Electronic Supplementary Information (ESI)

Antiprotozoal Dimeric Naphthylisoquinolines, Mbandakamines B_3 and B_4, and Related 5,8'-Coupled Monomeric Alkaloids, Ikelacongolines A-D, from a Congolese *Ancistrocladus* liana

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5. Ikelacongoline C (6)

6. Ikelacongoline D (7)

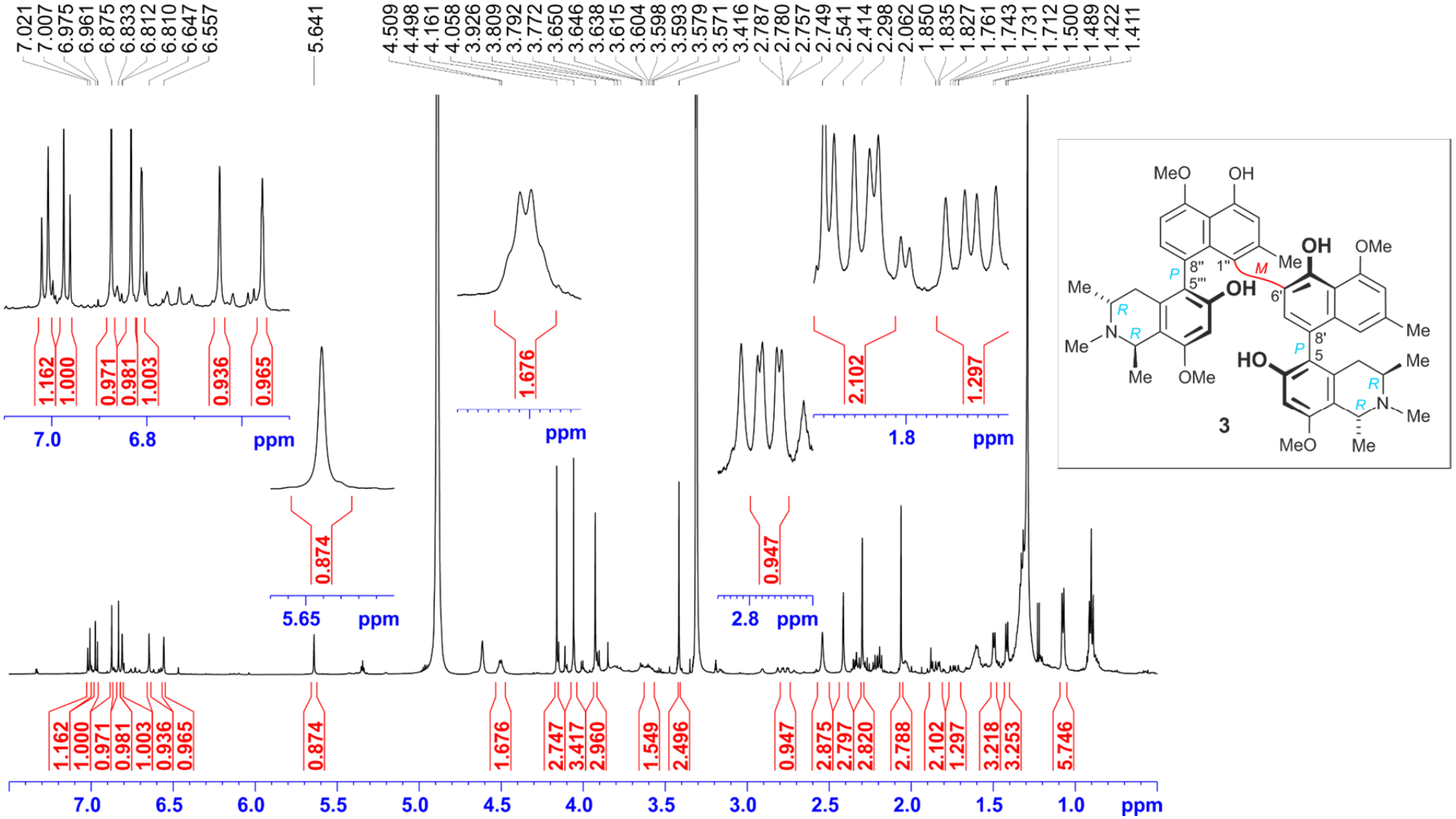


Figure S1. ^{1}H NMR spectrum of mbandakamine B_3 (**3**)

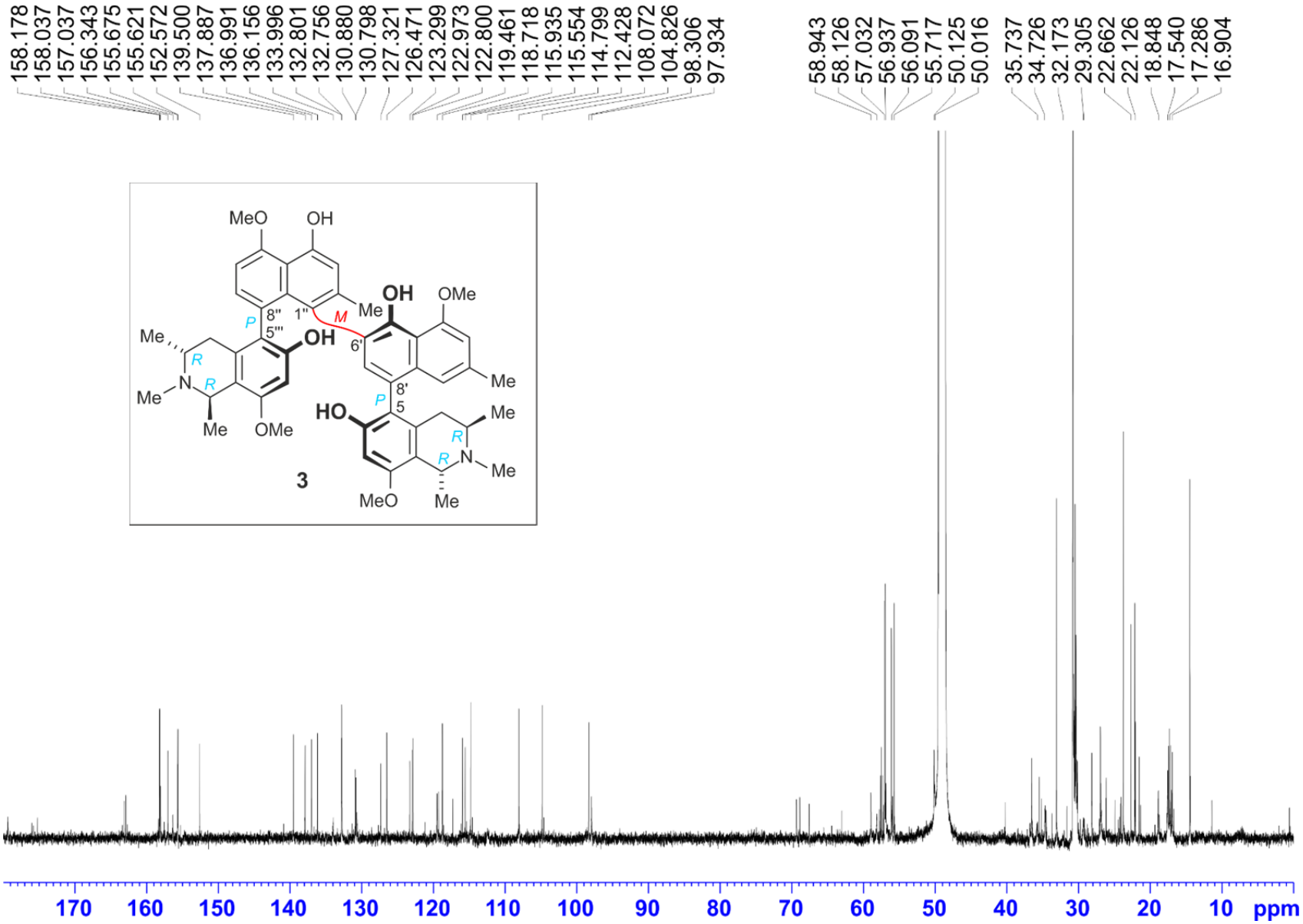


Figure S2. ^{13}C NMR spectrum of mbandakamine B_3 (**3**)

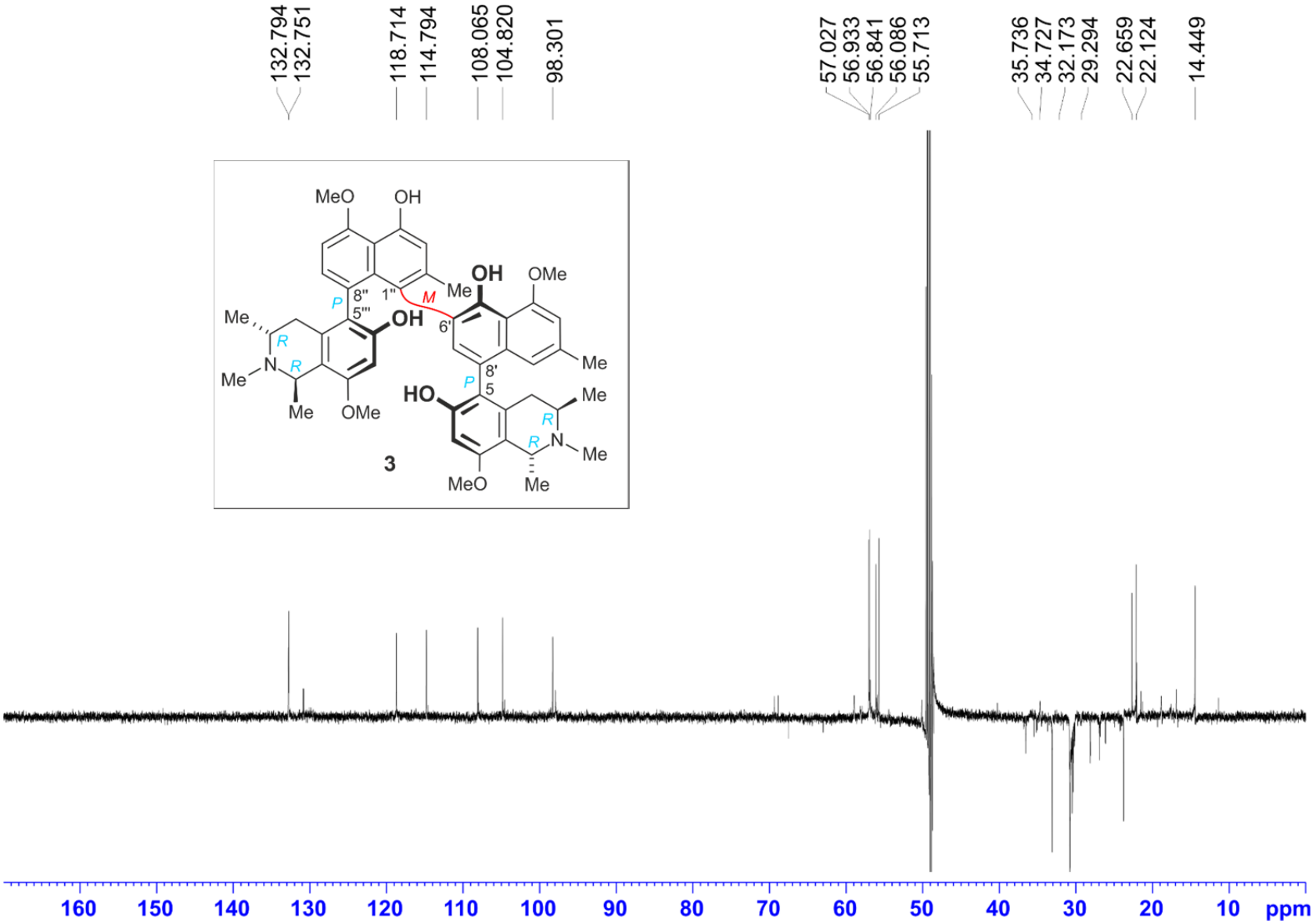
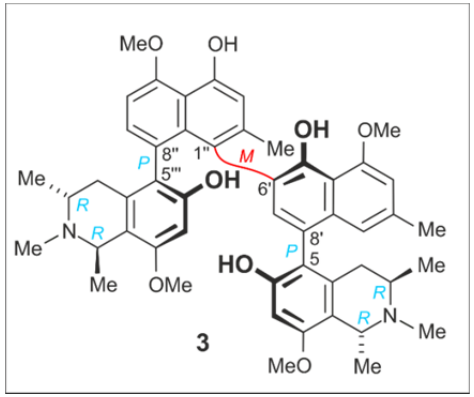


Figure S3. ^{13}C DEPT 135 NMR spectrum of mbandakamine B_3 (**3**



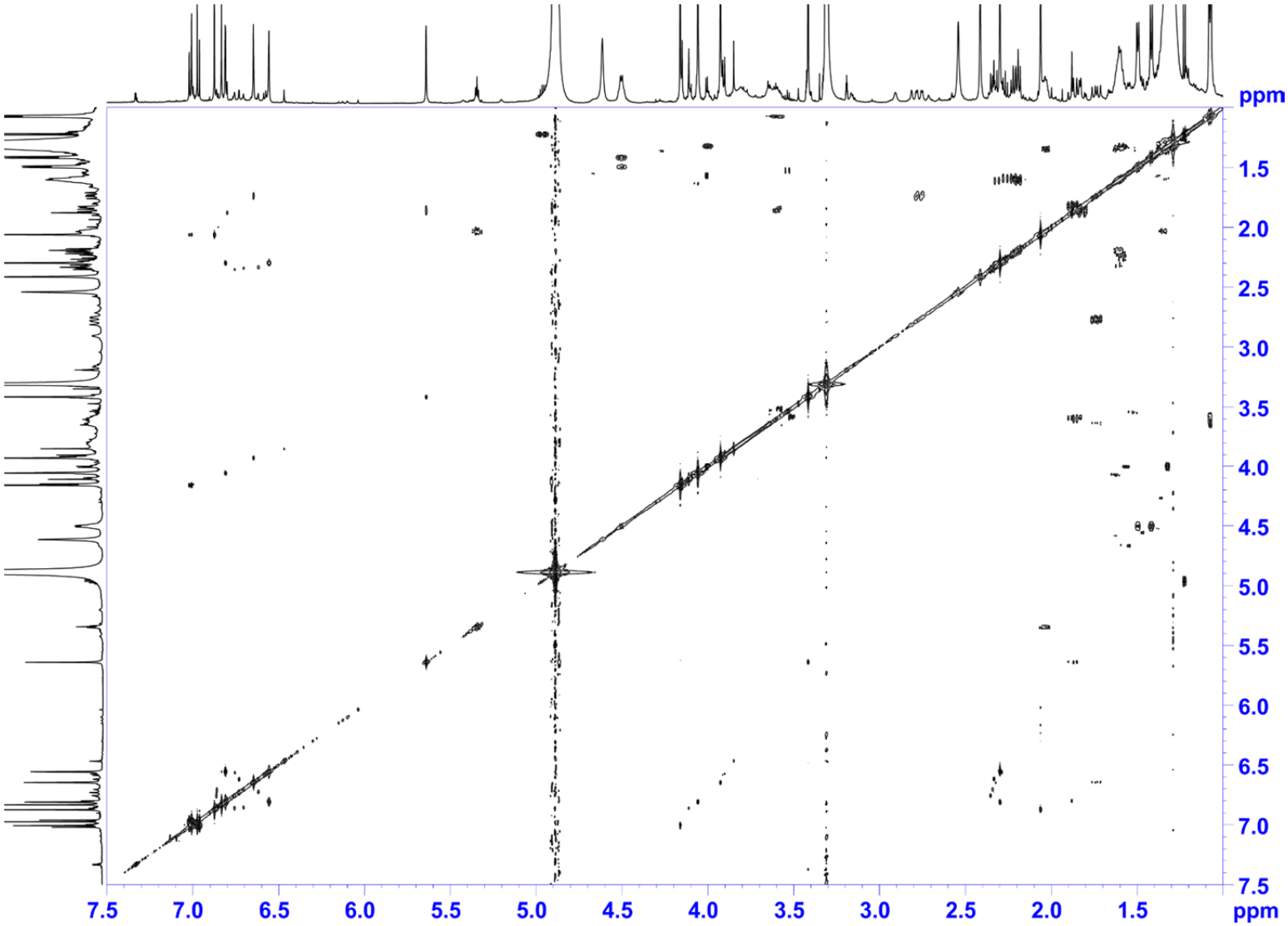
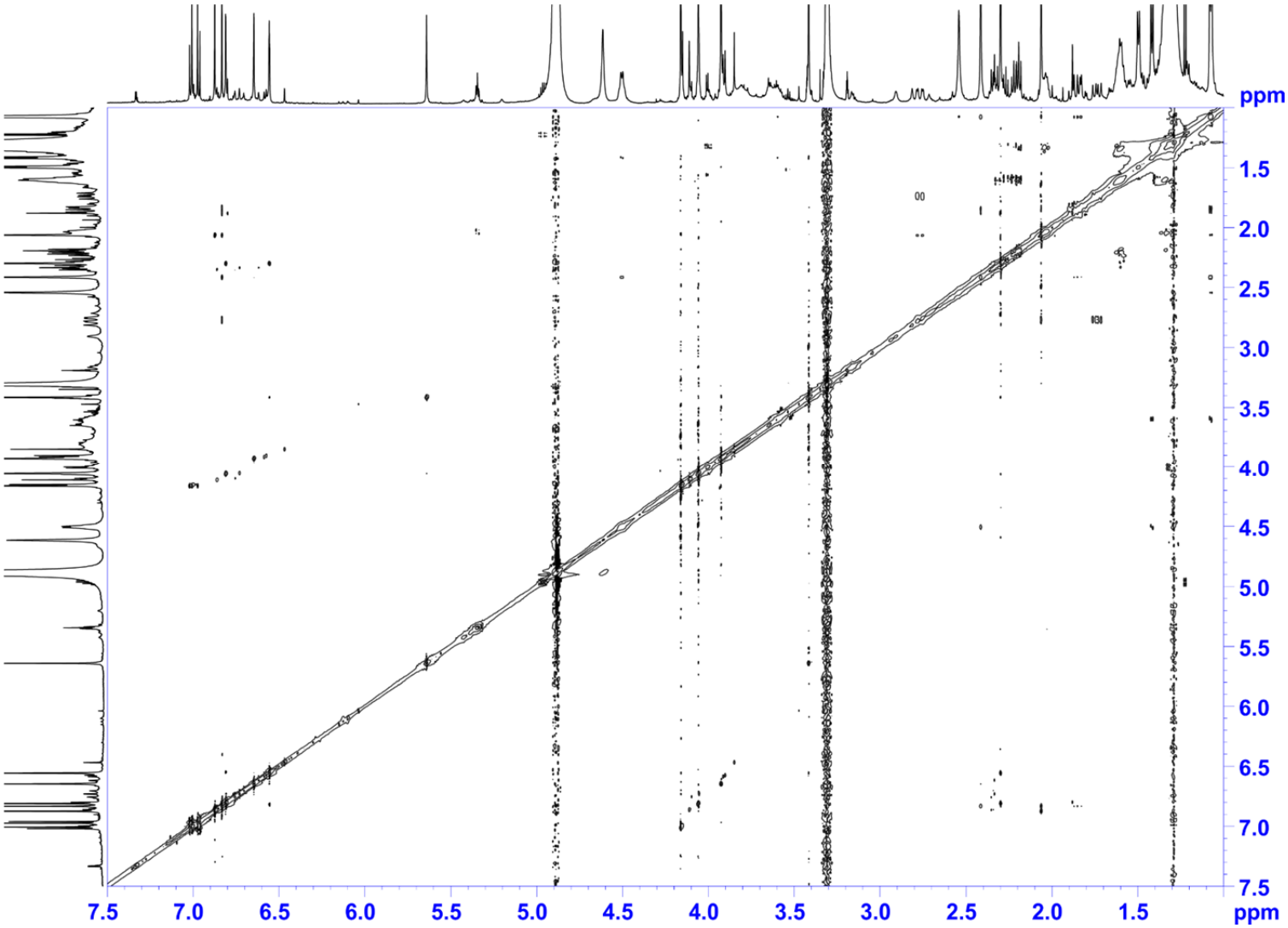


Figure S4. ^{1}H-^{1}H COSY spectrum of mbandakamine B_3 (**3**)



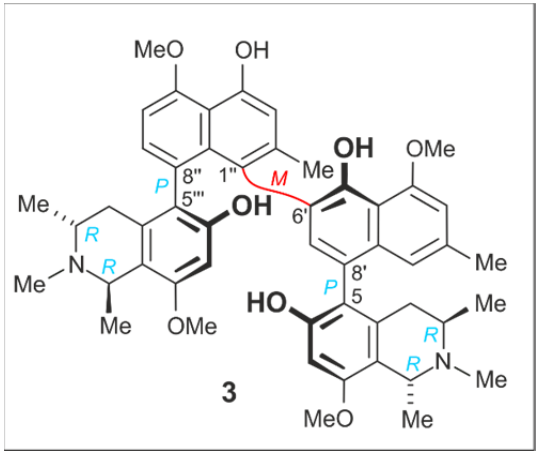
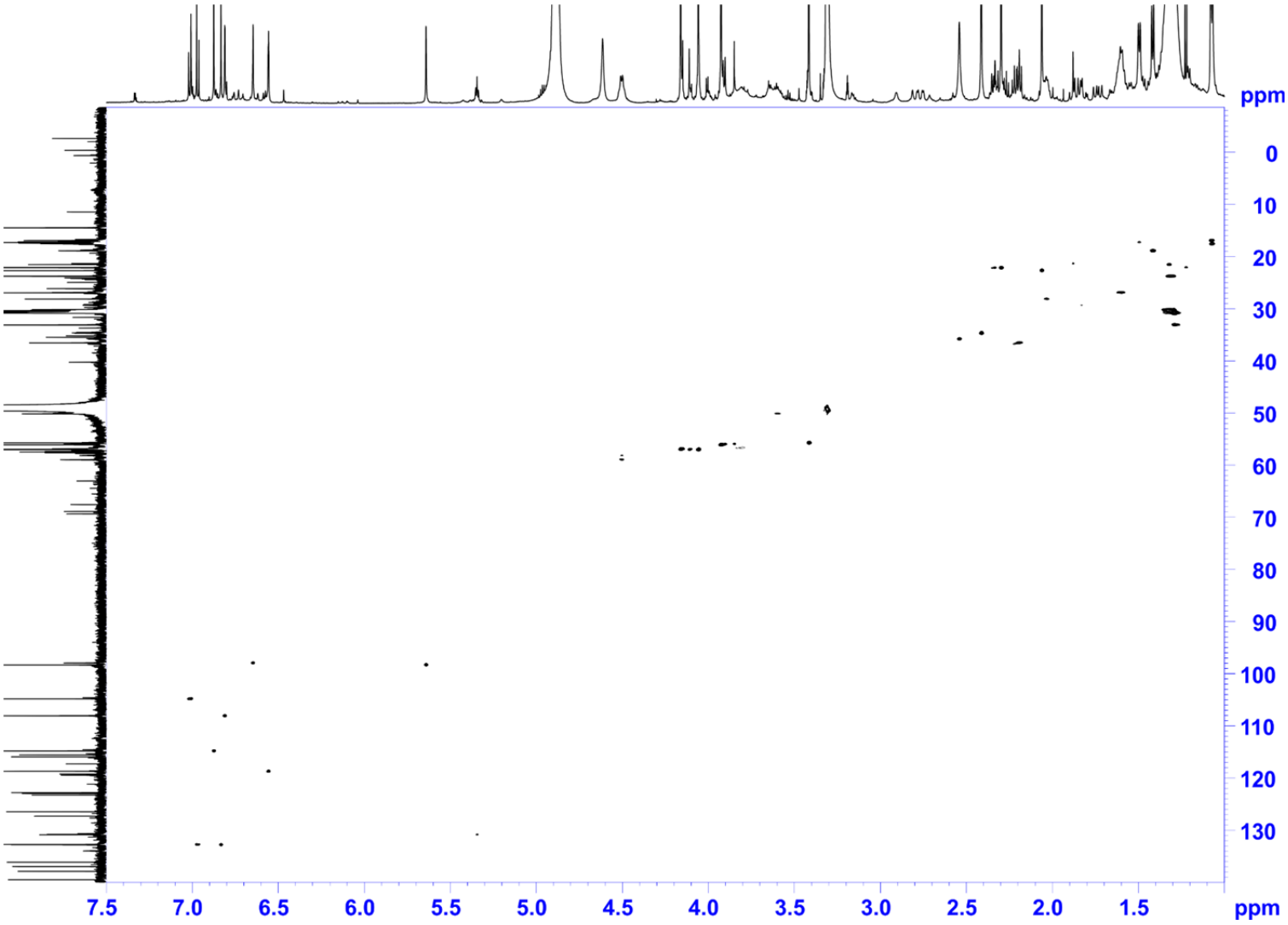


Figure S5. ^{1}H-^{1}H ROESY spectrum of mbandakamine B3 (**3**)



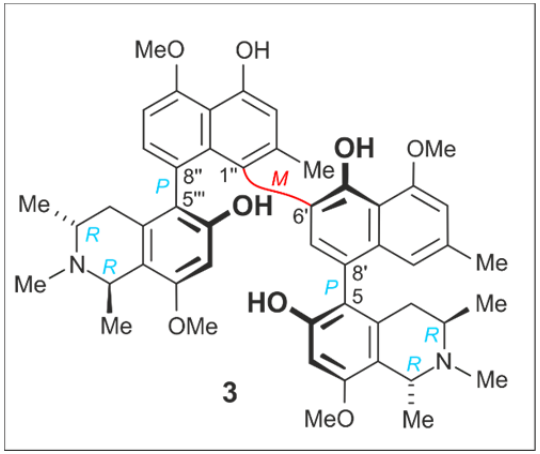
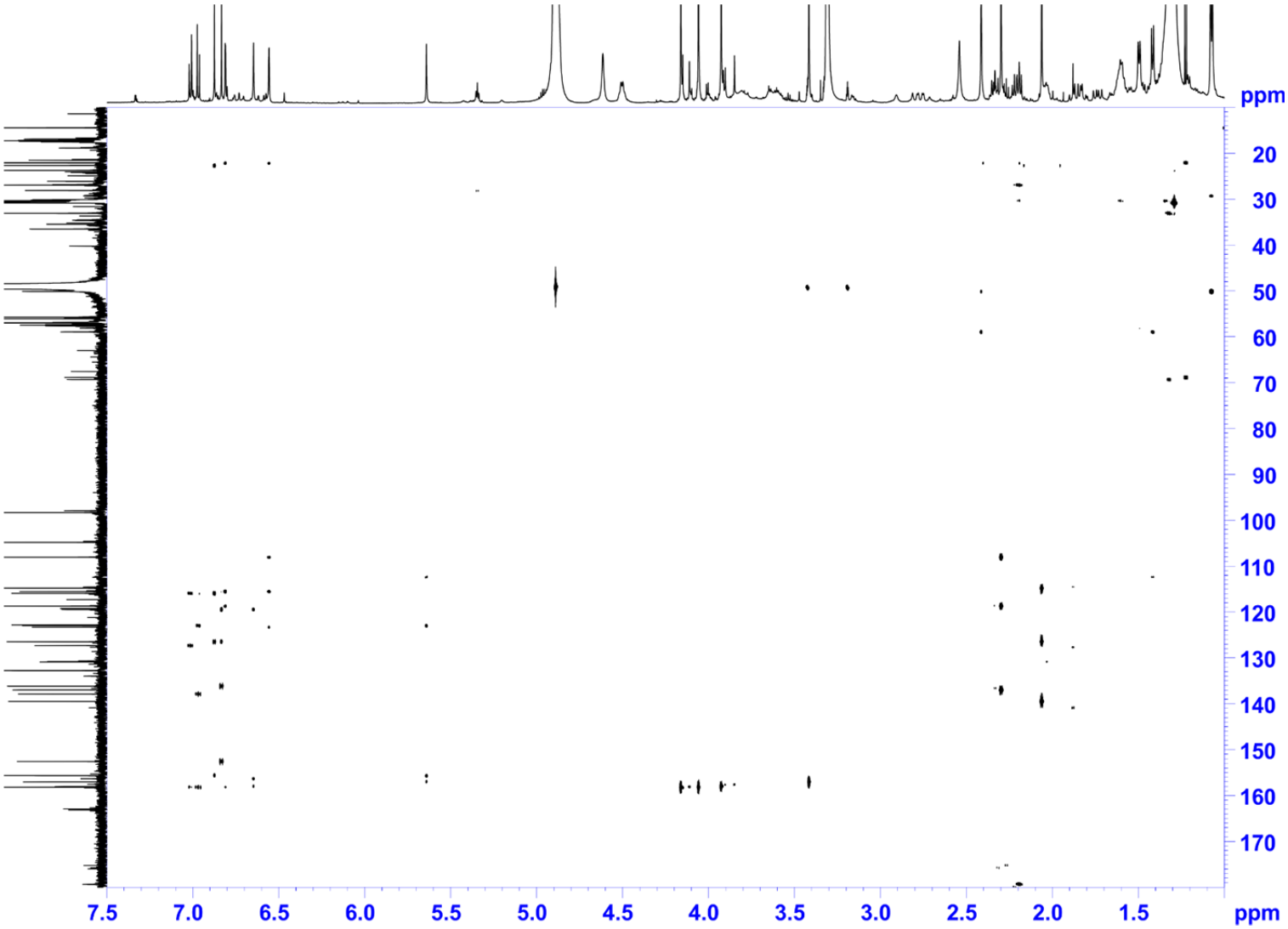
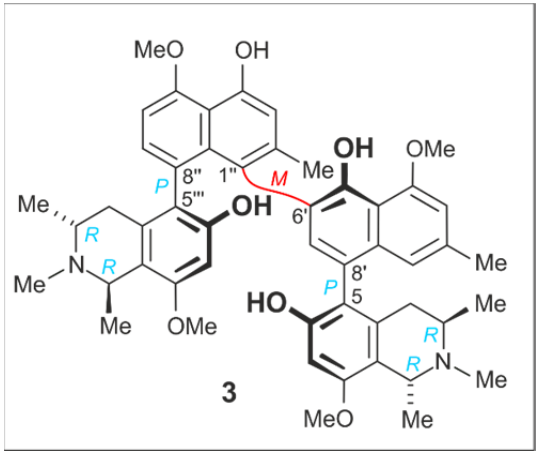


Figure S6. ^{1}H-^{13}C HSQC spectrum of mbandakamine B_3 (**3**).





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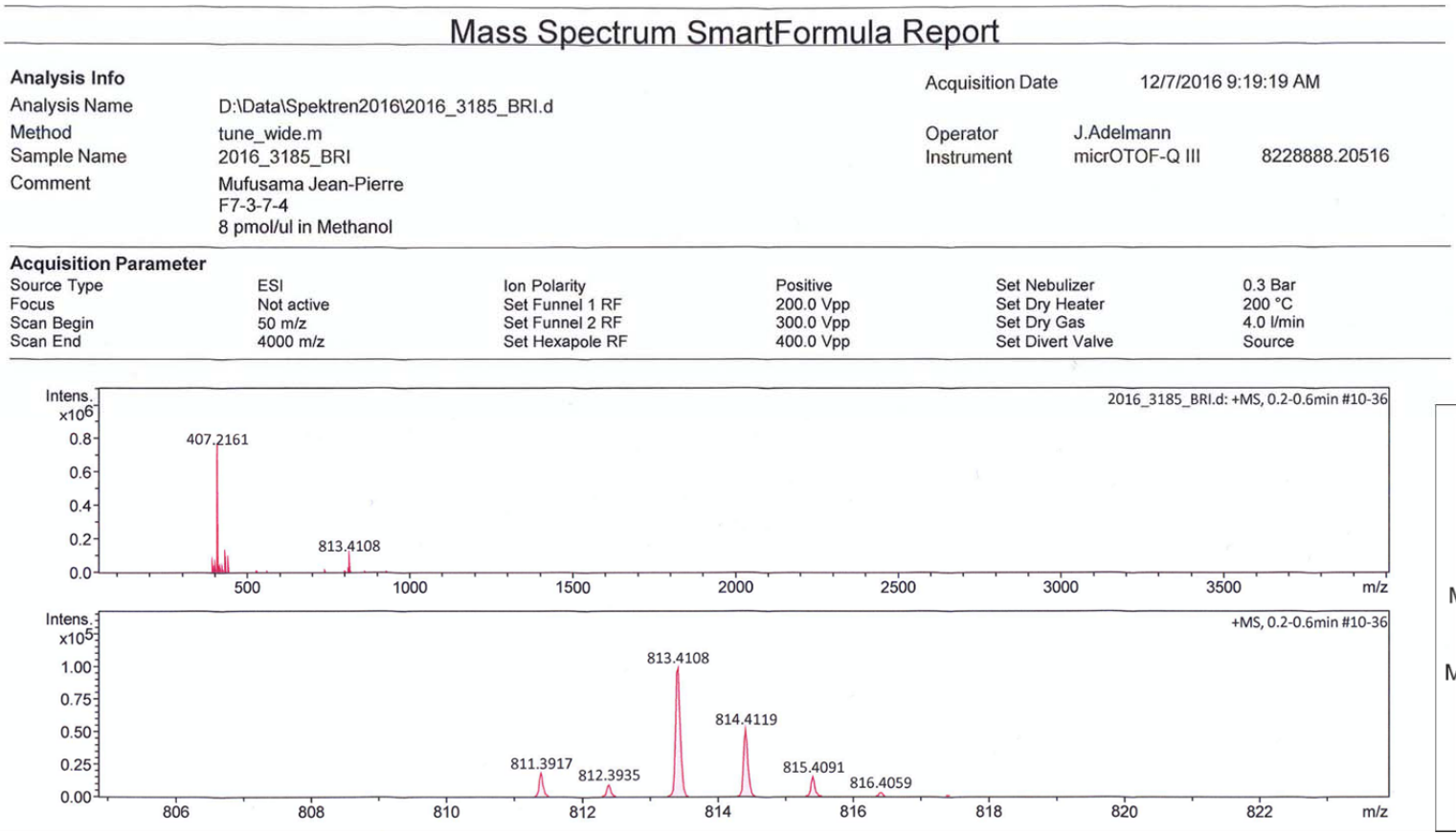


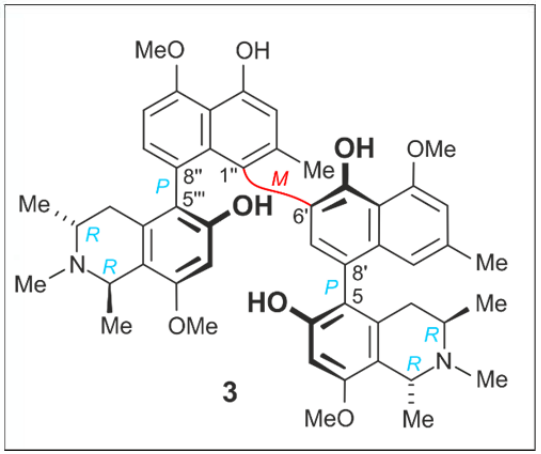
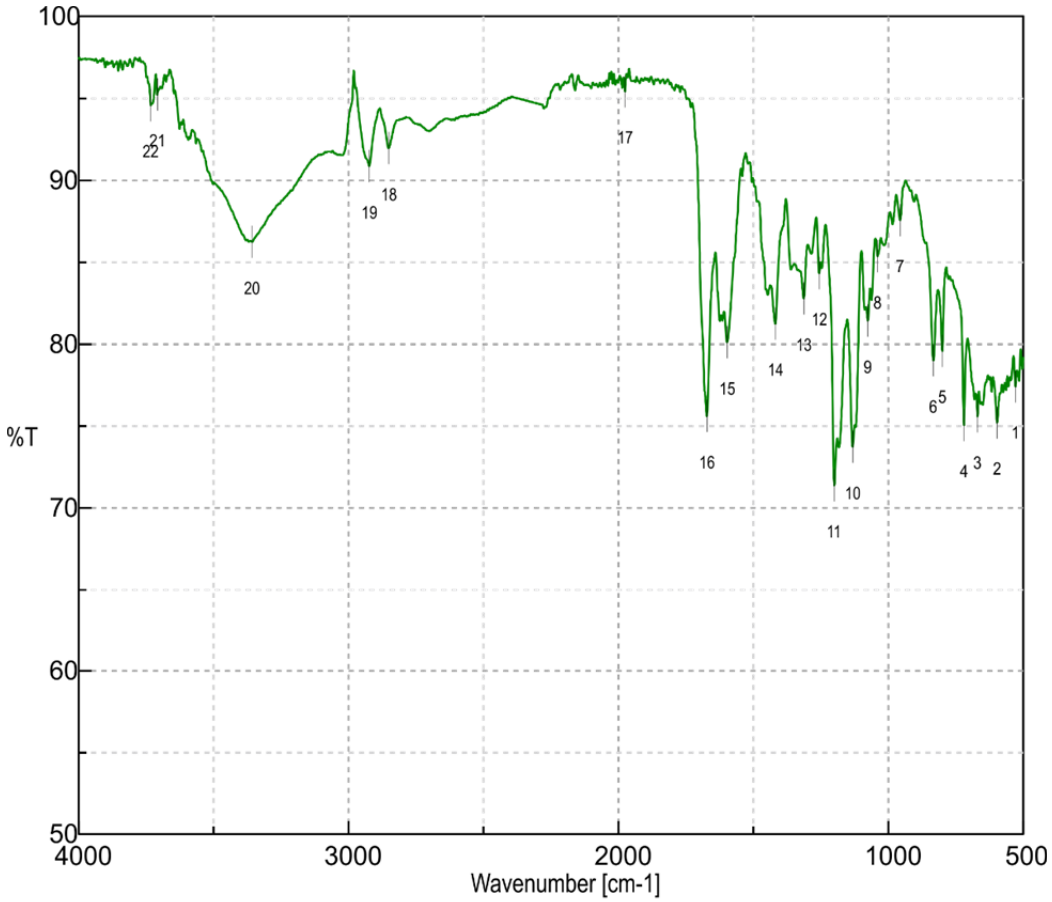


Figure S8. HRESIMS spectrum of mbandakamine B_3 (**3**).



