

1 *Supplementary Materials*

2 **Marine microorganism-derived macrolactins inhibit**  
3 **inflammatory mediator effects in LPS-induced**  
4 **macrophage and microglial cells by regulating**  
5 **BACH1 and HO-1/Nrf2 signals through inhibition of**  
6 **TLR4 activation**

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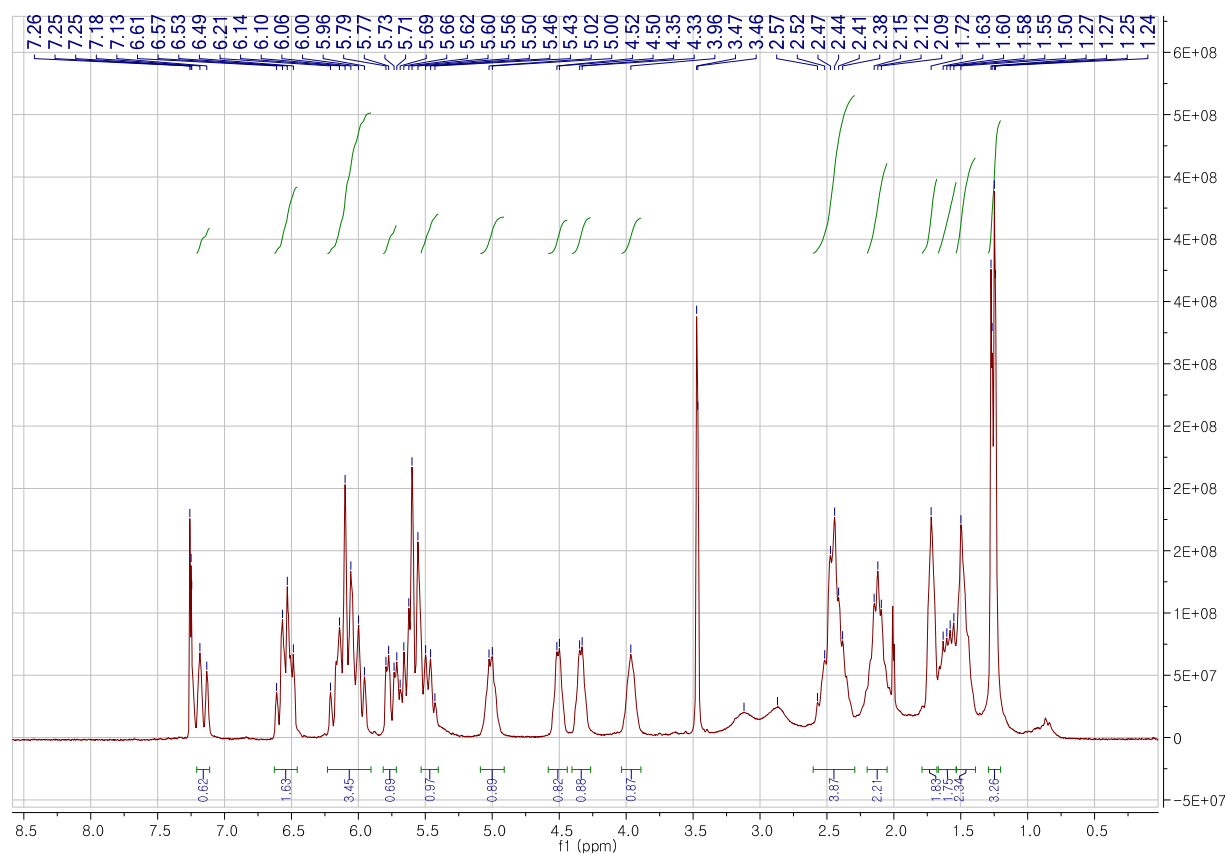
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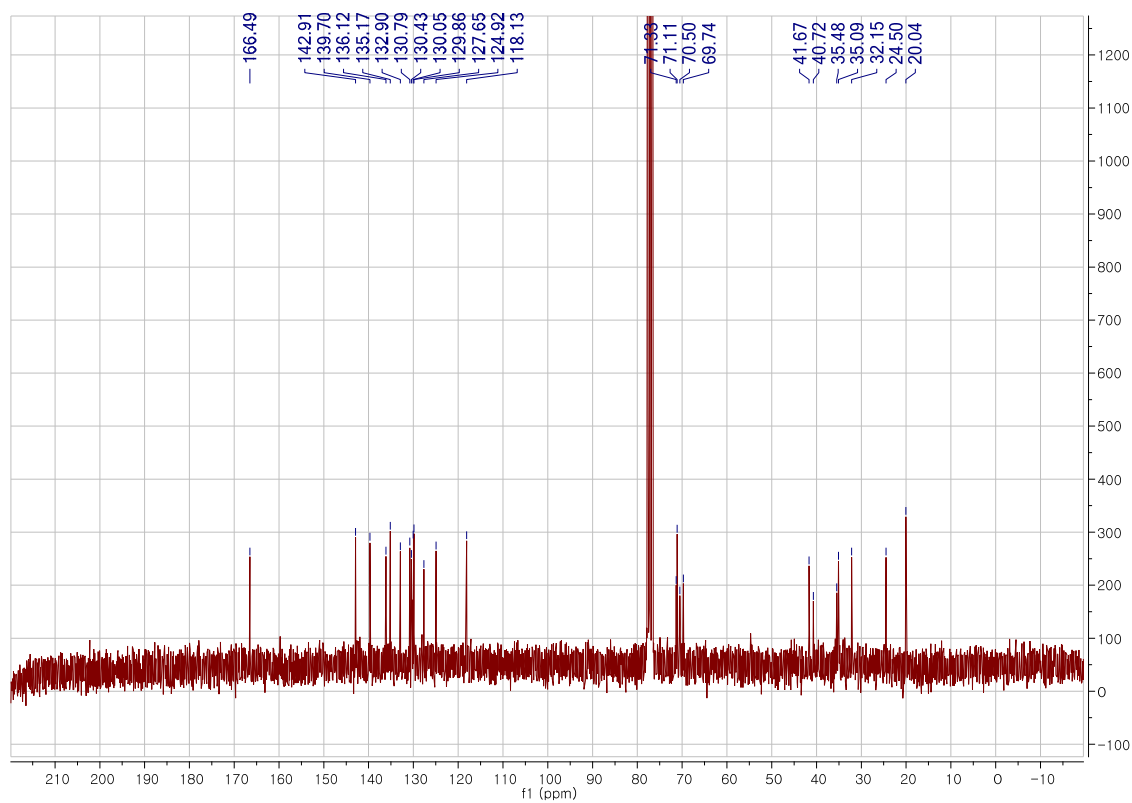
**Figure S19:** HMQC (500 MHz, CD<sub>3</sub>OD) spectrum of macrolactin F (3)

