Supporting Information

Isolation, Structure Elucidation, and First Total Synthesis of Quinomycins K and L, Two New Octadepsipeptides from the Maowei Sea Mangrove-derived *Streptomyces* sp. B475

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Contents

Table S1. The physicochemical properties of natural-**1**, synthetic-**1**, natural-**2**, and synthetic-**2**.

Table S2. The antibacterial activities of synthetic-**1** and synthetic-**2** (MIC, μg/mL).

Table S3. The cytotoxic activity of synthetic-**1** and synthetic-**2** against H460 lung cancer cells.

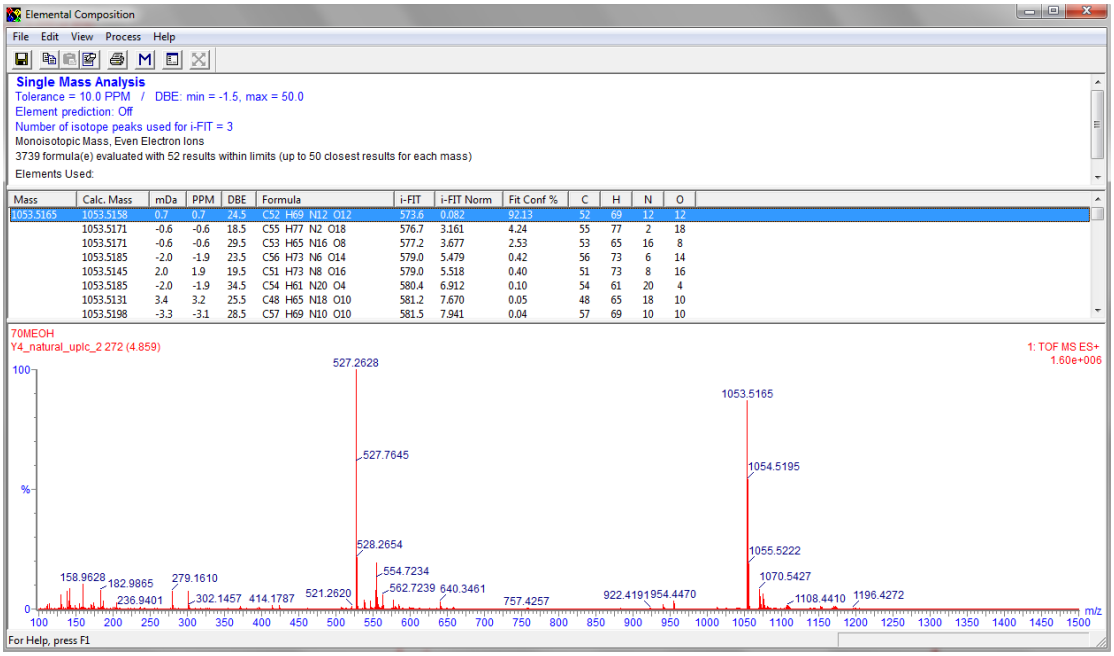

Figure S1. The HRESIMS of compound **1**.

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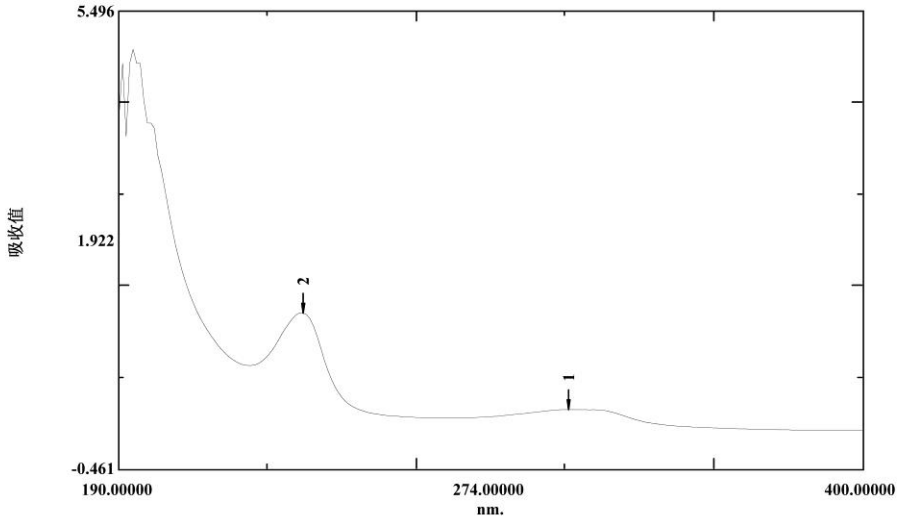
2020-11-11 11:55:06

数据集: Y4_2 - RawData



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自动采样间隔: 停用
扫描模式: 自动

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测定方式: 吸收值
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光源转换波长: 350.0 nm
S/R 转换: 标准

附件属性
附件: 6联池
池数目: 1

样品准备属性
重量: 0.03MG
体积: 1.5ML
稀释:
光程长: 10
附加信息: mg/ml

Figure S2. The UV spectrum of compound **1**.

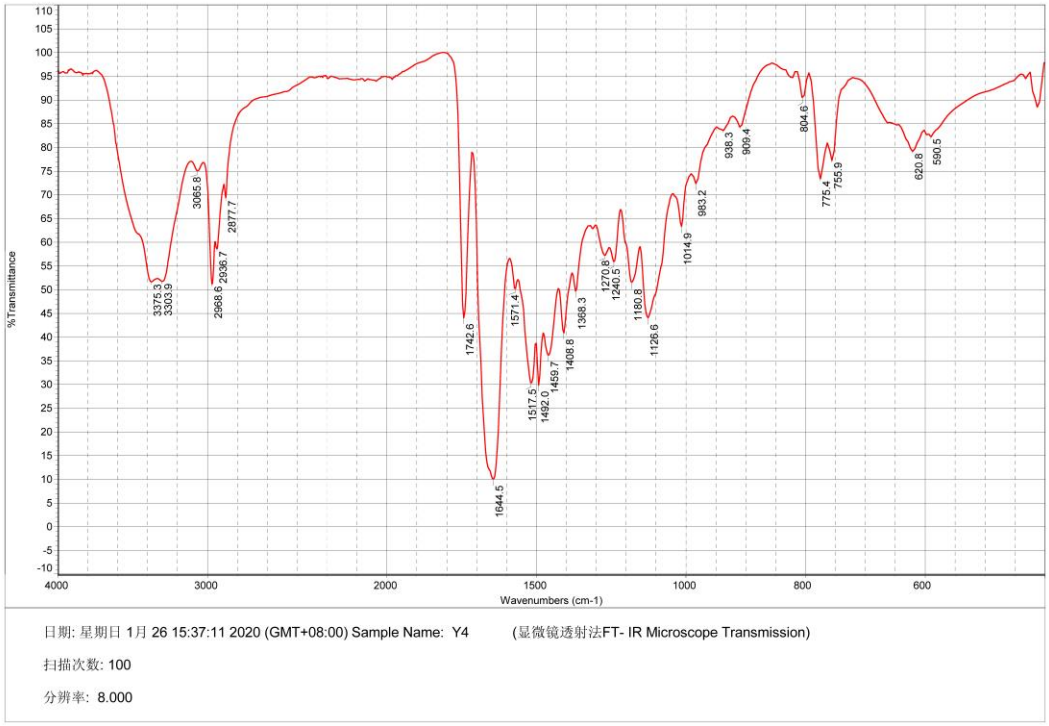
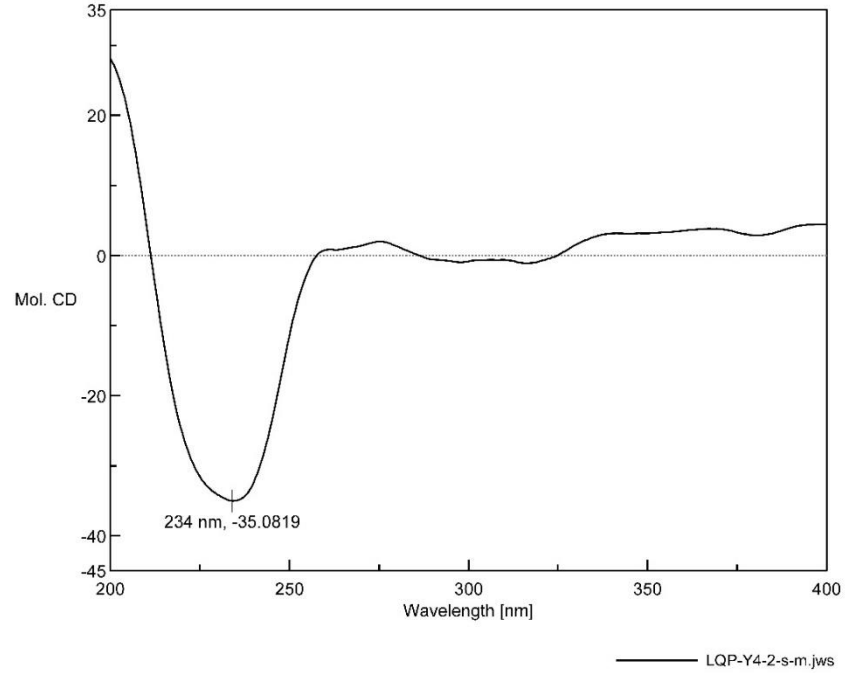


Figure S3. The IR spectrum of compound **1**.



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Sensitivity	Standard
D.I.T.	1 sec
Bandwidth	1.00 nm
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Shutter Control	Auto
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Solvent	MEOH
Concentration	0.02 (w/v)%

Figure S4. The ECD spectrum of compound **1**.

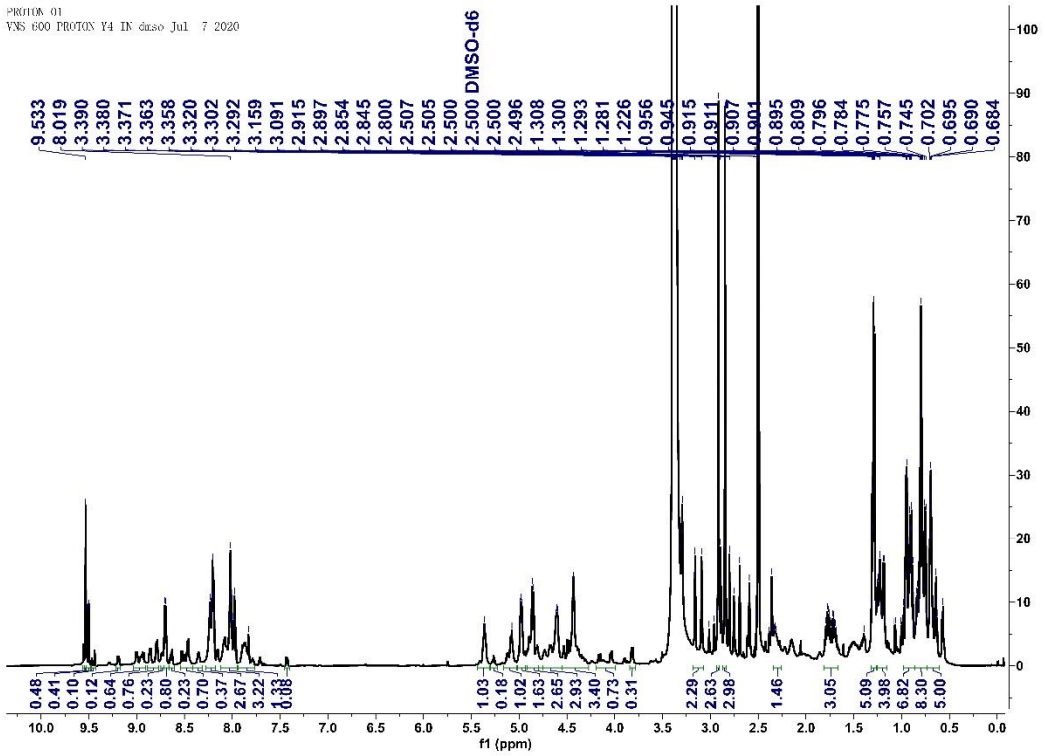

Figure S5. The ^{1}H NMR (600 MHz) spectrum of compound **1** in DMSO-*d*$_6$.