Results of Peak Find

No.	Position	Intensity	No.	Position	Intensity
1	529.364	77.3743	2	596.861	75.1845
3	669.178	75.5513	4	720.282	75.0211
5	800.314	79.5673	6	833.098	78.9996
7	956.52	87.5568	8	1039.44	85.3481
9	1076.08	81.4289	10	1132.01	73.7022
11	1199.51	71.353	12	1256.4	84.3026
13	1313.29	82.7669	14	1418.39	81.2313
15	1597.73	80.0801	16	1671.98	75.5936
17	1975.71	95.3963	18	2851.24	91.9372
19	2923.56	90.8525	20	3356.5	86.2178
21	3708.44	95.2063	22	3732.55	94.5595

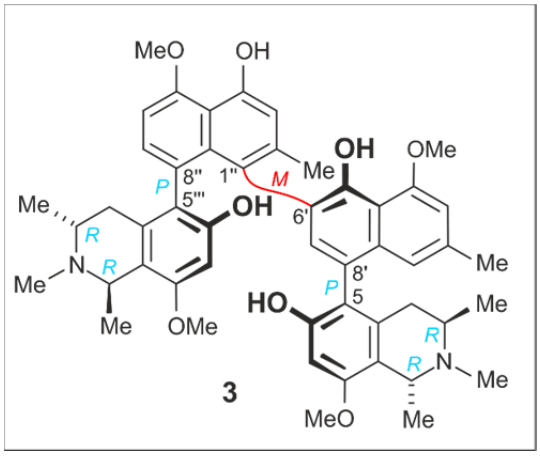
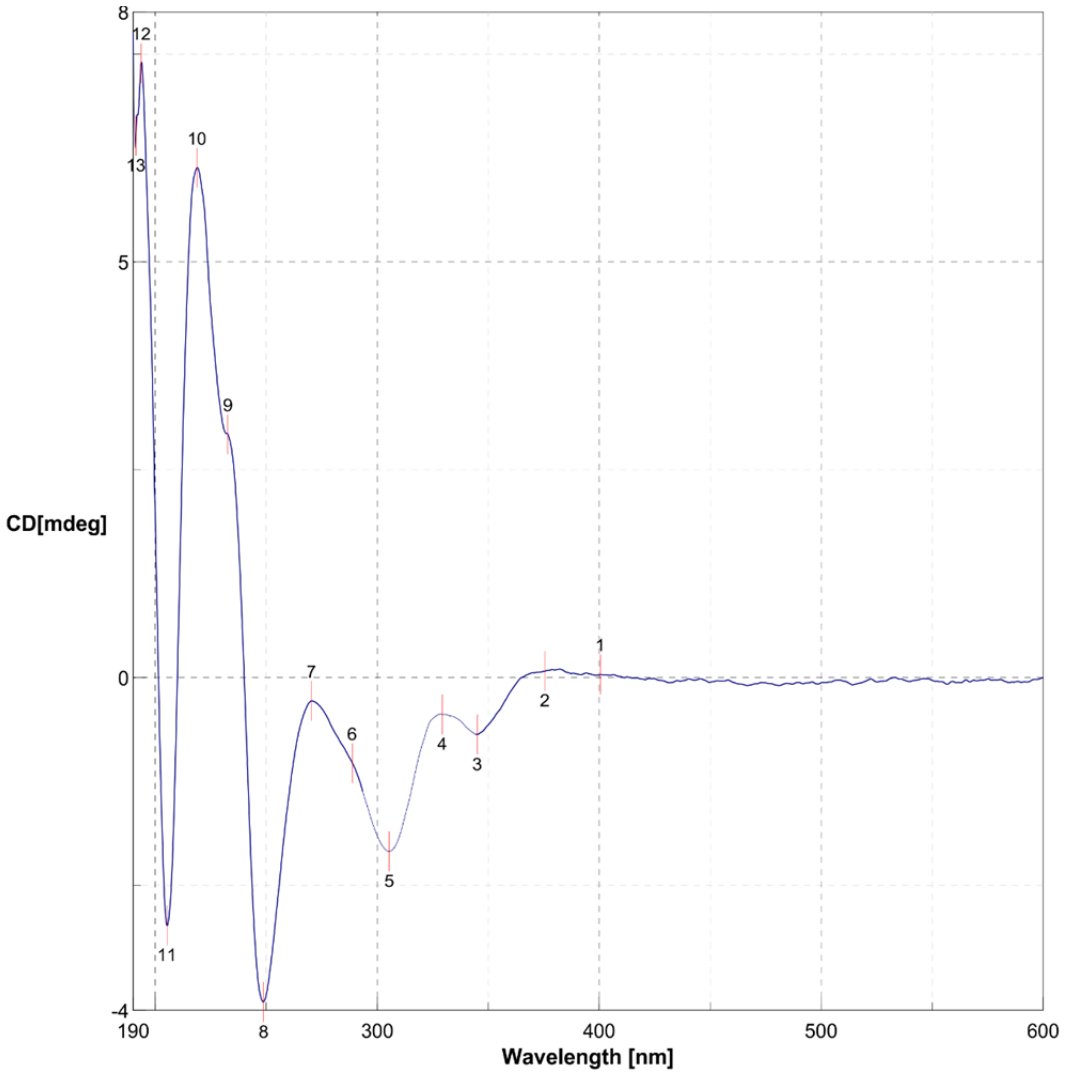


Figure S9. IR spectrum of mbandakamine B_3 (**3**).



No.	nm	CD[mdeg]	No.	nm		CD[mdeg]	No.	nm	CD[mdeg]
1	400.5	0.0354843	2	375.6	367	0.0789807	3	345.1	-0.683
4	329.3	-0.442441	5	305.4	1	-2.08736	6	288.8	-1.0254
7	270.4	-0.280467	8	248.8		-3.89769	9	232.7	2.92464
10	218.8	6.12982	11	205.3		-2.97964	12	193.6	7.38501
13	191.3	6.51525							

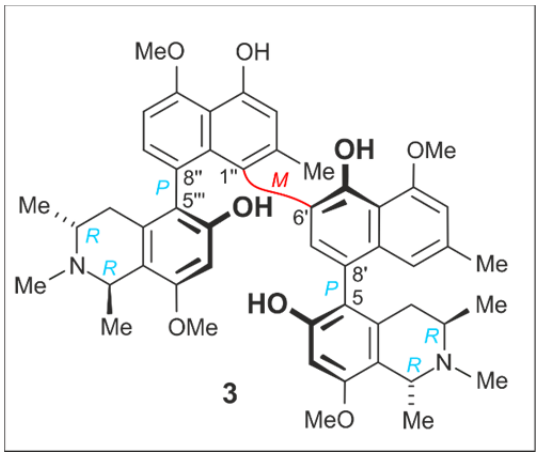
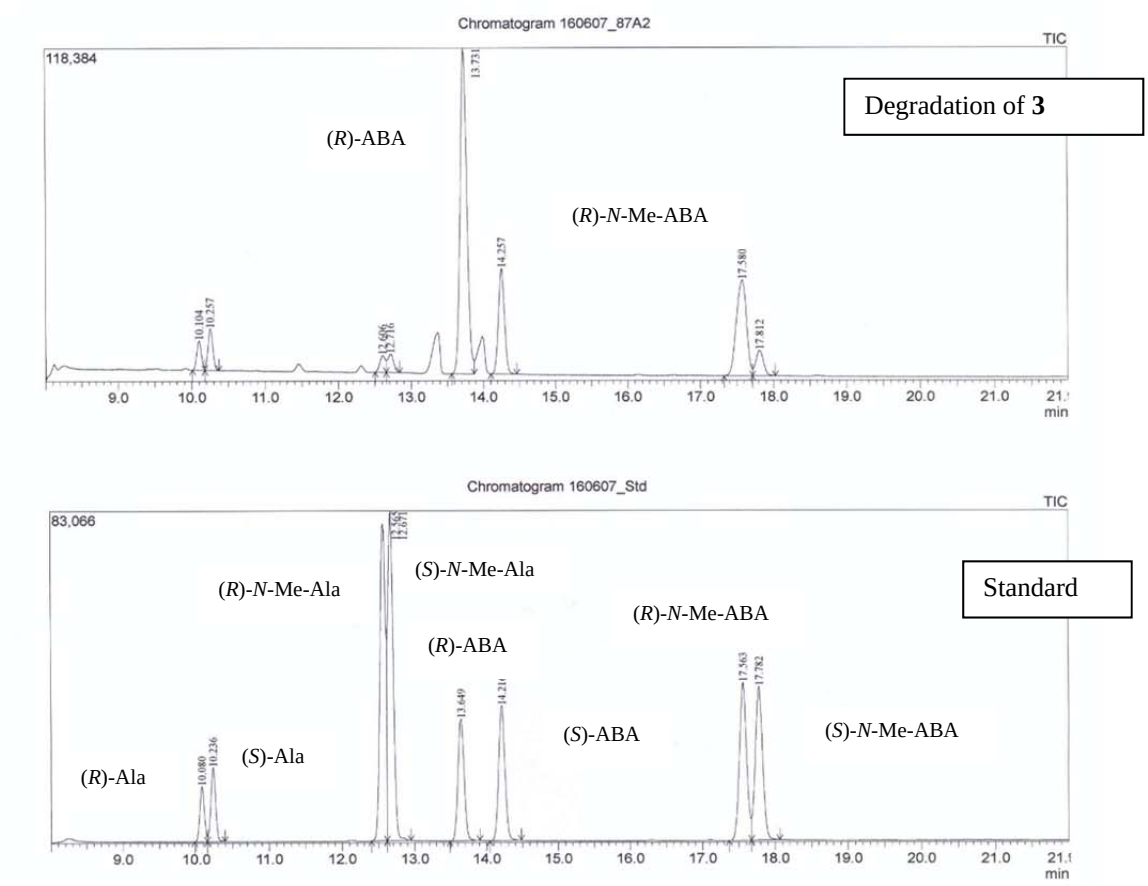
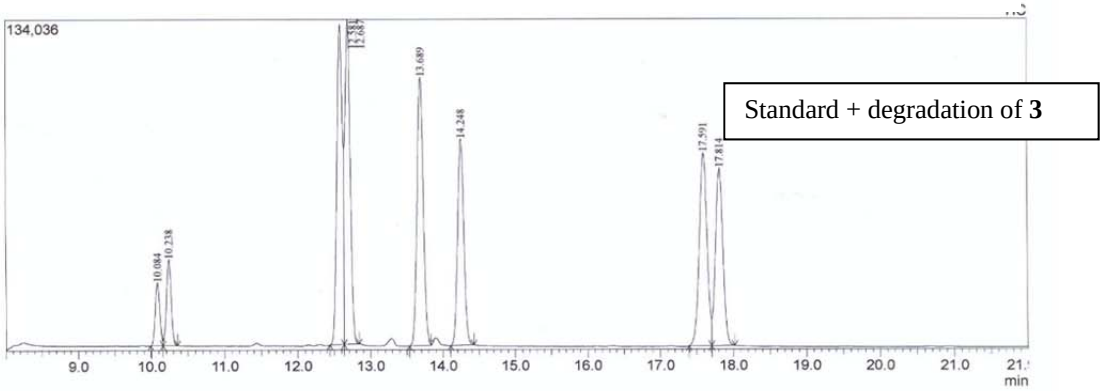


Figure S10. ECD spectrum of mbandakamine B_3 (**3**)



Where: Ala = alanine; *N*-Me-Ala = *N*-methyl alanine;
ABA = 3-aminobutyric acid; *N*-Me-ABA = *N*-methyl-3-aminobutyric acid



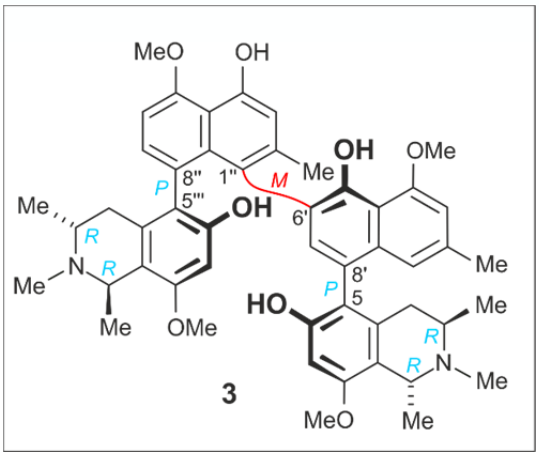


Figure S11: Oxidative degradation products of mbandakamine B_3 (**3**).

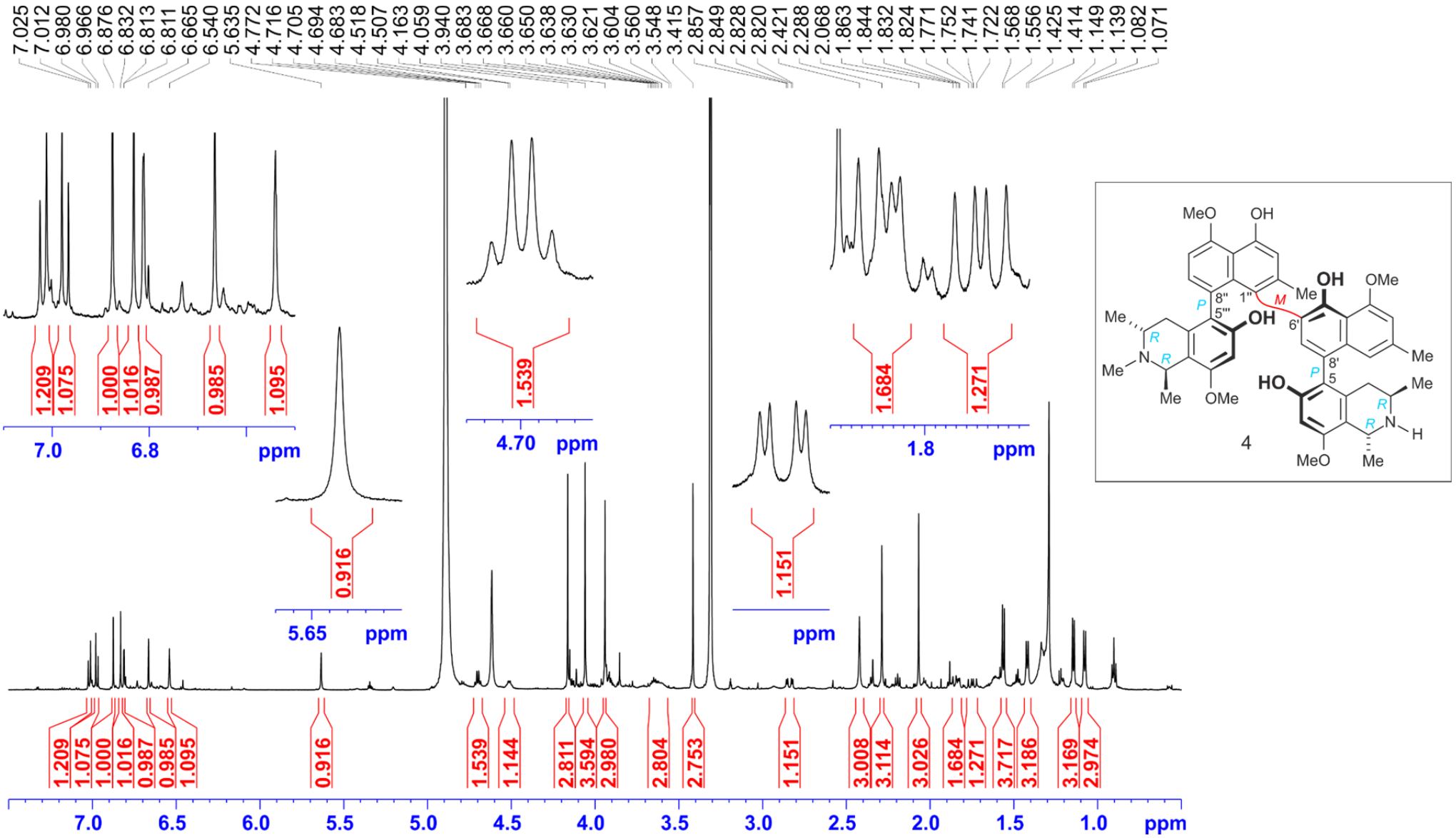


Figure S12. ^{1}H NMR spectrum of mbandakamine B_4 (**4**).

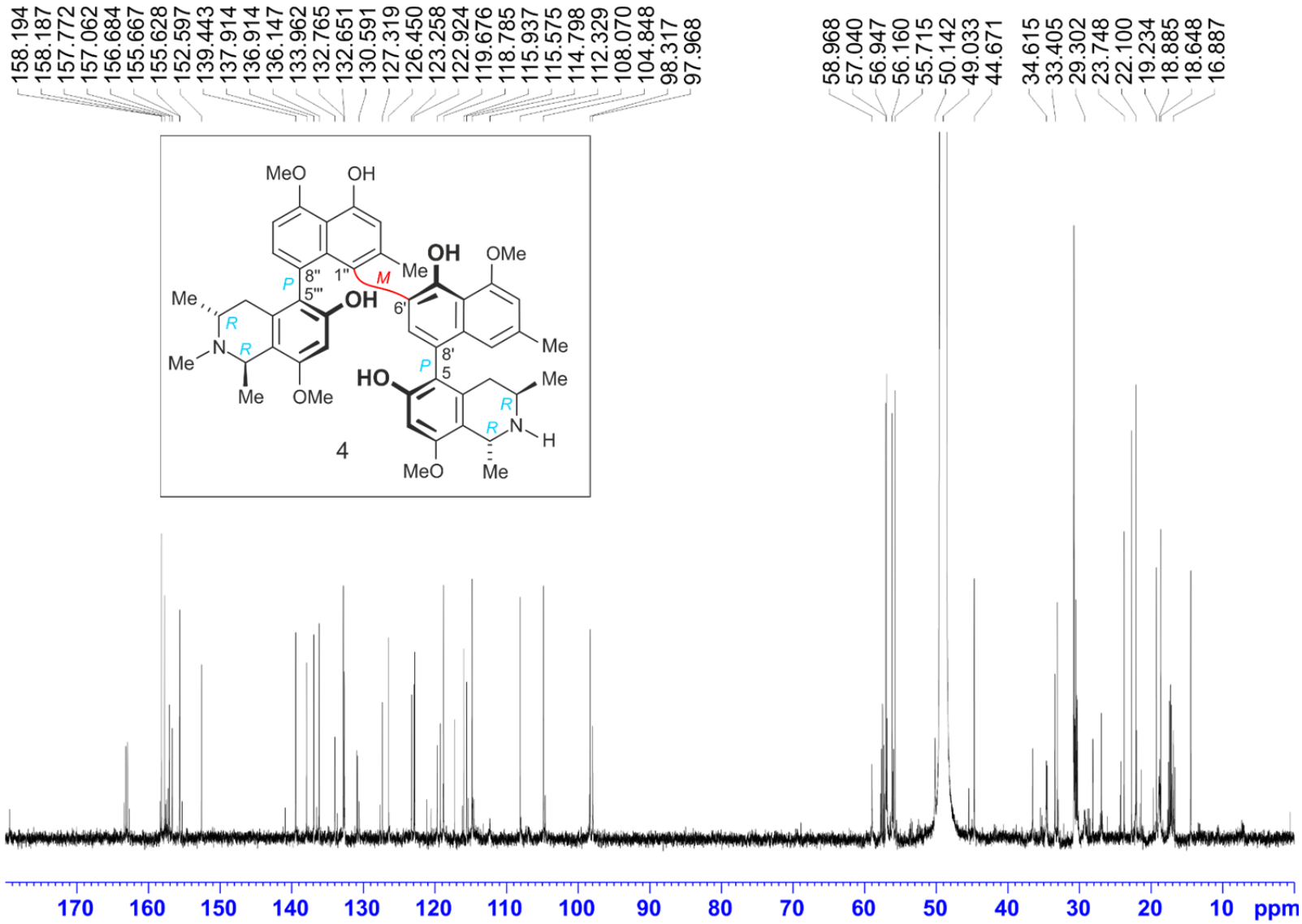


Figure S13. ^{13}C NMR spectrum of mbandakamine B_4 (**4**).

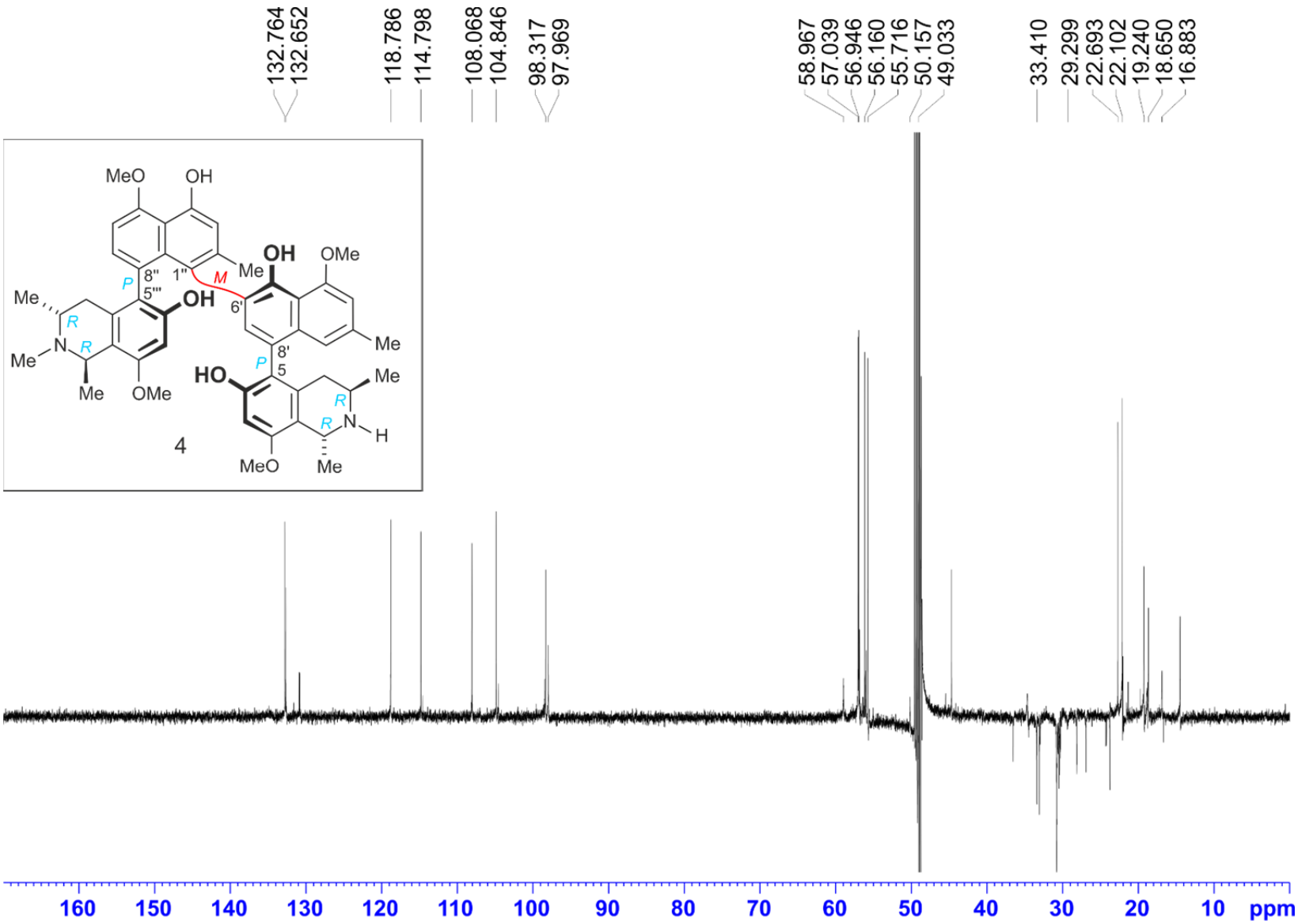
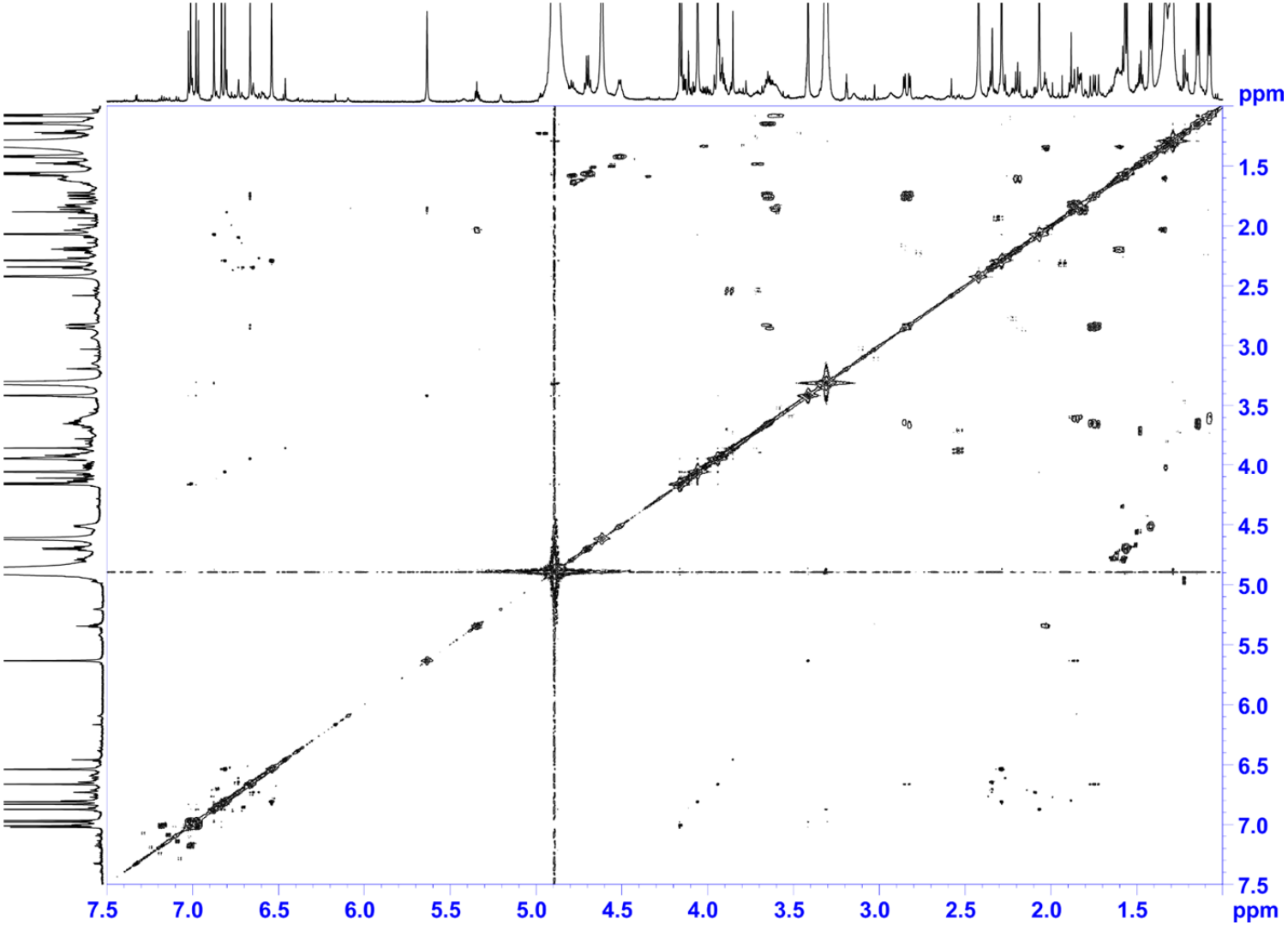


Figure S14. ^{13}C DEPT 135 spectrum of mbandakamine B_4 (**4**).



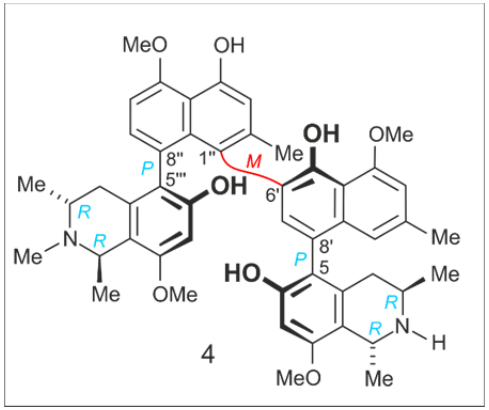
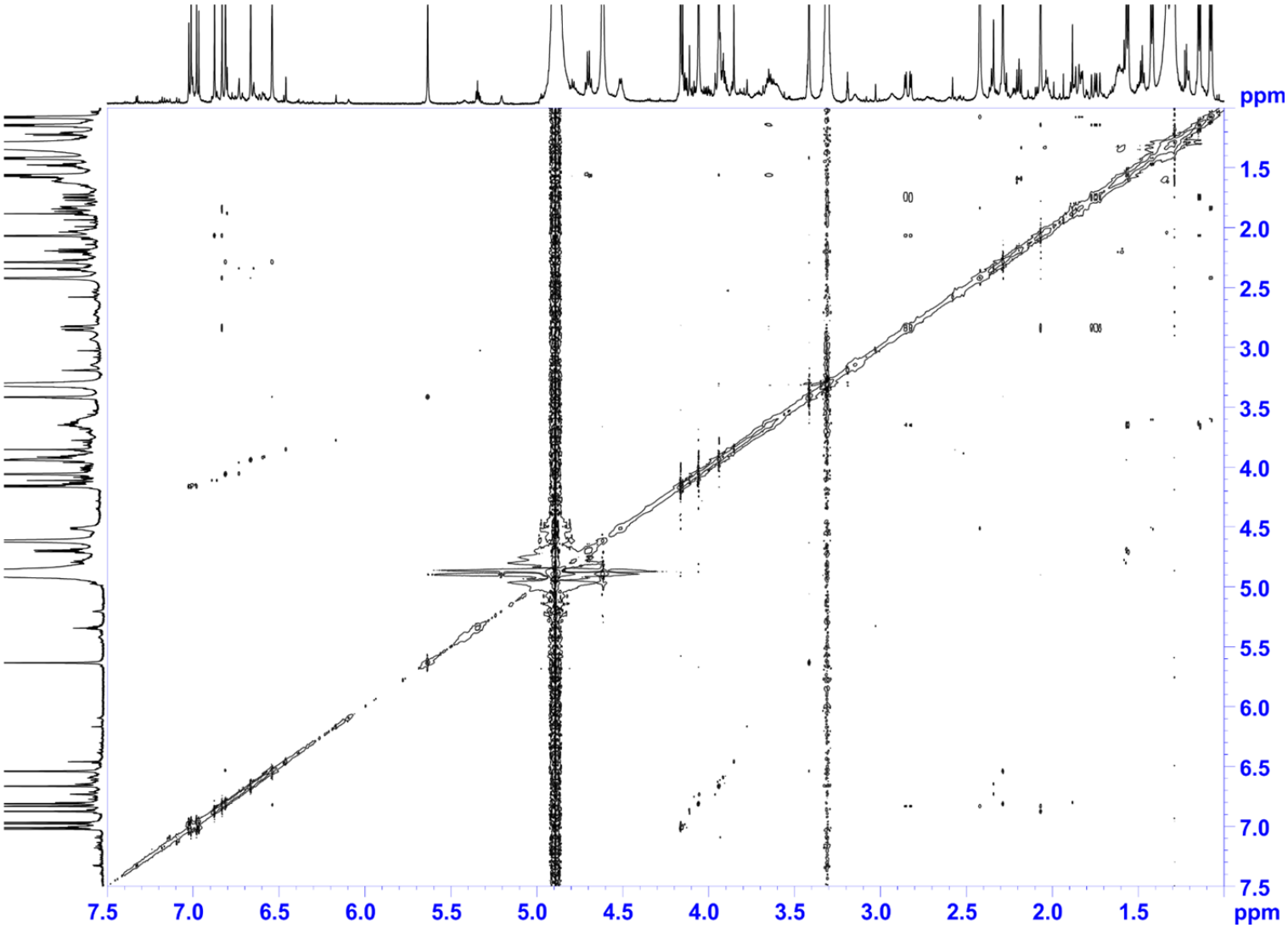


Figure S15. ^{1}H-^{1}H COSY spectrum of mbandakamine B_4 (**4**).



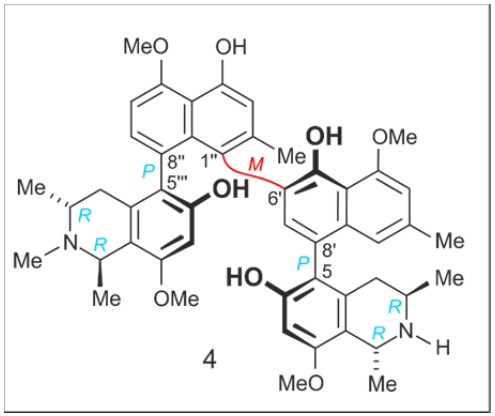


Figure S16. ^{1}H-^{1}H ROESY spectrum of mbandakamine B_4 (**4**).

