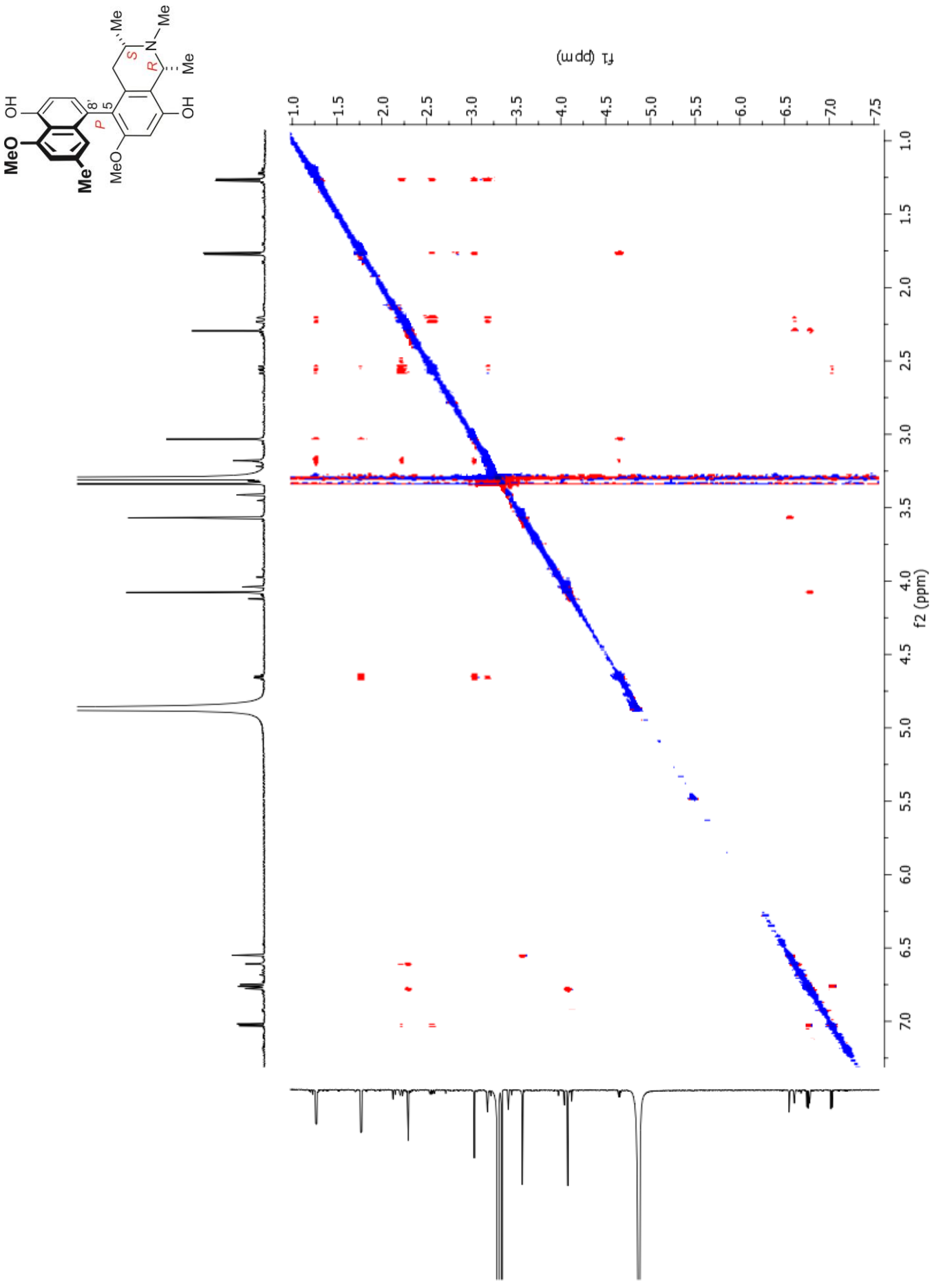


Figure S81. NOESY spectrum of ancistrolikokine H (**15**).

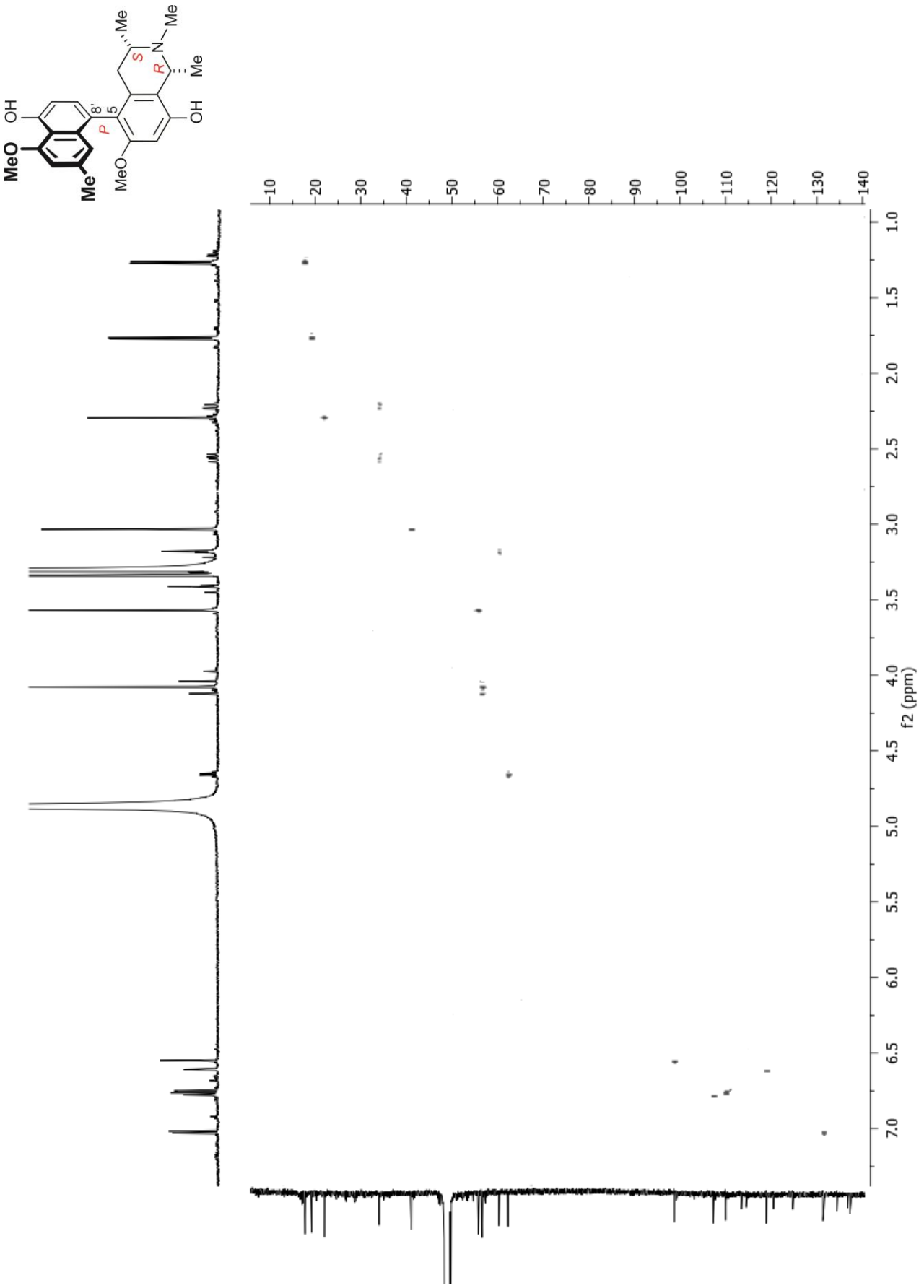


Figure S82. HSQC spectrum of ancistrolikokine H (**15**).

