Supporting Information

Rec. Nat. Prod. **17:2 (2023) 343-351**

Secondary Metabolites from Marine-Derived Fungus *Aspergillus carneus* GXIMD00519

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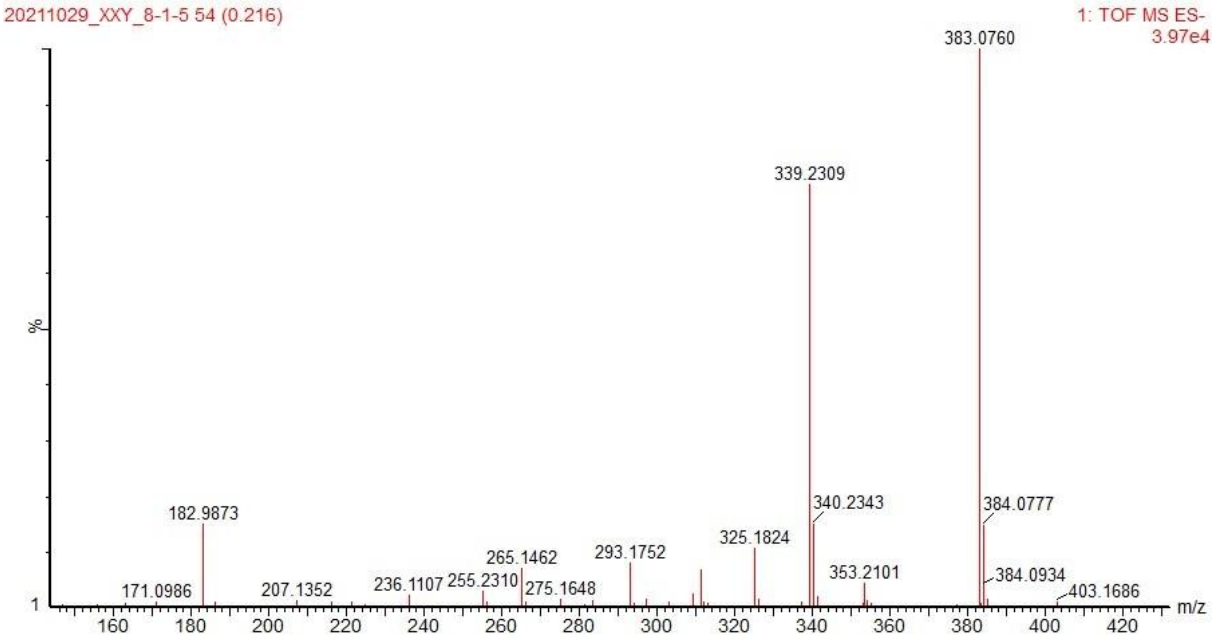


Figure S1: HR-ESI-MS spectrum of **1** (carneusin A)

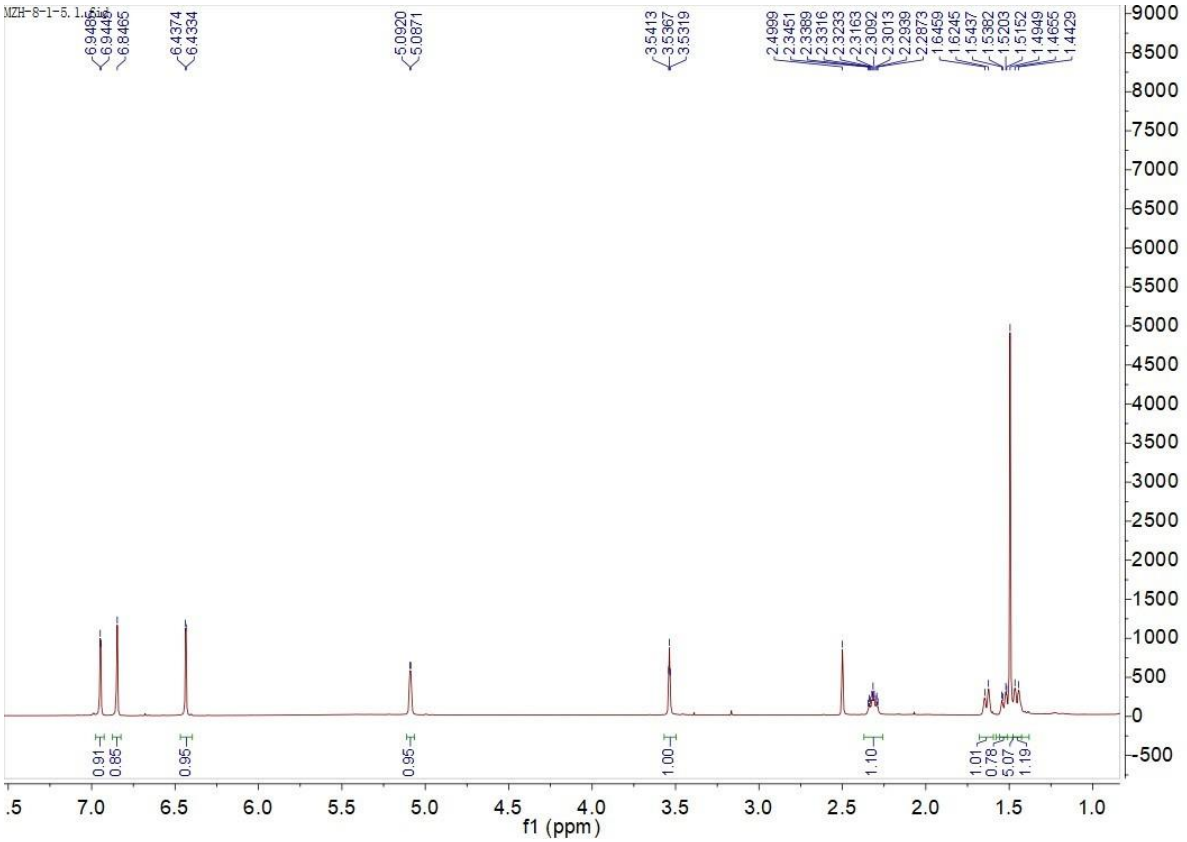


Figure S2: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of **1** (carneusin A)

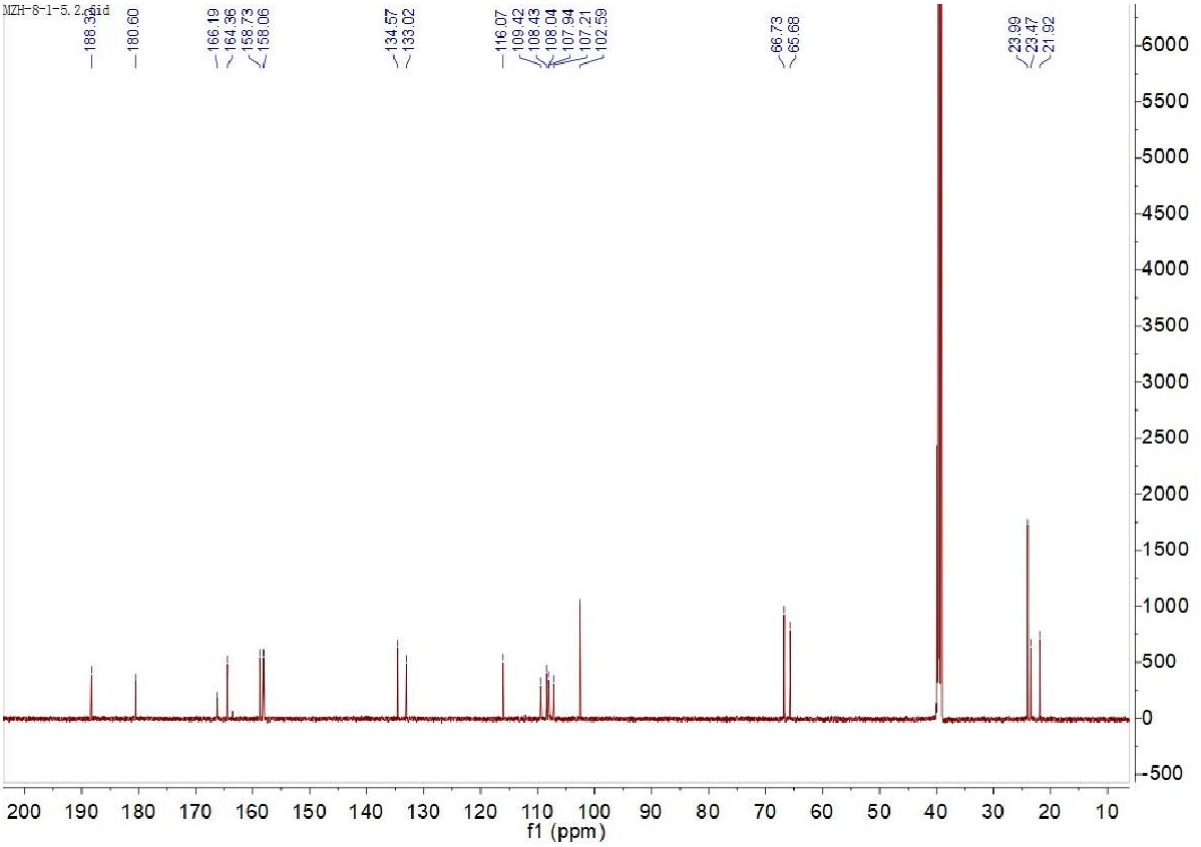


Figure S3: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of **1** (carneusin A)

