

Supporting Information

Inhibitory Effects of Epipolythiodioxopiperazine Fungal Metabolites on Isocitrate Lyase in the Glyoxylate Cycle of *Candida albicans*

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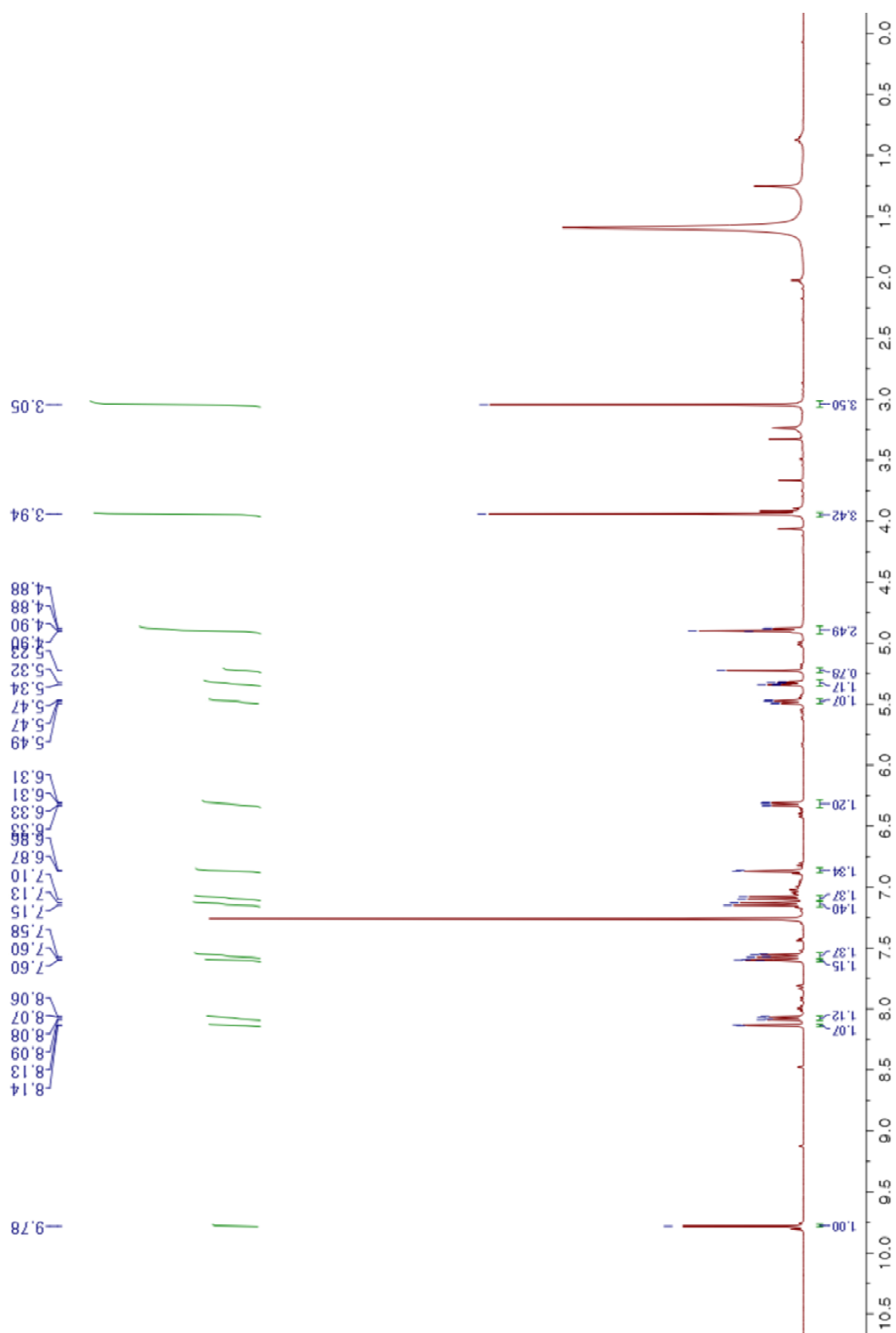


Figure S1. The ^1H NMR spectrum of secoemestrin C (1) (400MHz, CDCl_3)

