Supporting Information

Corallorazines from the Myxobacterium *Corallococcus coralloides*

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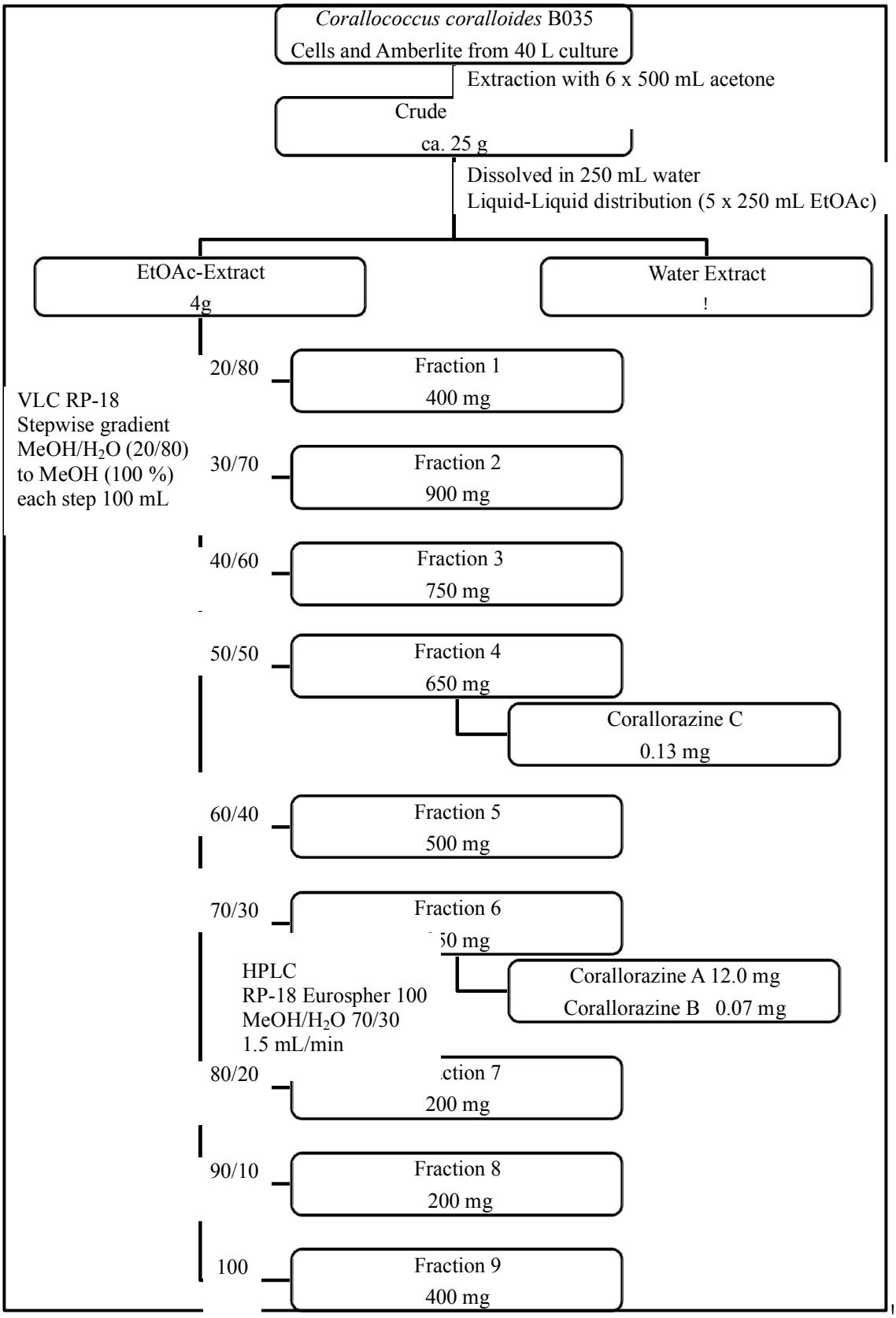

Figure S1. Extraction scheme for the corallorazines, exemplified for a 40 L culture.

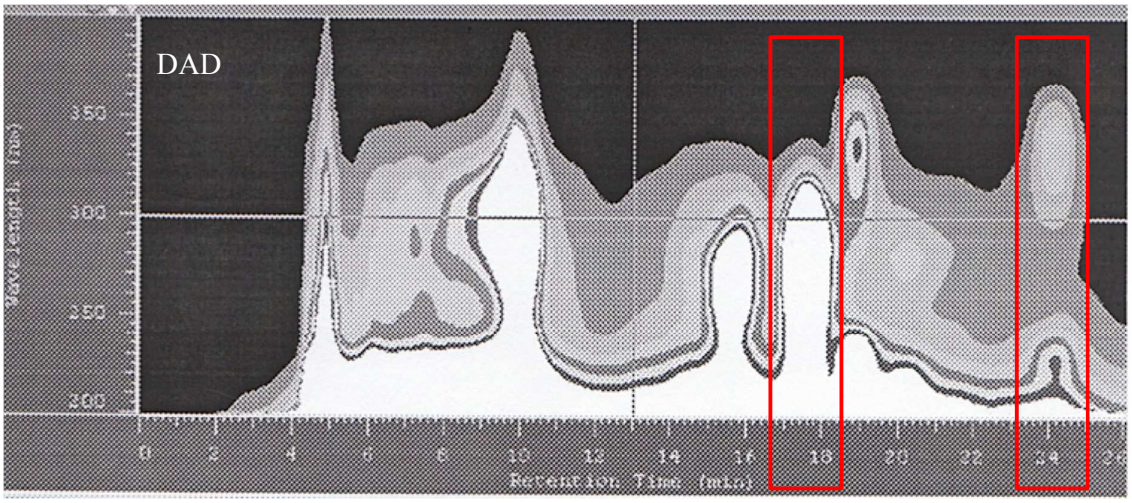

Figure S2. HPLC chromatogram of VLC fraction 6.

Merck HPLC system, Knauer Eurospher 100 RP_{18} semi-preparative column, MeOH/H_2O 70/30, 1.5 mL min^{-1}, DAD-Detection. R_t = 10 min: corallopyronin A, R_t = 17.5 min: corallorazine A (**1**), R_t = 24.5 min: corallorazine B (**2**).

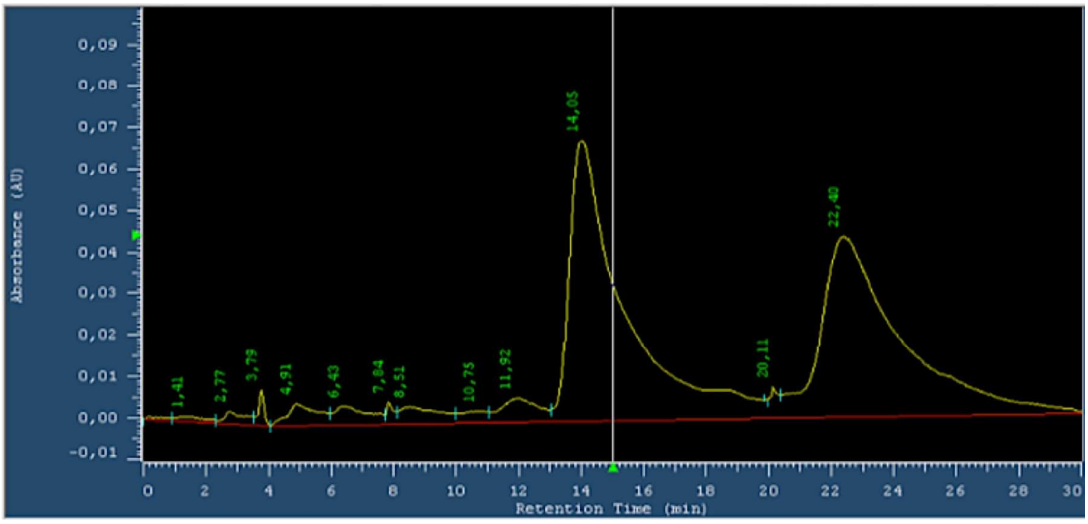

Figure S3. HPLC chromatogram of chiral separation of corallorazine A (**1**) enantiomers (Merck HPLC system, Phenomenex Cellulose 3 column, hexane/isopropanol 90/10, 1.0 mL min^{-1}, UV-Detection (λ_{max} = 275 nm)). R_{t1} = 14.05 min:, R_{t2} = 22.40 min.