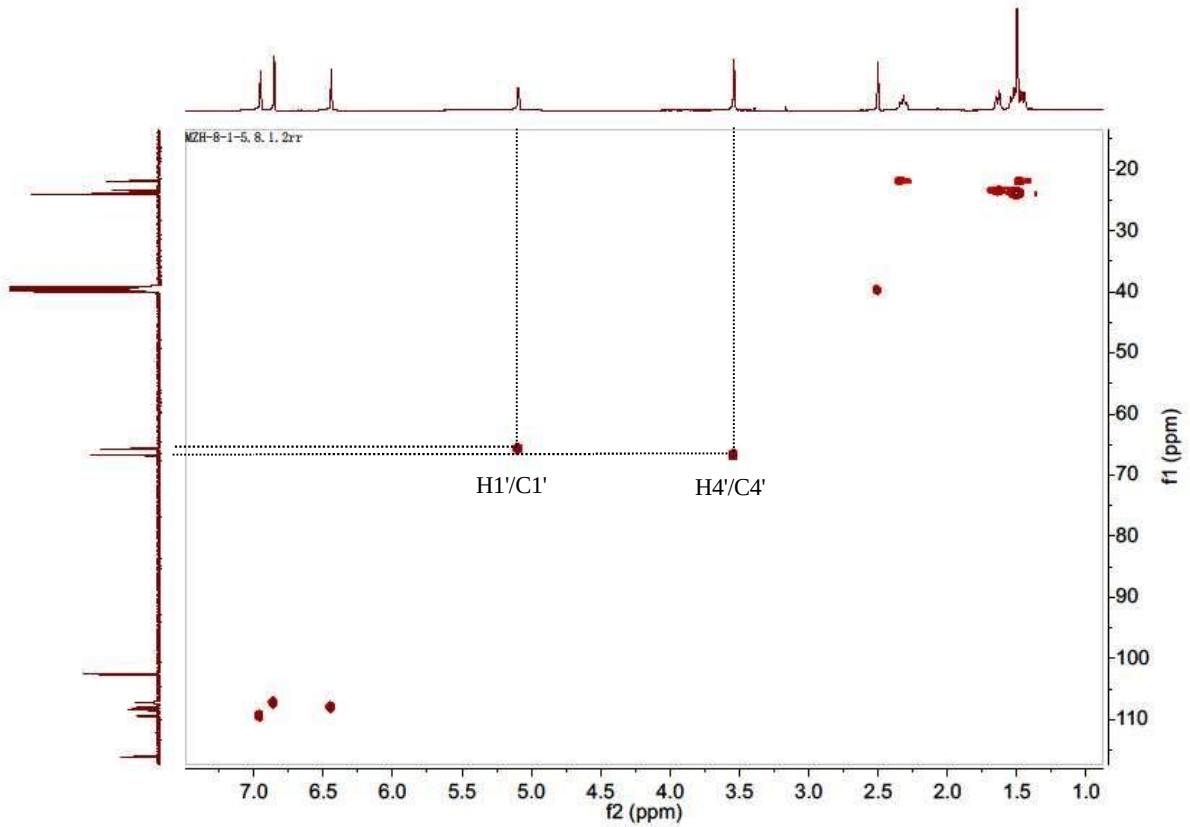


Figure S4: HSQC spectrum of **1** (carneusin A)

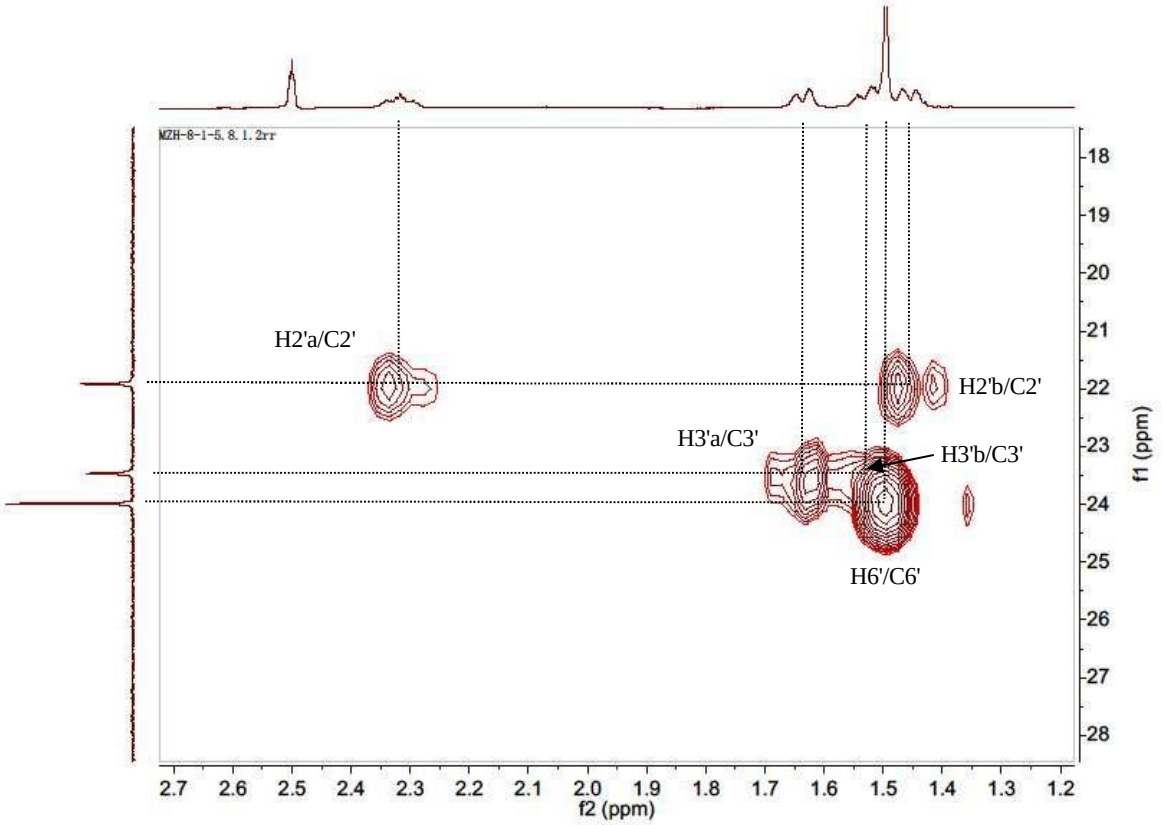


Figure S5: HSQC spectrum of **1** (carneusin A) (From δ_C18 ppm to δ_C 28 ppm)

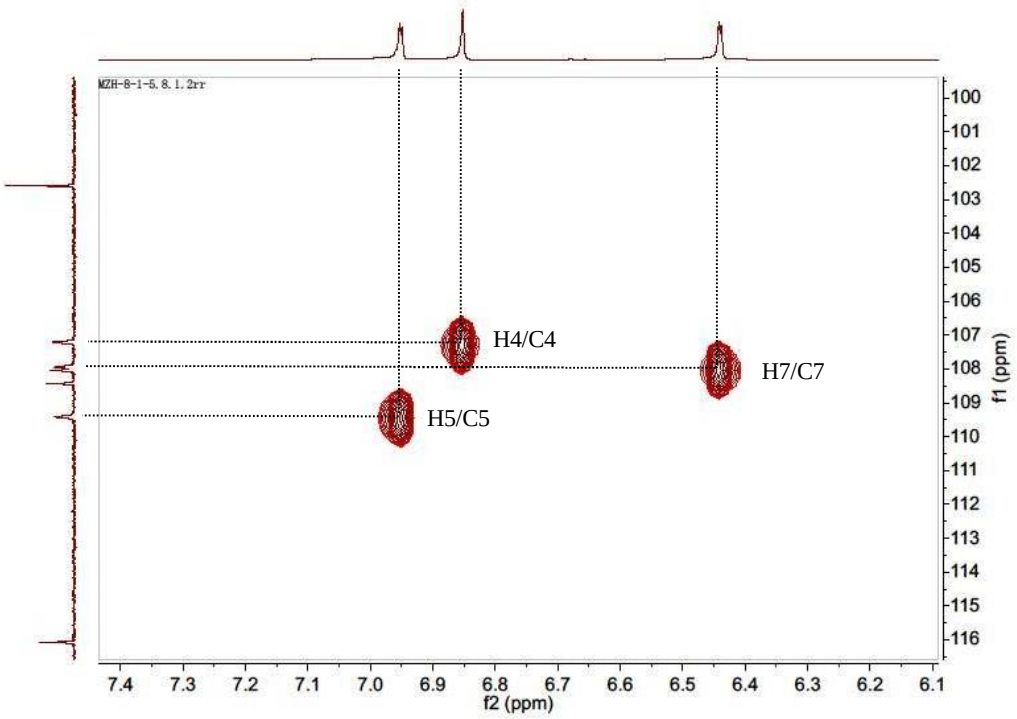


Figure S6: HSQC spectrum of **1** (carneusin A) (From δ_C100 ppm to δ_C 116 ppm)

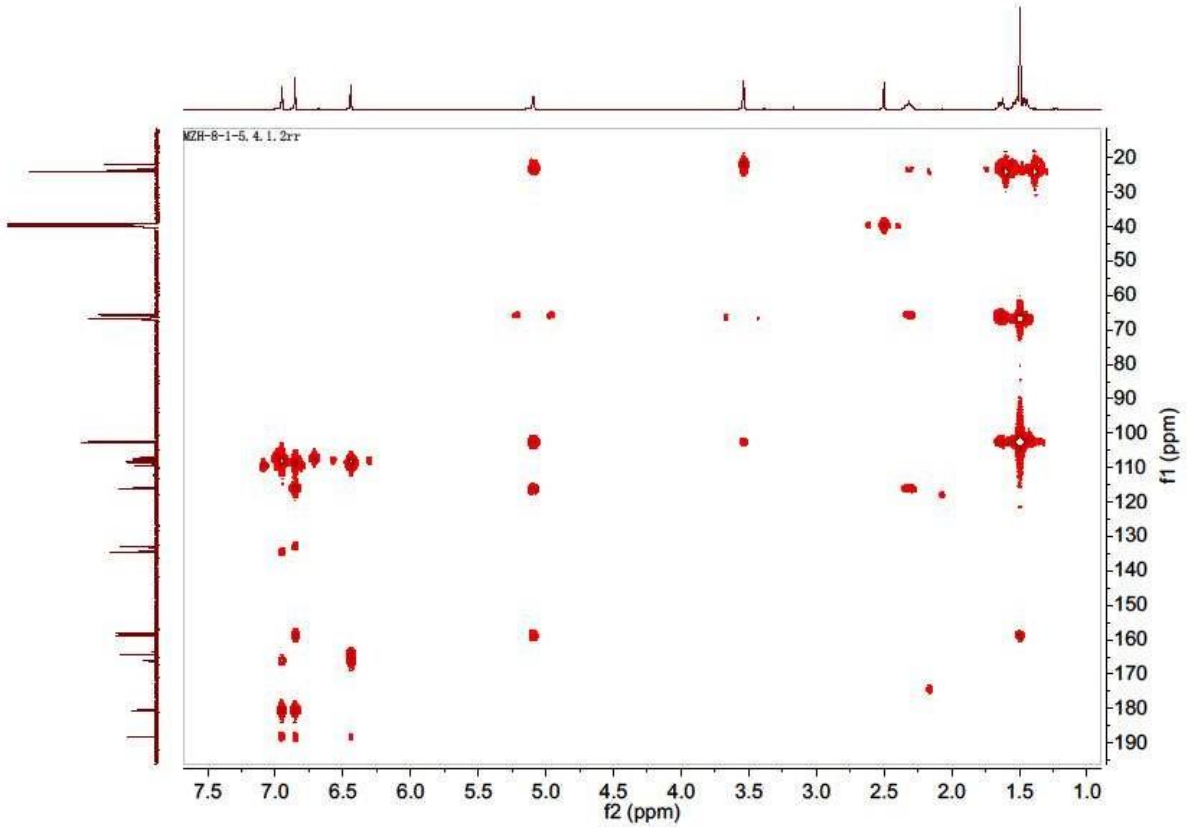


Figure S7: HMBC spectrum of **1** (carneusin A)

