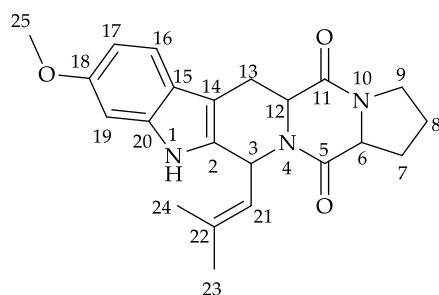


Table S1. NMR data for fumitremorgin C (**1**) [1], [2]

Position	δ_C , mult.	δ_C (Reported)	δ_H , mult. (<i>J</i> in Hz)	COSY	HMBC (H→C)
1-NH					
2	133.5, C	133.6			
3	51.9, CH	52.4	6.0, d (<i>J</i> = 9.6 Hz)	21	5, 2, 22, 21, 14, 12
4- N					
5	171.5, C	171.6			
6	60.2, CH	60.4	4.27, dd (<i>J</i> = 12.6, 6.5 Hz)	7	11
7, 7'	29.0, CH ₂	29.5	2.4, 2.1, m	6, 8	5, 9
8	23.5, CH ₂	24.0	2.1, m	7, 9	6
9	46.1, CH ₂	46.4	3.6, m	8	
10-N					
11	167.8, C	168.1			
12	57.7, CH	57.9	4.30, dd (<i>J</i> = 12.6, 6.5 Hz)	13	
13, 13'	22.2, CH ₂	22.8	3.58, m ; 3.0, dd (<i>J</i> = 15.7, 11.6 Hz)	12	2, 11, 12, 14, 15
14	106.0, C	106.1			
15	121.0, C	121.9			
16	119.1, CH	119.2	7.4, d (<i>J</i> = 6.8 Hz)	17	15, 14, 18, 20
17	109.7, CH	110.1	6.77, dd (<i>J</i> = 8.6, 2.3 Hz)	16, 19	15, 19
18	157.5, C	157.6			
19	94.2, CH	95.9	6.87, d (<i>J</i> = 2.3 Hz)	17	15, 17, 18, 20
20	138.8, C	138.9			
21	125.1, CH	125.2	4.9, d (<i>J</i> = 9.6 Hz)	3	w
22	135.1, C	135.1			
23	25.3, CH ₃	25.9	1.7, s		2, 21, 24
24	18.0, CH ₃	18.3	2.0, s		2, 21, 23
25	55.8, OCH ₃	55.9	3.8, s		18

NMR solvents used for fumitremorgin C (**1**) and that reported in the literature were CD₃OD and CDCl₃ at 600 MHz and 500 MHz, respectively. w= weak HMBC intensity.



Chemical Formula: $C_{22}H_{25}N_3O_3$

Exact Mass: 379.1896

Figure S1. Structure of fumitremorgin C (**1**)

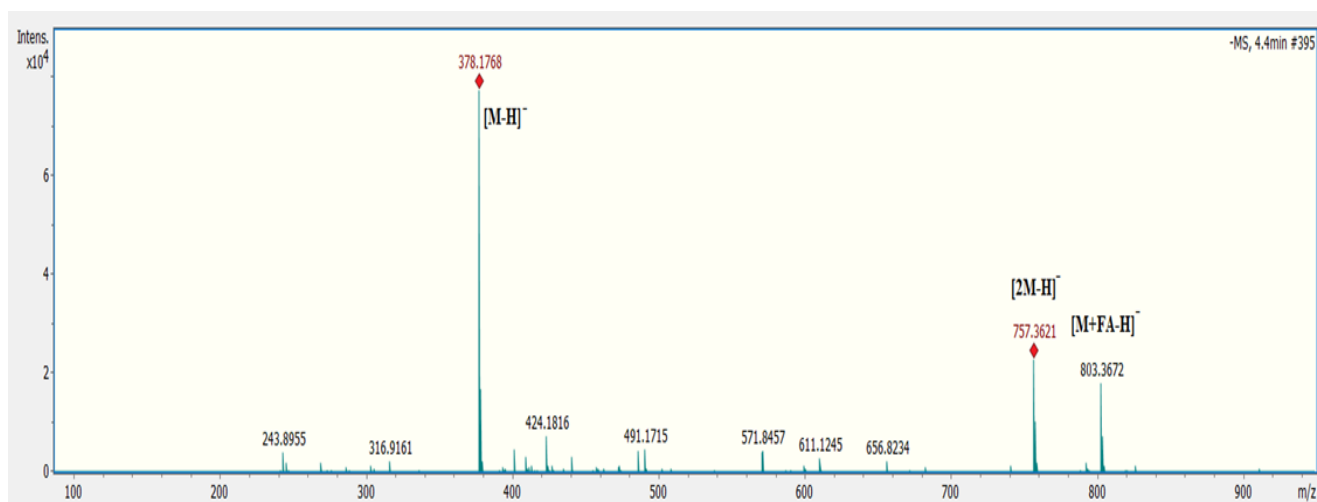


Figure S2. ESI MS (positive ionisation mode) of fumitremorgin C (**1**)

