Supporting Information

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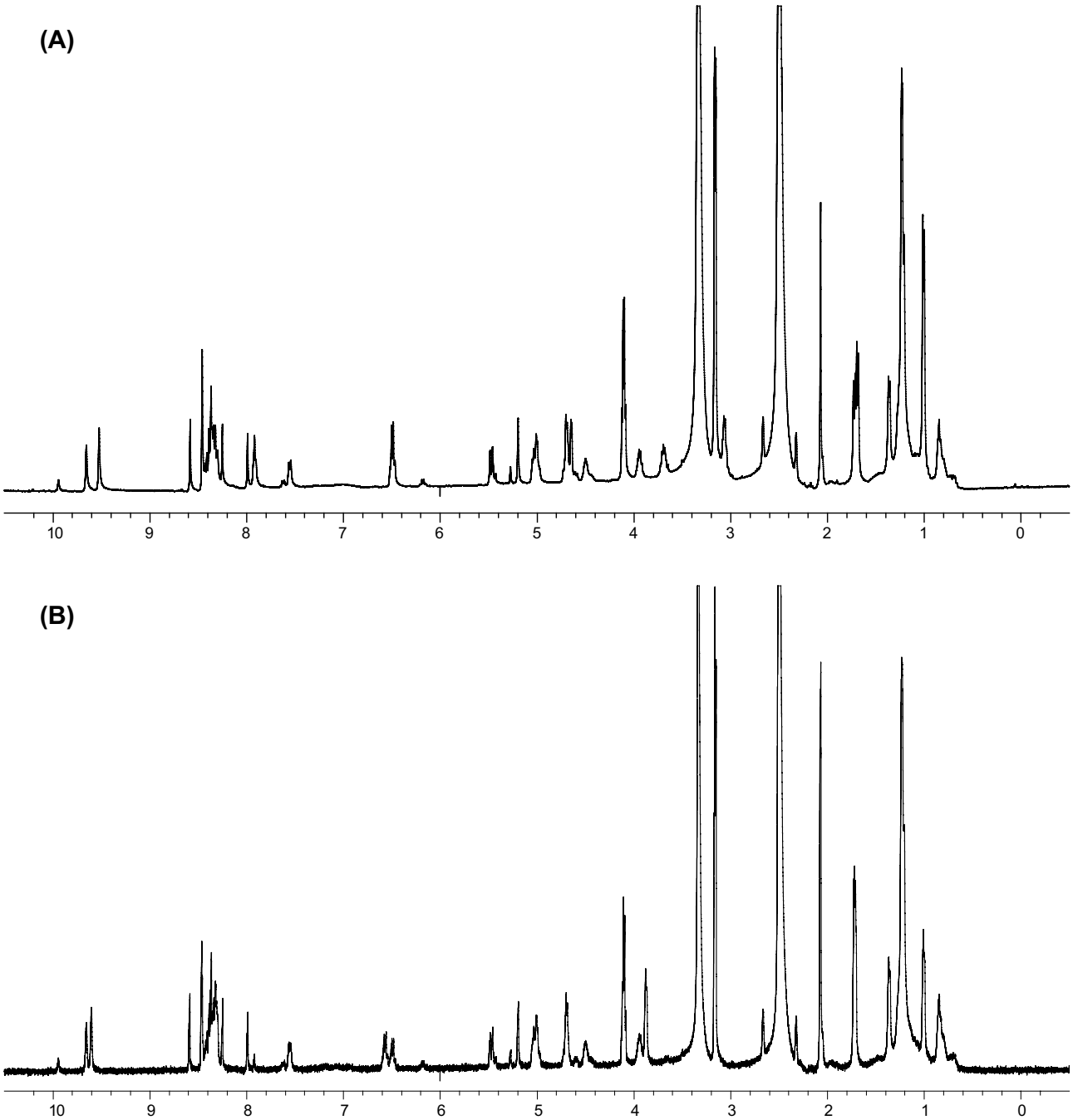

Fig. S1. Characterization of thiocillins by NMR. ^{1}H-NMR spectra of thiocillin I (compound **3**) (*A*) and YM-266183 [compound **6**, also known as QN3323A (1)] (*B*) are shown. Compounds were dissolved in DMSO-d_6, and data were collected on a Varian 400-MHz NMR spectrometer. Spectrum *A* contains minor peaks that are consistent with the presence of QN3323Y1 (1), which differs from 3 only in the olefin geometry at Dhb4, as a minor product.