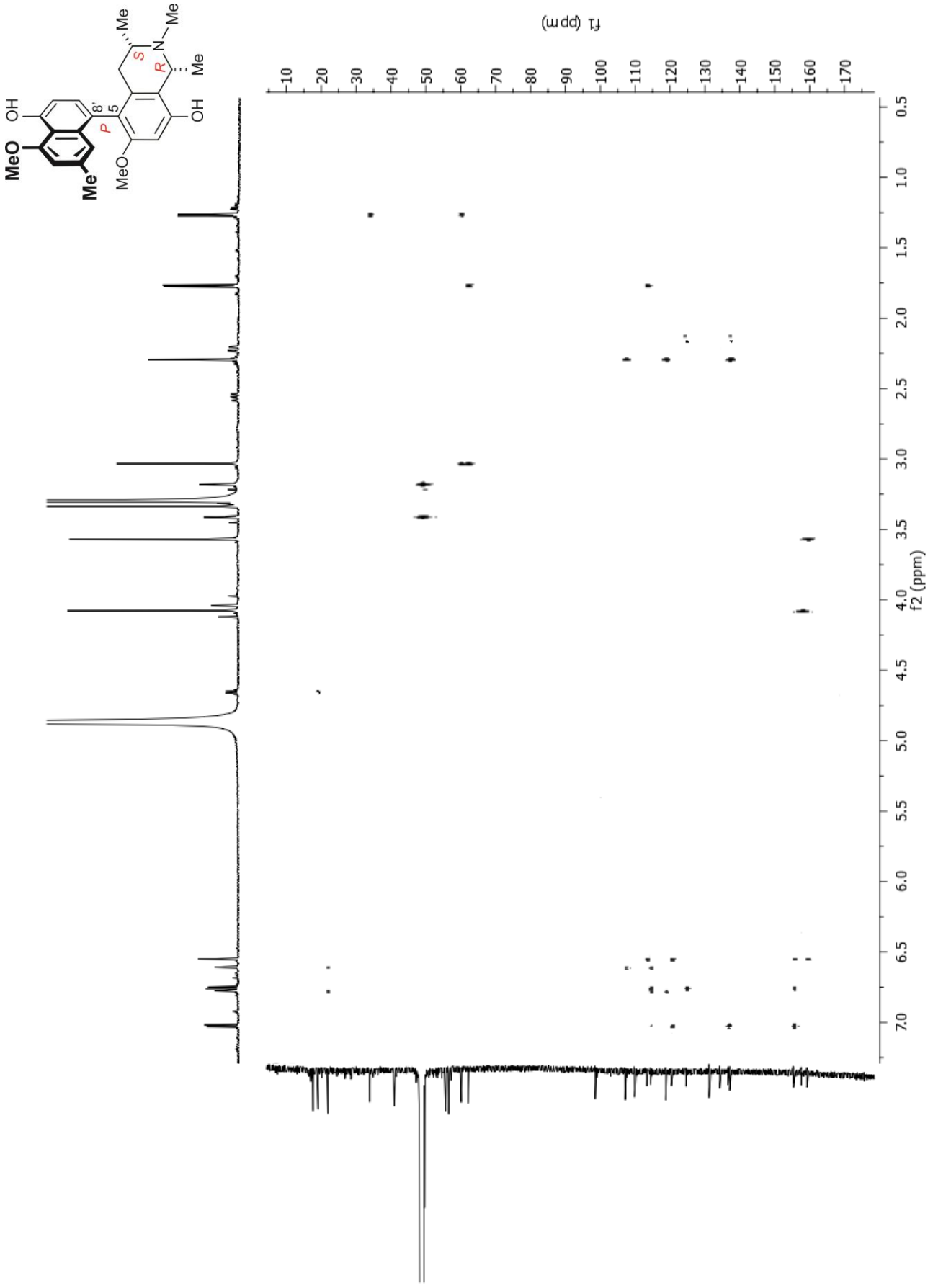
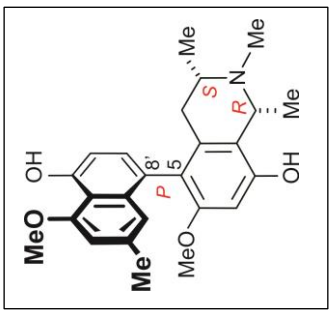


Figure S83. HMBC spectrum of ancistrolikokine H (**15**).



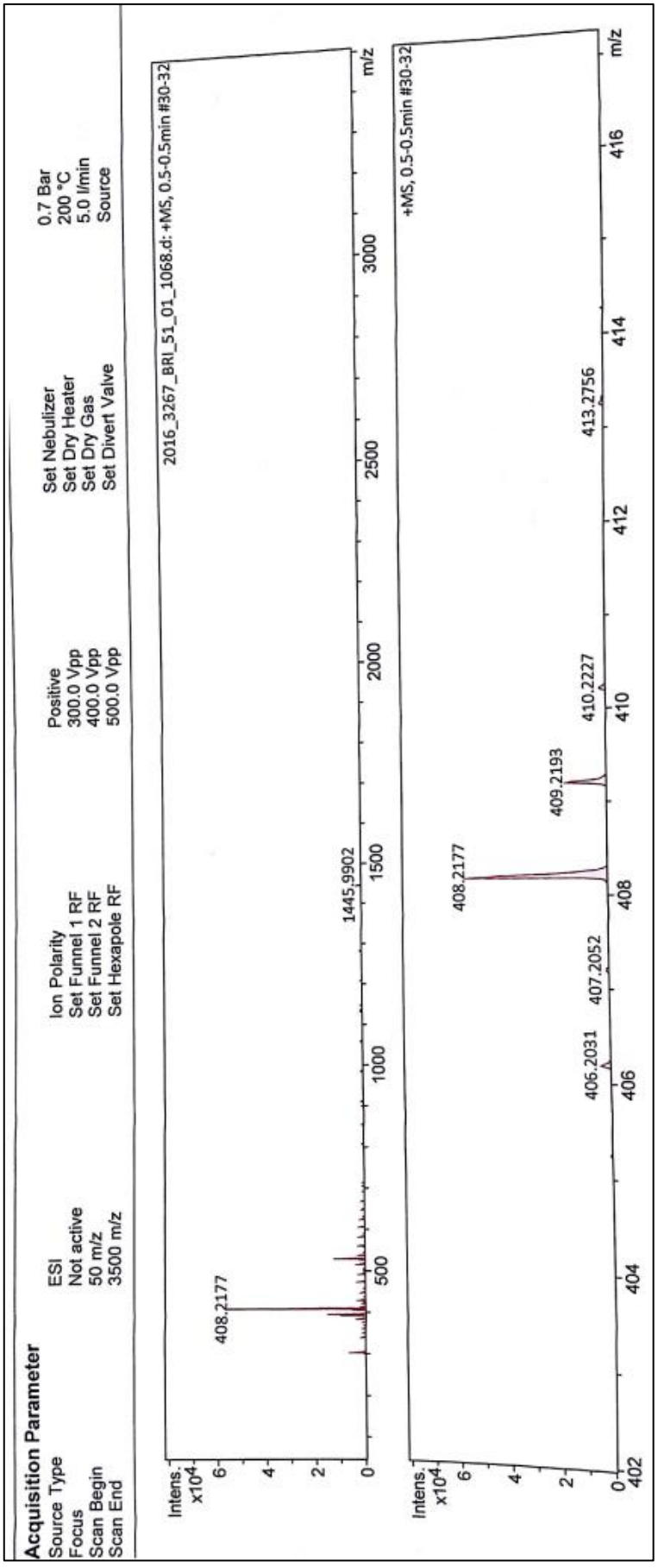
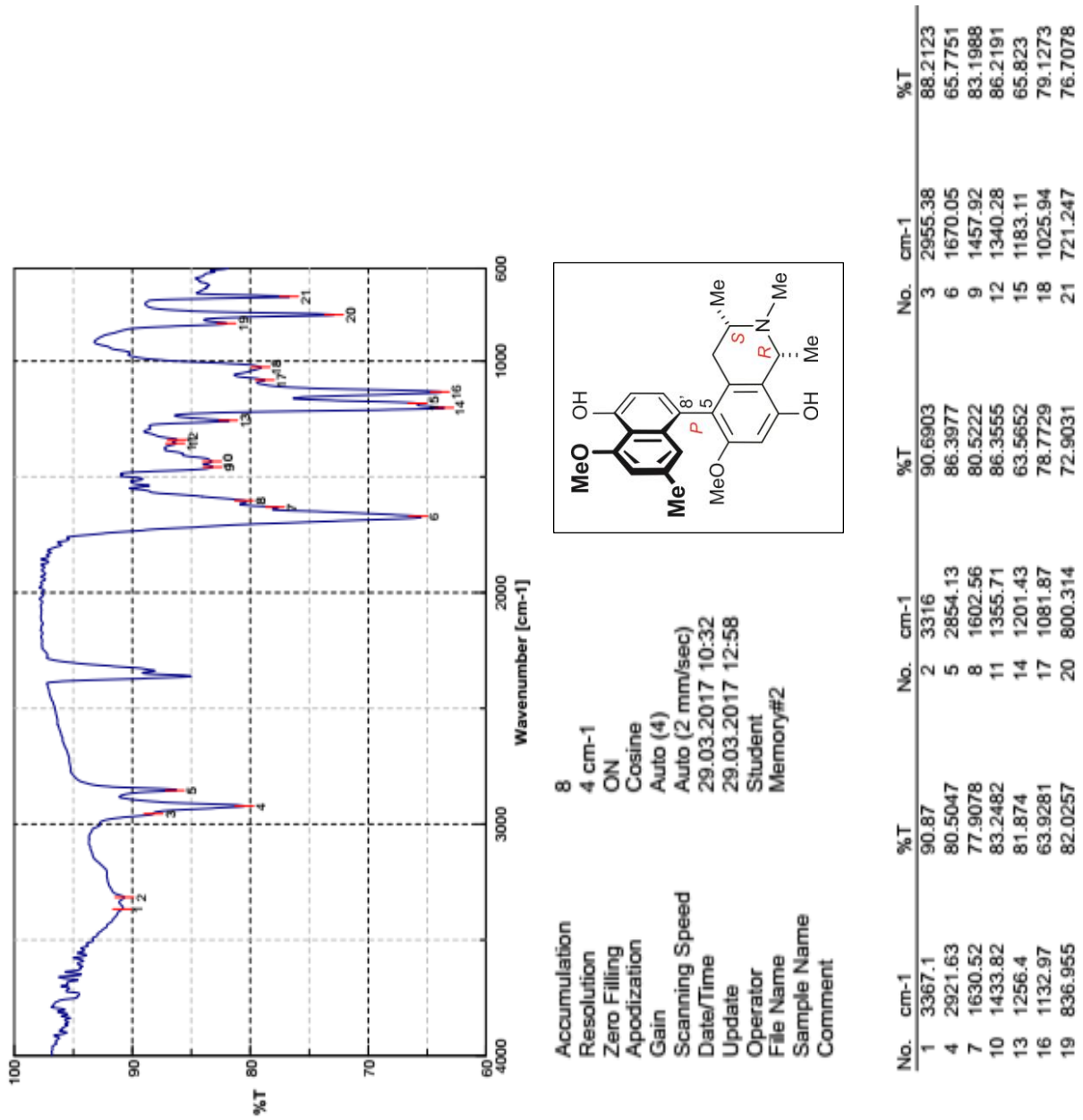


