Supporting Information

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A New Short Chain Acetamide from the Biosphere and Bioactive

Glycerolipids Extracted from the Marine Bivalve

Codakia orbicularis (Lucinidae).

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S1: General Experimental Procedures.

Gills of bivalve individuals freshly collected from the seagrass beds were extracted with ethyl acetate (EtOAc) (VWR Chemicals, CAS number 141-78-6). Column chromatography (63*3 cm) was performed on silica gel (MERCK silica gel, 70-230 mesh ASTM) and flash column was performed on Redisep®Rf (220-gram, 69-2203-422 TELEDYNE Isco). These were carried out using hexane (CAS number 110-54-3), ethyl acetate (CAS number 141-78-6) and methanol (CAS number 67-56-1). Thin layer chromatography (TLC) was performed on commercial TLC plates (pre-coated Kiesegel 60 F254 TLC, 20 x 20 mm, thickness 0.25 mm, Merck) and was visualized under UV (254nm and 366nm). Solvents used for chromatography (column, thin layer and HPLC) were purchased from MERCK and CARLO ERBA. HPLC-grade acetonitrile (MeCN, CAS number 75-05-8) and milliQ water, both acidified by 0.1% formic acid (noted HCOOH,) were used for analytical and semi-preparative HPLC analysis. LC/MS analyses were performed using Waters Alliance 2695 separation module equipped with mass spectrometer (Waters ZQ 2000 with a single-quadrupole and electrospray ionization source), ELS detector (Waters 2420) and photodiode array detector (Waters 996). Semi-preparative HPLC was performed using an Auto Prep system (Waters 600 controller and Waters 600 pump, equipped with a Waters 996 Photodiode Array Detector). Data acquisitions were dealt with two softwares from Waters company: Empower (analytical analysis) and Masslynx (semi-preparative analysis). High-resolution mass spectra were obtained on a Waters LCT Premier XE in electrospray ionization mode by direct infusion of the purified compounds. NMR experiences (1D and 2D) were operated on a Brucker 500 AVANCE II or on a Brucker AVANCE II 600 MHz spectrometer (TXI 1.7 mm probe) (CNRS-ICSN). Chemical shift values are given in δ (ppm) employing residual CDCl₃ signal as reference ($\delta_{\rm H}$ = 7.26 and $\delta_{\rm C}$ = 77.00). All measurements were analyzed with the software NMR notebook.



Figure S1: ¹H NMR spectrum of compound 1 (MeOD, 600 MHz).



Figure S2: ¹H-¹H COSY spectrum of compound 1 (MeOD, 600 MHz).

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Figure S3: ¹H-¹³C HSQC spectrum of compound 1(MeOD, 600 MHz).

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Figure S4: ¹H-¹³C HMBC spectrum of compound 1 (MeOD, 600 MHz).

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Figure S5: Overlays of ¹H NMR spectra of compounds 2 and 3 (CDCl₃, 600 MHz).

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Figure S6: ¹³C Spectrum of compound 2 (CDCl₃, 150 MHz).

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Figure S7: ¹H-¹H COSY spectrum of compound **2** (CDCl₃, 600 MHz).

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Figure S8: ¹H-¹³C HSQC spectrum of compound 2 (CDCl₃, 600 MHz).

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Figure S9: ¹H-¹³C HMBC spectrum of compound **2** (CDCl₃, 600 MHz).

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Figure S10: ¹H-¹H COSY spectrum of compound **3** (CDCl₃, 600 MHz).

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Figure S11: UHPLC – HRESIMS/SM spectra of compound 1.

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	vai.	Min	Max	Eimt	Val.	Min	Max	Eimt	Val.	Min Ma	x	Elmt Val.	Min Max	Use Ad	duct	
H	1	0	250	F	1	0	0	S	2	0	2	Br 1	0 0	Н		-
2H	1	0	0	Na	1	0	2	CI	1	0	2	1 3	0 0			
С	4	1	75	Mg	2	0	0	Ca	2	0	0	1.1.1	12			
N	3	0	5	Si	4	0	0	Ti	2	0	0					
0	2	0	50	Ρ	3	0	0	Fe	2	0	0					
Error N	Aargin (ppm):	30			D	BE Rar	nge: 0.0	50.0		E	Electron lons	: both			
	HC	Ratio: (0.0 - 5.0)		Ap	ply N R	ule: yes			L	Jse MSn Info				
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MS	in Iso R	l (%): !	5.00			MSn L	ogic Mo	de: ANE)			Max Results	: 50			
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2	0.0	0 C15	H31 N3	19			[M-H]	-		204	2213	284 2166	-1.0	16.54	0.00	
3	0.0	0 C17	H32 N (CI			IM-HI			284	2213	284 2151	6.2	21.81	0.00	
4	0.0	0 C18	H27 N3				IM-HI			284	2213	284 2132	81	28.50	0.00	
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lr _	nten. (x	<u>10,000</u>	<u>))</u>													
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lr - - 7.5-	nten. (x	<u>10,000</u> 20	7.1737			N	1S/M	S nega	tive n	node <i>i</i>	m/z 2	84.2187				
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Ir 7.5- 5.0-	nten. (x	20 181.16) 7.1737 362 25	4.2094		N	IS/M	S nega	tive m 54	node 7 4.0230	m/z 2	84.2187	746.6746			

