Supplementary Information

Structural diversity of terpenoids in the Soft Coral *Sinularia flexibilis*, evidence by a collection from the South China Sea

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Figure S1. ¹H NMR spectrum (400 MHz, CDCl₃) of 9α -hydroxy-flexibilide (1).



Figure S2. ¹³C NMR spectrum (100 MHz, CDCl₃) of 9α -hydroxy-flexibilide (1).



Figure S3. HMQC spectrum (400 MHz, CDCl₃) of 9α -hydroxy-flexibilide (1).



Figure S4. HMBC spectrum (400 MHz, CDCl₃) of 9α -hydroxy-flexibilide (1).



Figure S5. ¹H-¹H COSY spectrum (400 MHz, CDCl₃) of 9α -hydroxy-flexibilide (1).



Figure S6. ROESY spectrum (400 MHz, CDCl₃) of 9α -hydroxy-flexibilide (1).

Figure S7. HRESIMS spectrum of 9α -hydroxy-flexibilide (1).

MM-Shuying Peng	9	Q-Tof Ultima		27-Apr-201213:40:
1-24A 0427-1 190 (3 578) 4	M (Cen 5 80 00 Ht 9000 0 389	19.0.70): Sm (Mn. 2x0.00): Cm (189):196)	TOF MS FS
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	272 2187	373.1205	374 1986	
0	372.2187	373	374	
	012			
Elemental Co	omposition Report			Page 1
Telesense - 4		- 1 5 mov - 50 0		
Tolerance = 1	0.0 PPM / DBE: min	n = -1.5, max = 50.0	0%	
Tolerance = 1 Isotope cluste	0.0 PPM / DBE: min r parameters: Separati	a = -1.5, max = 50.0 ion = 1.0 Abundance = 1	.0%	
Tolerance = 1 Isotope cluste Monoisotopic Ma 18 formula(e) ev	0.0 PPM / DBE: mir. er parameters: Separati ass, Odd and Even Electron aluated with 1 results within	a = -1.5, max = 50.0 ion = 1.0 Abundance = 1 lons limits (up to 20 closest results	.0% for each mass)	
Tolerance = 1 Isotope cluste Monoisotopic Ma 18 formula(e) ev SIMM-Shuying Peng	0.0 PPM / DBE: mir er parameters: Separati ass, Odd and Even Electron aluated with 1 results within	a = -1.5, max = 50.0 ion = 1.0 Abundance = 1 lons limits (up to 20 closest results Q-Tof Ultima	.0% for each mass)	27-Apr-201213:40:11
Tolerance = 1 Isotope cluste Monoisotopic Ma 18 formula(e) ev SIMM-Shuying Peng G4-24A 120427-1190 (3 577	0.0 PPM / DBE: min r parameters: Separati ass, Odd and Even Electron aluated with 1 results within 1 3) AM (Cen. 5, 80.00, Ht.9000.0.38	a = -1.5, max = 50.0 ion = 1.0 Abundance = 1 lons limits (up to 20 closest results Q-Tof Ultima i9.19.0.70); Sm (Mn, 2x0.00); Cm (189	.0% for each mass)	27-Apr-201213:40:11 TOF MS ES+