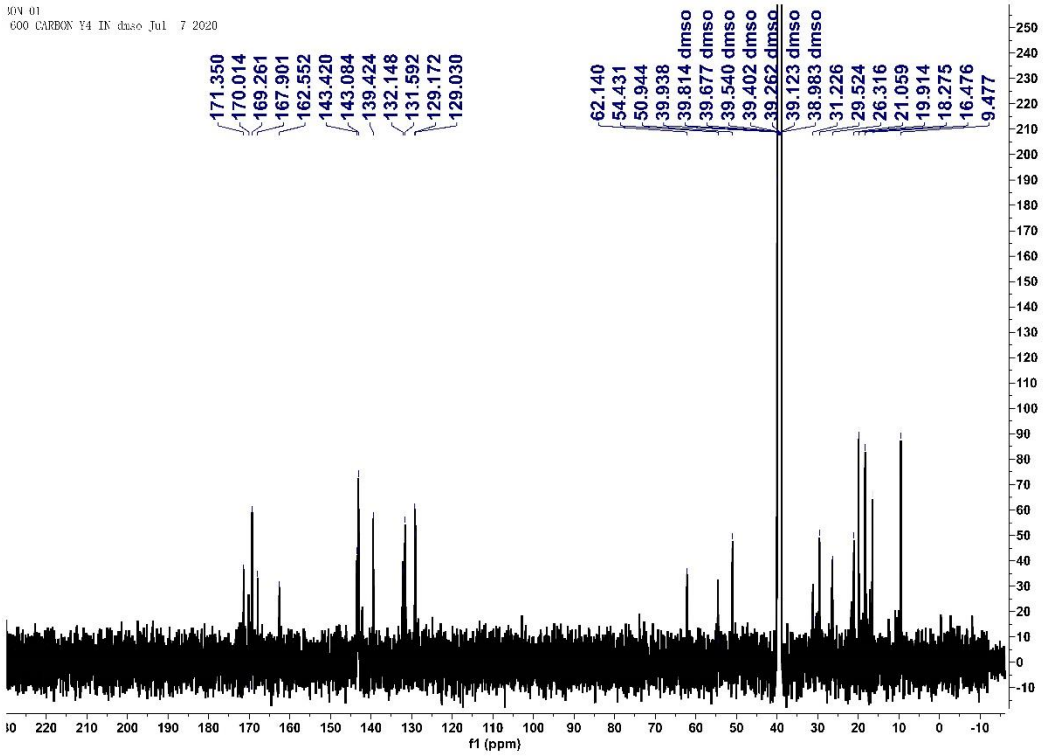

Figure S6. The ^{13}C NMR (150 MHz) spectrum of compound **1** in DMSO-*d*$_6$.

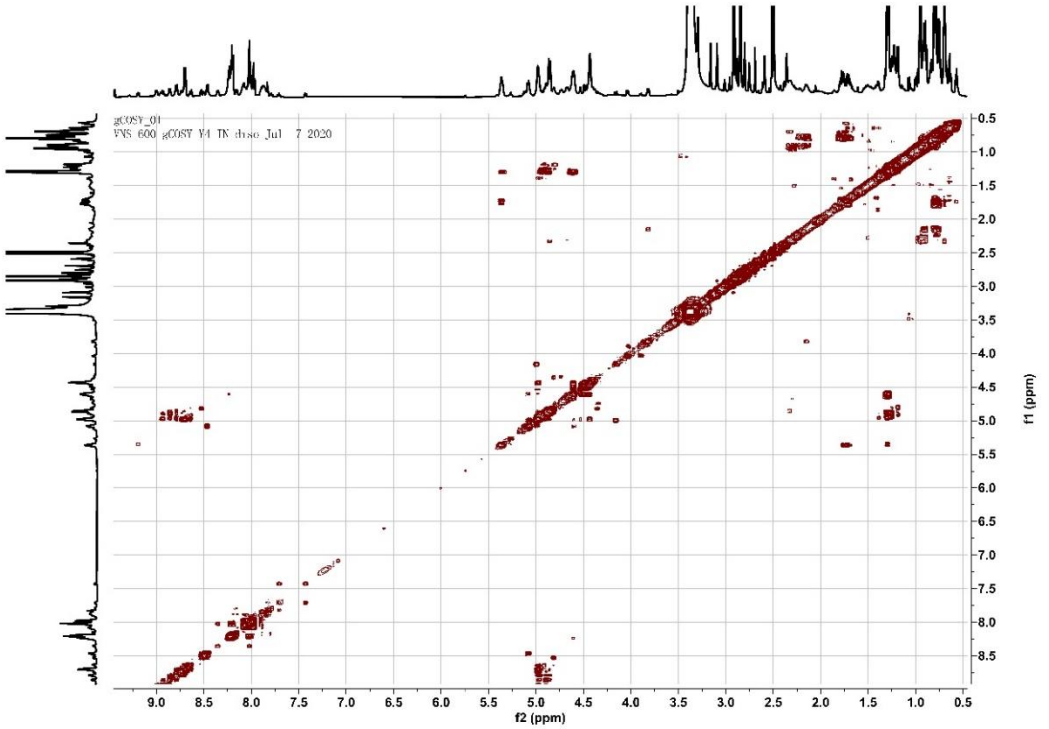

Figure S7. The ^{1}H-^{1}H COSY spectrum of compound **1**.

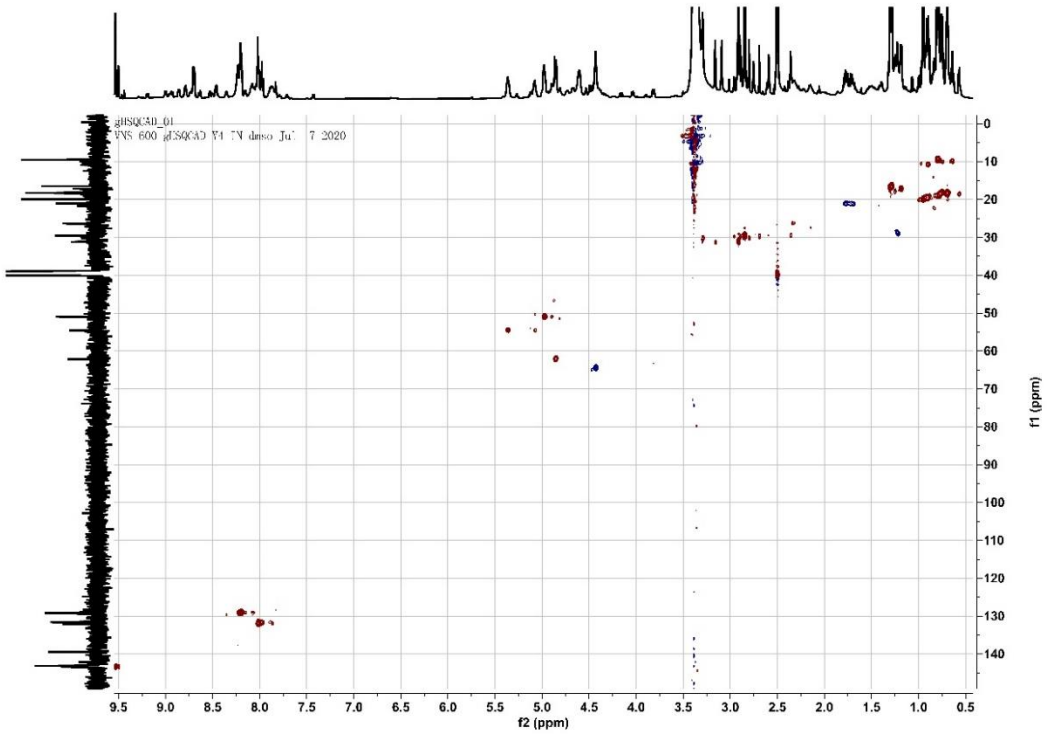

Figure S8. The HSQC spectrum of compound **1**.

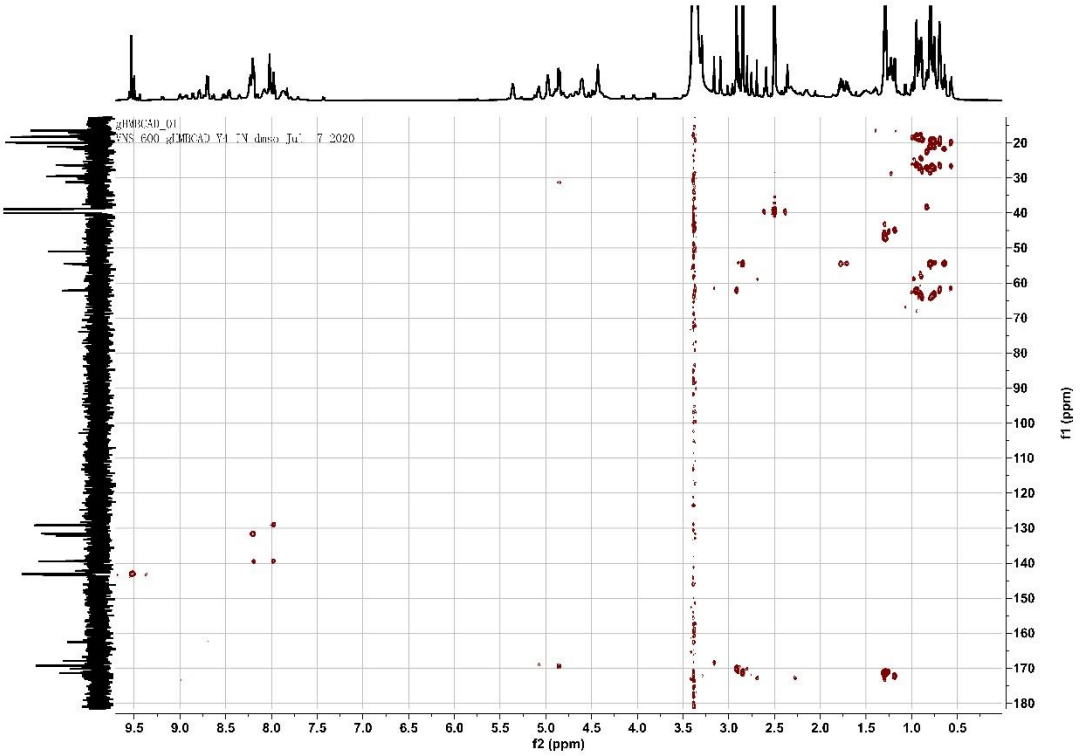

Figure S9. The HMBC spectrum of compound **1**.

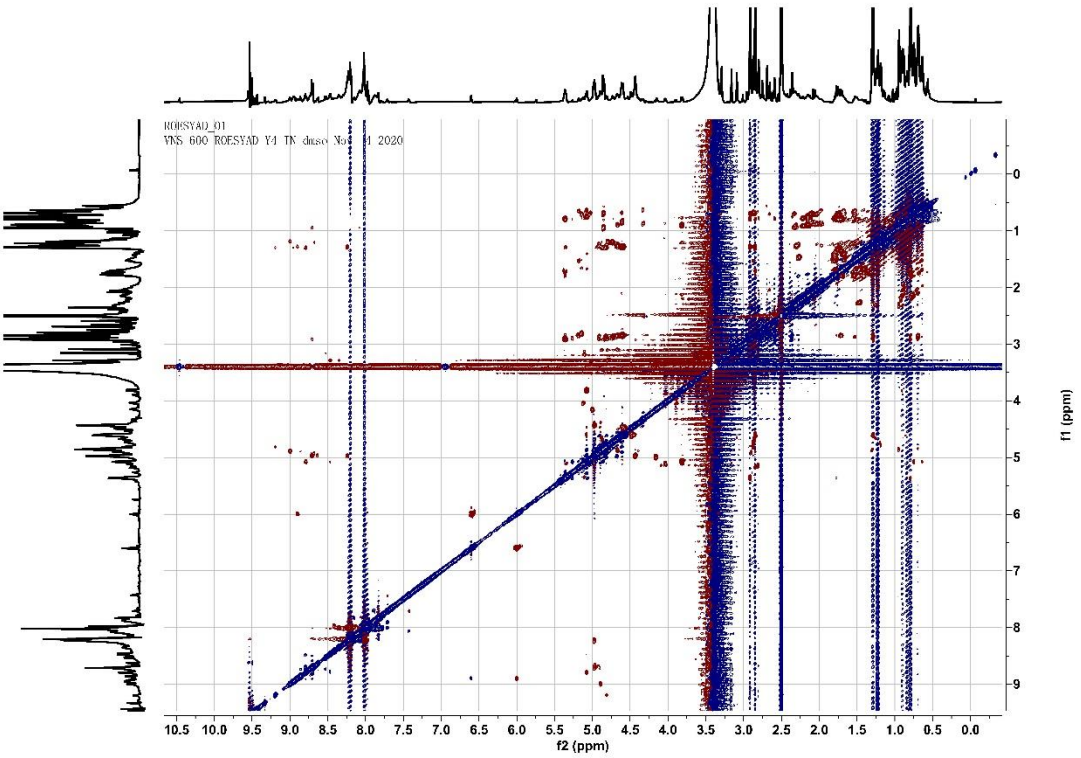

Figure S10. The ROESY spectrum of compound **1**.