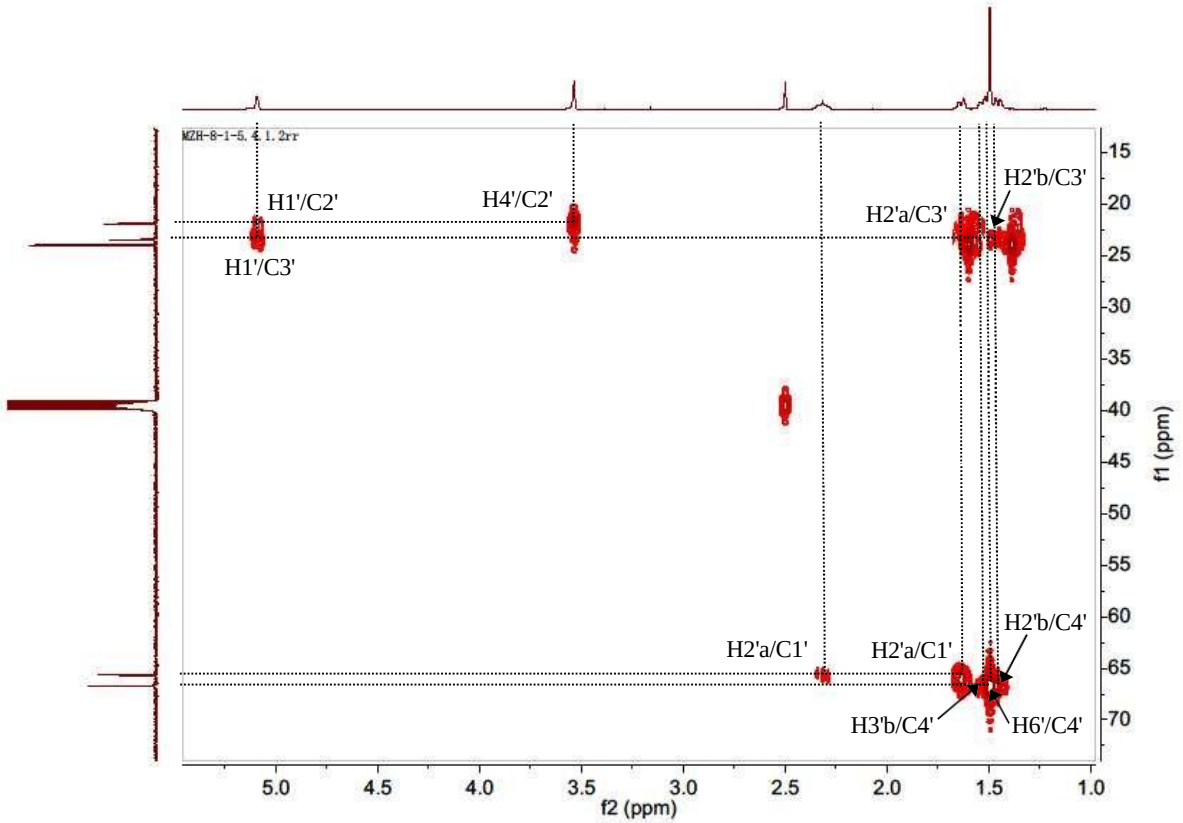


Figure S8: HMBC spectrum of **1** (carneusin A) (From δ_C 15 ppm to δ_C 70 ppm)

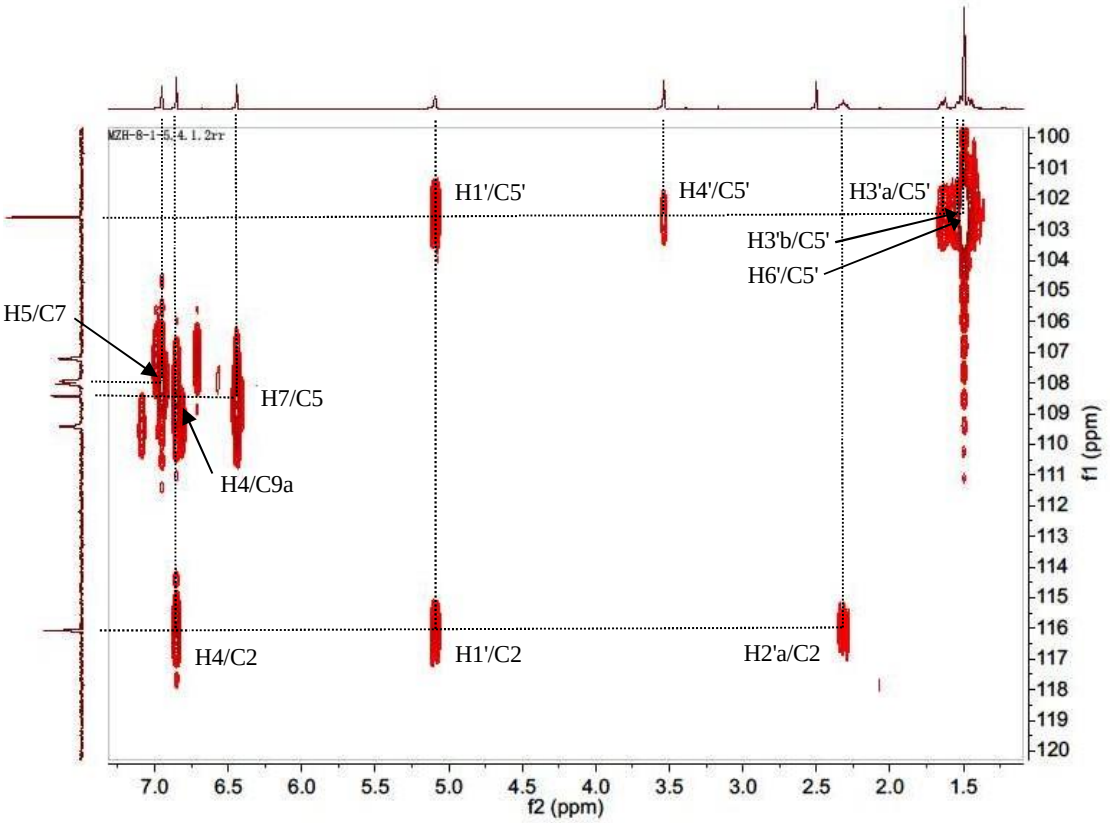


Figure S9: HMBC spectrum of **1** (carneusin A) (From δ_C 100 ppm to δ_C 120 ppm)

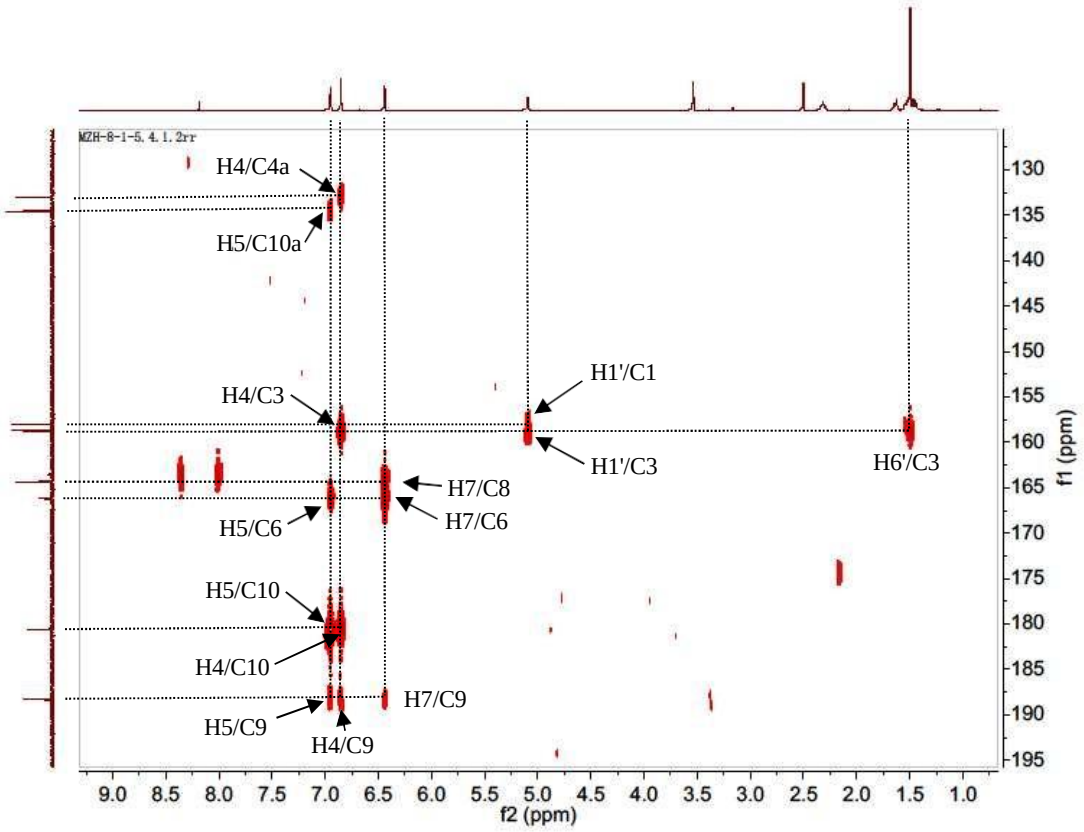


Figure S10: HMBC spectrum of **1** (carneusin A) (From δ_C 125 ppm to δ_C 195 ppm)

