Supporting information

Unstable tetramic acid derivatives from the deep-sea-derived fungus *Cladosporium sphaerospermum* EIODSF 008

Xiao Liang^{1, 2}, Zhong-Hui Huang^{1, 2}, Xuan Ma¹, Shu-Hua Qi^{1, *}

- ¹ CAS Key Laboratory of Tropical Marine Bio-resources and Ecology/Guangdong Key Laboratory of Marine Materia Medica/RNAM Center for Marine Microbiology, South China Sea Institute of Oceanology,
 - Chinese Academy of Sciences, 164 West Xingang Road, Guangzhou 510301, Guangdong, China; liangxiao213@mails.ucas.ac.cn (X.L.); zhonghui23@hotmail.com (Z.-H.H.); maxuan@scsio.ac.cn (X.M.)
- ² University of Chinese Academy of Sciences, Beijing 100049, China
- * Correspondence: shuhuaqi@scsio.ac.cn; Tel.: +86-20-8902-2112; Fax: +86-20-8445-8964

List of supporting information

Figure S1. The ¹ H-NMR spectrum of cladosporiumin I (1) in DMSO- d_6	
Figure S2. The ¹³ C NMR spectrum of cladosporiumin I (1) in DMSO- d_6	4
Figure S3. The HSQC spectrum of cladosporiumin I (1) in DMSO- d_6	5
Figure S4. The HMBC spectrum of cladosporiumin I (1) in DMSO- <i>d</i> ₆	6
Figure S5. The 1 H- 1 H COSY spectrum of cladosporiumin I (1) in DMSO- d_{6}	7
Figure S6. The (+)-HRESIMS spectrum of cladosporiumin I (1)	
Figure S7. The ¹ H-NMR spectrum of cladosporiumin J (2) in DMSO- d_6	9
Figure S8. The ¹³ C NMR spectrum of cladosporiumin J (2) in DMSO- d_6	
Figure S9. The HSQC spectrum of cladosporiumin J (2) in DMSO- d_6	11
Figure S10. The HMBC spectrum of cladosporiumin J (2) in DMSO- <i>d</i> ₆	
Figure S11. The ¹ H- ¹ H COSY spectrum of cladosporiumin J (2) in DMSO- d_6	
Figure S12. The IR spectrum of cladosporiumin J (2)	
Figure S13. The (+)-HRESIMS spectrum of cladosporiumin J (2)	
Figure S14. The ¹ H-NMR spectrum of cladosporiumin K (3) in DMSO- <i>d</i> ₆	
Figure S15. The ¹³ C NMR spectrum of cladosporiumin K (3) in DMSO- <i>d</i> ₆	
Figure S16. The HMBC spectrum of cladosporiumin K (3) in DMSO- <i>d</i> ₆	
Figure S17. The ¹ H- ¹ H COSY spectrum of cladosporiumin K (3) in DMSO- d_6	
Figure S18. The IR spectrum of cladosporiumin K (3)	
Figure S19. The (+)-HRESIMS spectrum of cladosporiumin K (3)	
Figure S20. The ¹ H-NMR spectrum of cladosporiumin L (4) in DMSO- <i>d</i> ₆	
Figure S21. The ¹³ C NMR spectrum of cladosporiumin L (4) in DMSO- d_6	
Figure S22. The HSQC spectrum of cladosporiumin L (4) in DMSO- <i>d</i> ₆	
Figure S23. The HMBC spectrum of cladosporiumin L (4) in DMSO- d_6	
Figure S24. The 1 H- 1 H COSY spectrum of cladosporiumin L (4) in DMSO- d_{6}	