Tolerance = 1 Isotope cluste Monoisotopic Ma 18 formula(e) ev SIMM-Shuying Peng G4-24A 120427-1 190 (3.57/ 100-	0.0 PPM / DBE: min r parameters: Separat ass, Odd and Even Electron aluated with 1 results within 3 3) AM (Cen,5, 80.00, Ht,9000.0,38	a = -1.5, max = 50.0 ion = 1.0 Abundance = 1 lons limits (up to 20 closest results Q-Tof Ultima 19.19.0.70); Sm (Mn, 2x0.00); Cm (189 373.1996	.0% for each mass) :196)	27-Apr-201213:40:11 TOF MS ES+ 919
Tolerance = 1 Isotope cluster Monoisotopic Ma 18 formula(e) ev SIMM-Shuying Peng G4-24A 120427-1 190 (3.576	0.0 PPM / DBE: min er parameters: Separati ass, Odd and Even Electron aluated with 1 results within 3 3) AM (Cen,5, 80.00, Ht,9000.0,38	a = -1.5, max = 50.0 ion = 1.0 Abundance = 1 lons limits (up to 20 closest results Q-Tof Ultima 9.19,0.70); Sm (Mn, 2x0.00); Cm (189 373.1998	.0% for each mass) :196)	27-Apr-201213:40:11 TOF MS ES+ 919
Tolerance = 1 Isotope cluste Monoisotopic Ma 18 formula(e) ev SIMM-Shuying Peng G4-24A 120427-1 190 (3.576	0.0 PPM / DBE: min er parameters: Separat ass, Odd and Even Electron aluated with 1 results within 3 B) AM (Cen,5, 80.00, Ht,9000.0,38	a = -1.5, max = 50.0 ion = 1.0 Abundance = 1 lons limits (up to 20 closest results Q-Tof Ultima i9.19,0.70); Sm (Mn, 2x0.00); Cm (189 373.1998	.0% for each mass)	27-Apr-201213:40:11 TOF MS ES+ 919
Tolerance = 1 Isotope cluste Monoisotopic Ma 18 formula(e) ev SIMM-Shuying Peng G4-24A 120427-1 190 (3.576	0.0 PPM / DBE: min er parameters: Separat ass, Odd and Even Electron aluated with 1 results within a b) AM (Cen,5, 80.00, Ht,9000.0,38	a = -1.5, max = 50.0 ion = 1.0 Abundance = 1 lons limits (up to 20 closest results Q-Tof Ultima i9.19,0.70); Sm (Mn, 2x0.00); Cm (189 373.1998	.0% for each mass) :196)	27-Apr-201213:40:11 TOF MS ES+ 919
Tolerance = 1 Isotope cluster Monoisotopic Ma 18 formula(e) ev SIMM-Shuying Peng G4-24A 120427-1 190 (3.576	0.0 PPM / DBE: min er parameters: Separat ass, Odd and Even Electron aluated with 1 results within 3 B) AM (Cen,5, 80.00, Ht,9000.0,38	n = -1.5, max = 50.0 ion = 1.0 Abundance = 1 lons limits (up to 20 closest results Q-Tof Ultima i9.19,0.70); Sm (Mn, 2x0.00); Cm (189 373.1998	.0% for each mass) :196)	27-Apr-201213:40:11 TOF MS ES+ 919
Tolerance = 1 Isotope cluste Monoisotopic Ma 18 formula(e) ev SIMM-Shuying Peng G4-24A 120427-1 190 (3.576	0.0 PPM / DBE: min er parameters: Separat ass, Odd and Even Electron aluated with 1 results within 3 B) AM (Cen,5, 80.00, Ht,9000.0,38	n = -1.5, max = 50.0 ion = 1.0 Abundance = 1 lons limits (up to 20 closest results Q-Tof Ultima 19.19,0.70); Sm (Mn, 2x0.00); Cm (189 373.1998	.0% for each mass) :196)	27-Apr-201213:40:11 TOF MS ES+ 919

