

Supplementary Materials for

New Antibacterial Bagremycins F and G from Marine-derived *Streptomyces* sp. ZZ745

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Table S1. Sequences producing significant alignments of strain ZZ745

Accession	Description	Max score	Total score	Query coverage	Evalue	Ident
KC306504.1	<i>Streptomyces</i> sp. NEAU-YX9 16S ribosomal RNA gene, partial sequence	2734	2734	97%	0.0	99%
JX047057.1	<i>Streptomyces</i> sp. OAct 127 16S ribosomal RNA gene, partial sequence	2730	2730	96%	0.0	99%
KU877596.1	<i>Streptomyces filipinensis</i> strain WJA67 16S ribosomal RNA gene, partial sequence	2689	2689	94%	0.0	100%
KU877593.1	<i>Streptomyces filipinensis</i> strain WJA60 16S ribosomal RNA gene, partial sequence	2689	2689	94%	0.0	100%
KU877590.1	<i>Streptomyces filipinensis</i> strain WJA55 16S ribosomal RNA gene, partial sequence	2687	2687	94%	0.0	100%
LC381941.1	<i>Streptomyces</i> sp. MR 602 gene for 16S ribosomal RNA, partial sequence	2673	2673	96%	0.0	99%

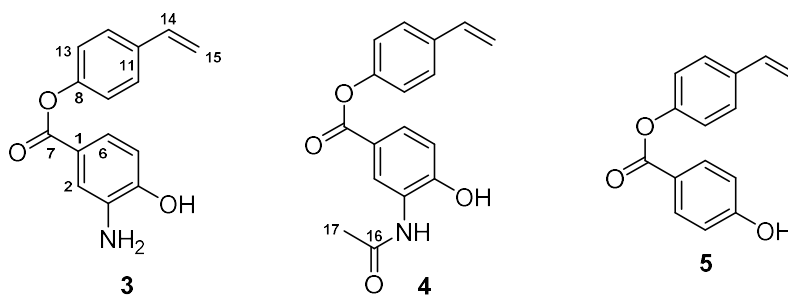


Table S2. NMR data of bagremycins A (**3**), B (**4**), and E (**5**) (in DMSO-*d*₆)

No.	3		4		5	
	¹³ C, type	¹ H (<i>J</i> in Hz)	¹³ C, type	¹ H (<i>J</i> , Hz)	¹³ C, type	¹ H (<i>J</i> , Hz)
1	119.2, C	–	119.1, C	–	119.0, C	–
2	114.9, CH	7.37, d (2.0)	123.8, CH	8.64, d (2.0)	132.2, CH	7.97, d (8.8)
3	137.0, C	–	127.0, C	–	115.7, CH	6.91, d (8.8)
4	149.9, C	–	153.0, C	–	163.0, C	–
5	113.8, CH	6.76, d (8.3)	115.3, CH	7.01, d (8.5)	115.7, CH	6.91, d (8.8)
6	119.8, CH	7.25, dd (8.3, 2.0)	126.6, CH	7.74, dd (8.5, 2.0)	132.2, CH	7.97, d (8.8)
7	164.9, C	–	164.3, C	–	164.3, C	–
8	150.6, C	–	150.4, C	–	150.4, C	–
9	122.2, CH	7.17, d (8.5)	122.1, CH	7.20, d (8.6)	122.2, CH	7.21, d (8.6)
10	127.1, CH	7.53, d (8.5)	127.2, CH	7.54, d (8.6)	127.1, CH	7.53, d (8.6)
11	134.6, C	–	134.8, C	–	134.7, C	–
12	127.1, CH	7.53, d (8.5)	127.2, CH	7.54, d (8.6)	127.1, CH	7.52, d (8.6)
13	122.2, CH	7.17, d (8.5)	122.1, CH	7.20, d (8.6)	122.2, CH	7.21, d (8.6)
14	135.8, CH	6.73, dd (17.6, 11.0)	135.8, CH	6.74, dd (17.7, 11.0)	135.8, CH	6.73, dd (17.7, 11.0)
15	114.3, CH ₂	5.26, dd (11.0, 0.7); 5.81, dd (17.6, 0.7)	114.4, CH ₂	5.26, dd (11.0, 0.6); 5.82, dd (17.7, 0.6)	114.4, CH ₂	5.26, dd (11.0, 0.7); 5.81, dd (17.7, 0.7)
16			169.1, C	–		
17			23.7, CH ₃	2.12, s		
NH				9.38, s		

Figure S1. Colony picture of strains ZZ745

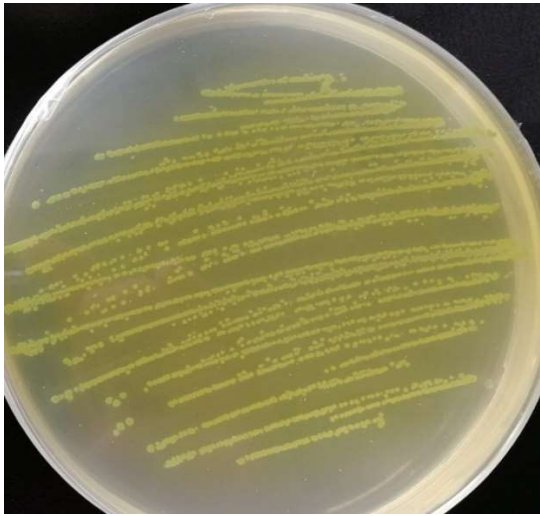


Figure S2. 16S rDNA sequence of *Streptomyces* sp. ZZ745

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GAGCCTCCCAGGCATCTGGGAGGCTGTAAAGCTCCGGCGGTGAAGGATGAGCCCGCGGCCTA
TCAGCTTGTTGGTGAGGTAATGGCTCACCAAGGCGACGACGGGTAGCCGGCCTGAGAGGGCG
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Figure S3. ^1H NMR spectrum of bagremycin F (**1**, 500 MHz, in $\text{DMSO-}d_6$)

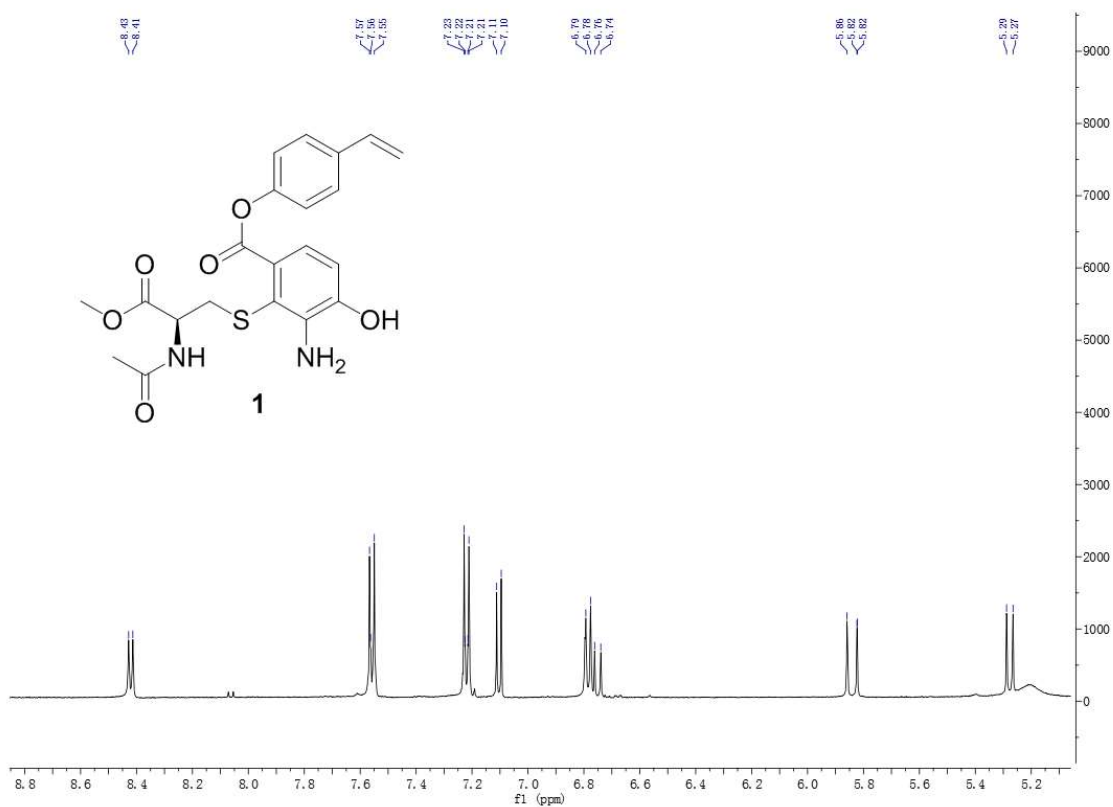
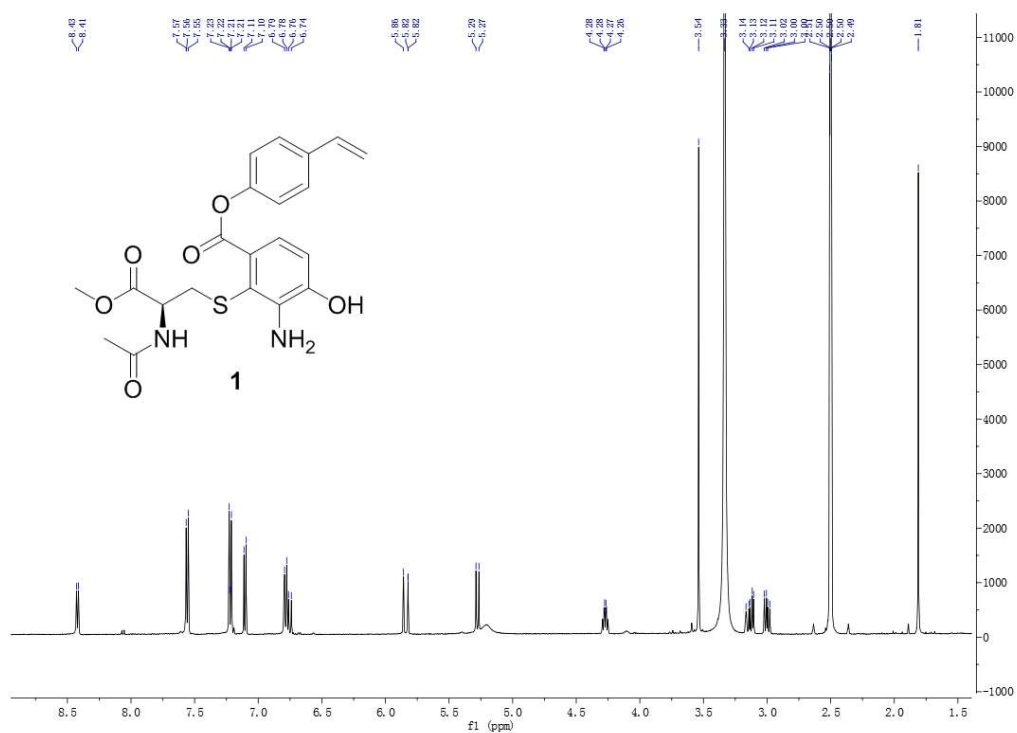


Figure S4. ^{13}C NMR spectrum of bagremycin F (**1**, 125 MHz, in $\text{DMSO-}d_6$)