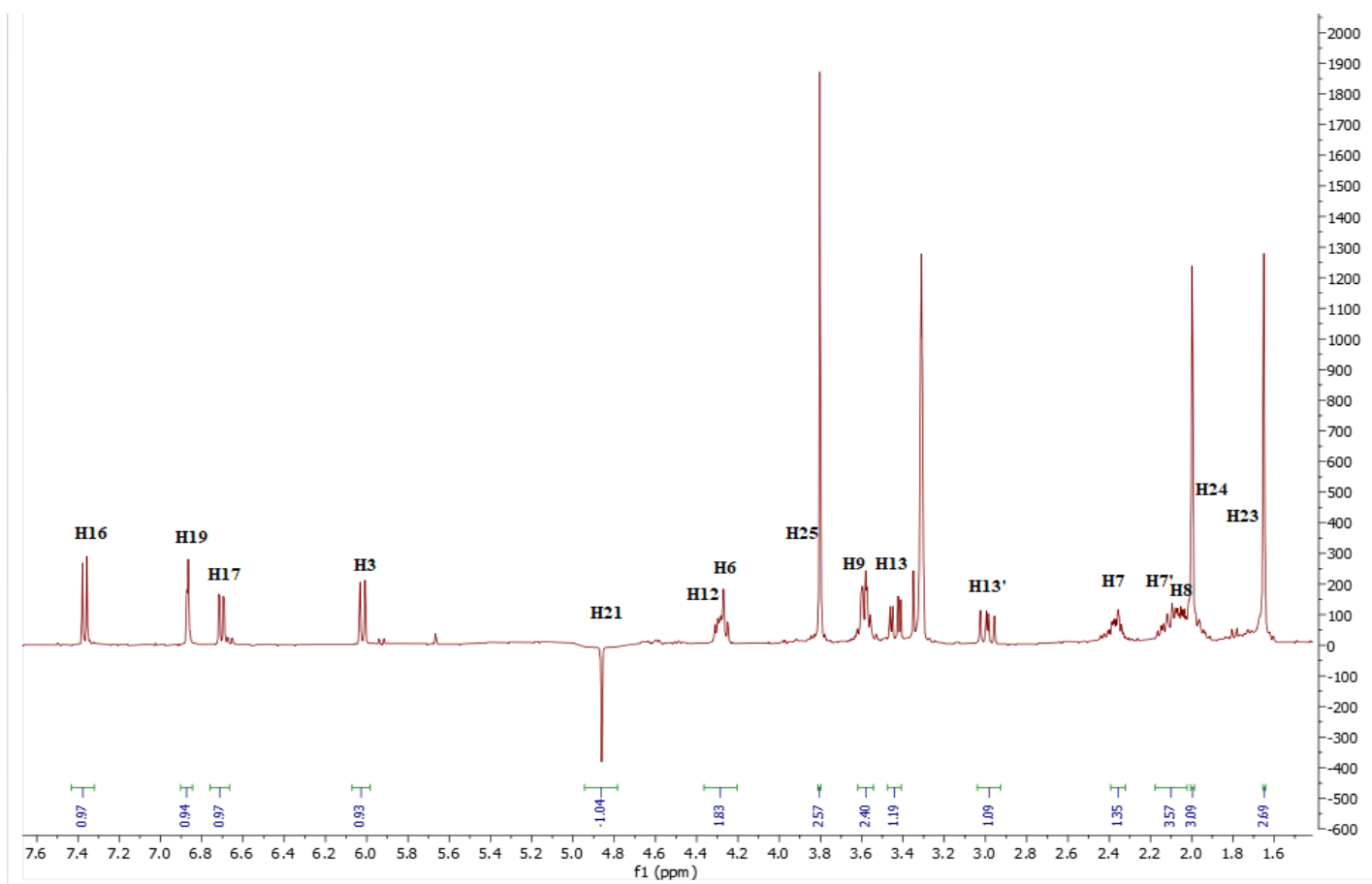


Figure S3. ^1H NMR spectrum of fumitremorgin C (**1**) at 600 MHz in CD_3OD

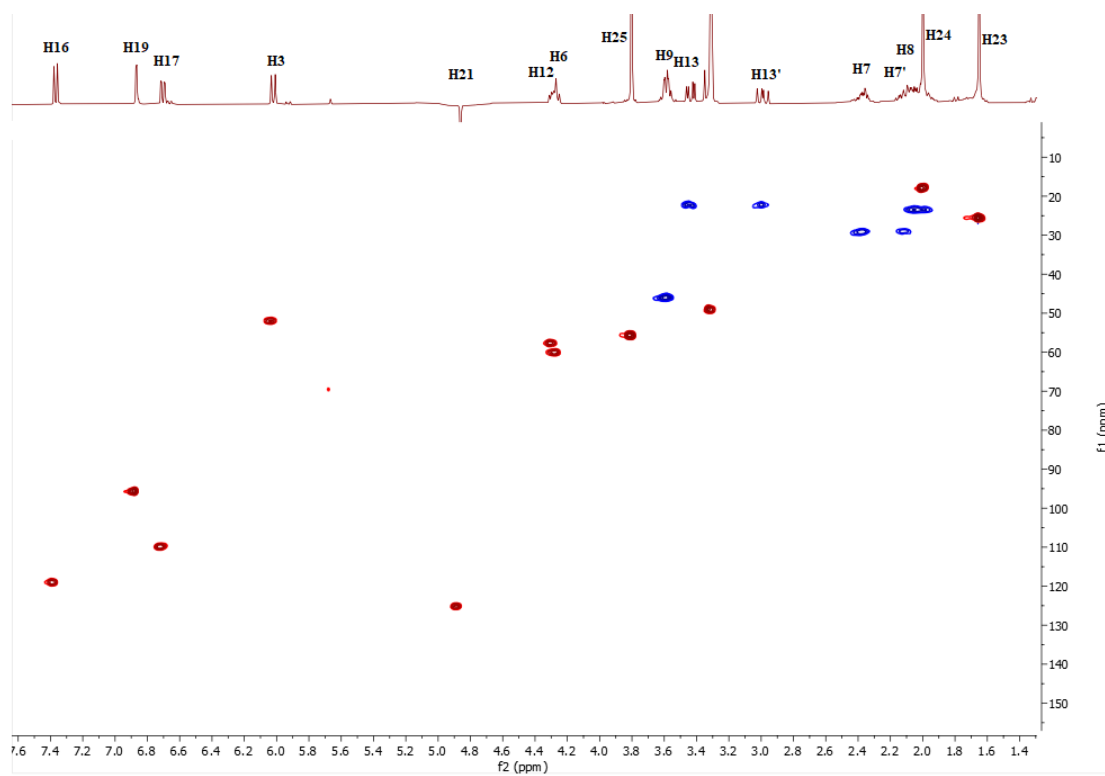