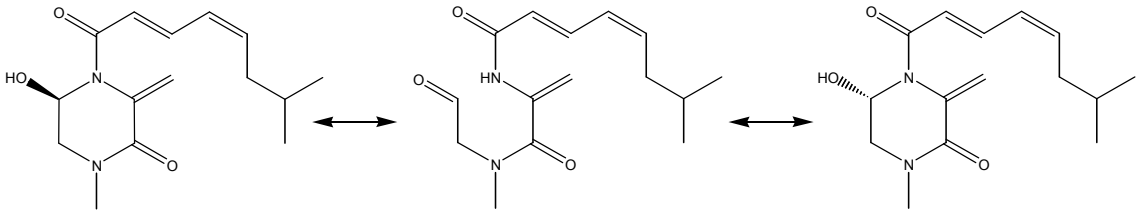

Figure S4. Interconversion of corallorazine A (**1**) enantiomers.

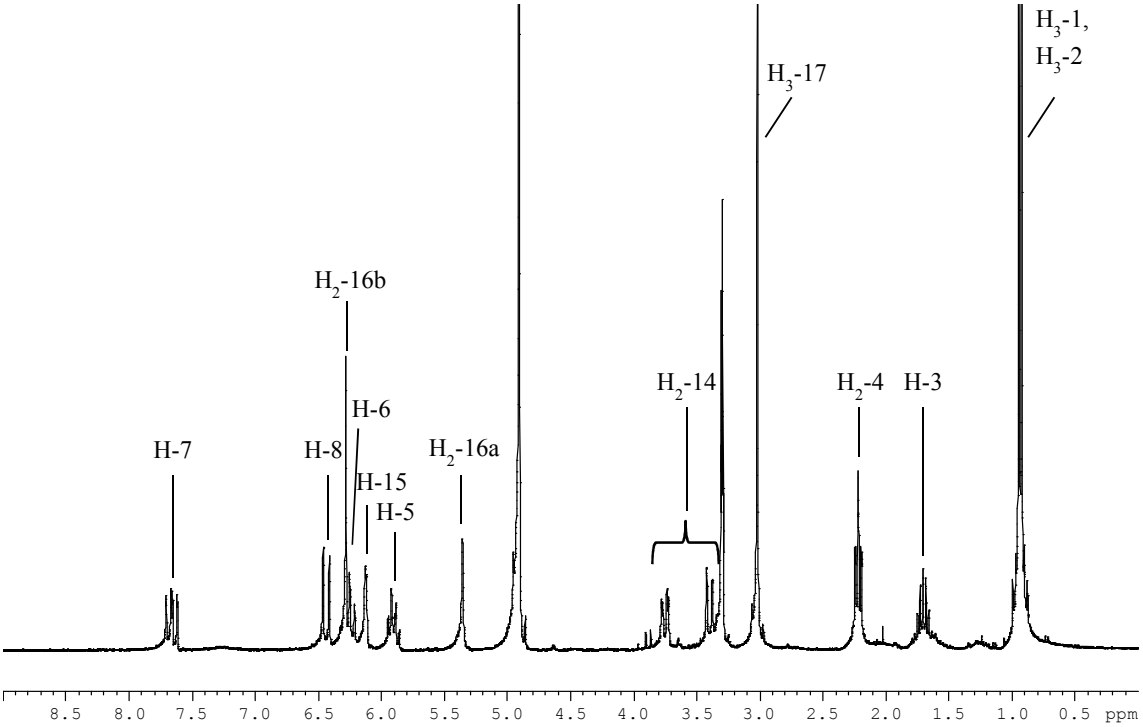

Figure S5. ^{1}H NMR spectrum of corallorazine A (**1**) in MeOH-d_4, 300 MHz.

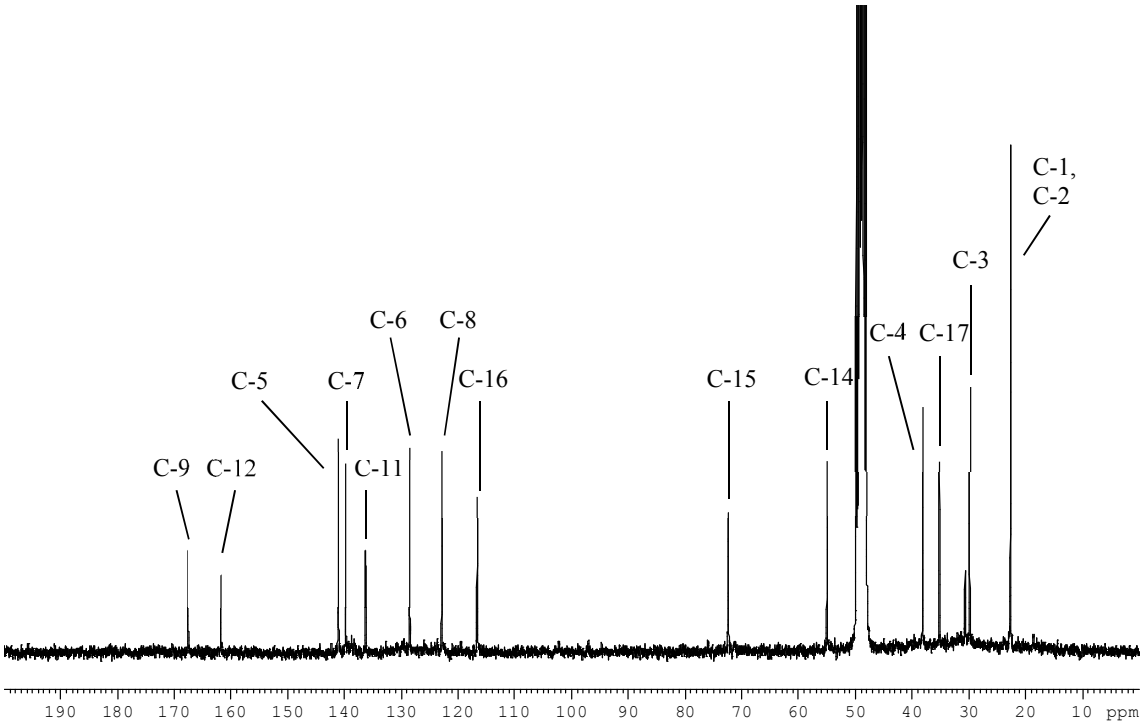

Figure S6. ^{13}C NMR spectrum corallorazine A in MeOH-d_4, 75 MHz.

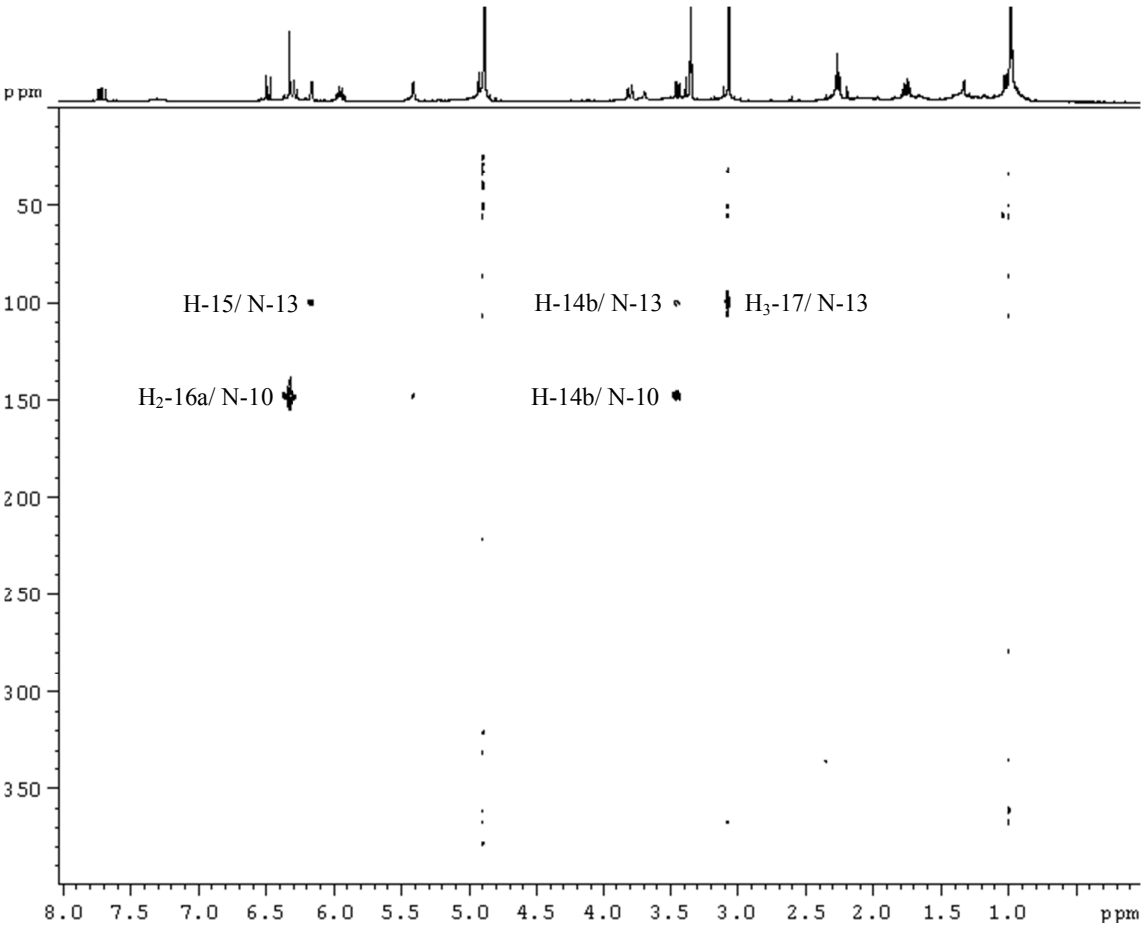

Figure S7. ^{1}H-^{15}N HMBC spectrum corallorazine A in MeOH-d_4, 500 MHz.