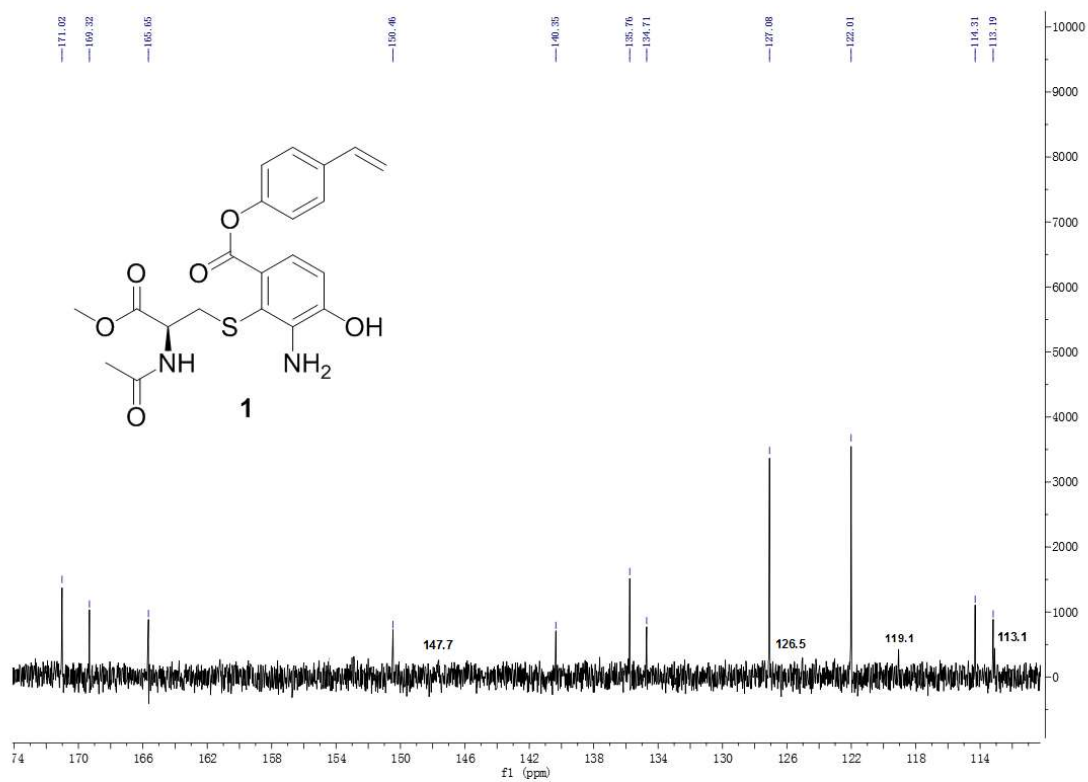
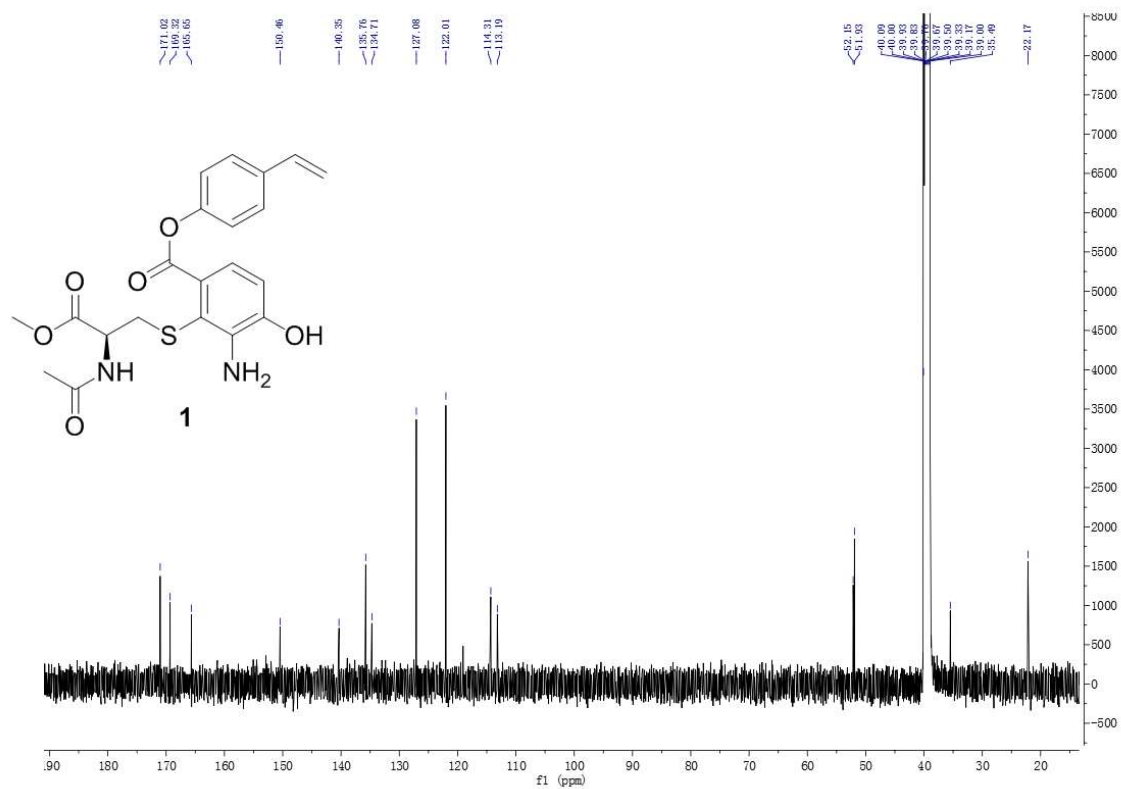


Figure S5. HSQC spectrum of bagremycin F (**1**, in DMSO-*d*₆)

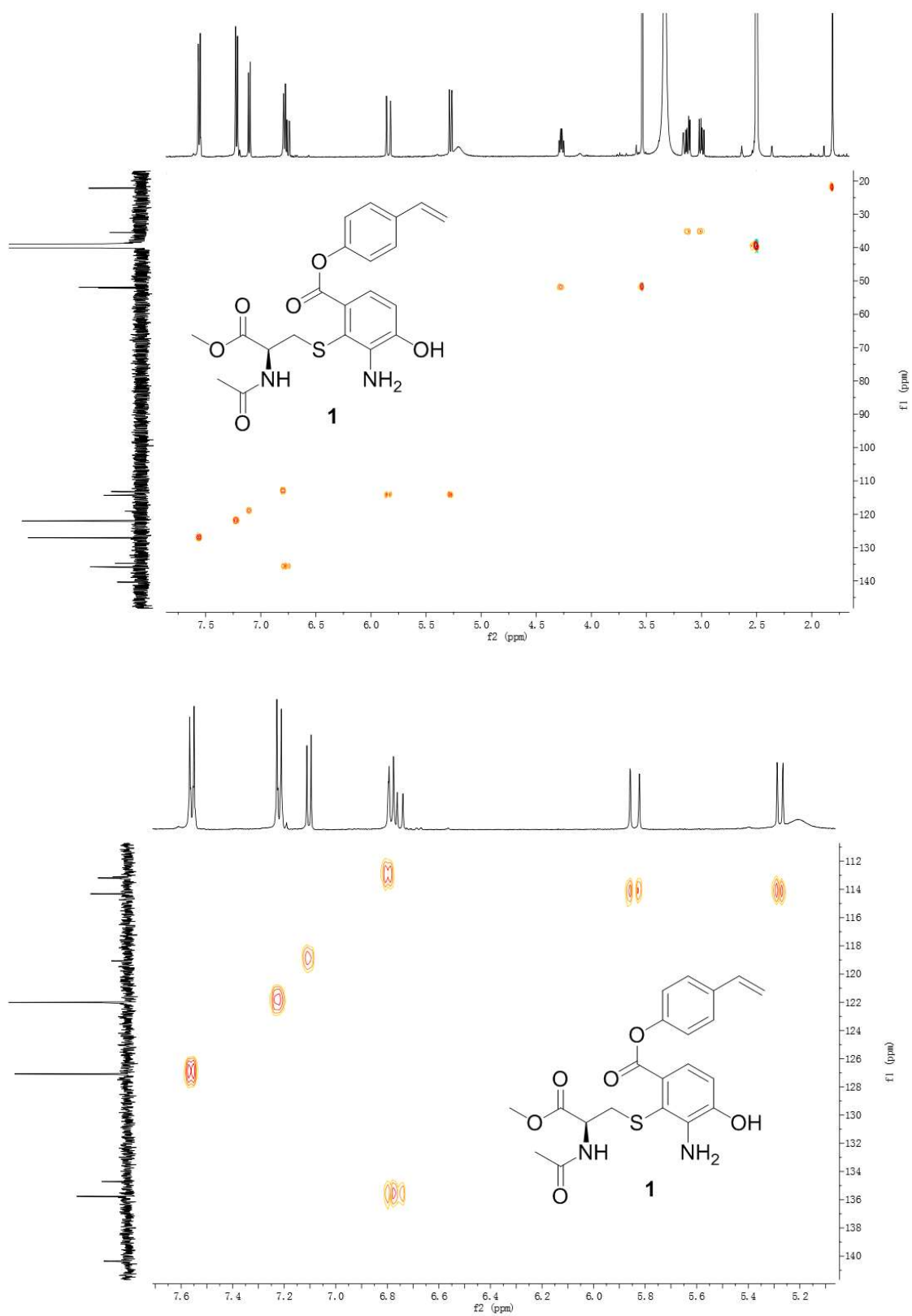


Figure S6. HMBC spectrum of bagremycin F (**1**, in DMSO-*d*₆)