Figure S4. HSQC spectrum of fumitremorgin C (**1**) at 600 MHz in CD₃OD

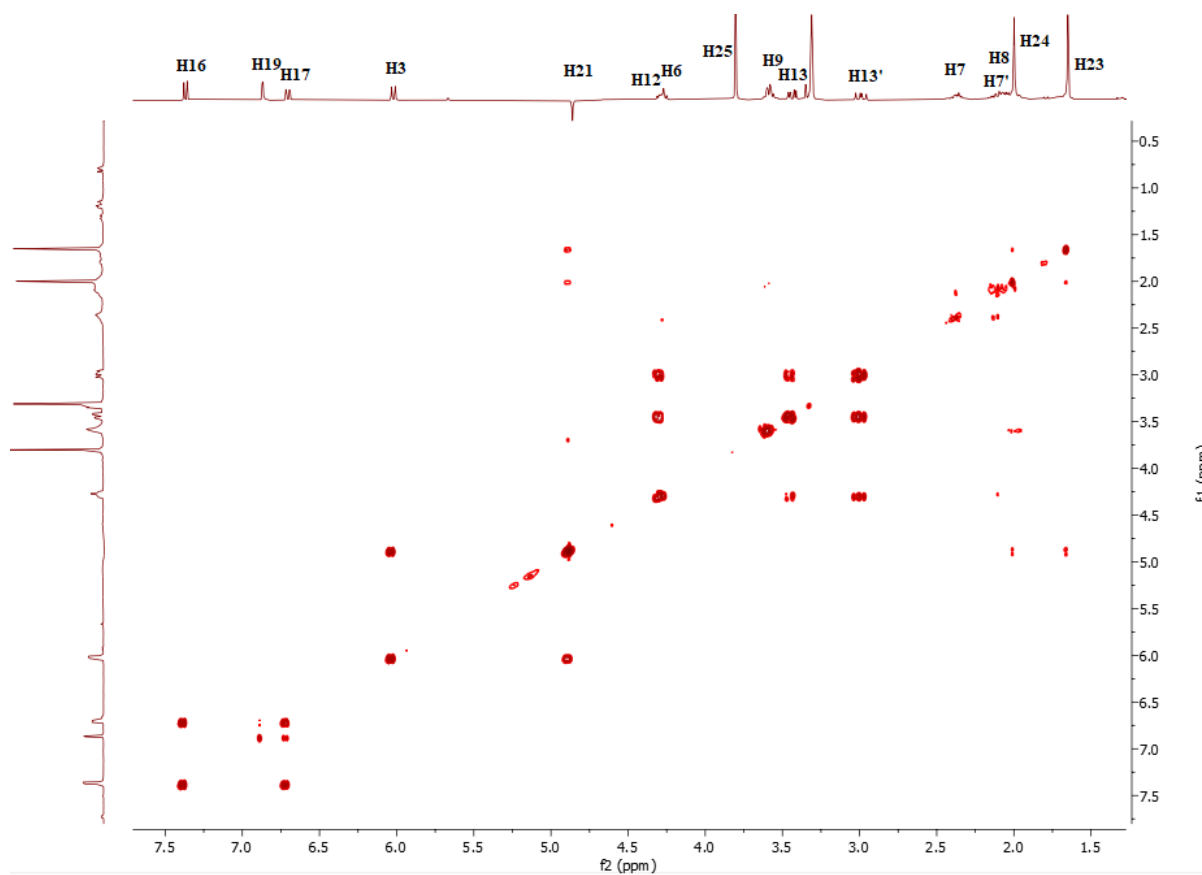