1

Figure S25. The IR spectrum of cladosporiumin L (4)	27
Figure S26. The (+)-HRESIMS spectrum of cladosporiumin L (4)	28
Figure S27. The ¹ H-NMR spectrum of cladosporiumin M (5) in CDCl ₃	29
Figure S28. The ¹³ C NMR spectrum of cladosporiumin M (5) in CDCl ₃	30
Figure S29. The HSQC spectrum of cladosporiumin M (5) in CDCl ₃	31
Figure S30. The HMBC spectrum of cladosporiumin M (5) in CDCl ₃	32
Figure S31. The ¹ H- ¹ H COSY spectrum of cladosporiumin M (5) in CDCl ₃	33
Figure S32. The IR spectrum of cladosporiumin M (5)	34
Figure S33. The (+)-HRESIMS spectrum of cladosporiumin M (5)	35
Figure S34. The ¹ H-NMR spectrum of cladosporiumin N (6) in DMSO- <i>d</i> ₆	36
Figure S35. The ¹³ C NMR spectrum of cladosporiumin N (6) in DMSO- <i>d</i> ₆	37
Figure S36. The HSQC spectrum of cladosporiumin N (6) in DMSO- <i>d</i> ₆	38
Figure S37. The HMBC spectrum of cladosporiumin N (6) in DMSO- <i>d</i> ₆	39
Figure S38. The ¹ H- ¹ H COSY spectrum of cladosporiumin N (6) in DMSO- d_6	40
Figure S39. The (+)-HRESIMS spectrum of cladosporiumin N (6)	41
Figure S40. The ¹ H-NMR spectrum of cladosporiumin O (7) in DMSO- <i>d</i> ₆	42
Figure S41. The ¹³ C NMR spectrum of cladosporiumin O (7) in DMSO- d_6	43
Figure S42. The HMBC spectrum of cladosporiumin O (7) in DMSO- <i>d</i> ₆	44
Figure S43. The (+)-HRESIMS spectrum of cladosporiumin O (7)	45
Figure S44. The ¹ H-NMR spectrum of cladodionen (8) in DMSO- <i>d</i> ₆	46
Figure S45. The ¹³ C NMR spectrum of cladodionen (8) in DMSO- d_6	47
Figure S46. The IR spectrum of cladodionen (8)	48
Figure S47. The (+)-HRESIMS spectrum of cladodionen (8)	49
Figure S48. HPLC analysis of FDAA derivates of acidic hydrolysates of cladosporiumin L (4) (Colum	n:
YMC-Pack ODS-A column, 250×4.6 mml.D. , S-5 $\mu m,$ 12 nm)	50
Figure S49. HPLC analysis of FDAA derivates of D-Val and L-Val (Column: YMC-Pack ODS-A colum	n,
250×4.6 mml.D. , S-5 μm, 12 nm)	50
Figure S50. HPLC chromatograms of compound cladosporiumin L (4) before and after acid treatment	50
Figure S51. The ICP-AES analysis report of magnesium content in compound cladosporiumin L (4)	51
Figure S52. The (+)-HRESIMS spectrum of cladosporiumin E	52
Figure S53. The (+)-HRESIMS spectrum of cladosporiumin G	52
Figure S54. The (+)-HRESIMS spectrum of cladosporiumin F	53
Figure S55. The (+)-HRESIMS spectrum of cladosporiumin H	53
Figure S56. Pictures of inhibition zones in the disc diffusion test	54
Table S1. Free energies (G) and equilibrium populations (P) of stable conformers of 1a and 1b with	R
configuration at C-10 in CH ₃ OH	55
Table S2. Free energies (G) and equilibrium populations (P) of stable conformers of 1a and 1b with	S
configuration at C-10 in CH ₃ OH	56
Table S3. Free energies (G) and equilibrium populations (P) of stable conformers of 2 with R configuration at C	-8
in CH ₃ OH	57







Figure S2. The ¹³C NMR spectrum of cladosporiumin I (1) in DMSO- d_6



Figure S3. The HSQC spectrum of cladosporiumin I (1) in DMSO- d_6



Figure S4. The HMBC spectrum of cladosporiumin I (1) in DMSO- d_6





Figure S6. The (+)-HRESIMS spectrum of cladosporiumin I (1)