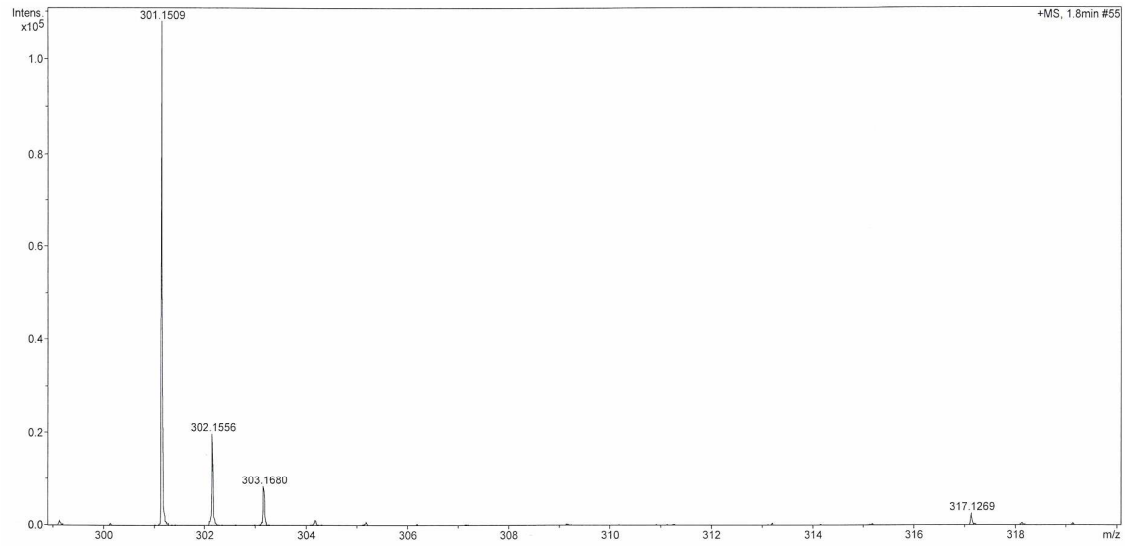

Figure S8. High resolution mass spectrum of corallorazine A.

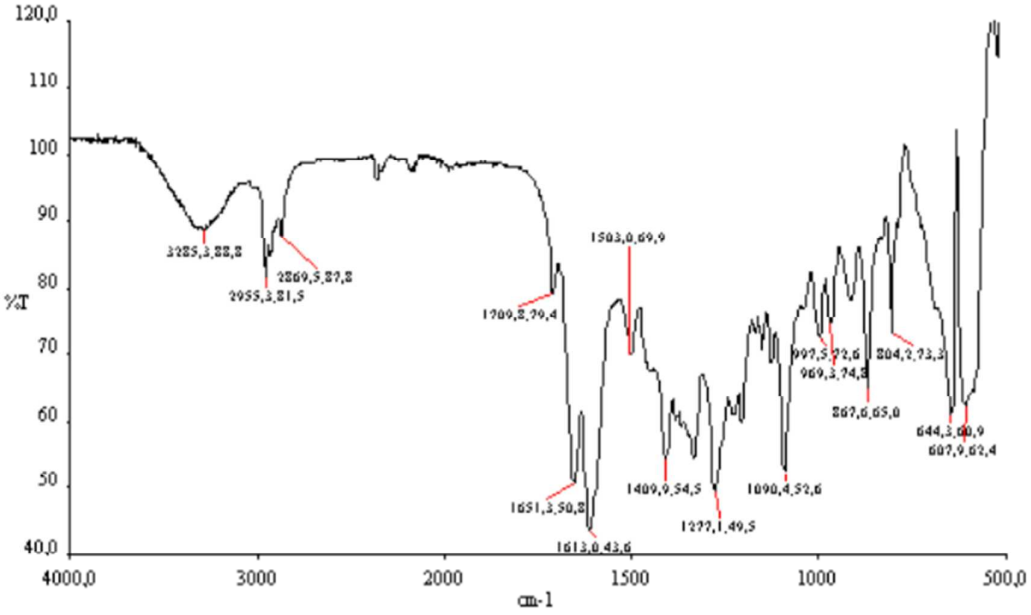

Figure S9. IR spectrum of corallorazine A.

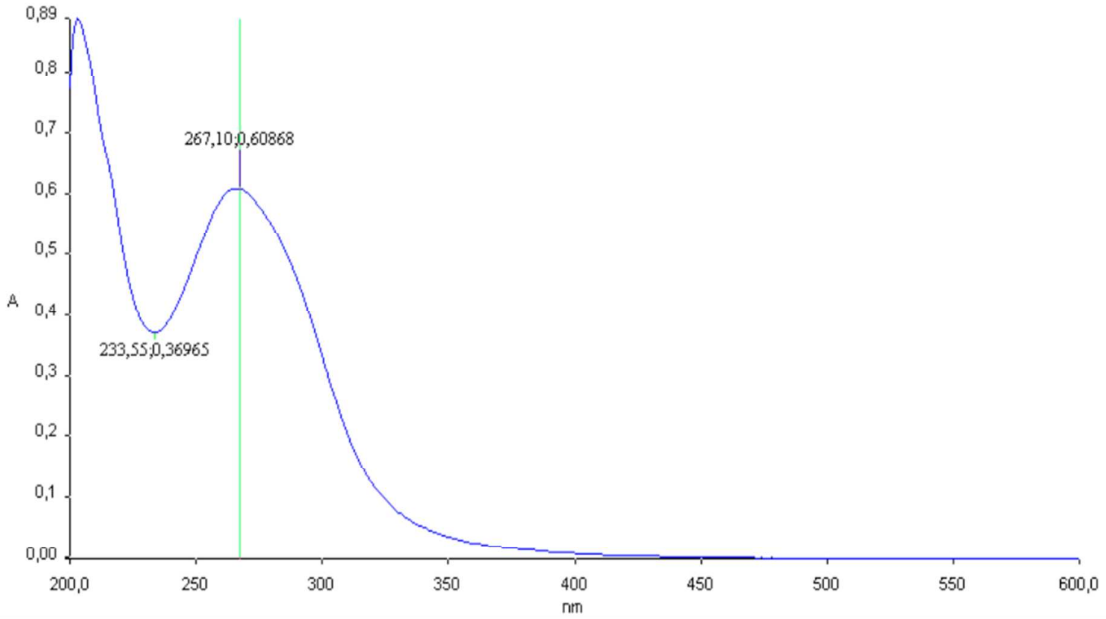

Figure S10. UV spectrum of corallorazine A (MeOH).

