

Supporting Information

Discovery, Antitumor Activity and Fermentation Optimization of Roquefortines from Marine-derived Fungi

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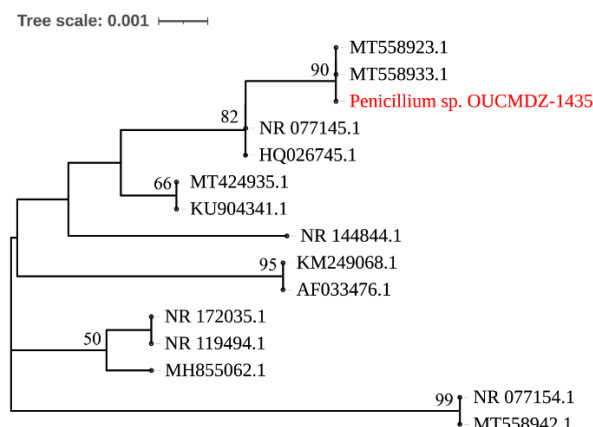


Figure S1.: Phylogenetic relationship based on ITS rDNA gene sequences using the neighbor-joining method. The scale bar represents 0.001 substitutions per nucleotide. Strain Number Notes: *Penicillium goetzii* isolate 2010F20 (MT558933.1), *Penicillium rubens* isolate 2010F5 (MT558923.1), *Penicillium chrysogenum* CBS 306.48 (NR_077145.1), *Penicillium chrysogenum* strain ATCC 10106 (HQ026745.1), *Penicillium fimorum* strain DTO149-B8 (MT424935.1), *Penicillium fimorum* strain CBS 140575 (KU904341.1), *Penicillium compactum* CGMCC 3.15411 (NR_144844.1), *Penicillium cellarum* isolate F727 (KM249068.1), *Penicillium aurantiogriseum* strain NRRL 971 (AF033476.1), *Penicillium speluncae* DAOMC 251701 (NR_172035.1), *Penicillium solitum* FRR 937 (NR_119494.1), *Penicillium fuscoglaucum* culture CBS:261.29 (MH855062.1), *Penicillium expansum* ATCC 7861 (NR_077154.1), *Penicillium fimorum* isolate 2011F12 (MT558942.1).

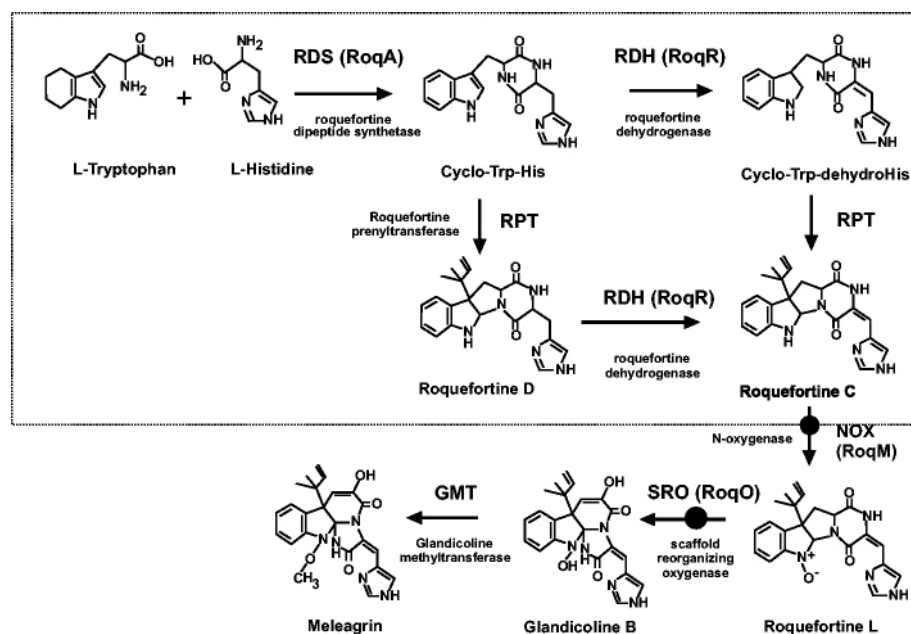


Figure S2. The biosynthetic pathway of diketopiperazine alkaloids¹

¹Kosalková, K.; Domínguez-Santos, R. A natural short pathway synthesizes roquefortine C but not meleagrins in three different *Penicillium roqueforti* strains. *Appl Microbiol Biot* 2015, 99, 7601-7612.