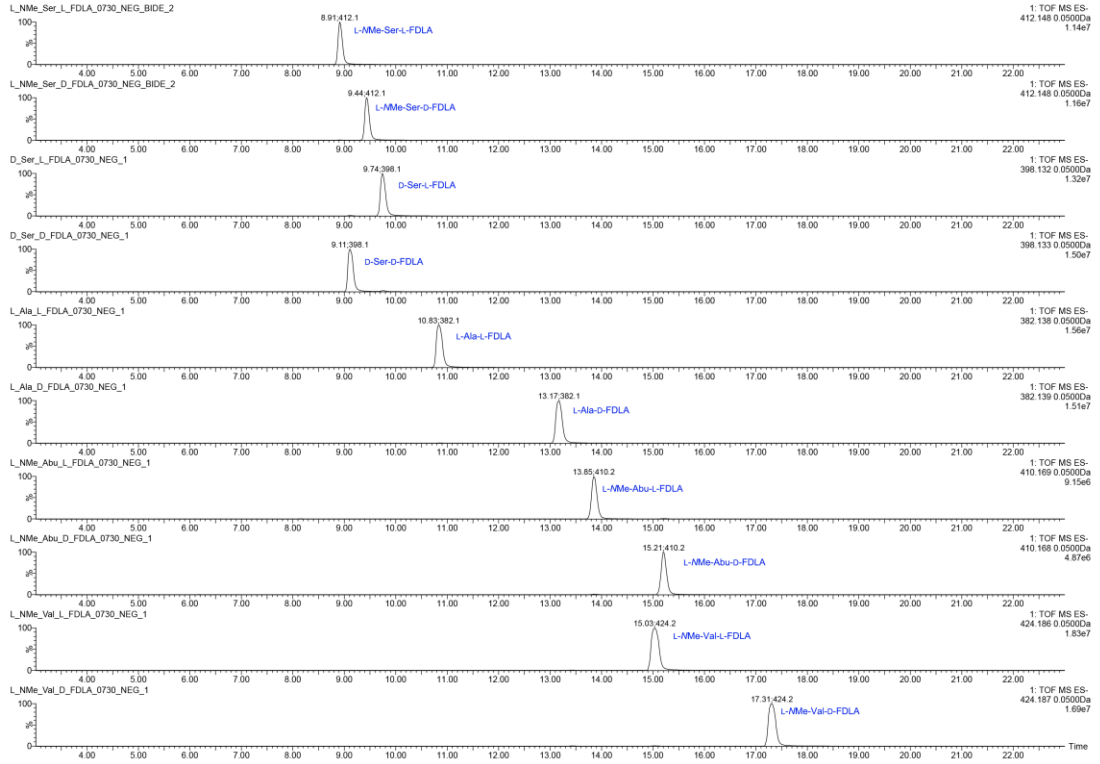

Figure S11. The Extracted Ion Chromatogram (EIC) of L-FDLA and D-FDLA derivatives of amino acid standards.

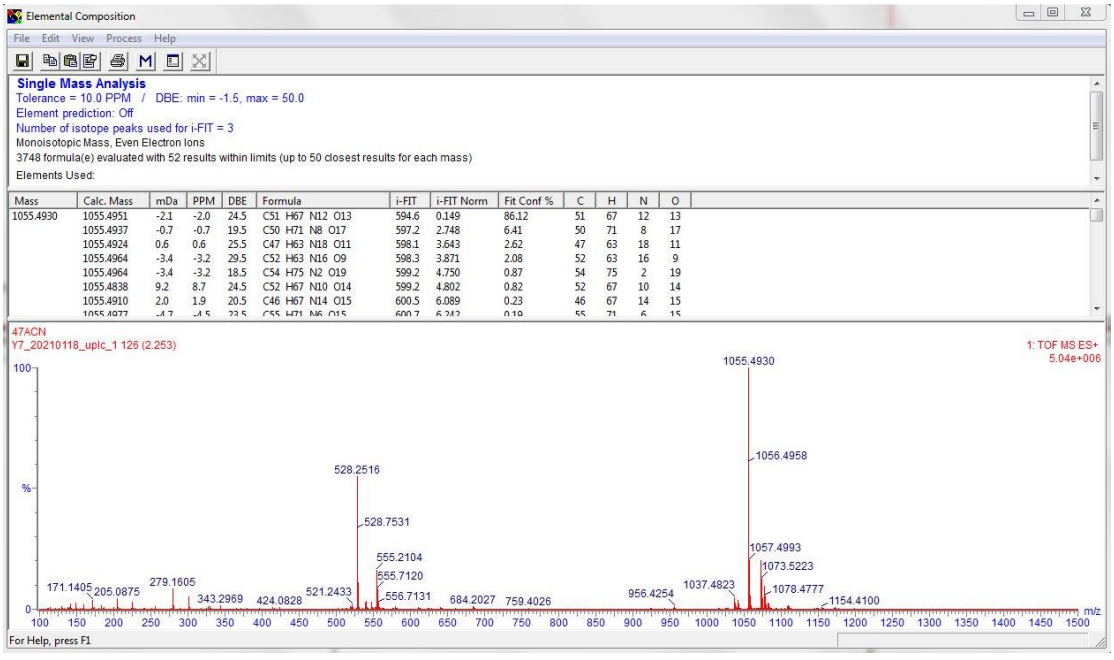

Figure S12. The HRESIMS of compound **2**.

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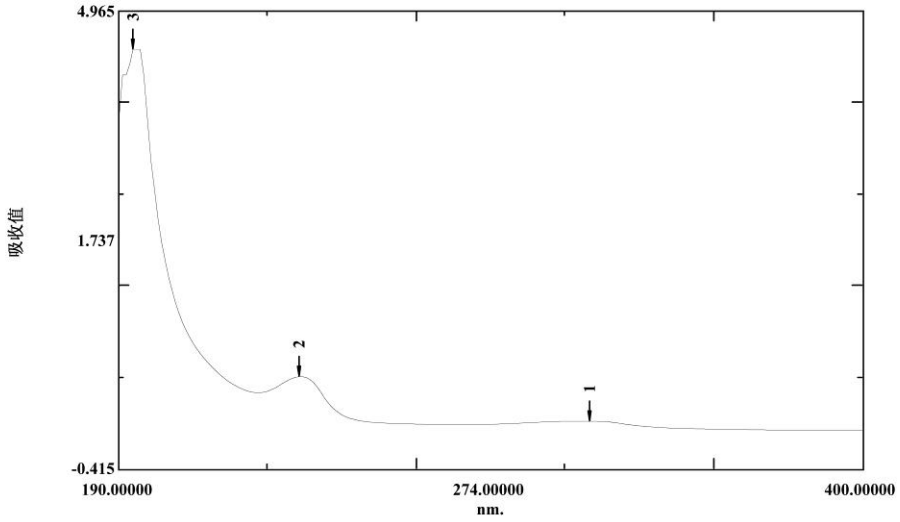
数据集: Y7_20210111 - RawData



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自动采样间隔: 停用
扫描模式: 自动

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测定方式: 吸收值
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光源转换波长: 350.0 nm
S/R 转换: 标准

附件属性
附件: 6联池
池数目: 1

样品准备属性
重量: 0.02
体积: 1
稀释:
光程长: 10
附加信息: 0.018mg/ml

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Figure S13. The UV spectrum of compound **2**.

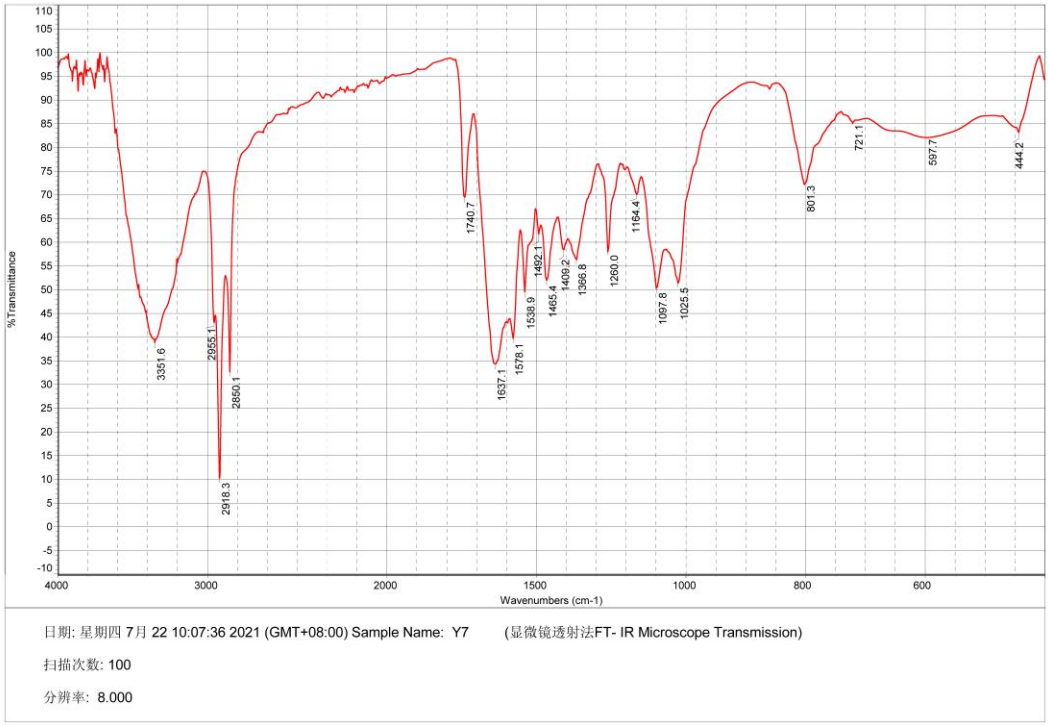
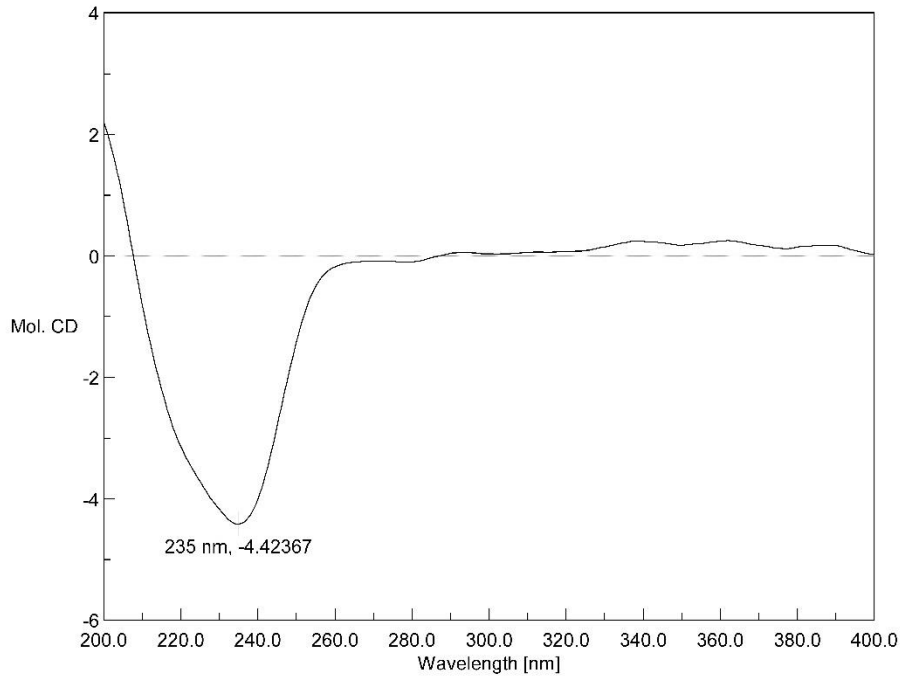


Figure S14. The IR spectrum of compound **2**.



Y7-1-s-m.jws

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Sample name Y7
Comment

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Serial No. A024461168

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Measurement date 2021-01-11 11:25

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D.I.T. 1 sec
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Shutter Control Auto
CD Detector PMT
PMT Voltage Auto
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Solvent MEOH
Concentration 0.018 (w/v)%

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Figure S15. The ECD spectrum of compound **2**.