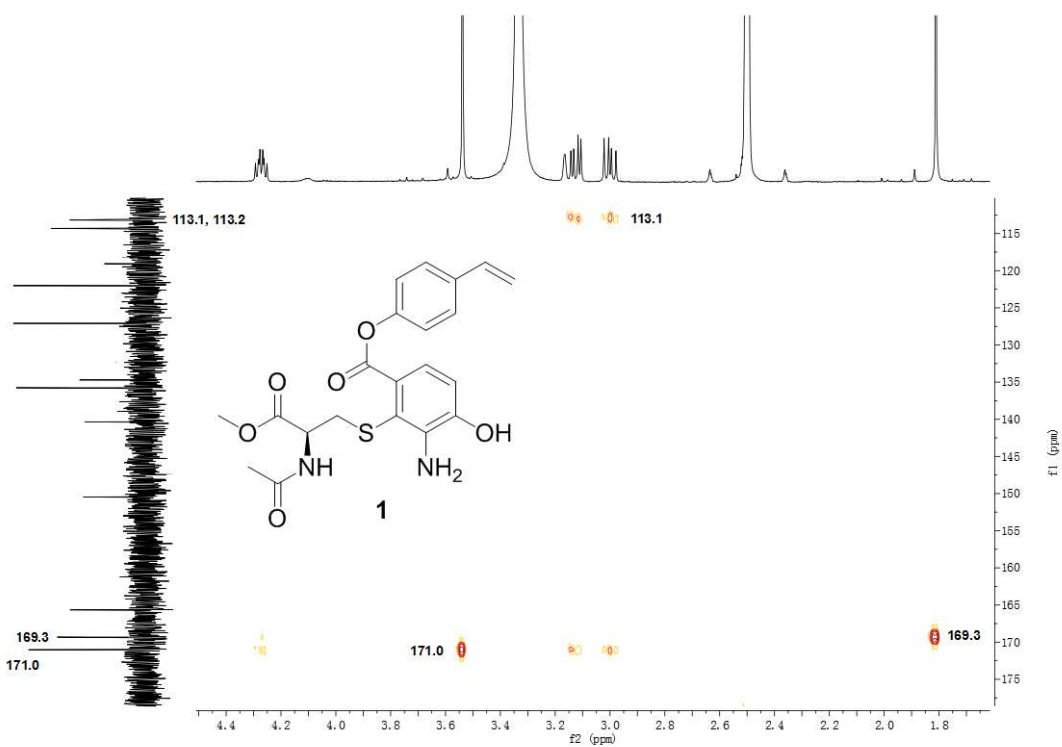
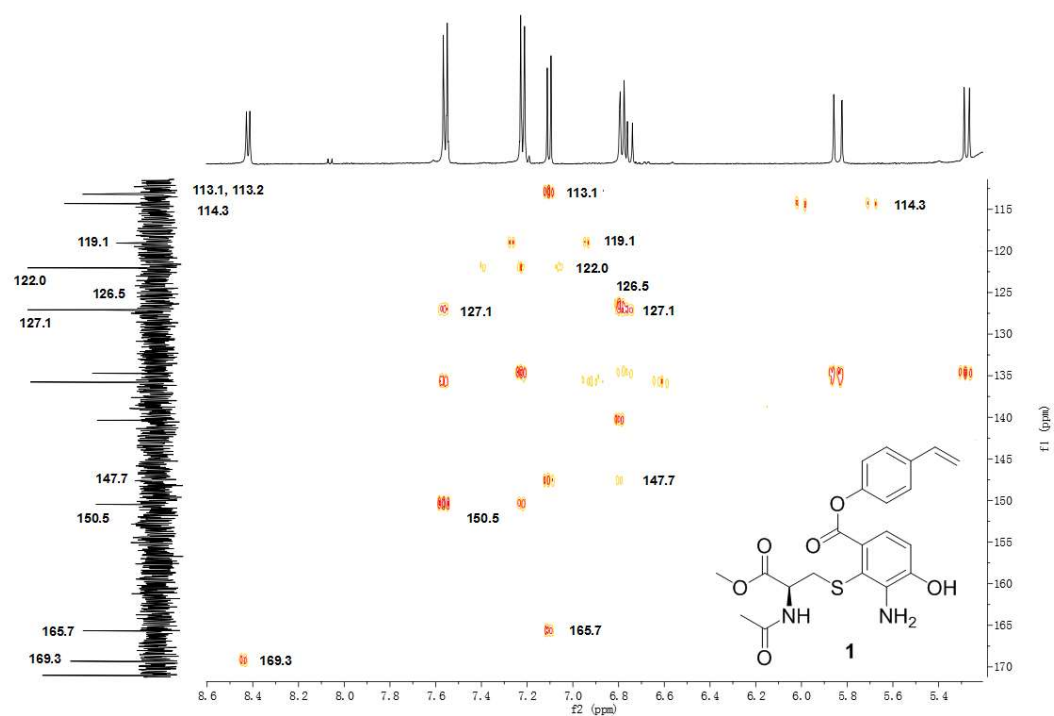


Figure S7. HRESIMS spectrum of bagremycin F (1)

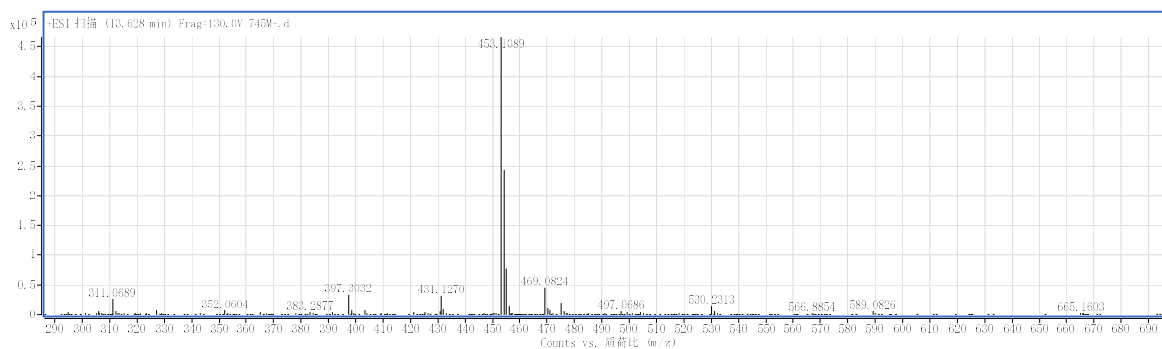


Figure S8. UV spectrum of bagremycin F (1)

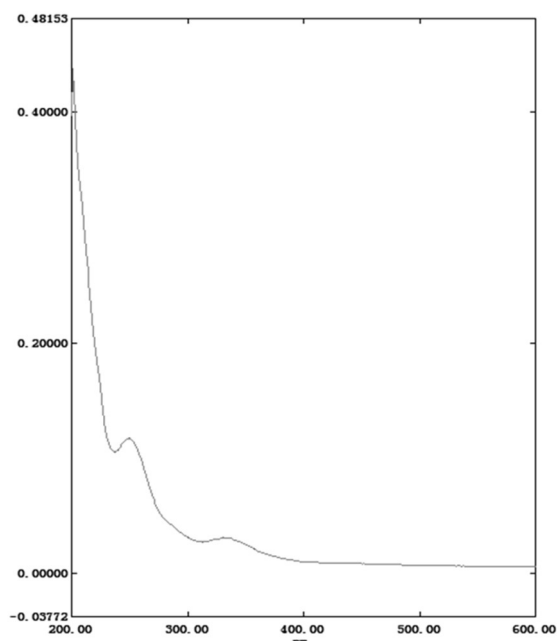


Figure S9. IR spectrum of bagremycin F (1)

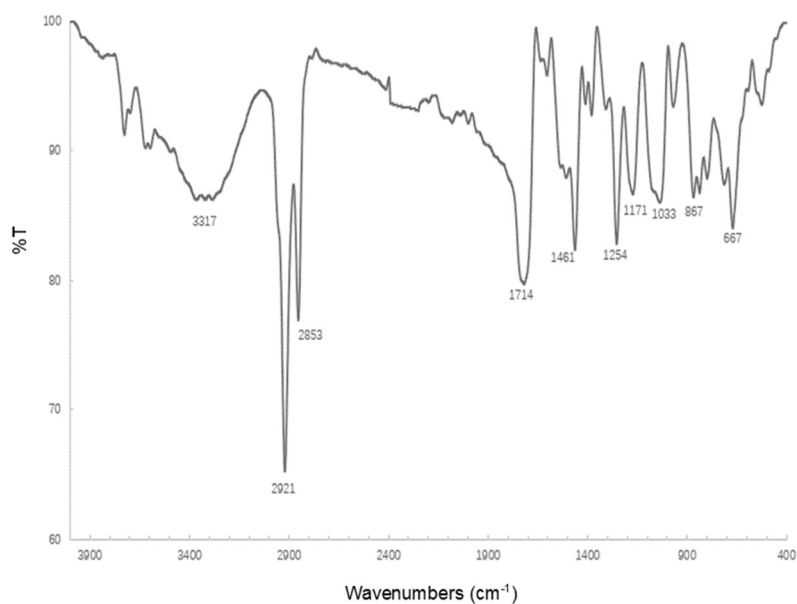


Figure S10. ^1H NMR spectrum of bagremycin G (**2**, 500 MHz, in $\text{DMSO-}d_6$)

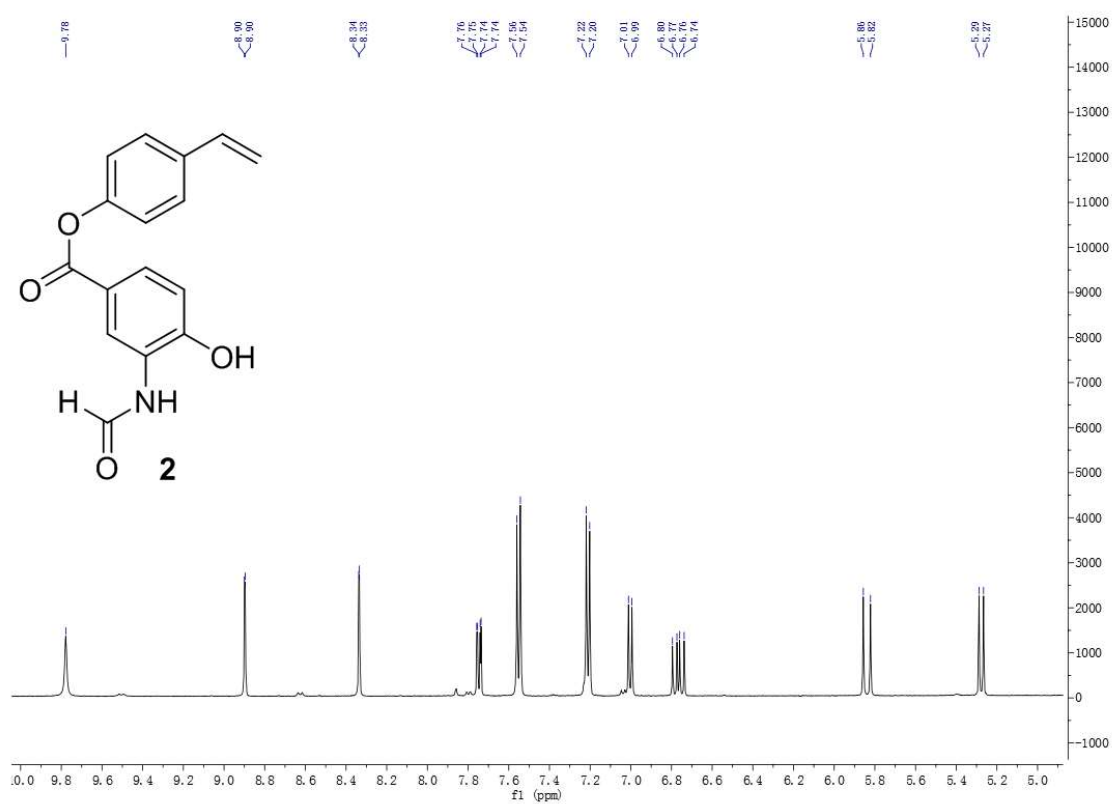
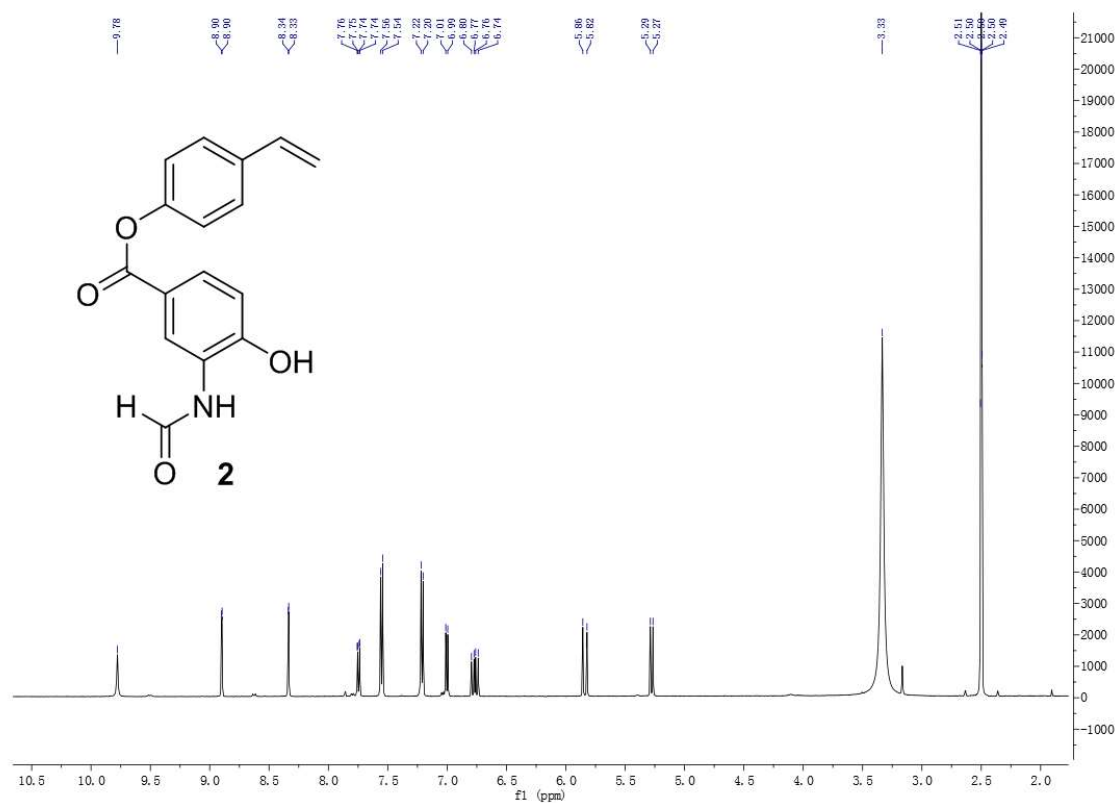