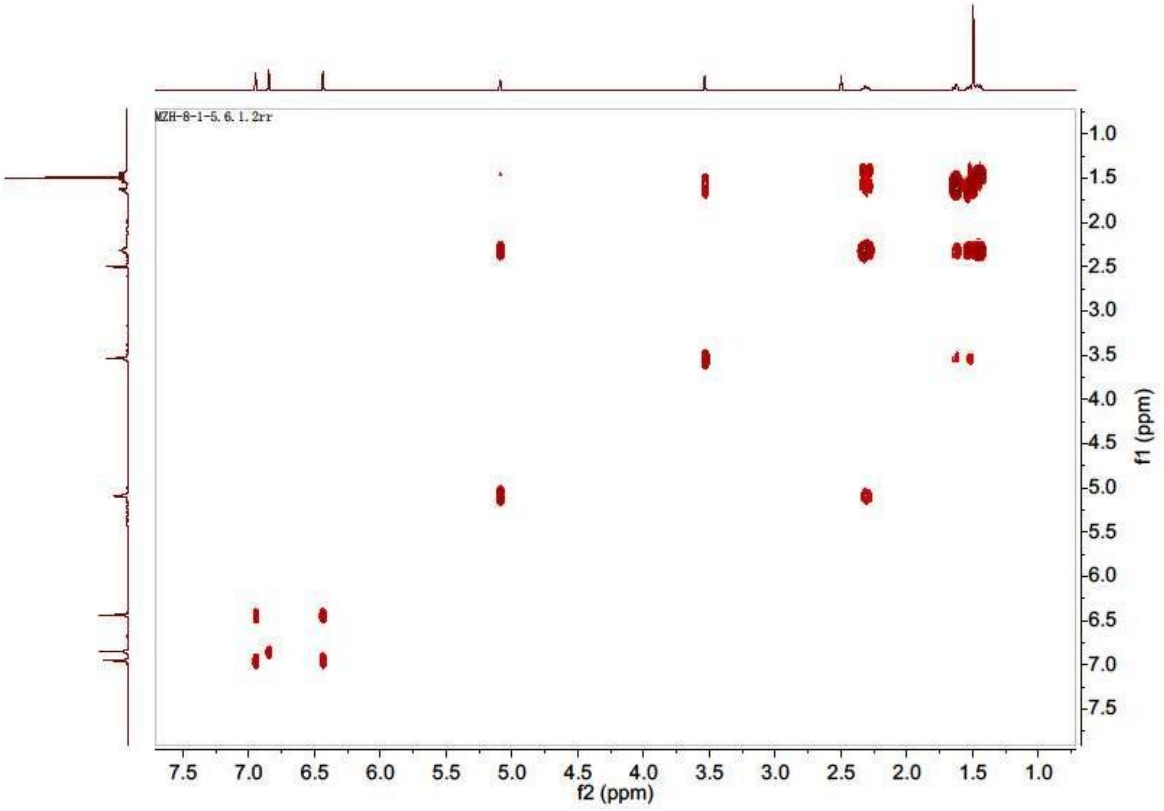


Figure S11: ^{1}H-^{1}H COSY spectrum of **1** (carneusin A)

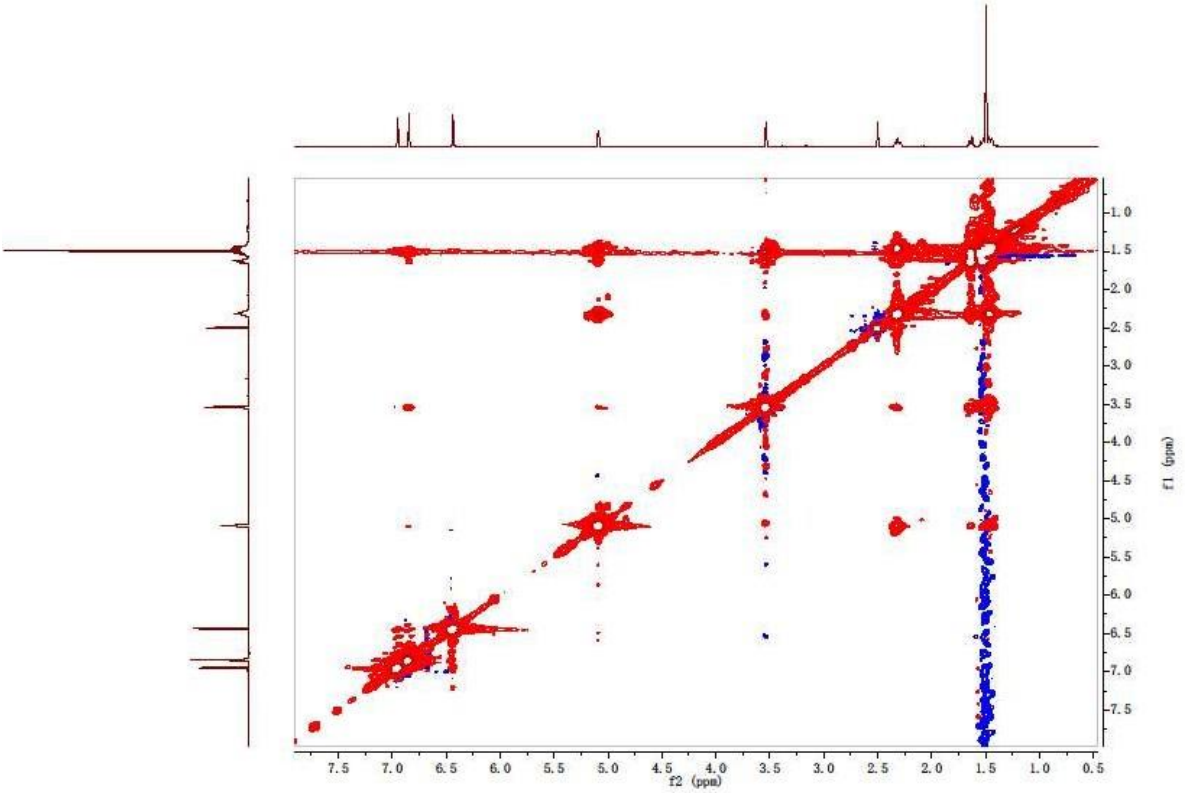


Figure S12: NOESY spectrum of **1** (carneusin A)

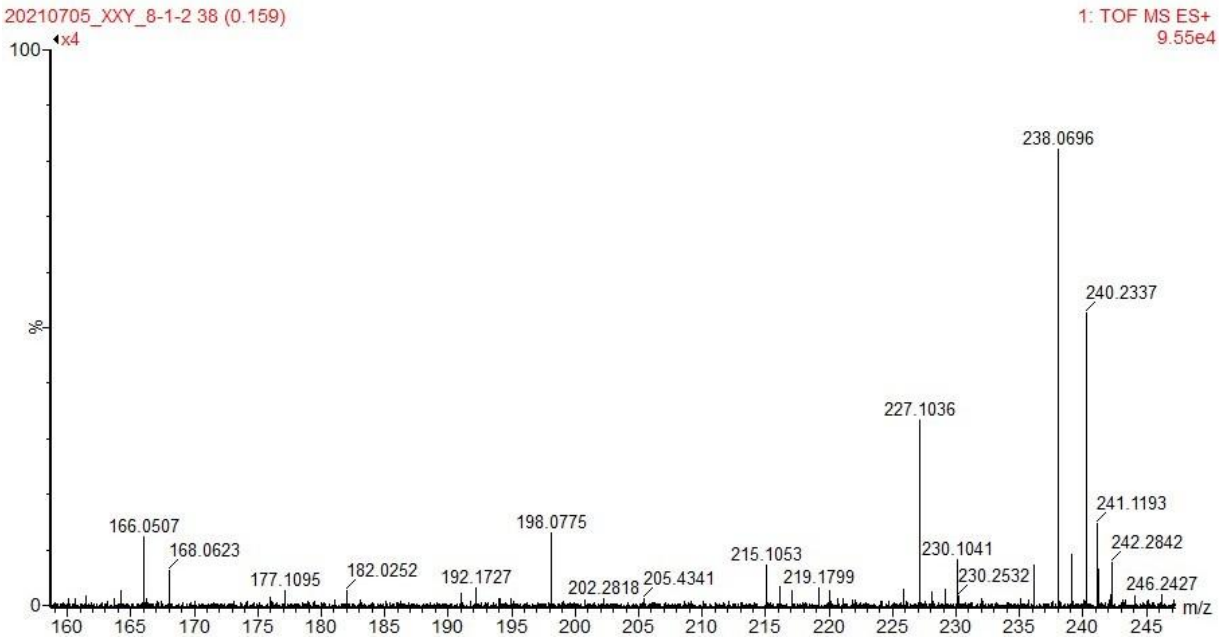


Figure S13: HR-ESI-MS spectrum of **2** (carneusin B)