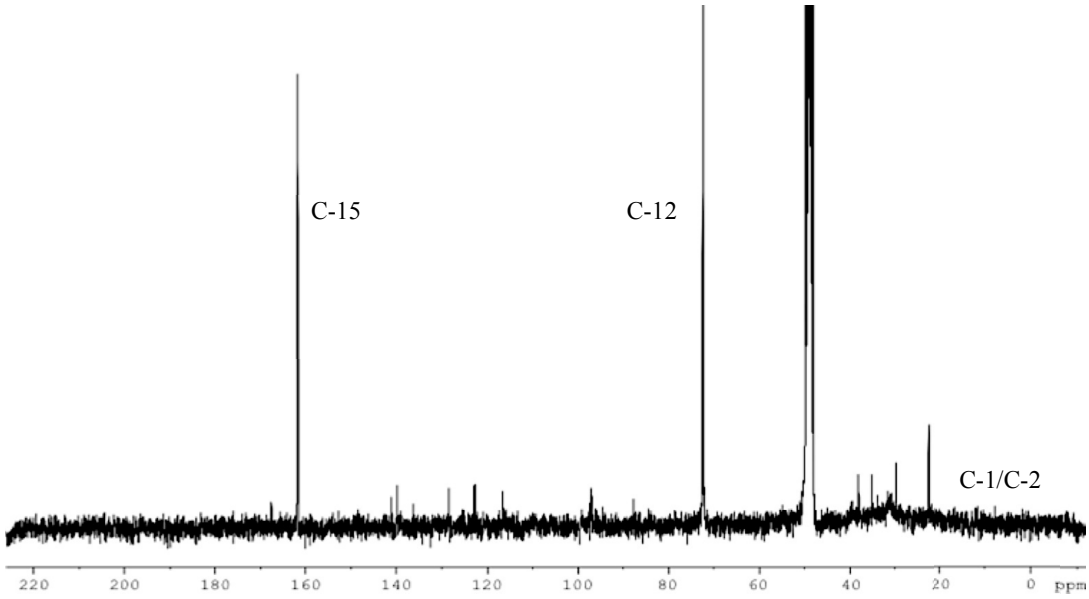

Figure S11. Result of the feeding experiment with 1-^{13}C labeled glycine, ^{13}C NMR spectrum of corallorazine A in MeOH-d_4 (75 MHz).

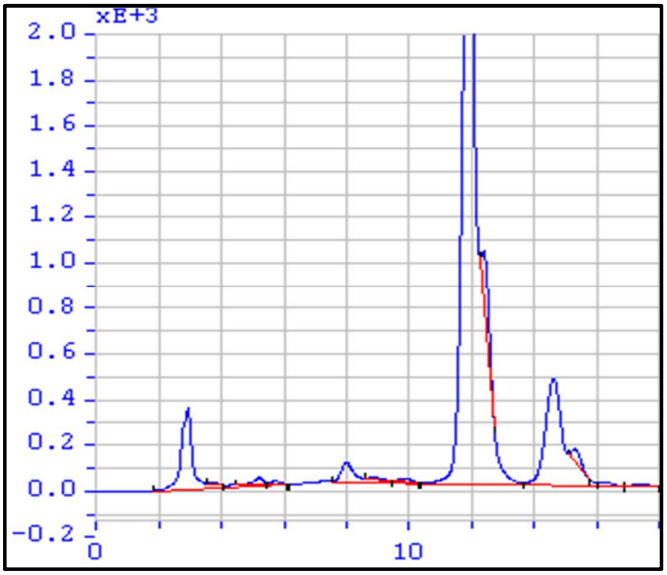

Figure S12. HPLC chromatogram of iso-octa-dienoic acid (**4**) containing extract (VLC fraction 6 of fermenter experiment) (Merck HPLC system, Waters Xterra RP_{18} analytical column (250 mm x 4.6 mm), MeOH/H_2O 48/52, 0.9 mL min^{-1}, UV-Detection (280 nm). R_t = 11 min: iso-octa-dienoic acid.

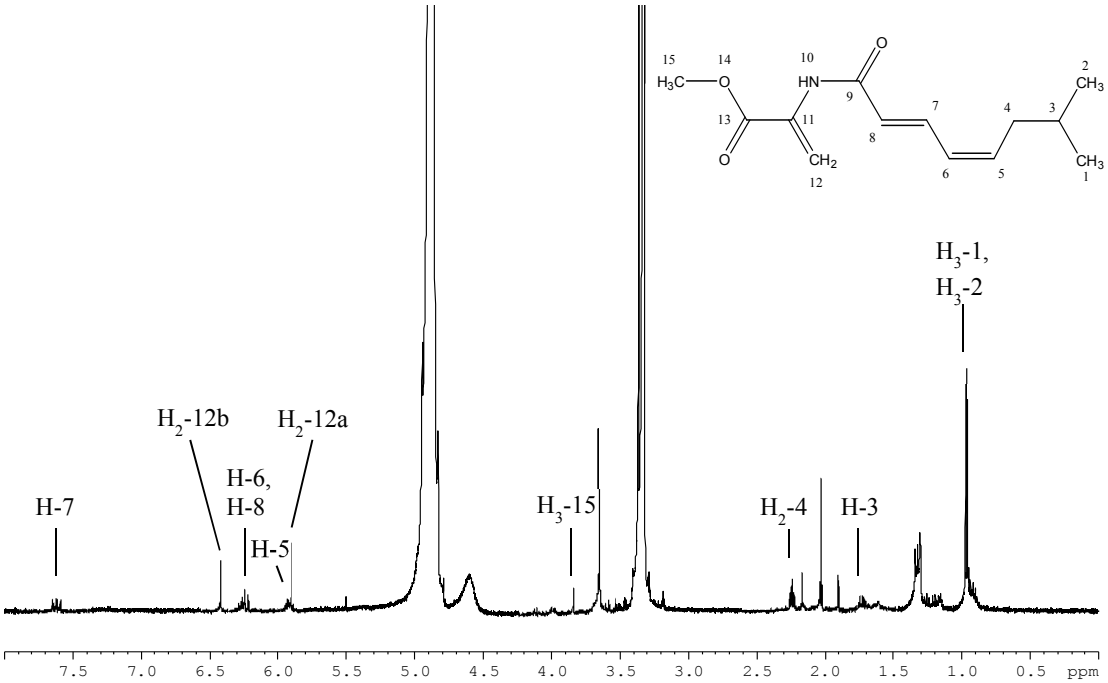

Figure S13. ^{1}H NMR spectrum of corallorazine B (**2**) in MeOH-d_4, 300 MHz.

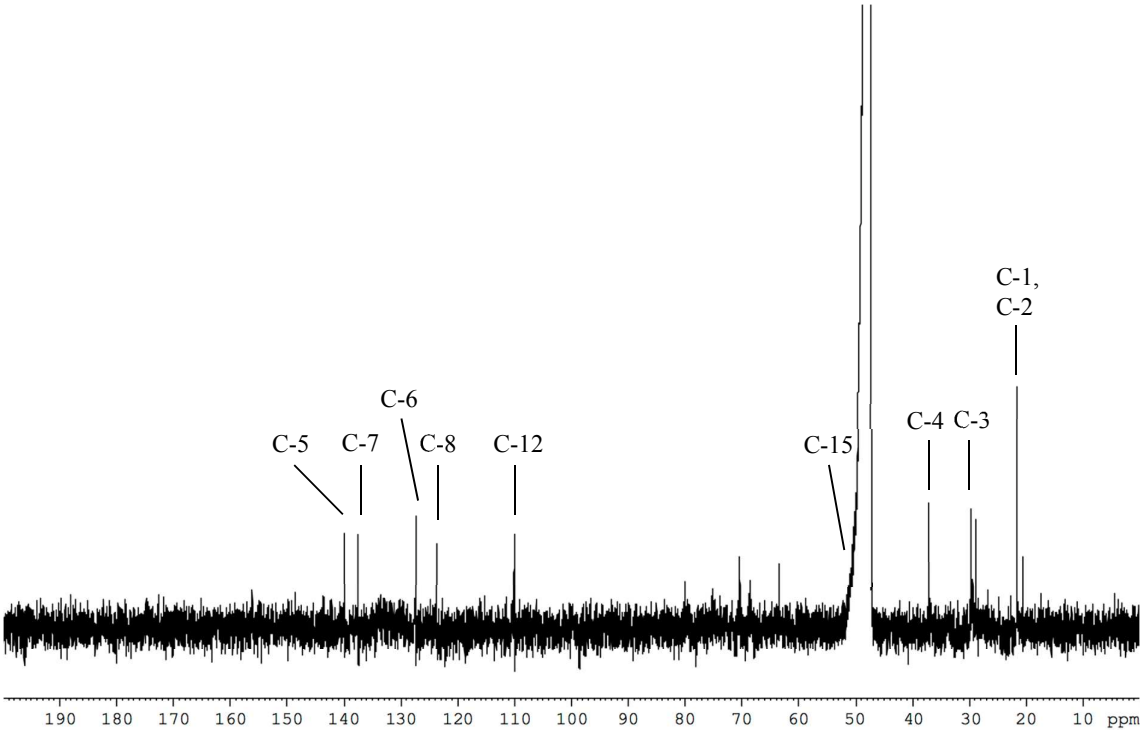

Figure S14. ^{13}C NMR spectrum corallorazine B in MeOH-d_4, 75 MHz.