%- 	7		····	373.1205					374.1986
	372.40	372.60 372.8	373.00	373.20	373.40	373.60	373.80	374.00	
Minimum: Maximum:	50.00 100.00		200.0	10.0	-1.5 50.0				
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula		
373.1998	100.00	373.1991	0.7	1.9	5.5	1	C20 H30	05 Na	



Figure S8. ¹H NMR spectrum (400 MHz, CDCl₃) of 15(17)-dehydromanaarenolide E (2)



Figure S9. ¹³C NMR spectrum (100 MHz, CDCl₃) of 15(17)-dehydromanaarenolide E (2)

MM-Shuying Peng					Q-Tof	Ultima					20-Ma	r-201213	:40::
L-F4-4Ed	(Can E 00		0 0 415 24	0.70). 6	m (Mn 2	0.00). Ca	(258-26)	3)				TOF M	S ES
0320-1 261 (4.913) AM	(Cen,5, 60.	00, HI,900	0.0,415.21	,0.70), 31	389.192	7	1 (200.200	.,					9
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			387.1871	389	1127 3	5.2051 390	3.2023 39	1.1898					
0						000	204	202	202	394	395	396	

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Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0 Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron lons 15 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

SIMM-Shuving	Peng			Q-Tof I		20-Mar-201213:40:25					
YAL-F4-4Ed 120320-1 261	(4.913) AM (C	ien,5, 80.00, Ht,900	0.0,415.21,0.7	0); Sm (Mn, 2 389.	x0.00); Cm (258 1927	:268)				TOF MS ES+ 904	
387.1871				389.1127	389.2657	39	0.2023			391.1898	
0 	87.50	388.00	388.50	389.00	389.50	390.00		390.5	0	391.00	
Minimum: Maximum:	50.00 100.00		200.0	100.0	-1.5 50.0						
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Form	ula			
389.1927	100.00	389.1940	-1.3	-3.4	5.5	1	C20	H30	06	Na	



Figure S11. ¹H NMR spectrum (400 MHz, CDCl₃) of 8-dehydroxy-15(17)-dehydromanaarenolide E (**3**)



Figure S12. ¹³C NMR spectrum (100 MHz, CDCl₃) of 8-dehydroxy-15(17)-dehydromanaarenolide E (**3**)



Figure S13. HMQC spectrum (400 MHz, CDCl₃) of 8-dehydroxy-15(17)-dehydromanaarenolide E (**3**)



Figure S14. HMBC spectrum (400 MHz, CDCl₃) of 8-dehydroxy-15(17)-dehydromanaarenolide E (**3**)



Figure S15. ¹H-¹H COSY spectrum (400 MHz, CDCl₃) of 8-dehydroxy-15(17)-dehydromanaarenolide E (**3**)

Figure S16. HRESIMS spectrum of 8-dehydroxy-15(17)-dehydromanaarenolide E (3)

SIMM-Shuying Per	M-Shuying Peng		of Ultima		09-Apr-201213:47:33		
20409-1 489 (9.201)	AM (Cen,5, 80.00, Ht,9	000.0,396.12,0.70); Sm (Mn	, 2x0.00); Cm (463:490)		TOF MS ES+		
00			373.2000		11		
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% -							
1							
0-1	373,160	373.180	373.200	373.220	373.240 m		
				An one distant contraction of the			
Flemental (composition Rer	oort			Page 1		
Lionionian	in pool of the p				· · · · · ·		
Tolerance =	10.0 PPM / DE	3E: min = -1.5, max =	= 50.0				
Isotope clus	ter parameters: S	eparation = 1.0 Abi	undance = 1.0%				
Monoisotopic I 13 formula(e)	lass, Odd and Even evaluated with 1 resu	Electron lons Its within limits (up to 20	closest results for each m	nass)			
SIMM-Shuying Pe	ang	Q-To	fUltima	09	-Apr-201213:47:33		
G4-24C	201) AM (Cen 5, 80 00, Ht	9000 0 396 12 0 70): Sm (Mn	2x0 00); Cm (463:490)		TOF MS ES+		
373 2000	,	,0000.0,000.12,0.10), Oll (Will,	210.00/, 011 (400.400)		110		
100 07 5.2000					110		
100_575.2000							

SIMM-Shuying Peng	MM-Shuying Peng I-24C				Q-Tof Ultima				
G4-24C 120499-1 489 (9.201) AM (Cen.5, 8 100- ^{373,2000}	0.00, Ht,9000.0	0,396.12,0.70); Sm (Mn, 2x	0.00); Cm (463:4	90)				TOF MS ES+ 110
0 373.200					3				373.201
Minimum: Maximum:	200.0	10.0	-1.5 50.0						
Mass Calc. Mass	mDa	PPM	DBE	Score	Formula				
373.2000 373.1991	0.9	2.4	5.5	1	C20 H30	05	Na		



Figure S17. ¹H NMR spectrum (400 MHz, CDCl₃) of 15,17-dedihydromanaarenolide A (4)



Figure S18. ¹³C NMR spectrum (100 MHz, CDCl₃) of 15,17-dedihydromanaarenolide A (4)



Figure S19. HRESIMS spectrum of 15,17-dedihydromanaarenolide A (4)

Figure S20. ¹H NMR spectrum (400 MHz, CDCl₃) of 15,17-dedihydromanaarenolide C (5)



Figure S21. ¹³C NMR spectrum (100 MHz, CDCl₃) of 15,17-dedihydromanaarenolide C (5)