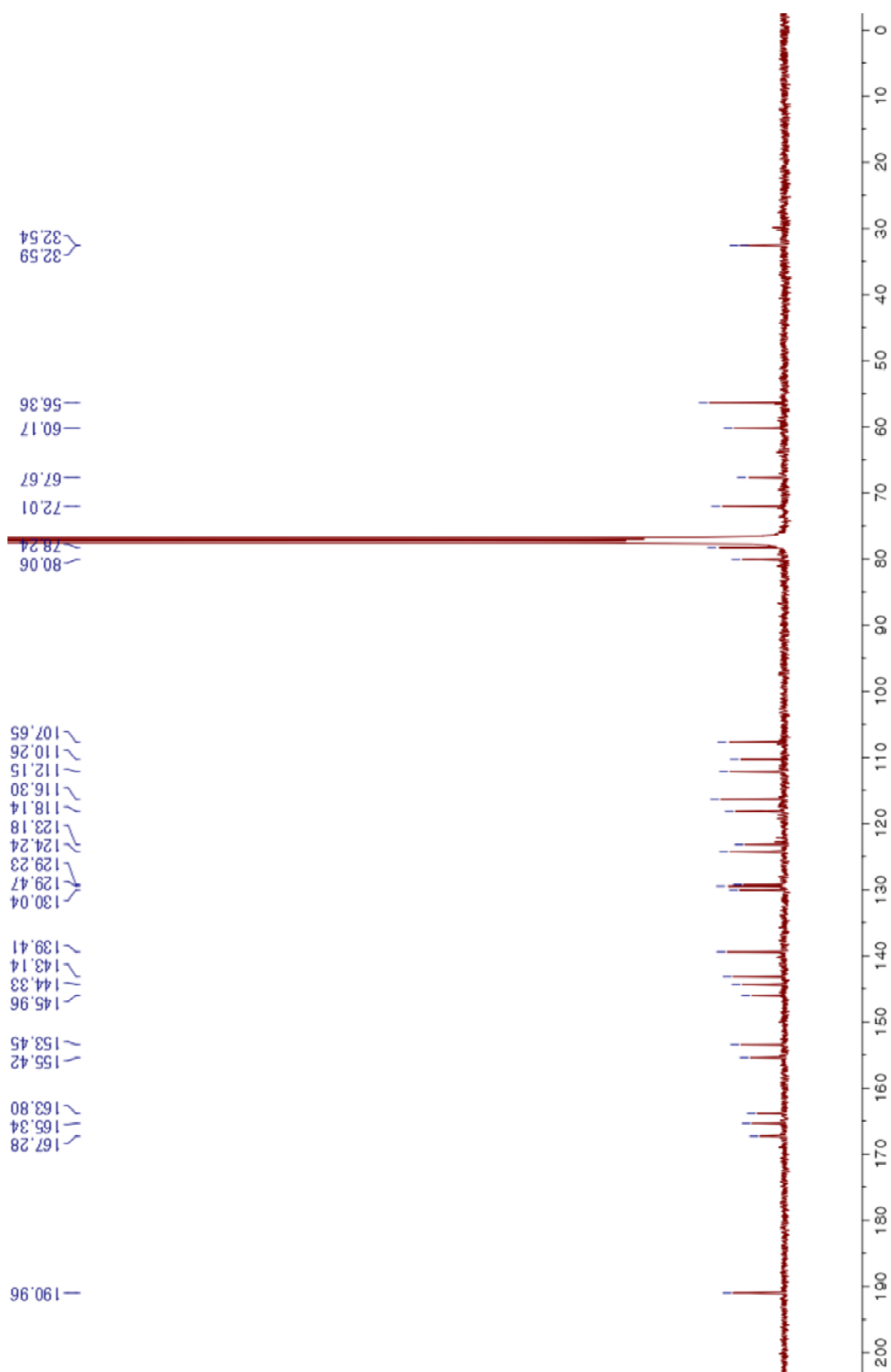


Figure S2. The ¹³C NMR spectrum of secoemestrin C (1) (100MHz, CDCl₃)