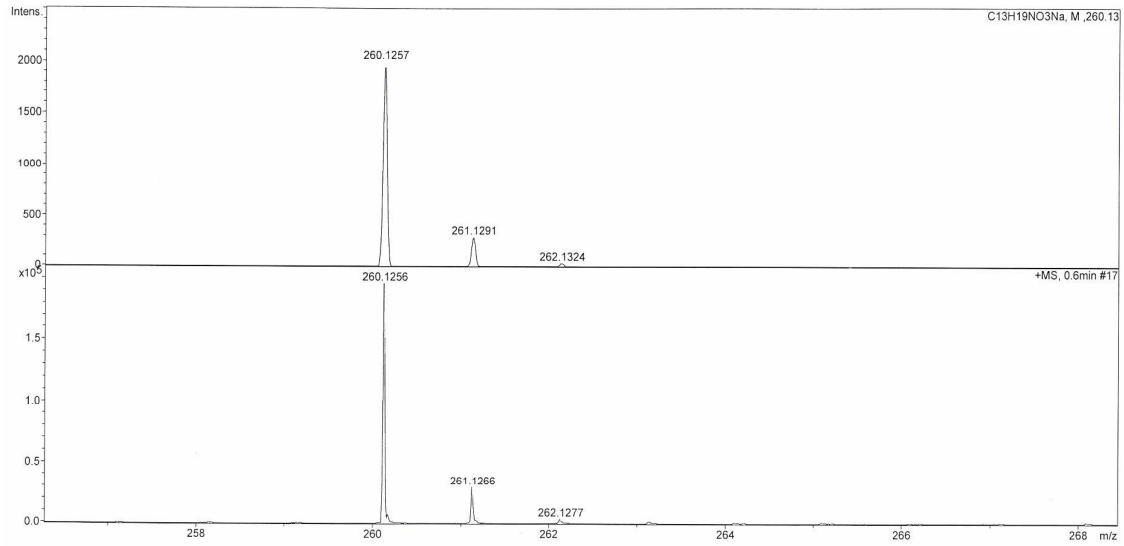

Figure S15. High resolution mass spectrum of corallorazine B.

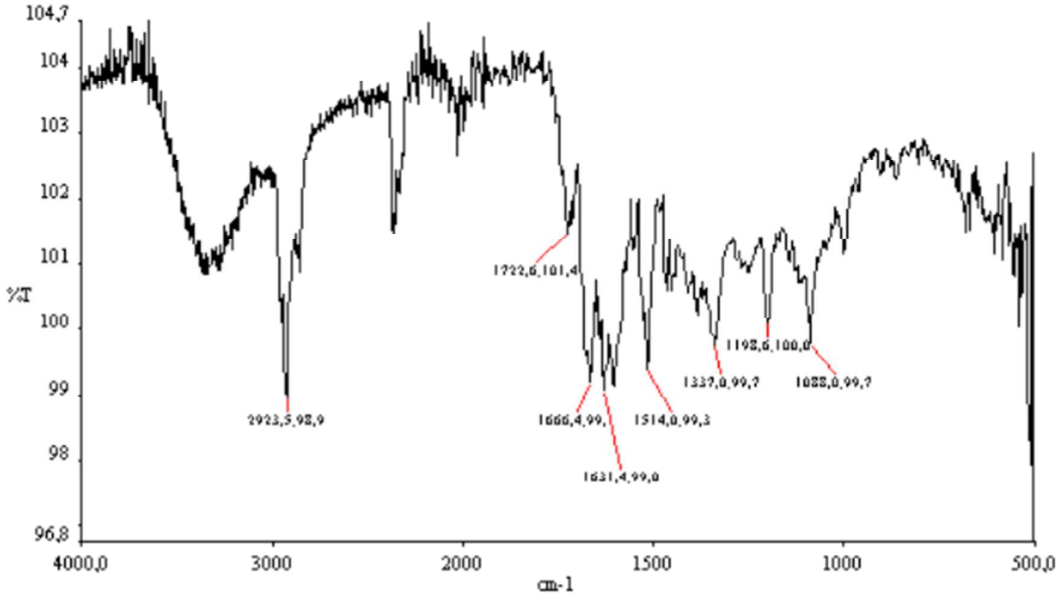

Figure S16. IR spectrum of corallorazine B.

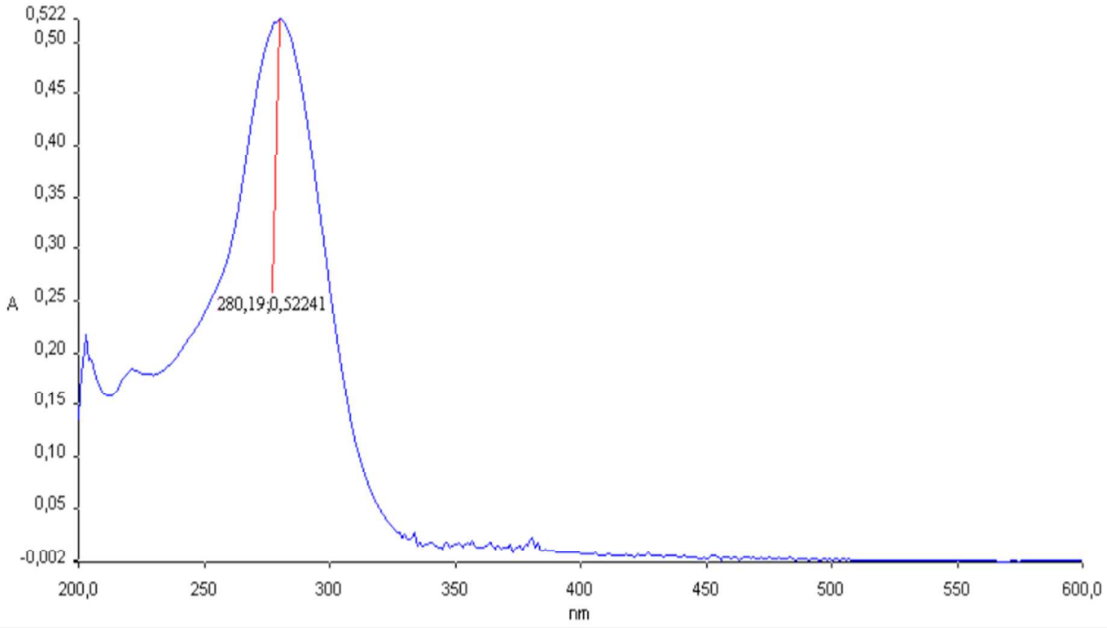

Figure S17. UV spectrum of corallorazine B (MeOH).

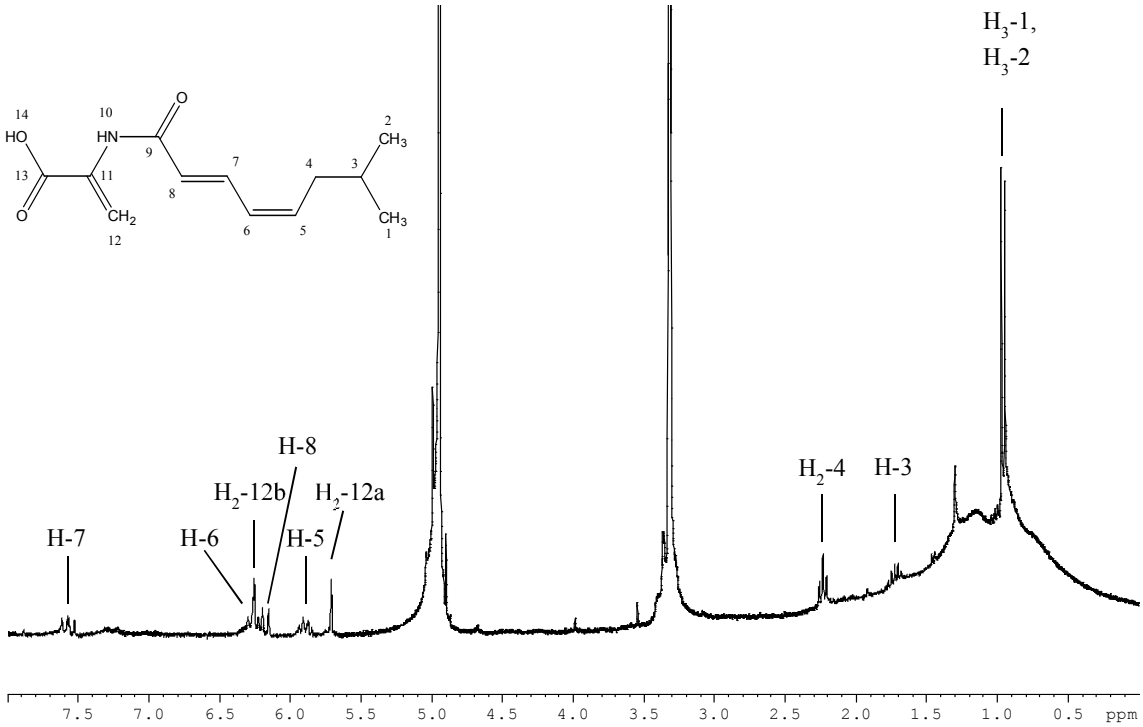

Figure S18. ^{1}H NMR spectrum of corallorazine C in MeOH-d_4, 300 MHz.