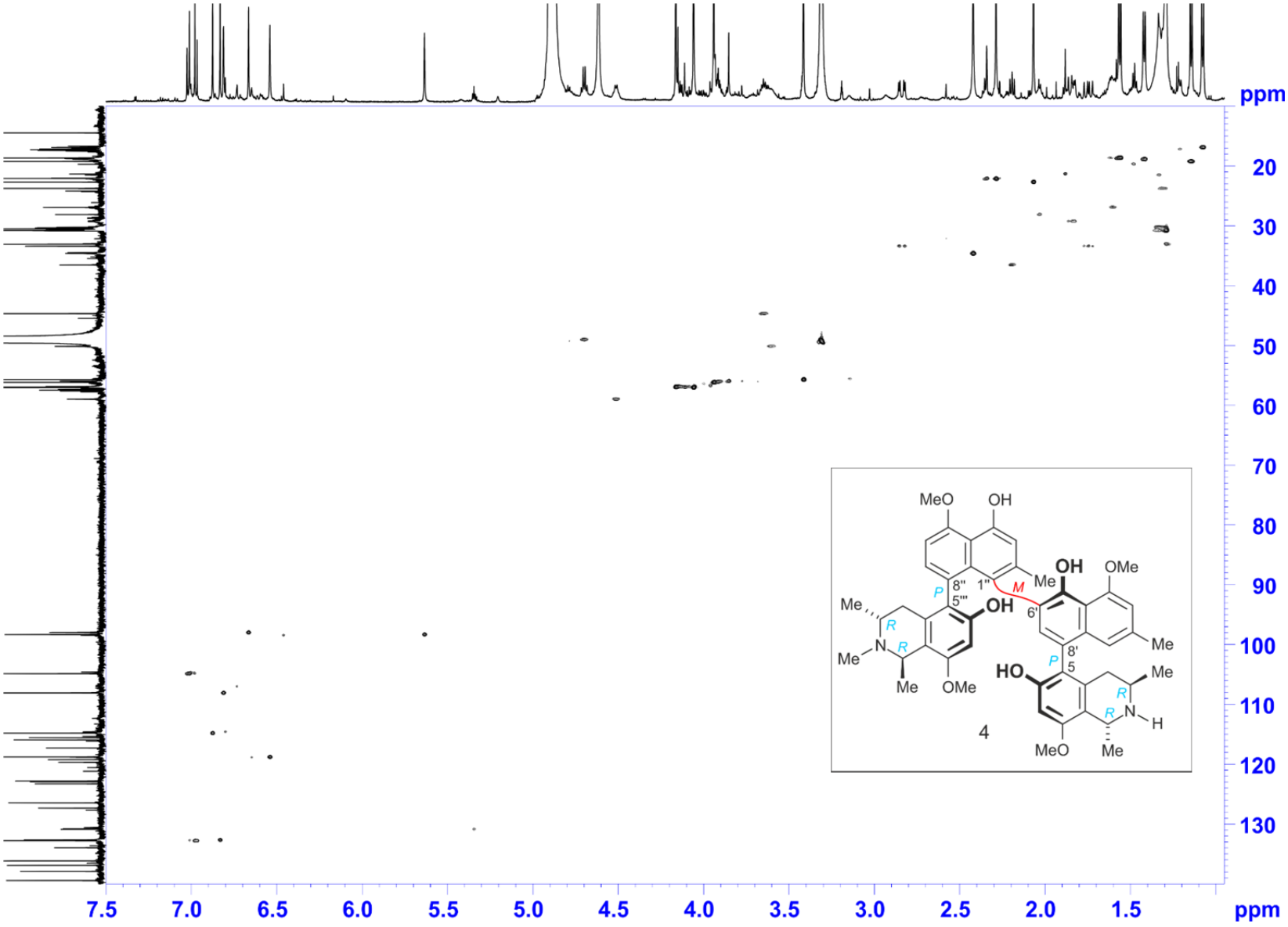
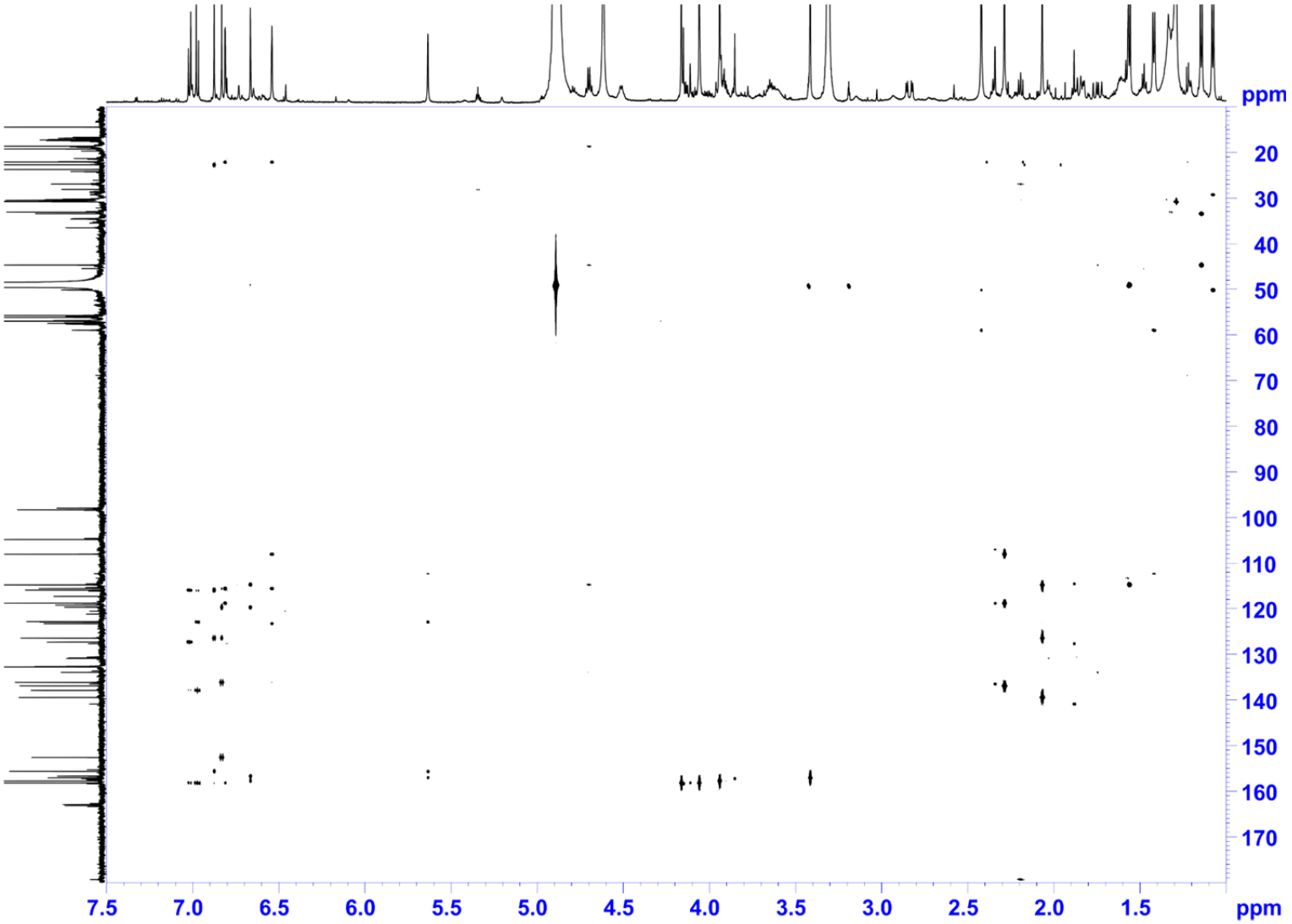


Figure S17. ^{1}H-^{13}C HSQC spectrum of mbandakamine B_4 (**4**).



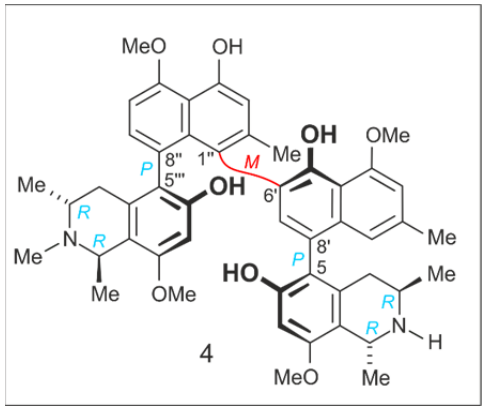
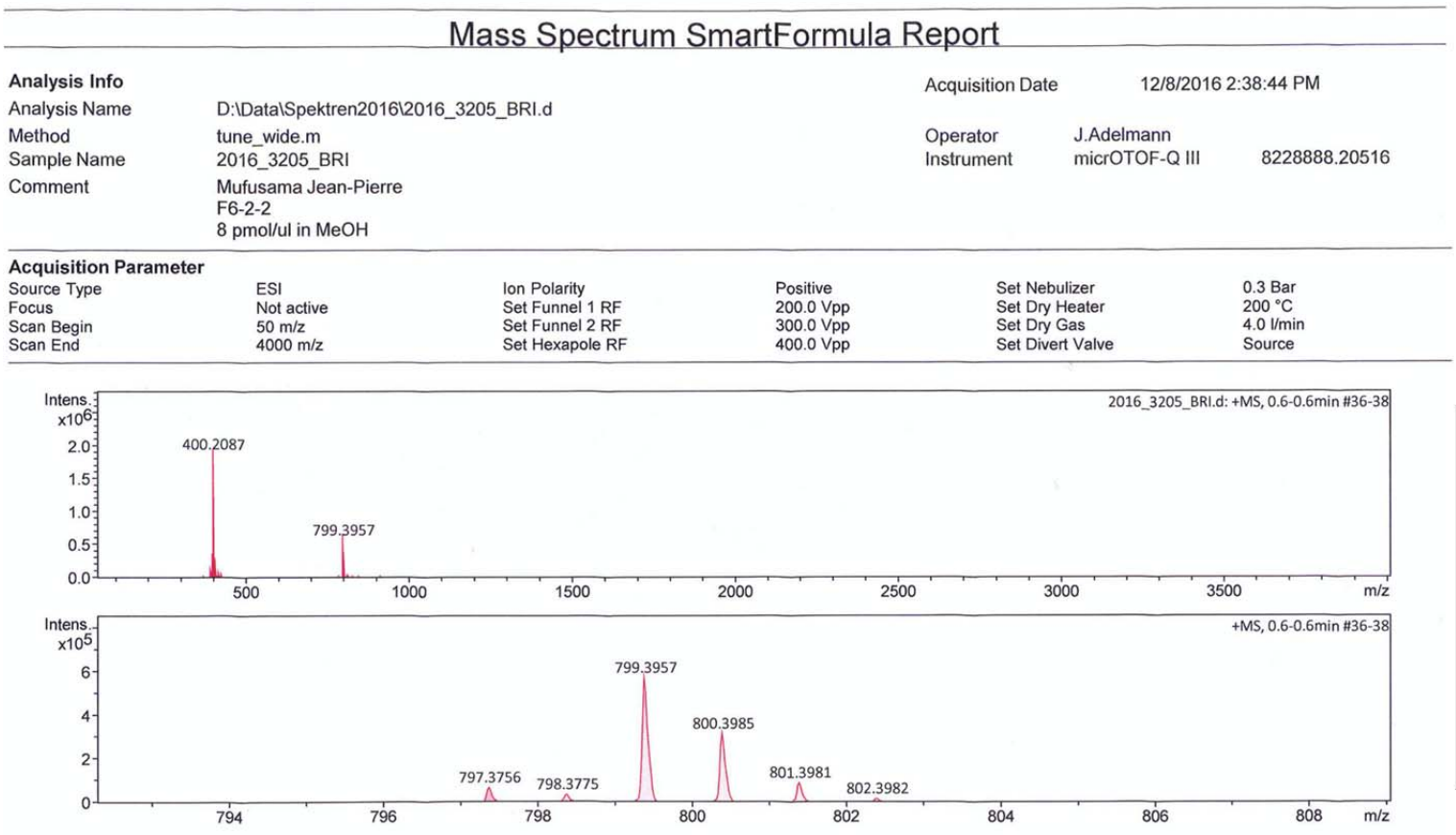


Figure S18. ^{1}H-^{13}C HMBC spectrum of mbandakamine B_4 (**4**).



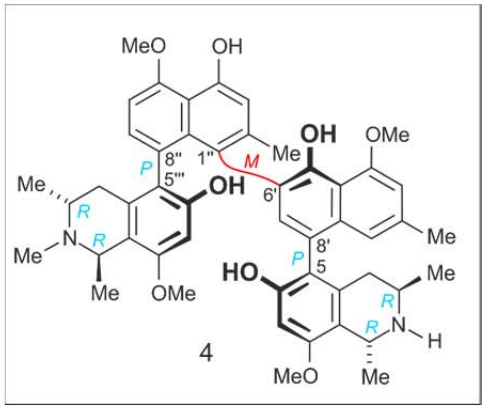
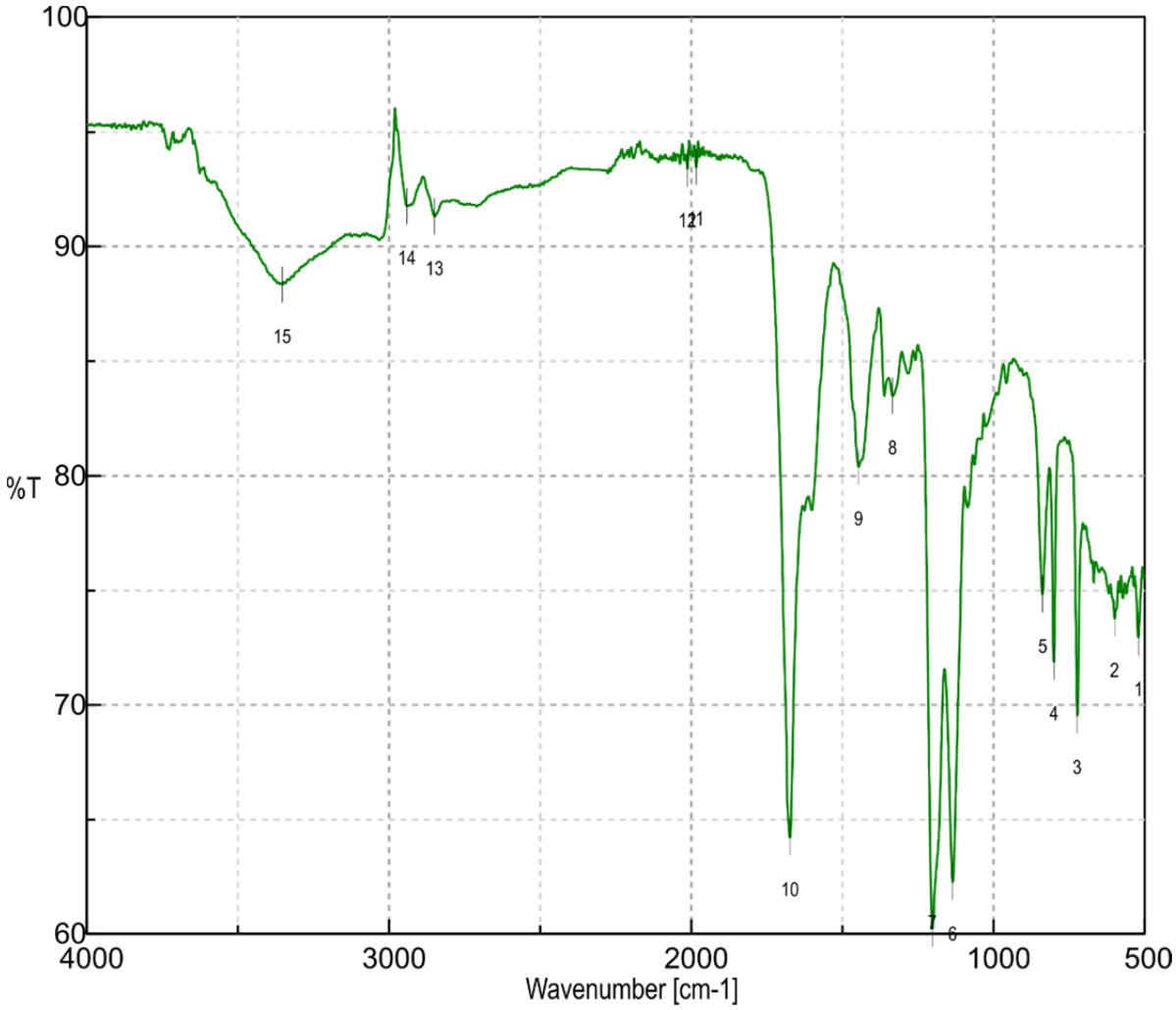


Figure S19. HRESIMS spectrum of mbandakamine B_4 (**4**).



Results of Peak Find

No.	Position	Intensity	No.	Position	Intensity
1	521.65	72.9289	2	599.753	73.7579
3	723.175	69.546	4	800.314	71.8864
5	837.919	74.8178	6	1134.9	62.2758
7	1201.43	60.2296	8	1333.53	83.4739
9	1446.35	80.3844	10	1673.91	64.1936
11	1983.43	93.4565	12	2013.32	93.3813
13	2848.35	91.2996	14	2939.95	91.7512
15	3353.6	88.3156			

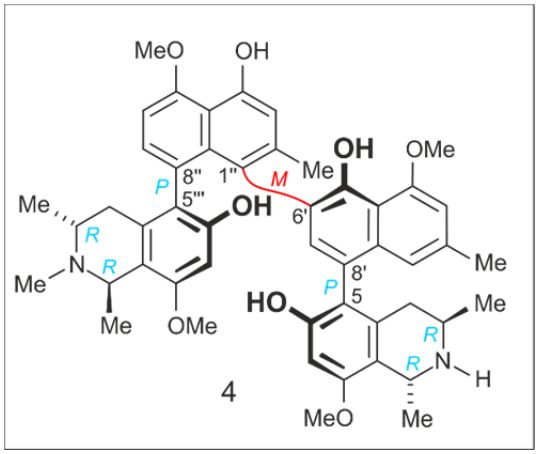
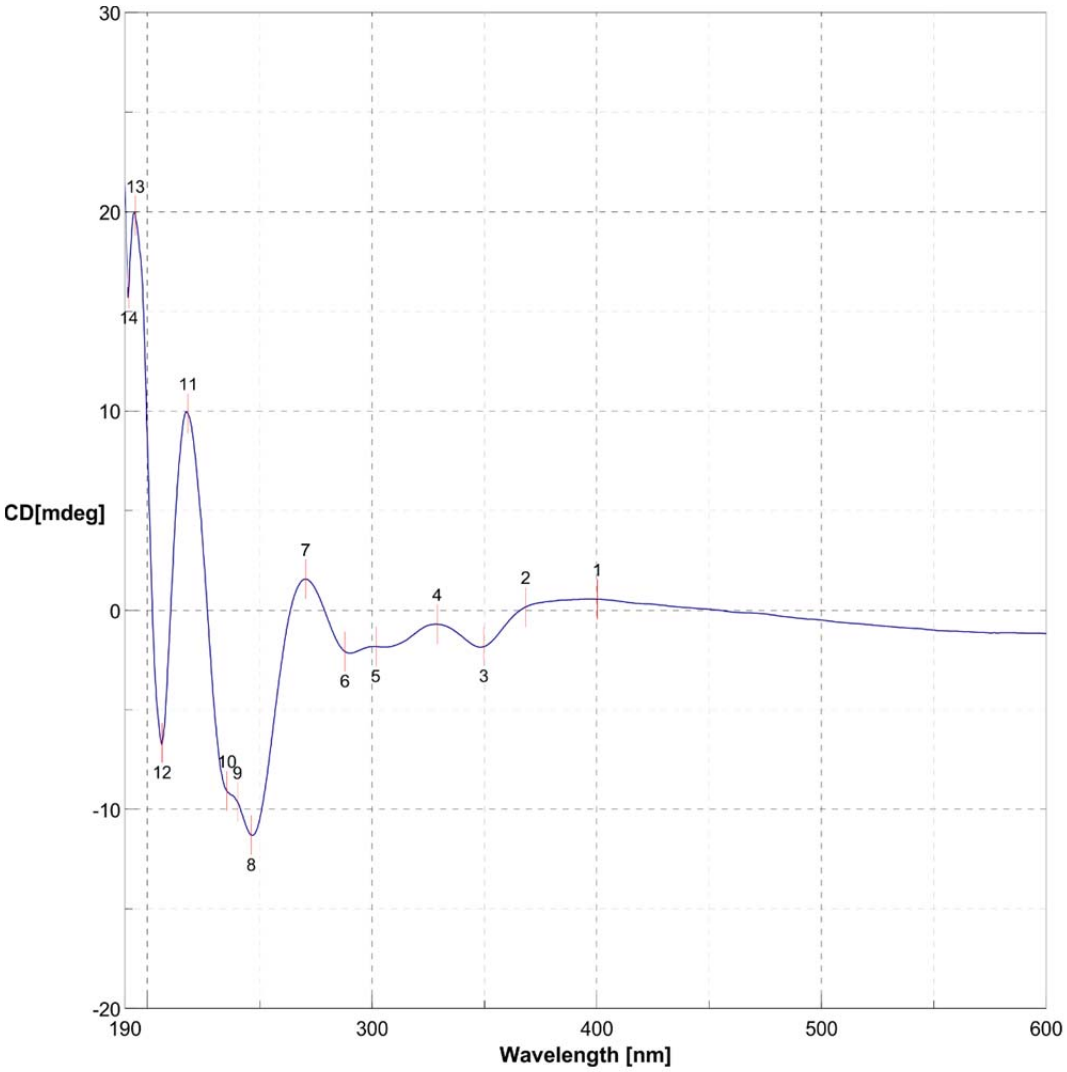


Figure S20. IR spectrum of mbandakamine B_4 (**4**).



No.	nm	Mol. CD	No.	nm	Mol. CD	No.	nm	Mol. CD
1	400.2	0.5523	2	368.3	0.157411	3	349.8	-1.82699
4	329	-0.703144	5	301.7	-1.82544	6	288	-2.08338
7	270.5	1.55812	8	246.3	-11.2948	9	240.2	-9.63675
10	235.4	-9.07438	11	218	9.87138	12	206.6	-6.66029
13	194.6	19.8189	14	191.7	16.1465			

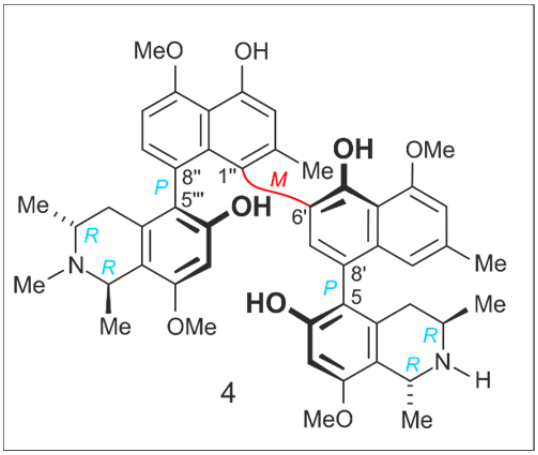
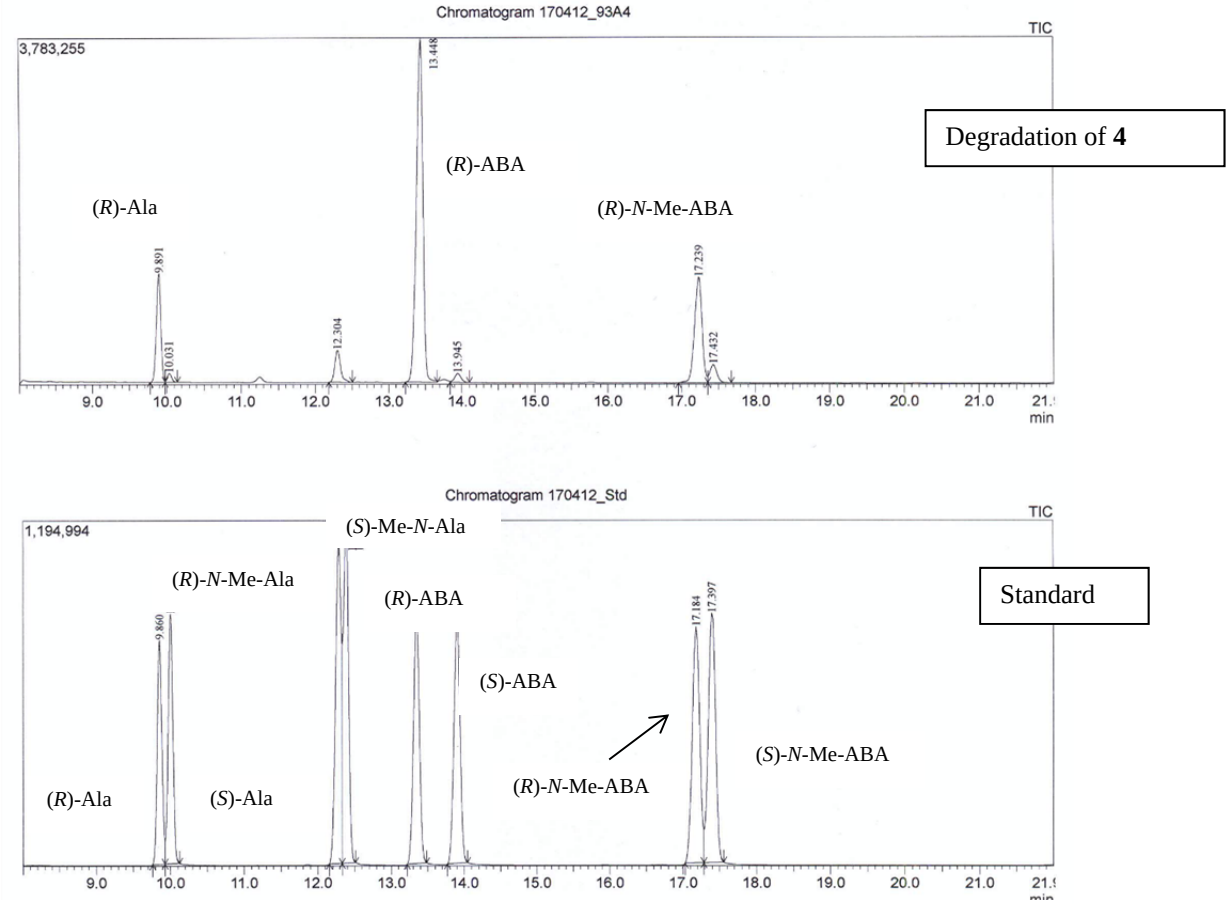


Figure S21. ECD spectrum of mbandakamine B_4 (**4**)



Where: Ala = alanine; *N*-Me-Ala = *N*-methylalanine;
ABA = 3-aminobutyric acid; *N*-Me-ABA = *N*-methyl-3-aminobutyric acid

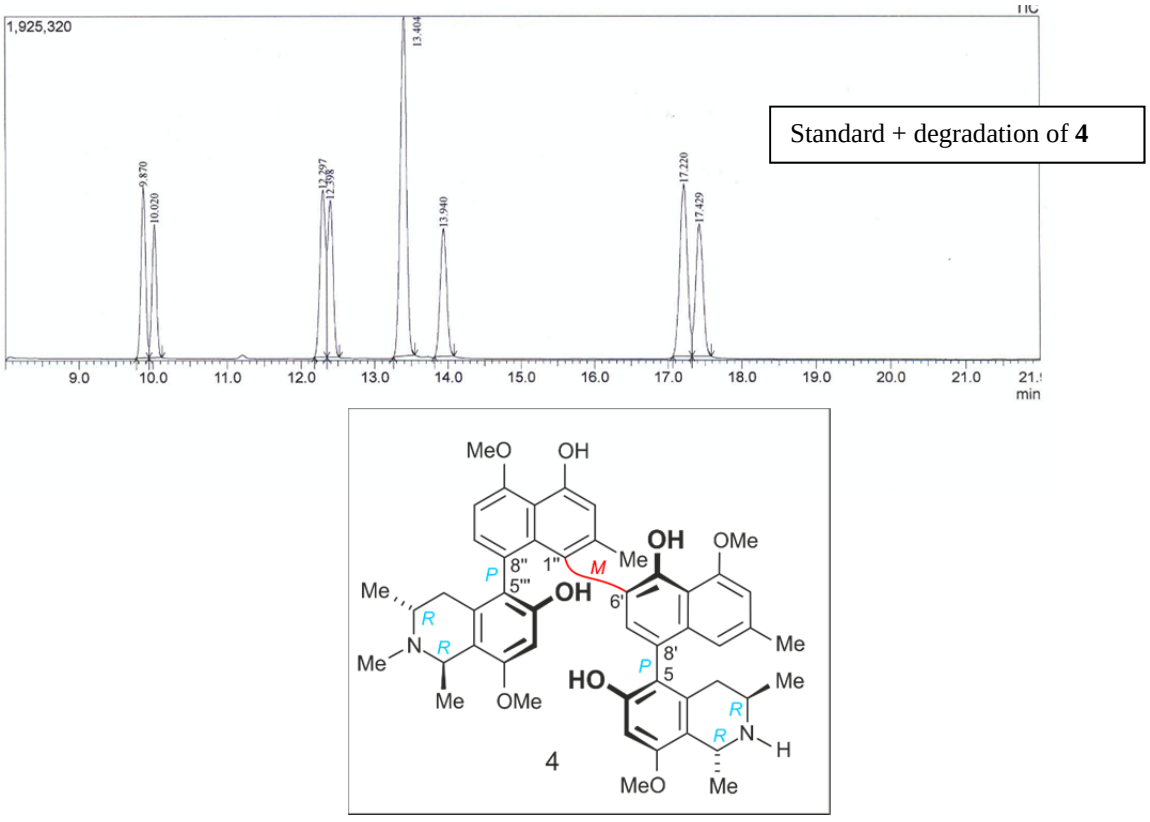


Figure S22: Oxidative degradation products of mbandakamine B_4 (**4**).

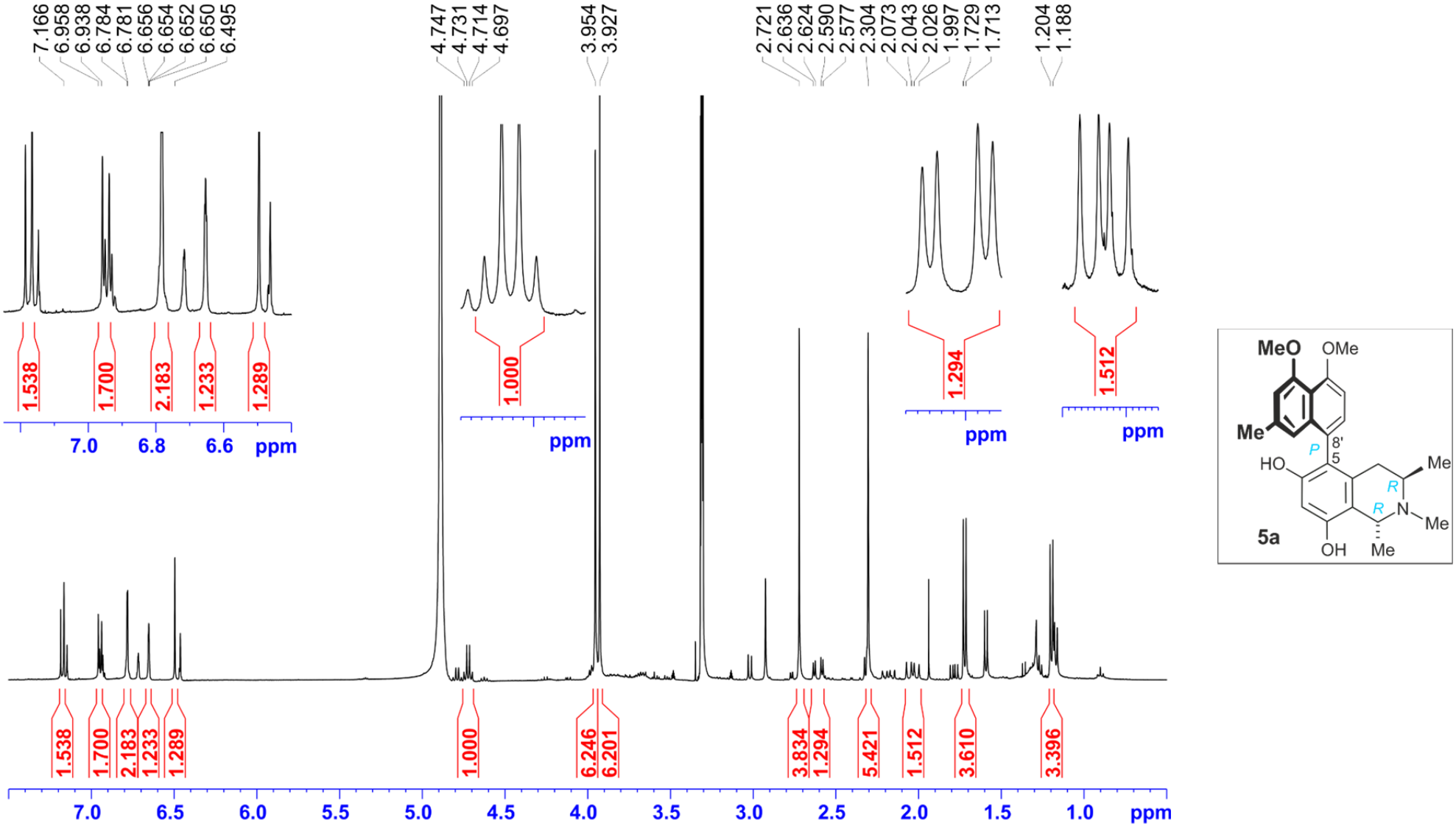


Figure S23. ^{1}H NMR spectrum of ikelacongoline A (**5a**).

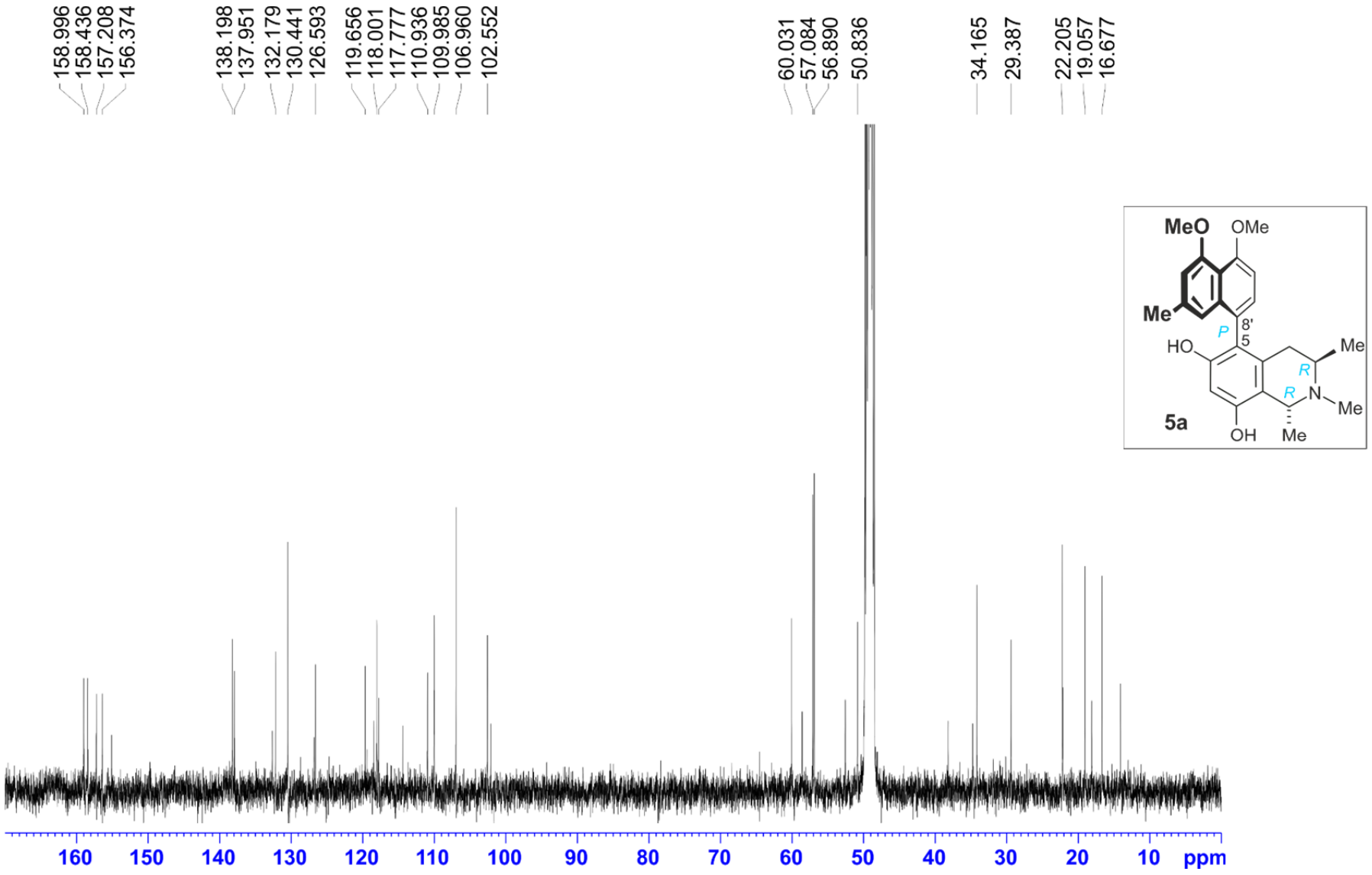


Figure S24. ^{13}C NMR spectrum of ikelacongoline A (**5a**).