Figure S84. HRESI-MS spectrum of ancistrolikokine H (**15**).



No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3367.1	90.87	2	3316	90.6903	3	2955.38	88.2123
4	2921.63	80.5047	5	2854.13	86.3977	6	1670.05	65.7751
7	1630.52	77.9078	8	1602.56	80.5222	9	1457.92	83.1988
10	1433.82	83.2482	11	1355.71	86.3555	12	1340.28	86.2191
13	1256.4	81.874	14	1201.43	63.5652	15	1183.11	65.823
16	1132.97	63.9281	17	1081.87	78.7729	18	1025.94	79.1273
19	836.955	82.0257	20	800.314	72.9031	21	721.247	76.7078

Figure S85. IR spectrum of ancistrolikokine H (**15**).

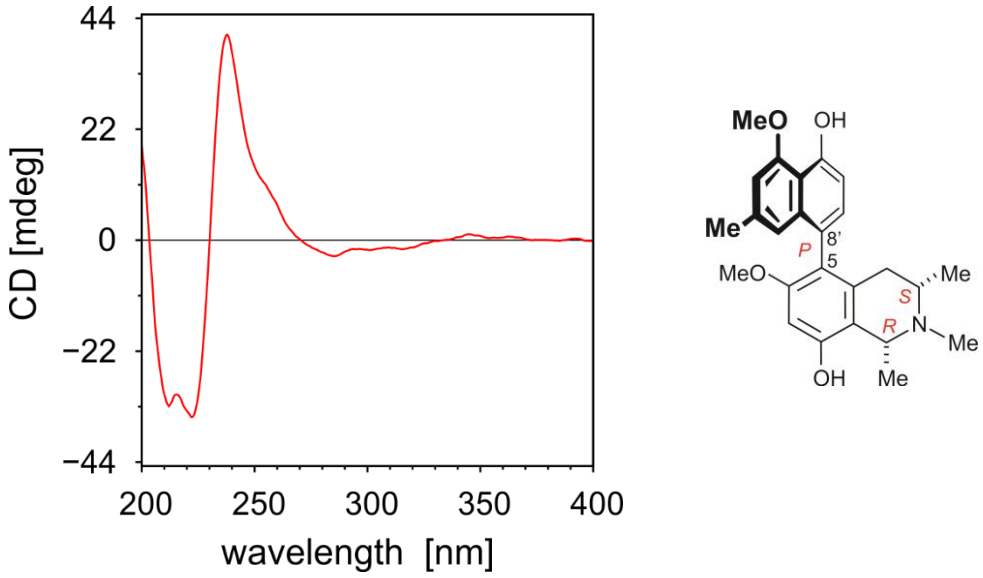
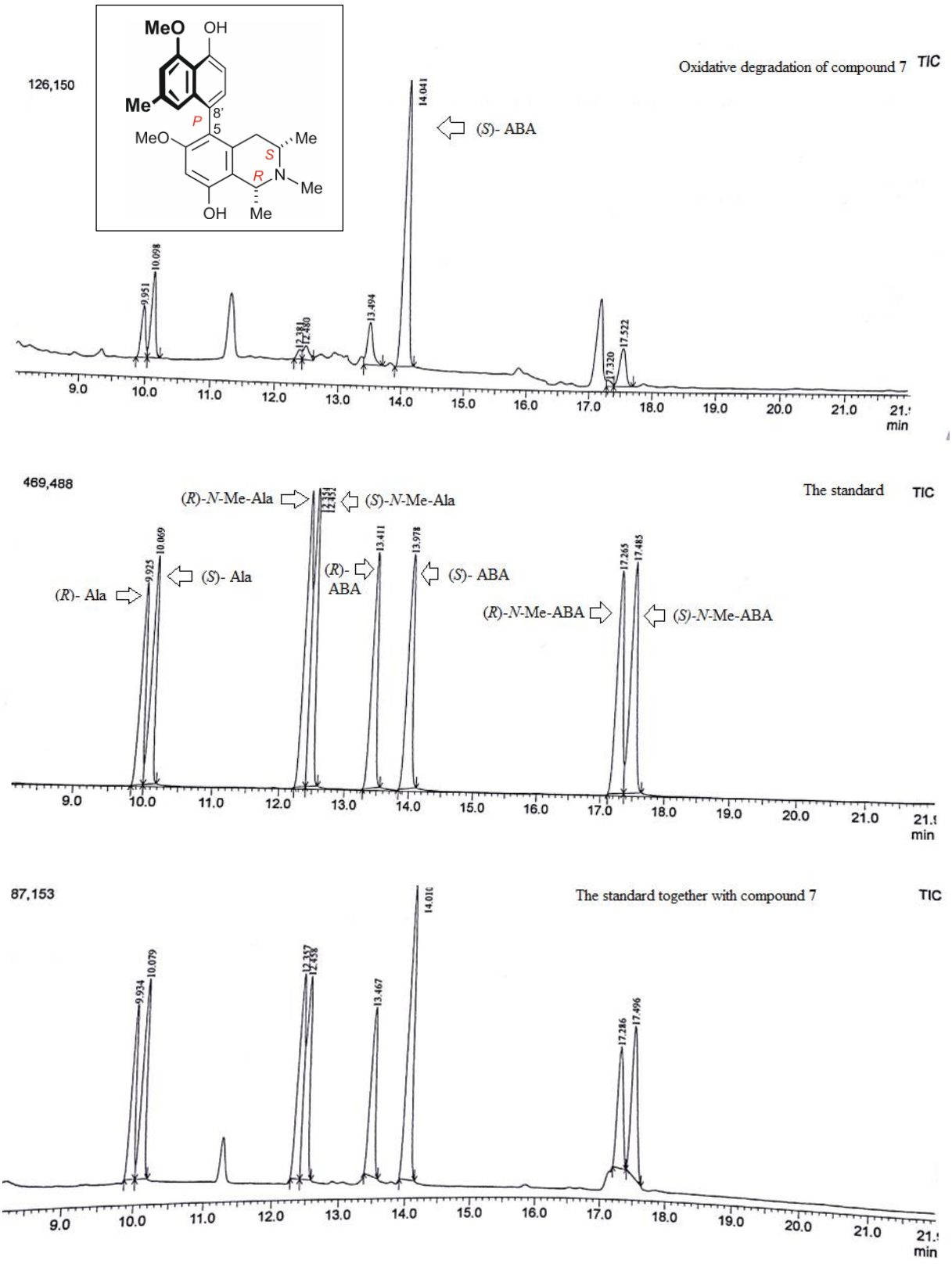


Figure S86. ECD spectrum of ancistrolikokine H (**15**).