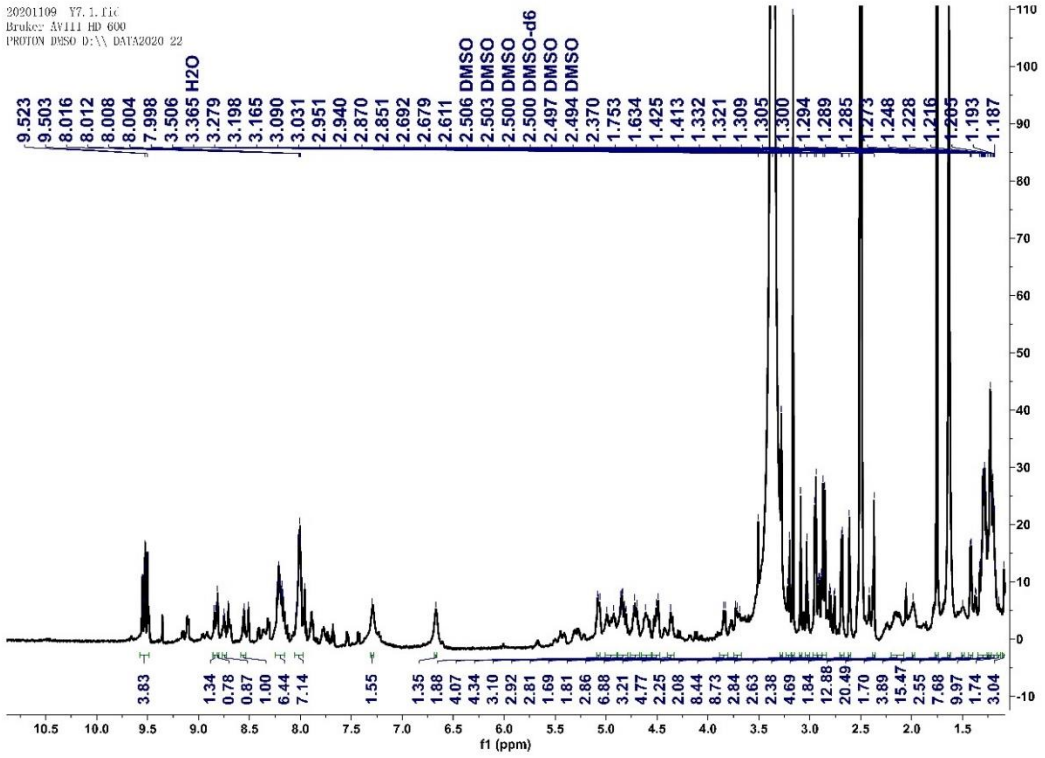

Figure S16. The ^{1}H NMR (600 MHz) spectrum of compound **2** in DMSO-*d*$_6$.

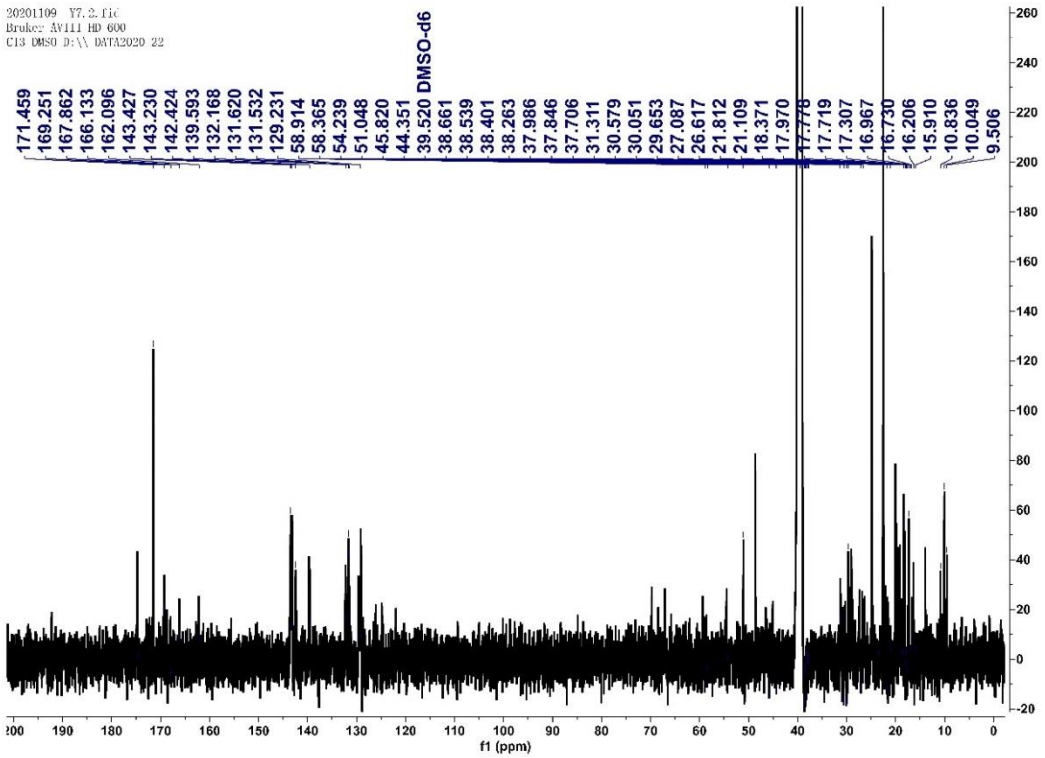

Figure S17. The ^{13}C NMR (150 MHz) spectrum of compound **2** in DMSO-*d*$_6$.

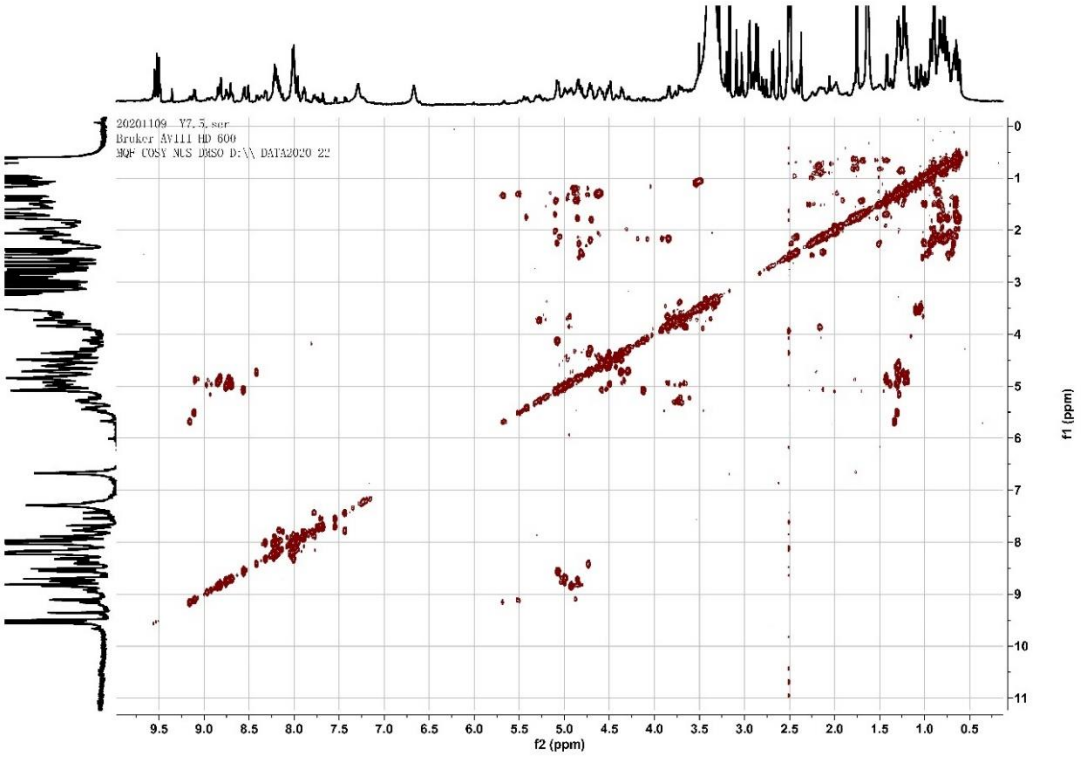

Figure S18. The ^{1}H-^{1}H COSY spectrum of compound **2**.

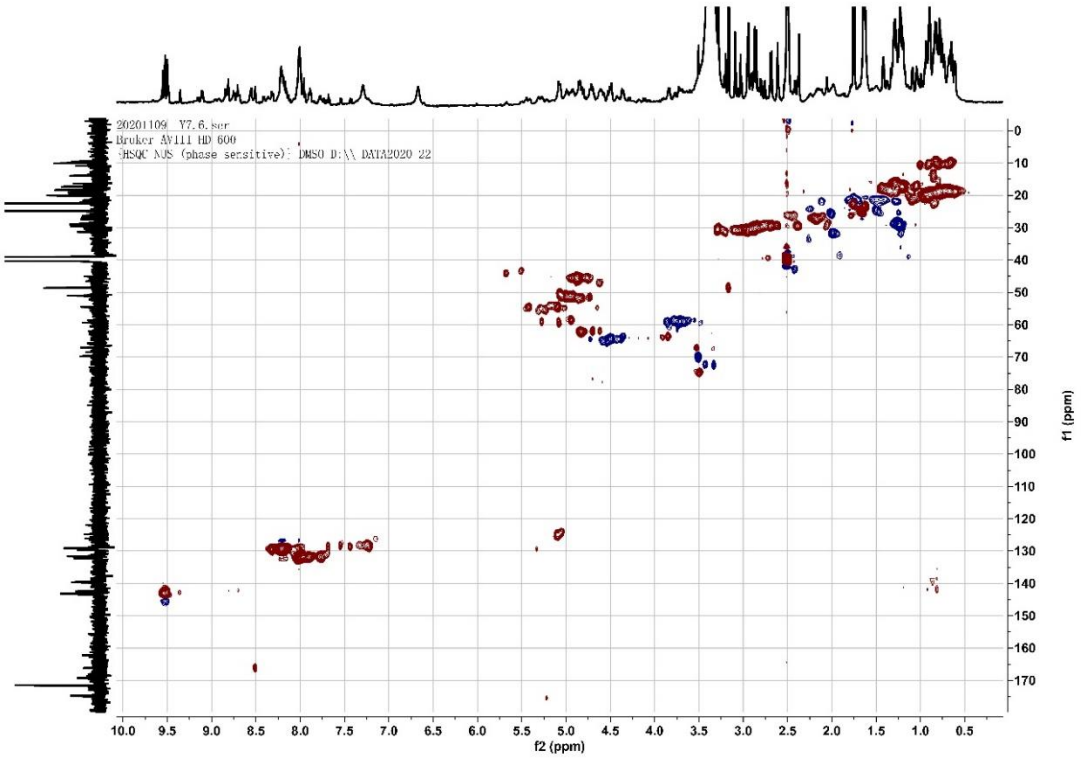

Figure S19. The HSQC spectrum of compound **2**.

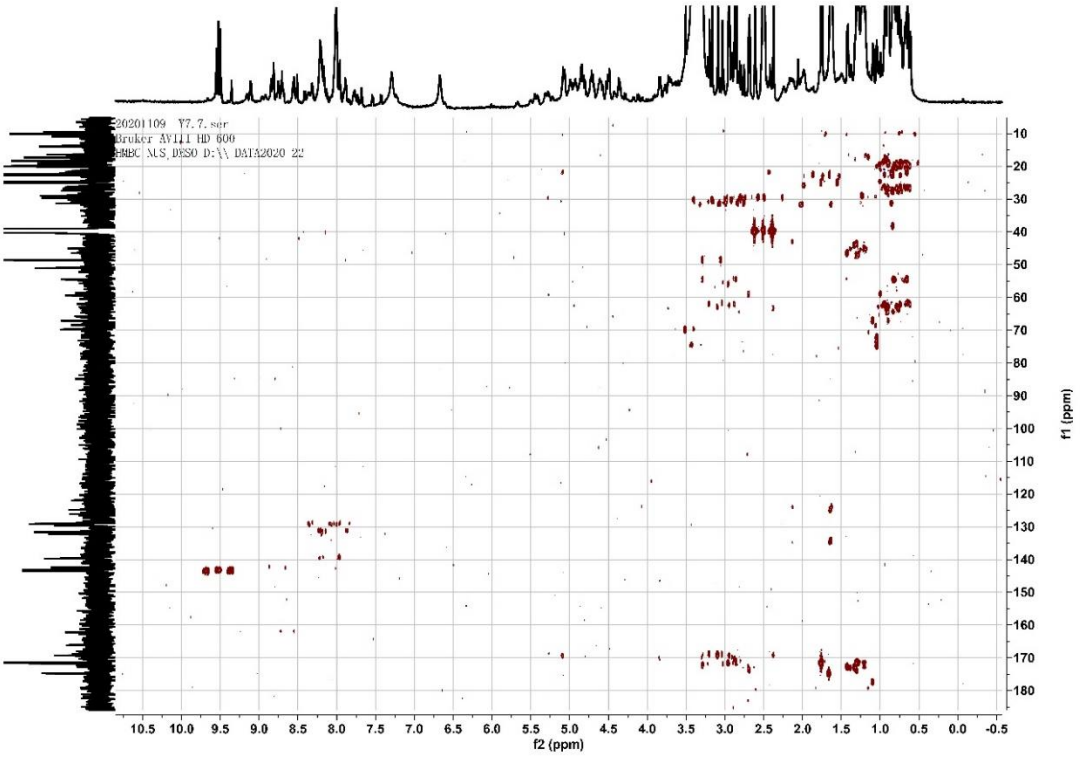

Figure S20. The HMBC spectrum of compound **2**.