Figure S12: Molecular formula propositions for ion [M-H]⁻ m/z 284.2187 and SM/SM fragmentations.

<u>m/z 284.2187</u>

ESI (-)

[M-H]⁻

<u>Ion *m/z* 286.2390 [M+H]</u>⁺

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Eimt	Val.	Min	Max	Elmt	Val.	Min	Min Max	Use Adduct		
н	1	0	250	F	1	0	0	S	2	0	2	Br	1	0	0	н		-
2H	1	0	0	Na	1	0	0	CI	1	0	2	1	3	0	0	Na		
С	4	1	75	Mg	2	0	0	Ca	2	0	0		ð					
N	3	0	5	Si	4	0	0	Ti	2	0	0							
0	2	0	50	Ρ	3	0	0	Fe	2	0	0							
Error M	largin ((mag	30			D	BE Rar	nae: 0.0	- 50.0			Electro	n lons:	both				
	HC	Ratio:	0.0 - 5.0)		Apply N Rule: yes					Use MSn Info: yes							
M	ax Isot	opes:	all			Isote	ope RI (%): 1.00)		Isotope Res: 8000							
MS	n Iso B	1 (%)	5.00			MSn L	onic Mo	de ANI	2			May F	Pesults.	50				

Figure S13: Molecular formula propositions for ion $[M+H]^+ m/z 286.2390$.

<u>m/z 268.2176</u> [M-H₂0+H]

Figure S14: Molecular formula proposition for ion $[M-H_2O + H]^+ m/z 268.2176$ and SM/SM fragmentations.

ESI (+)

<u>m/z 250.2078</u>

 $\underline{[M-2(H_{\underline{2}}0)+H]}^+$

Figure S15: Molecular formula proposition for ion $[M-2(H_2O) + H]^+ m/z 250.2078$ and SM/SM fragmentations.

Sing Toler Elem Num	gle Mass rance = 20 lent predict ber of isoto	Analysis 0 PPM / 1 tion: Off ope peaks u	DBE: min = - sed for i-FIT	-1.5, max = 3 = 3	0.0						
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0	120 140	160 180	200 220	240 260	280 300	320 340	360 380	400 420	440 460	, 480	
Minin Maxir	mum:		10.0	20.0	-1.5 30.0						
	17.0	La Mass	mDa	PPM	DBE	i - FIT	1-FT	r (Norm)	Formula		
Mass 357.3	3009 35	7.3005	0.4	1.1	1.5	415.4	0.0		C21 H4	0 du	

Figure S16: HRESIMS spectrum of compound 2 (positive mode).

Figure S17: HRESIMS spectrum of compound 3 (positive mode).

Bioassays. A: Bioassay on *Micrococcus luteus* ATCC 10240 (Gram⁺).

E: cellulose disc on which 20 μ L of the crude extract of *Codakia orbicularis* (diameter of inhibition de 10 mm). T⁺: Antibiogram of colistin (50 μ g; positive control). T⁻: cellulose disc containing 20 μ L ethyl acetate (negative control).

B: **Bioassay on** *Escherichia coli* **ATCC 35218 (Gram**). **E**: cellulose disc on which 20 μ L of the crude extract of *Codakia orbicularis* (diameter of inhibition de 15 mm). **T**⁺: Antibiogram of vancomycin (50 μ g; positive control). **T**⁻: cellulose disc containing 20 μ L ethyl acetate (negative control).

Figure S18: Bioassays on Escherichia coli ATCC 35218 and Micrococcus luteus ATCC 10240 with

the crude extract of endosymbiotic gills of Codakia orbicularis.