Ala = Alanine *N*-Me-Ala = *N*-Methylalanine

ABA = 3-Aminobutyric acid *N*-Me-ABA = *N*-Methyl-3-aminobutyric acid

Figure S87. Oxidative degradation products of ancistrolikokine H (**15**).

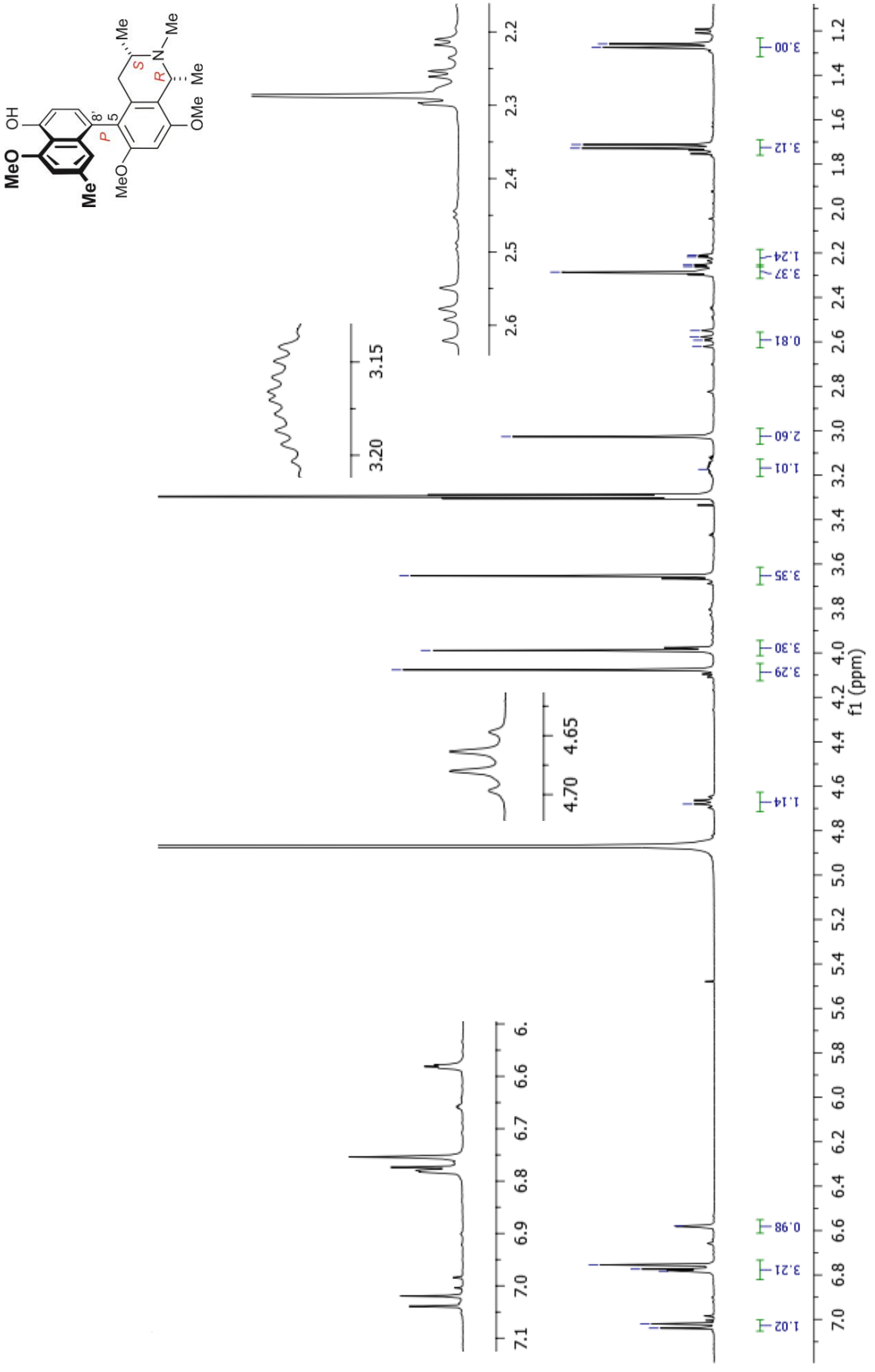


Figure S88. ^{1}H NMR spectrum of ancistrolikokine H_2 (**16**).

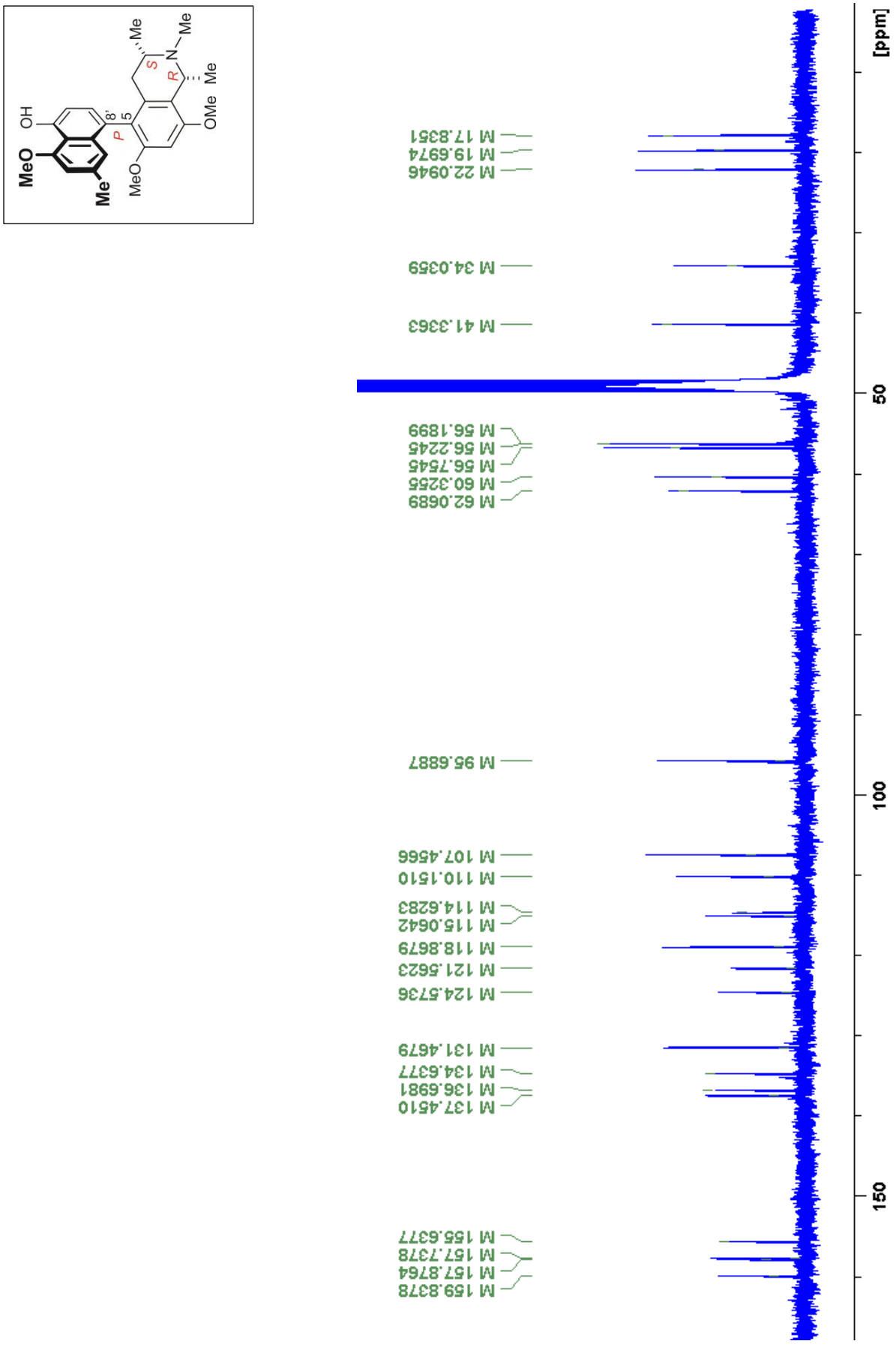


Figure S89. ^{13}C NMR spectrum of ancistrolikokine H_2 (**16**).