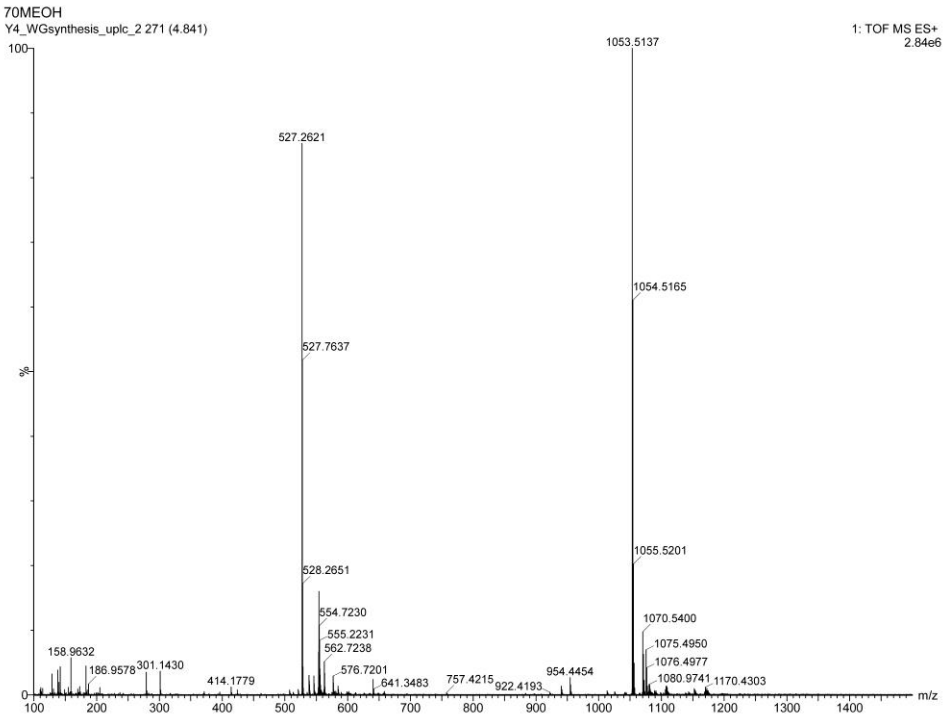

Figure S21. The HRESIMS of synthetic-**1**.

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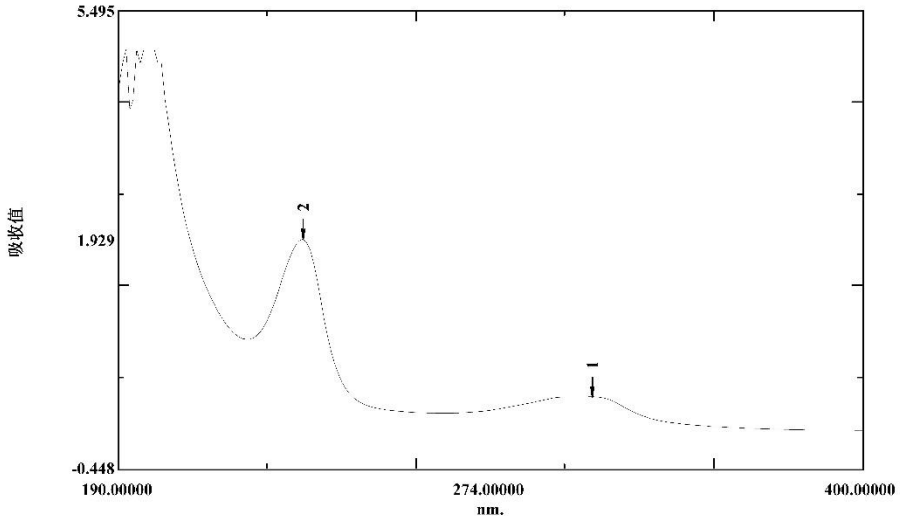
数据集: Y4s_20210111 - RawData



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采样间隔: 1.0
自动采样间隔: 停用
扫描模式: 自动

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3	↓	282.00000	0.269
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仪器属性
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测定方式: 吸收值
狭缝宽: 2.0 nm
光源转换波长: 350.0 nm
S/R 转换: 标准

附件属性
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池数目: 1

样品准备属性
重量: 0.02
体积: 1
稀释:
光程长: 10
附加信息: 0.04mg/ml

Figure S22. The UV spectrum of synthetic-**1**.

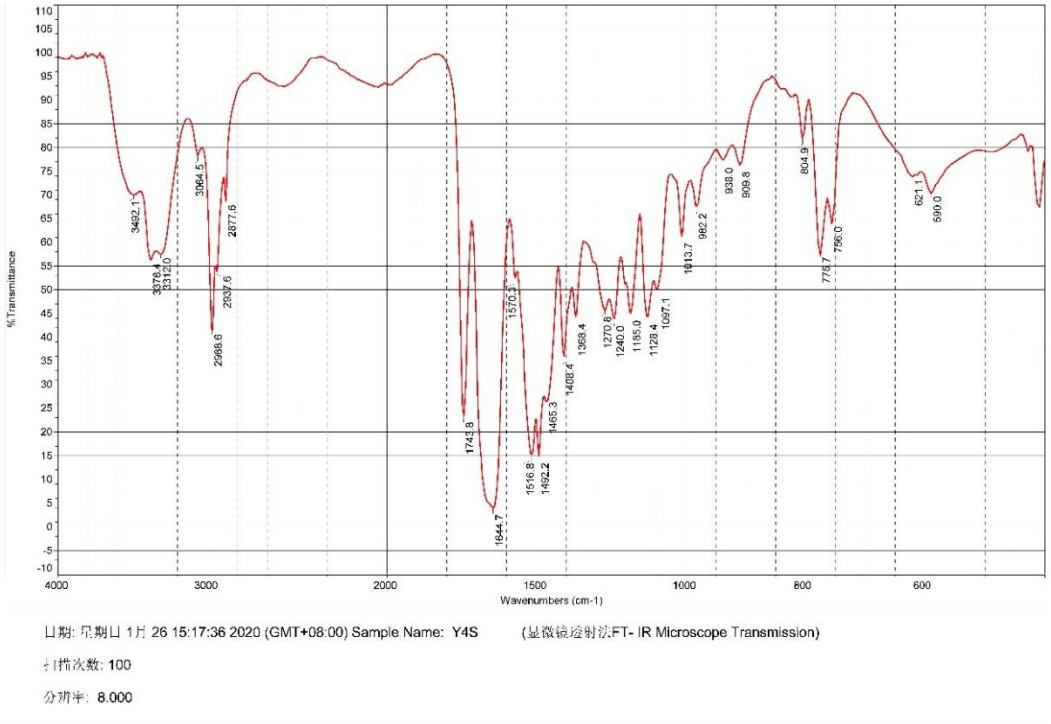


Figure S23. The IR spectrum of synthetic-**1**.

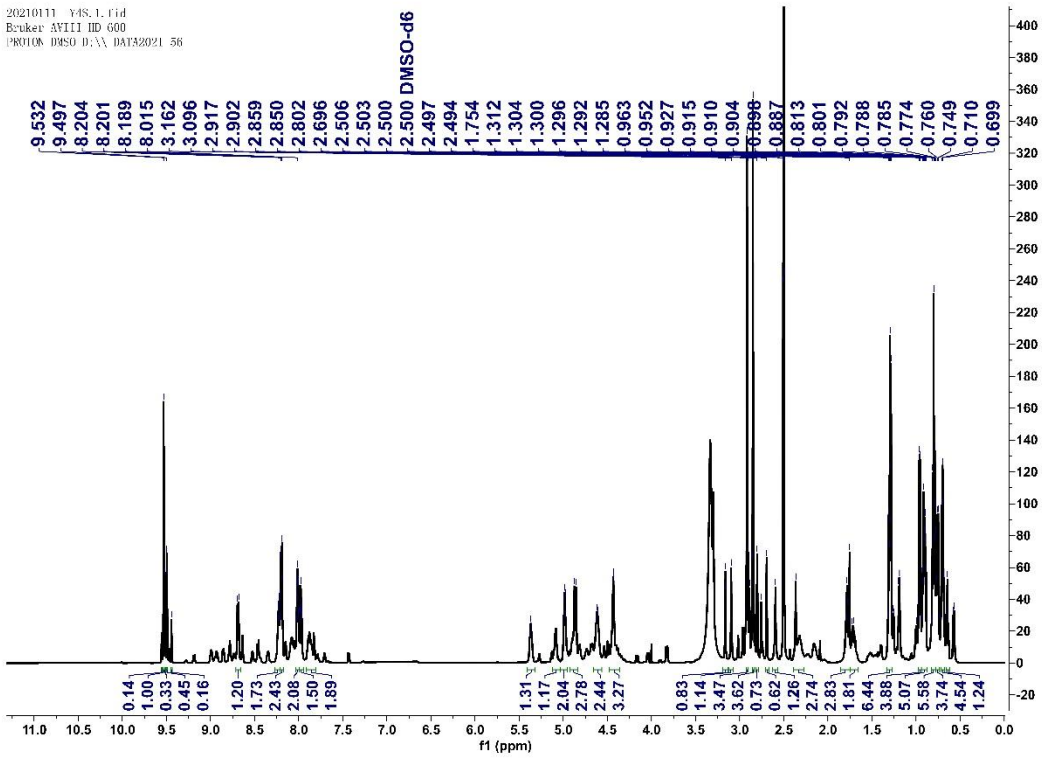


Figure S24. The ^{1}H NMR (600 MHz) spectrum of synthetic-**1** in DMSO-d_6.

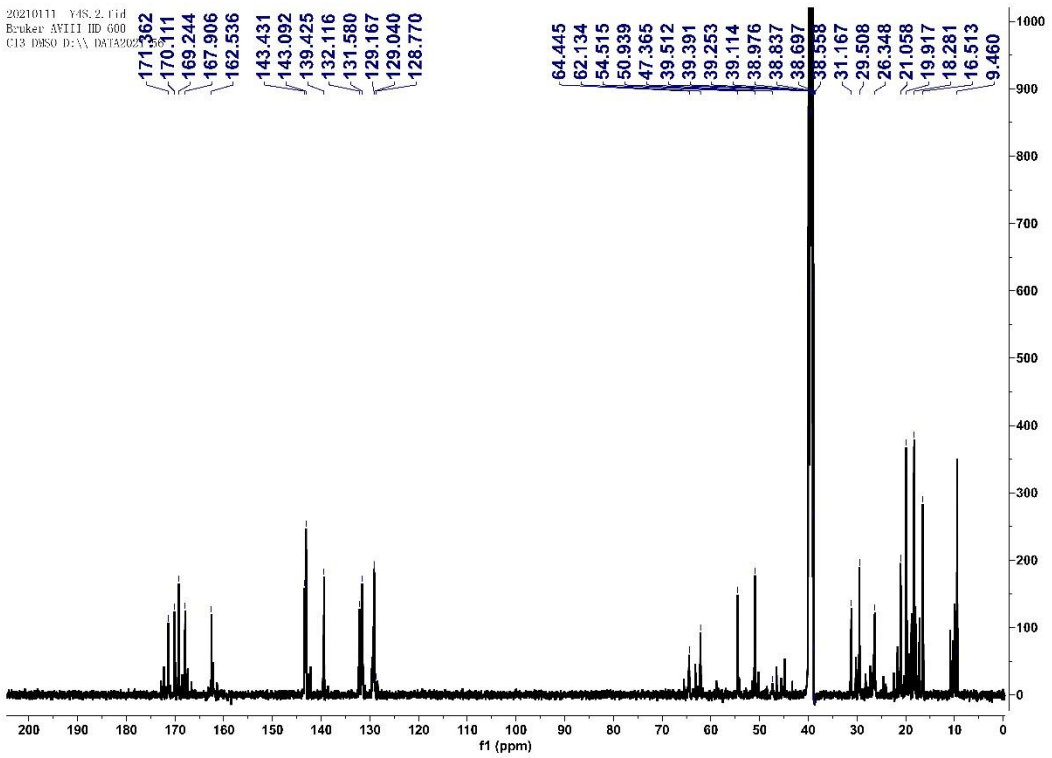


Figure S25.4 The ^{13}C NMR (150 MHz) spectrum of synthetic-**1** in DMSO-d_6.