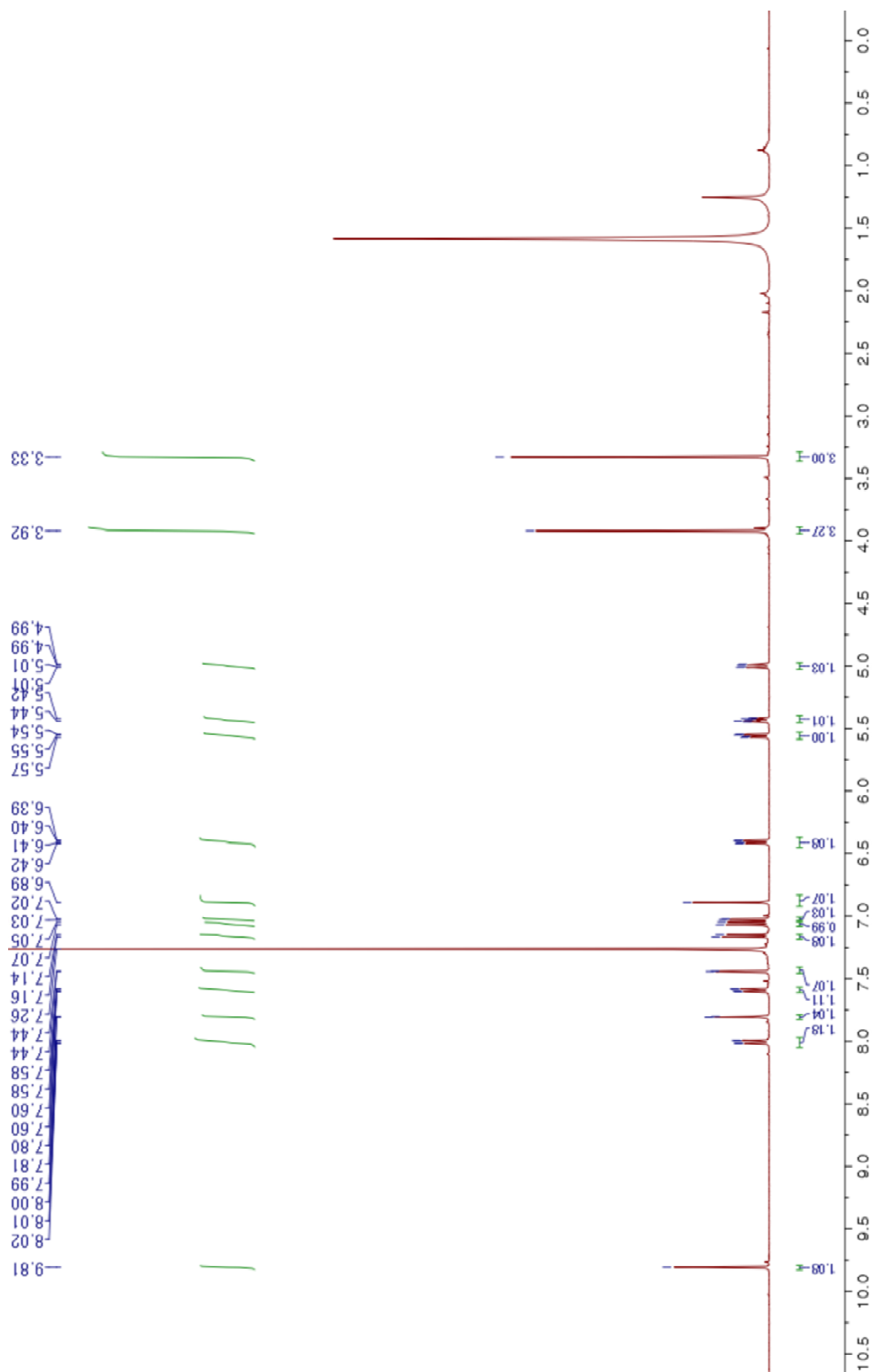


Figure S3. The ^1H NMR spectrum of dethiosecoemestrin (2) (400MHz, CDCl_3)