and the start of

		Mass Spectr	um Smart	Formula	Report		
Analysis Info			1. 1501 -		Acquisition Date	4/1/2016 6:24:20 PM	N
Analysis Name Method Sample Name Comment	LC_Direct Infusion_p liangxiao_LX-C-6	bos_100-1000mz.m	Л_1564.d		Operator Instrument / Ser#	SCSIO maXis	29
Acquisition Paran	neter				.		
Source Type Focus Scan Begin Scan End	ESI Active 100 m/z 2000 m/z	Ion Polarity Set Capillary Set End Plate O Set Collision Cel	Pos 450 ffset -500 II RF 800	itive 0 V 0 V 0 V 0 Vpp	Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve	0.4 Bar 180 °C 4.0 I/min Waste	
Intens							+MS, 0.2min #12
1.5-							
1.0-					258.1098		
0.5		246	.1100				
0.0	236.1281			254.1	378	262.1023 265.106	3
230	235	240 245	250)	255 260	265	m/z
Meas. m 236.128 258.109	/z # Formula 31 1 C 13 H 18 N O 3 38 1 C 13 H 17 N Na O 3	Score m/z err [100.00 236.1281 100.00 258.1101	[ppm] err [mDa] -0.1 -0.0 1.0 0.3	mSigma rdb 28.9 5.9 10.2 5.9	b e Conf N-Rule 5 even ok 5 even ok		



Figure S7. The ¹H-NMR spectrum of cladosporiumin J (2) in DMSO- d_6



Figure S8. The 13 C NMR spectrum of cladosporiumin J (2) in DMSO- d_6



Figure S9. The HSQC spectrum of cladosporiumin J (2) in DMSO- d_6



Figure S10. The HMBC spectrum of cladosporiumin J (2) in DMSO- d_6



Figure S11. The ¹H-¹H COSY spectrum of cladosporiumin J (2) in DMSO- d_6





			was	s Spe	ctrum a	Smanr	ormula		epon				
Analysis Info								Acc	quisition D	ate	4/1/2016 6	:31:09 PN	1
Analysis Name Method Sample Name Comment	D Lu lia	:\Data\MS\data\2016 C_Direct Infusion_po angxiao_LX-C-8	04\liangxia s_100-100	10_LX-C-8_ 00mz.m	_4_01_1566	.d		Op Ins	erator trument / S	Ser#	SCSIO maXis		29
Acquisition Parar	neter												
Source Type Focus Scan Begin Scan End		ESI Active 100 m/z 2000 m/z		Ion Polarity Set Capillan Set End Pla Set Collision	y te Offset n Cell RF	Positiv 4500 V -500 V 800.0 V	e V Vpp		Set No Set Di Set Di Set Di	ebulizer ry Heater ry Gas ivert Valve		0.4 Bar 180 °C 4.0 l/min Waste	
Intens. x10 ⁵ 1.0- 0.8-													+MS, 0.1min #
0.6-										274.1053			
0.4- 0.2-													
0.0 		250	255	26	60	265		270		275		280	m/
Meas. m 252.12 274.10 525.22	n/z # 30 1 53 1 03 1	Formula C 13 H 18 N O 4 C 13 H 17 N Na O 4 C 26 H 34 N 2 Na O 8	Score 100.00 100.00 100.00	m/z 252.1230 274.1050 525.2207	err [ppm] 0.3 -1.2 0.8	err [mDa] 0.1 -0.3 0.4	mSigma 10.8 8.4 5.4	rdb 5.5 5.5 10.5	e Conf even even even	N-Rule ok ok ok			

Mass Spectrum SmartFormula Poport



Figure S14. The ¹ H-N	NMR spectrum of cladosr	poriumin K (3) in DMSO-a	d_6
----------------------------------	-------------------------	--------------------------	-------



Figure S15. The ¹³C NMR spectrum of cladosporiumin K (3) in DMSO- d_6



Figure S16. The HMBC spectrum of cladosporium in K (3) in DMSO- d_6



Figure S17. The ¹H-¹H COSY spectrum of cladosporiumin K (3) in DMSO- d_6

Figure S18. The IR spectrum of cladosporiumin K (3)

G SHIMADZU



Figure S19. The (+)-HRESIMS spectrum of cladosporiumin K (3)