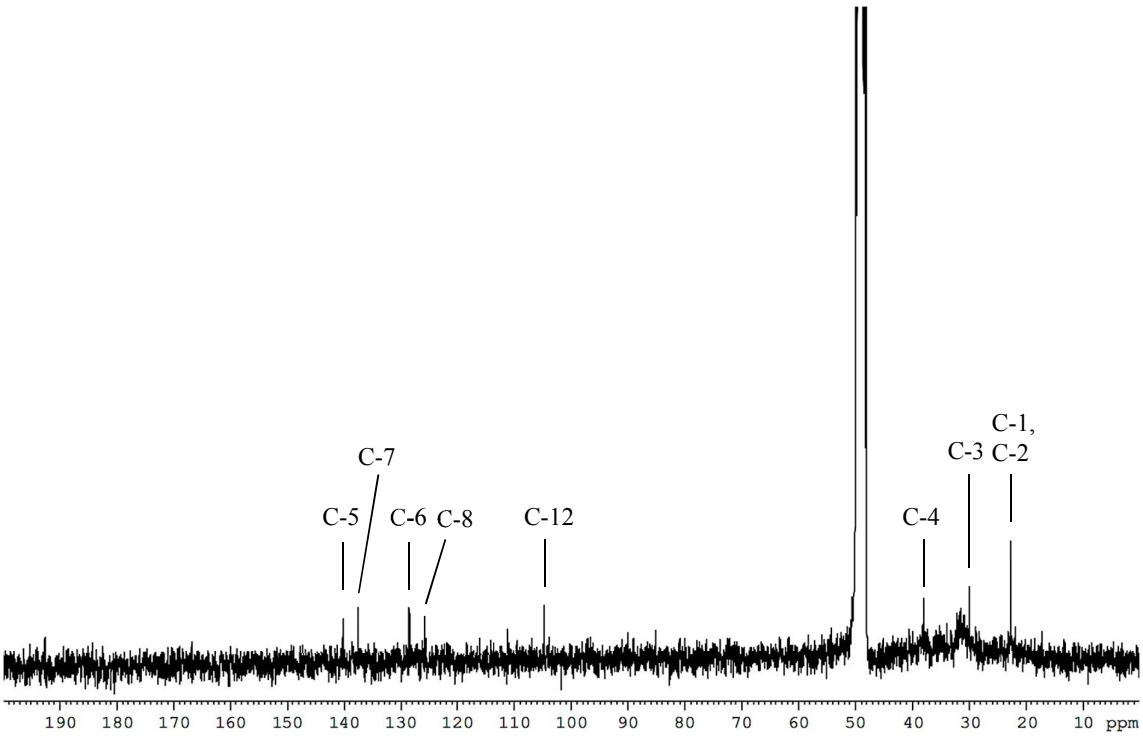

Figure S19. ^{13}C NMR spectrum corallorazine C in MeOH-d_4, 75 MHz.

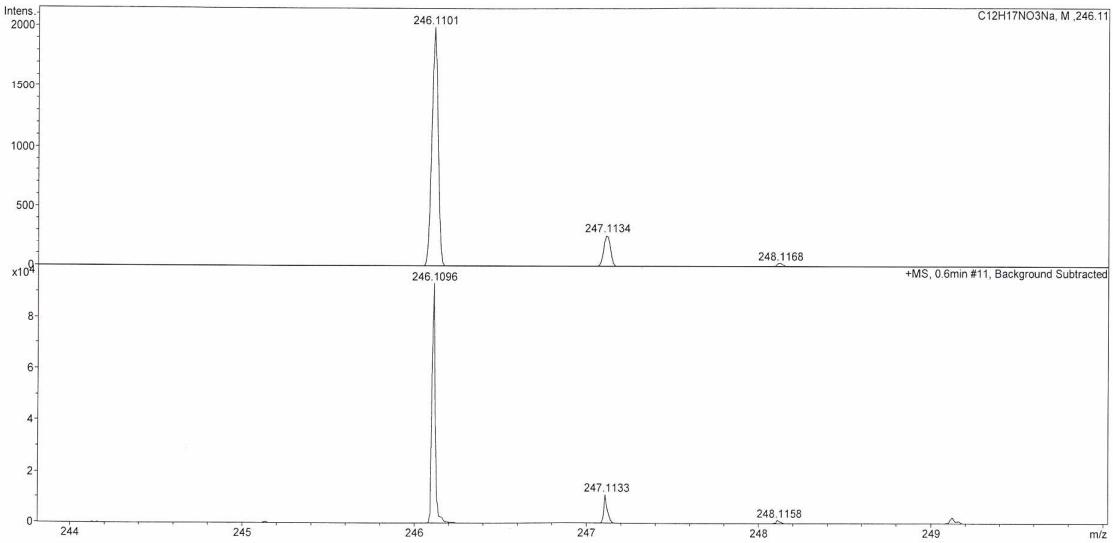

Figure S20. High resolution mass spectrum of corallorazine C.

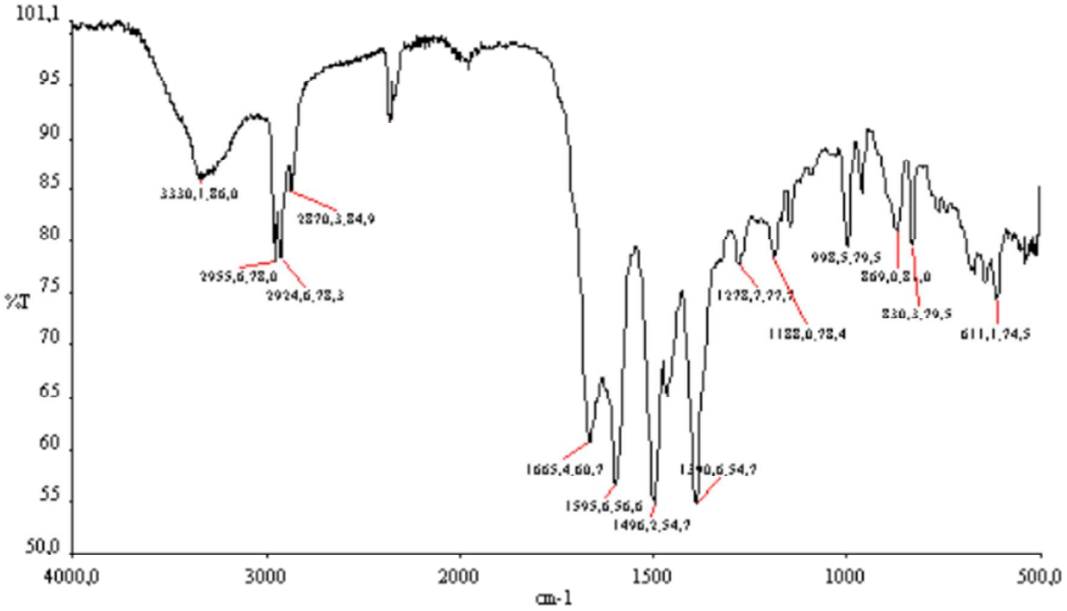

Figure S21. IR spectrum of corallorazine C.