Figure S11. ^{13}C NMR spectrum of bagremycin G (**2**, 125 MHz, in $\text{DMSO-}d_6$)

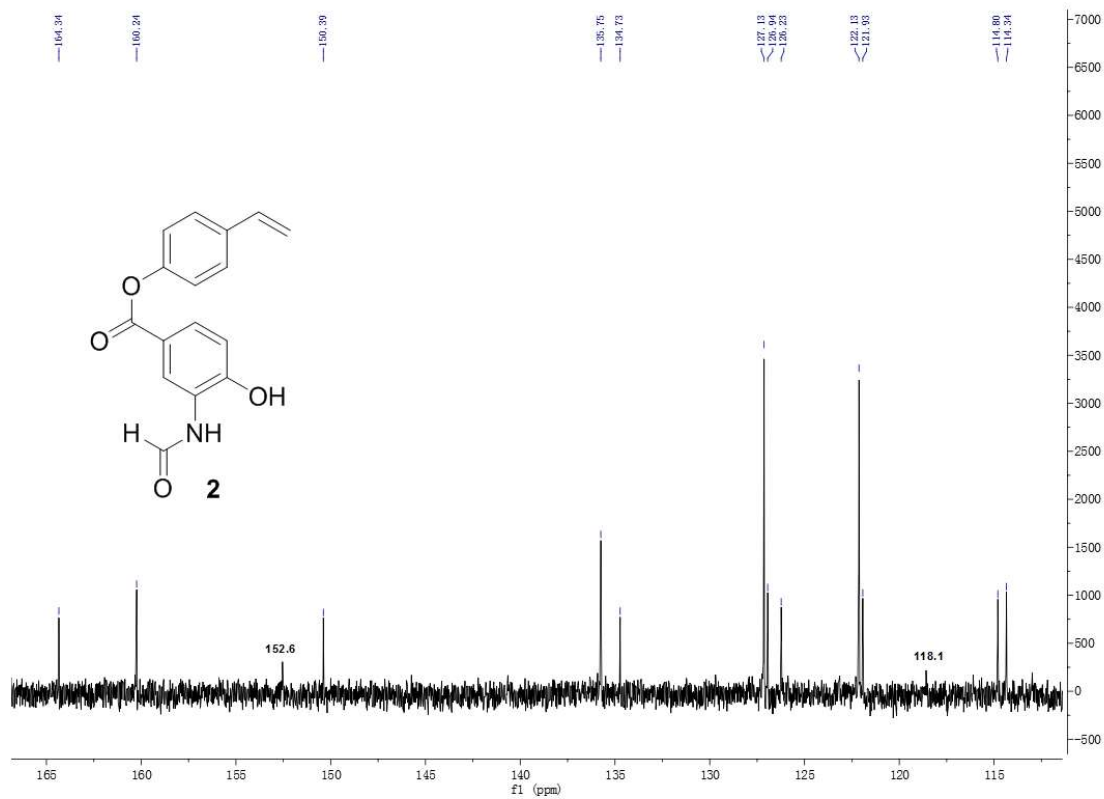
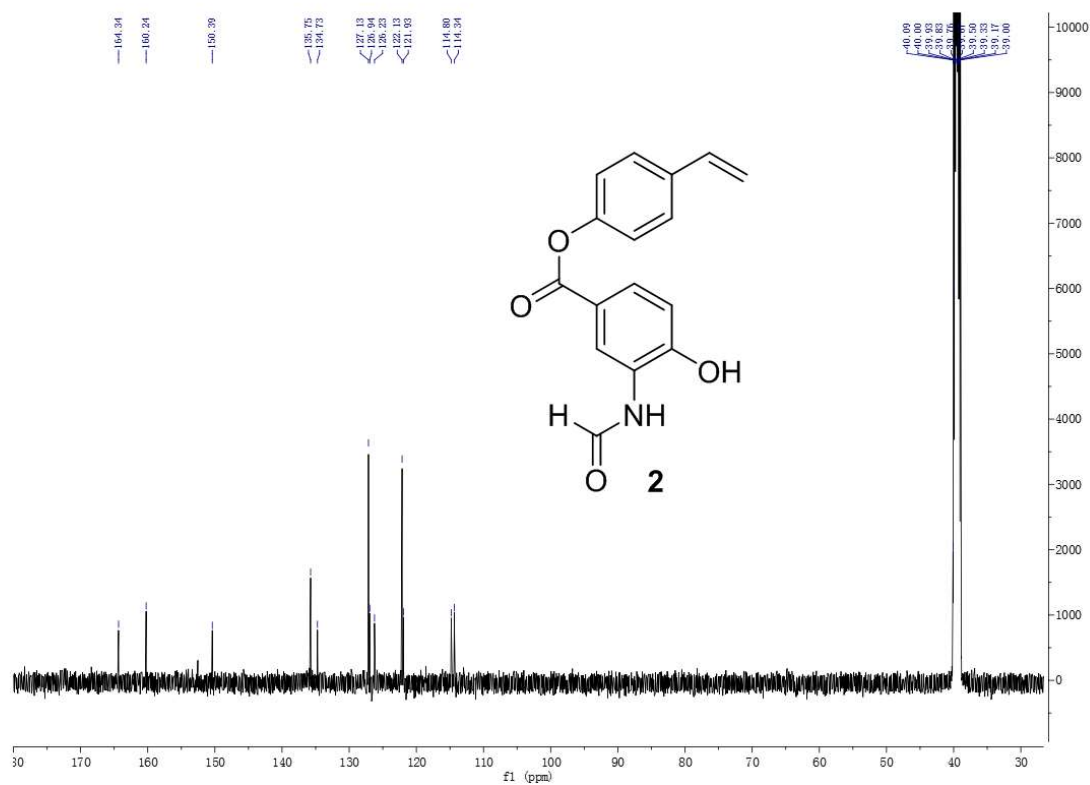


Figure S12. HSQC spectrum of bagremycin G (**2**, in DMSO-*d*₆)

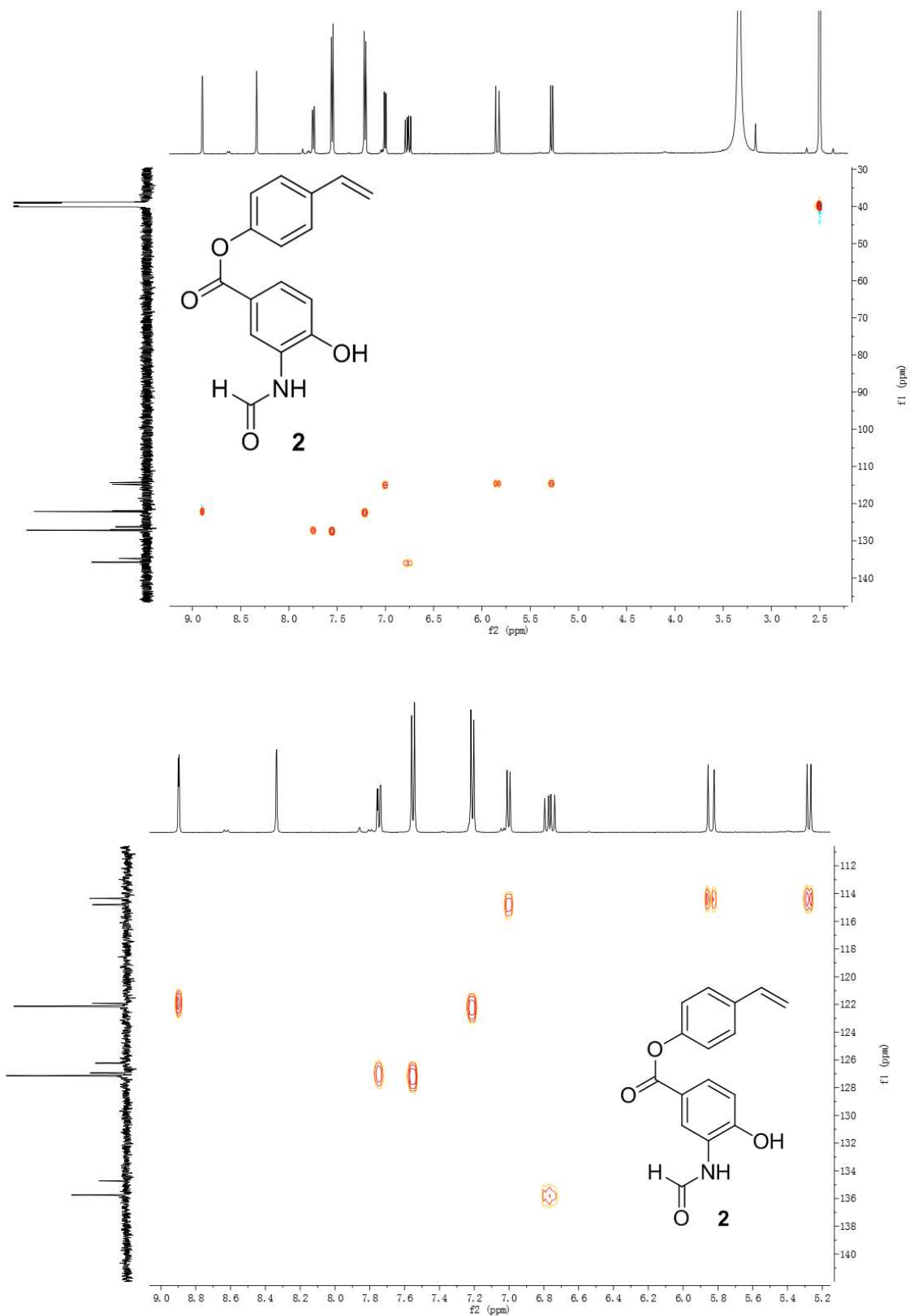


Figure S13. HMBC spectrum of bagremycin G (**2**, in DMSO-*d*₆)