			Mas	s Spe	ctrum \$	SmartF	ormula	a Re	eport				
Analysis Info								Acc	quisition D	ate	4/1/2016 6	5:45:29 PN	1
Analysis Name Method Sample Name Comment		D:\Data\MS\data\2(LC_Direct Infusion_ iangxiao_LX-C-7)1604\liangxi _pos_100-10	ao_LX-C-7_ 00mz.m	_3_01_1568	i.d		Op Ins	erator trument / S	Ser#	SCSIO maXis		29
Acquisition Para Source Type Focus Scan Begin Scan End	meter	ESI Active 100 m/z 2000 m/z		Ion Polarity Set Capillar Set End Pla Set Collision	y te Offset n Cell RF	Positiv 4500 V -500 V 800.0 V	e ∕ √pp		Set N Set D Set D Set D	ebulizer ry Heater ry Gas ivert Valve		0.4 Bar 180 °C 4.0 l/min Waste	
Intens. x10 ⁵													+MS, 0.5min #32
1.0-													
0.8-										274.1055			
0.6-													
0.4-													
0.2-		252 1236											
0.0- 245		250	255	20	60	265		270		275	*****	280	m
Meas. n 252.12 274.10 525.22	m/z # 236 / 055 / 215 /	Formula C 13 H 18 N O 4 C 13 H 17 N Na O C 26 H 34 N 2 Na	Score 78.59 4 100.00 0 8 100.00	m/z 252.1230 274.1050 525.2207	err [ppm] -2.3 -2.0 -1.5	err [mDa] -0.6 -0.5 -0.8	mSigma 37.0 11.9 7.4	rdb 5.5 5.5 10.5	e ⁻ Conf even even even	N-Rule ok ok ok			



Figure S20. The ¹H-NMR spectrum of cladosporiumin L (4) in DMSO- d_6

195.48 195.46	- 192. 67	- 177. 70							61 601	CT '701			66, 20 66, 04 65, 38 65, 31	- 63. 45 - 63. 33	46.73 46.57 46.13	8	- 29. 89	- 24, 99 - 24, 89	- 20. 02	- 15. 87	- - 28000 -
	\square	Ŷ																Ŷ			-26000
																				-	-24000
																				-	- 22000
																					- 20000
																				-	- 18000
																				-	-16000 -
																				-	-14000
																				-	- 12000 -
																		I		-	- 10000 -
															I					-	- 8000
									ļ				h							-	-6000 -
																				-	- 4000 -
															,					-	- 2000
adingbanashiribaliyadi	Hay ^l hainidhadapanhanta	hainina kini kini kan	Yan (population and a second	n na hain na ha Na hain na hain n	alihalihadharihadharih	iyaninidhaiwi	vininan levilyinin polo	hand elselandⁱ h aderen	innin nindra serie	ninhainealte (₁₆ 10)(1911)(141)	HALPHAN HANA HANA HANA HANA HANA HANA HANA	linin phatan	MMMM	n <mark>inininininininininininininininininini</mark>	intelligence of the second	iyini <mark>iyadida</mark> a	(mwini wwini	(),((⁾ la ine prin e	(Waangadiw)	alininyii	-0
200	190	180	170	160	150	140	130	120	110 f1 (ppm)	100	90	80	70	60	50	40	30		20	10	

Figure S21. The ¹³C NMR spectrum of cladosporiumin L (4) in DMSO- d_6



Figure S22. The HSQC spectrum of cladosporiumin L (4) in DMSO- d_6

Figure S23. The HMBC spectrum of cladosporiumin L (4) in DMSO- d_6

Figure S24. The ¹H-¹H COSY spectrum of cladosporiumin L (4) in DMSO- d_6

26

Figure S25. The IR spectrum of cladosporiumin L (4)

3 SHIMADZU

Figure S26. The (+)-HRESIMS spectrum of cladosporiumin L (4)

HN

28

Figure S27. The ¹H-NMR spectrum of cladosporiumin M (**5**) in CDCl₃

Figure S28. The ¹³C NMR spectrum of cladosporiumin M (**5**) in CDCl₃

Figure S29. The HSQC spectrum of cladosporiumin M (5) in CDCl₃

Figure S30. The HMBC spectrum of cladosporiumin M (5) in CDCl₃

Figure S31. The ¹H-¹H COSY spectrum of cladosporiumin M (5) in CDCl₃

Figure S32. The IR spectrum of cladosporiumin M (5)

Figure S33. The (+)-HRESIMS spectrum of cladosporiumin M (5)