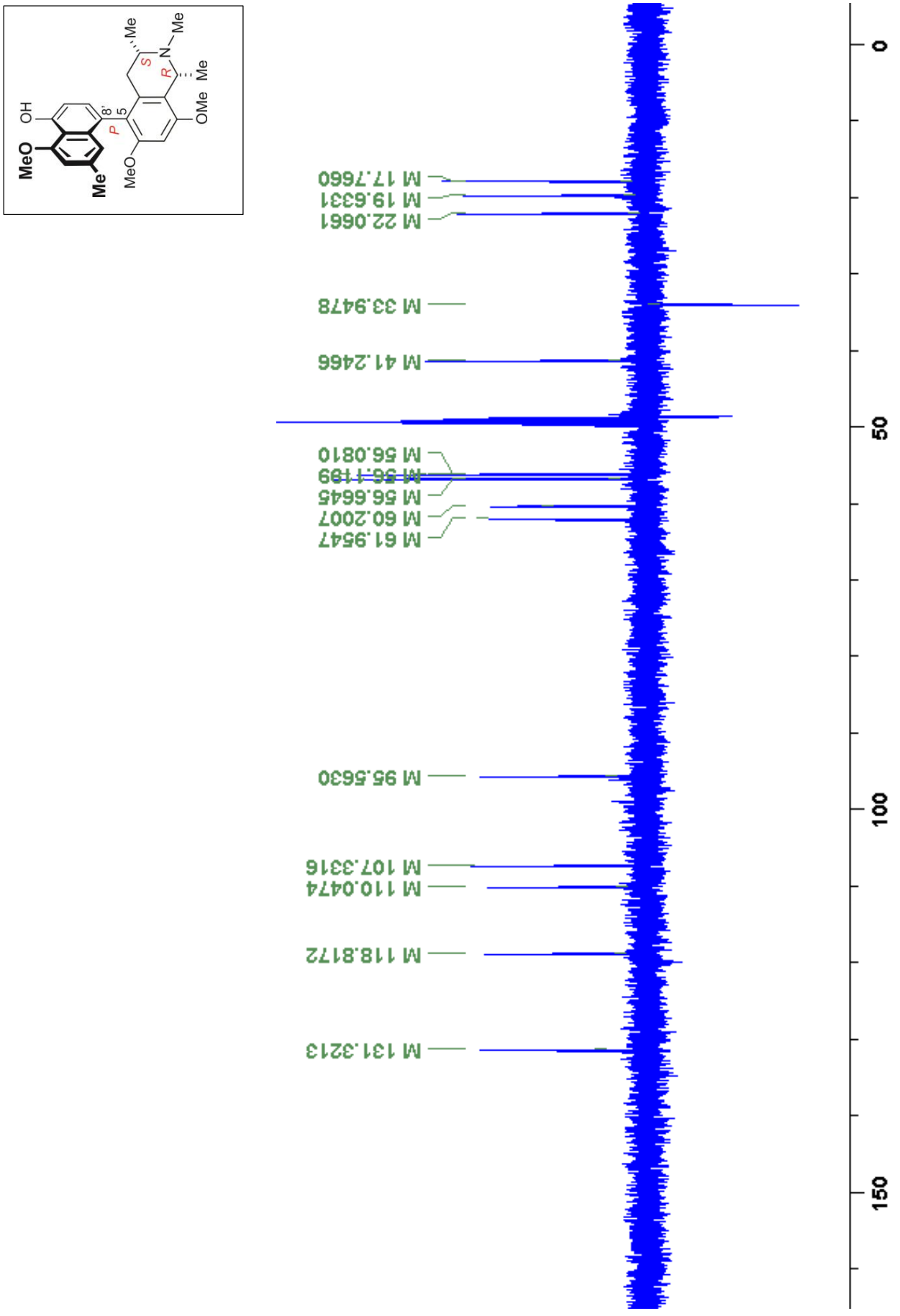


Figure S90. ^{13}C DEPT spectrum of ancistrolikokine H_2 (**16**).

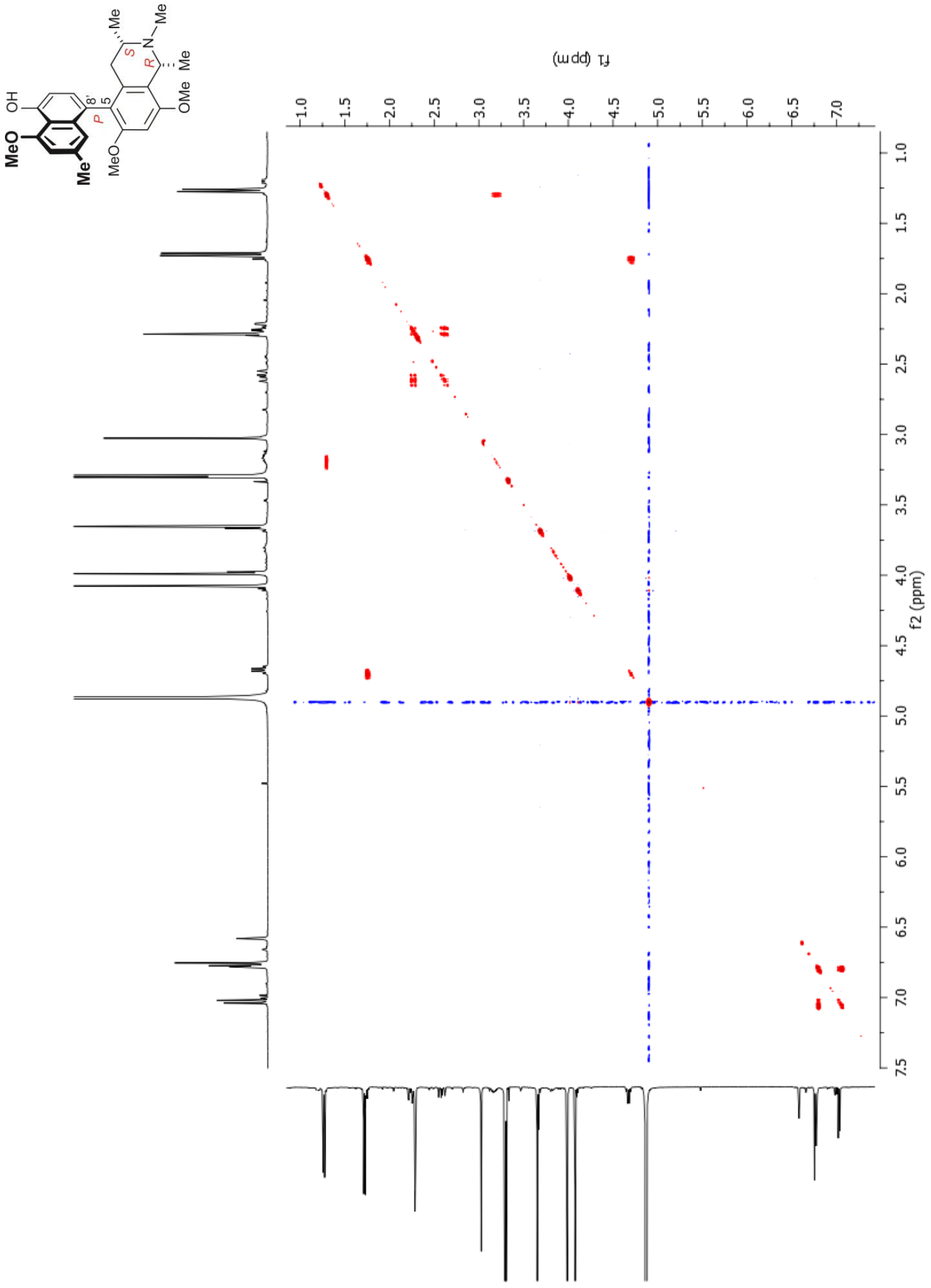


Figure S91. COSY spectrum of ancistrolikokine H_2 (**16**).