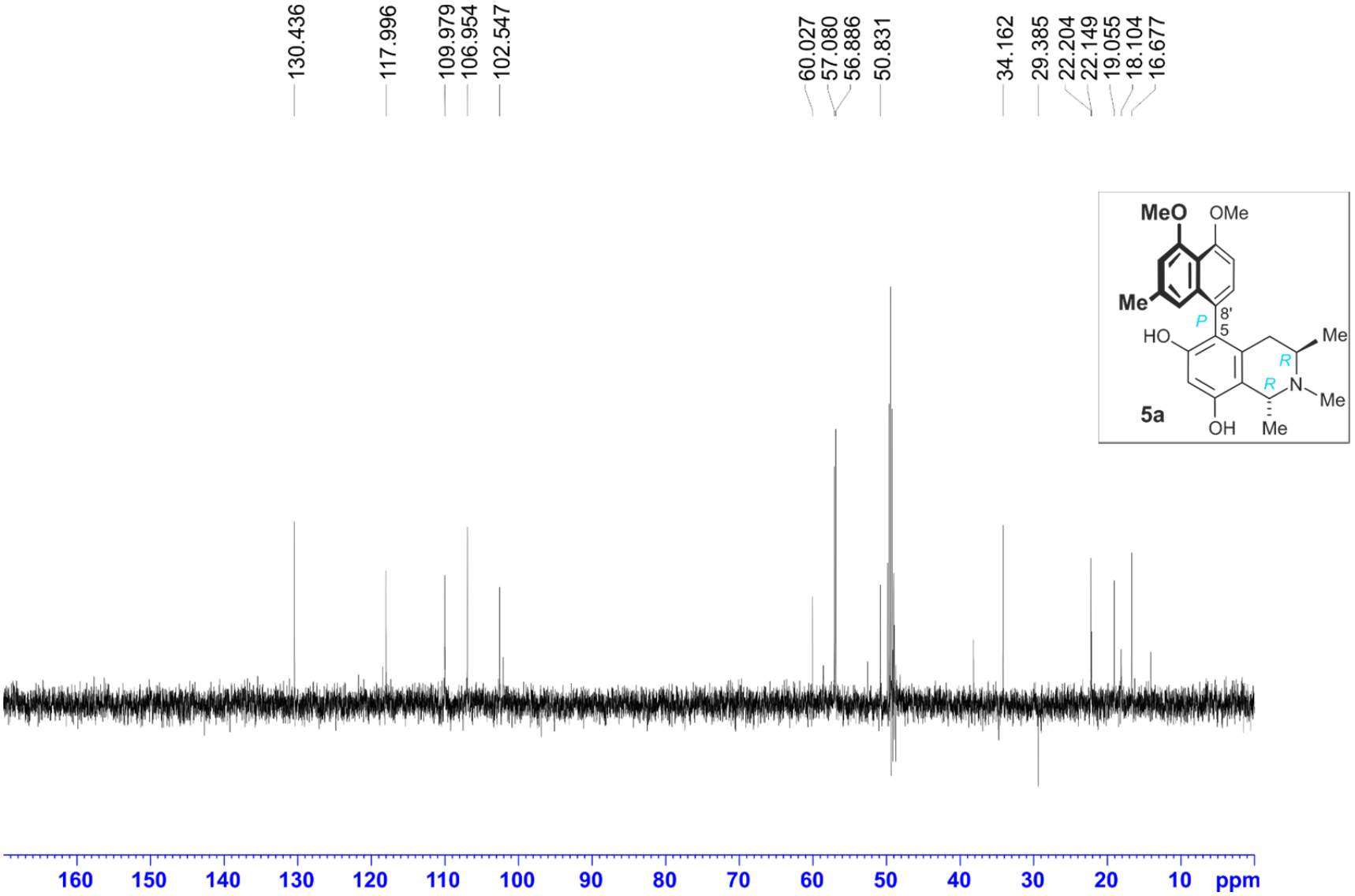
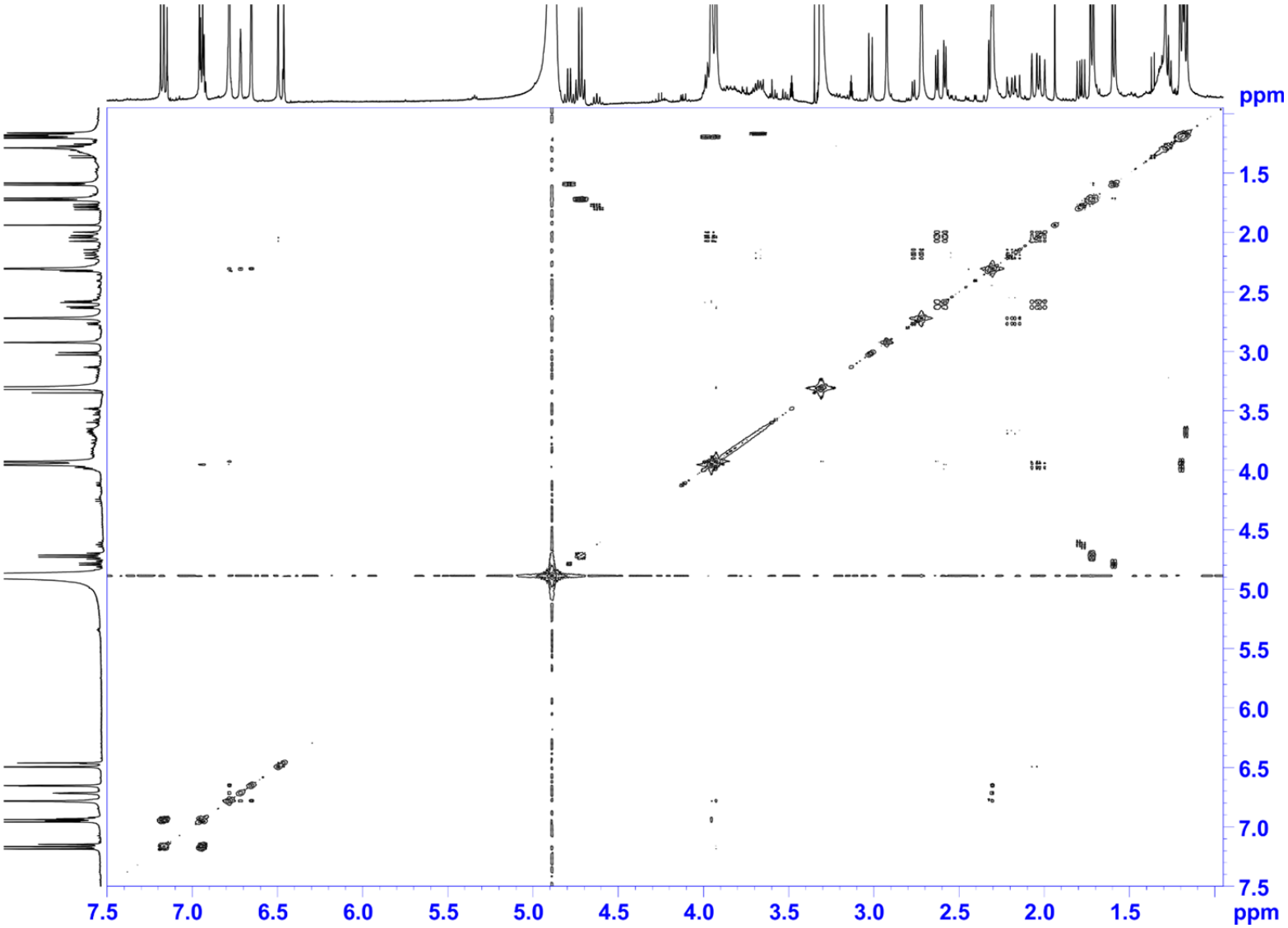


Figure S25. ^{13}C DEPT 135 spectrum of ikelacongoline A (**5a**).



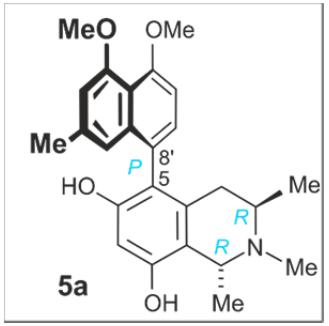
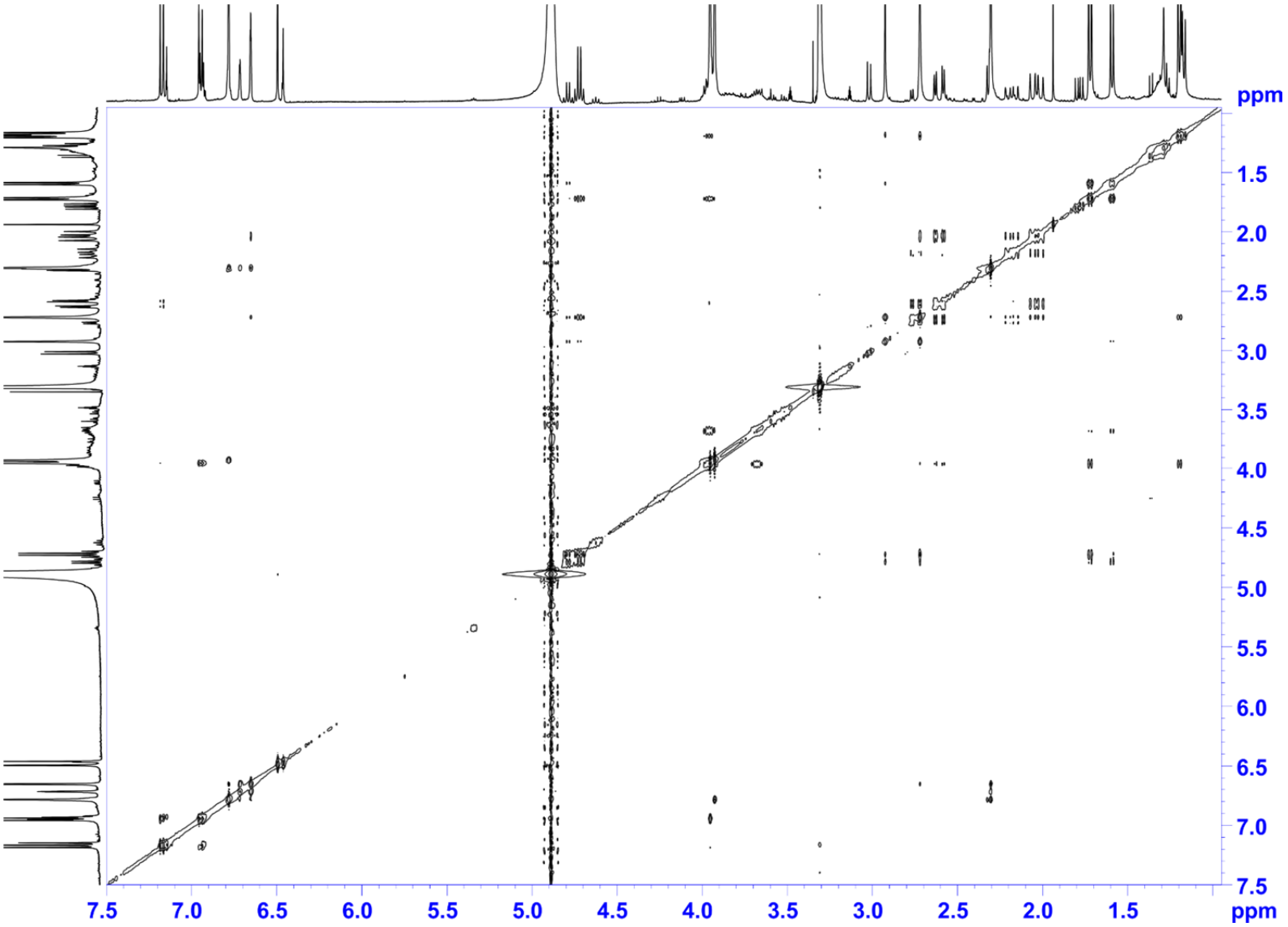


Figure S26. ^{1}H-^{1}H COSY spectrum of ikelacongoline A (**5a**).



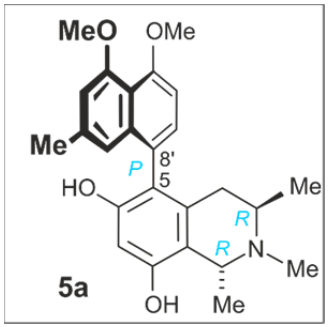


Figure S27. ^{1}H-^{1}H NOESY spectrum of ikelacongoline A (**5a**).

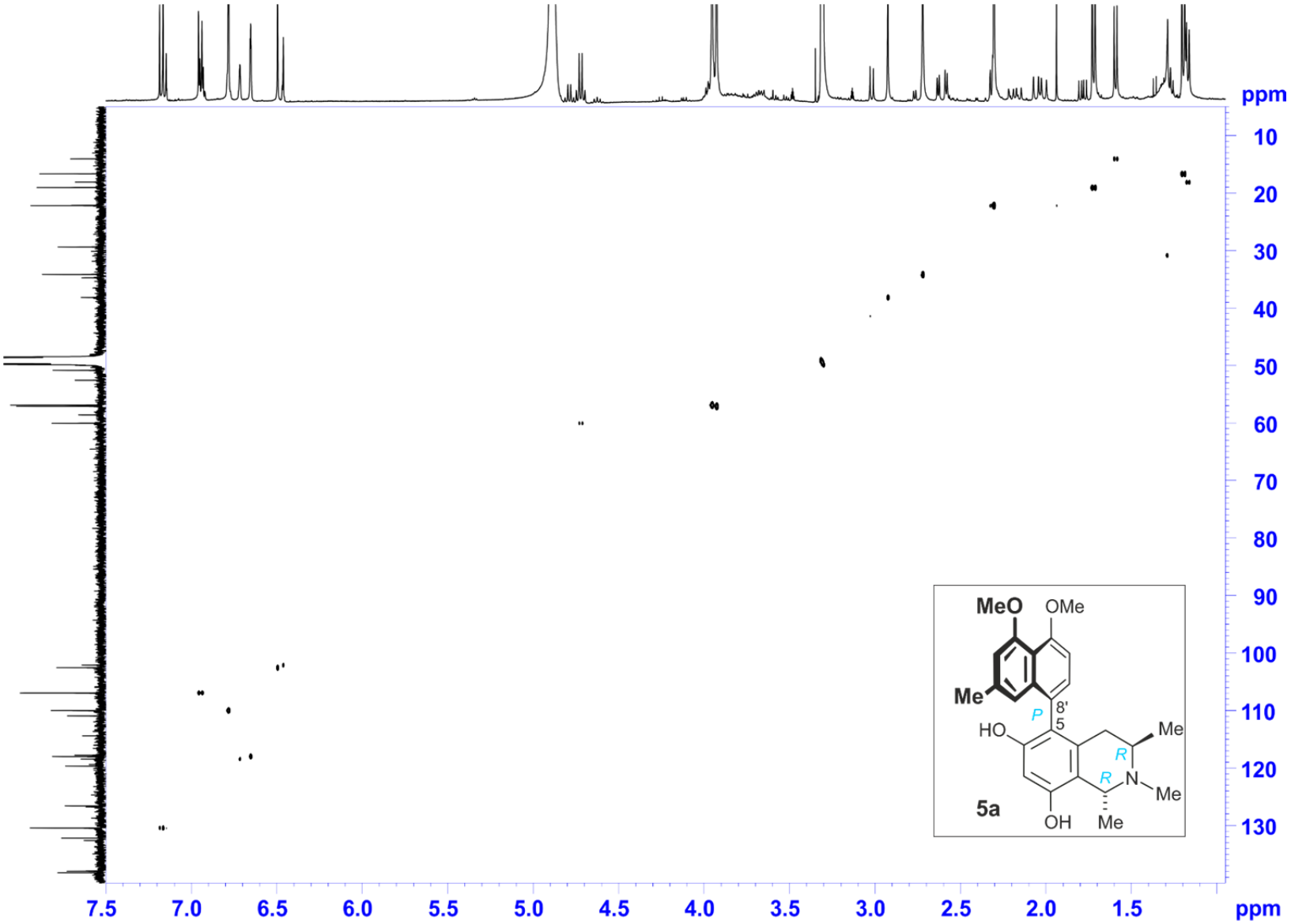


Figure S28. ^{1}H-^{13}C HSQC spectrum of ikelacongoline A (**5a**).

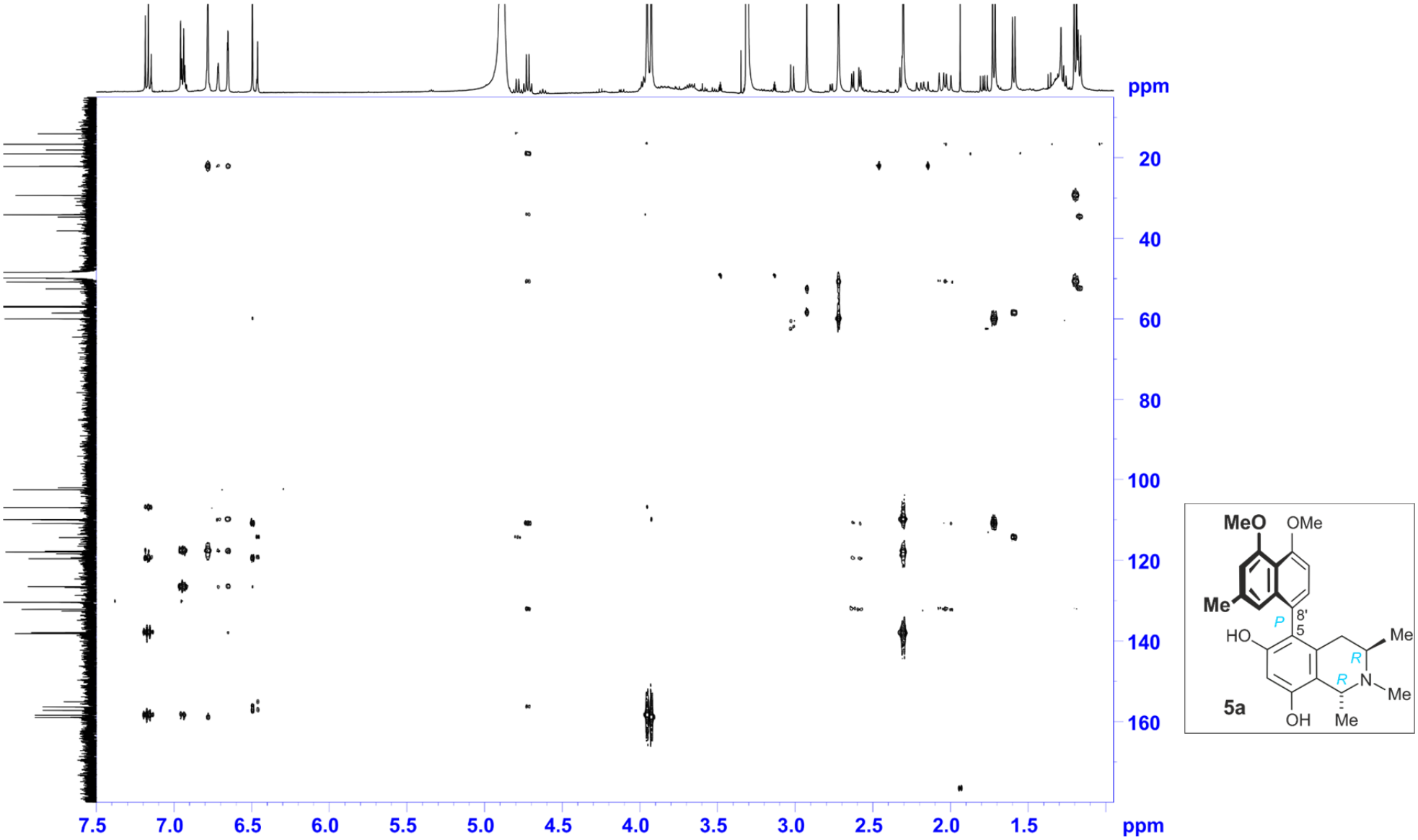


Figure S29. ^{1}H-^{13}C HMBC spectrum of ikelacongoline A (**5a**).

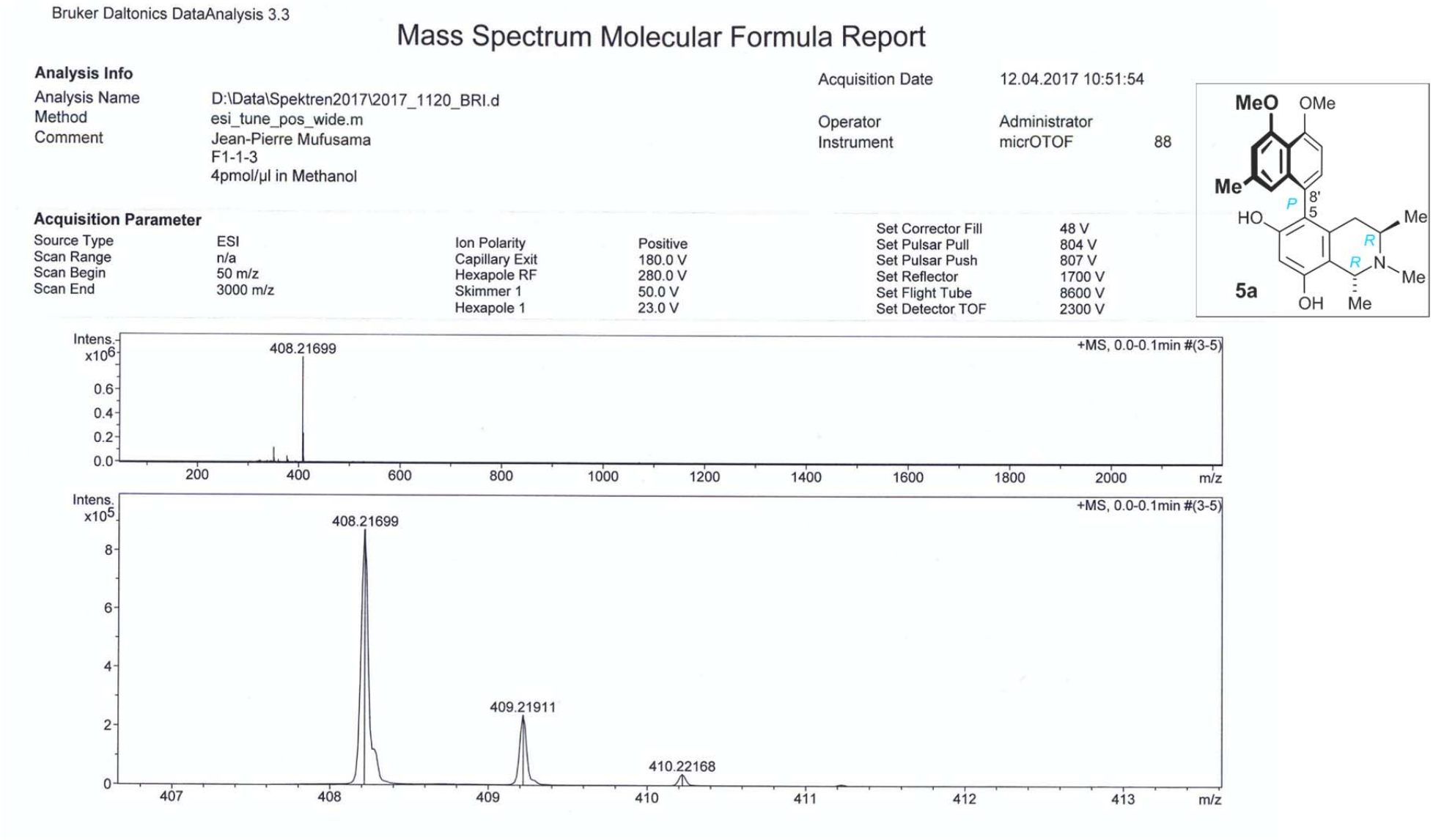
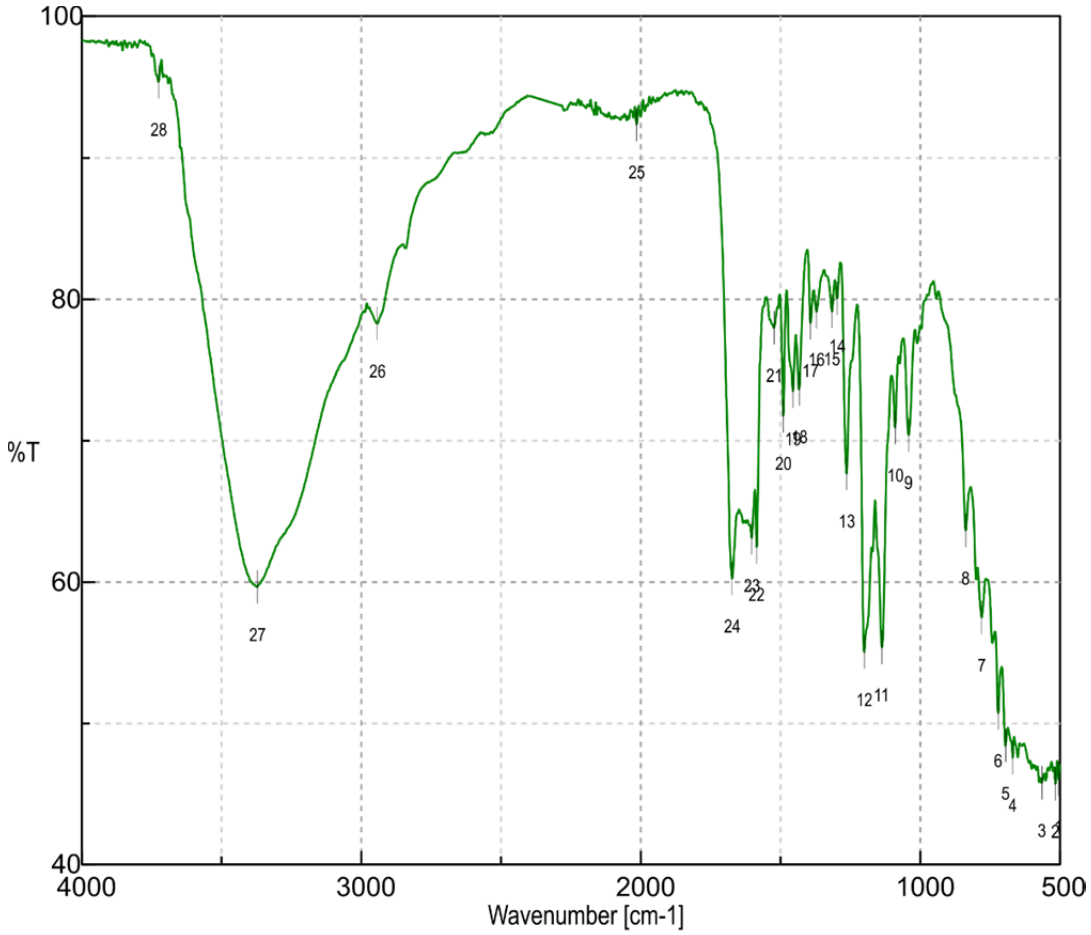


Figure S30. HRESIMS spectrum of ikelacongoline A (**5a**).



Results of Peak Find

No.	Position	Intensity	No.	Position	Intensity
1	505.258	46.0563	2	516.829	45.7118
3	565.041	45.7908	4	669.178	47.5409
5	695.212	48.4206	6	722.211	50.6981
7	780.065	57.4783	8	836.955	63.6077
9	1041.37	70.3784	10	1090.55	70.9039
11	1136.83	55.3656	12	1200.47	55.0365
13	1264.11	67.6507	14	1297.86	80.0462
15	1316.18	79.1392	16	1372.1	79.109
17	1392.35	78.2942	18	1433.82	73.6081
19	1455.99	73.4898	20	1489.74	71.7504
21	1523.49	77.9616	22	1585.2	62.4629
23	1603.52	63.0958	24	1672.95	60.2367
25	2015.25	92.3419	26	2942.84	78.2652
27	3372.89	59.6251	28	3725.8	95.365

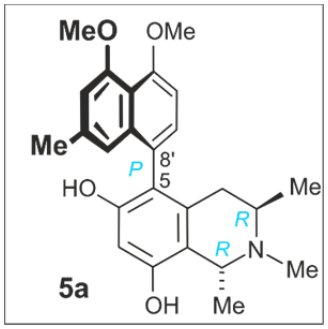
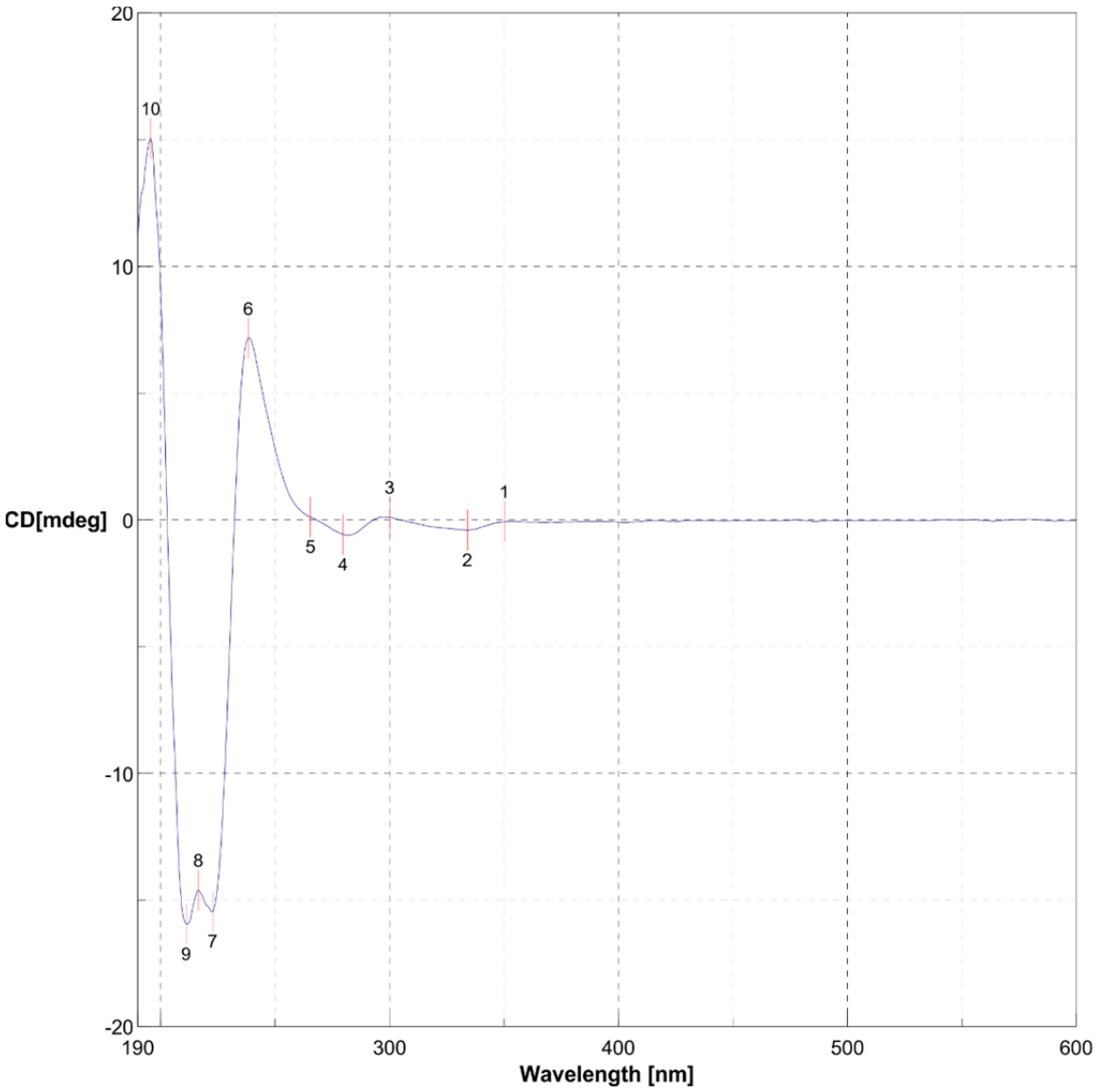


Figure S31. IR spectrum of ikelacongoline A (**5a**).



No.	nm	Mol. CD	No.	nm	Mol. CD	No.	nm	Mol. CD
1	350.2	-0.0712503	2	334.1	-0.4023	3	300.1	0.10304
4	279.8	-0.574268	5	265.5	0.108164	6	238.3	7.16546
7	222.8	-15.4525	8	216.6	-14.6128	9	211.2	-15.9326
10	195.7	15.0507						

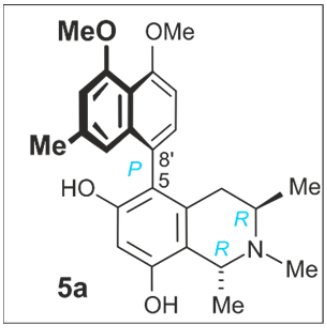
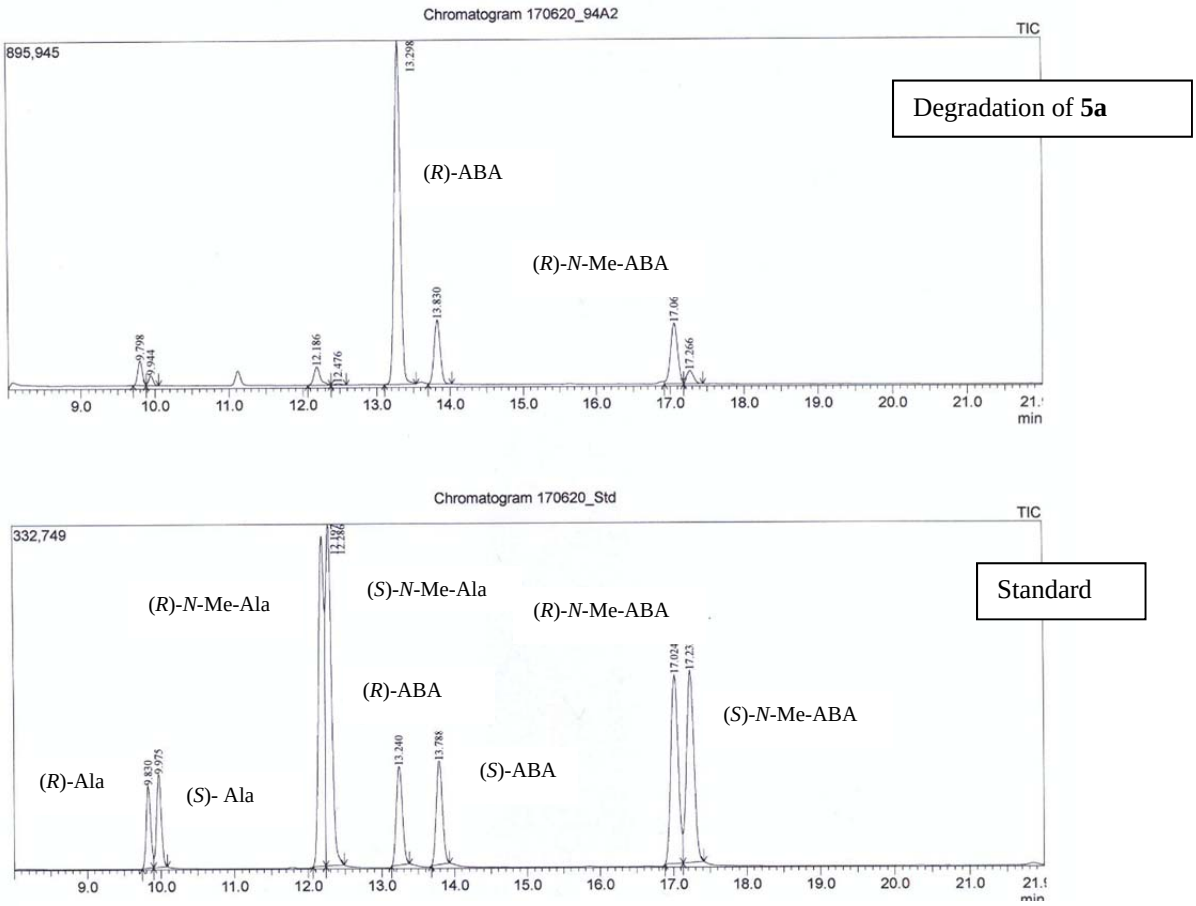


Figure S32. ECD spectrum of ikelacongoline A (**5a**).



Where: Ala = alanine; *N*-Me-Ala = *N*-methylalanine;
ABA = 3-aminobutyric acid; *N*-Me-ABA = *N*-methyl-3-aminobutyric acid

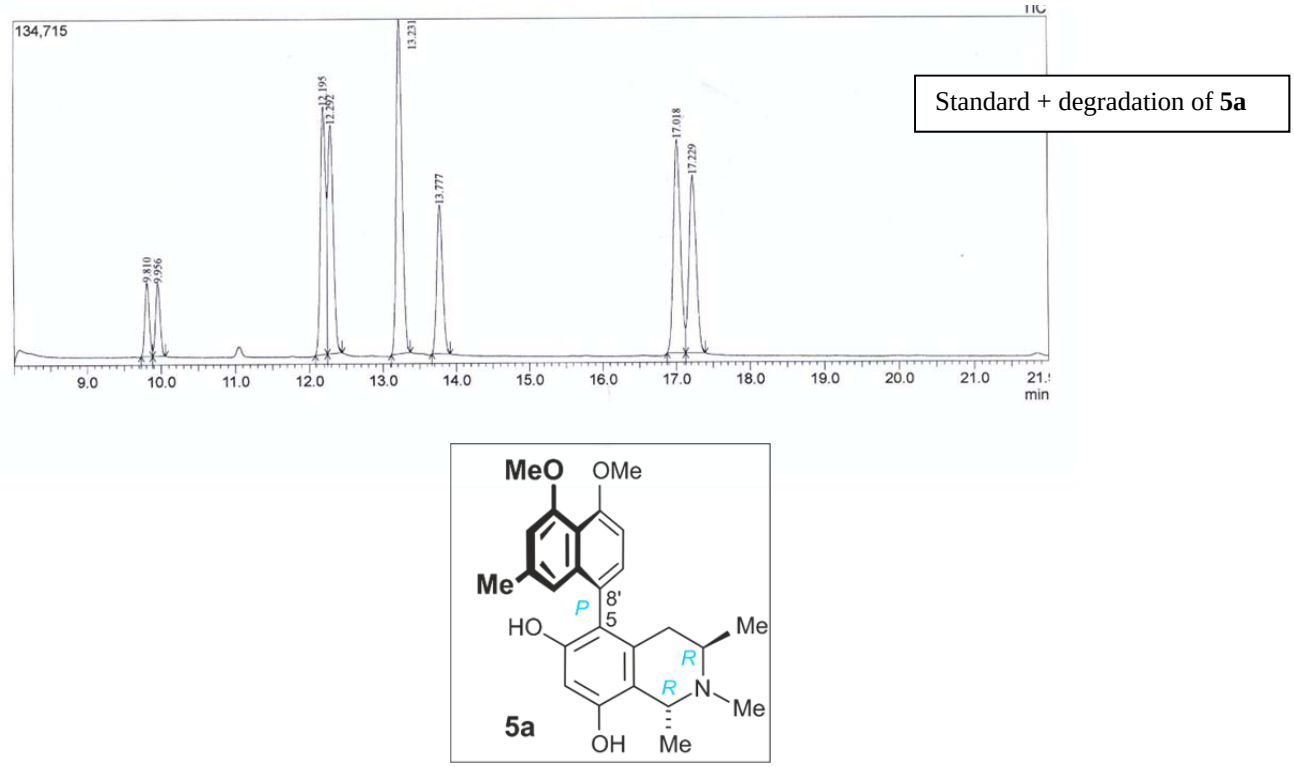


Figure S33. Oxidative degradation of ikelacongoline A (**5a**).