				Mass	Spect	rum Sr	nartFo	ormu	ula Re	port		11		
Analysis Info									Ac	quisition Da	te 6/9/	/2018 4:13:	30 PM	
Analysis Name		D:\Data\MS\data\	201806\lia	angxiao_LX	-C-9B-1_po	s_92_01_49	922.d							
Method Sample Name Comment		LC_DirectInfusion liangxiao_LX-C-9	n_pos_70 B-1_pos	-500mz.m					Op Ins	erator strument	SCSIO maXis		255552.0	0029
Acquisition Param	neter													
Source Type Focus Scan Begin Scan End		ESI Active 70 m/z 1500 m/z		lon Set Set Set	Polarity Capillary End Plate Off Charging Vol Corona	set tage	Positi 4500 -500 0 V 0 nA	ve V V			Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater		0.4 Bar 180 °C 4.0 l/m Waste 0 °C	in
Intens. x10 ⁵ 2.5								•					+	MS, 0.2min #13
1.5		234.1	135			.*								
1.0						· ·								
0.5		232.0967	1.					250.10	79	256.09	50	262.1060		268.1199
225	r - r	230	235		240	245		250		255	260		265	m/z
Meas. m 234.113 256.099 467.218 489.199	/z # 35 1 50 1 30 1 95 1	lon Formula C13H16NO3 C13H15NNaO3 C26H31N2O6 C26H30N2NaO6	Score 100.00 100.00 100.00 100.00	m/z 234.1125 256.0944 467.2177 489.1996	err [ppm] 4.2 -2.5 -0.7 0.3	err [mDa] 1.0 -0.6 -0.3 0.1	mSigma 16.5 23.8 31.1 26.0	rdb 6.5 6.5 12.5 12.5	e ⁻ Conf even even even even	N-Rule ok ok ok ok				

Figure S34. The ¹H-NMR spectrum of cladosporiumin N (6) in DMSO- d_6

Figure S35. The ¹³C NMR spectrum of cladosporiumin N (6) in DMSO- d_6

Figure S36. The HSQC spectrum of cladosporium in N (6) in DMSO- d_6

Figure S39. The (+)-HRESIMS spectrum of cladosporiumin N (6)

		Mass	s Spec	trum S	martFo	ormula	Re	port				
Analysis Info							Acqu	uisition Dat	te	3/22/2010	6 11:40:18	AM
Analysis Name Method Sample Name Comment	D:\Data\MS\data LC_Direct Infusio liangxiao_LX-C-{	a\201603\liangxiad on_pos_100-1000 5	o_LX-C-5_4)mz.m	1_01_1507	′.d		Ope Instr	rator ument / Se	er#	SCSIO maXis		29
Acquisition Param Source Type Focus Scan Begin Scan End	eter ESI Active 100 m/z 2000 m/z		on Polarity Set Capillary Set End Plate Set Collision	e Offset Cell RF	Positive 4500 V -500 V 800.0 V	ор		Set Net Set Dry Set Dry Set Div	oulizer Heater Gas ert Valve		0.4 Bar 180 °C 4.0 I/min Waste	
Intens.												+MS, 0.4min #21
XIO												
1.25												
1 00												
1.00									276.120	5		
0.75												
0.50												
0.25		258 1100										
3	254.1388							274.274	13	1		
0.00 250	255	260	, , , , , , , , , , , , , , , , , , , 	265	,	270	·····	2	75		280	m/z
Meas, m/	z # Formula	Score	m/z	err (ppm)	err [mDa]	mSigma	rdb	e ⁻ Conf	N-Rule			
254.138	1 C 13 H 20 N O	4 100.00	254.1387	-0.6	-0.2	6.3	4.5	even	ok			
	2 C 9 H 16 N 7 C	13.28	254.1360	-11.2	-2.8	17.7	5.5	even	ok			
070 400	3 C 8 H 20 N 3 C	0.6 2.33	254.1347	-16.5	-4.2	30.7	0.5	even	ok	-		
276.120	5 1 C 13 H 19 N N	a O 4 100.00	276.1206	0.6	0.2	6.7	4.5	even .	OK			
	2 C9H 15N / N 3 C8H 19N 3N	a 0 2 21.02	276 1166	-9.1	-2.5	20.8	0.5	even	ok			
529 251	2 1 C 26 H 38 N 2	Na O 8 100.00	529.2520	1.5	0.8	46.6	8.5	even	ok	7		
020.201	2 C 20 H 42 Na C	D 14 2.95	529.2467	-8.6	-4.6	50.4	-0.5	even	ok			
	3 C 22 H 34 N 8	Na O 6 42.81	529.2494	-3.6	-1.9	52.0	9.5	even	ok			
	4 C 18 H 30 N 14	4 Na O 4 2.17	529.2467	-8.6	-4.6	59.5	10.5	even	ok			
	5 C 32 H 34 N 4	Na O 2 0.18	529.2574	11.6	6.2	62.9	17.5	even	ok			