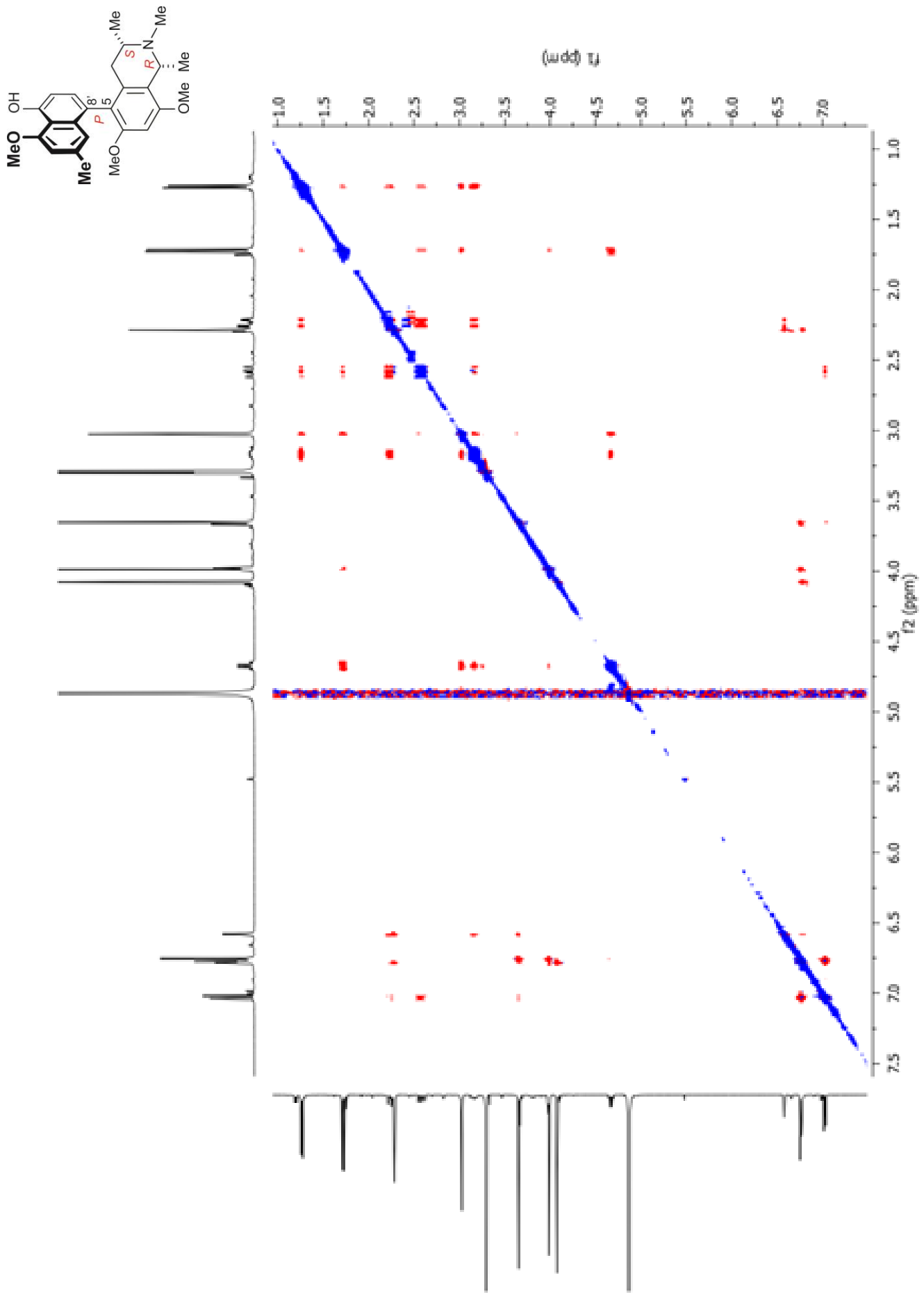


Figure S92. NOESY spectrum of ancistrolikokine H_2 (**16**).

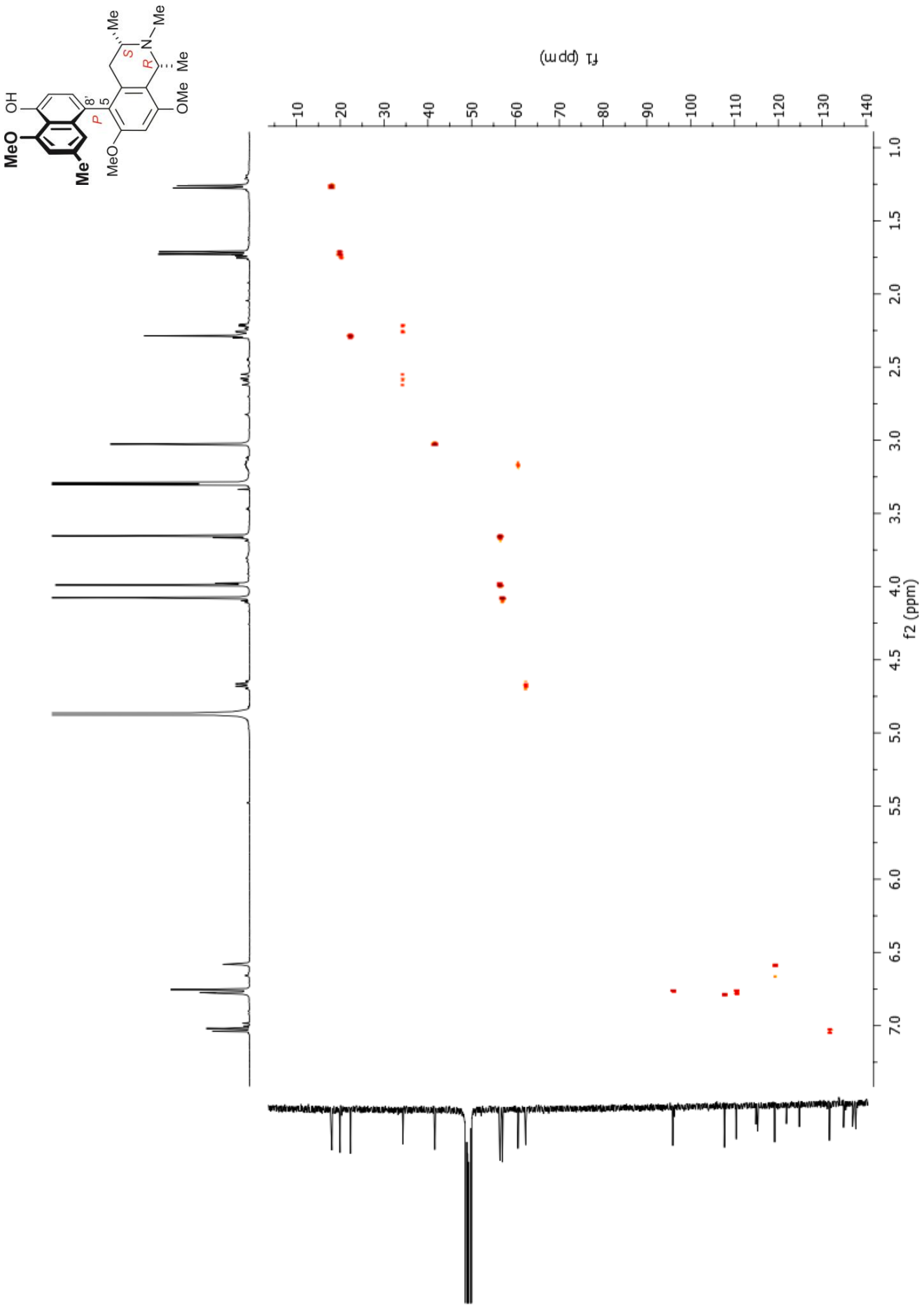


Figure S93. HSQC spectrum of ancistrolikokine H_2 (**16**).