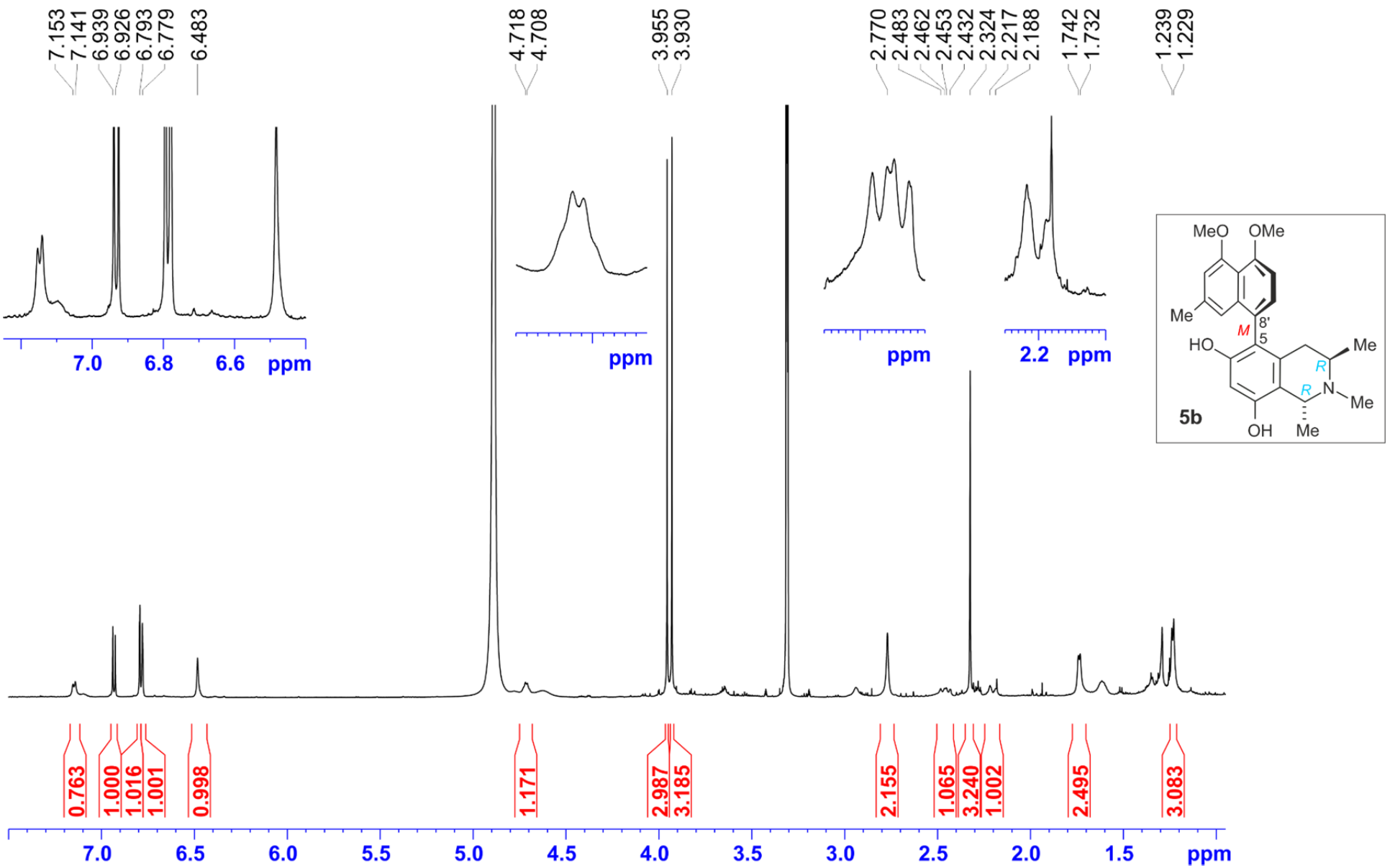


Figure S34. ^{1}H NMR spectrum of ikelacongoline B (**5b**).

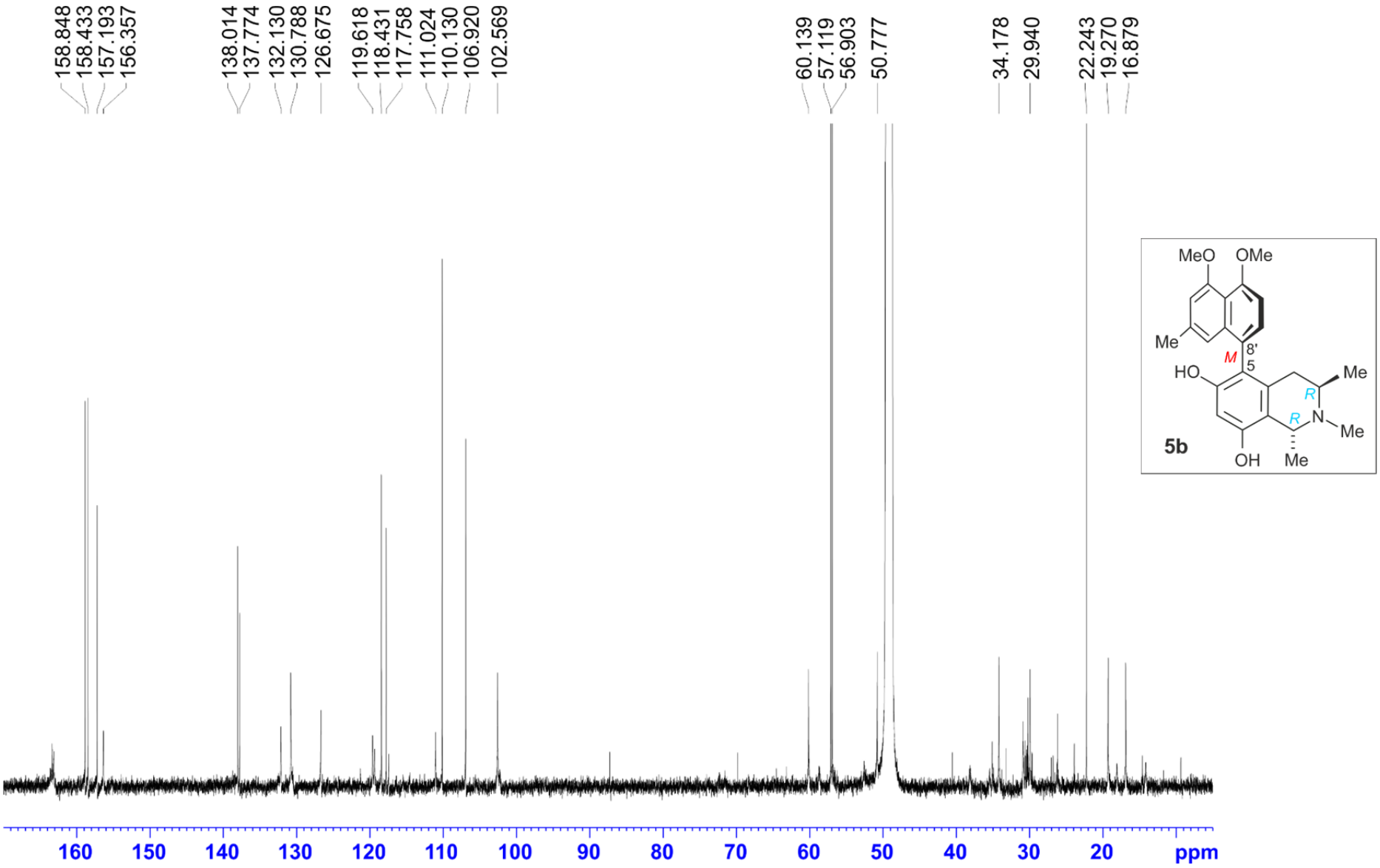


Figure S35. ^{13}C NMR spectrum of ikelacongoline B (**5b**).

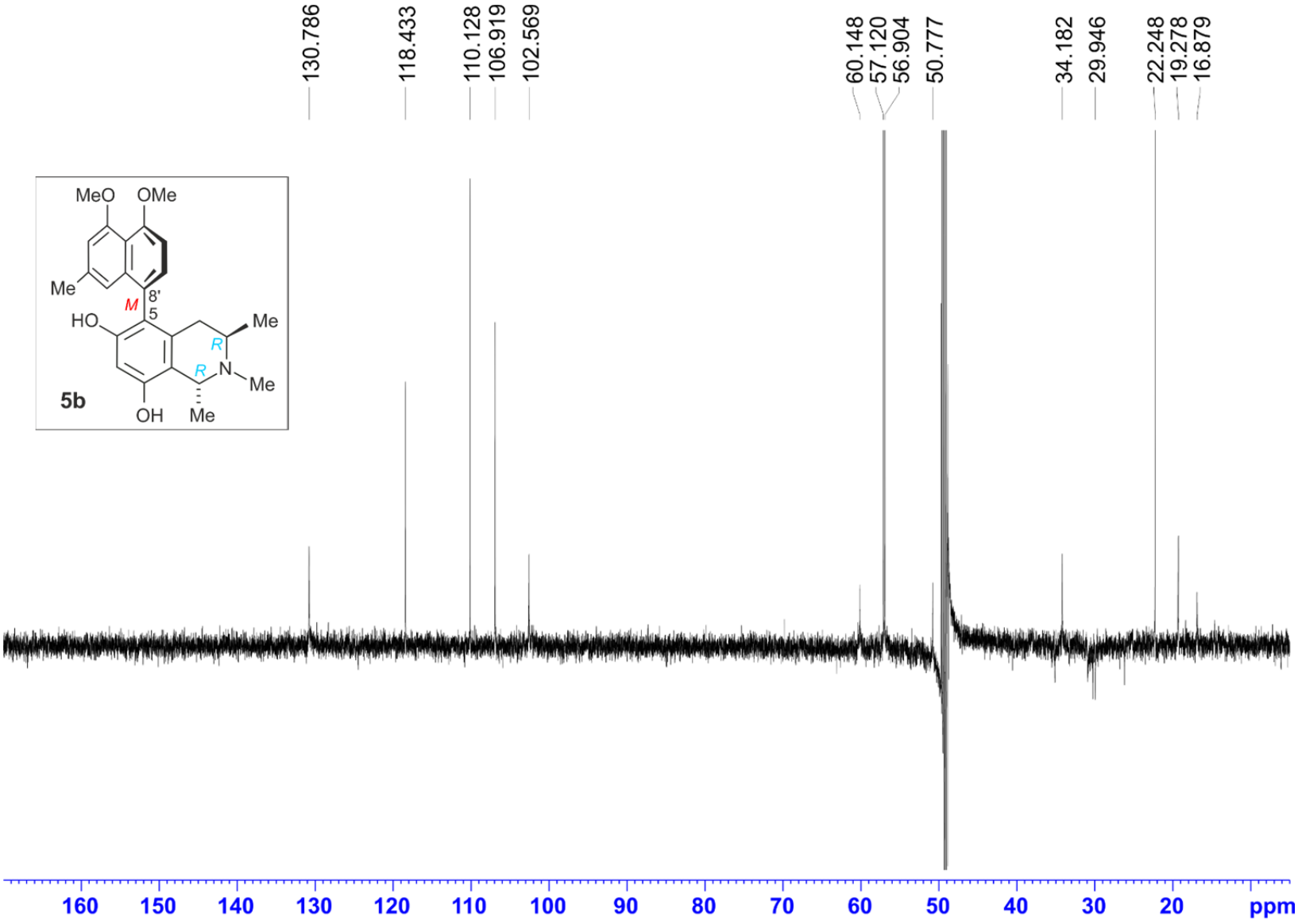
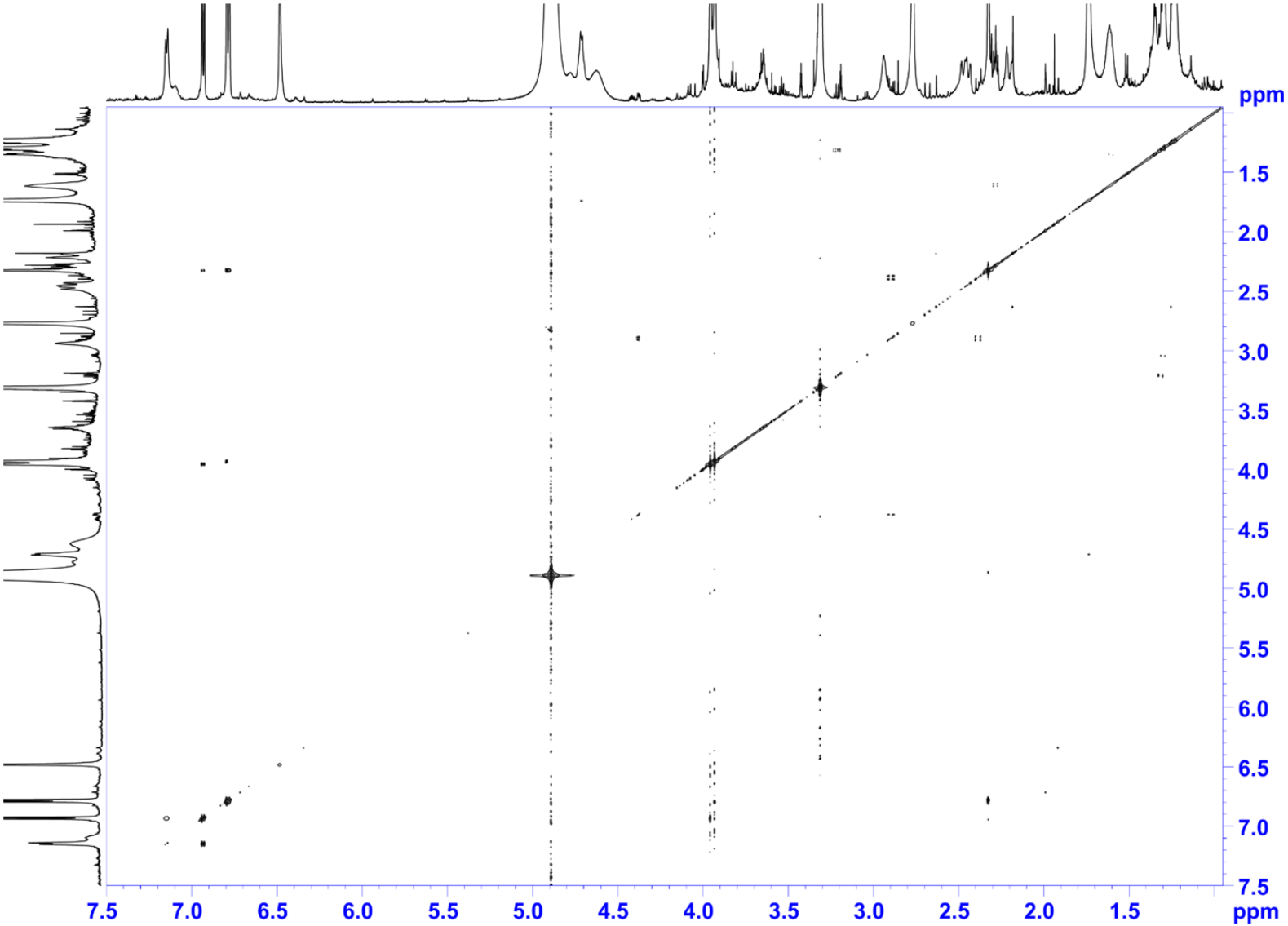


Figure S36. ^{13}C DEPT 135 NMR spectrum of ikelacongoline B (**5b**).



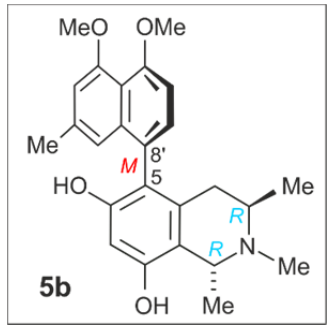
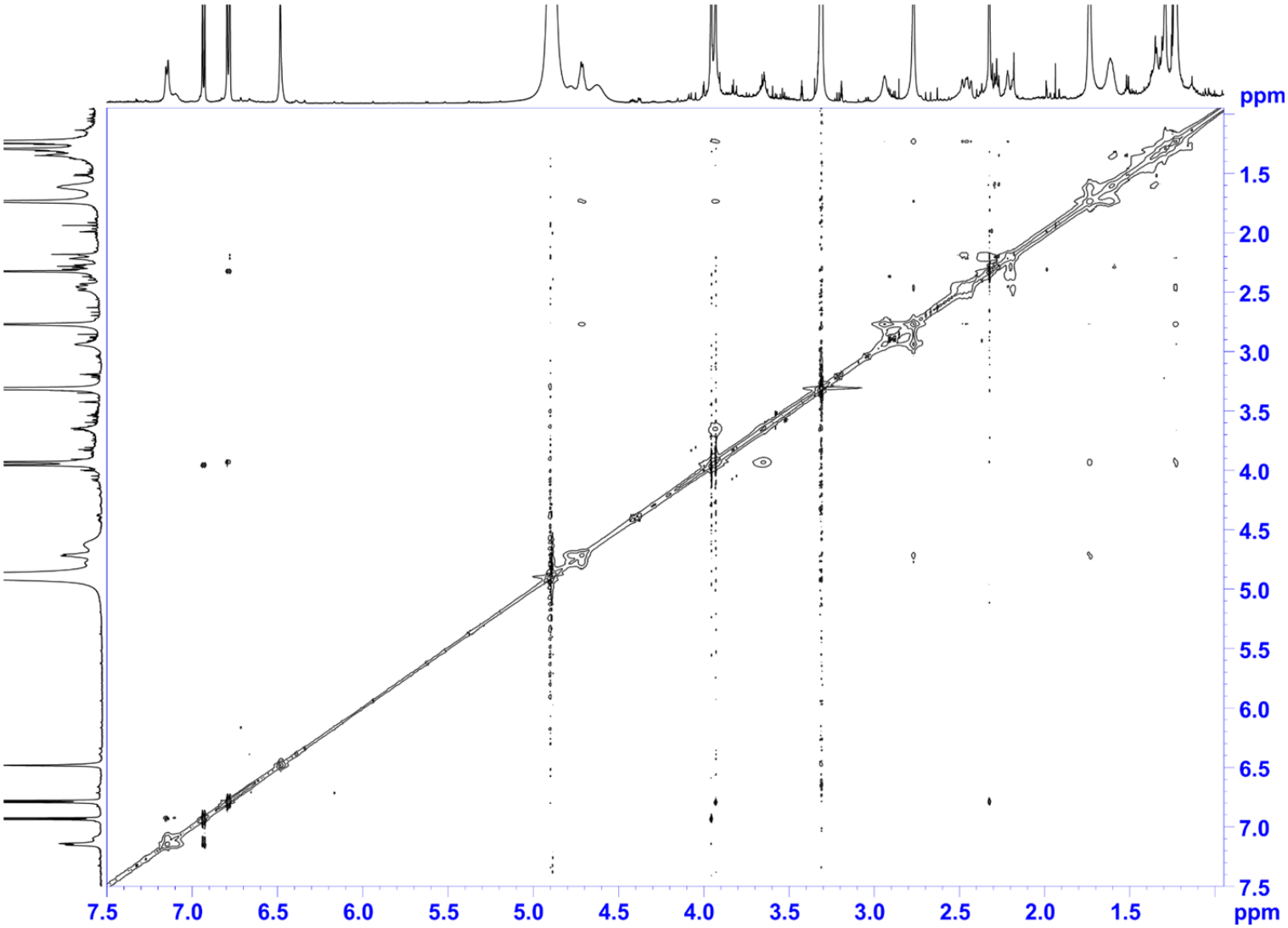


Figure S37. ^{1}H-^{1}H COSY spectrum of ikelacongoline B (**5b**).



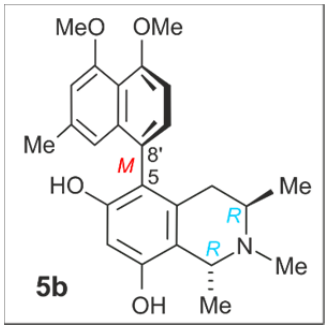
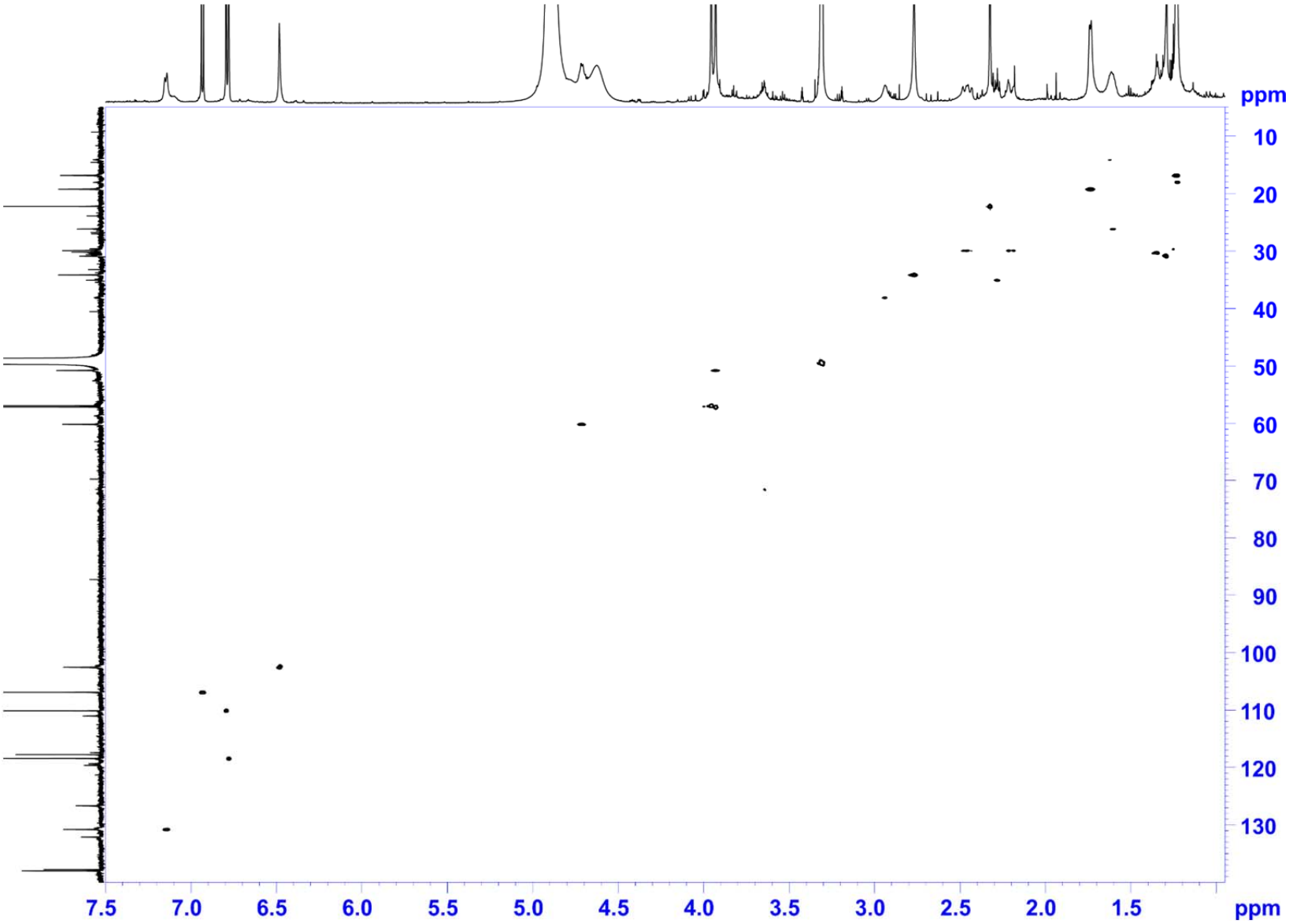


Figure S38. ^{1}H-^{1}H NOESY spectrum of ikelacongoline B (**5b**).



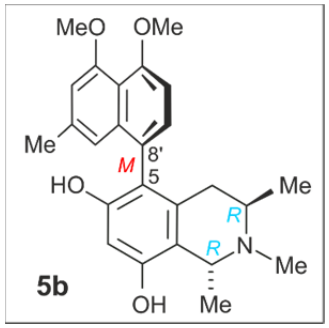
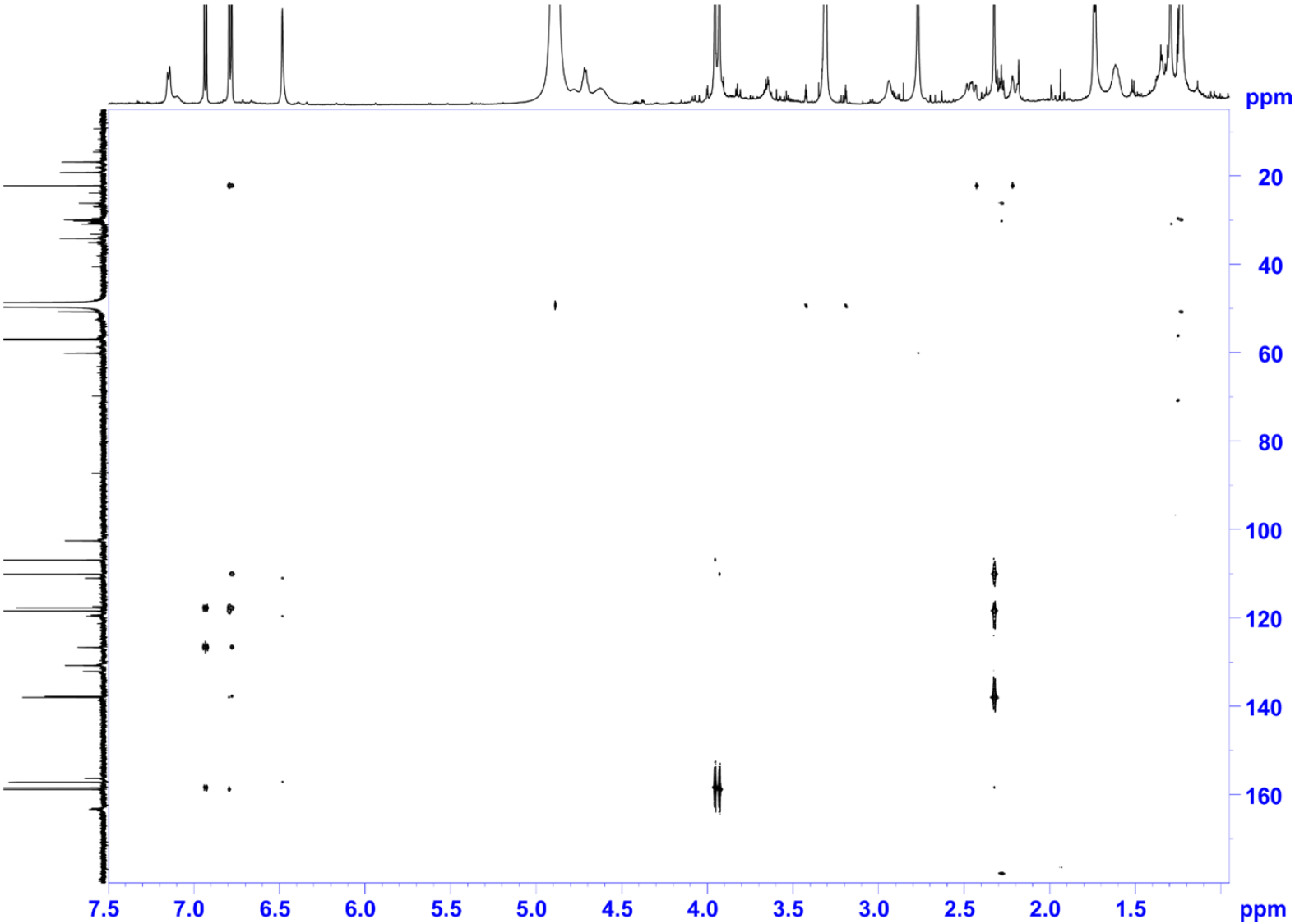


Figure S39. ^{1}H-^{13}C HSQC spectrum of ikelacongoline B (**5b**).



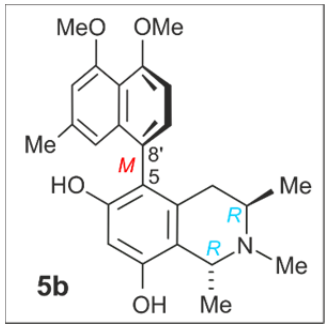


Figure S40. ^{1}H-^{13}C HMBC spectrum of ikelacongoline B (**5b**).

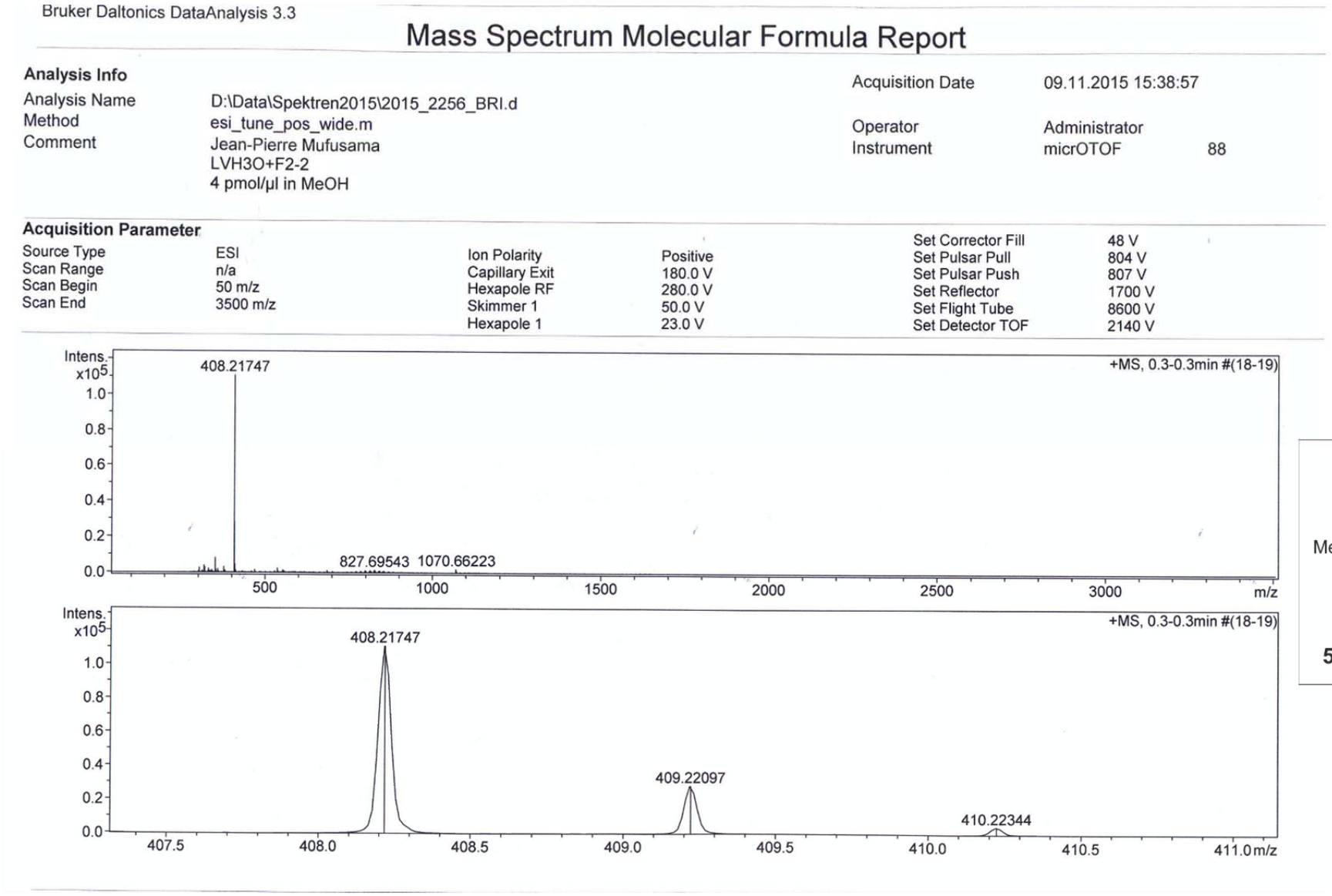
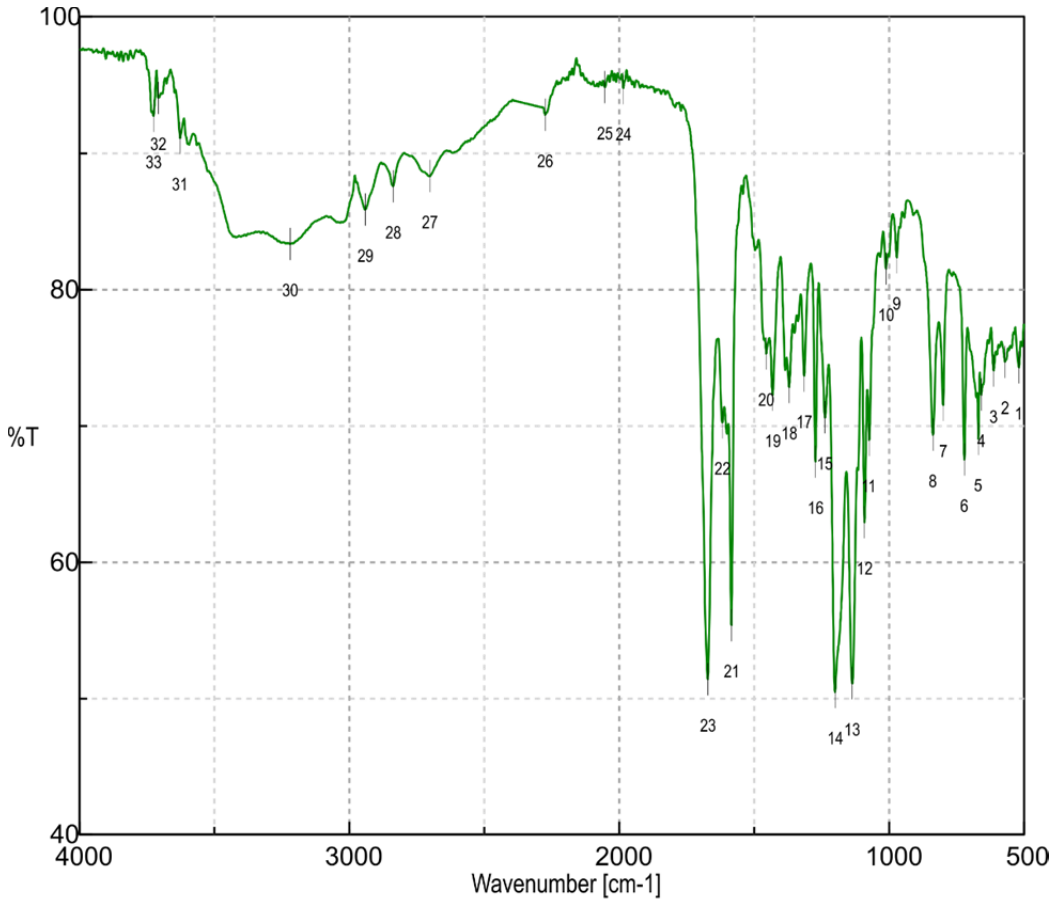


Figure S41. HRESIMS spectrum of ikelacongoline B (**5b**).