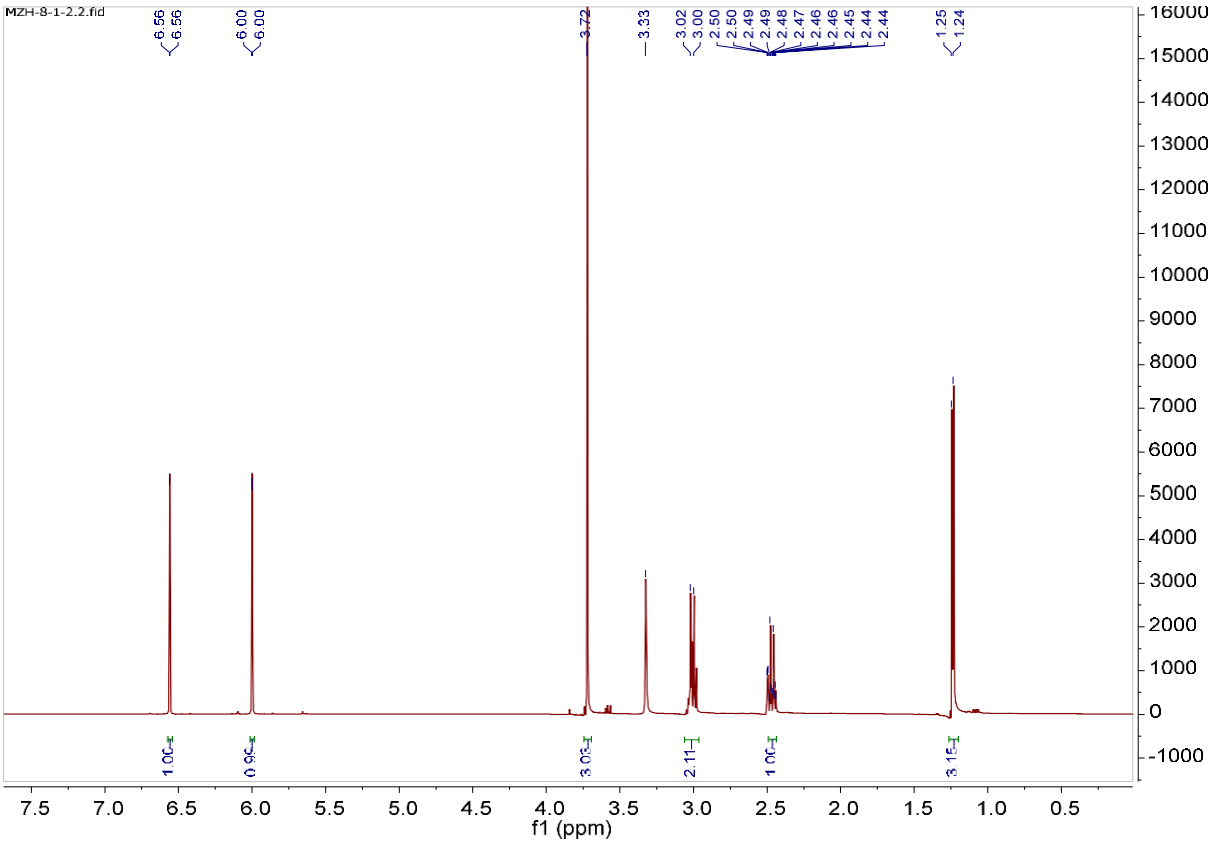


Figure S14: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of **2** (carneusin B)

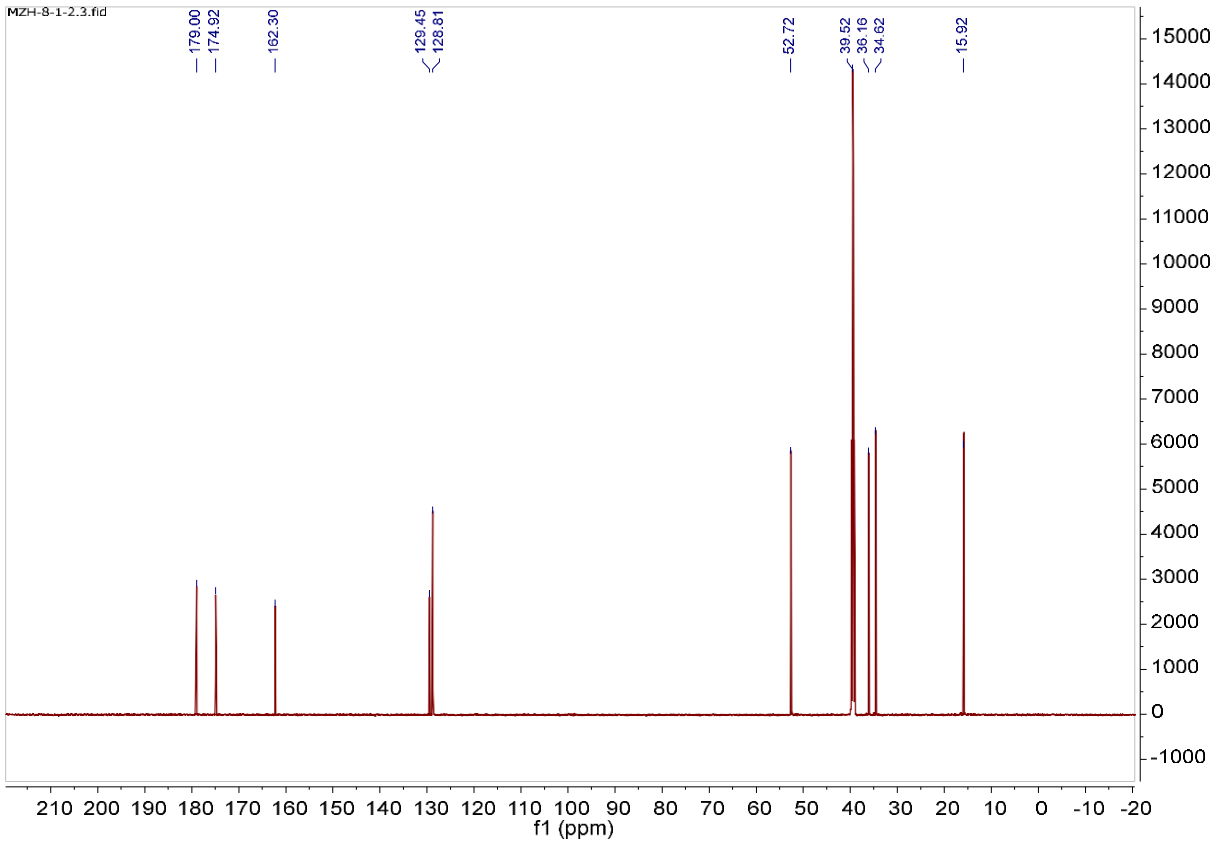


Figure S15: ^{13}C-NMR (150 MHz, $CDCl_3$) spectrum of **2** (carneusin B)

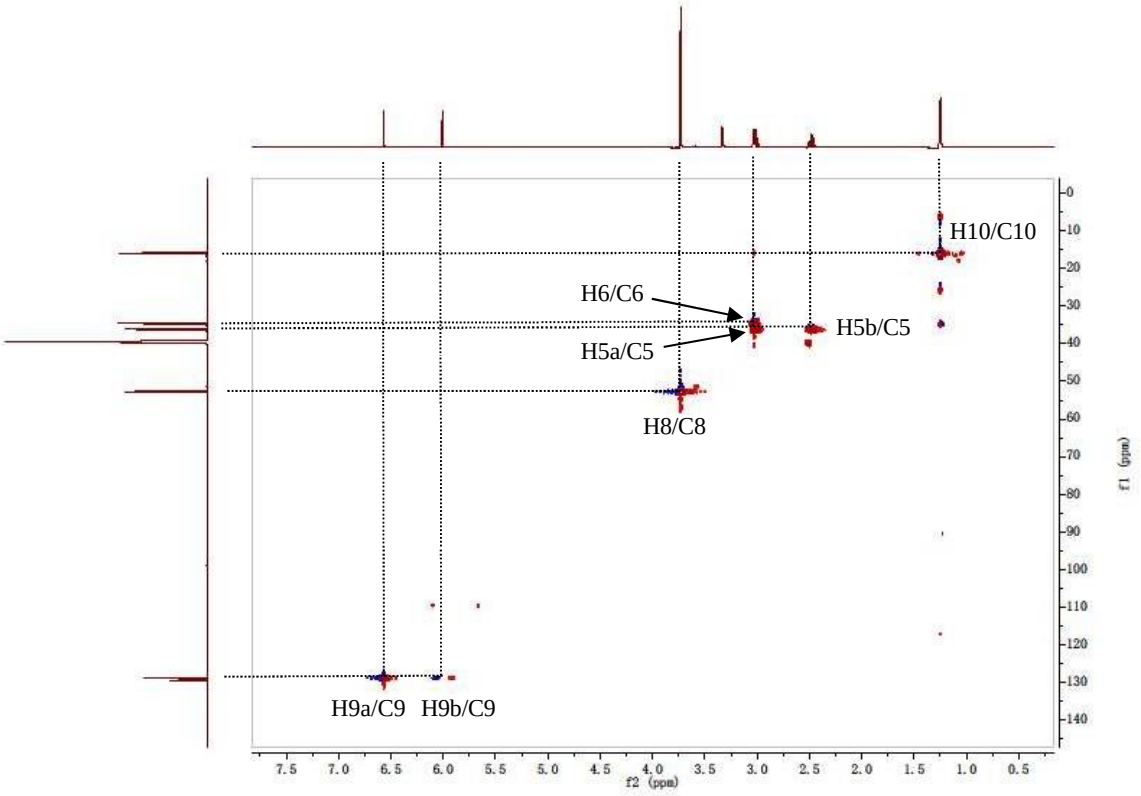


Figure S16: HSQC spectrum of **2** (carneusin B)