Figure S5. COSY spectrum of fumitremorgin C (**1**) at 600 MHz in CD₃OD

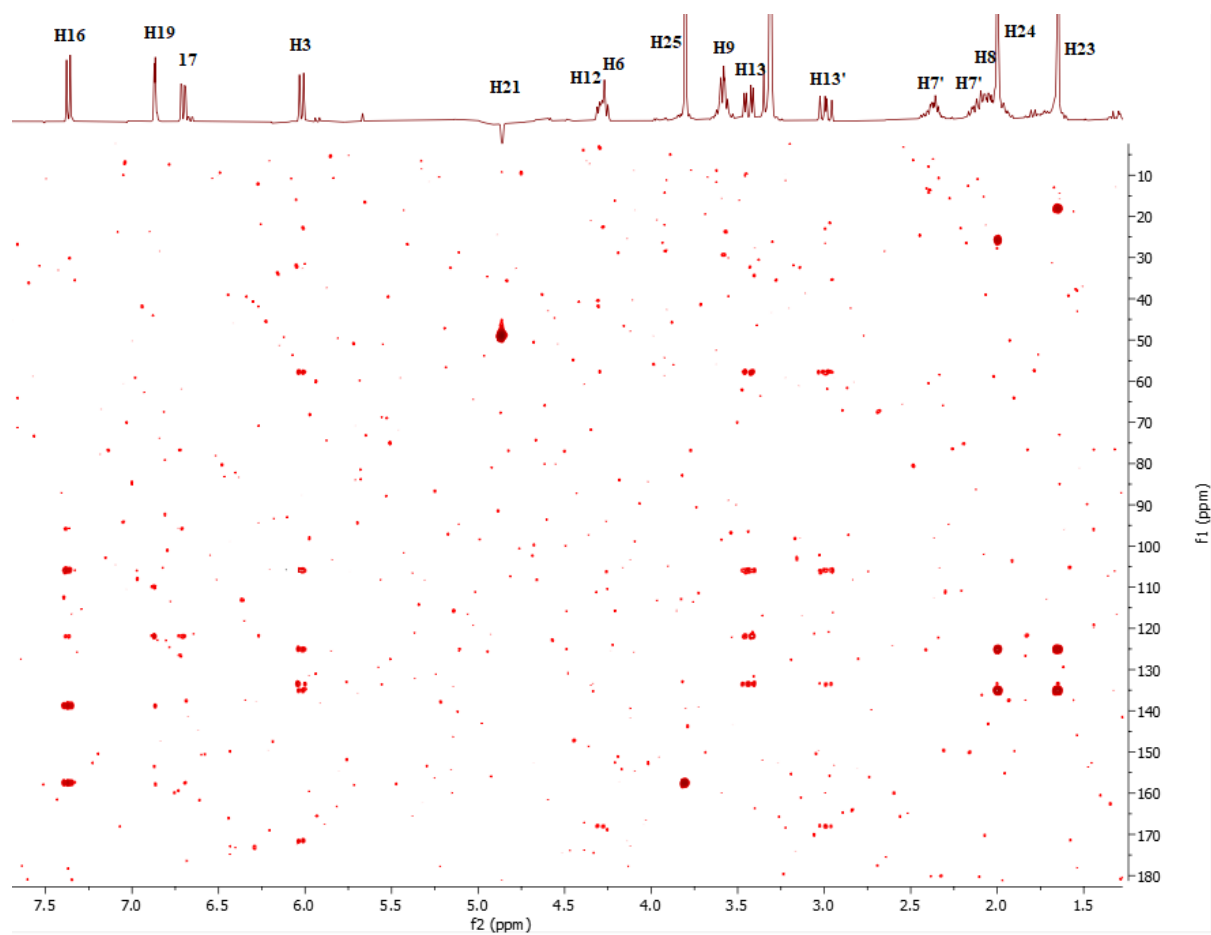
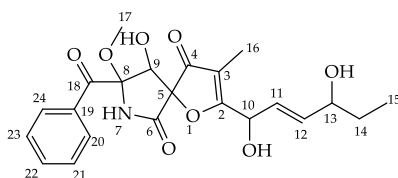