Results of Peak Find

No.	Position	Intensity	No.	Position	Intensity
1	519.722	74.2628	2	570.826	74.6781
3	613.252	74.0286	4	658.571	72.265
5	669.178	69.014	6	722.211	67.5055
7	800.314	71.5006	8	836.955	69.3198
9	971.947	82.3419	10	1011.48	81.5273
11	1074.16	68.944	12	1091.51	62.9075
13	1136.83	51.0842	14	1200.47	50.4704
15	1238.08	70.6108	16	1273.75	67.3408
17	1315.21	73.6501	18	1371.14	72.8199
19	1431.89	72.2791	20	1455.99	75.2895
21	1584.24	55.3551	22	1617.98	70.2109
23	1671.98	51.3856	24	1985.36	94.7554
25	2052.85	94.8325	26	2274.63	92.7985
27	2701.78	88.2884	28	2838.7	87.5624
29	2940.91	85.8428	30	3219.58	83.315
31	3627.45	91.0775	32	3708.44	94.034
33	3725.8	92.7317			

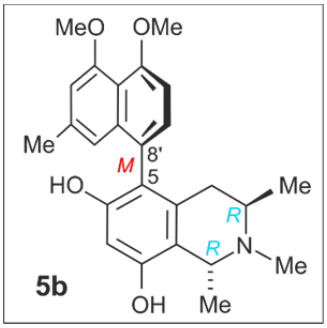
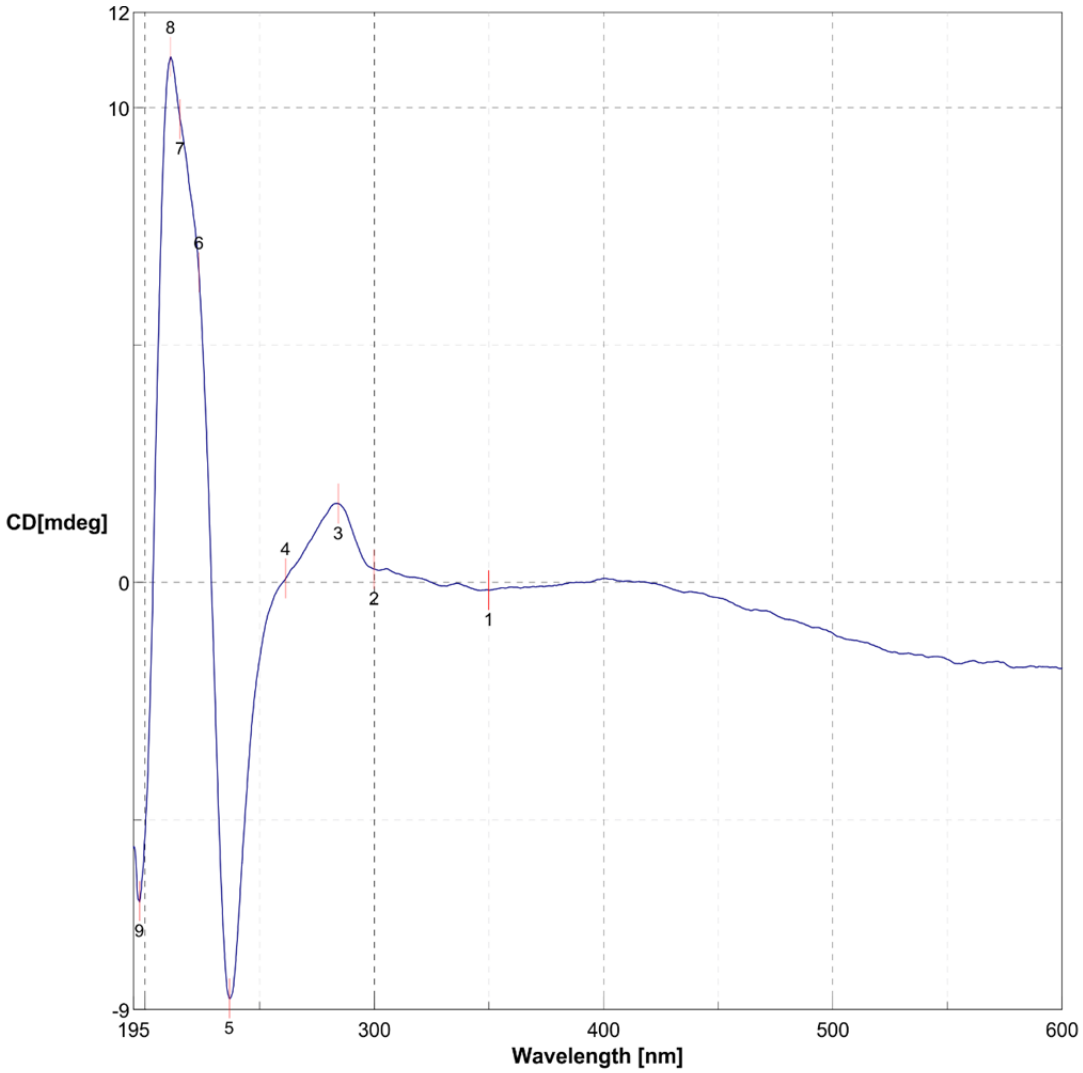


Figure S42. IR spectrum of ikelacongoline B (**5b**).



No.	nm	Mol. CD	No.	nm	Mol. CD	No.	nm	Mol. CD
1	349.9	-0.163176	2	299.9	0.277695	3	284.3	1.65682
4	261.4	0.0818669	5	236.8	-8.76205	6	223.5	6.52628
7	215.3	9.75589	8	211.2	11.0706	9	197.6	-6.71186

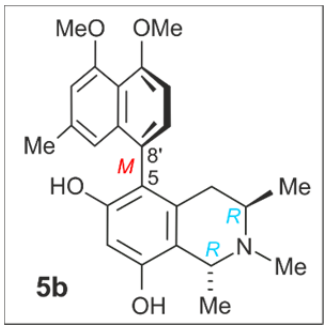
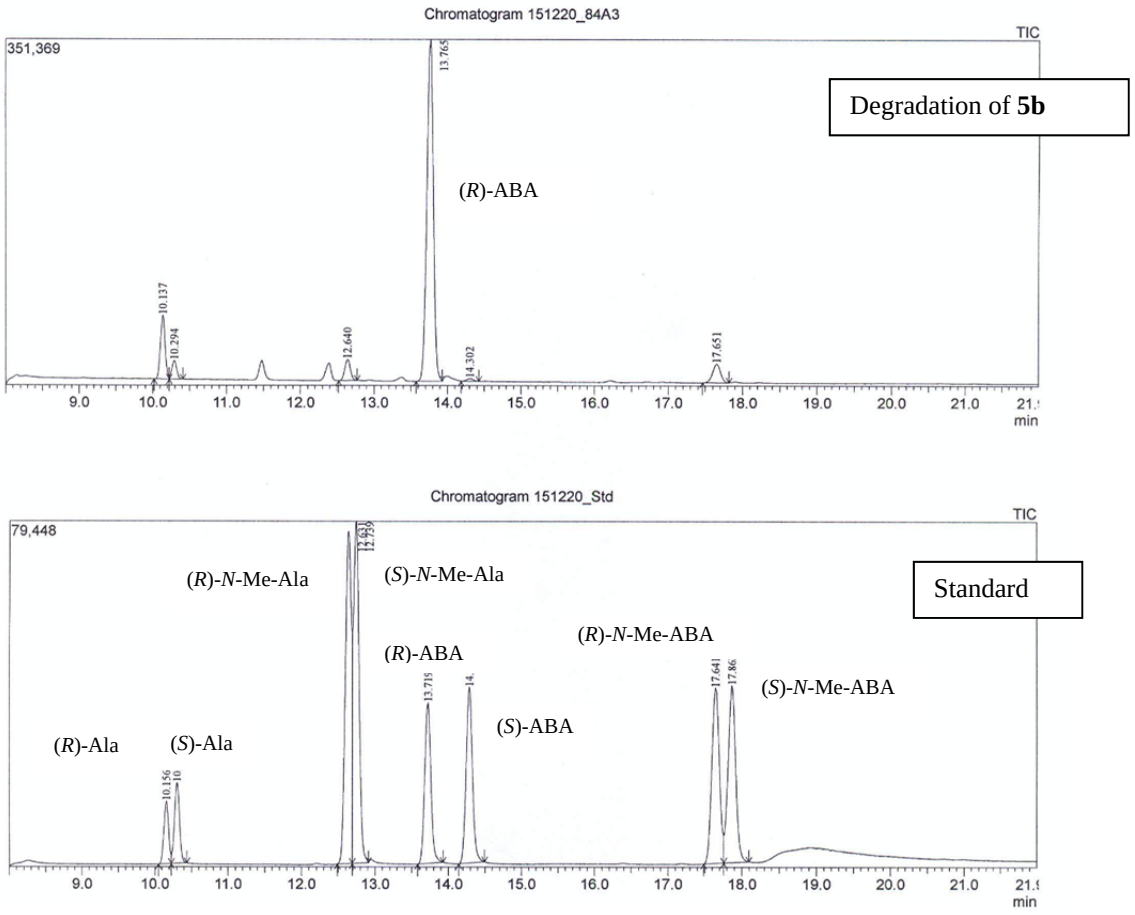
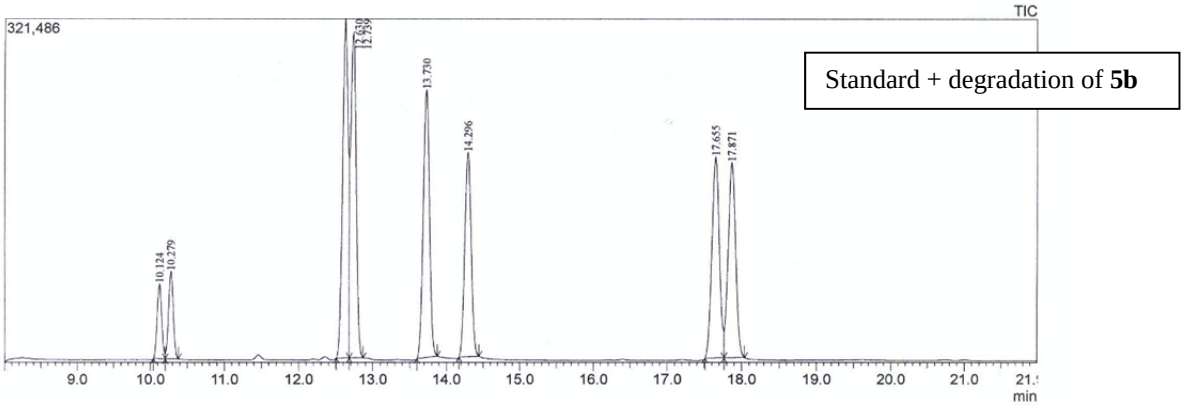


Figure S43. ECD spectrum of ikelacongoline B (**5b**)



Where: Ala = alanine; *N*-Me-Ala = *N*-methylalanine;
ABA = 3-aminobutyric acid; *N*-Me-ABA = *N*-methyl-3-aminobutyric acid



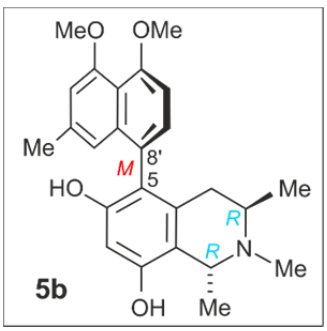


Figure S44. Oxidative degradation of ikelacongoline B (**5b**).

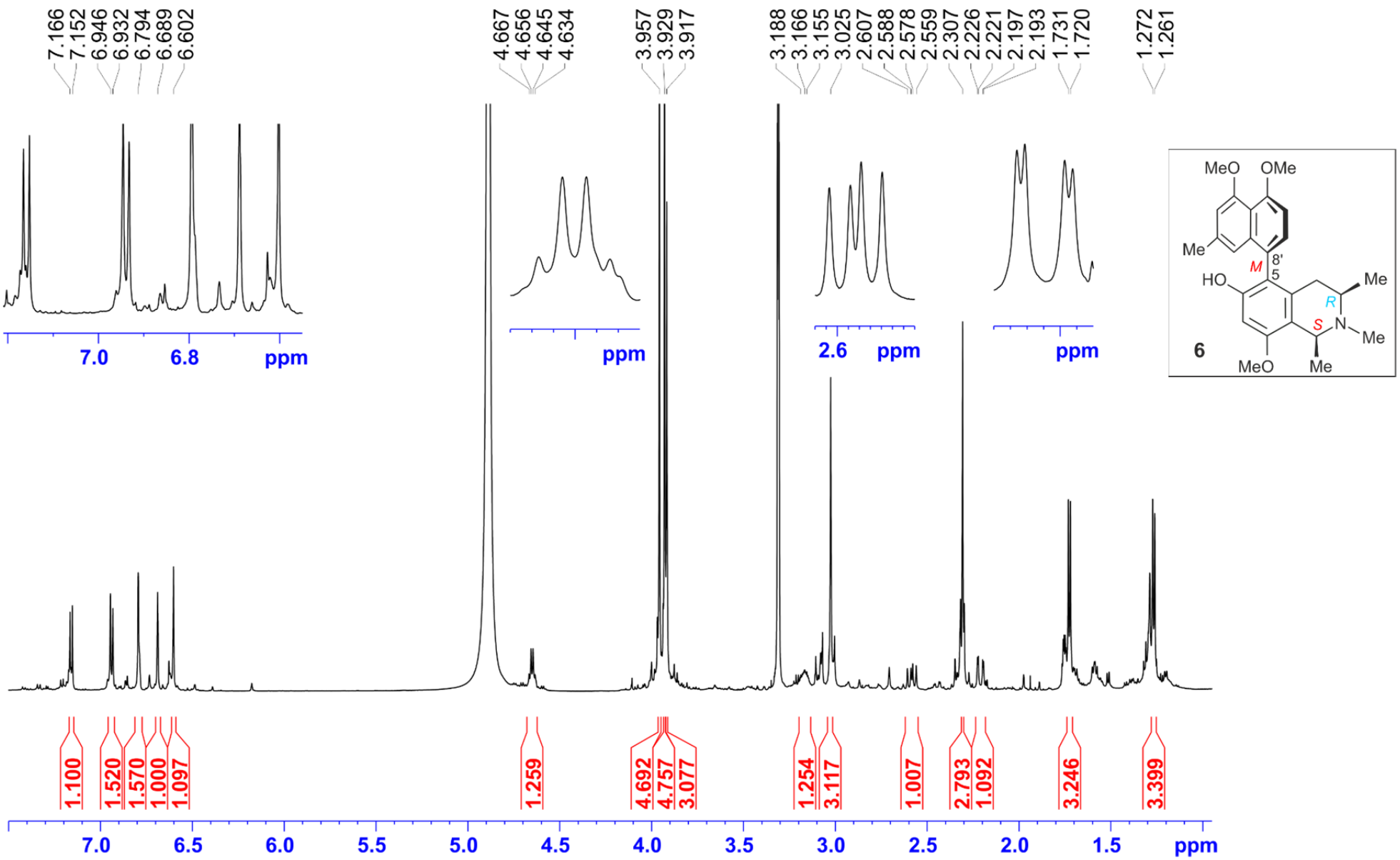


Figure S45. ^{1}H NMR spectrum of ikelacongoline C (**6**).

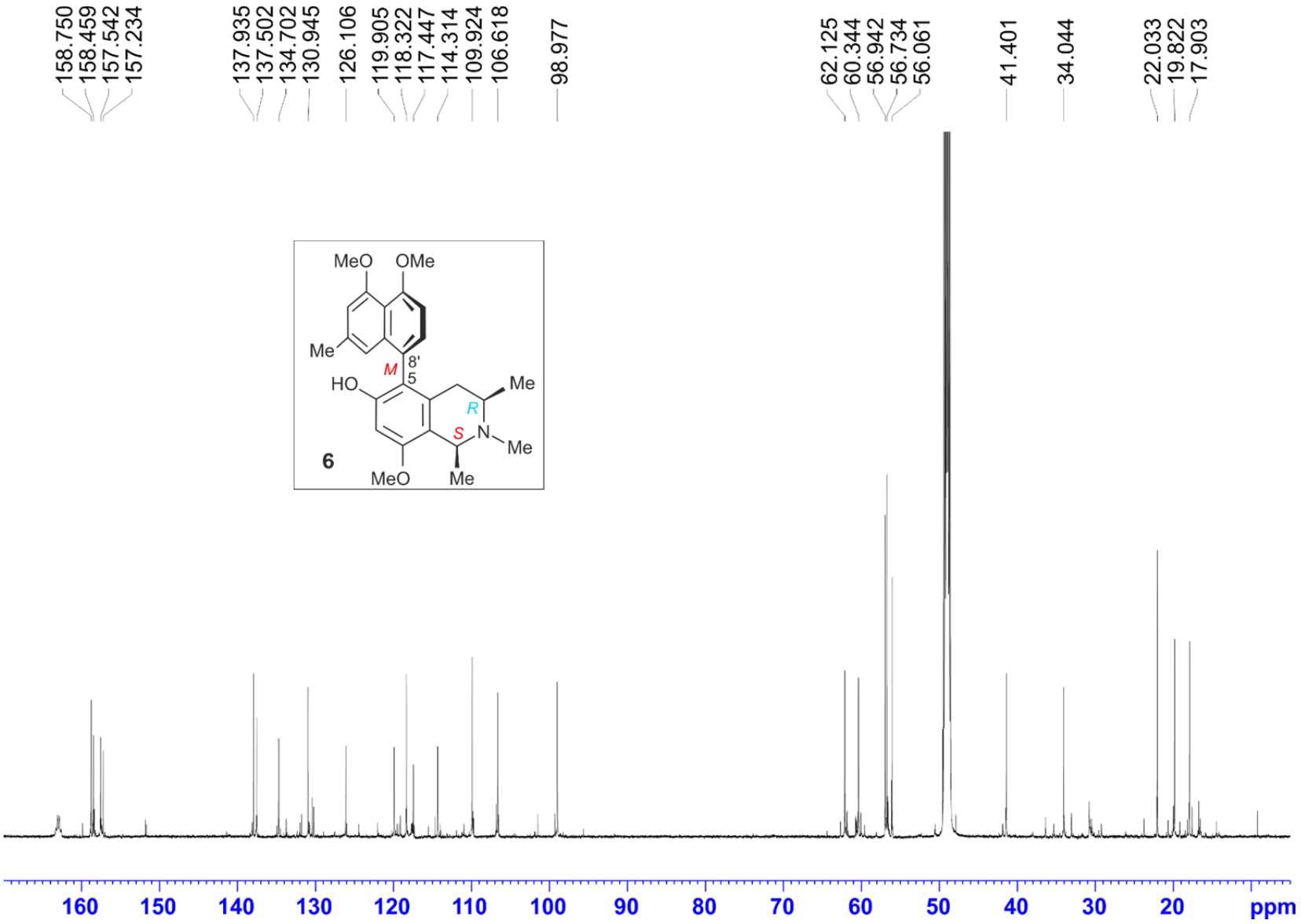


Figure S46. ^{13}C NMR spectrum of ikelacongoline C (**6**).

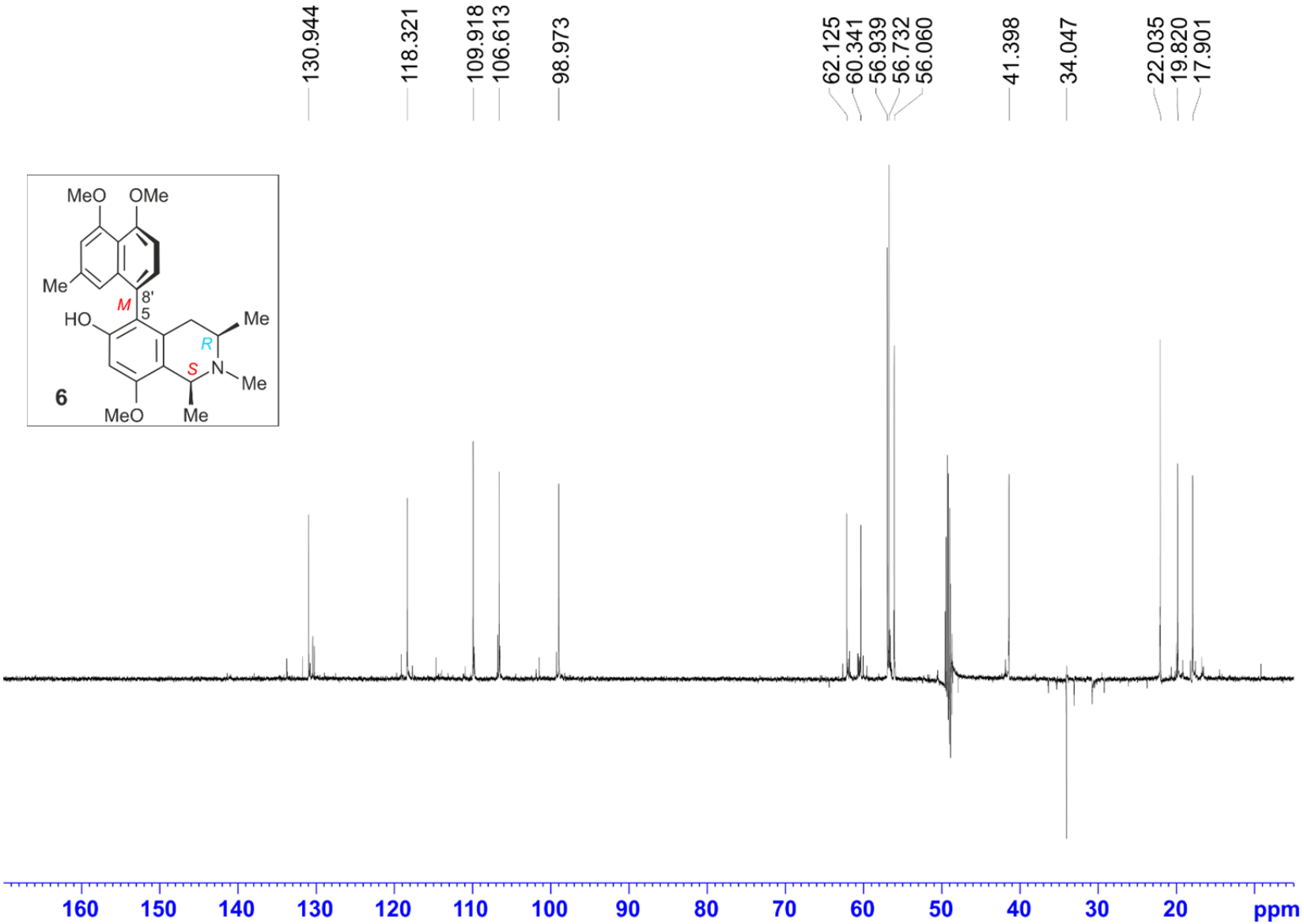


Figure S47. ^{13}C DEPT 135 NMR spectrum of ikelacongoline C (**6**).

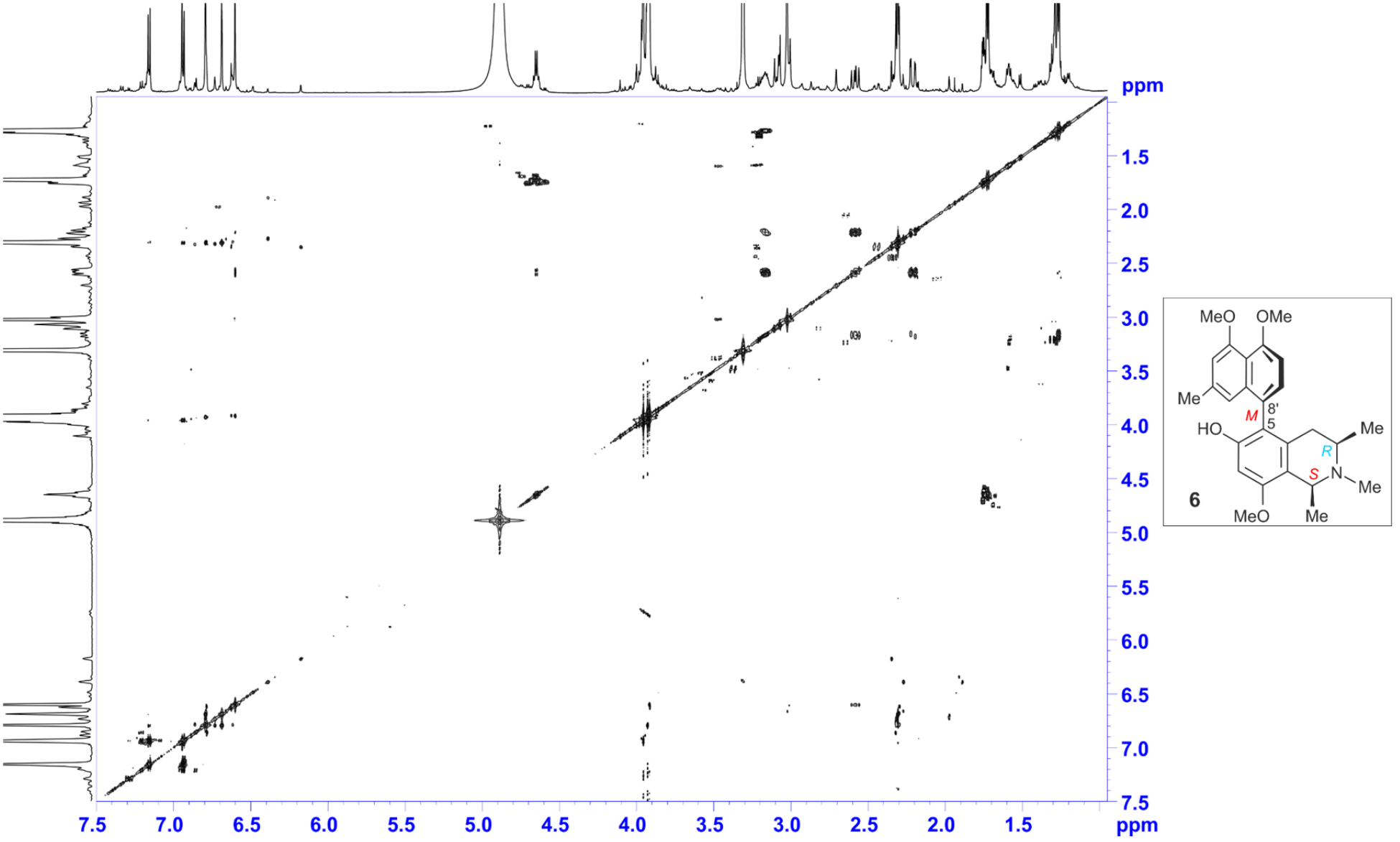
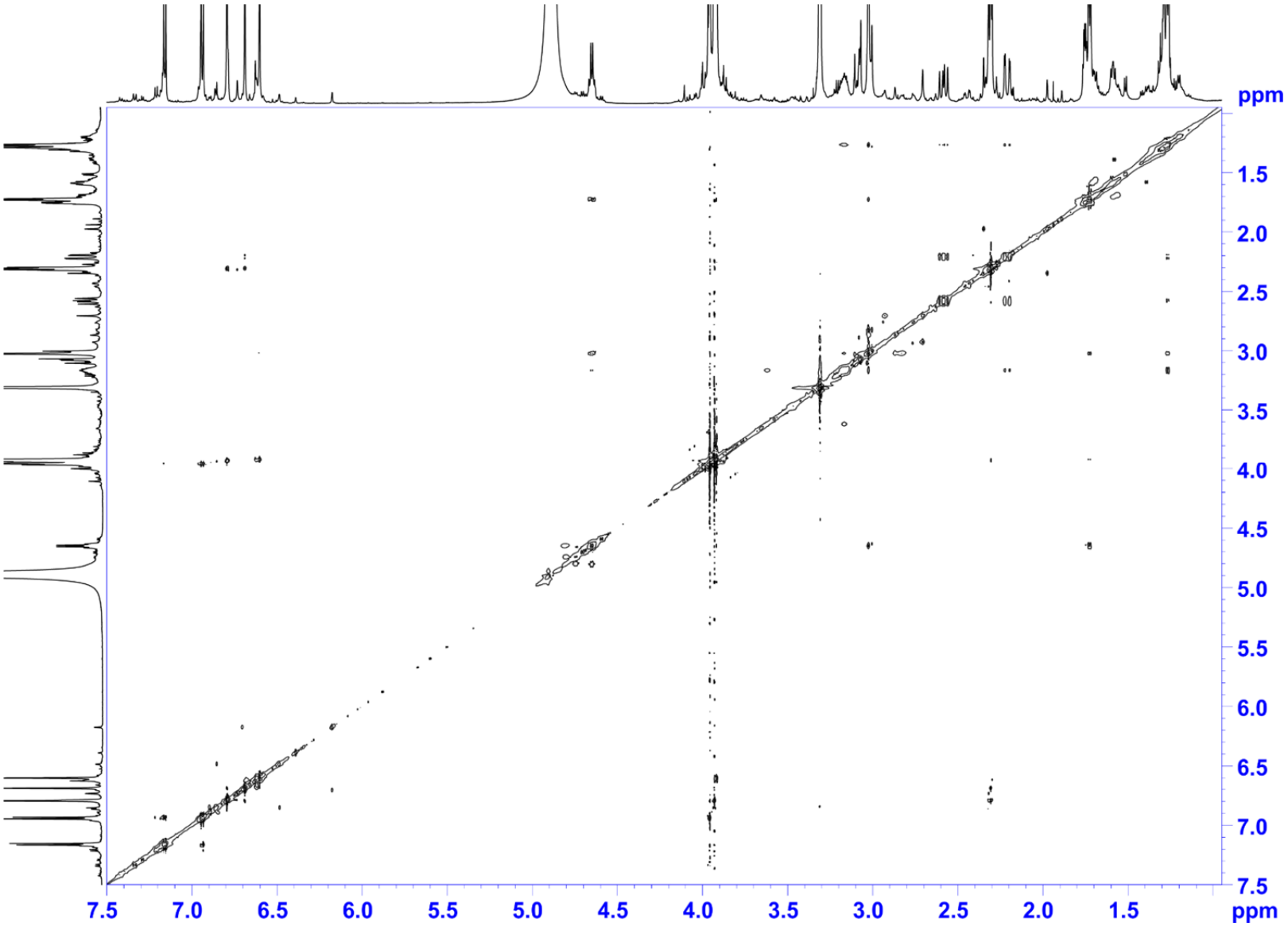


Figure S47. ^{1}H-^{1}H COSY spectrum of ikelacongoline C (**6**)



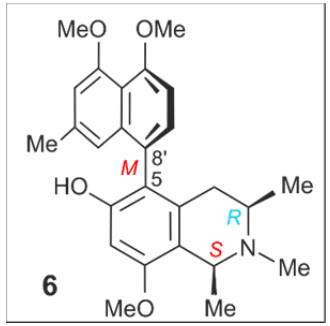
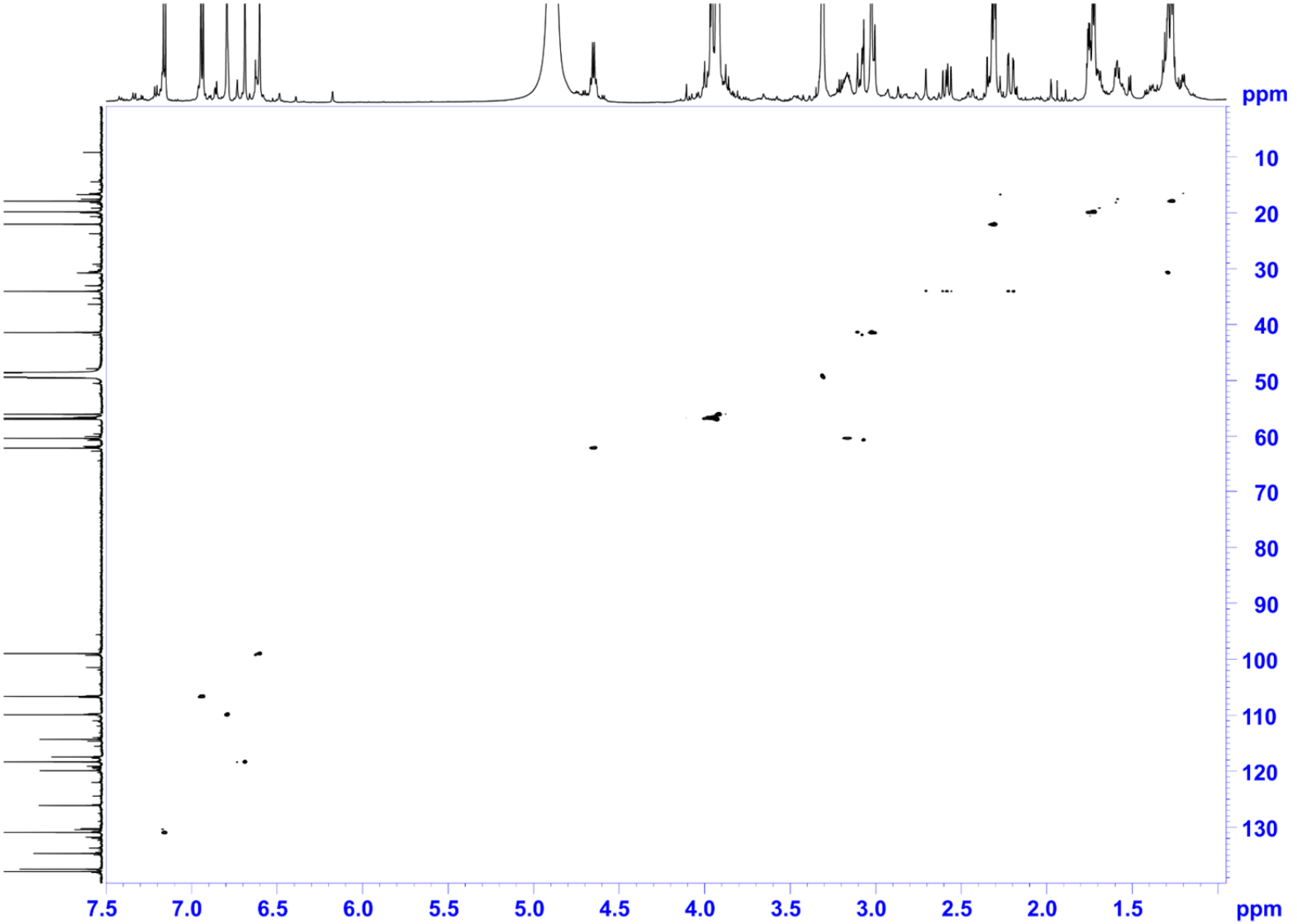


Figure S49. ^{1}H-^{1}H NOESY spectrum of ikelacongoline C (**6**).



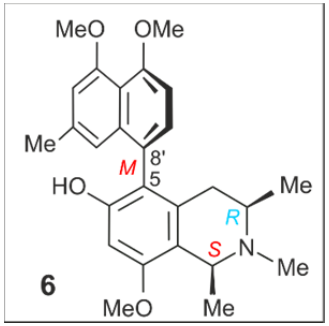
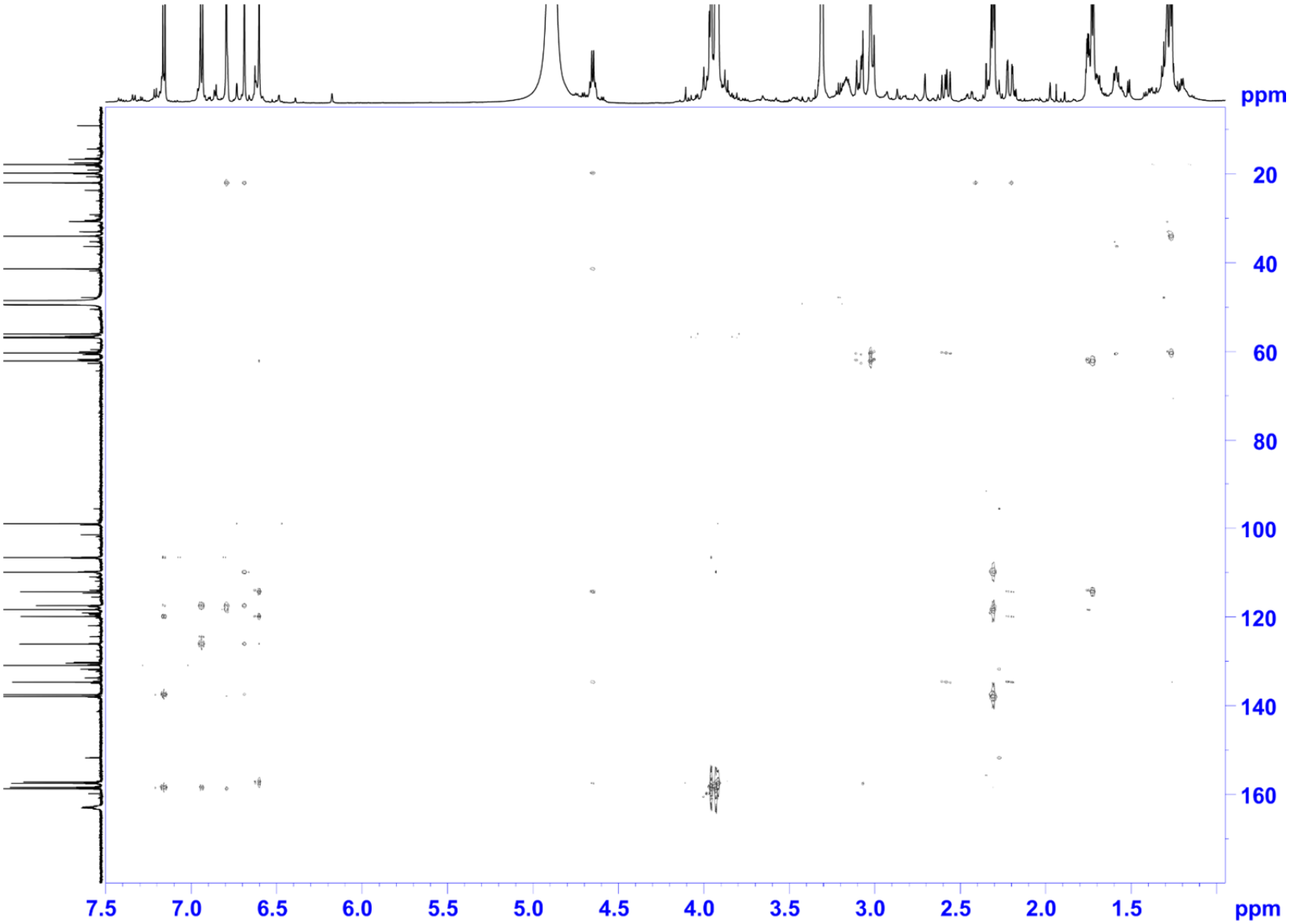


Figure S50. ^{1}H-^{13}C HSQC spectrum of ikelacongoline C (**6**).