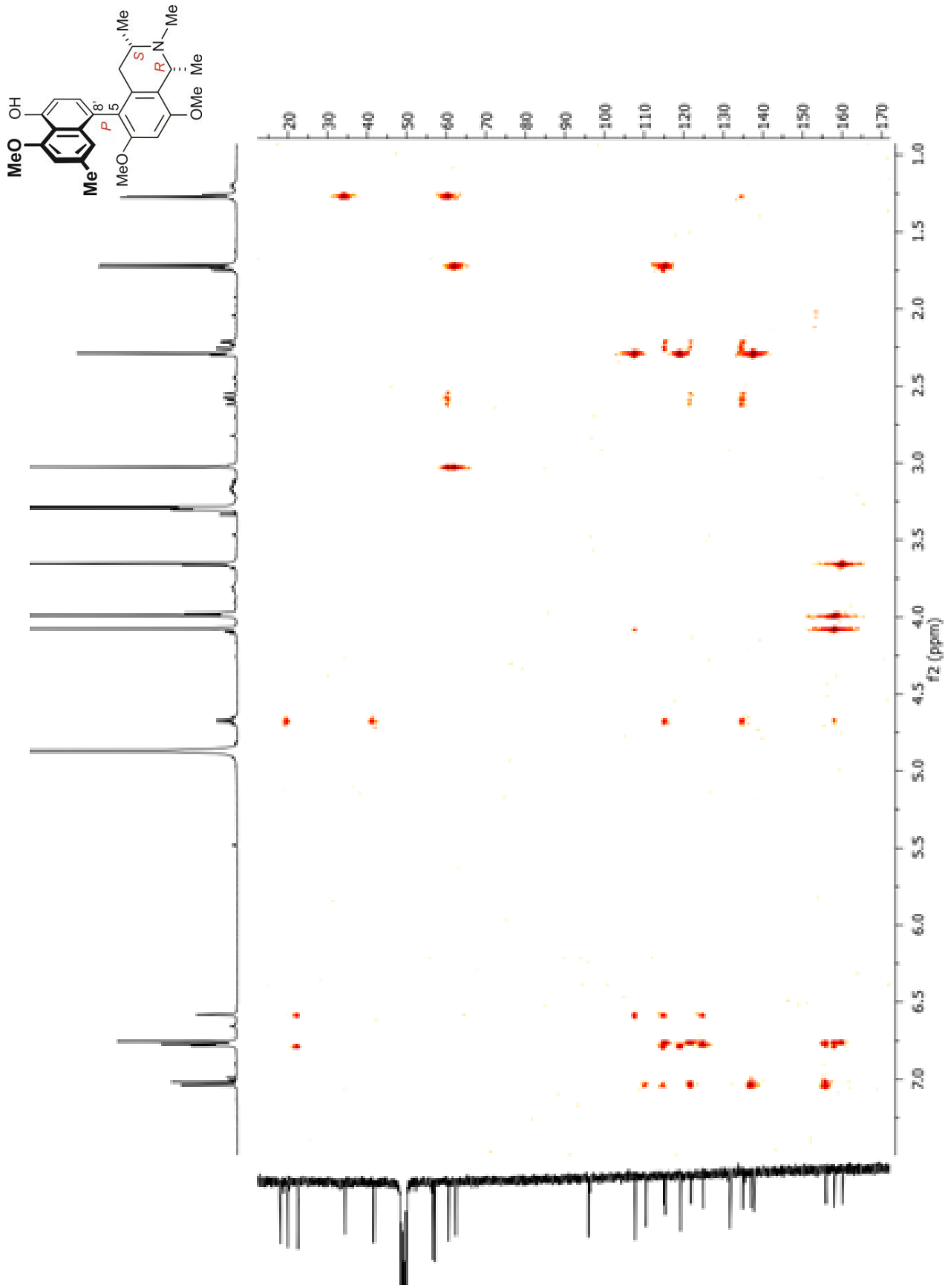
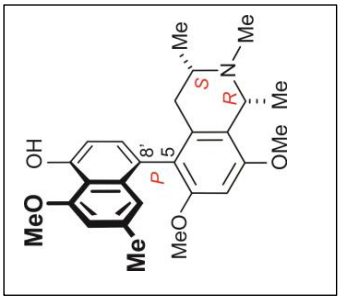


Figure S94. HMBC spectrum of ancistrolikokine H_2 (**16**).



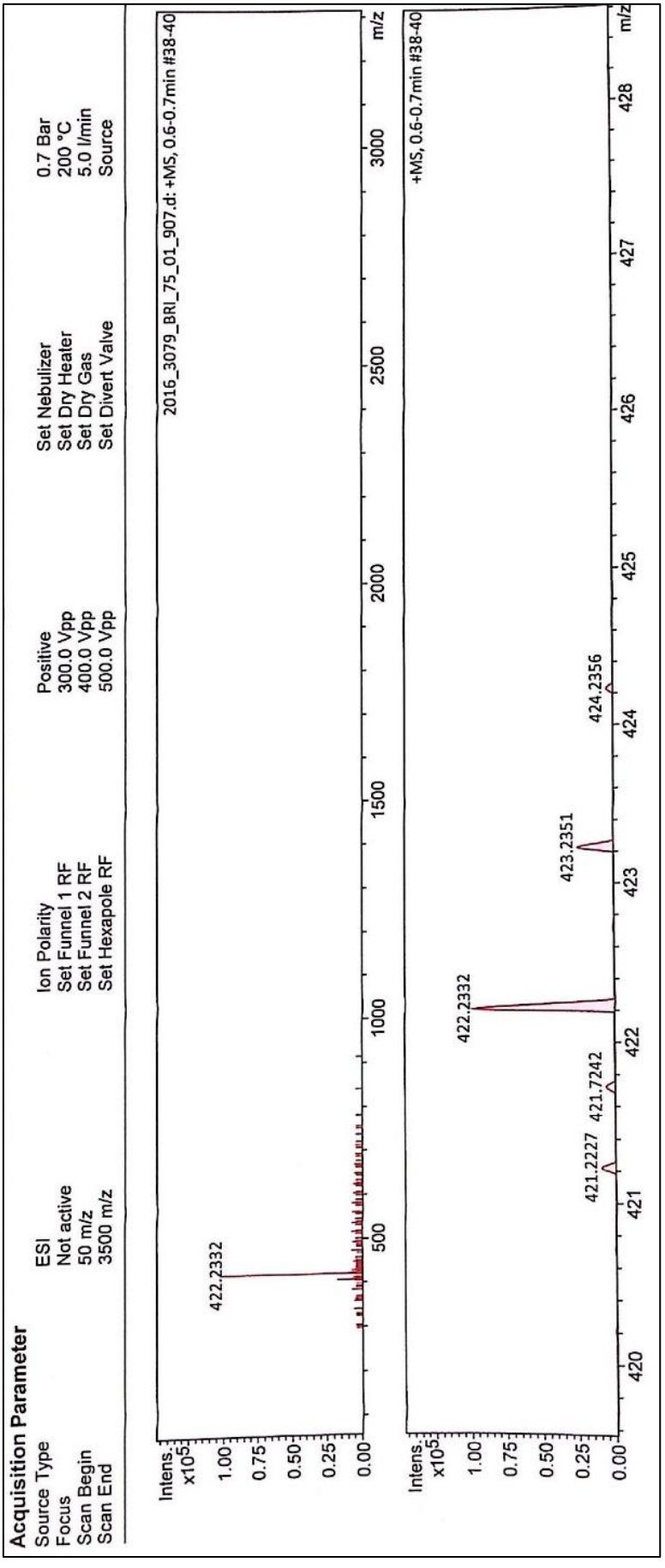
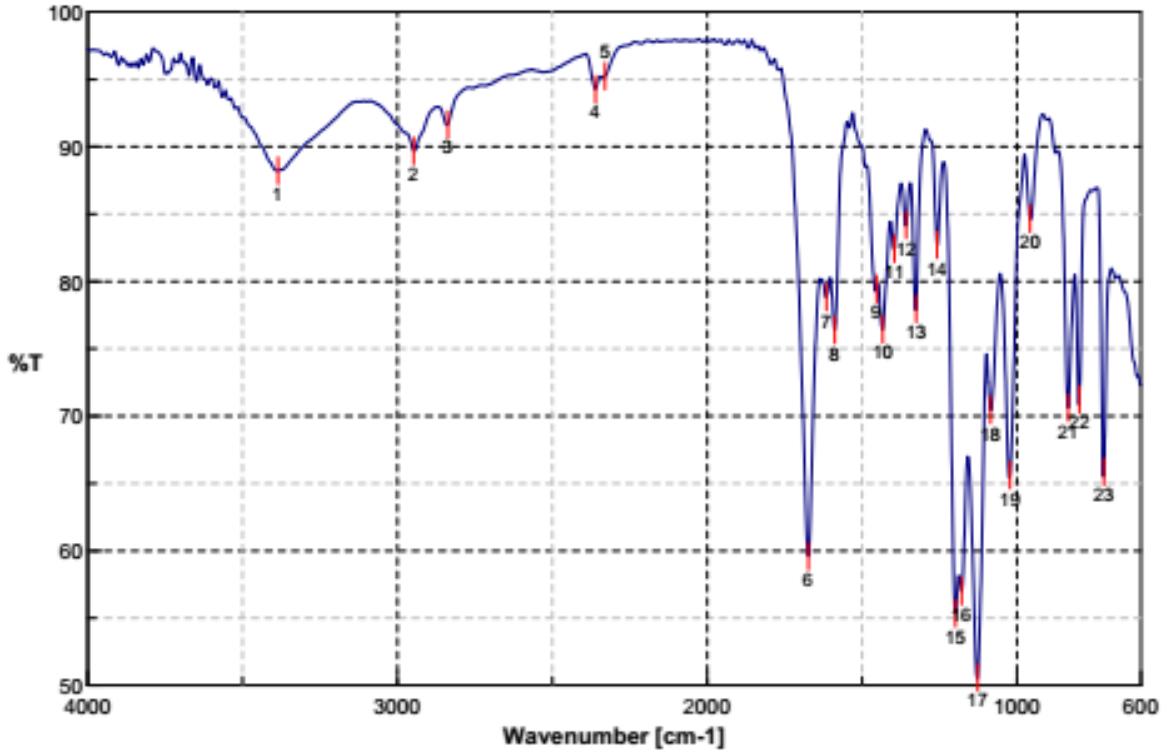