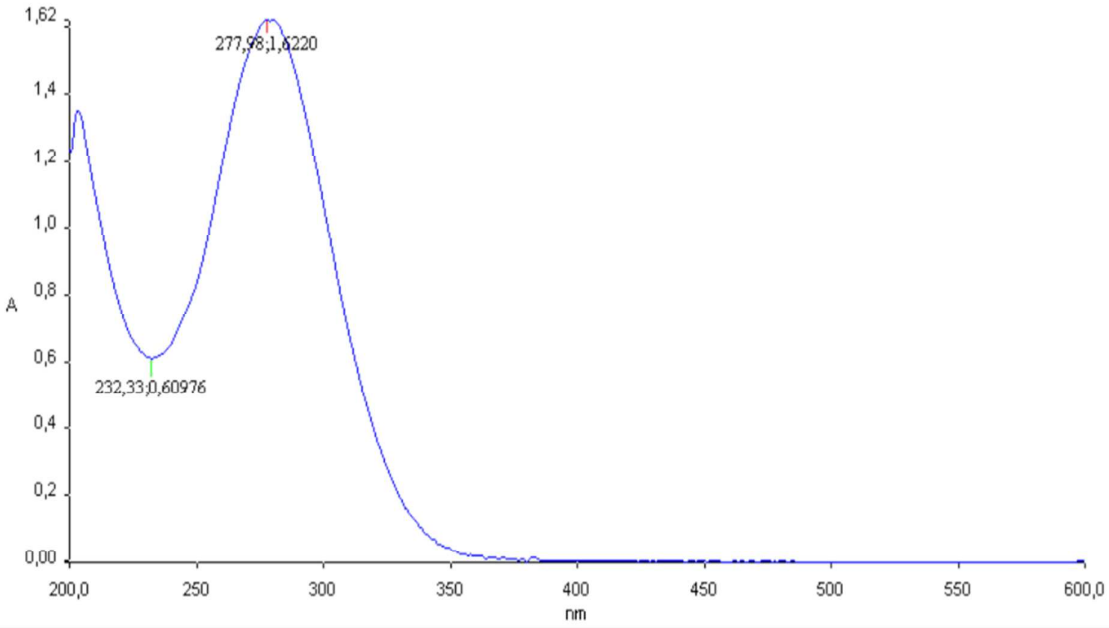

Figure S22. UV spectrum of corallorazine C (MeOH).

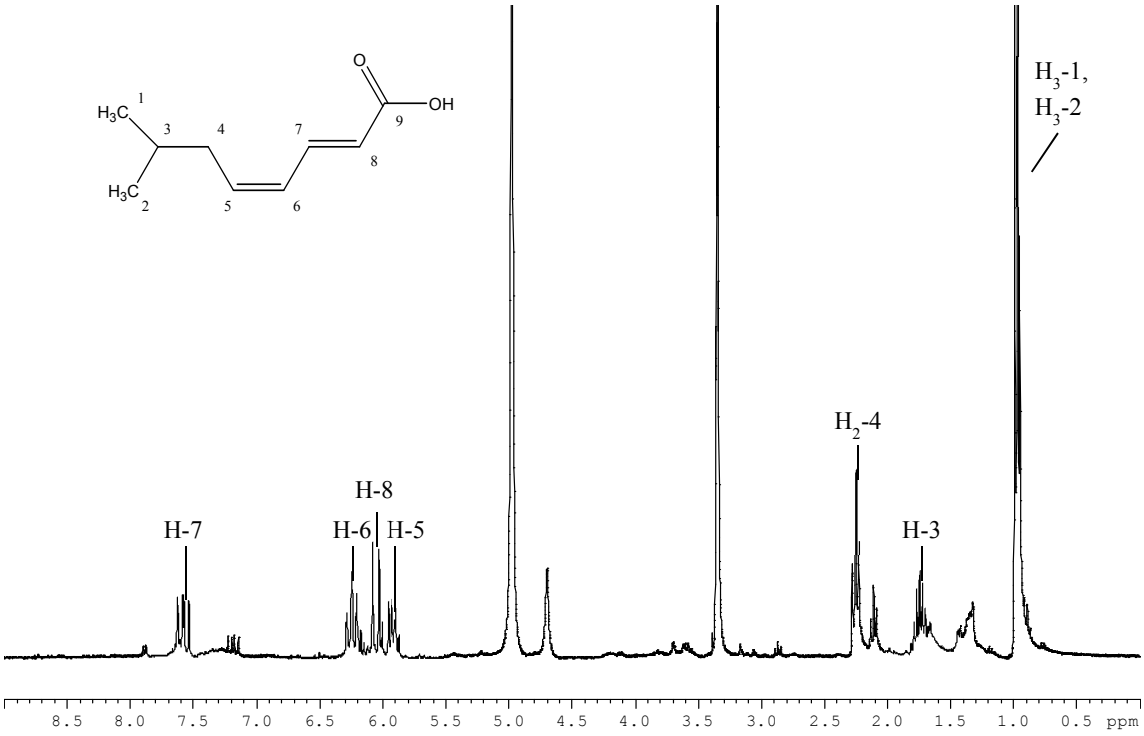

Figure S23. ^{1}H NMR spectrum of iso-oct-dienoic acid in MeOH-d_4, 300 MHz.

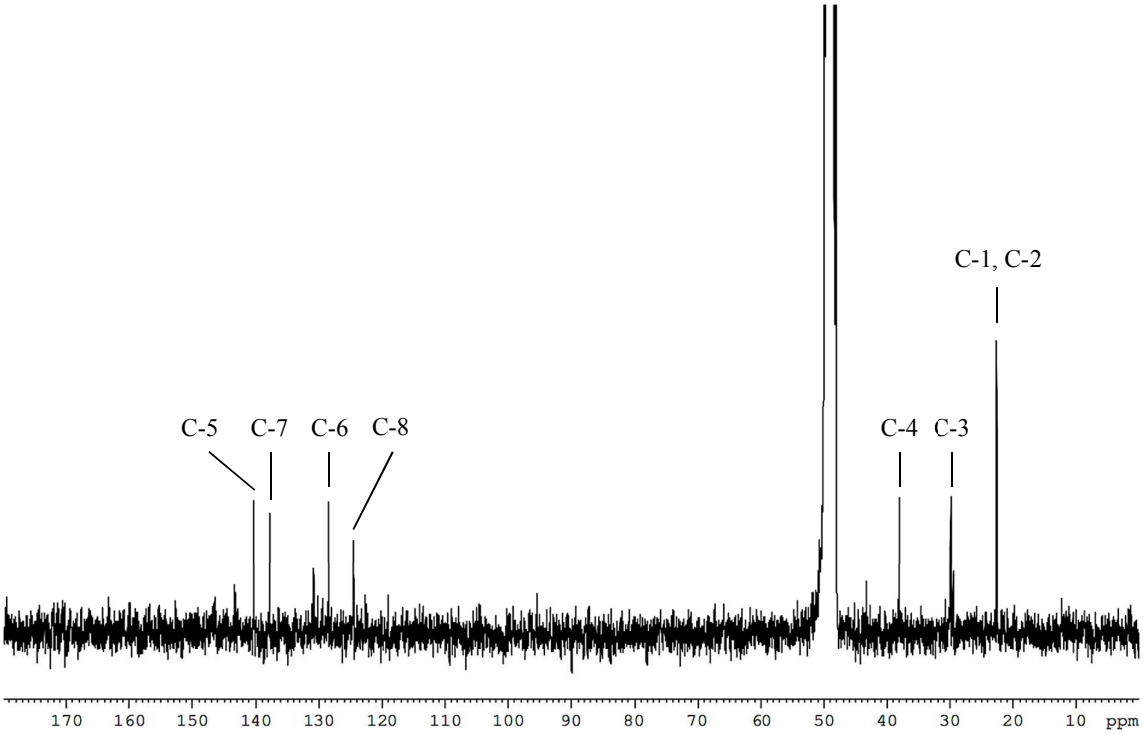

Figure S24. ^{13}C NMR spectrum iso-oct-dienoic acid in MeOH-d_4, 75 MHz.