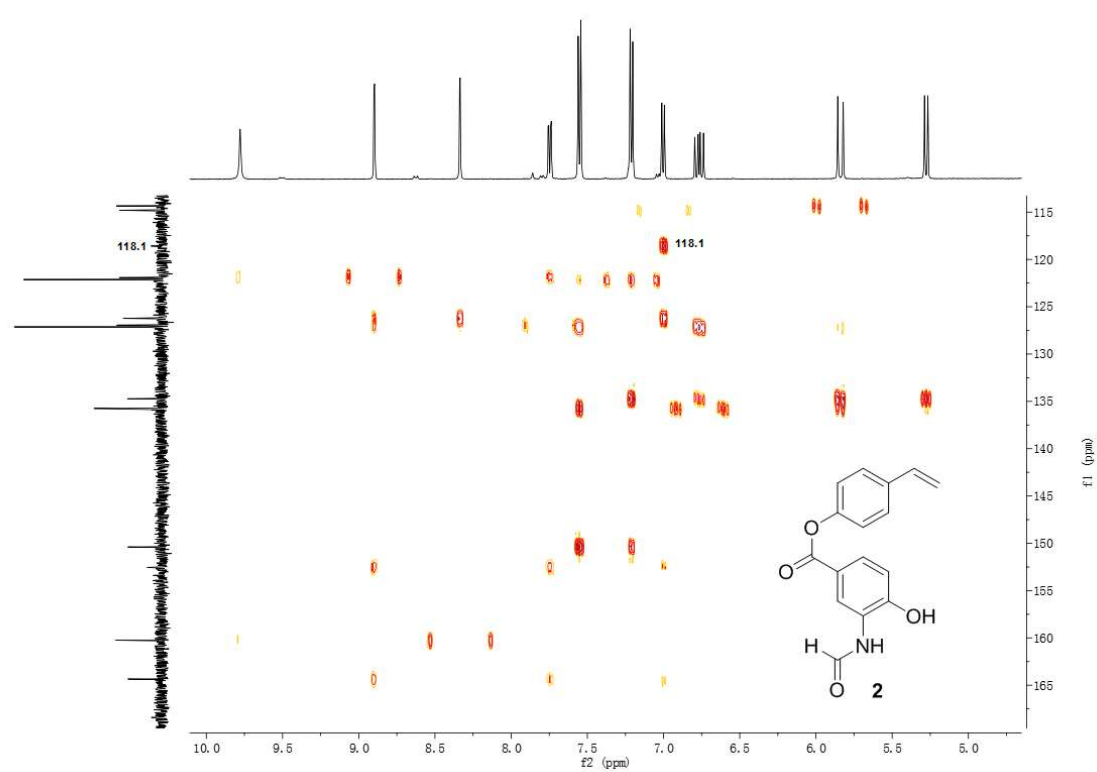
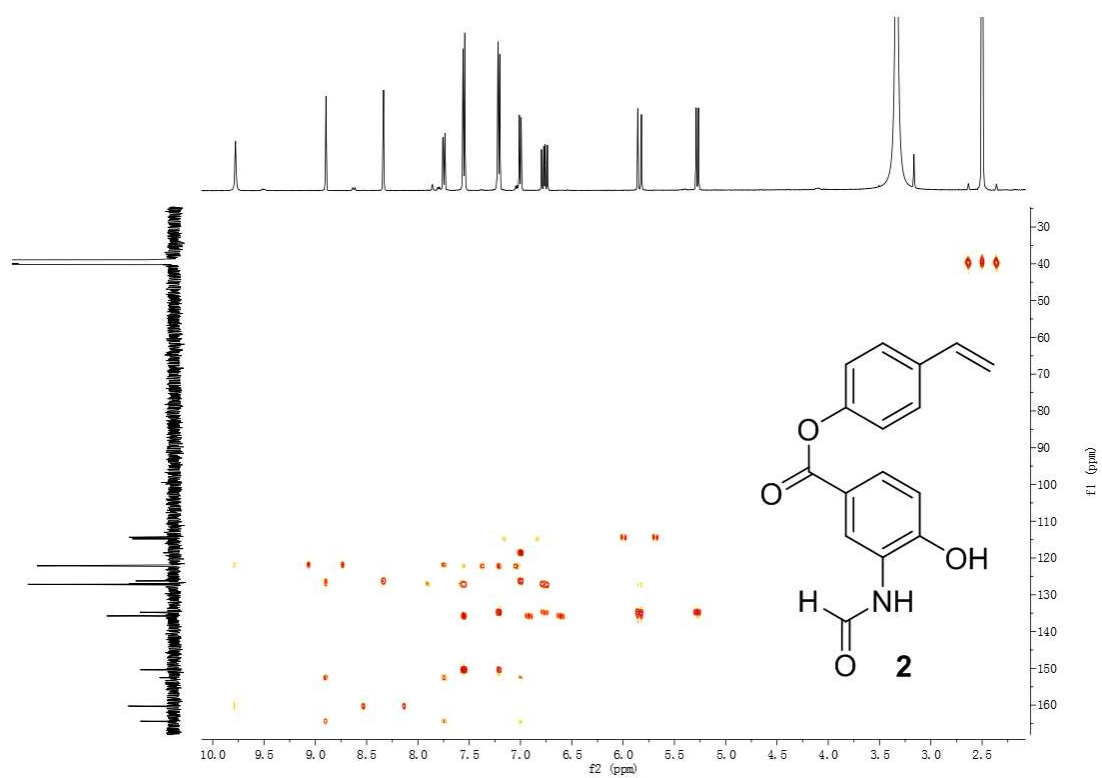


Figure S14. HRESIMS spectrum of bagremycin G (2)

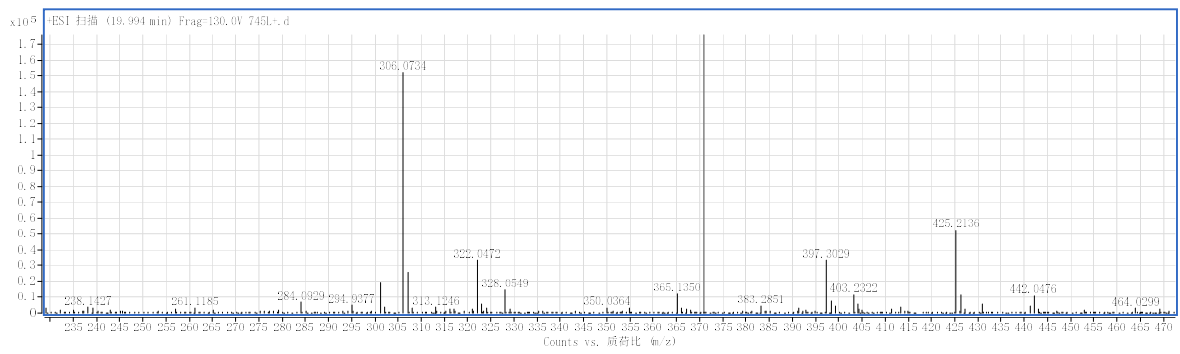


Figure S15. UV spectrum of bagremycin G (2)

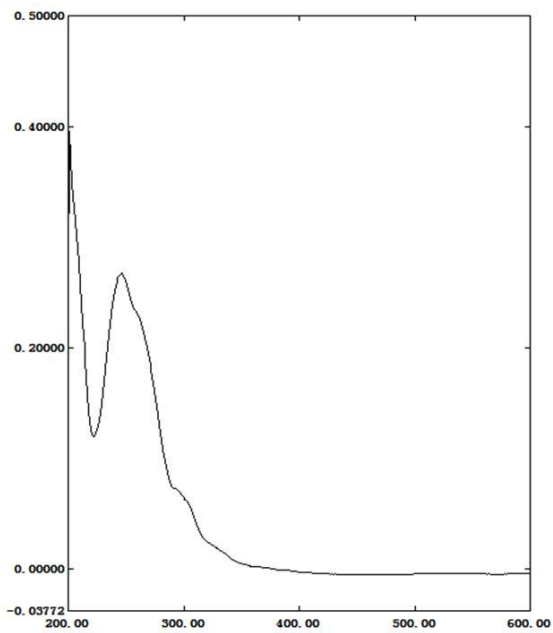


Figure S16. IR spectrum of bagremycin G (2)

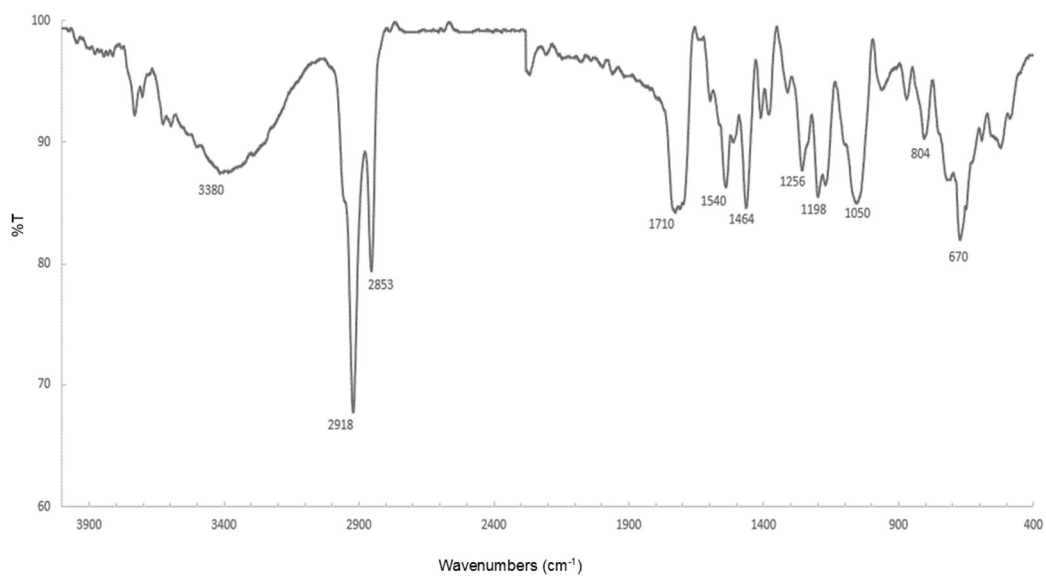


Figure S17. ^1H NMR spectrum of bagremycin A (**3**, 500 MHz, in $\text{DMSO-}d_6$)