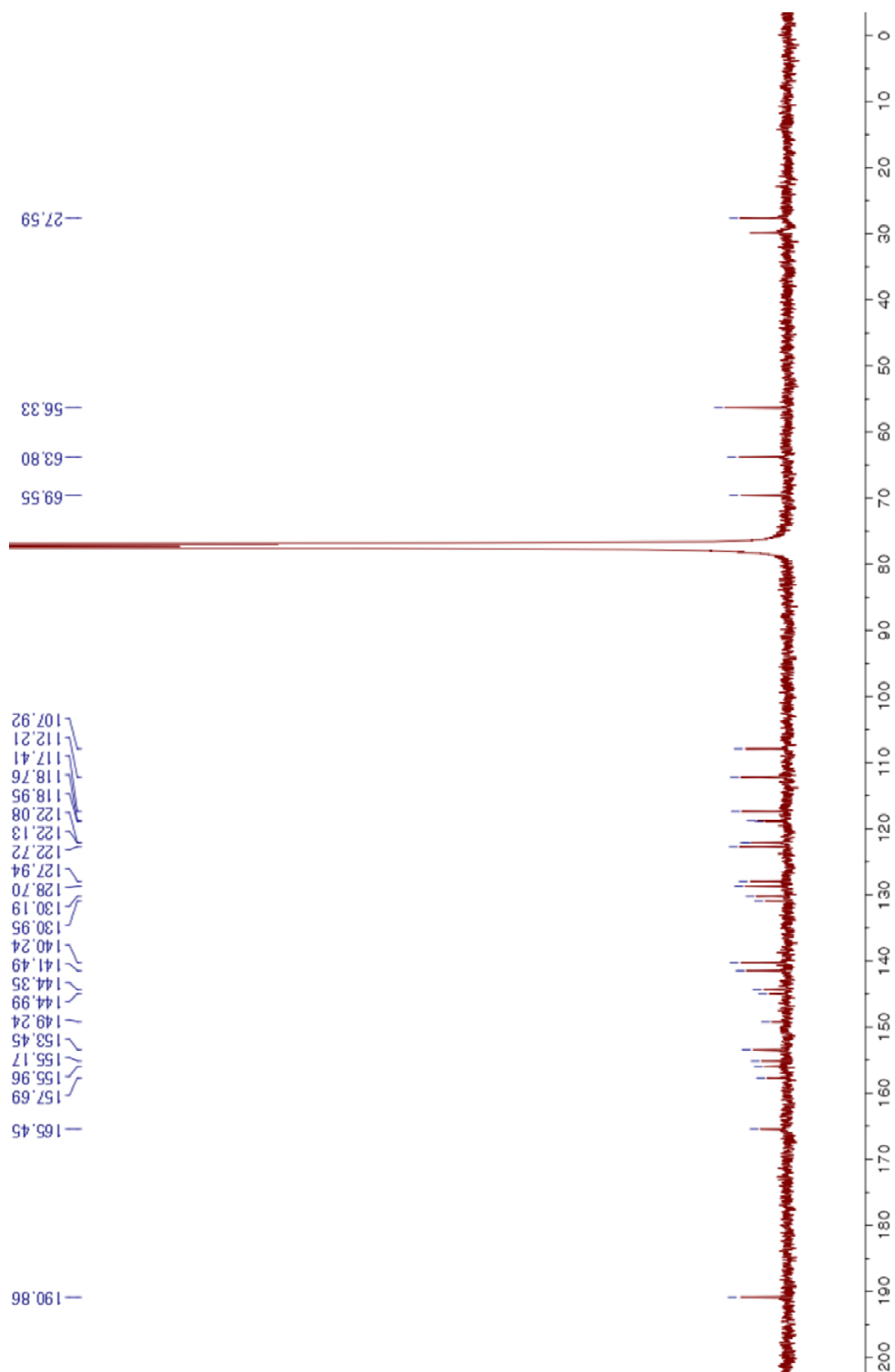


Figure S4. The ^{13}C NMR spectrum of dethiosecoemestrin (**2**) (100MHz, CDCl_3)