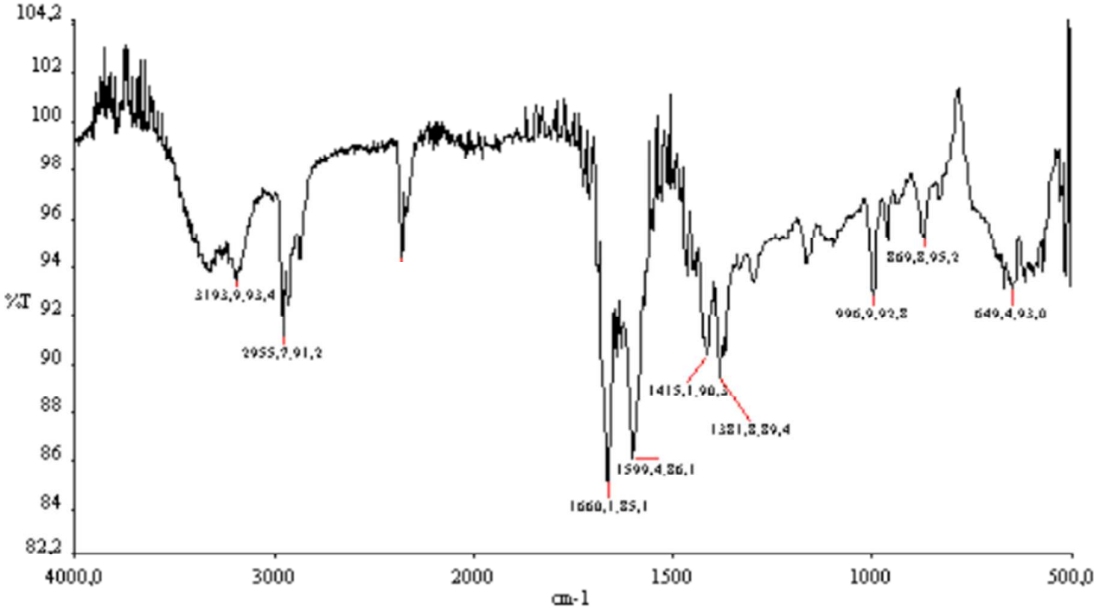

Figure S25. IR spectrum of iso-oct-dienoic acid.

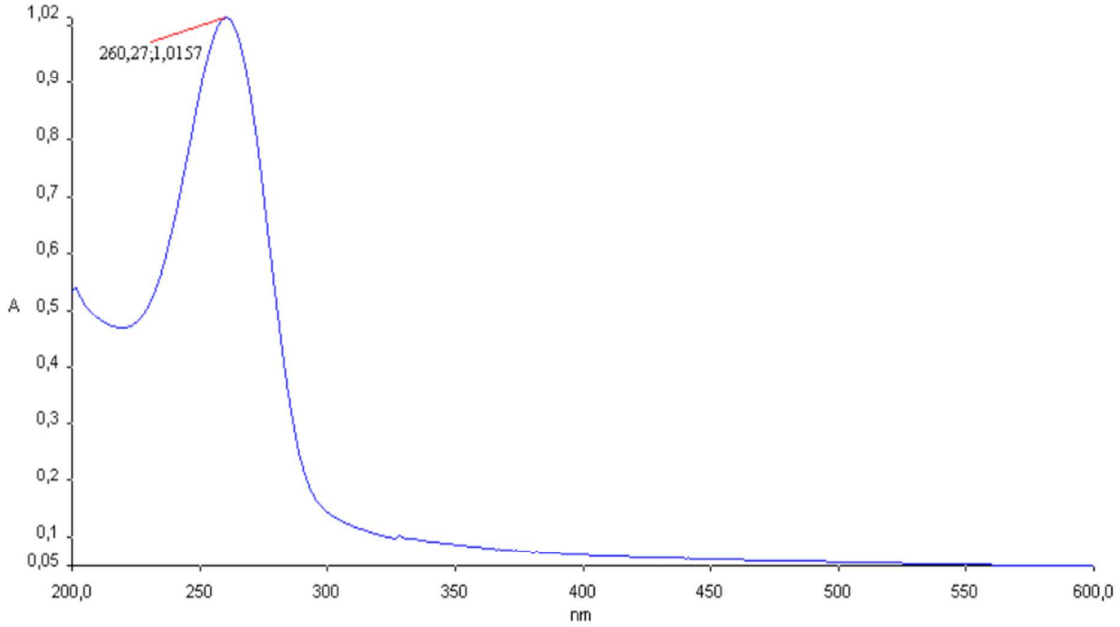

Figure S26. UV spectrum of iso-oct-dienoic acid (MeOH).

Table S1. NMR spectroscopic data of corallorazine A (**1**) in MeOH-d_4 (^{1}H: 300 MHz; ^{13}C: 75 MHz).

pos.	$\delta_{C/N}$, mult	δ_H (J in Hz)	COSY	HMBC (H to C/N)
1	22.7, CH_3	0.99, d (6.8)	3	3, 4
2	22.7, CH_3	0.99, d (6.8)	3	3, 4
3	29.9, CH	1.76, m	1, 2, 4	1, 2, 4, 5
4	38.2, CH_2	2.27, td (7.9, 1.0)	3, 5	1, 2, 3, 5, 6
5	141.1, CH	5.95, dt (11.0, 7.9)	4, 6	4, 6, 7
6	128.6, CH	6.30, br t (11.3)	5, 7	4, 7, 8
7	139.9, CH	7.72, ddd (1.0, 11.6, 15.0)	6, 8	5, 6, 8, 9
8	122.9, CH	6.49, d (15.0)	7	6, 9
9	167.6, C	-		
10	149.0, N	-		
11	136.3, C	-		
12	161.8, C	-		
13	100.5, N	-		
14	55.0, CH_2	a: 3.81, dd (3.1, 13.2)	14b, 15	15, 17
		b: 3.45, dd (1.1, 13.2)	14a, 15	15, 17, N-10/13
15	72.4,CH	6.17, dd (1.1, 3.1)	14a/b	N-13
16	116.6, CH_2	a: 6.33, s		12, N-10
		b: 5.41, s		11, 12
17	35.3, CH_3	3.07, s		12, 14, N-13

Table S2. ^{13}C enrichment of individual carbons of corallorazine A (feeding with 1-^{13}C glycine).

carbon	integral (labeled compound)	integral (non-labeled compound)	enhancement (labeled/ non- labeled)	enrichment (%)[1]
12	4.58	0.14	32.71	34.88
15	16.59	0.46	36.06	38.57
1/2	1.00	1.00	1.00	0

[1]enrichment = enhancement of the signal x 1.1% - 1.1%; The integral of carbon 1/2 was set to 1.00.

Table S3. NMR spectroscopic data of corallorazine B (**2**) in MeOH-d_4. (^1H: 300 MHz; ^{13}C: 75 MHz).

pos.	δ_C,[1] mult	δ_H (*J* in Hz)	COSY	HMBC
1	22.7, CH_3	0.99, d (6.9)	3, 4	3, 4
2	22.7, CH_3	0.99, d (6.9)	3, 4	3, 4
3	29.9, CH	1.75, m	1, 2, 4	1, 2, 4, 5
4	38.1, CH_2	2.26, t (7.5)	5	1, 2, 3, 5, 6
5	140.9, CH	5.96, m	4, 6	
6	128.4, CH	6.30, t (11.6)	5, 7	4, 7, 8
7	138.5, CH	7.62, ddd (1.1, 11.6, 15.0)	6, 8	5, 8, 9
8	124.7, CH	6.27, d (15.0)	7	6, 7, 9
9	167.7, C	-		
11	133.9, C	-		
12	111.2, CH_2	a: 5.92, s	8	13
		b: 6.41, s		11, 13
13	165.6, C	-		
15	53.2, CH_3	3.87, s		13

[1]Assignments are based on extensive 1D and 2D NMR measurements (HMBC, HSQC).

Table S4. NMR spectroscopic data of corallorazine C (**3**) in MeOH-d_4 (^1H: 300 MHz; ^{13}C: 75 MHz).

pos.	δ_C, mult	δ_H (*J* in Hz)
1	22.6, CH_3	0.99, d (6.6)
2	22.6, CH_3	0.99, d (6.6)
3	29.9, CH	1.73, m
4	38.1, CH_2	2.27, td (8.1, 1.5)
5	140.2, CH	5.92, dt (11.6, 8.1)
6	128.5, CH	6.29, t (11.6)
7	137.5, CH	7.60, ddd (1.1, 11.6, 15.0)
8	125.8, CH	6.20, d (15.0)
9	-*, C	
11	-*, C	
12	104.7, CH_2	a: 6.28, s
		b: 5.74, s
13	-*, C	

*^{13}C NMR signals not detectable

Table S5. NMR spectroscopic data of iso-oct-dienoic acid (**4**) in MeOH-d_4. (^{1}H: 300 MHz ^{3}C: 75 MHz).

pos.	δ_C, mult	δ_H (J in Hz)	COSY	HMBC
1	22.7, CH_3	0.98, d (6.6)	3	3, 4
2	22.7, CH_3	0.98, d (6.6)	3	3, 4
3	29.9, CH	1.75, m	1, 2, 4	
4	38.1, CH_2	2.25, td (8.1; 1.5)	3, 5, 6	5, 6
5	140.2, CH	5.92, dt (11.0; 8.1)	4	
6	128.4, CH	6.24, t (11.0)	4	
7	137.8, CH	7.58, ddd (1.1, 11.0, 15.0)	6, 8	5, 6, 9
8	124.5, CH	6.05, d (15.0)	7	9
9	171.5, C	-		