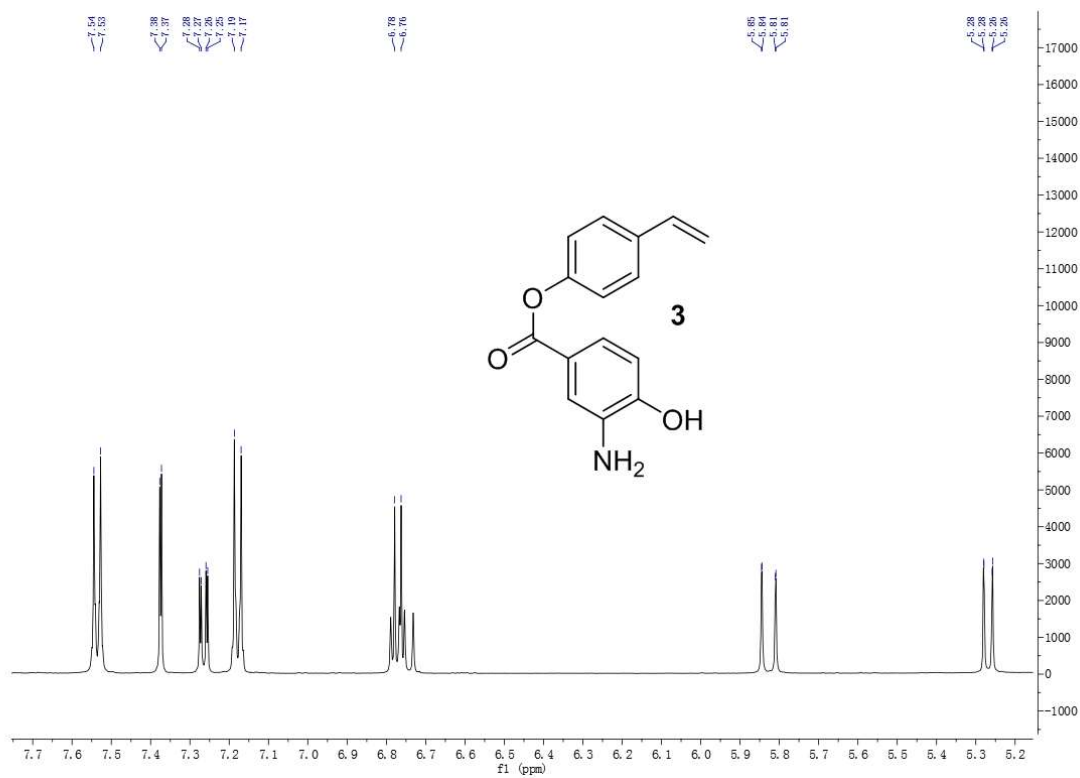
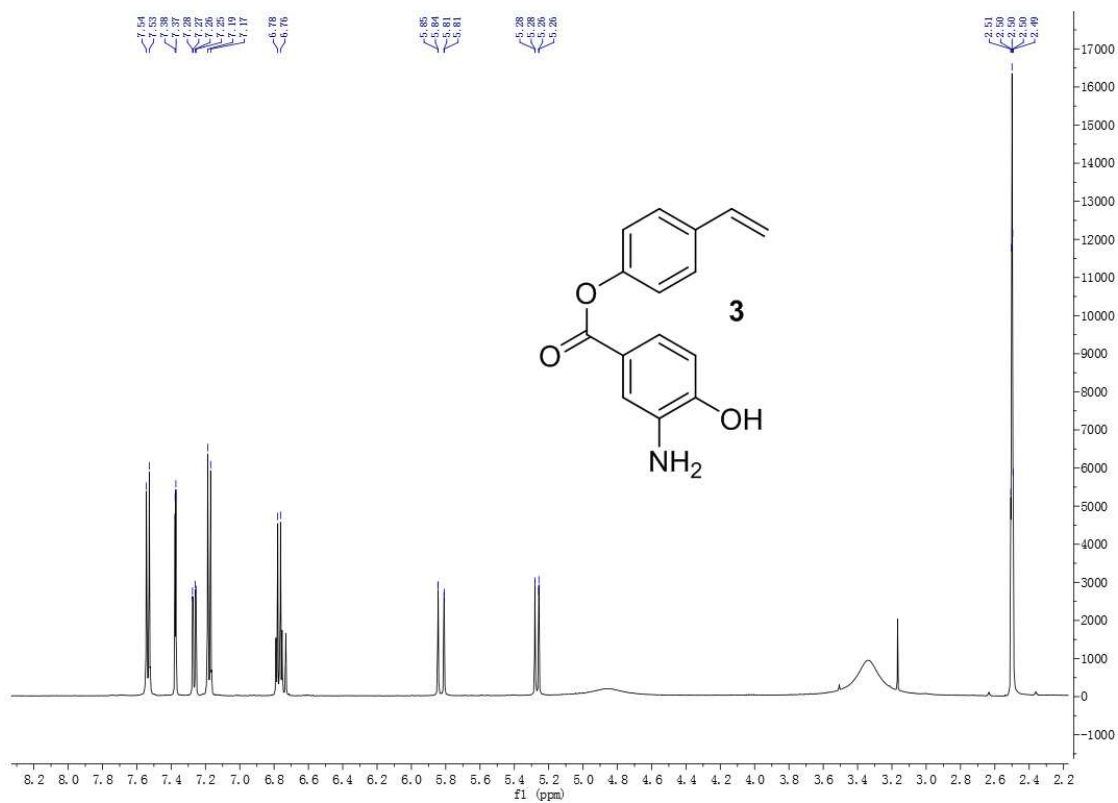


Figure S18. ^{13}C NMR spectrum of bagremycin A (**3**, 125 MHz, in $\text{DMSO-}d_6$)

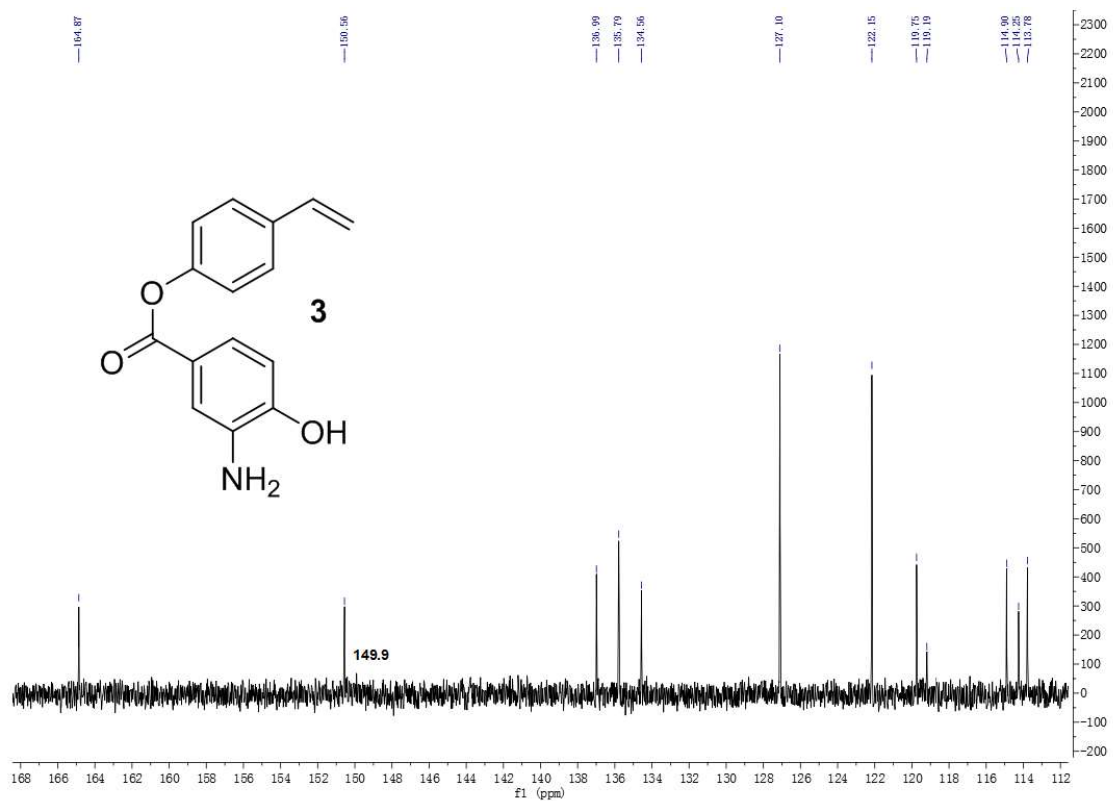
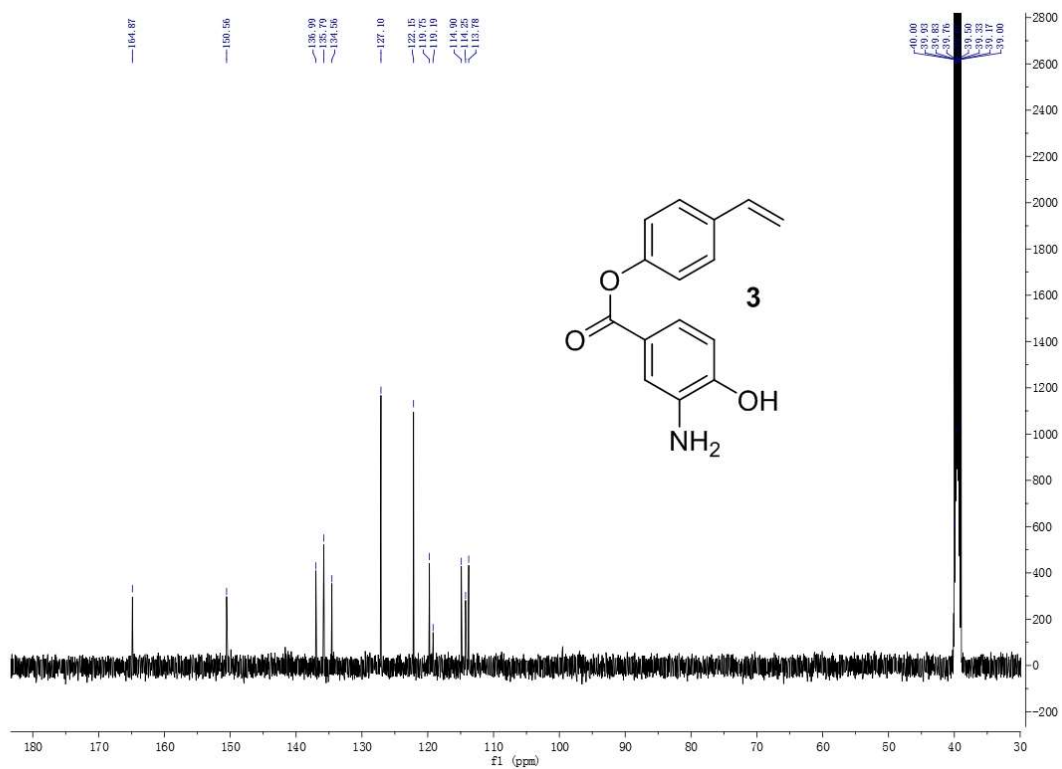


Figure S19. ^1H NMR spectrum of bagremycin B (**4**, 500 MHz, in $\text{DMSO-}d_6$)