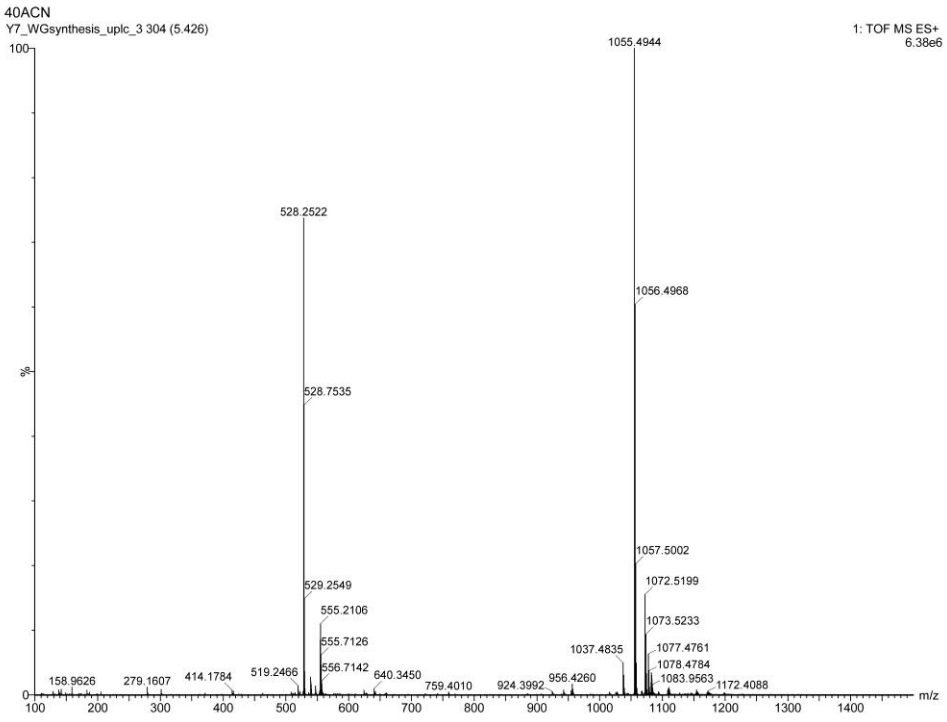
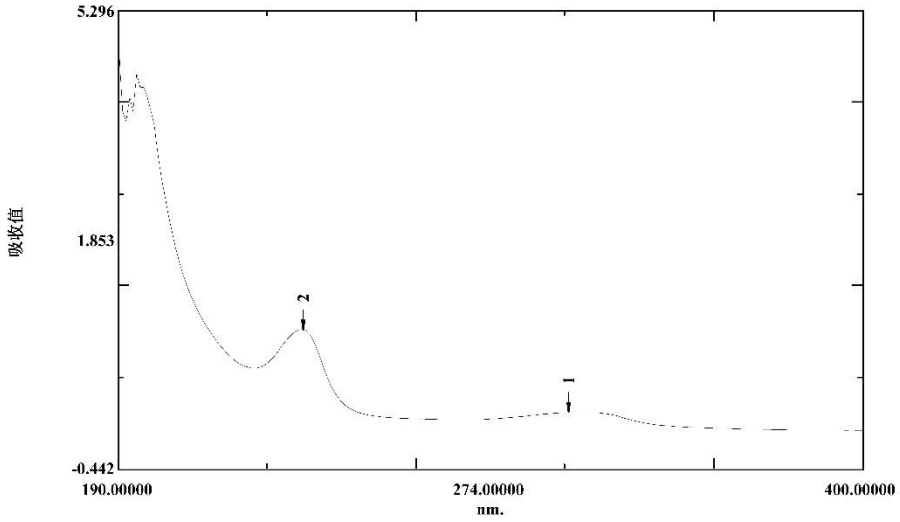


Figure S26. The HRESIMS of synthetic-**2**.

光谱峰值检测报告

2012-08-21 02:46:23

数据集: Y7S_gaonongdu20210111 - RawData



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自动采样间隔: 停用
扫描模式: 自动

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1	↑	317.00000	0.258
2	↑	242.00000	1.302
3	↓	287.00000	0.169
4	↓	228.00000	0.816

仪器属性
仪器类型: UV-2500PC 系列
测定方式: 吸收值
狭缝宽: 2.0 nm
光源转换波长: 350.0 nm
S/R 转换: 标准

附件属性
附件: 6联池
池数目: 1

样品准备属性
重量: 0.02
体积: 1
稀释:
光程长: 10
附加信息: 0.04mg/ml

Figure S27. The UV spectrum of synthetic-**2**.

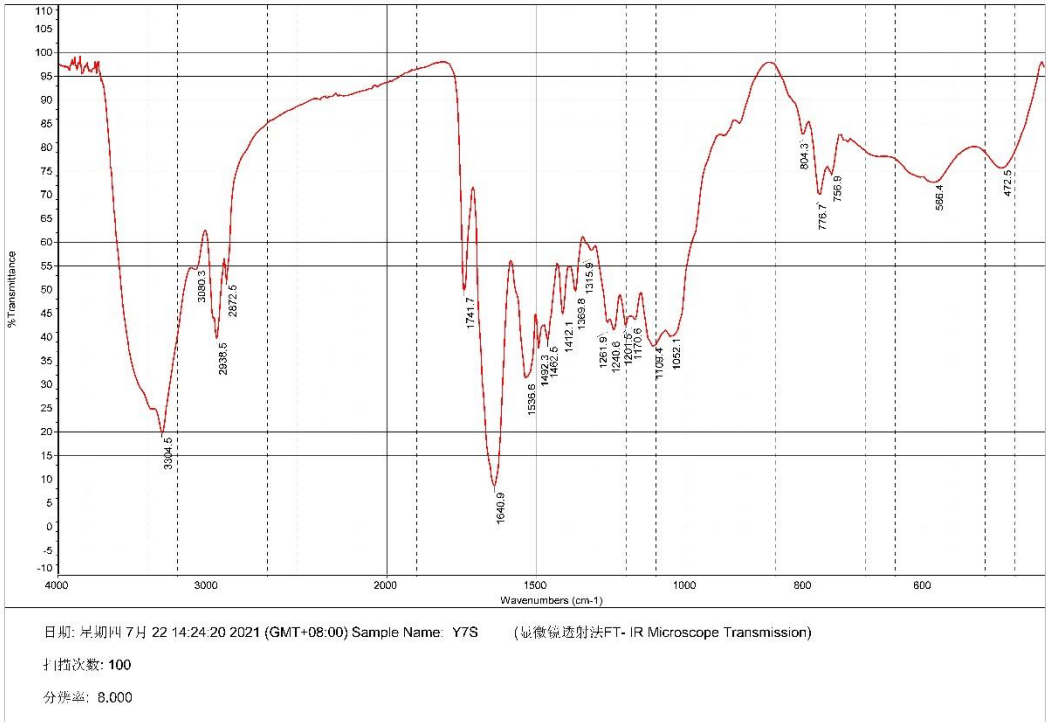

Figure S28.5 The IR spectrum of synthetic-**2**.

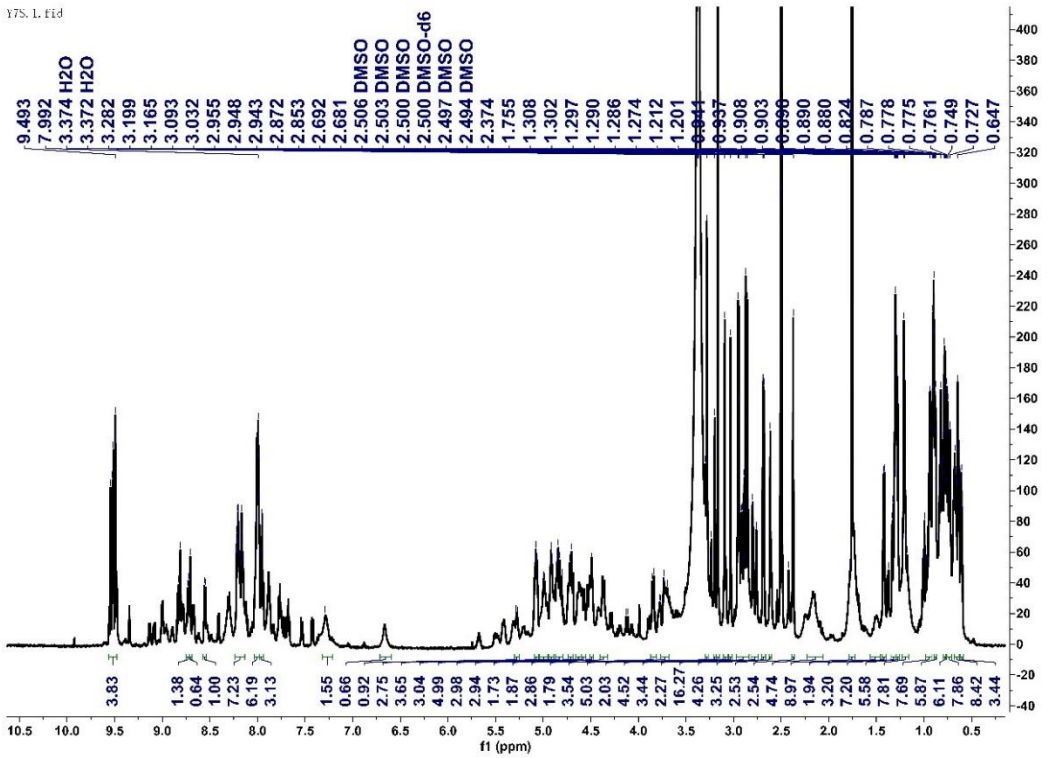

Figure S29.6 The ^{1}H NMR (600 MHz) spectrum of synthetic-**2** in DMSO-*d*$_6$.

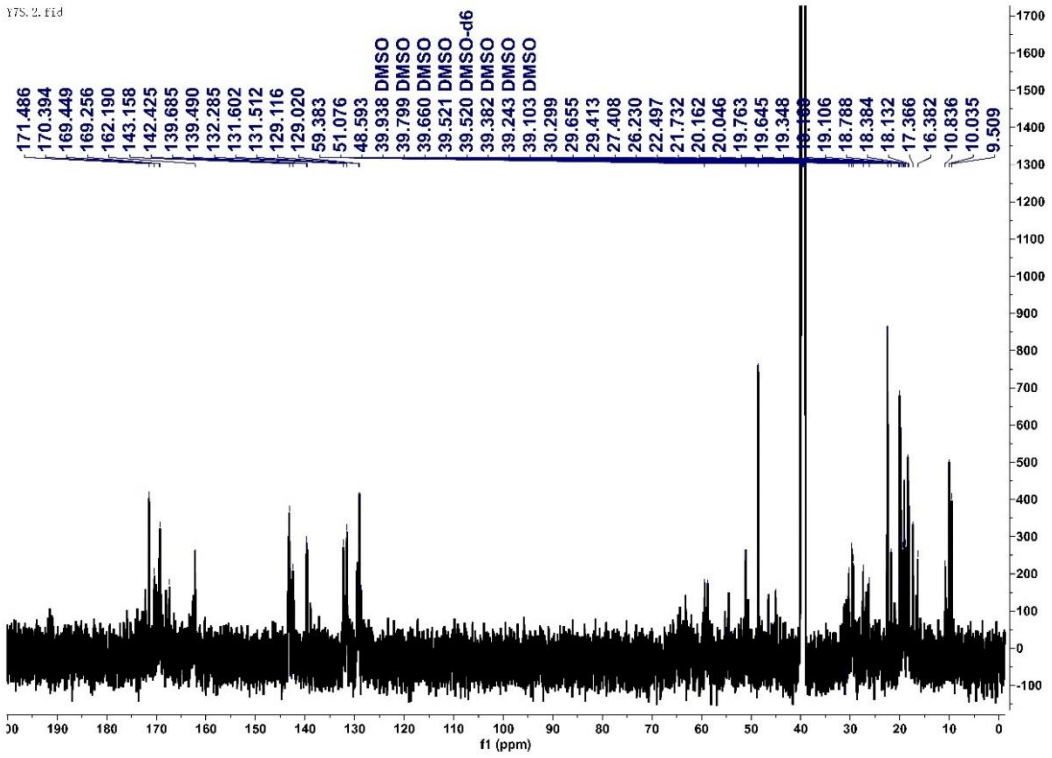

Figure S30. The ^{13}C NMR (150 MHz) spectrum of synthetic-**2** in DMSO-d_6.

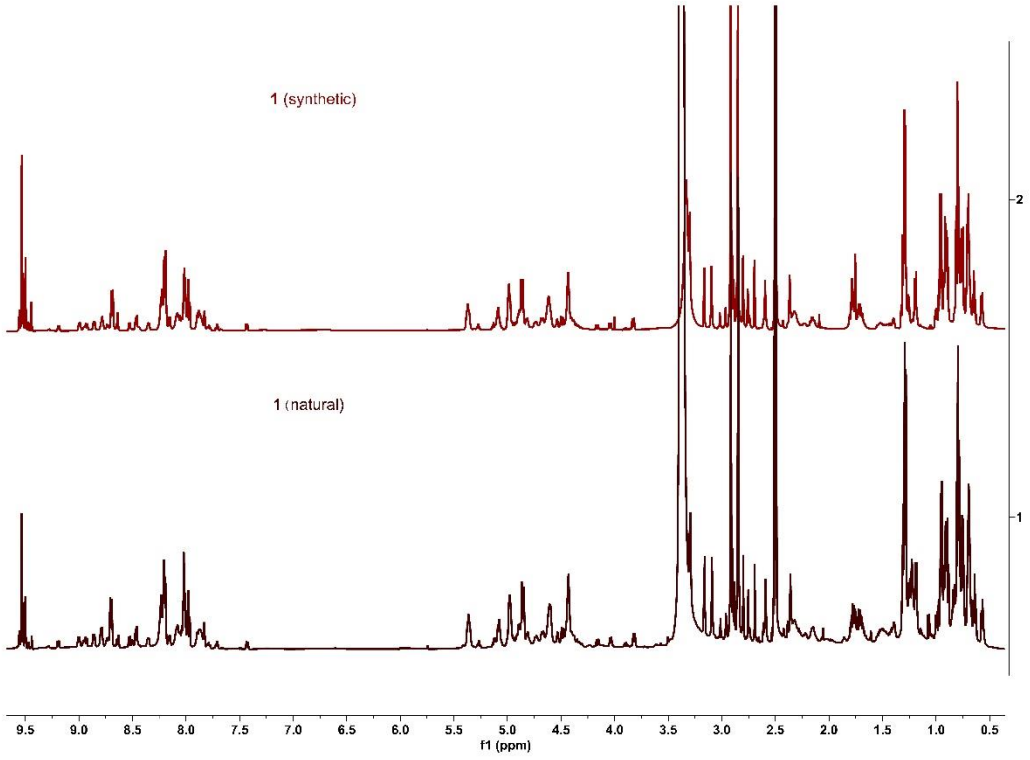

Figure S31. Comparison of ^{1}H NMR spectra (600 MHz) of natural and synthetic of **1**.