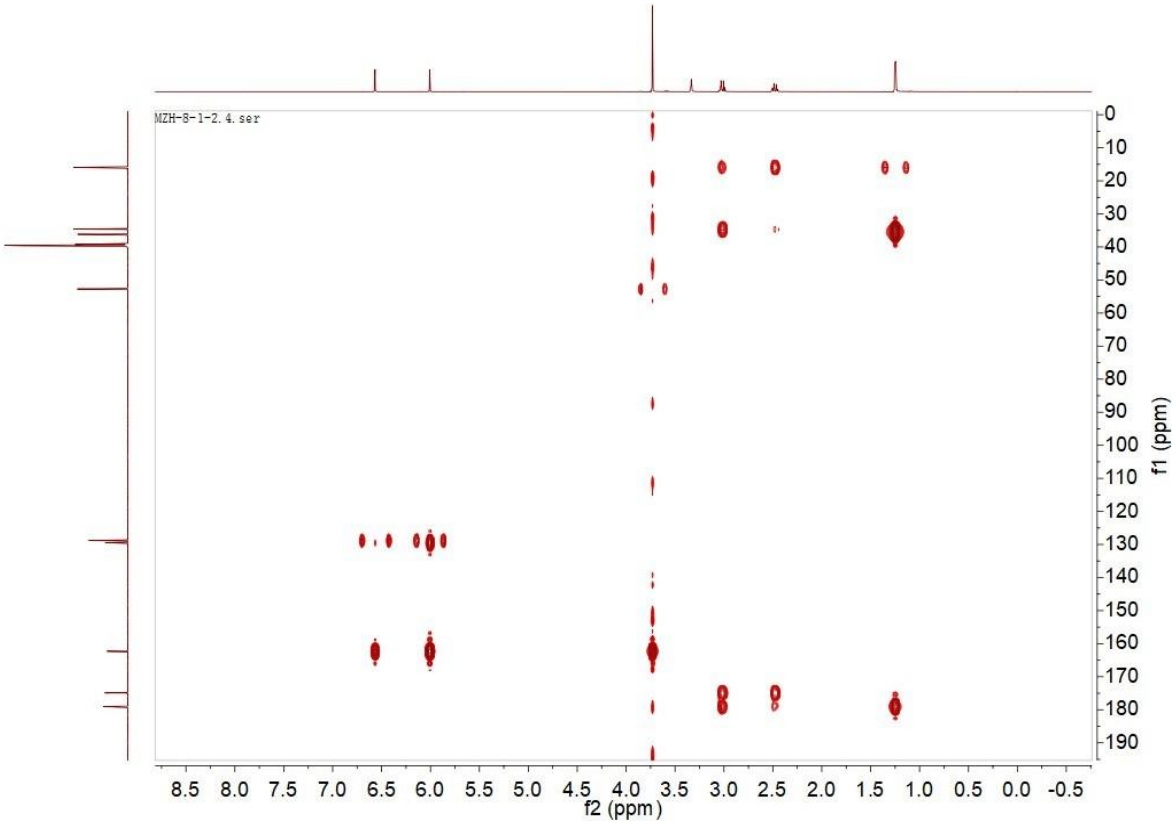


Figure S17: HMBC spectrum of **2** (carneusin B)

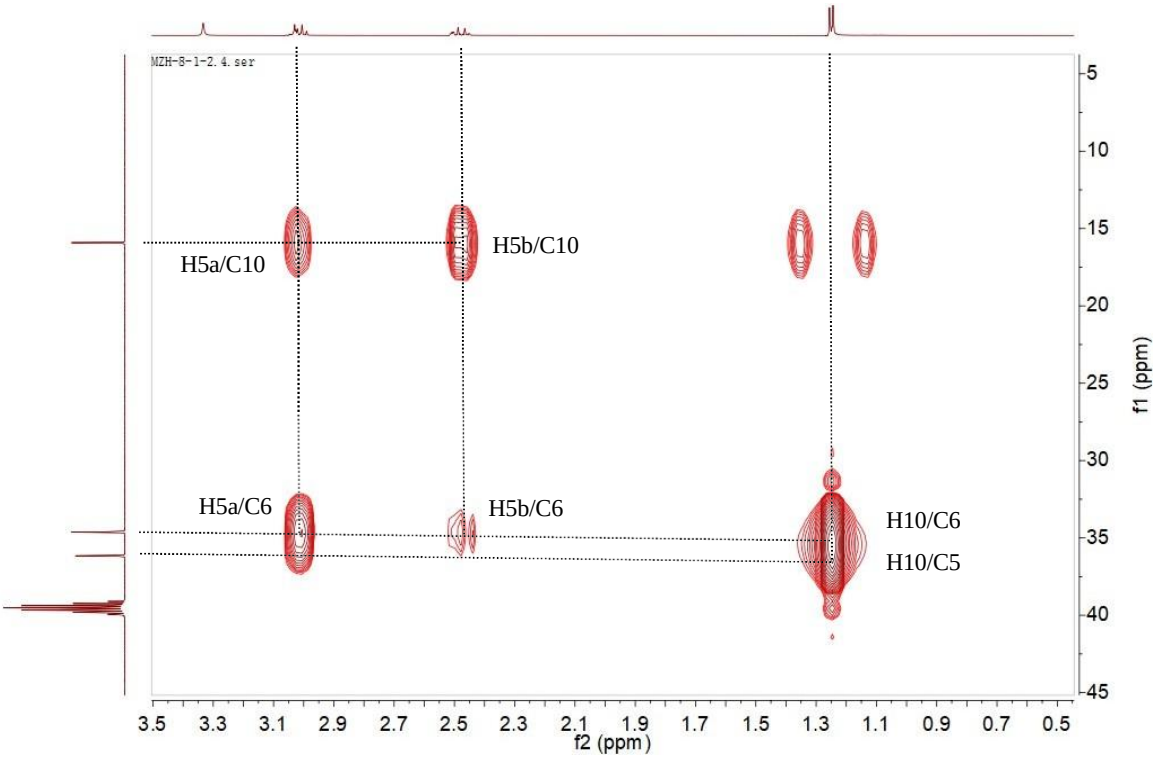


Figure S18: HMBC spectrum of **2** (carneusin B) (From δ_C 5 ppm to 45 ppm)

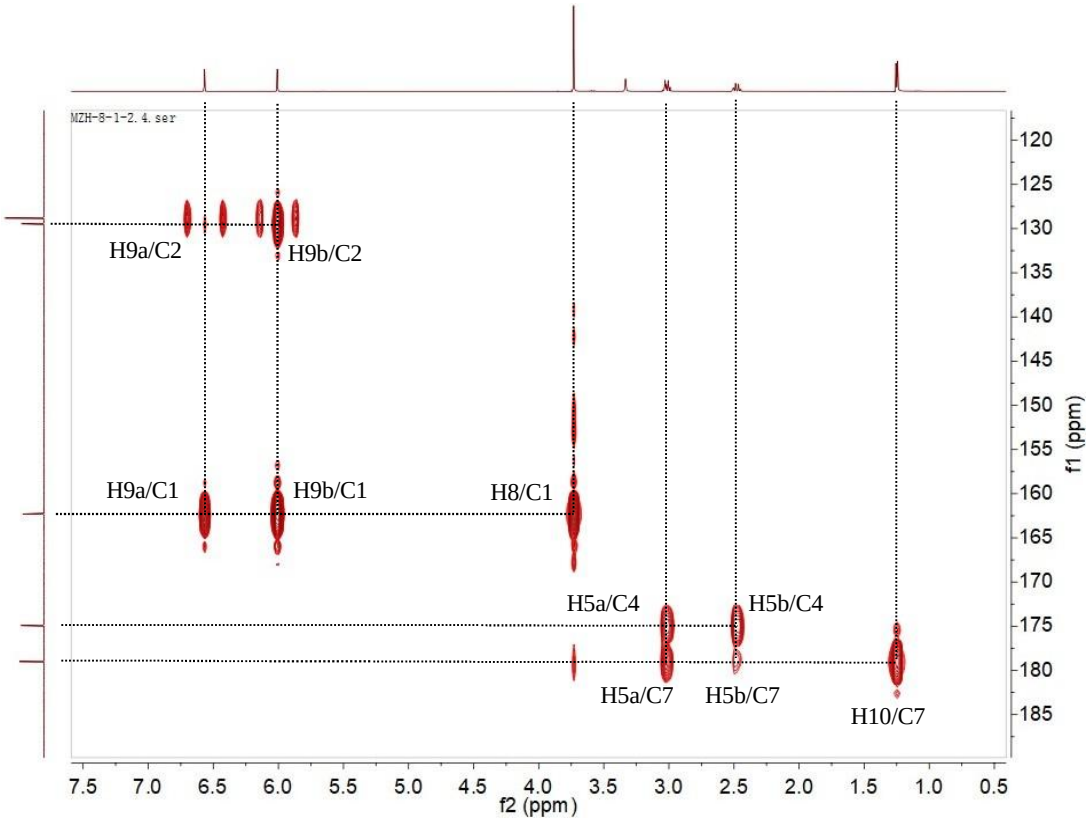
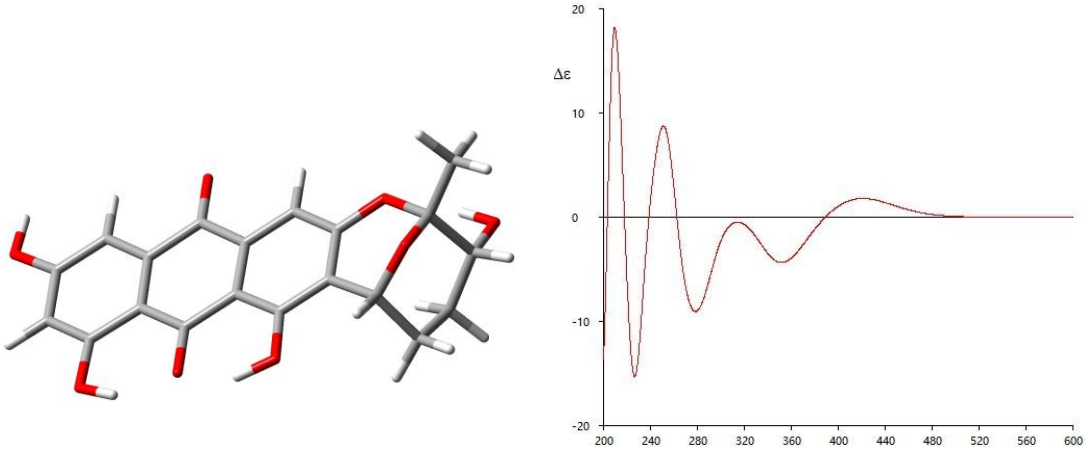


Figure S19: HMBC spectrum of **2** (carneusin B) (From δ_C 120 ppm to 190 ppm)

Table S1: Relative free energies[a] and equilibrium populations[b] of conformers for (1'*S*, 4'*S*, 5'*S*)-**1**[c]

conformer	□*G*	P (%)
1a	0.00	100.00

[a] B3LYP/6-31G(d), in kcal/mol. [b] From □*G* values at 298.15 K. [c] in MeOH, no imaginary frequency