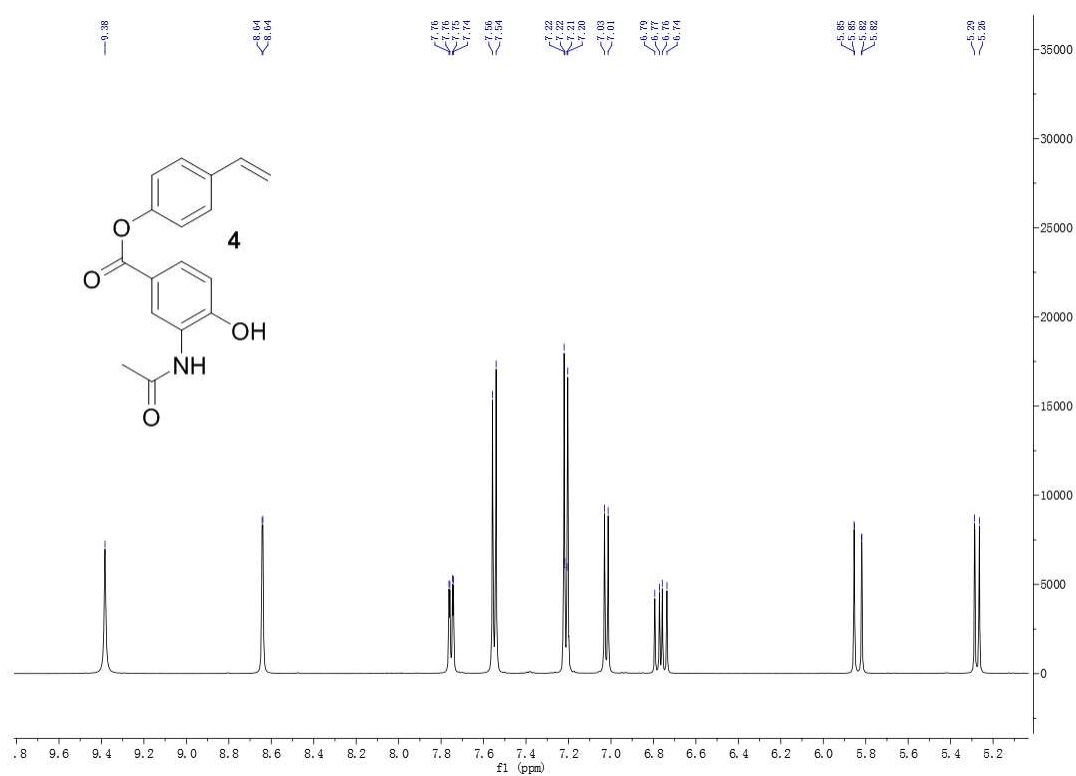
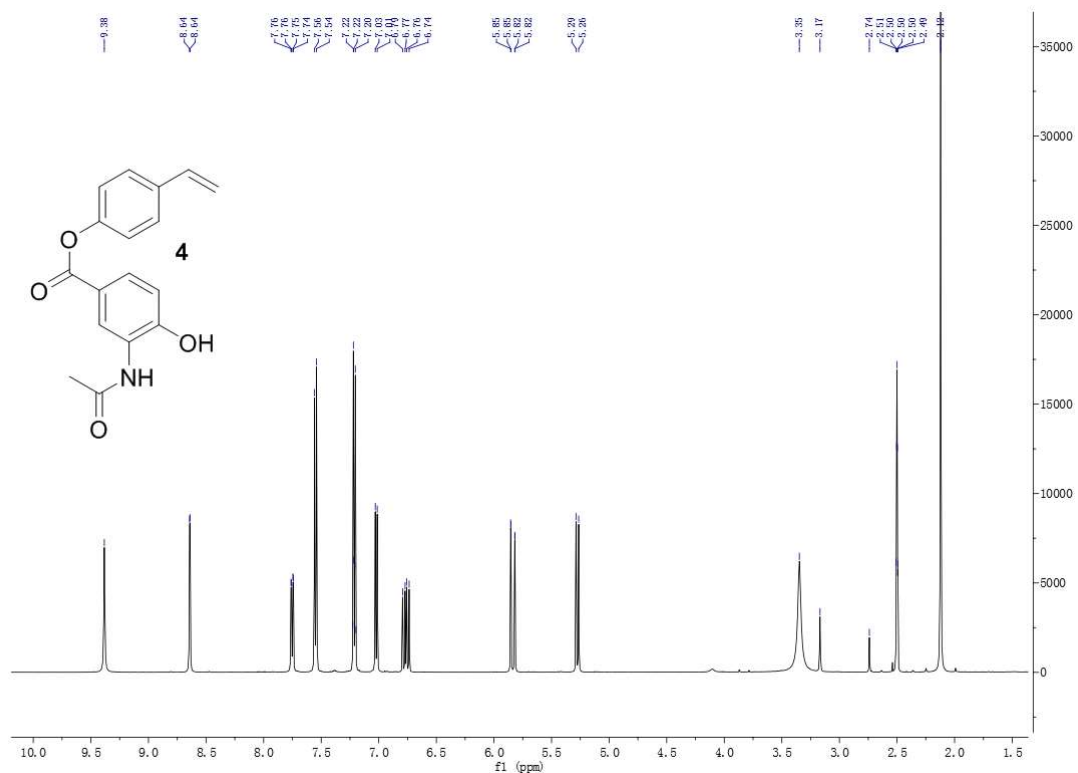


Figure S20. ^{13}C NMR spectrum of bagremycin B (**4**, 125 MHz, in $\text{DMSO-}d_6$)

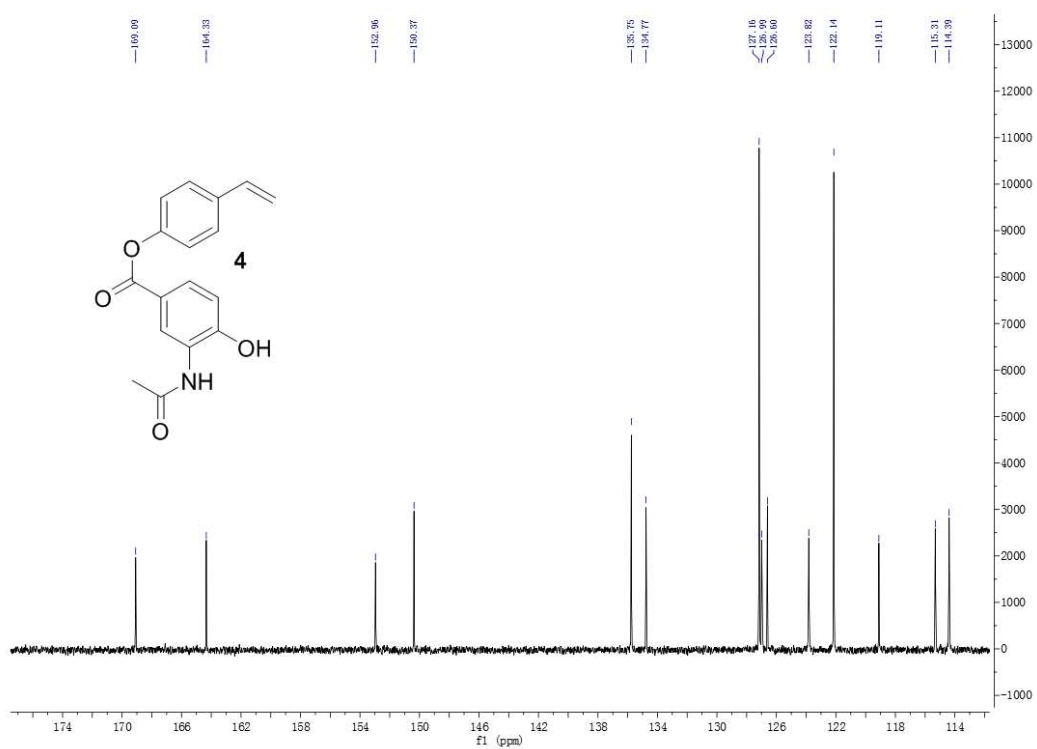
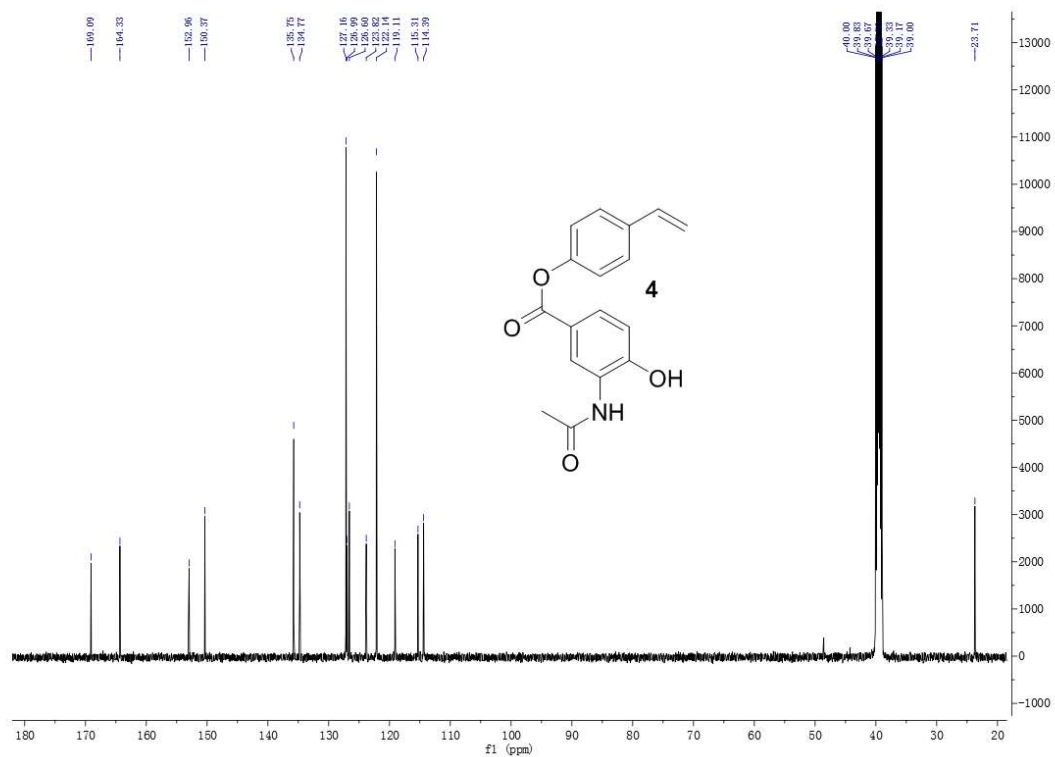


Figure S21. ^1H NMR spectrum of bagremycin E (**5**, 500 MHz, in $\text{DMSO-}d_6$)

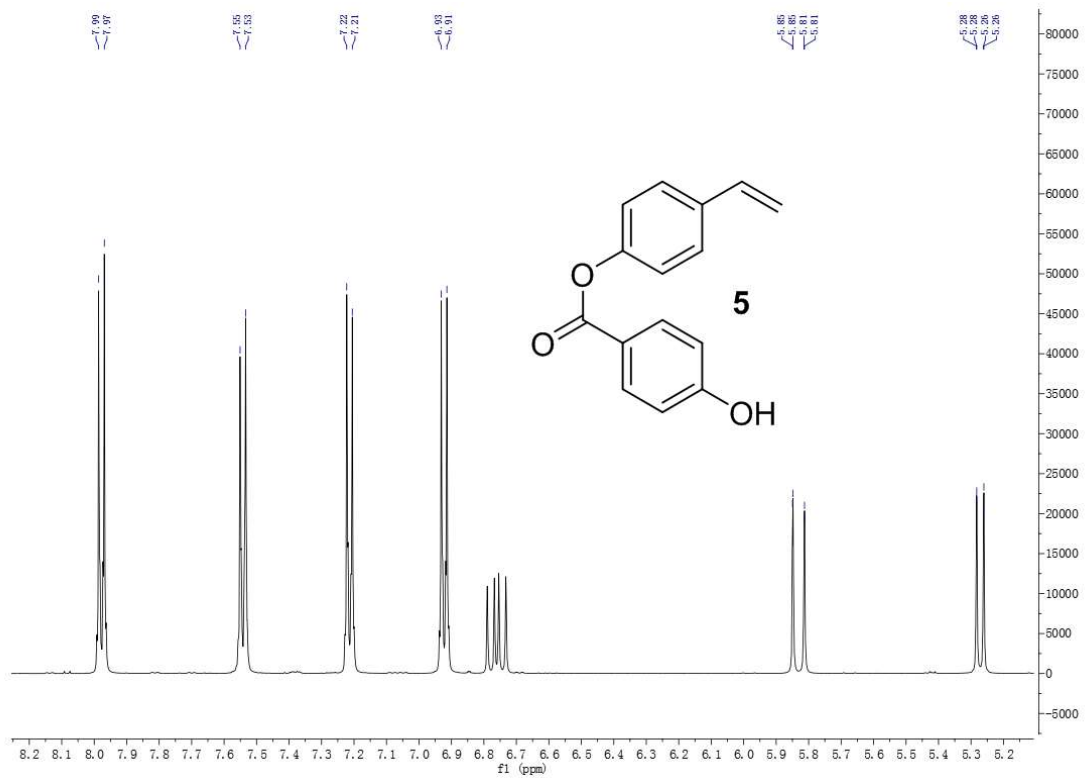
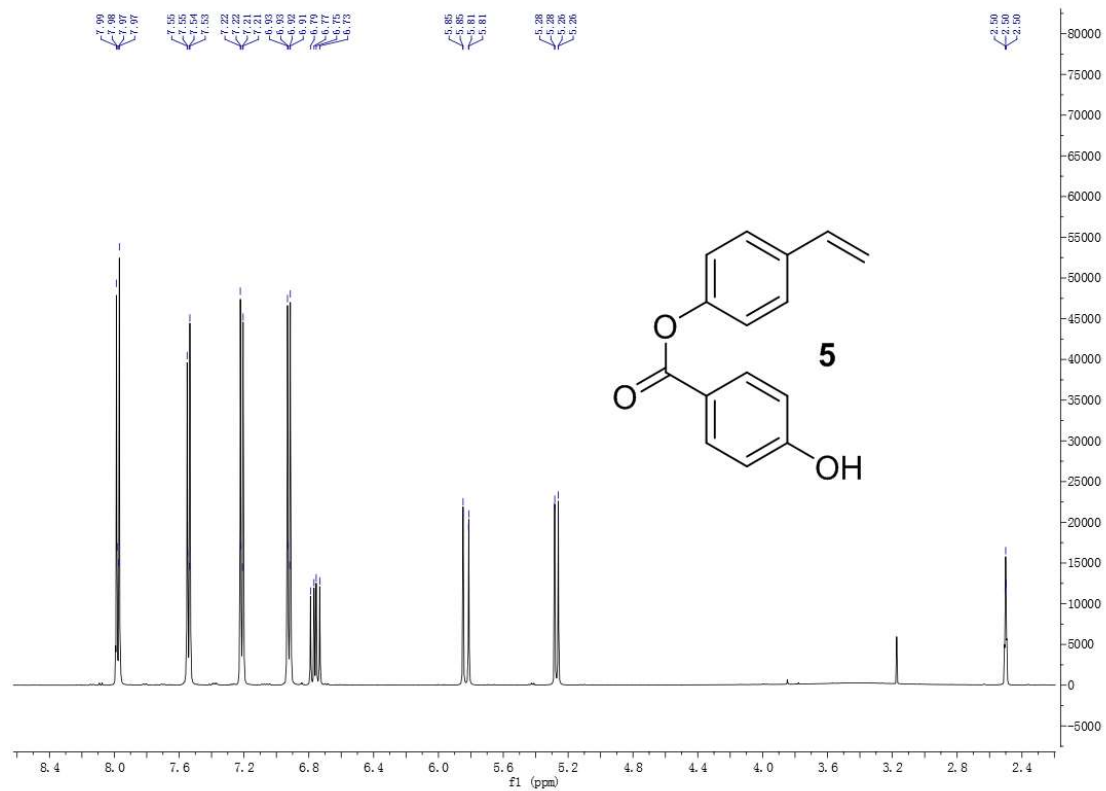