Figure S3. ^1H (400MHz)-NMR spectrum of compound **1** in DMSO

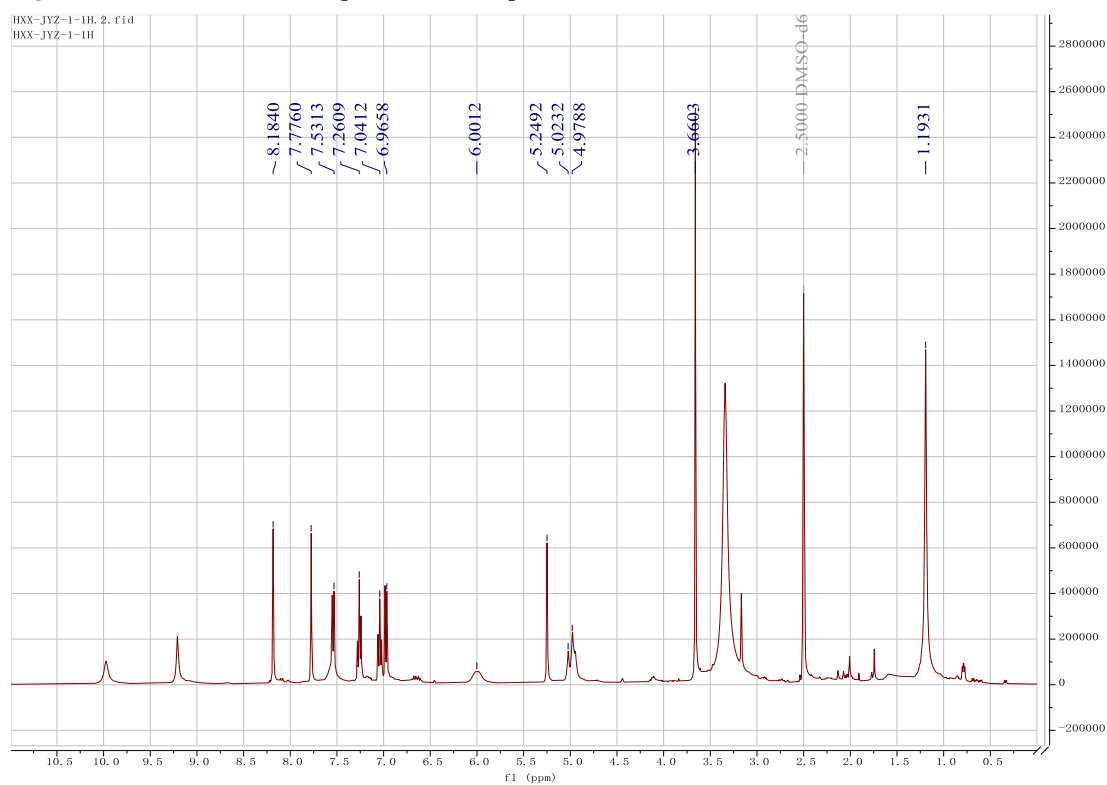


Figure S4. ^{13}C (125MHz)-NMR spectrum of compound **1** in DMSO

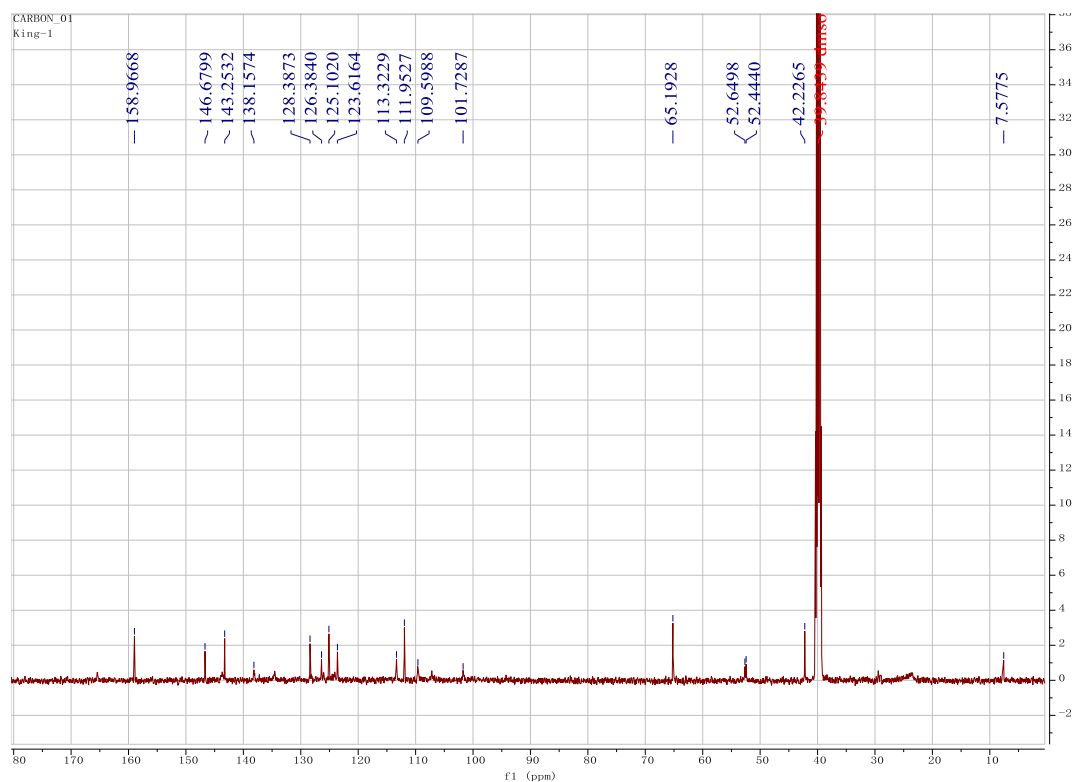


Figure S5. ^1H (500MHz)-NMR spectrum of compound **2** in DMSO

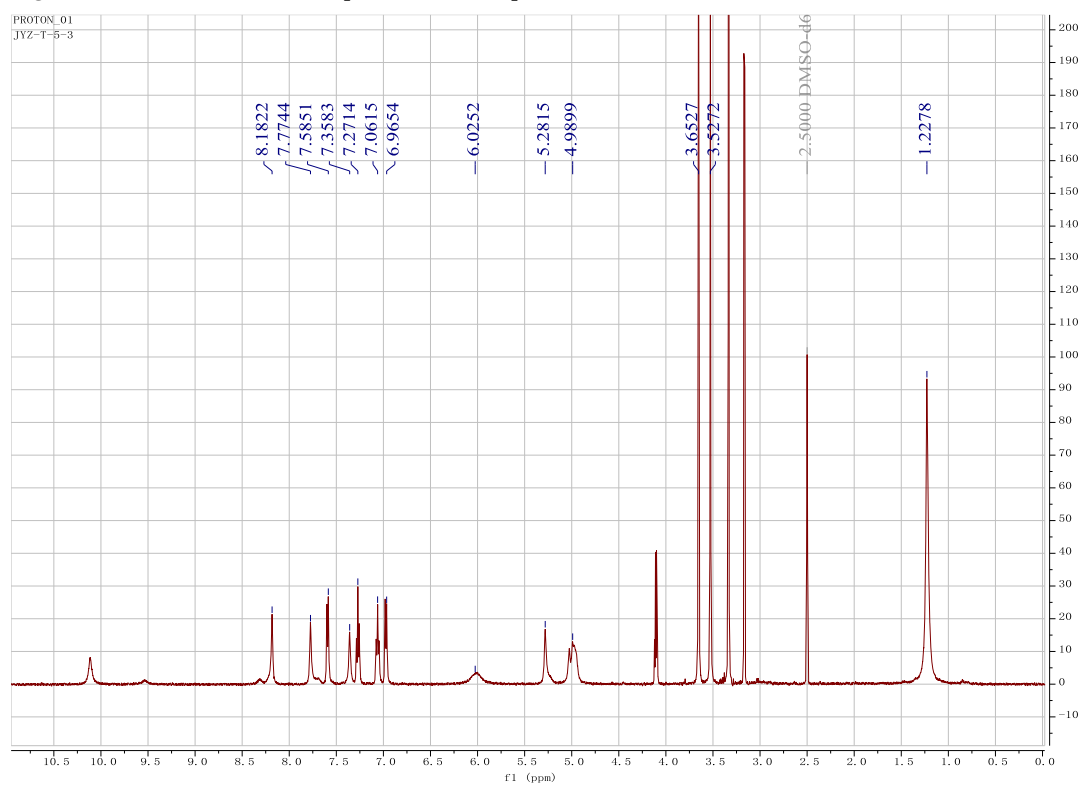


Figure S6. ^{13}C (125MHz)-NMR spectrum of compound **2** in DMSO

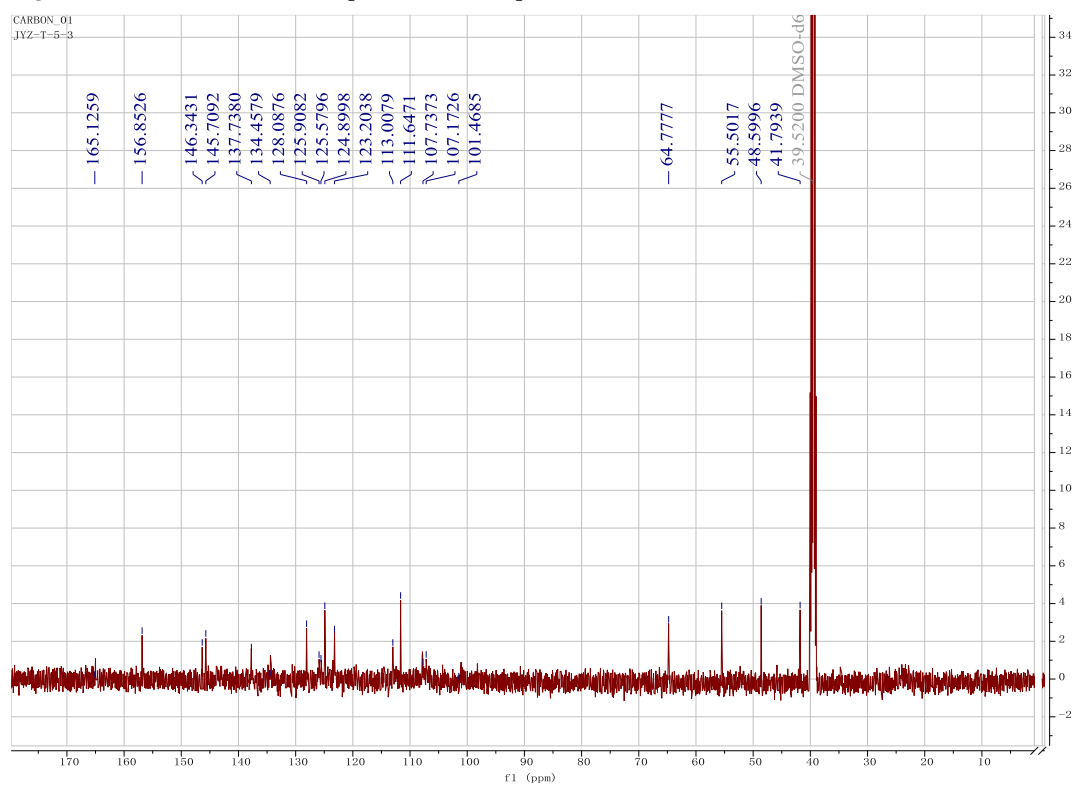