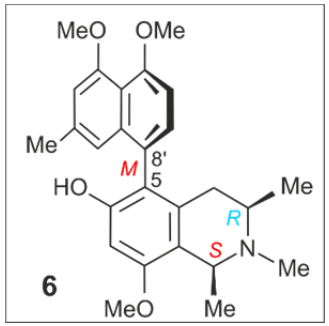


Figure S51. ^{1}H-^{13}C HMBC spectrum of ikelacongoline C (**6**).

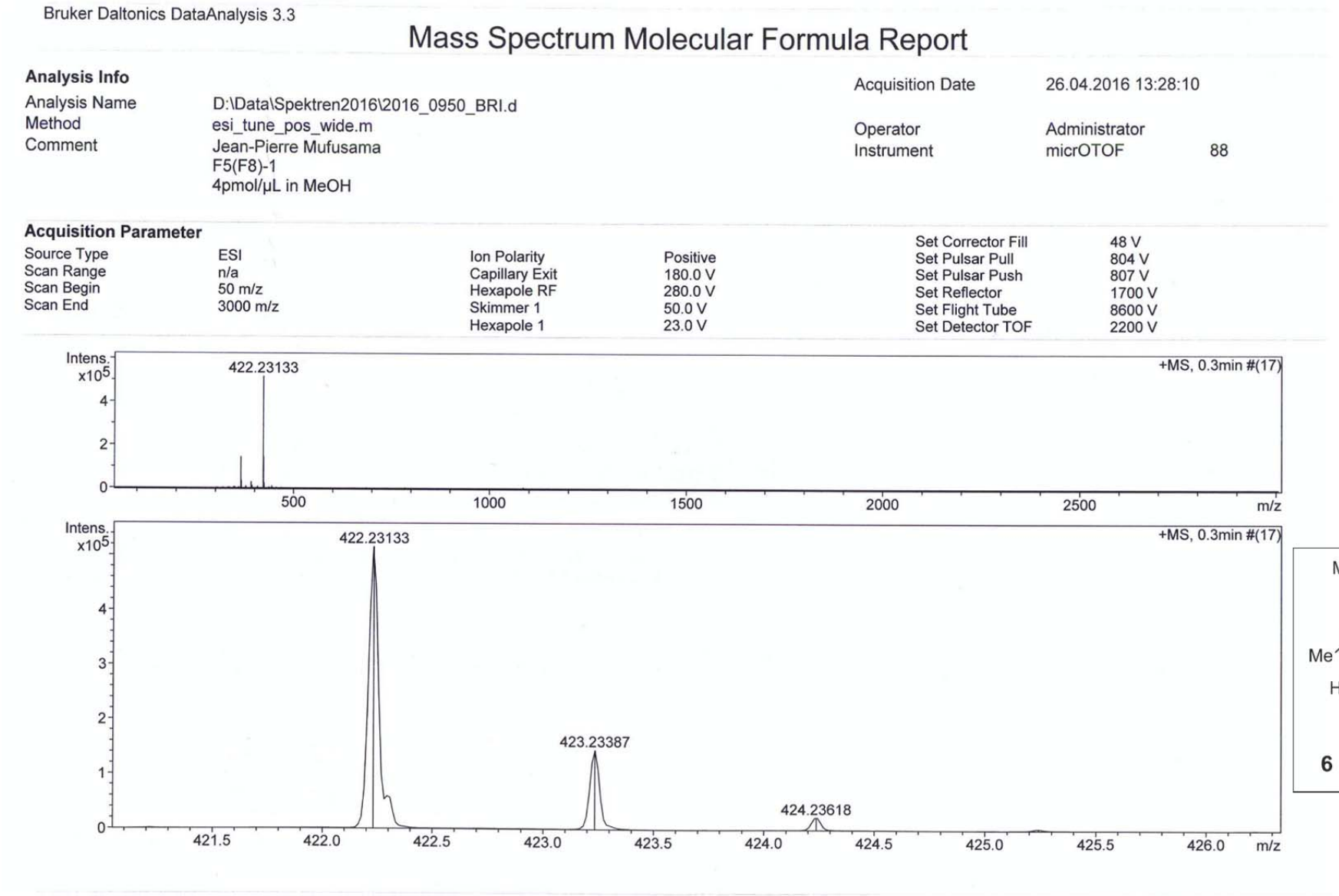
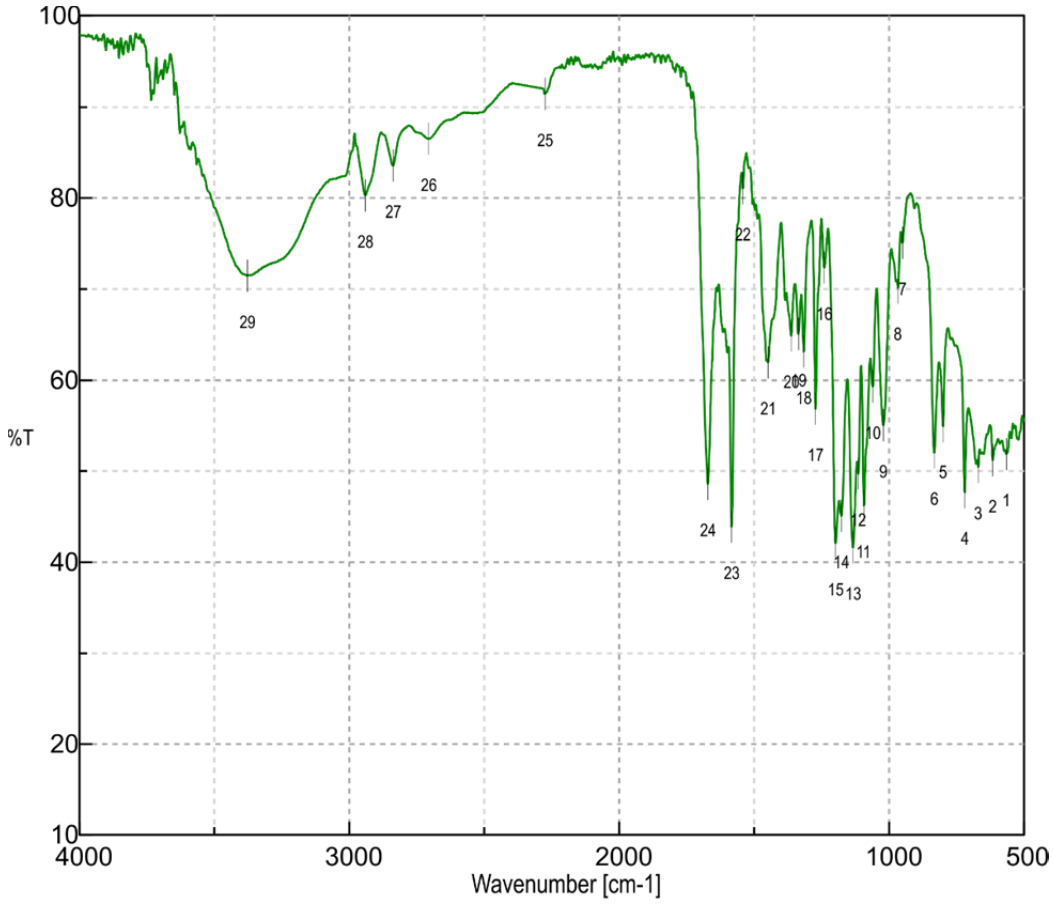


Figure S52. HRESIMS spectrum of ikelacongoline C (**6**).



Results of Peak Find

No.	Position	Intensity	No.	Position	Intensity
1	565.041	51.8232	2	616.145	51.1542
3	669.178	50.3984	4	720.282	47.6333
5	800.314	54.8899	6	832.133	51.982
7	950.734	75.0185	8	967.126	70.0929
9	1021.12	55.0187	10	1060.66	59.2346
11	1093.44	46.1831	12	1113.69	49.7067
13	1133.94	41.5843	14	1177.33	45.059
15	1197.58	42.0289	16	1240	72.3072
17	1272.79	56.7944	18	1316.18	63.0906
19	1336.43	64.992	20	1363.43	64.8323
21	1449.24	61.8914	22	1541.81	81.0372
23	1583.27	43.8362	24	1671.02	48.5487
25	2275.59	91.4061	26	2705.64	86.4569
27	2838.7	83.5149	28	2940.91	80.257
29	3378.67	71.4406			

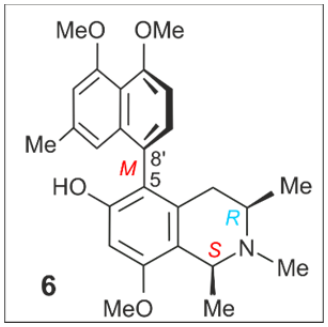
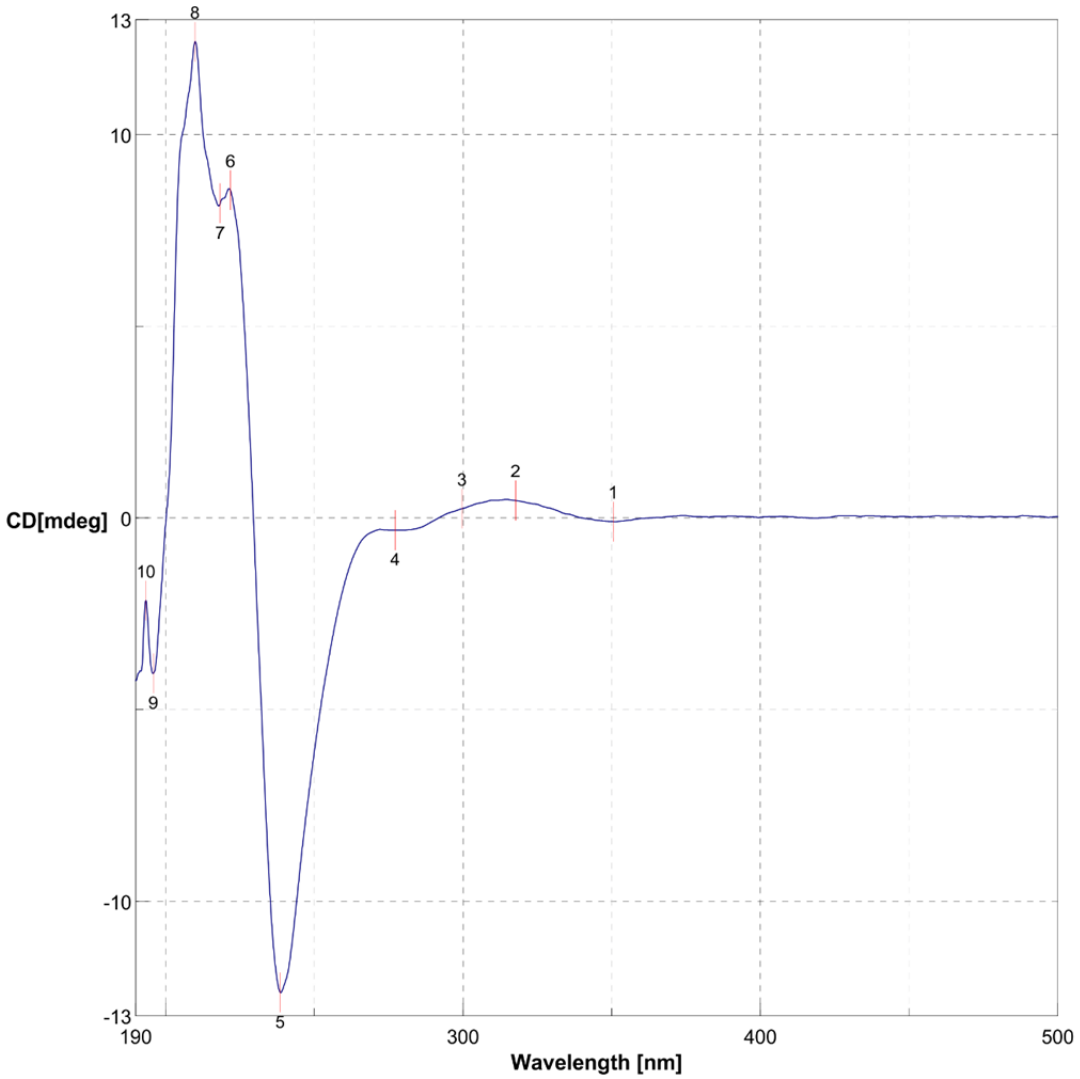


Figure S53. IR spectrum of ikelacongoline C (**6**).



No.	nm	Mol. CD	No.	nm		Mol. CD	No.	nm	Mol. CD
1	350.6	-0.0933689	2	317.7	5	0.45587	3	299.7	0.24543
4	277.2	-0.317781	5	238.6		-12.3836	6	221.8	8.55817
7	218.4	8.21624	8	209.9		12.4271	9	195.9	-4.05193
10	193.4	-2.15666							

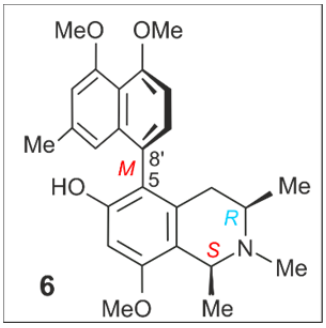
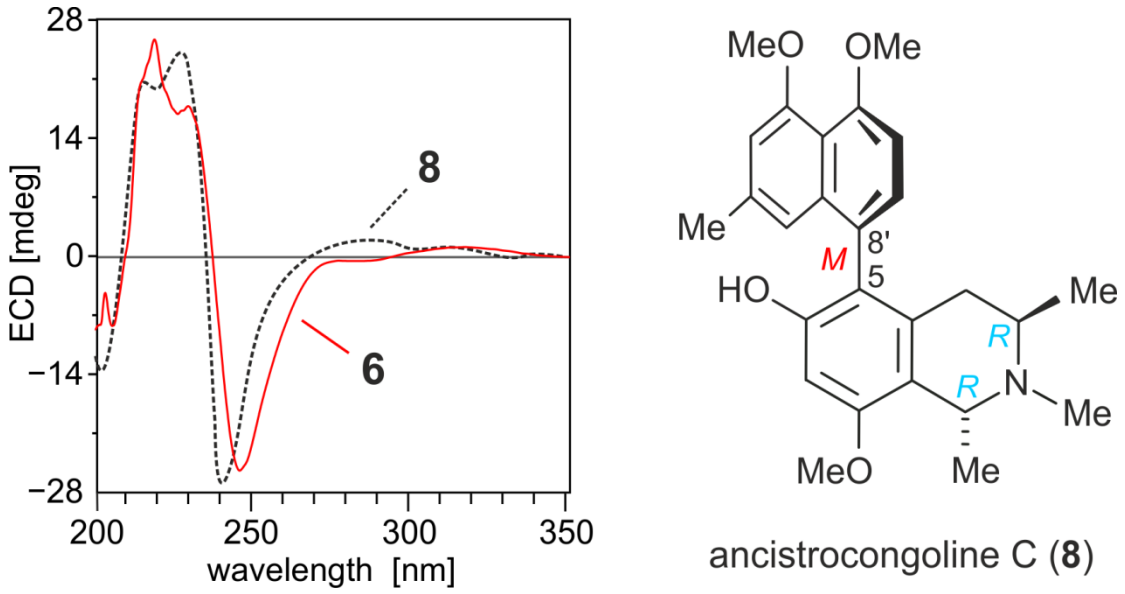
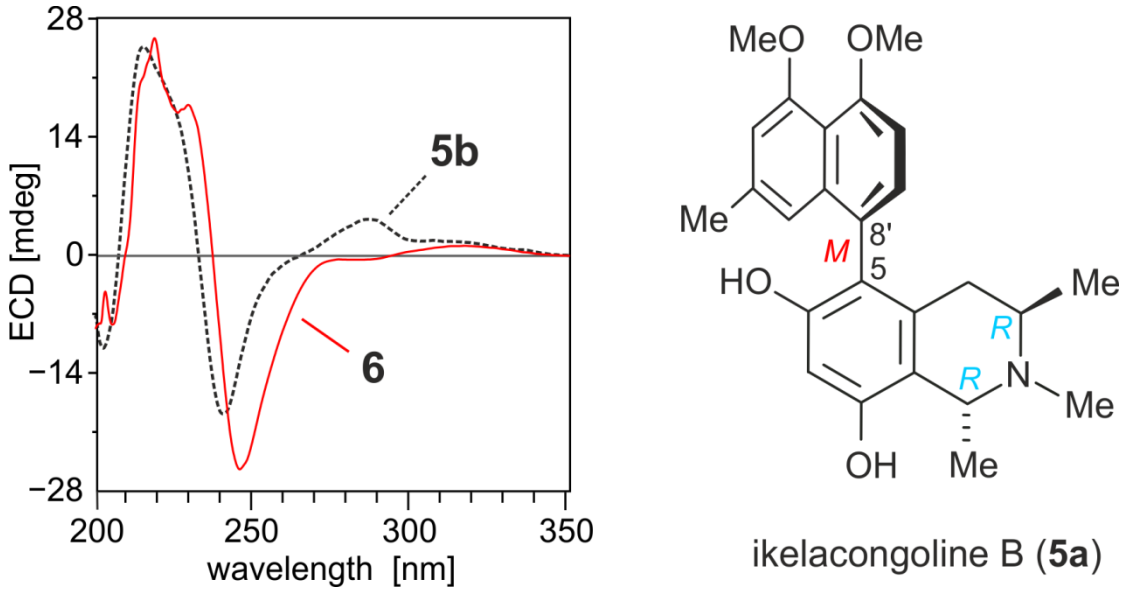


Figure S54a. ECD spectrum of ikelacongoline C (**6**).



S54b. Comparison of the ECD spectrum of ikelacongoline C (**6**) with that of the structurally related and likewise *M*-configured 5,8'-coupled alkaloid ancistrocongoline C (**8**).



S54c. Comparison of the ECD spectrum of ikelacongoline C (**6**) with that of the structurally related and likewise *M*-configured 5,8'-coupled alkaloid ikelacongoline B (**5b**).

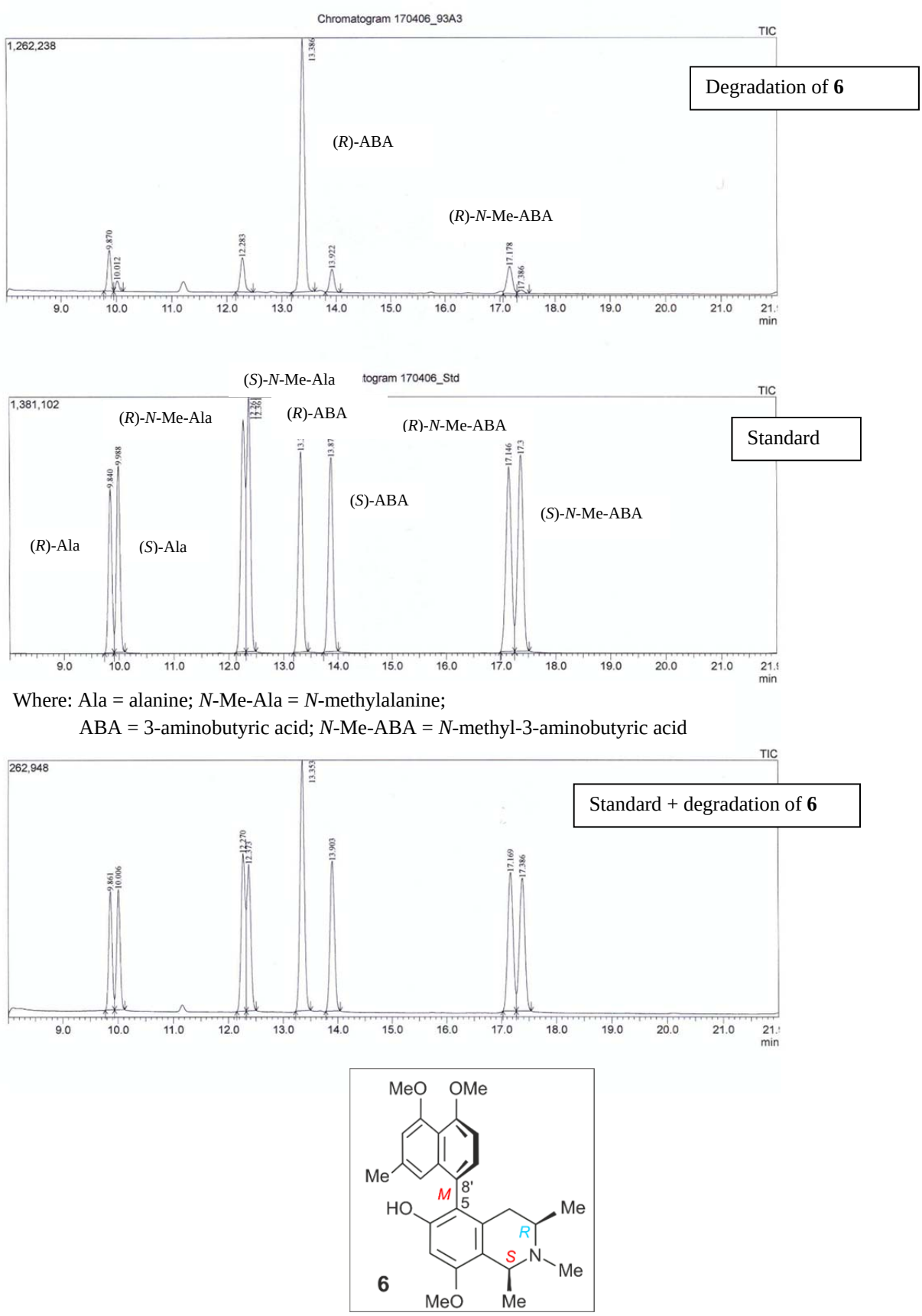


Figure S55: Oxidative degradation products of ikelacongoline C (**6**).

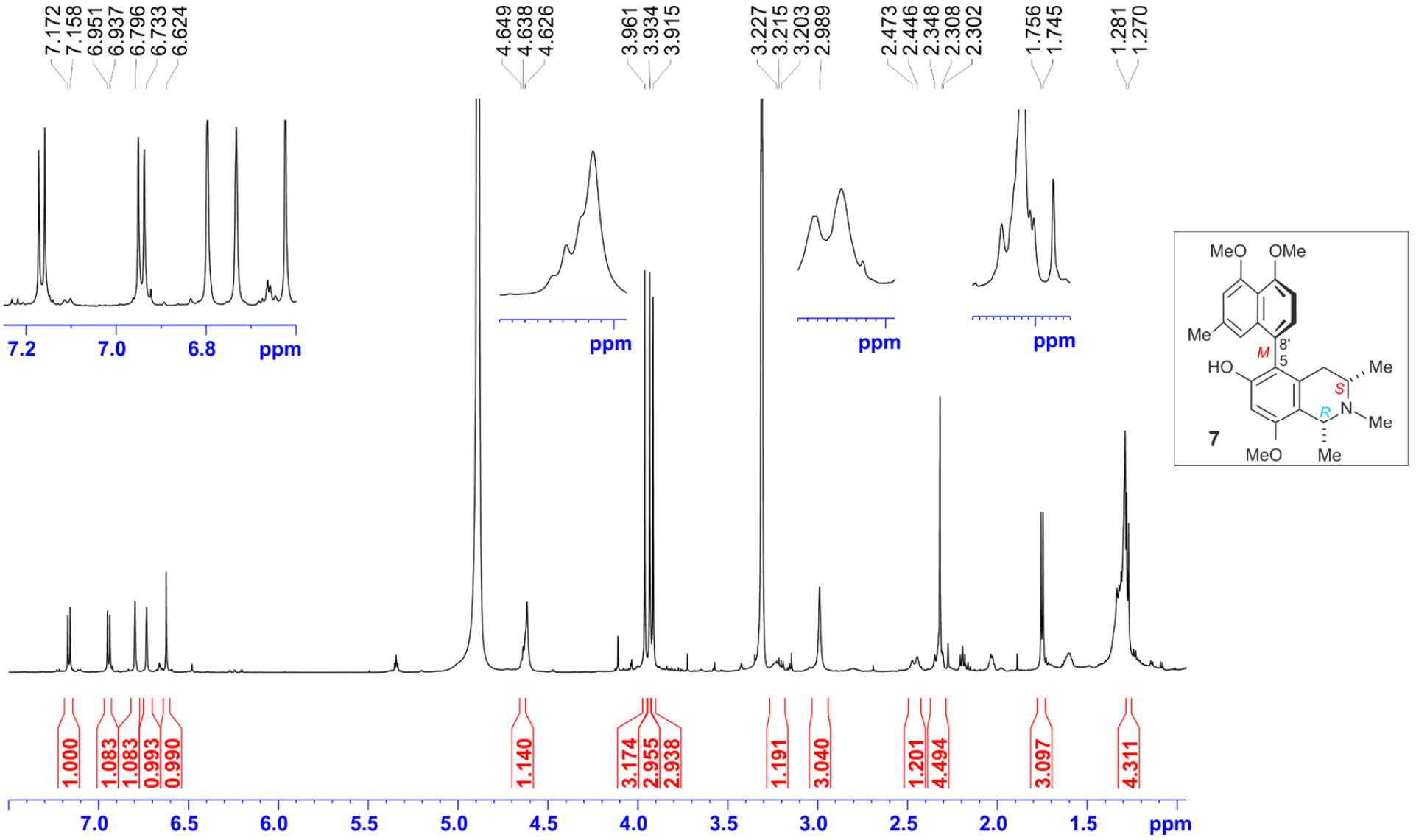


Figure S56. ^{1}H NMR spectrum of ikelacongoline D (**7**).

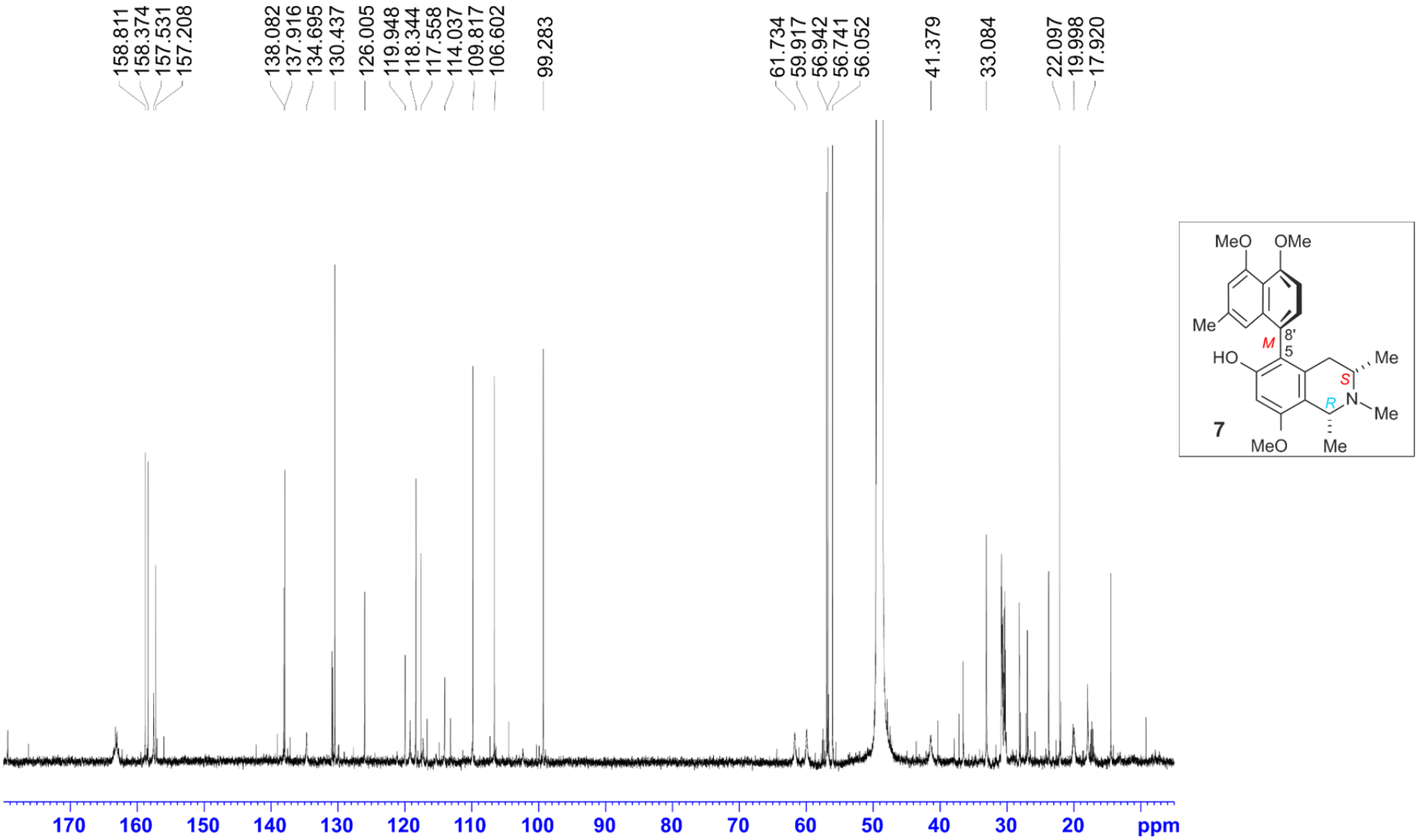
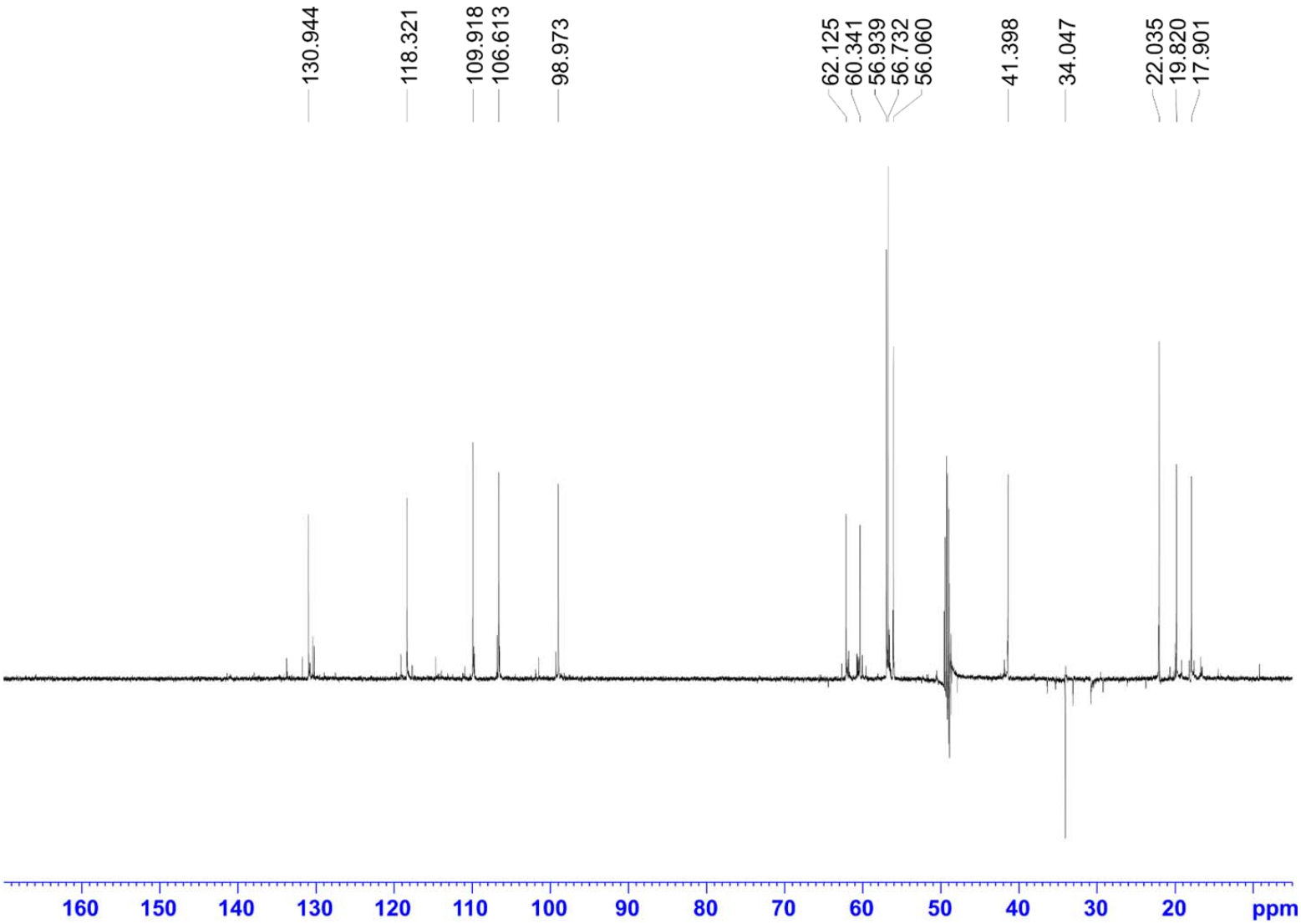


Figure S57. ^{13}C NMR spectrum of ikelacongoline D (**7**).



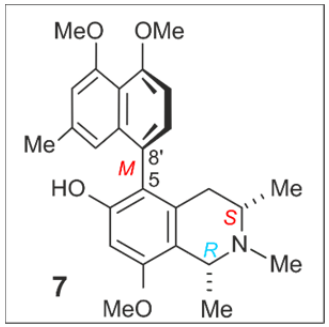
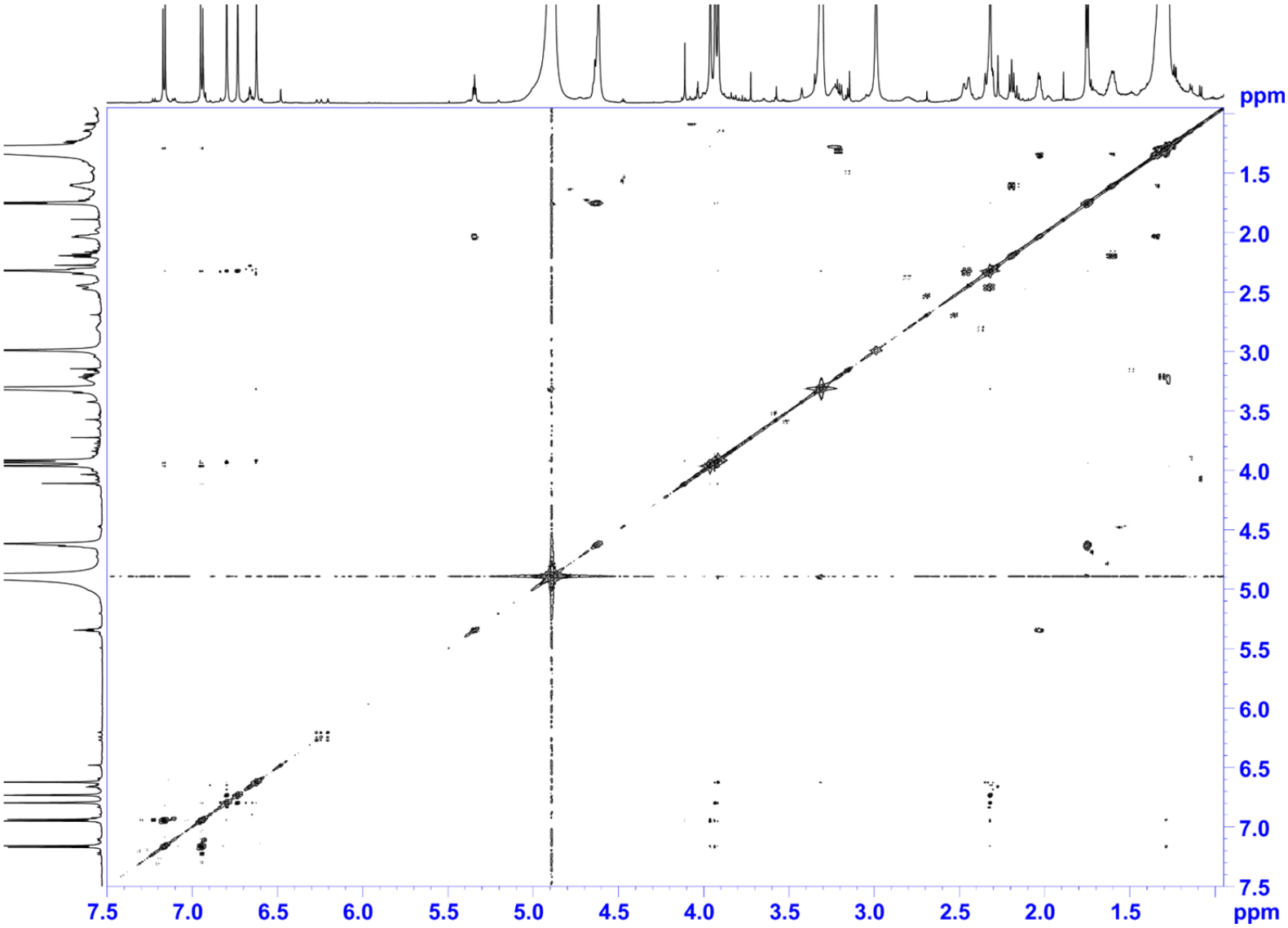


Figure S58. ^{13}C DEPT 135 NMR spectrum of ikelacongoline D (**7**).