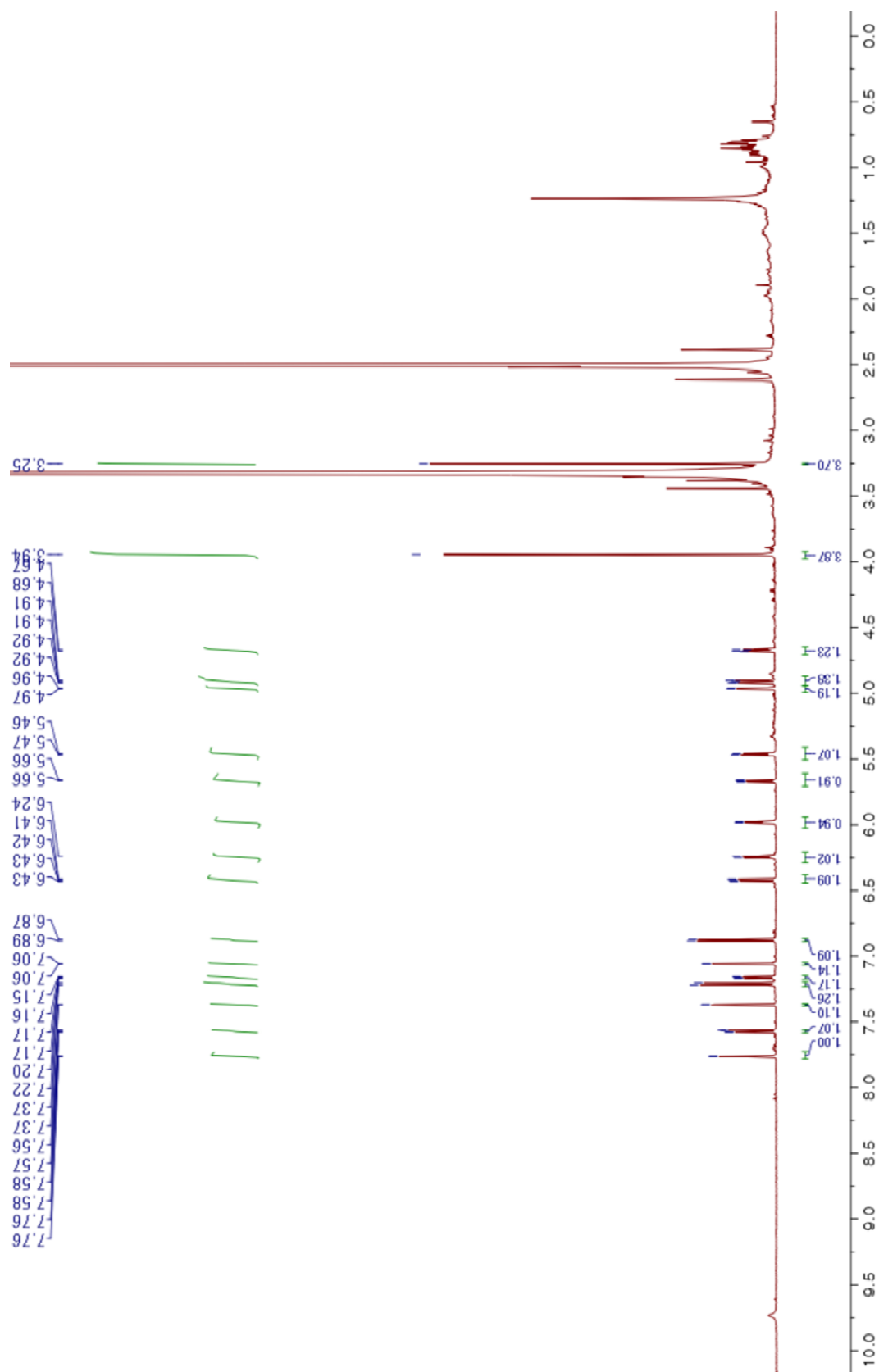


Figure S5. The ^1H NMR spectrum of emestrin (**3**) (800MHz, $\text{DMSO}-d_6$)

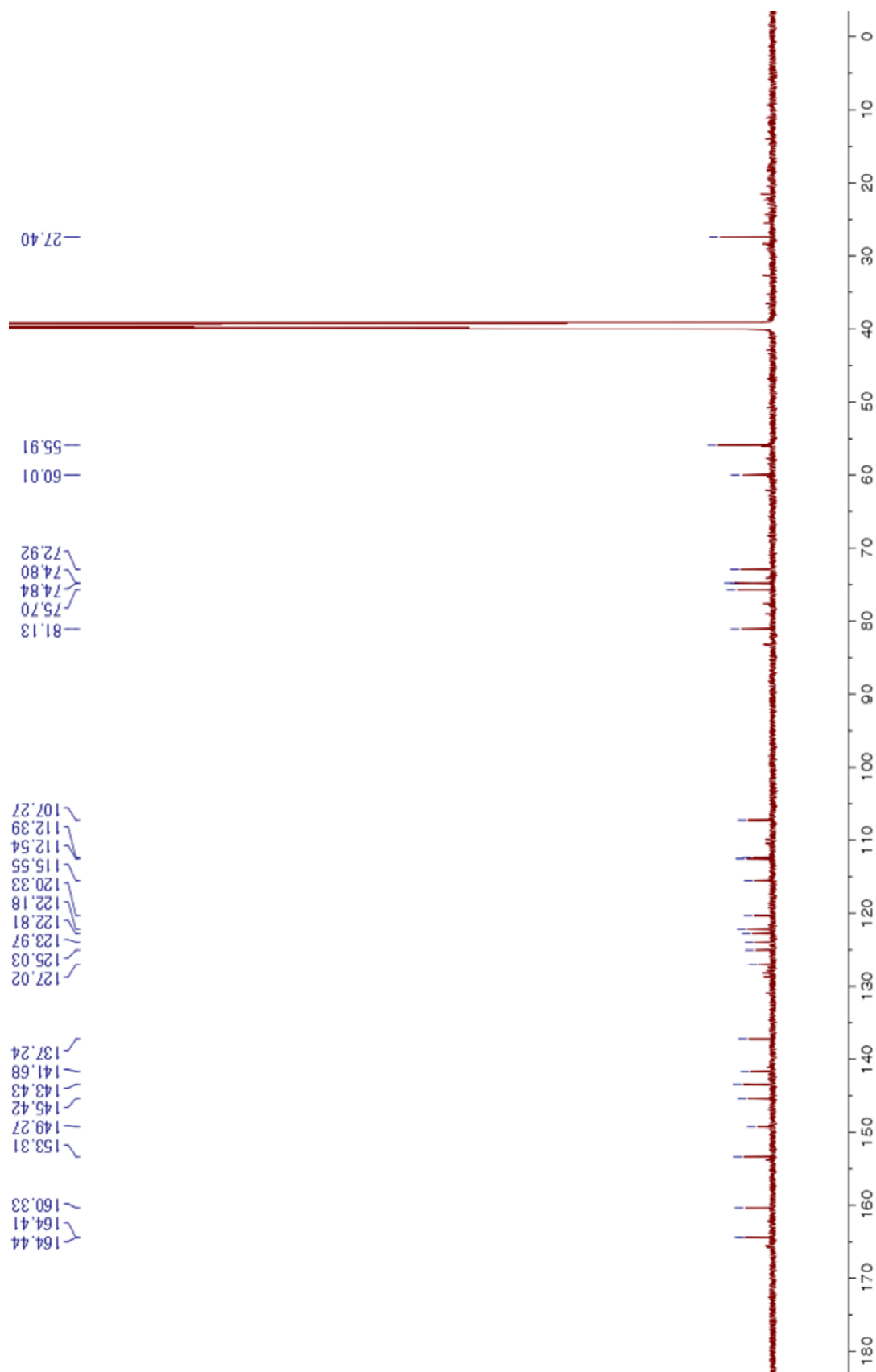


Figure S6. The ^{13}C NMR spectrum of emestrin (3) (200MHz, $\text{DMSO}-d_6$)