1. Kamigiri K, *et al.* (2006) US Patent 7030085 (April 18, 2006).

Table S1. Primers used in this study

Primer	Sequence	Comments
LCW001	5′-gtacggatcccatactcccagattatttgcagtcgtaac-3′	BamHI (LF-5′)
LCW002	5′-gtacgtcgacgagaggagtatacatatgcttactg-3′	SalI (LF-3′)
LCW010	5′-gtacggatccgaaataaactctatttcagaaattgag-3′	BamHI (cam1–5′)
LCW011	5′-gtacctcgaggtccgattgttcggacacacctaagc-3′	XhoI (cam1–3′)
LCW012	5′-gtacggatccgccaactcccttcagttcatttacagg-3′	BamHI (cam2–5′)
LCW013	5′-gtacctcgagcttactcttcaataaatcagggaacttg-3′	XhoI (cam2–3′)
LCW014	5′-gtacggatccggacgattatgaaagtcctttcgcag-3′	BamHI (cam3–5′)
LCW015	5′-gtacctcgagccatcgtccgtacaagtgaataattc-3′	XhoI (cam3–3′)
LCW028	5′-gctgaattcataagcttatactagtgtc-3′	IMX_check1_3′
LCW029	5′-gtgtagcatgtctcattcaattttgagg-3′	IMX_check2_5′
LCW032	5′-gtgatataacatgaaaccaataaactatg-3′	IM2_check1_5′
LCW033	5′-ctacaaggtgtgagaccgatttttcaac-3′	IM2_check2_3′
LCW034	5′-catgaataactataccgttatgaaatcc-3′	IM3_check1_5′
LCW035	5′-cacctacaagaaatttttggaaactaac-3′	IM3_check2_3′
LCW040	5′-gttagaagactatgatgtaccgtggatc-3′	IM4_check1_5′
LCW041	5′-ccgcggtttgatcgactacgatgatatc-3′	IM4_check2_3′
LCW042	5′-caaagcacgctacatctgatgagagaaac-3′	IM1_check1a_5′
LCW043	5′-gtgcttacctaatcctggccctatctta-3′	IM1_check2a_3′

Restriction sites are underlined.

Table S2. Plasmids used in this study

Plasmid	Comments	Source
pKM082	Carries MLS resistance gene.	David Rudner, Harvard Medical School
pLW106	Derived from pKM082. Transformed into *B. cereus* ATCC14579 to generate IM1. (pKM082 + cam2)	This study
pLW105	Derived from pKM082. Transformed into *B. cereus* ATCC14579 to generate IM2. (pKM082 + cam1)	This study
pLW111	Derived from pKM082. Transformed into *B. cereus* ATCC14579 to generate IM3. (pKM082 + LF)	This study
pLW107	Derived from pKM082. Transformed into *B. cereus* ATCC14579 to generate IM4. (pKM082 + cam3)	This study

Table S3. Strains used in this study

Strain	Comments	Source
B. cereus ATCC 14579	Thiocillin producer	ATCC
B. cereus ATCC 14579 IM1	Derivative of *B. cereus* ATCC 14579 harboring pLW106 (MLS resistance)	This study
B. cereus ATCC 14579 IM2	Derivative of *B. cereus* ATCC 14579 harboring pLW105 (MLS resistance)	This study
B. cereus ATCC 14579 IM3	Derivative of *B. cereus* ATCC 14579 harboring pLW111 (MLS resistance)	This study
B. cereus ATCC 14579 IM4	Derivative of *B. cereus* ATCC 14579 harboring pLW107 (MLS resistance)	This study

Table S4. 400-MHz ^{1}H NMR data of 3 in d_6-DMSO at 25 °C

δ, ppm	Description	Integration	J, Hz
9.65	s	1	
9.52	s	1	
8.58	s	1	
8.46–8.30	m	7	
8.25	s	1	
7.99	s	1	
7.92–7.90	m	1	
7.55	d	1	7.8
6.52–6.47	m	2	
5.48	d	1	10.2
5.19	s	1	
5.05–4.97	m	2	
4.72–4.58	m	3	
4.50–4.48	m	1	
3.98–3.90	m	1	
3.75–3.65	m	1	
3.07–3.03	m	2	
2.07	s	3	
1.73–1.71	m	6	
1.37	m	3	
1.24–1.20	m	6	
1.01	d	3	6.0

s, singlet; d, doublet; t, triplet; q, quartet; br, broad; m, multiplet.

Table S5. 400-MHz ^{1}H NMR data of 6 in d_6-DMSO at 25 °C

δ, ppm	Description	Integration	J, Hz
9.65	s	1	
9.60	s	1	
8.58	s	1	
8.46–8.32	m	8	
8.25	s	1	
7.99	s	1	
7.55	d	1	8.0
6.58–6.55	m	1	
6.50–6.47	m	1	
5.48–5.44	m	1	
5.19	s	1	
5.04–4.98	m	2	
4.70–4.67	m	2	
4.51–4.98	m	1	
3.96–3.91	m	1	
3.88–3.86	m	2	
2.07	s	3	
1.73–1.71	m	6	
1.37	m	3	
1.24–1.20	m	6	
1.01	d	3	6.0

s, singlet; d, doublet; t, triplet; q, quartet; br, broad; m, multiplet.