Figure S6. HMBC spectrum of fumitremorgin C (**1**) at 600 MHz in CD₃OD

Table S2. NMR data for pseurotin D (**2**) [3]

Position	δ_C , mult.	δ_C reported	δ_H , mult. (J in Hz)	HMBC (H \rightarrow C)
2	189.1, C	187.8		
3	112.1, C	111.2		
4	199.3, C	197.4		
5	93.6, C	91.0		
6	168.8, C	166.8		
8	93.8, C	91.9		
9	76.3, CH	74.1	4.52, d ($J = 2.3$ Hz)	4, 8
10	69.8, CH	68.7	5.20, dd ($J = 6.1, 3.5$ Hz)	2, 3, 11, 12
11	127.9, CH	126.4	5.87, m	2, 10, 11, 13
12	137.9, CH	137.3	5.94, m	10, 12, 13, 14
13	74.0, CH	73.1	4.02, q ($J = 6.3$ Hz)	11, 12, 14, 15
14	30.9, CH	29.7	1.52, m	12, 13, 16
15	5.5, CH ₃	5.4	0.91, s	
16	10.1, CH ₃	9.8	1.76, s	
17	52.5, OCH ₃	52.0	3.36, s	8
18	197.1, C	195.2		
19	139.2, C	134.6		
20, 24	131.7, CH	130.8	8.37, d ($J = 7.4$ Hz)	18, 22
21, 23	129.5, CH	128.7	7.52, t ($J = 7.4$ Hz)	19
22	134.8, CH	132.7	7.66, t ($J = 7.4$ Hz)	20, 24

NMR solvents used for pseurotin D (**2**) and that reported in the literature were CD₃OD and CDCl₃ at 600 MHz, respectively.



Chemical Formula: C₂₂H₂₅NO₈

Exact Mass: 431.1580

Figure S7. Structure of pseurotin D (**2**)