Figure S22. ^{13}C NMR spectrum of bagremycin E (**5**, 125 MHz, in $\text{DMSO-}d_6$)

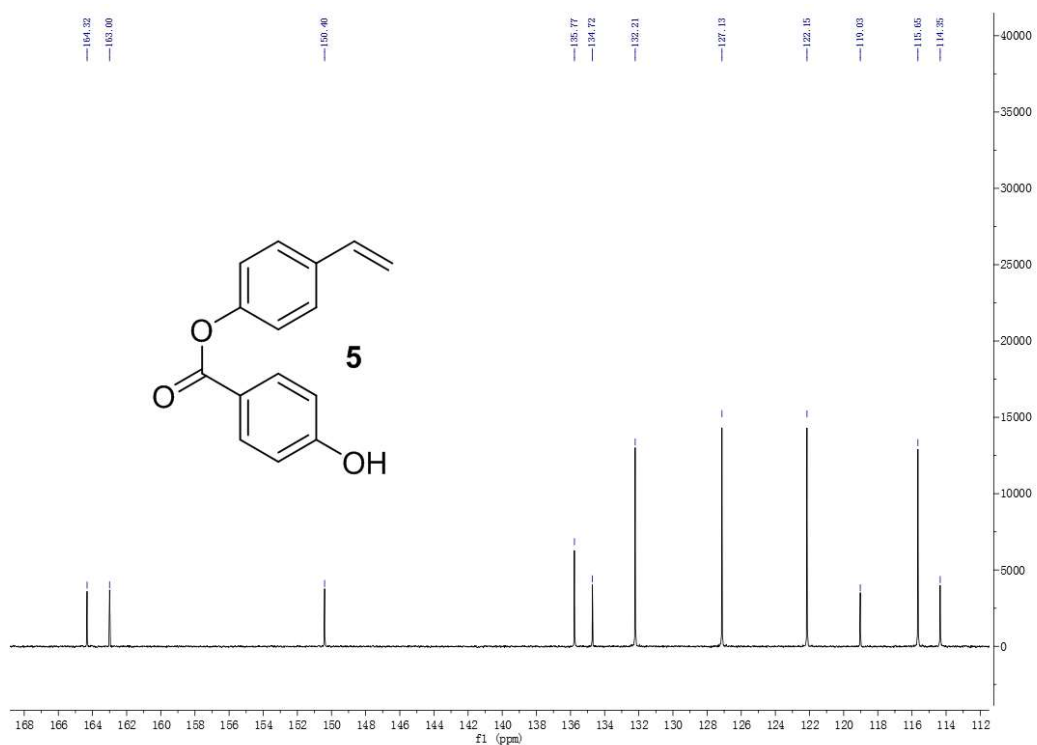
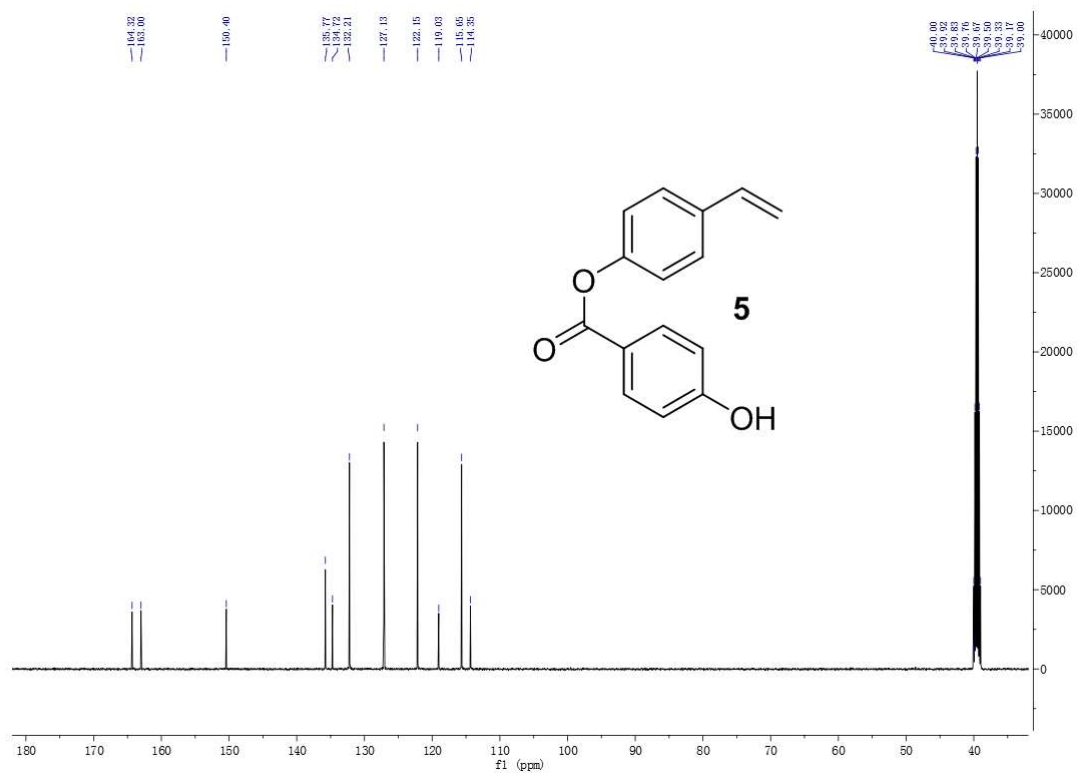


Figure S23. HPLC profile of bagremycin F (**1**) and ethanol crude extract (A: compound **1** + crude extract; B: crude extract; C: compound **1**). The separation of compounds was conducted on a ZORBAX SB-C18 HPLC column (250 × 4.6 mm, 5 μm) on the conditions of UV detection at 256 nm and flow rate at 1.0 mL/min. Acetonitrile and water were used as mobile phases A and B, respectively. The binary gradient program was 0.0–40.0 min with 20–100% A, 40.1–48.0 min with 100% A, and 48.1–60.0 min with 20% A.

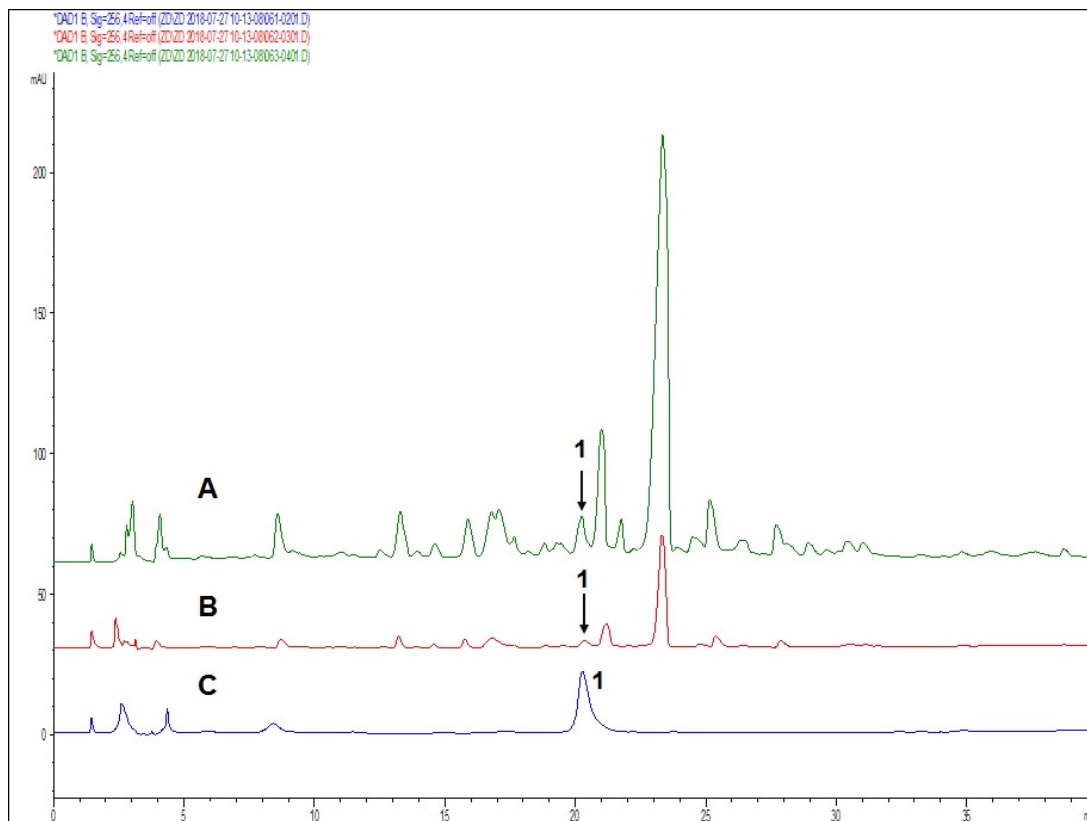


Figure S24. The analytic result of the ethanol crude extract by HPLC-HRESIMS. The separation was conducted on an Agilent Poroshell 120 EC-18 column (50 × 4.6 mm, 2.7 μm) with UV detection at 256 nm and flow rate at 0.6 mL/min. Acetonitrile and water were employed as mobile phases A and B, respectively. The binary gradient program was 0.0–10.0 min with 10–50% A, 10.1–15.0 min with 100% A, and 15.1–18.0 min with 10% A. Bagremycin F (**1**) was detected at t_R 12.44 min with a $[M + Na]^+$ ion at m/z 453.1092 (calcd for $C_{21}H_{22}N_2NaO_6S$, 453.1096).