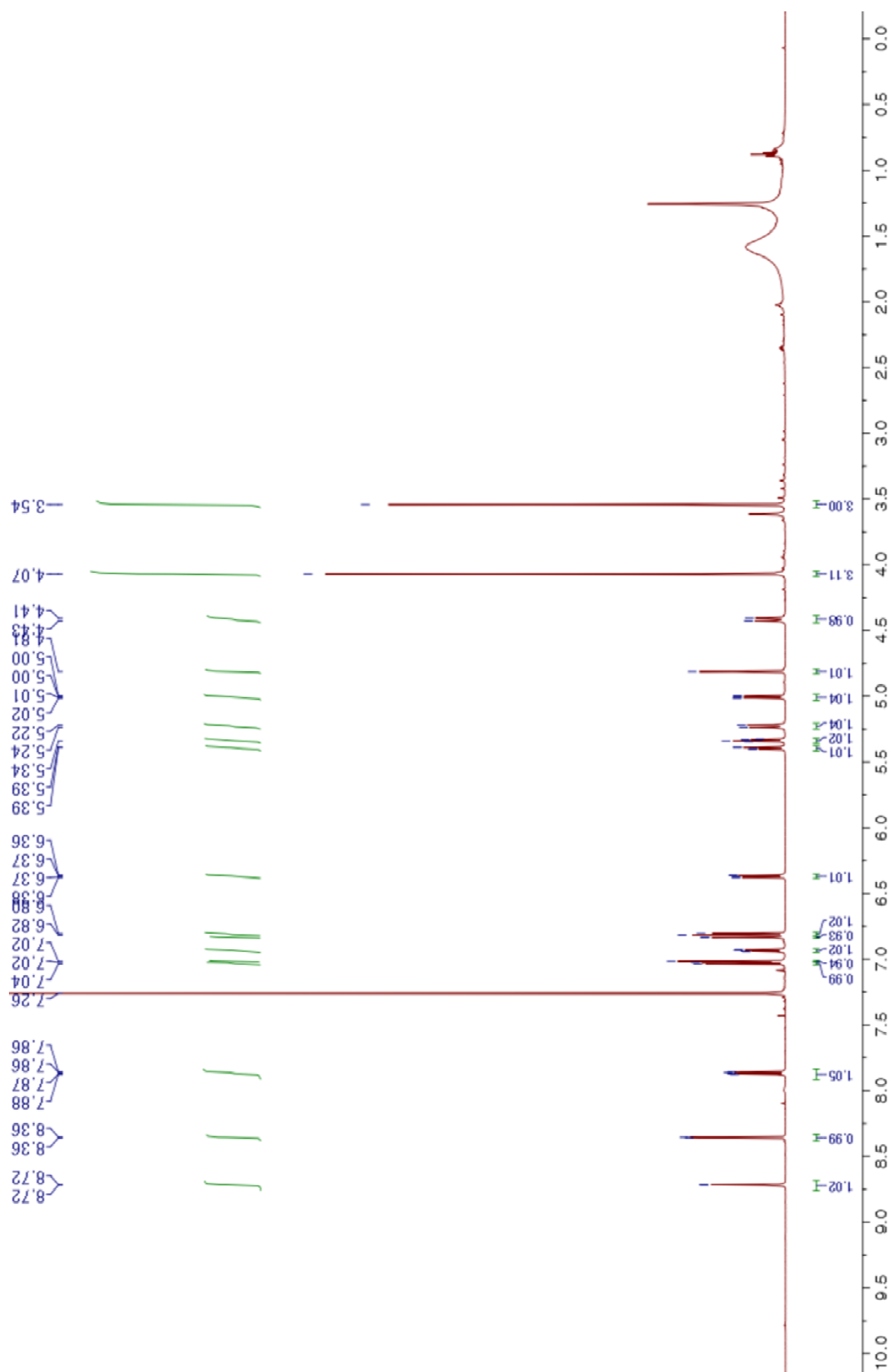


Figure S7. The ¹H NMR spectrum of emestrin B (4) (600MHz, CDCl₃)