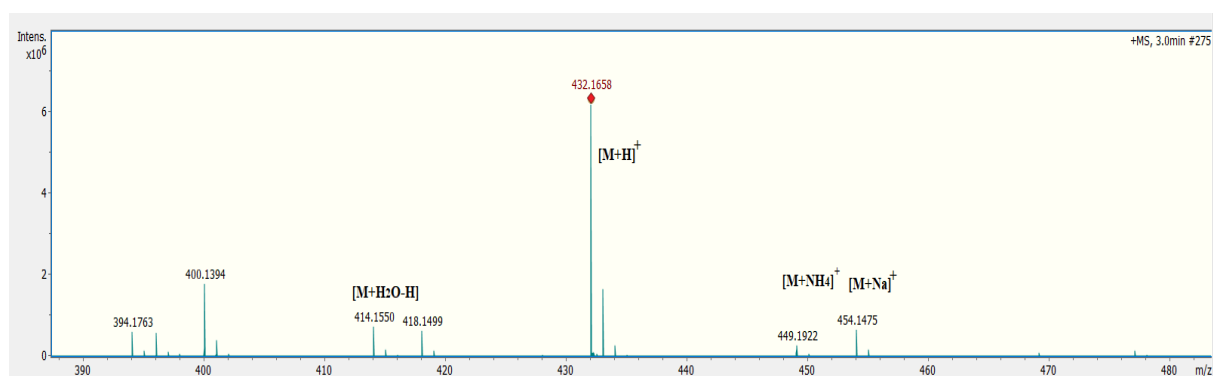


Figure S8. ESI MS (positive ionisation mode) of pseurotin D (2)