Figure S40. The ¹H-NMR spectrum of cladosporiumin O (7) in DMSO- d_6

Figure S41. The ¹³C NMR spectrum of cladosporiumin O (7) in DMSO- d_6

Figure S42. The HMBC spectrum of cladosporiumin O (7) in DMSO- d_6

Figure S43. The (+)-HRESIMS spectrum of cladosporiumin O (7)

					Mas	s Spe	ctrum	SmartF	ormu	a Re	eport				
Analysis Info										Ac	quisition Da	ate	5/17/2016	6 5:39:56 P	M
Analysis Name Method Sample Name Comment		D: LC lia	\Data\MS\d C_Direct Inf ngxiao_LX-	ata\20160 usion_pos_ C-9B_pos	4\liangxia _100-100	io_LX-C-9E 00mz.m	3_pos_23_	01_1834.d		Op Ins	erator trument / S	Ser#	SCSIO maXis		29
Acquisition Pa	ramete	r						D			0	- h - 1 ¹		0.4 Dec	
Source Type Focus Scan Begin Scan End			ESI Active 100 m/z 2000 m/z			Set Capillar Set End Pla Set Collision	y te Offset n Cell RF	4500 \ -500 \ 800.0	ve V Vpp		Set No Set Di Set Di Set Di	ebulizer ny Heater ny Gas ivert Valve		0.4 Bar 180 °C 4.0 I/min Waste	
Intens. ⁻ x10 ⁵ -															+MS, 0.2min #12
0.8- - 0.6-											274	1.1051			
0.4-															
0.2-			256.0	945											
25	52.0243					262.104	9		270	0348 2	72.0896		-		
250			255	, ,	260	, ,	26	5	2	70		275		280	m/z
Meas 252 274 525	. m/z .1233 .1051 .2202	# 1 1	Formula C 13 H 18 M C 13 H 17 M C 26 H 34 M	N O 4 N Na O 4 N 2 Na O 8	Score 100.00 100.00 90.09	m/z 252.1230 274.1050 525.2207	err [ppm] -0.9 -0.4 0.9	err [mDa] -0.2 -0.1 0.5	mSigma 39.9 1.2 20.5	rdb 5.5 5.5 10.5	e ⁻ Conf even even even	N-Rule ok ok ok			

Figure S44. The ¹H-NMR spectrum of cladodionen (8) in DMSO- d_6

Figure S45. The ¹³C NMR spectrum of cladodionen (8) in DMSO- d_6

		Mass Spectrum	SmartFormula	a Report	
Analysis Info			1005 1	Acquisition Date	5/17/2016 5:43:18 PM
Analysis Name Method Sample Name Comment	D:\Data\MS\data\20160 LC_Direct Infusion_pos liangxiao_LX-C-2_pos	04\liangxiao_LX-C-2_pos_22_01 s_100-1000mz.m	I_1835.d	Operator Instrument / Ser#	SCSIO maXis 29
Acquisition Paran	neter				
Source Type Focus Scan Begin Scan End	ESI Active 100 m/z 2000 m/z	Ion Polarity Set Capillary Set End Plate Offset Set Collision Cell RF	Positive 4500 V -500 V 800.0 Vpp	Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve	0.4 Bar 180 °C 4.0 l/min Waste
Intens. x10 ⁵ 3- 2-	234.1127			256.09	+MS, 0.2min #11
230	235	240 245	250	255	260 m/z
Meas. m 234.11 256.09 489.20	l/z # Formula 27 1 C 13 H 16 N O 3 52 1 C 13 H 15 N Na O 3 06 1 C 26 H 30 N 2 Na O 6	Score m/z err [ppm] 100.00 234.1125 -1.0 100.00 256.0944 -3.2 42.98 489.1996 -2.1	err [mDa] mSigma -0.2 9.1 -0.8 1.7 -1.0 48.3	rdb e Conf N-Rule 6.5 even ok 6.5 even ok 12.5 even ok	

Figure S48. HPLC analysis of FDAA derivates of acidic hydrolysates of cladosporiumin L (4) (Column: YMC-Pack ODS-A column, 250×4.6 mml.D., S-5 μ m, 12 nm).