Figure S22. HRESIMS spectrum of 15,17-dedihydromanaarenolide C (5)

SIMM-	Shuying Per	ng			Q-Tof	Jitima			29-1	May-201213:4	47:37
H3-32 120529-	-1 114 (2.149)	AM (Cen,5,	80.00, Ht,9000.0,	362.27,0.70); S	5m (Mn, 2x	0.00); Cm (11	4:122)			TOF MS	ES+ 760
100-											
%-											
o		1		1		374.2034	Ii.				m/z
	367 3	368 369	370 3	371 372	373	374 3	75 376	377	378 37	9 380	
	Flomont	Compo	cition Pono	-+						Dono 1	
2	Liementa	a compo	stuon kepo	n						Page	
	Tolerance	e = 30.0 P	PM / DBE	: min = -1.5	max =	50.0					
	Isotope cl	luster par	ameters: Sep	paration = 1	.0 Abu	ndance =	1.0%				
	Monoisotop	ic Mass, Oo	dd and Even Ele	ectron lons			6				
		e) evaluate	u with Tresults	within infins (t	10 20 C	IUSESI TESUIIS	for each ma	55)			
	H3-32 120529-1 114	(2.149) AM (C	Cen,5, 80.00, Ht,90	00.0,362.27,0.70	; Sm (Mn, 2	2x0.00); Cm (11	4:122)		29-141ay	TOF MS ES+	
	100_373.19	85								760	
	-										
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	-										
	0									374.2034 m/z	
	373.20	373.30	373.40 37	3.50 373.6	0 373	.70 373.8	0 373.90	374.00	374.10	374.20	
	Minimum: Maximum:	50.00 100.00		200.0	30.0	-1.5 50.0					
	Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula			
	373.1985	100.00	373.1991	-0.6	-1.6	5.5	1	C20 H30	05 Na		

Figure S23 ¹H NMR spectrum (400 MHz, CDCl₃) of *epi*-flexilarin A (6)



Figure S24 HRESIMS spectrum of *epi*-flexilarin A (6)



Figure S25. ¹H NMR spectrum (400 MHz, CDCl₃) of epoxyflexibilene (7)



Figure S26. ¹³C NMR spectrum (100 MHz, CDCl₃) of epoxyflexibilene (7)



Figure S27. HMQC spectrum (400 MHz, CDCl₃) of epoxyflexibilene (7)



Figure S28. HMBC spectrum (400 MHz, CDCl₃) of epoxyflexibilene (7)



Figure S29. ¹H-¹H COSY spectrum (400 MHz, CDCl₃) of epoxyflexibilene (7)



Figure S30. HREIMS spectrum of epoxyflexibilene (7)