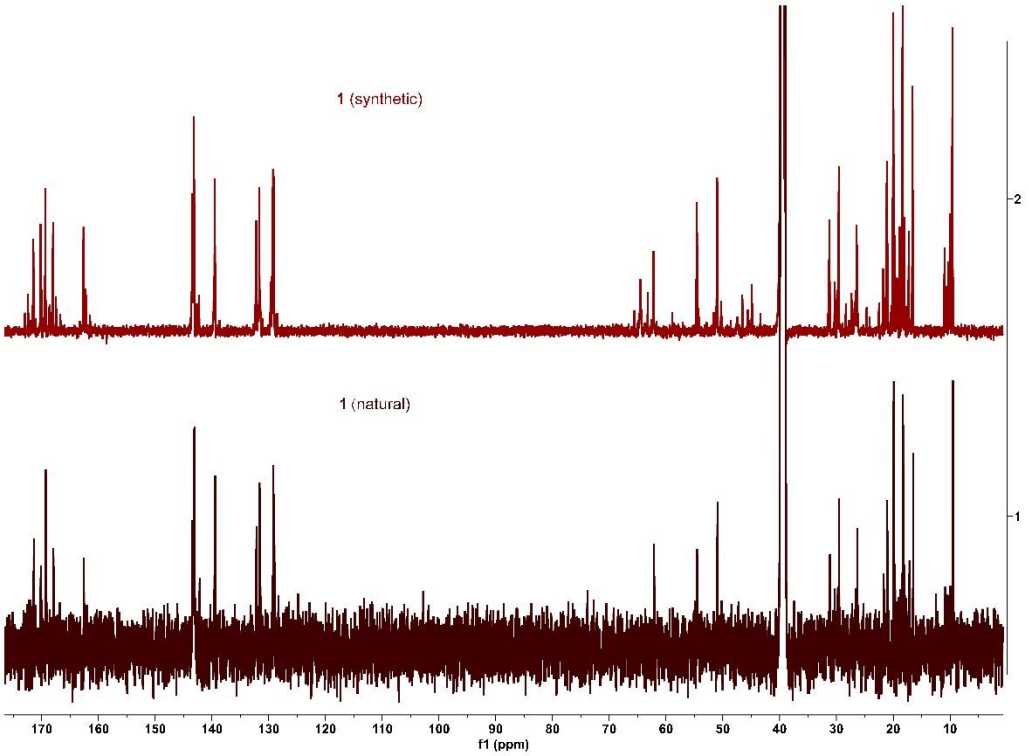

Figure S32. Comparison of ^{13}C NMR spectra (150 MHz) of natural and synthetic of **1**.

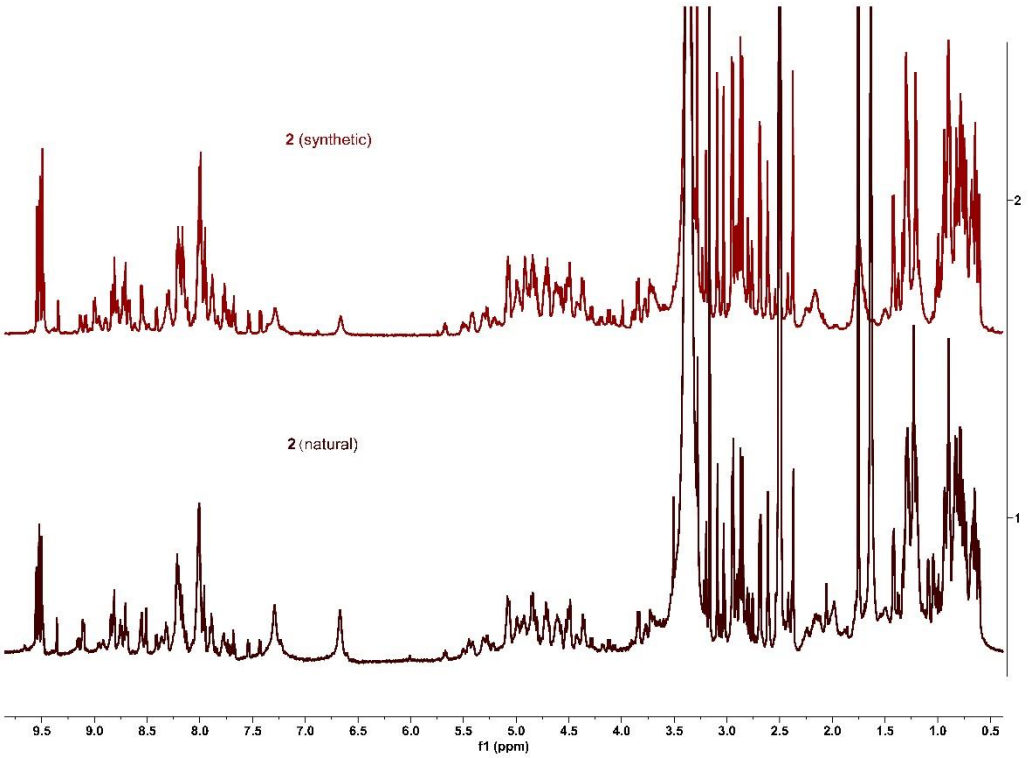

Figure S33. Comparison of ^{1}H NMR spectra (600 MHz) of natural and synthetic of **2**.

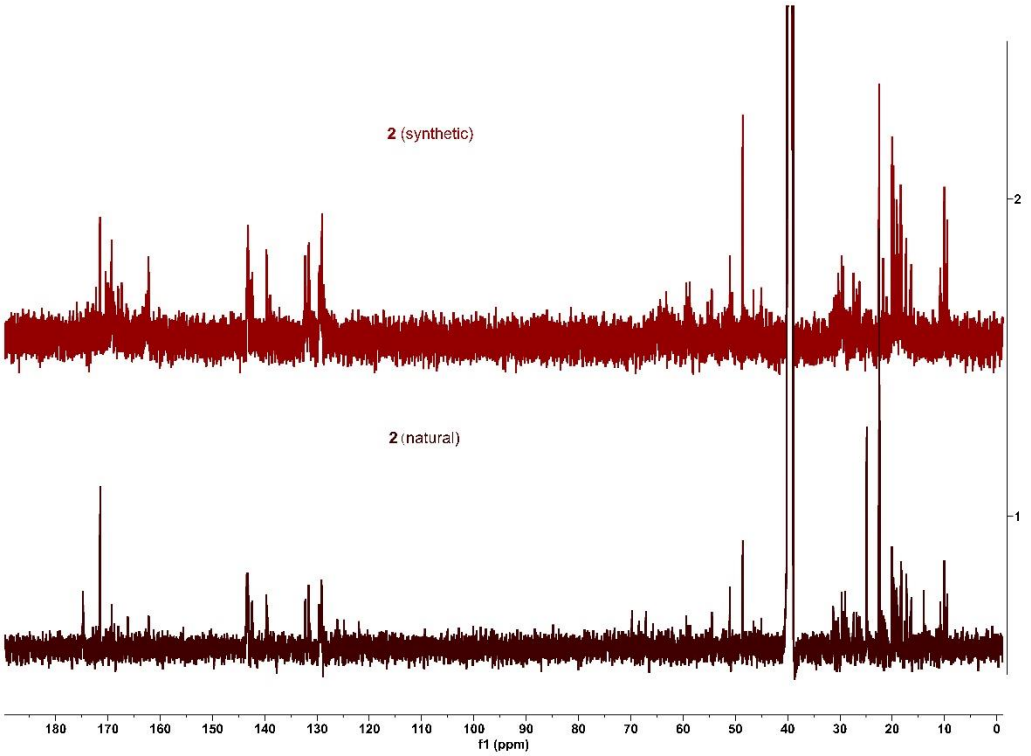

Figure S34. Comparison of ^{13}C NMR spectra (125 MHz) of natural and synthetic of **2**.

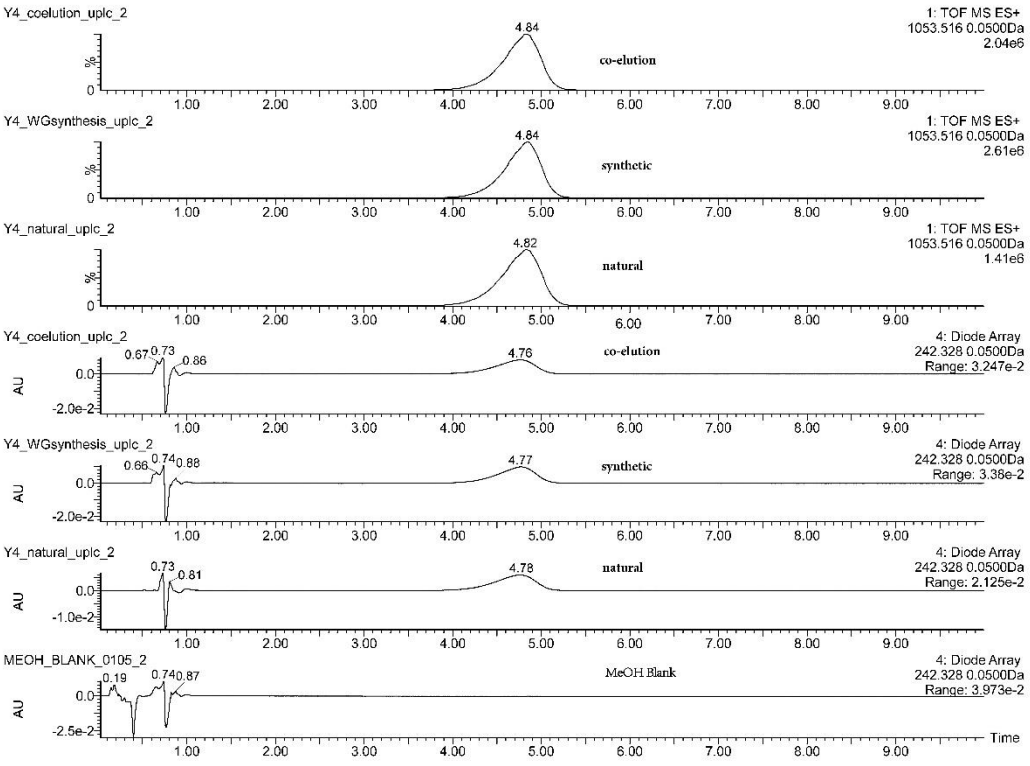

Figure S35. The UPLC-UV-MS chromatograms of **1** (natural, synthetic, and co-elution) in the condition of ACN/water with 0.1% formic acid.