Figure S49. HPLC analysis of FDAA derivates of D-Val and L-Val (Column: YMC-Pack ODS-A column, 250×4.6 mml.D., S-5 μ m, 12 nm).

Figure S50. HPLC chromatograms of compound cladosporiumin L (4) before and after acid treatment

Figure S51. The ICP-AES analysis report of magnesium content in compound cladosporiumin L (4)

			分	析	报	告		
モ 岸 单 位	:中国和	斗学院	南海海	羊研究所	听	来样日	期:	2018-05-03
羊品原标识	LX-C-	-4B、LX	K-C-4B	(空白))	样品外	观:	无色液体
▶析项目	:Mg					检测日	期 :	2018-05-04
检测仪器: 检测条件: 检测依据:	全谱直试 入射功 [™] JY/T(卖等离子 率: 1300)15-1990	←体原子) DW 等 6 (国	发射光谱 离子气流 家教委"	¥仪,Opt 〔量: 15 '感耦等	tima 8300 5L/min 雾 离子体原	(美 化气 注 子 发 5	国 PerkinElmer) 流量: 0.6 L/min 射光谱方法通则")
			枨	测结	果(mg	/L) —	► T	he concentration of Mg
			编号 LX-C-4 LX 【X	/元素 B(空白 C-C-4B) 以	Mg 0.073 6.79 下空白		 Blank control Compound 4

Figure S52. The (+)-HRESIMS spectrum of cladosporiumin E

		Mass	Spec	trum S	martFo	rmula	Re	port					
Analysis Info Analysis Name Method Sample Name Comment	D:\Data\MS\data\201608 LC_Direct Infusion_pos_ huangzhonghui_CL1	huangzho 100-1000n	nghui_CL nz.m	1_41_01_2	304.d		Acqu Oper Instru	isition Cat ator ument / Se	e r#	8/22/2 SCSIC maXis	016 5:03: D	27 PM 29	
Acquisition Paramet Scurce Type Focus Scan Begin Scan End	ESI Active 100 m/z 2000 m/z	lon Se Se	Polarity t Capillary t End Plate t Collision (Ofset Cel RF	Positive 4500 V -500 V 800.0 Vp	PP P		Set Neb Set Dry Set Dry Set Dive	ulizer Heater Gas ert Valve		0.4 E 180 4.0 I Was	Bar *C /min ite	
intens. x10 ⁵												+MS, 0.	4min #23
3									[M+	Na] ⁺			
2				+					296.	0873			
1			[M	I+HJ									
		27	0.0348	(4.1051						E.			
250	260		270	- J	280			290		1.	300		m/:
Meas. m/z 274.1051 296.0873 525.2203 547.2021	 # Formula 1 C13 H17 N Na 0.4 1 C13 H16 N Na 2.0.4 1 C26 H34 N 2 Na 0.8 1 C26 H33 N 2 Na 2.0.8 	Score 100.00 100.00 100.00 100.00	m/z 274.1050 296.0869 525.2207 547.2027	er [ppm] -0.5 -1.3 0.9 1.0	err [mDa] -0.1 -0.4 0.5 0.5	mSigma 2.6 4.0 3.5 20.9	rdb 5.5 5.5 10.5 10.5	e Conf even even even even	N-Rule ok ok ok				
Buker Compass Data	aAnalvsis 4.0			printed	8/22/2	2016 5:10:4	2 PM				P	age 1 of 1	

Figure S54. The (+)-HRESIMS spectrum of cladosporiumin F

Figure S55. The (+)-HRESIMS spectrum of cladosporiumin H

Figure S56. Pictures of inhibition zones in the disc diffusion test

Escherichia coli

Bacillus subtilis

Micrococcus luteus

The samples indicated by the arrow are EtOAc extracts of *Cladosporium sphaerospermum* EIODSF 008 obtained from the preliminary experiment. (100 μ g/disc)