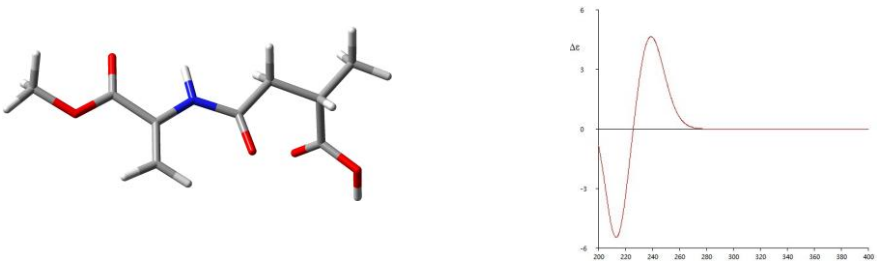
(1'*S*, 4'*S*, 5'*S*)-**1**a

Figure S20: . The optimized structures (left) and the calculated CD spectra of conformers (1'*S* 4'*S*, 5'*S*)-**1** in MeOH at M06-2X/def2TZVP level (right). σ =0.22 eV

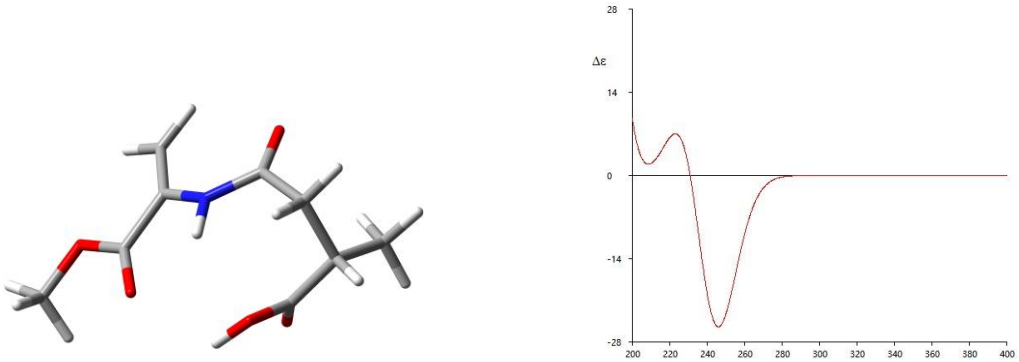
Table S2: Relative free energies[a] and equilibrium populations[b] of conformers for (6*S*)-**2**[c]

conformer	Δ*G*	P (%)
2a	0.00	69.13
2b	1.03	11.98
2c	1.15	9.86
2d	1.20	9.03

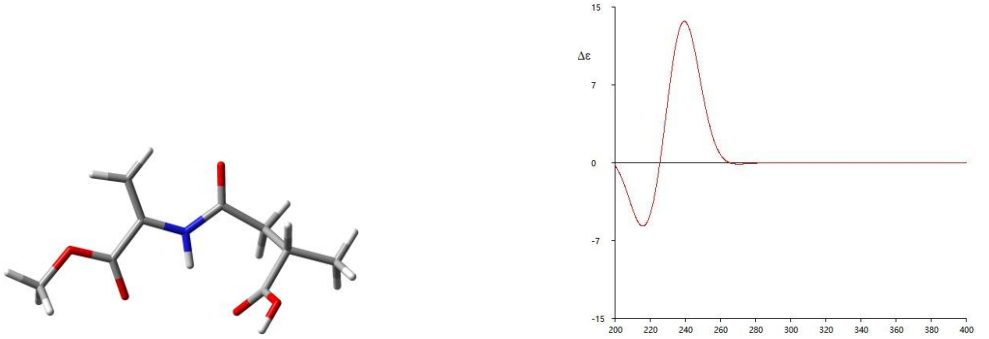
[a] B3LYP/6-31G(d), in kcal/mol. [b] From □*G* values at 298.15 K. [c] in MeOH, no imaginary frequency



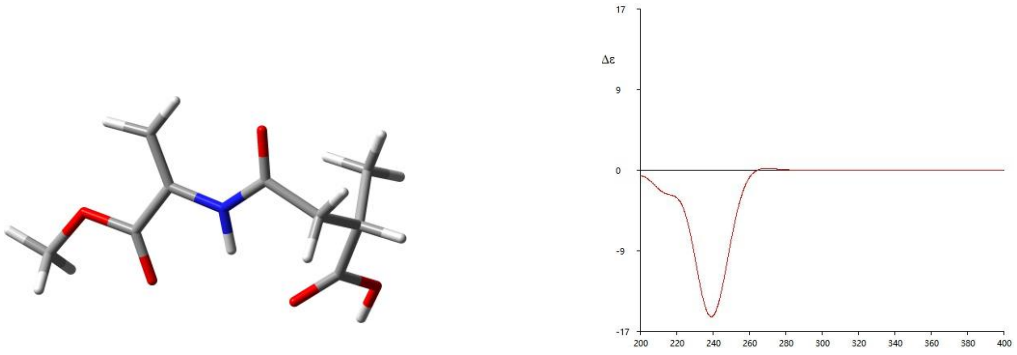
(6*S*)-**2a**



(6*S*)-**2b**



(6*S*)-**2c**



(6*S*)-**2d**

Figure S21: The optimized structures (left) and the calculated CD spectra of conformers (6*S*)-**2** in MeOH at M06-2X/def2TZVP level (right). σ =0.3 eV

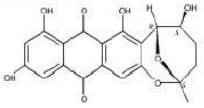
		DP4+	89.54%	10.46%
Nuclei	sp2?	xperimenta	Isomer 1	Isomer 2
C	x	174.92	173.925	173.405
C		36.16	40.254	39.546
C		34.62	36.852	35.959
C	x	179	182.141	181.509
C		15.92	15.798	15.255
C	x	129.45	134.359	134.334
C	x	162.3	168.816	168.733
C	x	128.81	106.88	106.844
C		52.72	53.321	53.359

Figure S22: DP4+ probabilities (%) for conformers (6*S*)-**2** (isomer 1) and (6*R*)-**2** (isomer 2)

Score: 95

1.

28458-23-3



Absolute stereochemistry.

$C_{20}H_{16}O_8$
2,6-Epoxy-2*H*-anthra[2,3-*b*]oxocin-8,13-dione, 3,4,5,6-tetrahydro-5,7,9,11-tetrahydroxy-2-methyl-, (2*S*,5*S*,6*R*)-

Key Physical Properties:

Molecular Weight
384.34
Melting Point (Experimental)
Value: 203-206 °C
Boiling Point (Predicted)
Value: 659.2±55.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.676±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 5.70±0.60 | Condition: Most Acidic Temp: 25 °C

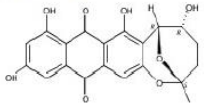
Related Info:

~ 55 References
Reactions
~ 2 Commercial Sources
Spectra
Experimental Properties

Score: 95

2.

93922-50-0



Absolute stereochemistry.

$C_{20}H_{16}O_8$
2,6-Epoxy-2*H*-anthra[2,3-*b*]oxocin-8,13-dione, 3,4,5,6-tetrahydro-5,7,9,11-tetrahydroxy-2-methyl-, [2*S*-(2α,5β,6α)]- (9CI)

Key Physical Properties:

Molecular Weight
384.34
Boiling Point (Predicted)
Value: 659.2±55.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.676±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 5.70±0.60 | Condition: Most Acidic Temp: 25 °C

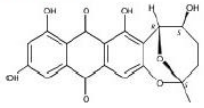
Related Info:

~ 1 References

Score: 95

3.

99528-66-2



Relative stereochemistry.

$C_{20}H_{16}O_8$
2,6-Epoxy-2*H*-anthra[2,3-*b*]oxocin-8,13-dione, 3,4,5,6-tetrahydro-5,7,9,11-tetrahydroxy-2-methyl-, (2*R*,5*R*,6*S*)-*rel*-

Key Physical Properties:

Molecular Weight
384.34
Boiling Point (Predicted)
Value: 659.2±55.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.676±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 5.70±0.60 | Condition: Most Acidic Temp: 25 °C

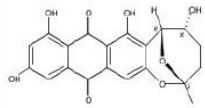
Related Info:

~ 2 References
Reactions

Score: 95

4.

99528-67-3



Relative stereochemistry.

$C_{20}H_{16}O_8$
2,6-Epoxy-2*H*-anthra[2,3-*b*]oxocin-8,13-dione, 3,4,5,6-tetrahydro-5,7,9,11-tetrahydroxy-2-methyl-, (2*R*,5*S*,6*S*)-*rel*-

Key Physical Properties:

Molecular Weight
384.34
Boiling Point (Predicted)
Value: 659.2±55.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.676±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 5.70±0.60 | Condition: Most Acidic Temp: 25 °C

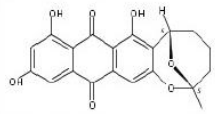
Related Info:

~ 1 References
Reactions
Spectra

Score: 93

5.

14016-29-6



Absolute stereochemistry.

$C_{20}H_{16}O_7$
2,6-Epoxy-2*H*-anthra[2,3-*b*]oxocin-8,13-dione, 3,4,5,6-tetrahydro-7,9,11-trihydroxy-2-methyl-, (2*S*,6*S*)-

Key Physical Properties:

Molecular Weight
368.34
Melting Point (Experimental)
Value: 288-293 °C
Boiling Point (Predicted)
Value: 602.9±55.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.585±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 5.83±0.40 | Condition: Most Acidic Temp: 25 °C

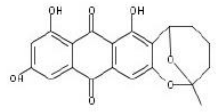
Related Info:

~ 201 References
Reactions
~ 7 Commercial Sources
Experimental Properties

Score: 93

6.

