

## SUPPLEMENTARY MATERIAL

### Isolation and structure elucidation of a novel symmetrical macrocyclic phthalate hexaester

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**Abstract:** A novel symmetrical macrocyclic hexaester (**1**) and a macrocyclic tetraester (**2**), were isolated during a natural product exploring program on the cyanobacterium *Moorea producens*. Their structures were elucidated based on spectroscopic data, including nuclear magnetic resonance and high-resolution mass spectra. In the antibacterial activity test, compounds **1** and **2** showed no bioactivity at the concentration tested.

**Keywords:** phthalate ester; cyanobacterium; *Moorea producens*, isolation; structural elucidation

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## Display Report

### Analysis Info

Analysis Name D:\Data\H.U\20160201\_Kou\20160201\_Kou2\Kou\_3\_18\_5\_4\_C4\_BA2\_01\_2359.d  
Method 20160129\_fe.ms.ms4.m  
Sample Name Kou\_3\_18\_5\_4\_C4  
Comment  
Acquisition Date 2/1/2016 2:38:42 PM  
Operator BDAL@DE  
Instrument micrOTOF-Q 10380

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste

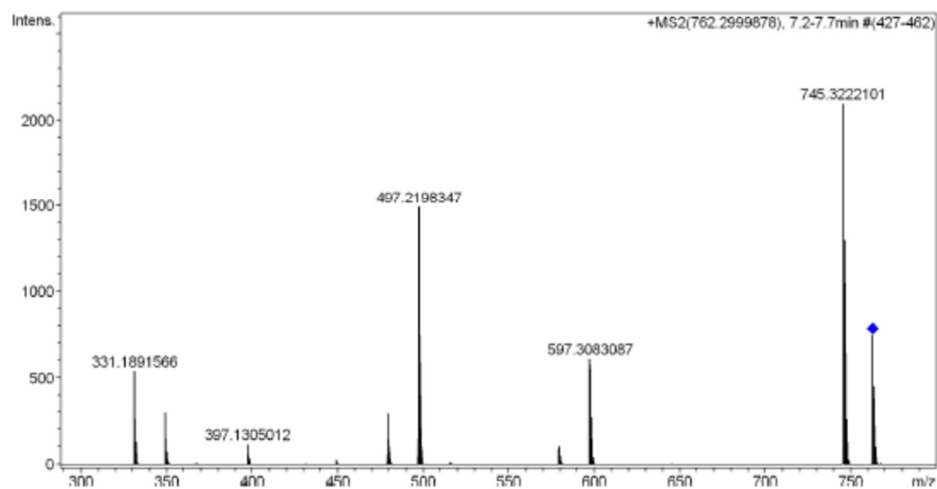
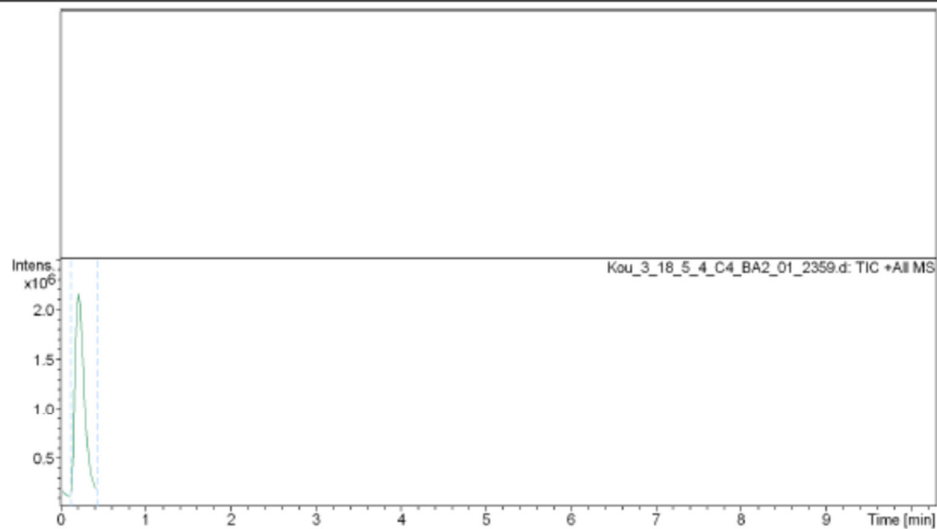