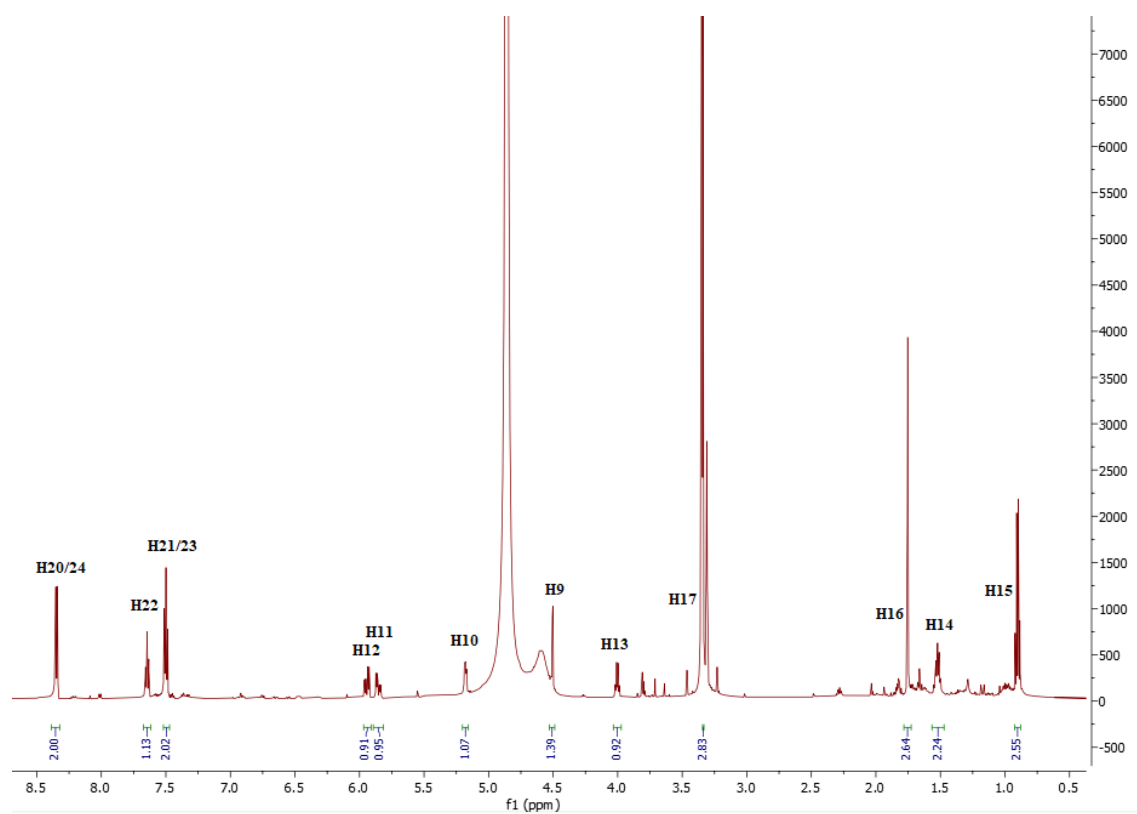


Figure S9. ¹H NMR spectrum of pseurotin D (2) at 600 MHz in CD₃OD

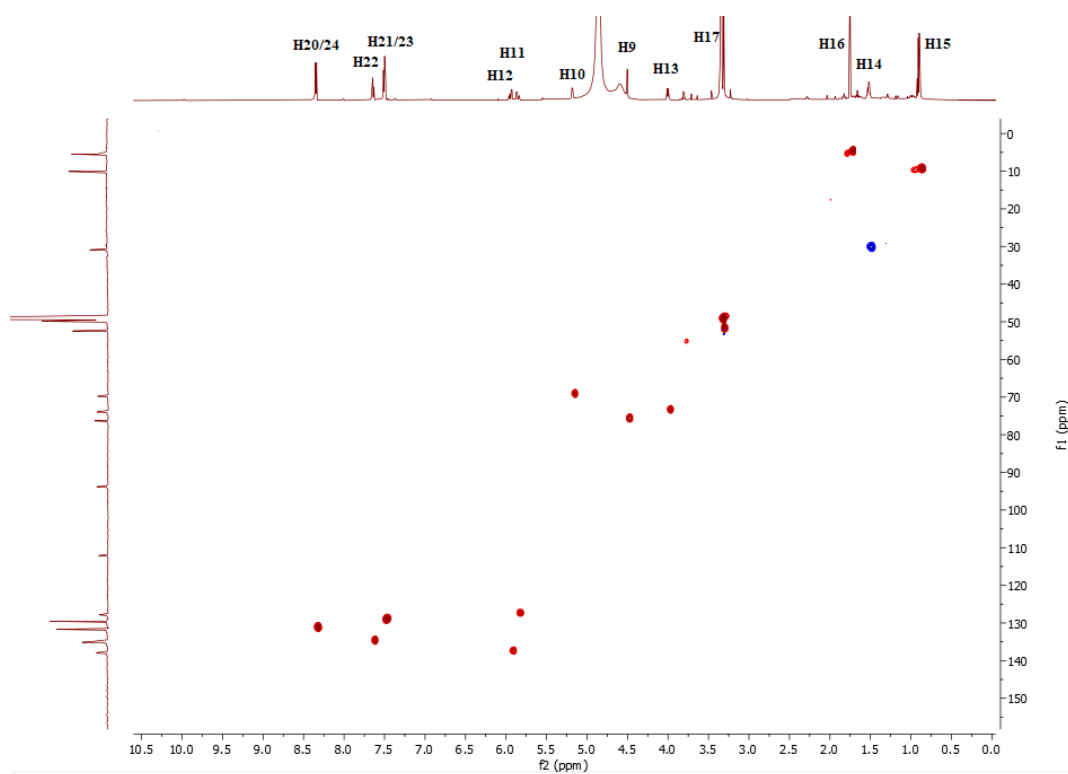


Figure S10. HSQC spectrum of pseurotin D (2) at 600 MHz in CD₃OD

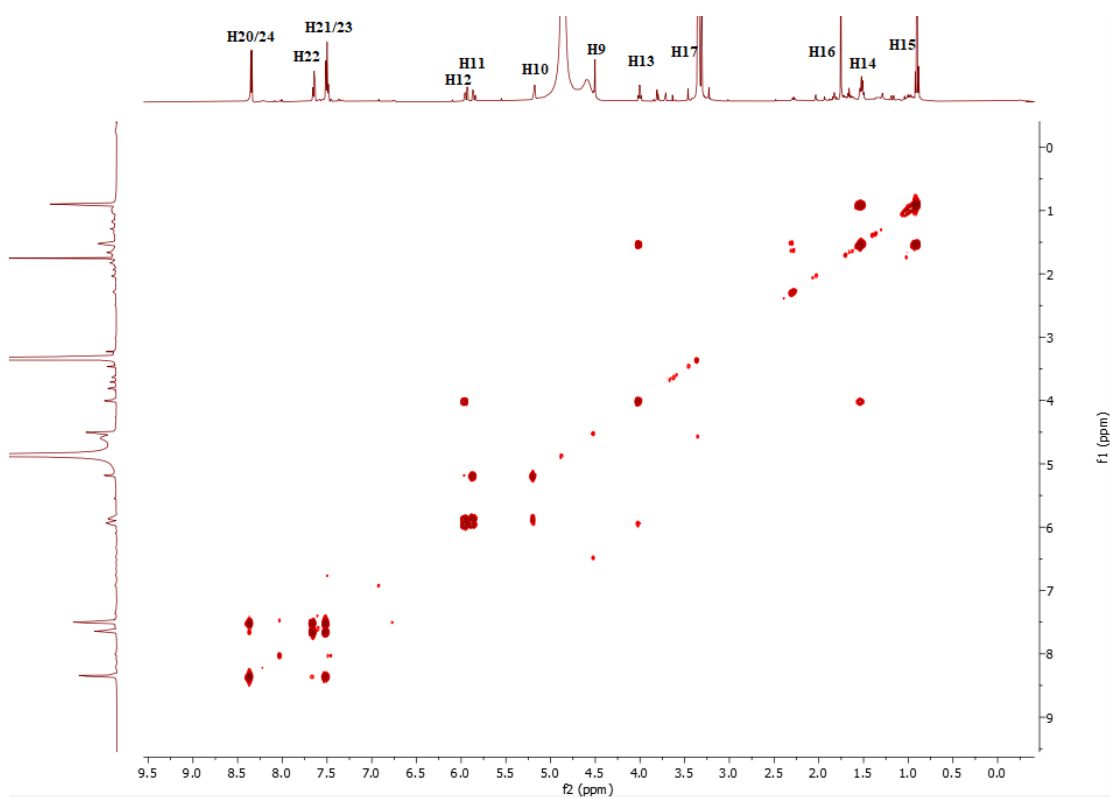


Figure S11. COSY spectrum of pseurotin D (2) at 600 MHz in CD₃OD

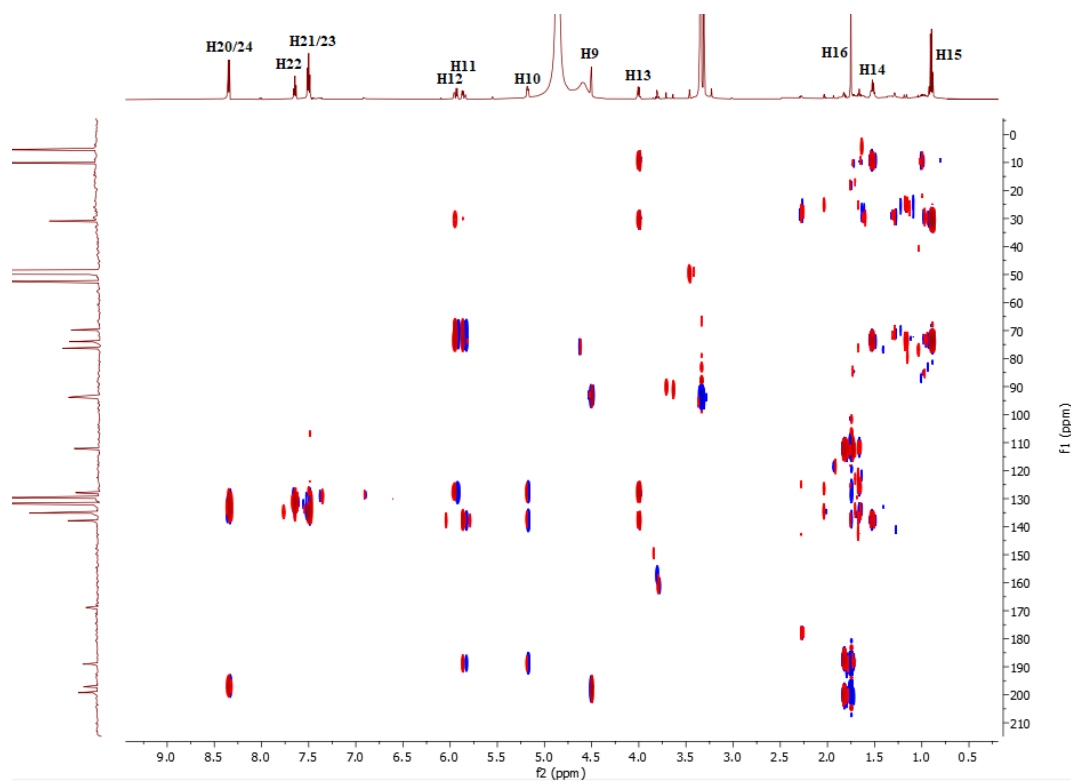


Figure S12. HMBC spectrum of pseurotin D (**2**) at 600 MHz in CD₃OD

References

- [1] X. Li *et al*, "Metabolites from *Aspergillus fumigatus*, an endophytic fungus associated with *Melia azedarach*, and their antifungal, antifeedant, and toxic activities," *J. Agric. Food Chem.*, vol. 60, (13), pp. 3424-3431, 2012.
- [2] Q. Lu *et al*, "Bioactive metabolites from the mycelia of the basidiomycete *Hericium erinaceum*," *Natural Product Research*, vol. 28, (16), pp. 1288-1292, 2014.
- [3] D. Copmans *et al*, "Zebrafish-based discovery of antiseizure compounds from the Red Sea: pseurotin A2 and azaspirofuran A," *ACS Chemical Neuroscience*, vol. 9, (7), pp. 1652-1662, 2018.