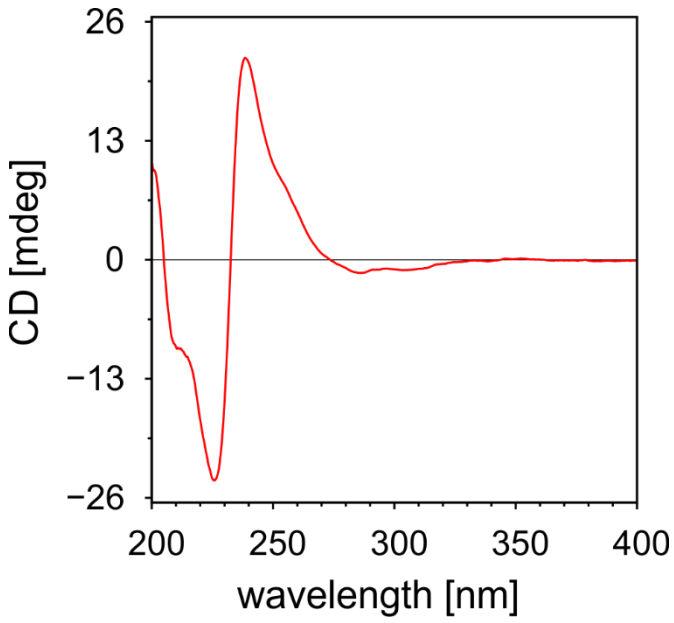
Figure S95. HRESI-MS spectrum of ancistrolikokine H_2 (**16**).



Accumulation	8
Resolution	4 cm-1
Zero Filling	ON
Apodization	Cosine
Gain	Auto (4)
Scanning Speed	Auto (2 mm/sec)
Date/Time	29.03.2017 10:29
Update	29.03.2017 13:01
Operator	Student
File Name	Memory#2
Sample Name	
Comment	

No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3385.42	88.2379	2	2947.66	89.7056	3	2837.74	91.6699
4	2360.44	94.2768	5	2330.55	95.2486	6	1673.91	59.6011
7	1615.09	78.8288	8	1588.09	76.4042	9	1453.1	79.4422
10	1433.82	76.44	11	1396.21	82.4439	12	1357.64	84.1885
13	1325.82	77.971	14	1258.32	82.7232	15	1198.54	55.3542
16	1179.26	56.9853	17	1127.19	50.5985	18	1085.73	70.4546
19	1023.05	65.6262	20	957.484	84.6526	21	835.026	70.6335
22	798.385	71.2437	23	719.318	65.857			

Figure S96. IR spectrum of ancistrolikokine H_2 (**16**).



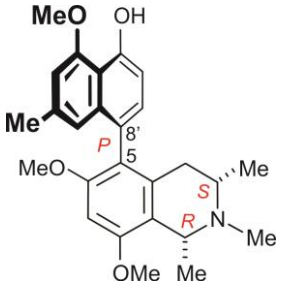
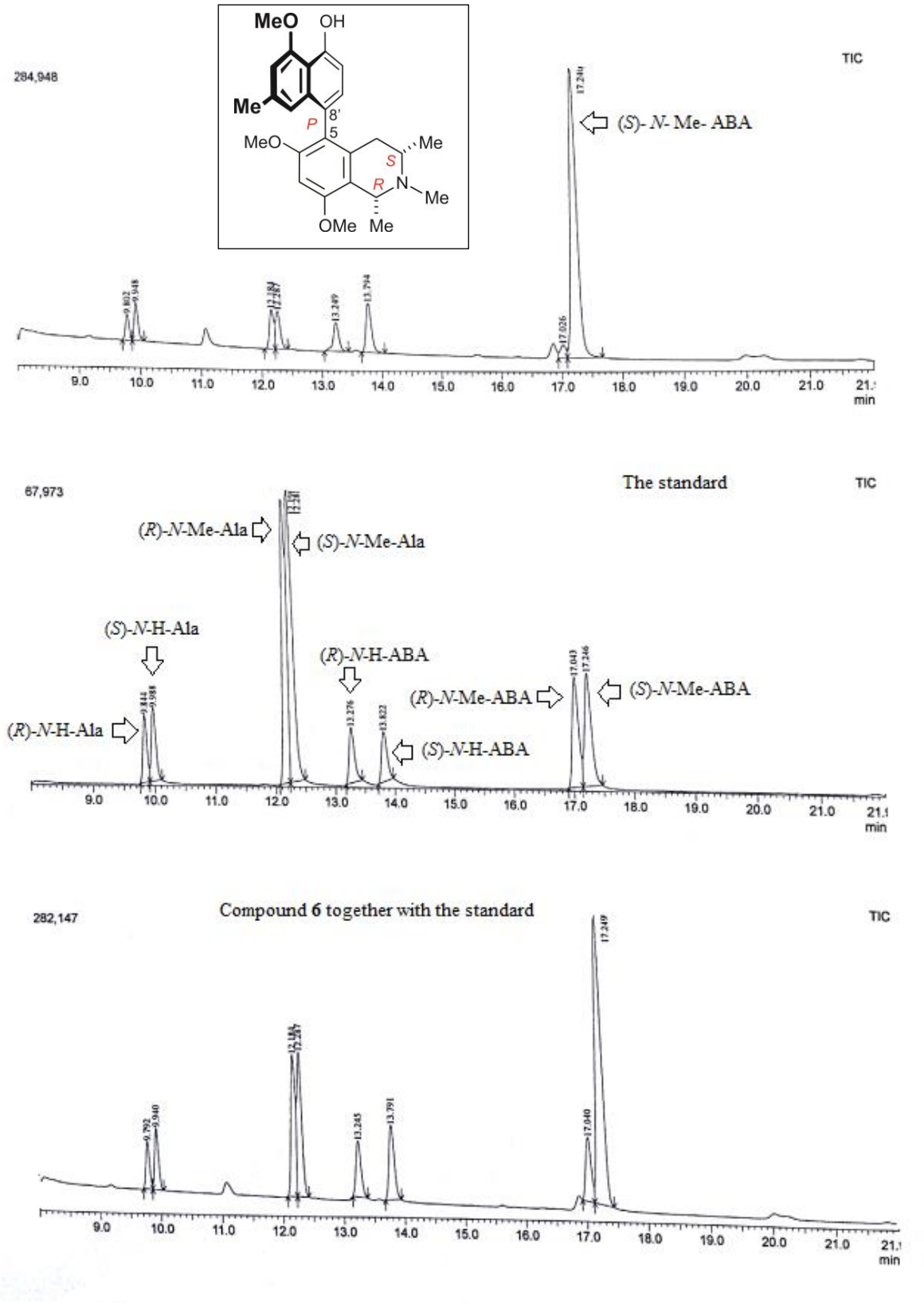


Figure S97. ECD spectrum of ancistrolikokine H_2 (**16**).



Ala = Alanine *N*-Me-Ala = *N*-Methylalanine

ABA = 3-Aminobutyric acid *N*-Me-ABA = *N*-Methyl-3-aminobutyric acid

Figure S98. Oxidative degradation products of ancistrolikokine H_2 (**16**).