Figure S1. HR-ESI-MS spectrum of compound 1

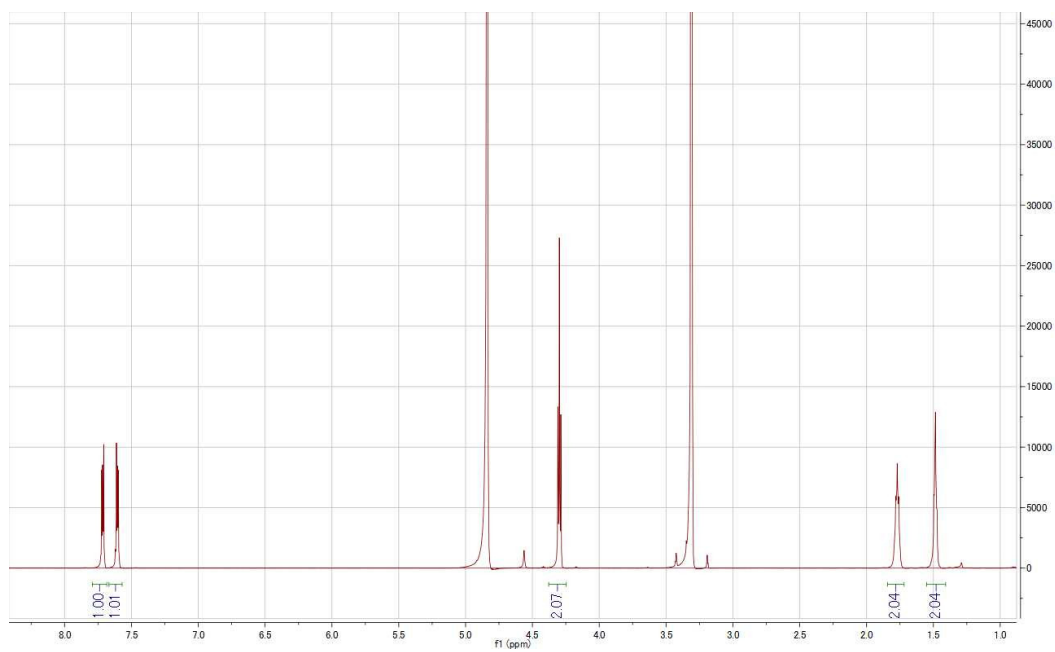


Figure S2.  $^1\text{H}$ -NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$