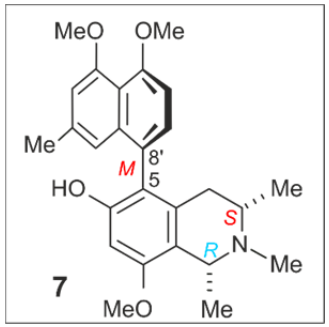
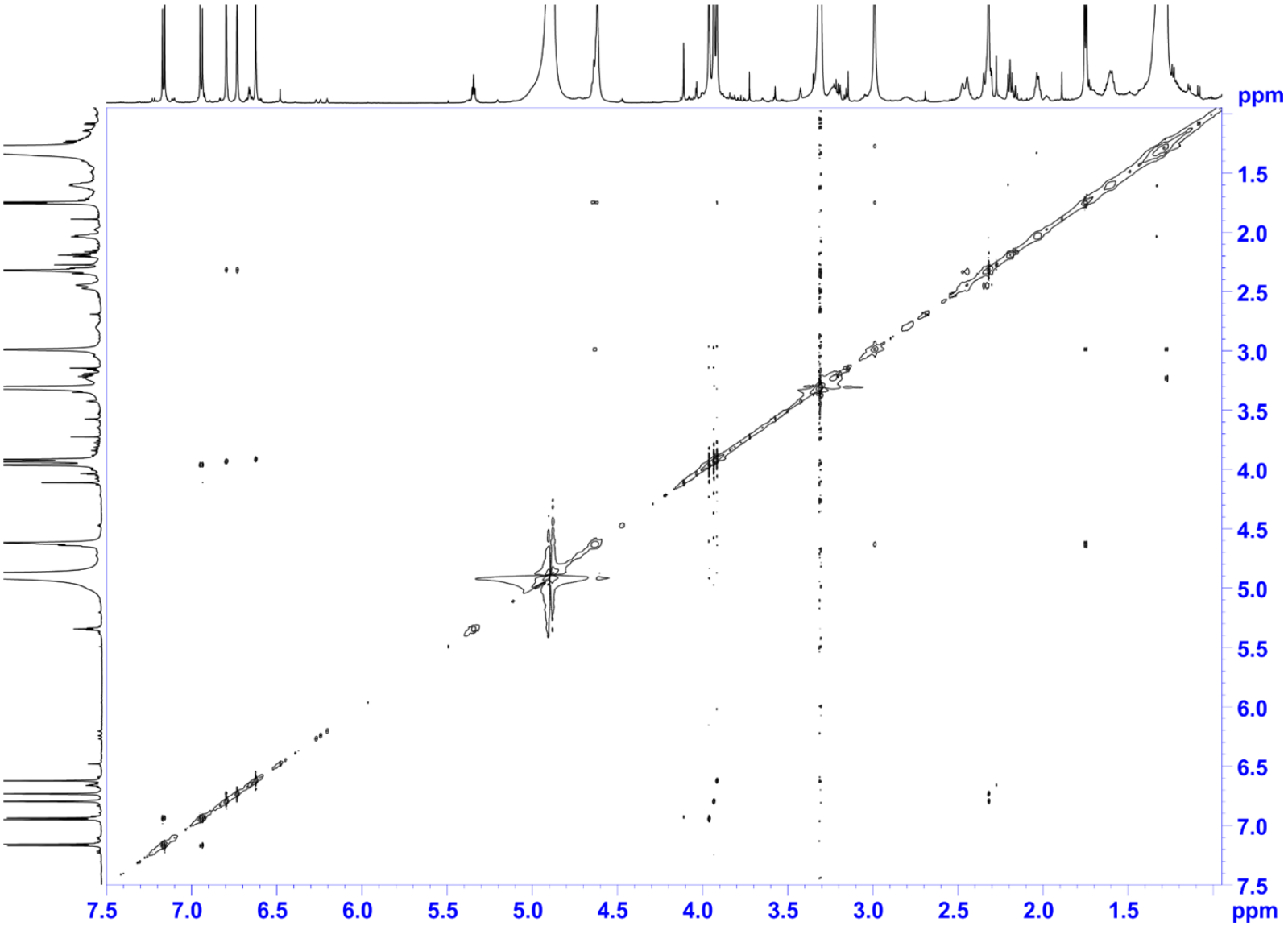


Figure S59. ^{1}H-^{1}H COSY spectrum of ikelacongoline D (**7**).



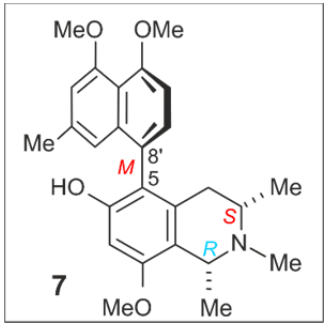
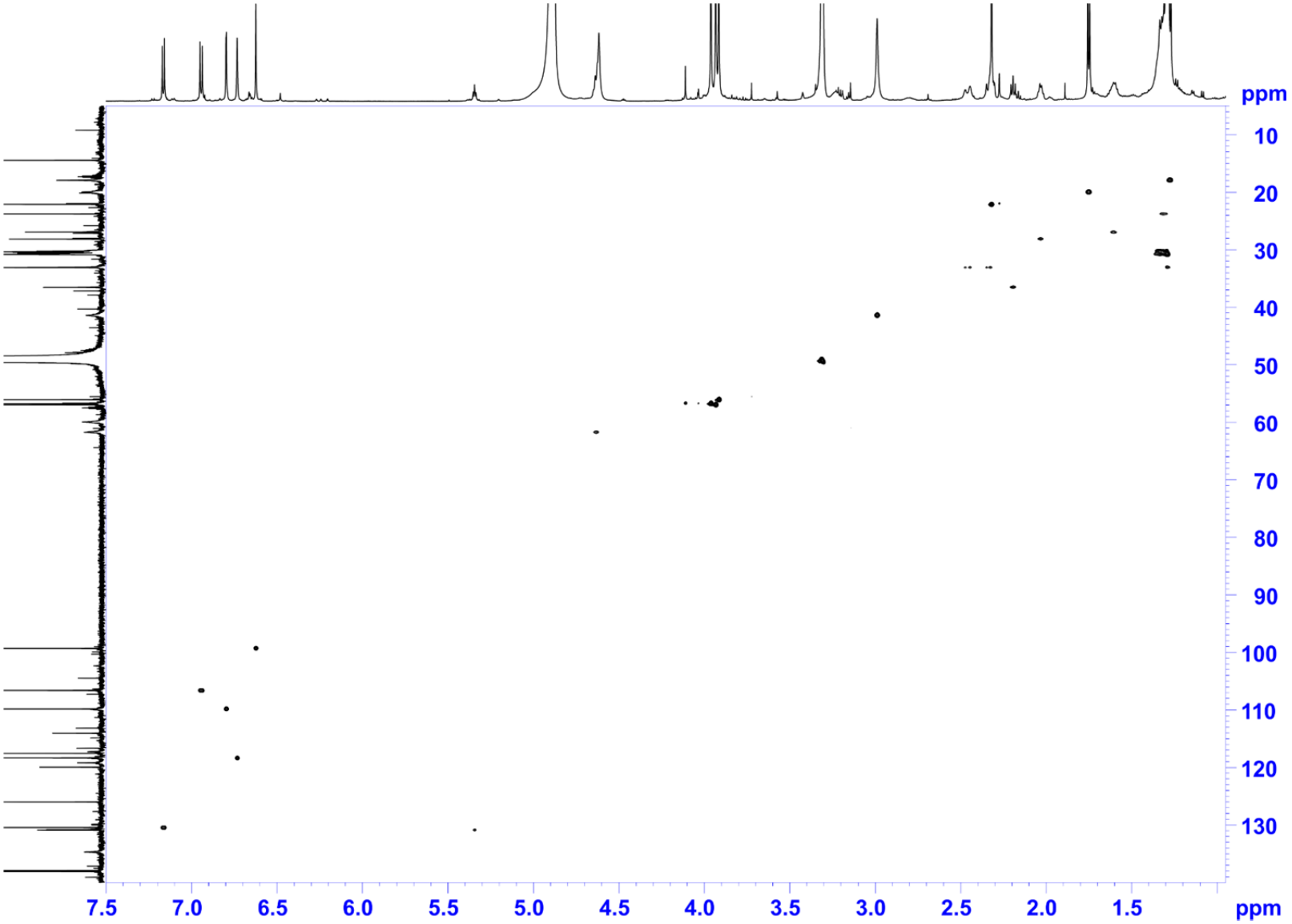


Figure S60. ^{1}H-^{1}H NOESY spectrum of ikelacongoline D (**7**).



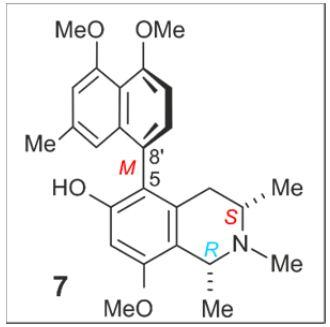
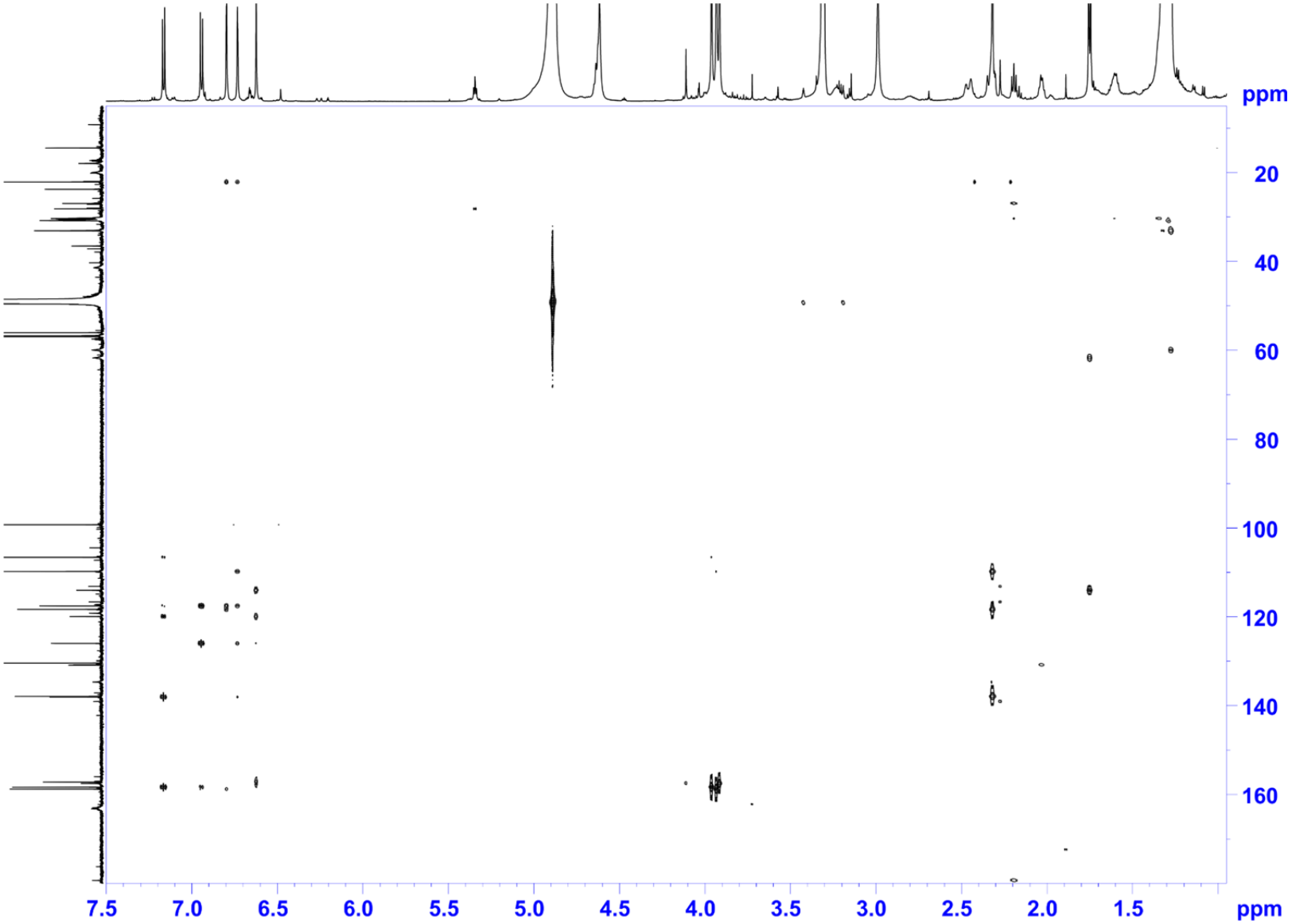


Figure S61. ^{1}H-^{13}C HSQC spectrum of ikelacongoline D (**7**).



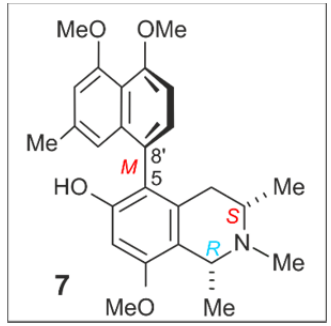


Figure S62. ^{1}H-^{13}C HMBC spectrum of ikelacongoline D (**7**).

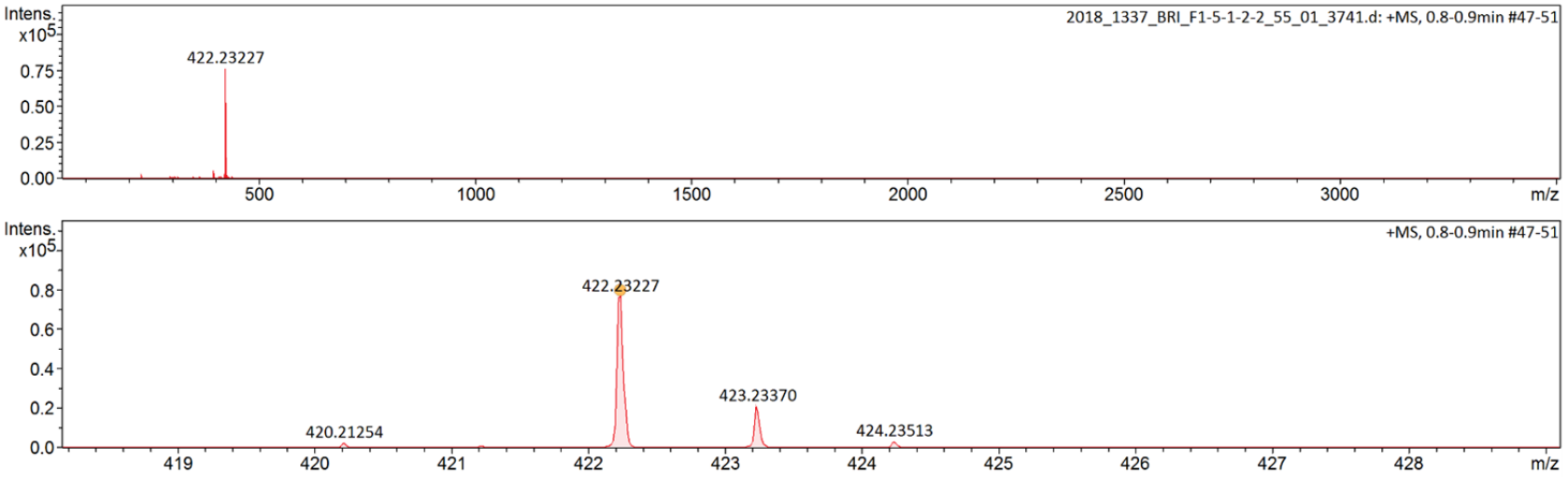
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Spektren2018\2018_1337_BRI_F1-5-1-2-2_55_01_3741.d	Acquisition Date	4/9/2018 2:06:28 PM
Method	automation_esi_tune_pos_low_ja_meoh.m	Operator	J.Adelmann
Sample Name	2018_1337_BRI_F1-5-1-2-2	Instrument	micrOTOF-Q III 8228888.20516
Comment	Mufusama Jean-Pierre F1-5-1-2-2 4 pmol/uL in MeOH		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Not active	Set Funnel 1 RF	100.0 Vpp	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Funnel 2 RF	200.0 Vpp	Set Dry Gas	5.0 l/min
Scan End	3500 m/z	Set Hexapole RF	300.0 Vpp	Set Divert Valve	Source



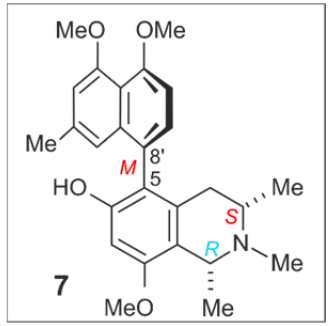
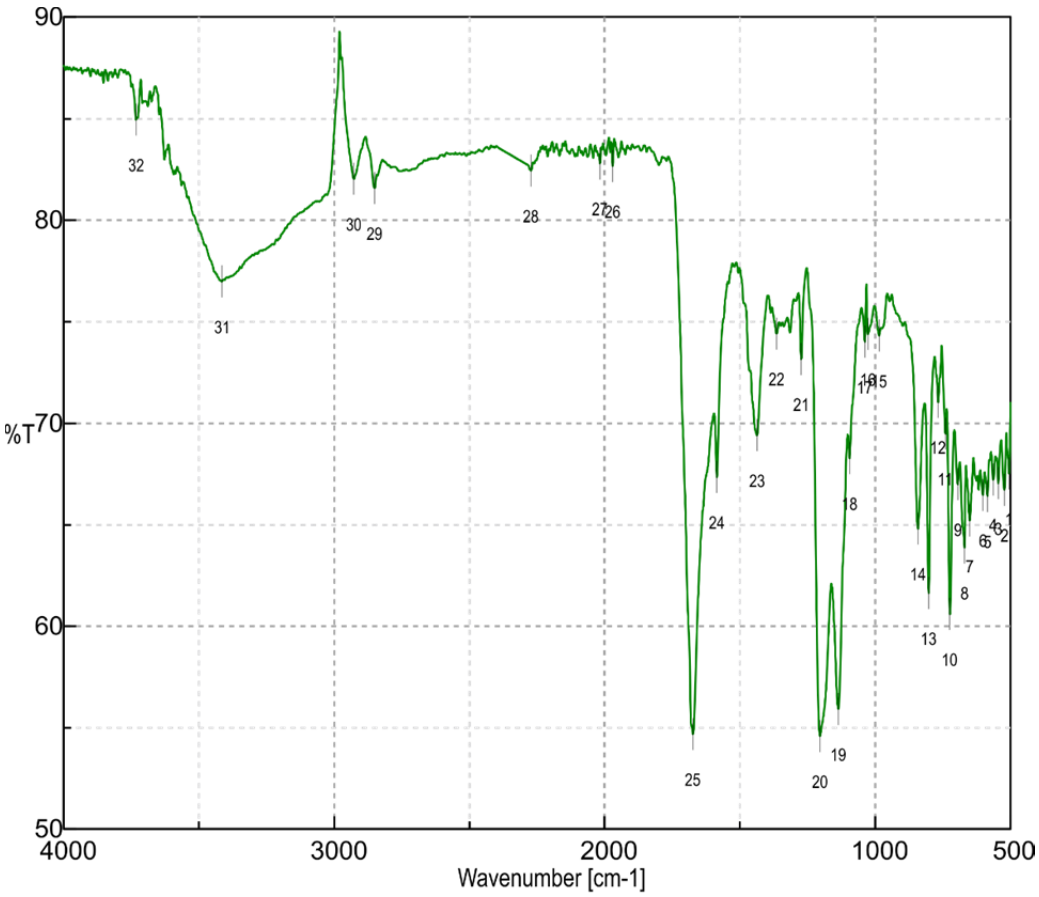


Figure S63. HRESIMS spectrum of ikelacongoline D (**7**).



Results of Peak Find

No.	Position	Intensity	No.	Position	Intensity
1	505.258	67.5079	2	523.579	66.7024
3	544.792	67.0419	4	564.077	67.22
5	585.29	66.401	6	602.646	66.4568
7	650.858	65.1923	8	670.142	63.8637
9	695.212	66.9876	10	724.139	60.5846
11	740.531	69.4776	12	767.53	71.0225
13	802.242	61.6352	14	841.776	64.8049
15	985.447	74.3105	16	1026.91	74.3752
17	1038.48	74.0103	18	1095.37	68.275
19	1136.83	55.9241	20	1204.33	54.579
21	1273.75	73.1355	22	1365.35	74.3948
23	1436.71	69.3872	24	1585.2	67.323
25	1673.91	54.68	26	1969.93	82.6605
27	2017.18	82.7754	28	2272.7	82.4303
29	2851.24	81.5686	30	2927.41	82.0204
31	3415.31	76.9678	32	3732.55	84.9425

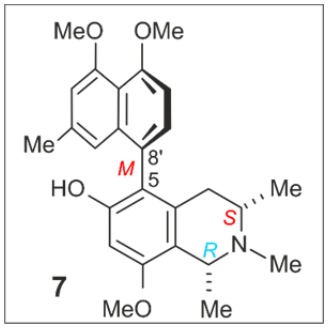
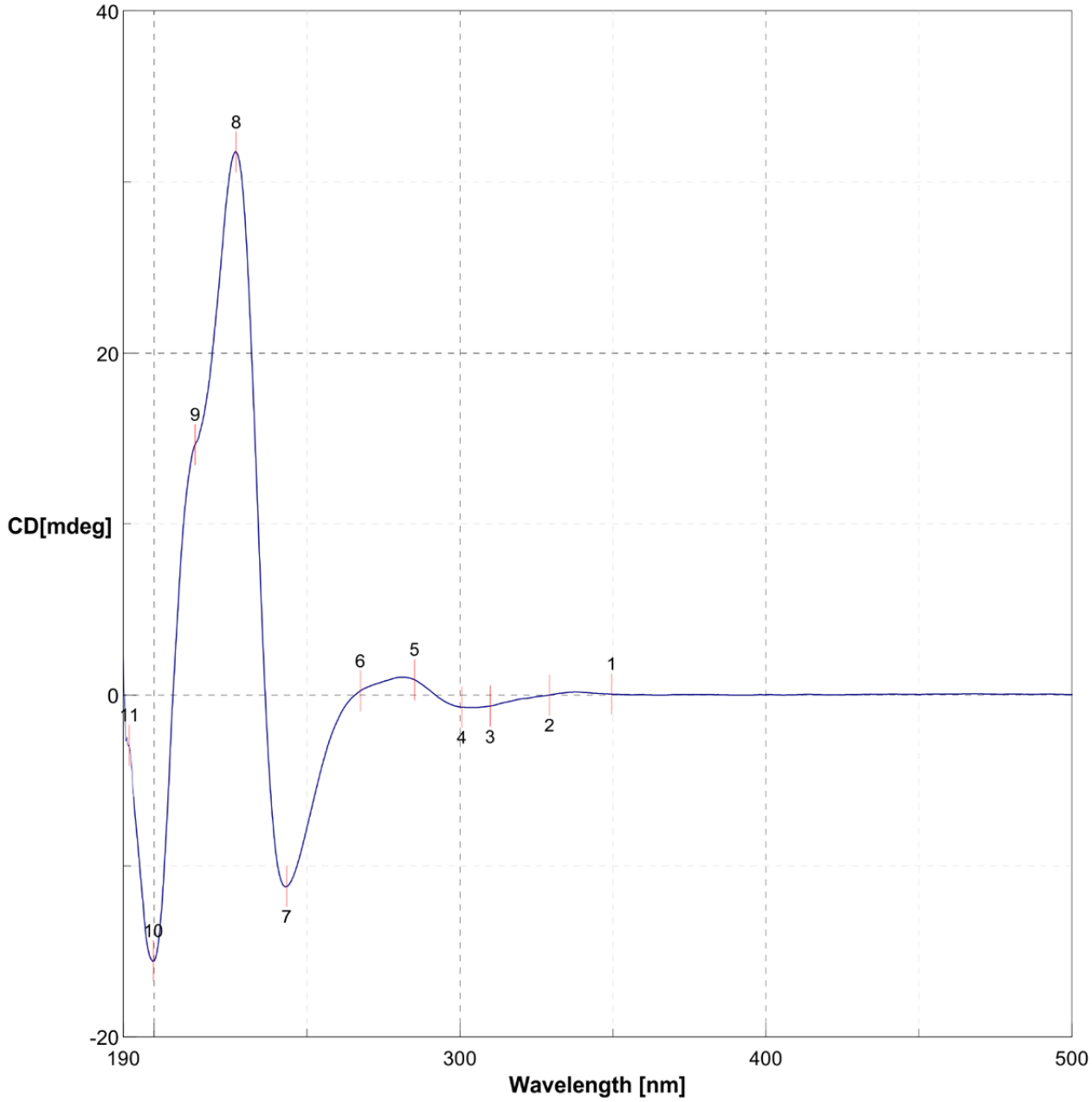


Figure S64. IR spectrum of ikelacongoline D (**7**).



No.	nm	Mol. CD	No.	nm		Mol. CD	No.	nm	Mol. CD
1	349.6	0.0547381	2	329.3	0334	0.00318183	3	309.9	-0.64
4	300.6	-0.7044	5	285.2		0.894308	6	267.5	0.25068
7	243.4	-11.1948	8	226.9		31.7576	9	213.5	14.6553
10	199.9	-15.5336	11	192		-2.93846			

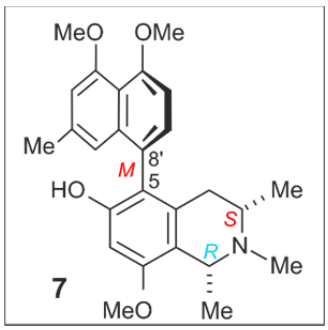
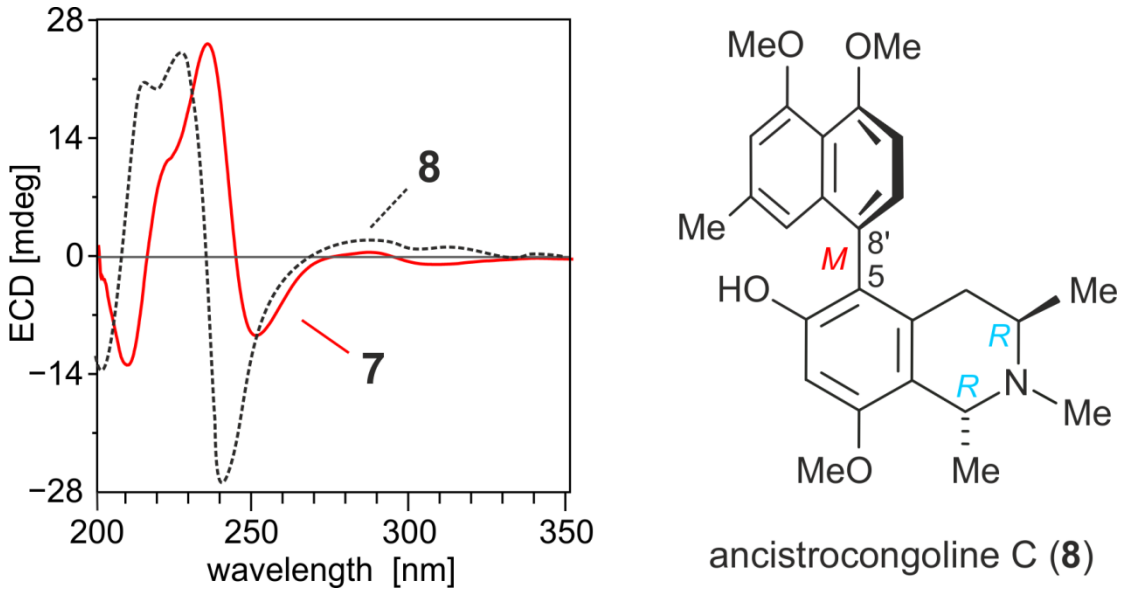
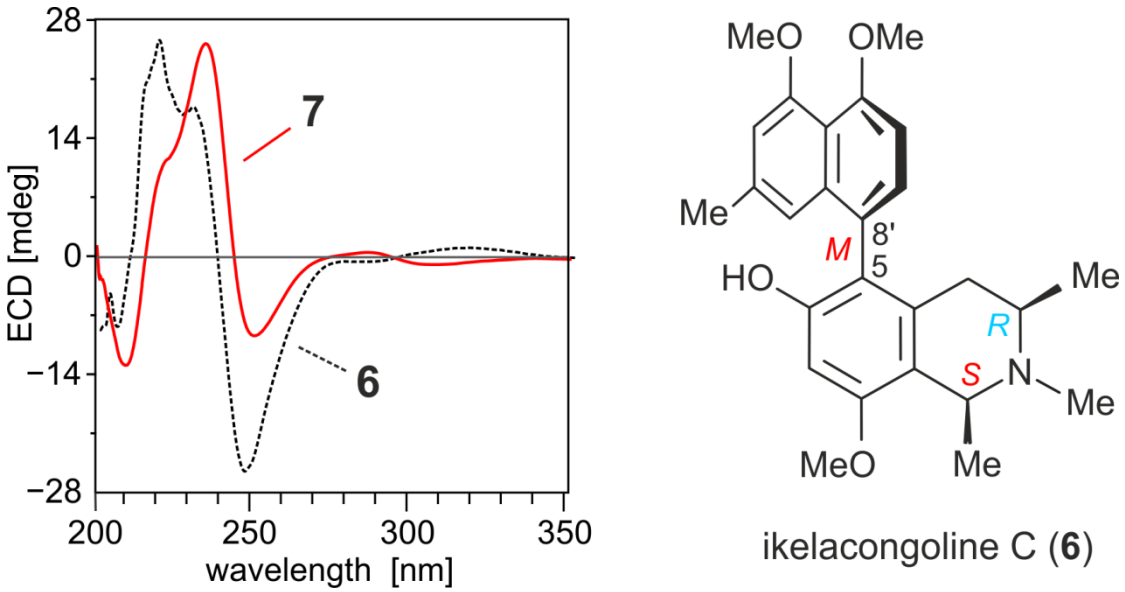


Figure S65a. ECD spectrum of ikelacongoline D (**7**)



S65b. Comparison of the ECD spectrum of ikelacongoline D (**7**) with that of the structurally related and likewise *M*-configured 5,8'-coupled alkaloid ancistrocongoline C (**8**).



S65c. Comparison of the ECD spectrum of ikelacongoline D (**7**) with that of the structurally related and likewise *M*-configured 5,8'-coupled alkaloid ikelacongoline C (**6**).

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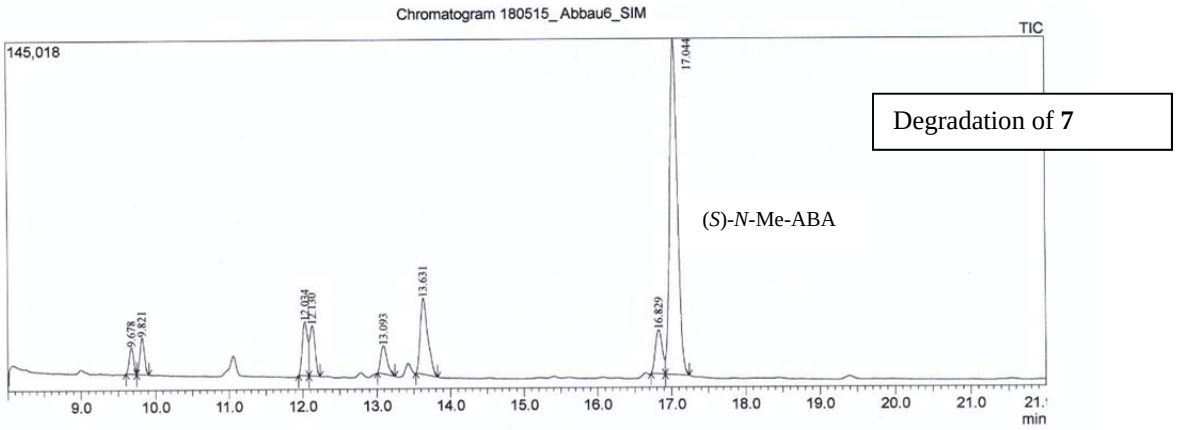
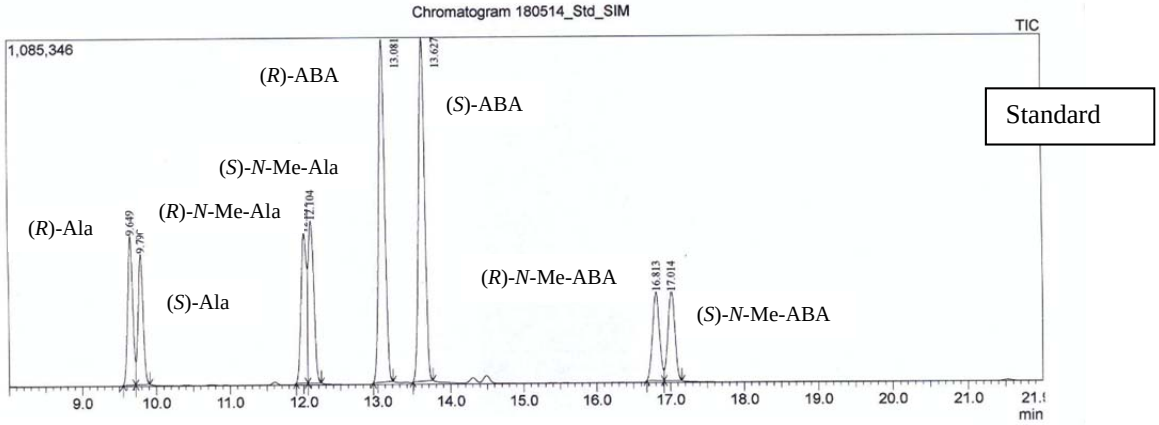
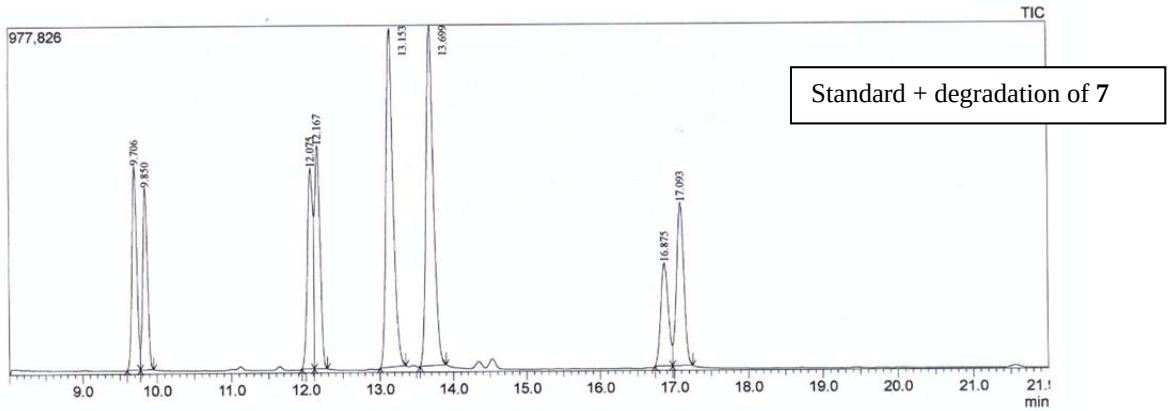




Where: Ala = alanine; *N*-Me-Ala = *N*-methylalanine;
ABA = 3-aminobutyric acid; *N*-Me-ABA = *N*-methyl-3-aminobutyric acid



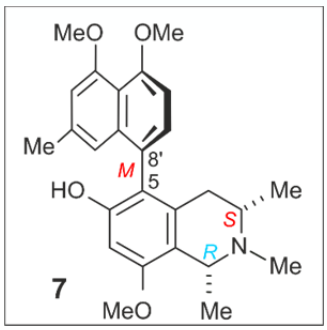


Figure S66. Oxidative degradation of ikelacongoline D (**7**).