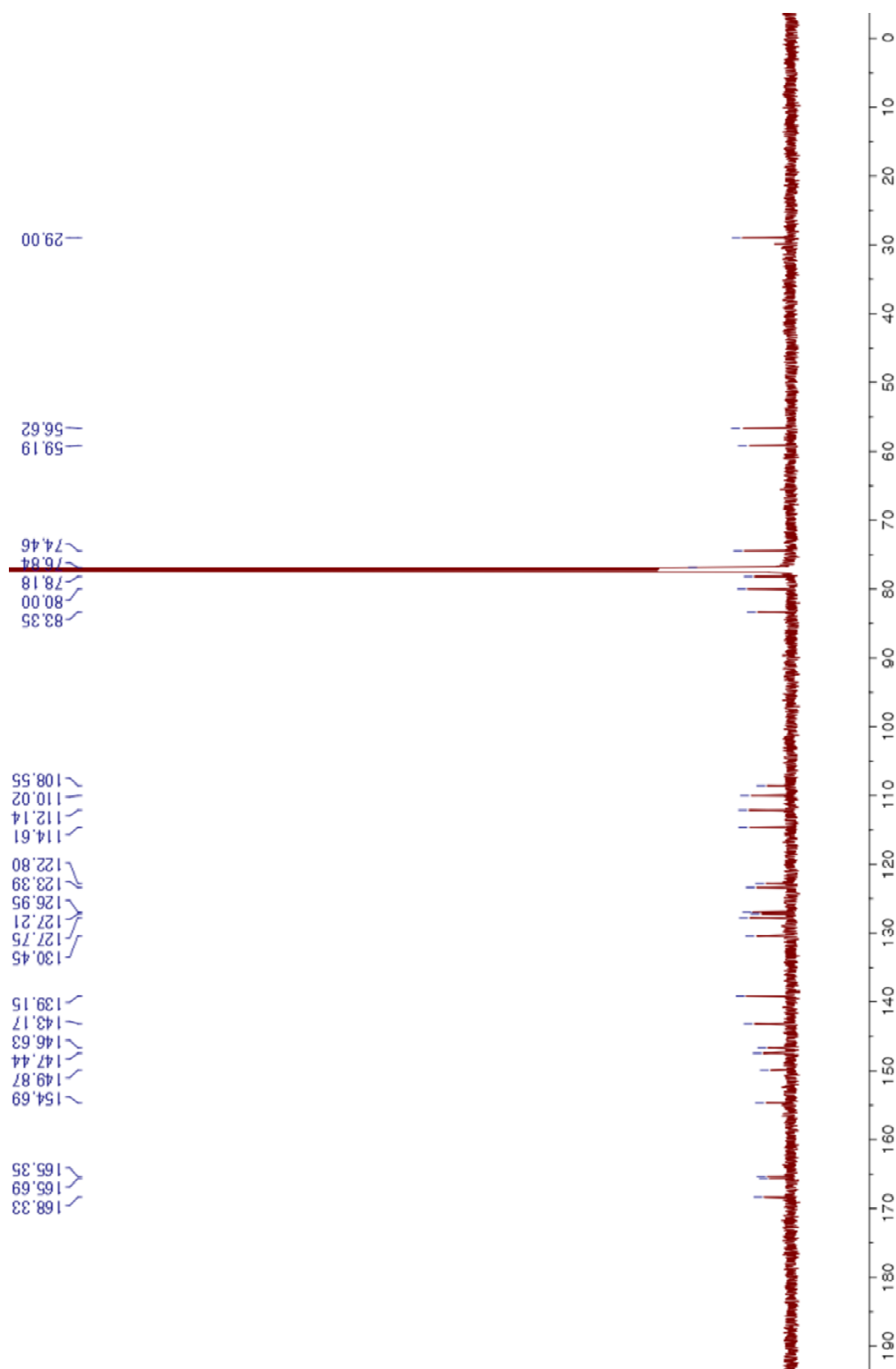
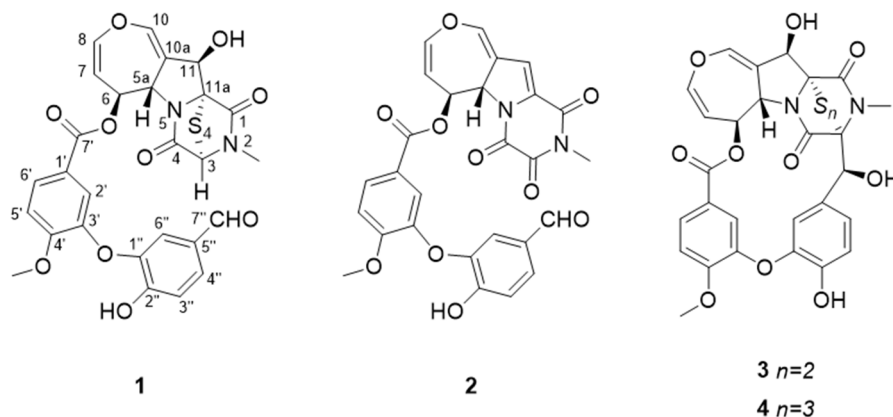