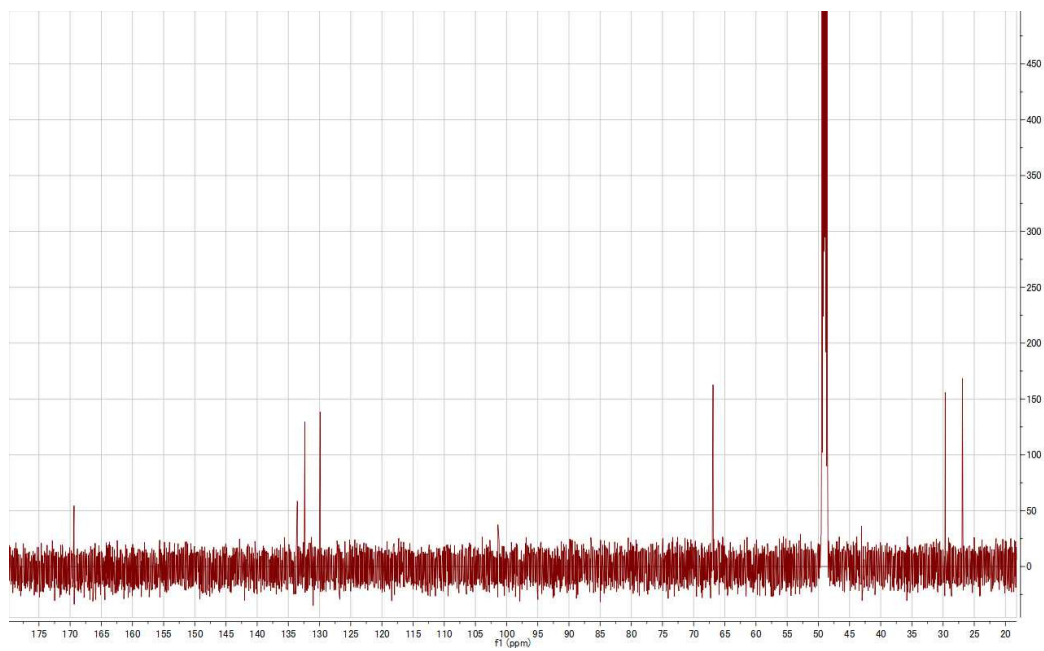


Figure S3.  $^{13}\text{C}$ -NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$

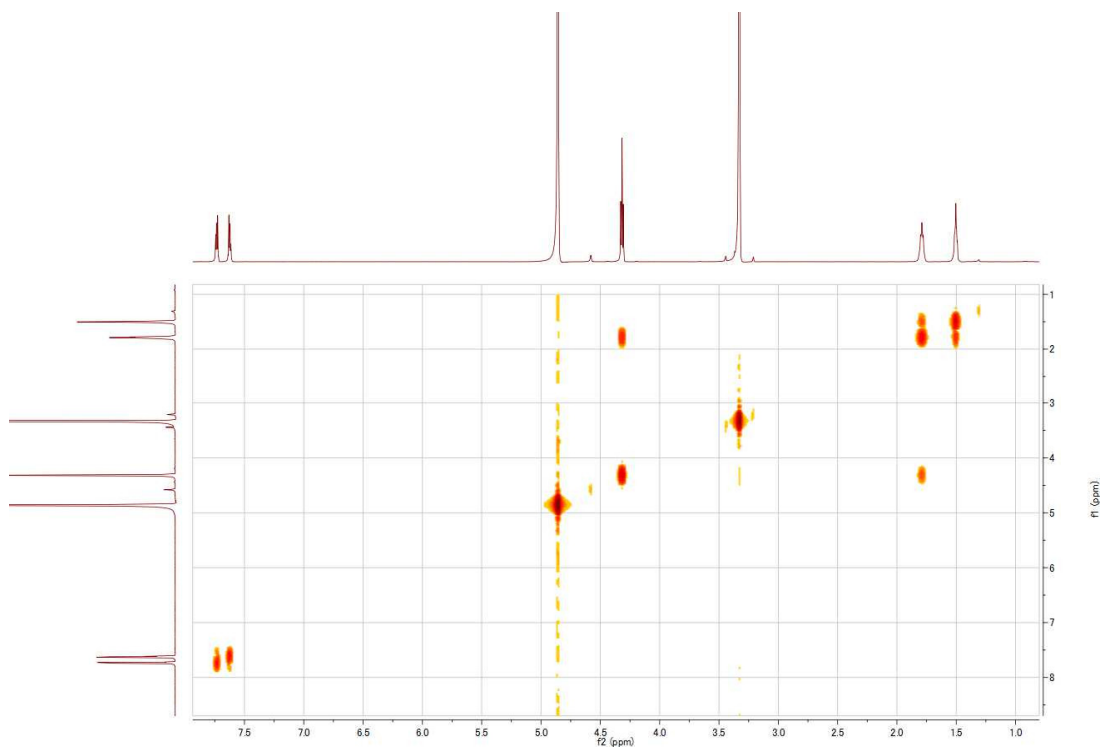


Figure S4.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1** in  $\text{CD}_3\text{OD}$