Table S1. ¹H and ¹³C NMR Data for Compounds **1** and **2** (¹H 500MHz, ¹³C 150 MHz, DMSO-d₆, TMS, δ ppm)

Position	Compound 1		Compound 2	
	δ _C	δ _H (J in Hz)	δ _C	δ _H (J in Hz)
1		3.66, s		3.65, s
2	101.7,C		101.1,C	
3	52.5,C		55.5,C	
4	125.1,CH	7.53,d	124.9,CH	7.59,d
4a	126.4,C		125.5,C	
5	123.7,CH	7.04,t	123.2,CH	7.06,t
6	128.4,CH	7.26,t	128.1,CH	7.27,t
7	111.9,CH	6.97, d	111.6,CH	6.97, d
7a	146.6,C		146.3,C	
8	109.3,CH	5.25,s	107.7,CH	5.28,s
9	143.2,CH		142.9,C	
9'			64.7,CH ₃	3.53,s
10	158.9,C		158.8,C	
11				
12	123.9,C	3.82, s	124.8,C	
13	165.4,C		165.0,C	
14				10.11,s
15	107.2,CH	8.18,s	107.1,CH	8.18,s
16	126.3,C		125.9,C	
17				
18	134.5,CH	7.34,s	134.4,CH	7.36,s
19				
20	138.5,CH	7.78,s	137.7,CH	7.78,s
21	41.9,C		41.8,C	
22	143.7,CH	6.00	143.8,CH	6.01,s
23	113.3,CH	4.98	113.0,CH	5.00
		5.02		5.28
24	23.7,CH ₃	1.19,s	24.0,CH ₃	1.23,s
25	23.7,CH ₃	1.19,s	24.0,CH ₃	1.23,s