79896-28-9



$C_{20}H_{16}O_7$
2,6-Epoxy-2*H*-anthra[2,3-*b*]oxocin-8,13-dione, 3,4,5,6-tetrahydro-7,9,11-trihydroxy-2-methyl-

Key Physical Properties:

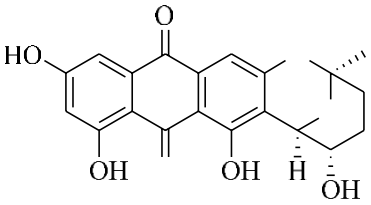
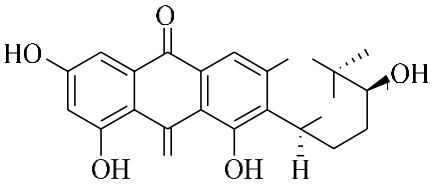
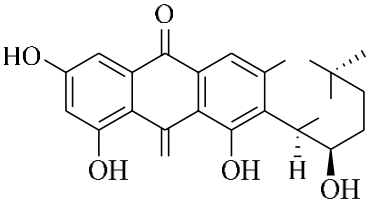
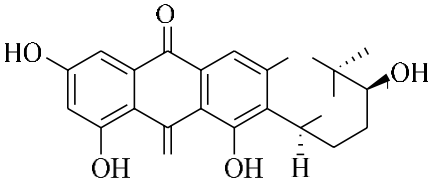
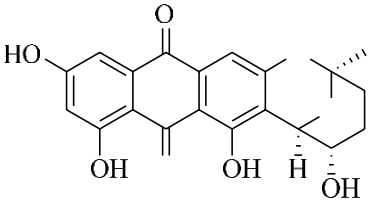
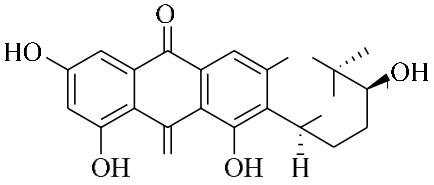
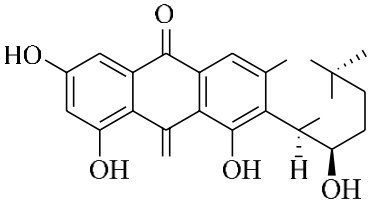
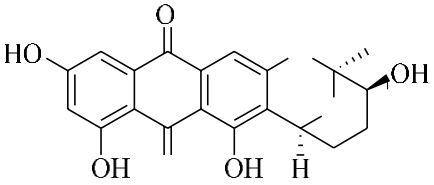
Molecular Weight
368.34
Melting Point (Experimental)
Value: 282-288 °C (decomp) | Condition: Solv: chloroform (67-66-3)
Boiling Point (Predicted)
Value: 602.9±55.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.585±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 5.83±0.40 | Condition: Most Acidic Temp: 25 °C

Related Info:

~ 16 References
Reactions
~ 3 Commercial Sources
Spectra
Experimental Properties

Figure S23 : The Scifinder searching results of compound **1**

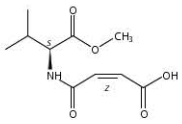
Table S3 : The structural comparison of similar comounds with **1**

No.	Similarity score	Similar chemical structure and CAS number	compound **1**
1	95	 CAS NO. 28458-23-3 Absolute stereochemistry	
2	95	 CAS NO. 93922-50-0 Absolute stereochemistry	
3	95	 CAS NO. 99528-66-2 Relative stereochemistry	
4	95	 CAS NO. 99528-67-3 Relative stereochemistry	

Score: 91

1.

824393-57-9



Double bond geometry as shown., Rotation (-)., Absolute stereochemistry.

$C_{10}H_{15}NO_5$
2-Butenoic acid, 4-[[(1*S*)-1-(methoxycarbonyl)-2-methylpropyl]amino]-4-oxo-, (2*Z*)-

Key Physical Properties:

Molecular Weight
229.23
Boiling Point (Predicted)
Value: 432.1±45.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.193±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 2.78±0.25 | Condition: Most Acidic Temp: 25 °C

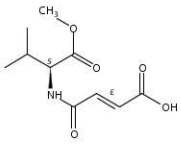
Related Info:

~ 3 References
Reactions

Score: 91

2.

2165716-67-4



Absolute stereochemistry., Double bond geometry as shown.

$C_{10}H_{15}NO_5$
2-Butenoic acid, 4-[[(1*S*)-1-(methoxycarbonyl)-2-methylpropyl]amino]-4-oxo-, (2*E*)-

Key Physical Properties:

Molecular Weight
229.23
Boiling Point (Predicted)
Value: 432.1±45.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.193±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 3.47±0.10 | Condition: Most Acidic Temp: 25 °C

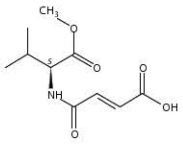
Related Info:

~ 0 References
~ 1 Commercial Sources

Score: 91

3.

2307909-20-0



Absolute stereochemistry., Double bond geometry unknown.

$C_{10}H_{15}NO_5$
INDEX NAME NOT YET ASSIGNED

Key Physical Properties:

Molecular Weight
229.23
Boiling Point (Predicted)
Value: 432.1±45.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.193±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 3.47±0.10 | Condition: Most Acidic Temp: 25 °C

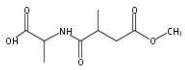
Related Info:

~ 0 References
~ 1 Commercial Sources

Score: 90

4.

65306-00-5



$C_9H_{15}NO_5$
Butanoic acid, 4-[(1-carboxyethyl)amino]-3-methyl-4-oxo-, 1-methyl ester

Key Physical Properties:

Molecular Weight
217.22
Boiling Point (Predicted)
Value: 438.1±30.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.194±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 3.52±0.10 | Condition: Most Acidic Temp: 25 °C

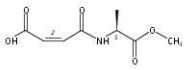
Related Info:

~ 2 References
~ 2 Commercial Sources

Score: 90

5.

124326-04-1



Double bond geometry as shown., Absolute stereochemistry.

$C_8H_{11}NO_5$
2-Butenoic acid, 4-[[(1*S*)-2-methoxy-1-methyl-2-oxoethyl]amino]-4-oxo-, (2*Z*)-

Key Physical Properties:

Molecular Weight
201.18
Boiling Point (Predicted)
Value: 429.0±45.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.268±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 2.79±0.25 | Condition: Most Acidic Temp: 25 °C

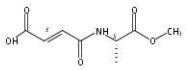
Related Info:

~ 5 References
Reactions
~ 1 Commercial Sources

Score: 90

6.

124326-05-2



Double bond geometry as shown., Absolute stereochemistry.

$C_8H_{11}NO_5$
2-Butenoic acid, 4-[(2-methoxy-1-methyl-2-oxoethyl)amino]-4-oxo-, [*S*-(*E*)]- (9CI)

Key Physical Properties:

Molecular Weight
201.18
Boiling Point (Predicted)
Value: 429.0±45.0 °C | Condition: Press: 760 Torr
Density (Predicted)
Value: 1.268±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr
pKa (Predicted)
Value: 3.47±0.10 | Condition: Most Acidic Temp: 25 °C

Related Info:

~ 1 References
~ 5 Commercial Sources

Figure S24 : The Scifinder searching results of compound **2**

Table S4 : The structural comparison of similar compounds with **2**

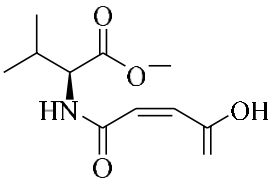
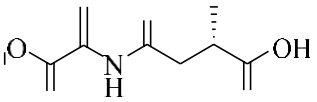
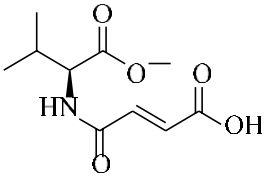
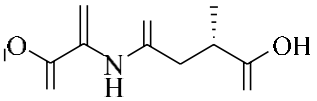
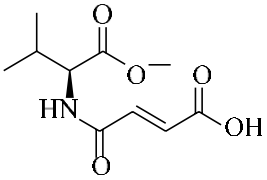
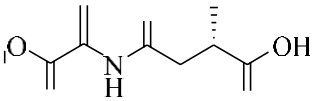
No.	Similarity score	Chemical structure and CAS number	Chemical structure of compound **2**
1	91	 CAS NO. 824393-57-9 Absolute stereochemistry	
2	91	 CAS NO. 2165716-67-4 Absolute stereochemistry	
3	91	 CAS NO. 2307909-20-0 Absolute stereochemistry	

Table S5: The NMR data comparison of similar compounds with **1**

Position	Compound **1** [a]		nidurufin [a, b] (CAS NO. 28458-23-3)		2'-epinidurufin [c] (CAS NO. 93922-50-0)	
	δ_H	δ_C (mult.)	δ_H	δ_C (mult.)	δ_H	δ_C (mult.)
1	-	158.1 (C)	-	159.8 (C)	NMR data is not available	
2	-	116.1 (C)	-	115.0 (C)		
3	-	158.7 (C)	-	158.4 (C)		
4	6.85, *s*	107.2 (CH)	6.85, s	107.4 (CH)		
4a	-	133.0 (C)	-	134.6 (C)		
5	6.94, *d, J* = 2.4	109.4 (CH)	6.97, s	108.9 (CH)		
6	-	166.2 (C)	-	164.2 (C)		
7	6.43, *d, J* = 2.4	107.9 (CH)	6.49, s	108.0 (CH)		
8	-	164.4 (C)	-	165.2 (C)		
8a	-	108.0 (C)	-	108.5 (C)		
9	-	188.3 (C)	-	188.6 (C)		
9a	-	108.4 (C)	-	108.2 (C)		
10	-	180.6 (C)	-	180.5 (C)		
10a	-	134.6 (C)	-	133.1 (C)		
1'	5.09, *d, J* = 3.0	65.7 (CH)	5.36, overlapped	70.7 (CH)		
2'	2.32, *ddt, J* = 17.3, 8.3, 3.8 1.45, *d, J* = 13.6	21.9 (CH_2)	3.75, m	63.5 (CH)		
3'	1.64, *d, J* = 13.0 1.53, *td, J* = 13.0, 3.2	23.5 (CH_2)	2.16, m 1.82, m	30.2 (CH_2)		
4'	3.55, *t, J* = 2.8	66.7 (CH)	1.57, m	22.7 (CH)		
5'	-	102.6 (C)	-	101.5 (C)		
6'	1.49, *s*	24.0 (CH_3)	1.54, s	27.2 (CH_3)		

[a] in DMSO-d_6.

[b] reference: X. W. Luo, H. M. Lu, X. Q. Chen, X. F. Zhou, C. H. Gao and Y. H. Liu (2020). Secondary metabolites and their biological activities from the sponge derived fungus *Aspergillus versicolor*, *Chem. Nat. Comp.* **56**, 716-719.

[c] reference: R. A. Murphy Jr and M. P. Cava (1984). Stereochemistry of nidurufin: synthesis of 6,8-dideoxynidurufin and 6,8-dideoxyepinidurufin, *J. Am. Chem. Soc.* **106**, 7630-7632.