Figure S8. The ^{13}C NMR spectrum of emestrin B (**4**) (150MHz, CDCl_3)

Table S1. The Deviations with literature of ^{13}C NMR Chemical shifts **1-4**

	secoemestrin C (1)			dethiosecoemestrin			emestrin (3)			emestrin B (4)		
No.	Ref. ¹	1	Dev	Ref. ²	2	Dev	Ref. ³	3	Dev	Ref. ⁴	4	Dev
1	166.7	167.3	-0.6	155.9	155.9	0	164.3	164.4	-0.1	165.7	165.7	0
2-NMe	32.3	32.6	-0.3	27.3	27.6	-0.3	27.3	27.4	-0.1	29.0	29.0	0
3	68.6	67.7	0.9	157.5	157.7	-0.2	75.6	75.7	-0.1	83.3	83.4	-0.1
4	164.3	163.8	0.5	149.2	149.2	0	160.6	160.3	0.3	165.4	165.4	0
5a	60.2	60.2	0	63.8	63.8	0	59.9	60.0	-0.1	59.2	59.2	0
6	72.7	72	0.7	69.4	69.6	-0.2	72.9	72.9	0	74.9	74.5	0.4
7	108.5	107.7	0.8	107.8	107.9	-0.1	107.2	107.3	-0.1	110.0	110.0	0
8	140.0	139.4	0.6	140.2	140.2	0	137.2	137.2	0	139.2	139.2	0
10	142.3	143.1	-0.8	141.2	141.5	-0.3	141.7	141.7	0	143.2	143.2	0
10a	113.2	110.3	2.9	118.9	118.9	0	112.4	112.5	-0.1	108.5	108.6	-0.1
11	78.6	78.2	0.4	122.2	122.1	0.1	74.8	74.8	0	76.8	76.8	0
11a	81.1	80.1	1.0	131.2	130.9	0.3	81.0	81.1	-0.1	78.1	78.2	-0.1
1'	123.8	124.2	-0.4	122.2	122.7	-0.5	122.2	122.2	0	122.8	122.8	0
2'	122.9	123.2	-0.3	122.2	122.1	0.1	123.9	123.9	0	130.5	130.5	0
3'	145.4	144.3	1.1	144.3	144.4	-0.1	143.4	143.4	0	146.6	146.6	0
4'	156.2	155.4	0.8	155.2	155.2	0	148.9	149.3	-0.4	149.9	149.9	0
4'-OMe	56.7	56.4	0.3	56.2	56.3	-0.1	55.8	55.9	-0.1	56.7	56.6	0.1
5'	113.2	112.2	1.0	112.2	112.2	0	115.4	115.5	-0.1	112.1	112.1	0
6'	129.0	129.5	-0.5	128.6	128.7	-0.1	124.9	125.0	-0.1	127.8	127.8	0
7'	165.8	165.3	0.5	165.2	165.5	-0.3	164.4	164.4	0	168.3	168.3	0
1''	146.5	145.9	0.6	145.1	144.9	0.2	145.3	145.4	-0.1	147.4	147.4	0
2''	154.6	153.5	1.1	153.3	153.5	-0.2	153.3	153.3	0	154.7	154.7	0
3''	117.7	116.3	1.4	117.2	117.4	-0.2	112.3	112.4	-0.1	114.6	114.6	0
4''	128.5	129.2	-0.7	127.6	127.9	-0.3	122.7	122.8	-0.1	126.9	126.9	0
5''	130.8	130.1	0.7	130.1	130.2	-0.1	127.1	127.0	0.1	127.2	127.2	0
6''	118.5	118.1	0.4	118.7	118.8	-0.1	120.4	120.3	0.1	123.4	123.4	0
7''	190.9	190.9	0	190.5	190.9	-0.4	74.8	74.8	0	79.9	80.0	-0.1

¹ Ooike, M.; Nozawa, K.; Kawai, K.-I. An epitetrahydrodioxopiperazine related to emestrin from *Emericella foveolata*. *Phytochemistry* **1997**, 46, 123–126.

² Seya, H.; Nozawa, K.; Udagawa, S.-I.; Nakajima, S.; Kawai, K.-I. Studies on fungal products. IX. dethiosecoemestrin, a new metabolite related to emestrin, from *Emericella striata*. *Chem. Pharm.*

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⁴ Nozawa, K.; Udagawa, S.; Nakajima, S.; Kawai, K. Studies on fungal products. XIV. emestrin B, a new epitritiodioxopiperazine, from *Emericella striata*. *Chem. Pharm. Bull.* **1987**, 35, 3460–3463.