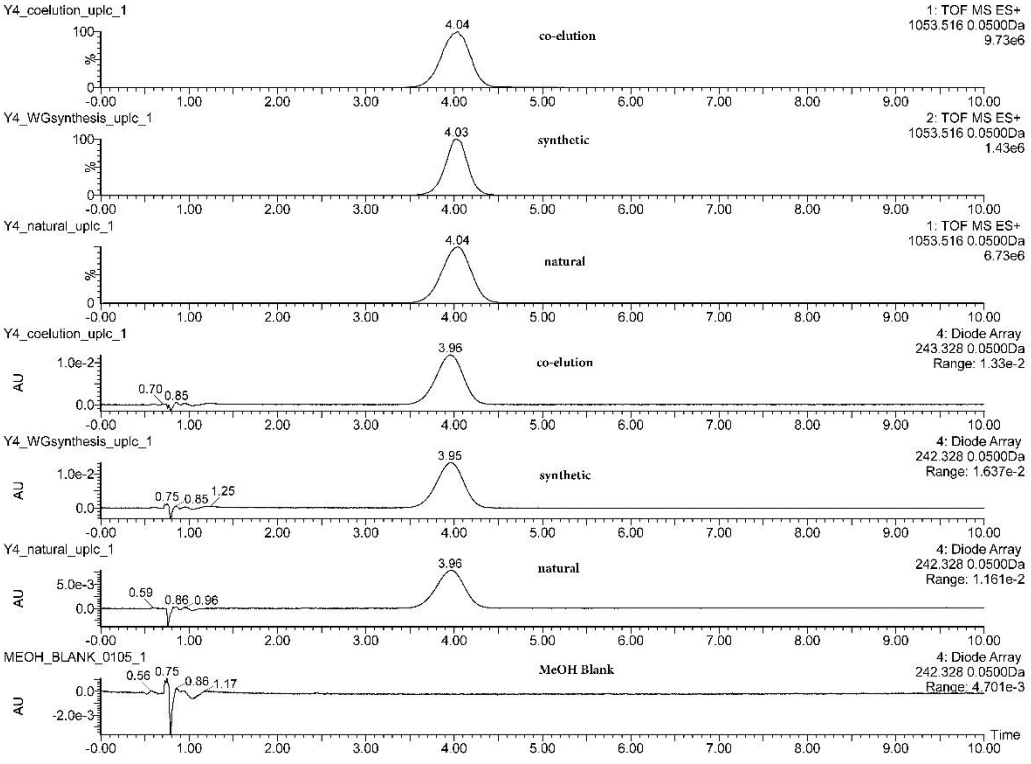

Figure S36. The UPLC-UV-MS chromatograms of **1** (natural, synthetic, and co-elution) in the condition of MeOH/water with 0.1% formic acid.

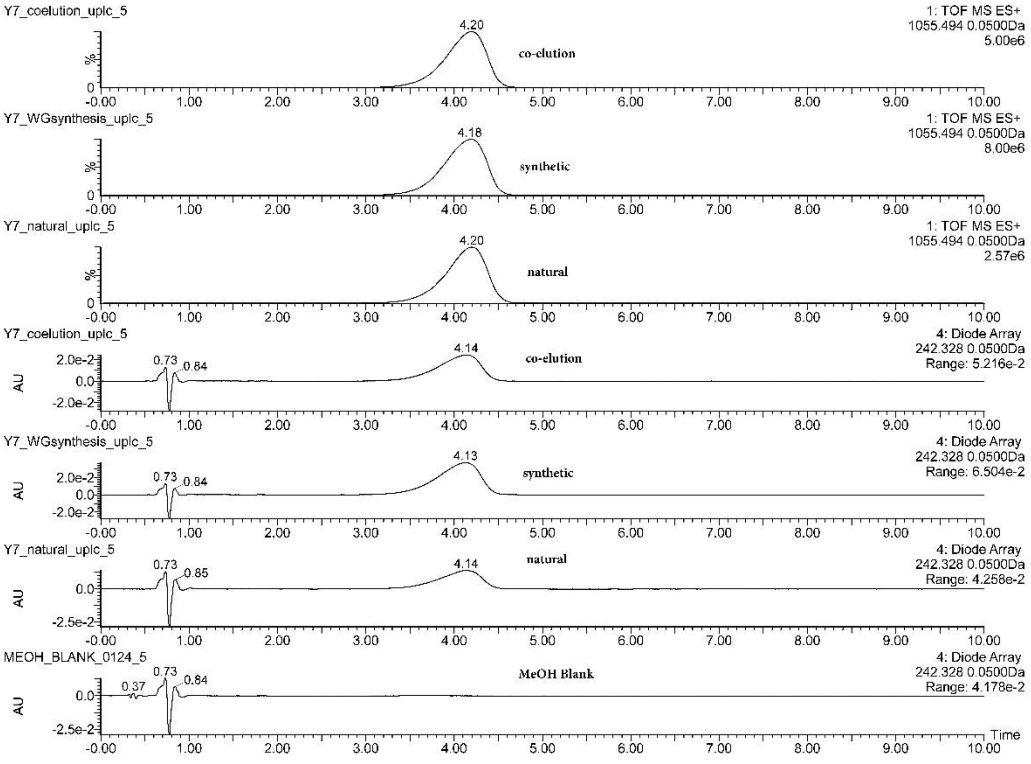

Figure S37. The UPLC-UV-MS chromatograms of **2** (natural, synthetic, and co-elution) in the condition of

ACN/ water with 0.1% formic acid.

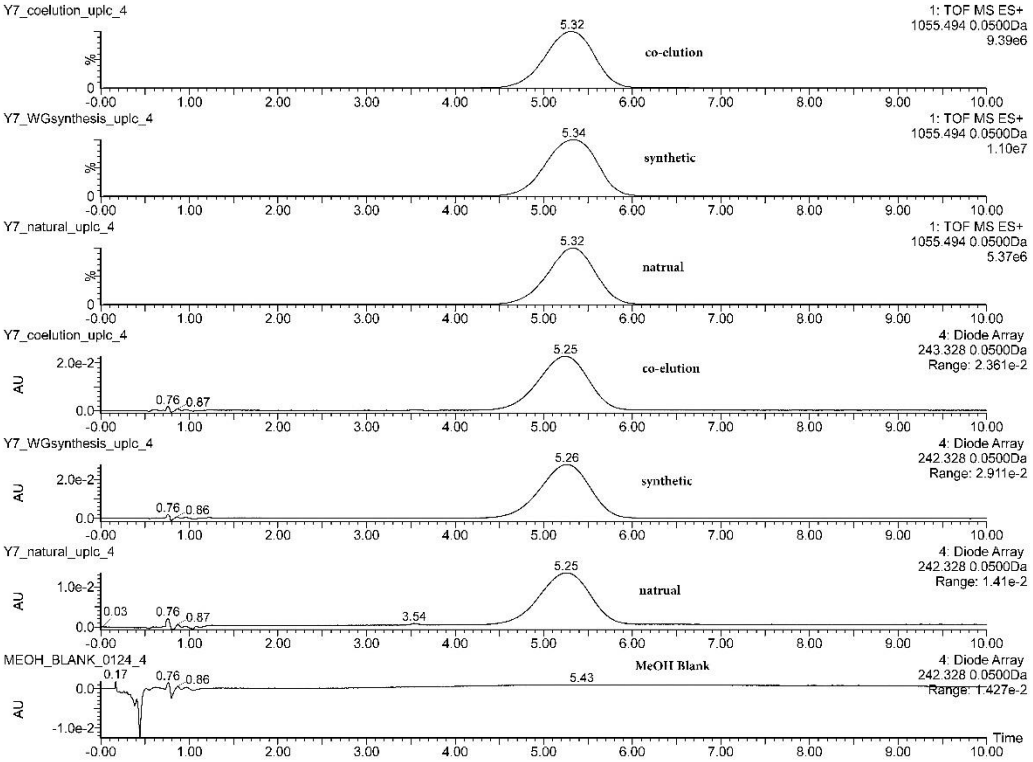

Figure S38. The UPLC-UV-MS chromatograms of **2** (natural, synthetic, and co-elution) in the condition of MeOH/ water with 0.1% formic acid.

Table S1. The physicochemical properties of natural-**1**, synthetic-**1**, natural-**2**, and synthetic-**2**.

	natural-**1**	synthetic-**1**	natural-**2**	synthetic-**2**
Properties	white amorphous powder	white amorphous powder	white amorphous powder	white amorphous powder
HRESIMS	1053.5165 $[M+H]^+$ (calcd for $C_{52}H_{69}N_{12}O_{12}$, 1053.5158)	1053.5139 $[M+H]^+$ (calcd for $C_{52}H_{69}N_{12}O_{12}$, 1053.5158)	1055.4930 $[M+H]^+$ (calcd for $C_{51}H_{67}N_{12}O_{13}$, 1055.4951)	1055.4944 $[M+H]^+$ (calcd for $C_{51}H_{67}N_{12}O_{13}$, 1055.4951)
Molecular formula	$C_{52}H_{68}N_{12}O_{12}$	$C_{52}H_{68}N_{12}O_{12}$	$C_{51}H_{66}N_{12}O_{13}$	$C_{51}H_{66}N_{12}O_{13}$
IR cm-1	3375, 3303, 2968, 2936, 2877, 1742, 1644, 1517, 1492, 1459, 1408, 1180, 1126, 1014	3378, 3312, 2968, 2937, 2877, 1743, 1644, 1517, 1492, 1465, 1408, 1180, 1128, 1014	3351, 2918, 2850, 1740, 1637, 1578, 1538, 1492, 1465, 1409, 1260, 1097, 1025	3304, 2938, 2872, 1741, 1640, 1536, 1492, 1462, 1412, 1261, 1109, 1052
UV(MeOH) λmax (log ε)	242 (4.92), 317 (4.21)	242 (4.82), 324 (4.10)	241 (4.59), 323 (3.91)	242 (4.54), 317 (3.83)
$[\alpha]_D^{25}$	-110.0° (c 0.08, ACN)	-110.0° (c 0.08, ACN)	-152.0° (c 0.05, ACN)	-155.0° (c 0.05, ACN)

Table S2. The antibacterial activities of synthetic-**1** and synthetic-**2** (MIC, μg/mL).

Test organisms	Strain No.	R/S[b]	synthetic-**1**	synthetic-**2**	Ec[c]	Lev[c]
Staphylococcus epidermidis	ATCC 12228	MSSE	>64	>32	0.25	0.25
	18-1[a]	MRSE	>64	>32	0.5	4
	17-13[a]	MSSE	>64	>32	0.12	0.25
Staphylococcus aureus	ATCC 29213	MSSA	>64	>32	0.12	0.5
	ATCC 33591	MRSA	>64	>32	0.25	0.25
	15[a]	MSSA	>64	>32	0.25	0.25
	18-2[a]	MRSA	>64	>32	0.25	>32
	18-3[a]	MSSA	>64	>32	0.12	1
	ATCC 43300	MRSA	>64	>32	0.12	0.5
	ATCC 700698	MRSA,VISA	>64	>32	0.12	16
Enterococcus faecalis	ATCC 29212	VSE	>64	>32	0.12	1
	ATCC 51299	VRE	>64	>32	0.12	1
	ATCC 51575	VRE	>64	>32	0.12	2
	18-6[a]	VSE	>64	>32	0.25	2
Enterococcus faecium	ATCC 700221	VRE	>64	>32	0.12	>32
	18-4[a]	VSE	>64	>32	0.25	4
	15-6[a]	VRE	>64	>32	0.25	>32
Escherichia coli	ATCC 25922	ESBLs(-)	>64	>32	8	0.06
	ATCC 35218	ESBLs(+)	>64	>32	1	0.06
	1515[a]	ESBLs(-)	>64	>32	2	0.06
	18-1[a]	ESBLs(-)	>64	>32	8	2
	18-4[a]	ESBLs(+)	>64	>32	16	16
Klebsiella pneumoniae	ATCC 700603	ESBLs(+)	>64	>32	32	1
	ATCC BAA-2146	NDM-1(+)	>64	>32	16	>32
	7[a]	ESBLs(-)	>64	>32	>32	0.12
	18-2[a]	ESBLs(-)	>64	>32	>32	0.25
	18-8[a]	ESBLs(+)	>64	>32	>32	1
Pseudomonas aeruginosa	ATCC 27853		>64	>32	>32	2
	PAO1		>64	>32	>32	1
Acinetobacter baumannii	ATCC 19606		>64	>32	4	0.5
	16-33[a]	CRAB	>64	>32	8	4
Enterobacter cloacae	ATCC 43560		>64	>32	4	≤0.03
Enterobacter aerogenes	ATCC 13048		>64	>32	16	0.12
Serratia marcescens	ATCC 21074		>64	>32	>32	0.25
Proteus mirabilis	ATCC 49565		>64	>32	>32	0.12
Stenotrophomonas maltophilia	ATCC 13636		>64	>32	4	2
Shigella flexneri	ATCC 12022		>64	>32	8	≤0.03

[a]clinical isolates; [b]drug-resistance; MSSE, methicillin-susceptible *S. epidermidis*; MRSE, methicillin-resistant *S. epidermidis*; MSSA, methicillin-susceptible *S. aureus*; MRSA, methicillin-resistant *S. aureus*; VISA, Vancomycin-intermediate *S. aureus*; VSE, Vancomycin-sensitive *Enterococcus*; VRE, Vancomycin-resistant *Enterococcus*; ESBLs, extended-spectrum beta-lactamases; NDM-1, New Delhi Metallo-beta-lactamase-1; CRAB, Carbapenem-resistant *A. baumannii*; [c]positive control, Ec, echinomycin, Lev, Levofloxacin.

Table S3 The cytotoxic activity of synthetic-**1** and synthetic-**2** against H460 lung cancer cells

	synthetic-**1**	synthetic-**2**	**echinomycin**
IC_{50} (nM)	>1000	>1000	1.5 ± 0.2

IC_{50}, 50% inhibitory concentration (mean ± SD, n=3). They were determined by MTT assay following 72 h of drug treatment.