LIST: h120684-c1	20-J	ul-12 E	lapse:	03:28	.9	16
Samp: B54 Comm: Finnigan/MAT95//70eV/Tsou:220c/	B-10000	S	tart :	14:01	:24	23
Mode: EI +VE +LMR BSCAN (EXP) UP HR	NRM	S	tudy :	S/N:	PT200712	-01-01
Oper: WANG_J@SIMM.CAS		I	nlet :			
Limt: (0)						
Peak: 1000.00 mmu R+D: $-2.0 > 60$	0.0					
Data: CMASS : converted						
79007	(mm))					
Mass Intensity %RA %RIC De	lta R+D	Composit	ion			
71.07406 * 208064 9.93 0.55						
77.00519 * 344109 16.42 0.91 -	2.5 5.5	C5.H.O				
79.01825 * 706990 33.74 1.87	0.1 4.5	C5.H3.O				
81_03134 * 1229042 58.66 3.25	2.7 3.5	C5.H5.0				
82.04390 * 414558 19.79 1.09 -	2.0 3.0	C5.H6.O				
83.02024 * 97072 4.63 0.26						
83.05672 * 323124 15.42 0.85						
85.08075 * 118914 5.68 0.31						
91.05135 * 528476 25.22 1.40						
92.06045 * 280654 13.40 0.74	2.2 4.0	C7.H8				
93.06998 * 2095203 100.00 5.53	0.4 3.5	C7.H9				
95.08729 * 949957 45.34 2.51 -	1.2 2.5	C7.H11				
96.05934 * 143325 6.84 0.38 -	1.8 3.0	C6.H8.O				
96.09433 * 200355 9.56 0.53 -	0.4 2.0	C7.H12				
97.06630 * 122054 5.83 0.32 -	1.0 2.5	C6.H9.O				
105 0341 * 517198 24 68 1.37	0.0 5.5	C7.H5.0				
106.0372 * 141754 6.77 0.37		0.1.0.0				
107.0435 * 931328 44.45 2.46						
108.0482 * 312346 14.91 0.82						
109.0204 * 206493 9.86 0.55						
110.0277 * 82940 3.96 0.22						
110.0628 * 237542 11.34 0.63						
111.0375 * 169235 8.08 0.45						
119 0869 * 467091 22.29 1.23 -	0.8 4.5	C9.H11				
120.0929 * 170020 8.11 0.45	1.0 4.0	C9.H12				
121.1021 * 802564 38.30 2.12 -	0.4 3.5	C9.H13				
122.1075 * 224909 10.73 0.59	2.0 3.0	C9.H14	、 、			
123.1168 * 285508 13.63 0.75	0.6 2.5	C9.H15	,			
125.0962 * 318056 15.18 0.84	0.4 2.5	C8.H13.0)			
133.1021 * 358170 17.09 0.95 -	0.3 4.5	C10.H13				
134.1091 * 339897 16.22 0.90	0.5 4.0	C10.H14				
$135.1172 \times 1222404 58.54 5.25$ $136.1230 \times 304566 14.54 0.80$	2.2 3.0	C10.H16				
137.0966 * 173374 8.27 0.46	0.0 3.5	C9.H13.0)			
137.1319 * 153246 7.31 0.40	1.1 2.5	C10.H17				
138.1042 * 134902 6.44 0.36	0.3 3.0	C9.H14.0)			
145,1009 * 120413 5,75 0.32	0.8 5.5	C11.H13	,			
147.1162 * 232974 11.12 0.62	1.2 4.5	C11.H15				
148.1229 * 184938 8.83 0.49	2.3 4.0	C11.H16				
149.0226 * 110277 5.26 0.29	2035	C11 U17				
151.1116 * 139970 6.68 0.37	0.7 3.5	C10.H15	0			
152.1178 * 105566 5.04 0.28	2.3 3.0	C10.H16.	0			
159.1165 * 135830 6.48 0.36	0.9 5.5	C12.H15				
161.1320 * 245037 11.70 0.65 163.1477 * 91434 4.36 0.24	1.0 4.5	C12.H17				
175.1477 * 109635 5.23 0.29	1.0 4.5	C13.H19				
219.1752 * 142183 6.79 0.38 -	0.3 4.5	C15.H23	0			
288.2466 * 92861 4.43 0.25 -	1.3 5.0	C20.H32.	0			

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Figure S31. ¹H NMR spectrum (400 MHz, Pyr-d₅) of sinulaflexiolide L (8)



Figure S32. ¹³C NMR spectrum (100 MHz, Pyr-d₅) of sinulaflexiolide L (8)



Figure S33. HMQC spectrum (400 MHz, Pyr-d₅) of sinulaflexiolide L (8)



Figure S34. HMBC spectrum (400 MHz, Pyr-d₅) of sinulaflexiolide L (8)



Figure S35. ¹H-¹H COSY spectrum (400 MHz, Pyr-d₅) of sinulaflexiolide L (8)

Figure S36. HRESIMS spectrum of sinulaflexiolide L (8)



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Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions 20 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

SIMM-Mass S	Spec			Q-Tof	Ultima			21	-Aug-201316	:00:11
130654 281 (5.298) AM (Ce 727.4396	en,5, 80.00, Ht,9000.0	0,430.91,0.70);	Sm (Mn, 2)	:0.00); Cm (27	2:284)			TOF MS 1	ES+ .13e3
727.307	72					s.		72	8.3637 728.	4541
0 1 1 1 1	727.40 72	27.50 727.60	727.70	727.80	727.90 72	28.00 728.10	728.20	728.30	728.40	nuz.
Minimum: Maximum:	50.00 100.00		200.0	10.0	-1.5 50.0					
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula			
727 4396	100.00	707 4207	-0.1	0.0	0.5	1	040 1164	010	Ne	