Conformer	Conformation	G (kcal/mol)	P (%)	Conformer	Conformation	G (kcal/mol)	P (%)
(5 <i>R</i> , 10 <i>R</i>)- 1a-1	474	-493102.1267	42.89	(5 <i>R</i> , 10 <i>R</i>)- 1b-1	444	-493101.8931	28.91
(5 <i>R</i> , 10 <i>R</i>)- 1a-2	444	-493101.1117	7.73	(5 <i>R</i> , 10 <i>R</i>)- 1b-2	A-A-A-	-493100.9144	5.54
(5 <i>R</i> , 10 <i>R</i>)- 1a-3	YHY	-493100.5243	2.86	(5 <i>R</i> , 10 <i>R</i>)- 1b-3	YYY	-493100.3143	2.01
(5 <i>R</i> , 10 <i>R</i>)- 1a-4	AHA	-493100.8912	5.32	(5 <i>R</i> , 10 <i>R</i>)- 1b-4	なな	-493100.5250	2.87
(5 <i>R</i> , 10 <i>R</i>)- 1a-5	XHX	-493099.8114	0.86	(5 <i>R</i> , 10 <i>R</i>)- 1b-5	XXX	-493099.4899	0.50
(5 <i>R</i> , 10 <i>R</i>)- 1a-6	YHY.	-493099.2133	0.31	(5 <i>R</i> , 10 <i>R</i>)- 1b-6	4AA	-493098.9320	0.19
			Total: 59.98				Total: 40.02

Table S1. Free energies (*G*) and equilibrium populations (P) of stable conformers of **1a** and **1b** with *R* configuration at C-10 in CH₃OH

Conformer	Conformation	G (kcal/mol)	P (%)	Conformer	Conformation	G (kcal/mol)	P (%)
(5 <i>R</i> , 10 <i>S</i>)- 1a-1	444	-493102.1865	47.77	(5 <i>R</i> , 10 <i>S</i>)- 1b-1	444	-493101.8078	25.19
(5 <i>R</i> , 10 <i>S</i>)- 1a-2	AAA	-493101.1329	8.06	(5 <i>R</i> , 10 <i>S</i>)- 1b-2	AA	-493100.7791	4.43
(5 <i>R</i> , 10 <i>S</i>)- 1a-3	YHY	-493100.5576	3.05	(5 <i>R</i> , 10 <i>S</i>)- 1b-3	44	-493100.1712	1.59
(5 <i>R</i> , 10 <i>S</i>)- 1a-4	474	-493100.8302	4.83	(5 <i>R</i> , 10 <i>S</i>)- 1b-4	4	-493100.5579	3.05
(5 <i>R</i> , 10 <i>S</i>)- 1a-5	AAA	-493099.7721	0.81	(5 <i>R</i> , 10 <i>S</i>)- 1b-5	AA.	-493099.6409	0.65
(5 <i>R</i> , 10 <i>S</i>)- 1a-6	YH4	-493099.2377	0.33	(5 <i>R</i> , 10 <i>S</i>)- 1b-6	YYY	-493099.0377	0.23
			Total: 64.85				Total: 35.15

Table S2. Free energies (*G*) and equilibrium populations (P) of stable conformers of **1a** and **1b** with *S* configuration at C-10 in CH₃OH

Conformer	Conformation	G (kcal/mol)	P (%)	Conformer	Conformation	G (kcal/mol)	P (%)
2-1	好	-540314.3871	19.71	2-6	+FF	-540313.4774	4.24
2-2	the t	-540314.3796	19.46	2-7	Y TX	-540313.1813	2.57
2 -3	J J J J J J J J J J J J J J J J J J J	-540314.1949	14.25	2-8	The second secon	-540313.1316	2.36
2-4	XXX	-540314.1882	14.08	2-9		-540313.0808	2.17
2 -5		-540314.1594	13.42	2 -10	14	-540313.0489	2.06

	Table S3. Free energies ((G) and e	auilibrium	populations	(\mathbf{P}) of	stable conform	ners of 2 w	ith R config	guration at C-8	in CH ₃ OH
--	---------------------------	-----------	------------	-------------	-------------------	----------------	-------------	--------------	-----------------	-----------------------

2-11		-540313.0194	1.96	2-3	t t	-540312.9645	1.78
2-12	大大	-540313.0174	1.95				