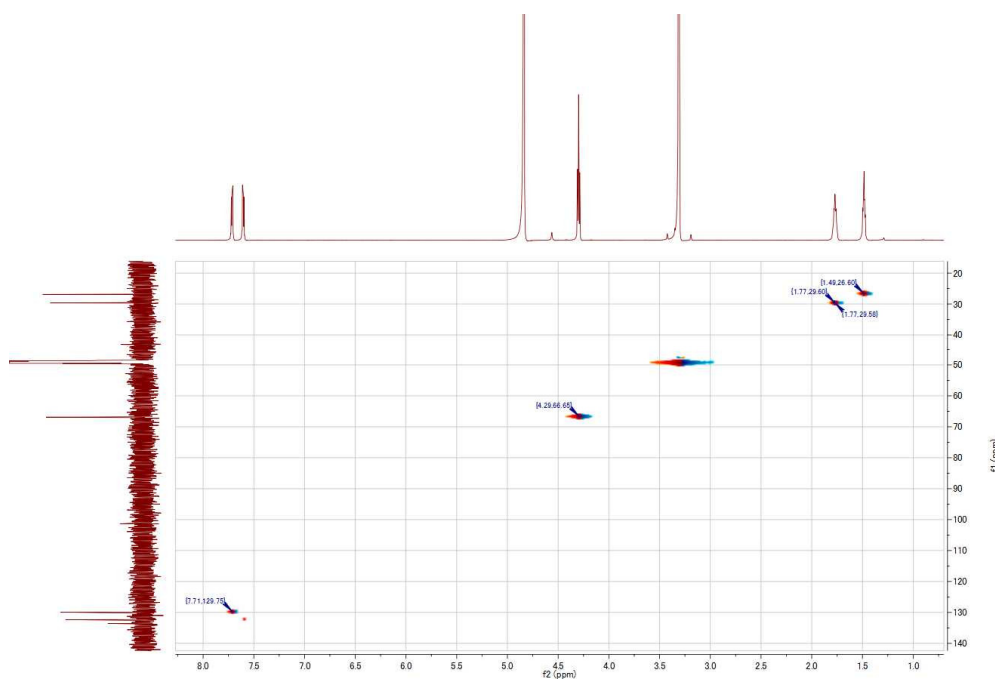


Figure S5.  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **1** in  $\text{CD}_3\text{OD}$

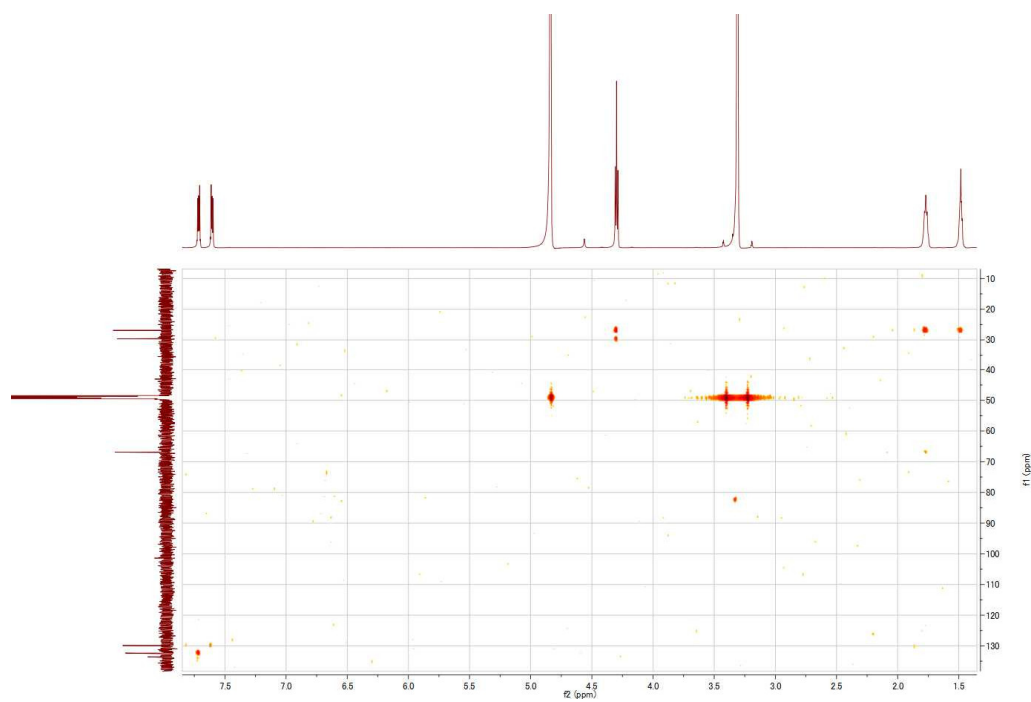


Figure S6.  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **1** in  $\text{CD}_3\text{OD}$