**Figure S20:** HMBC (500 MHz, CD<sub>3</sub>OD) spectrum of macrolactin F (3)

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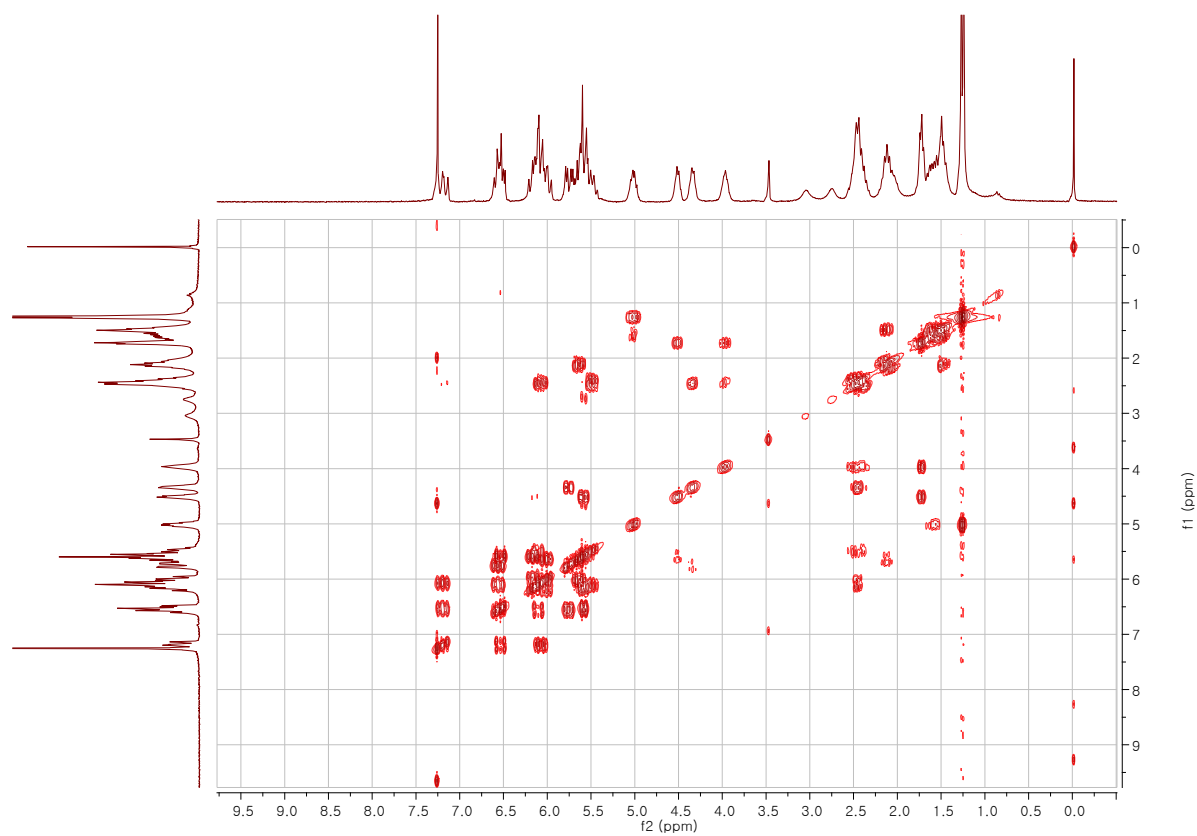


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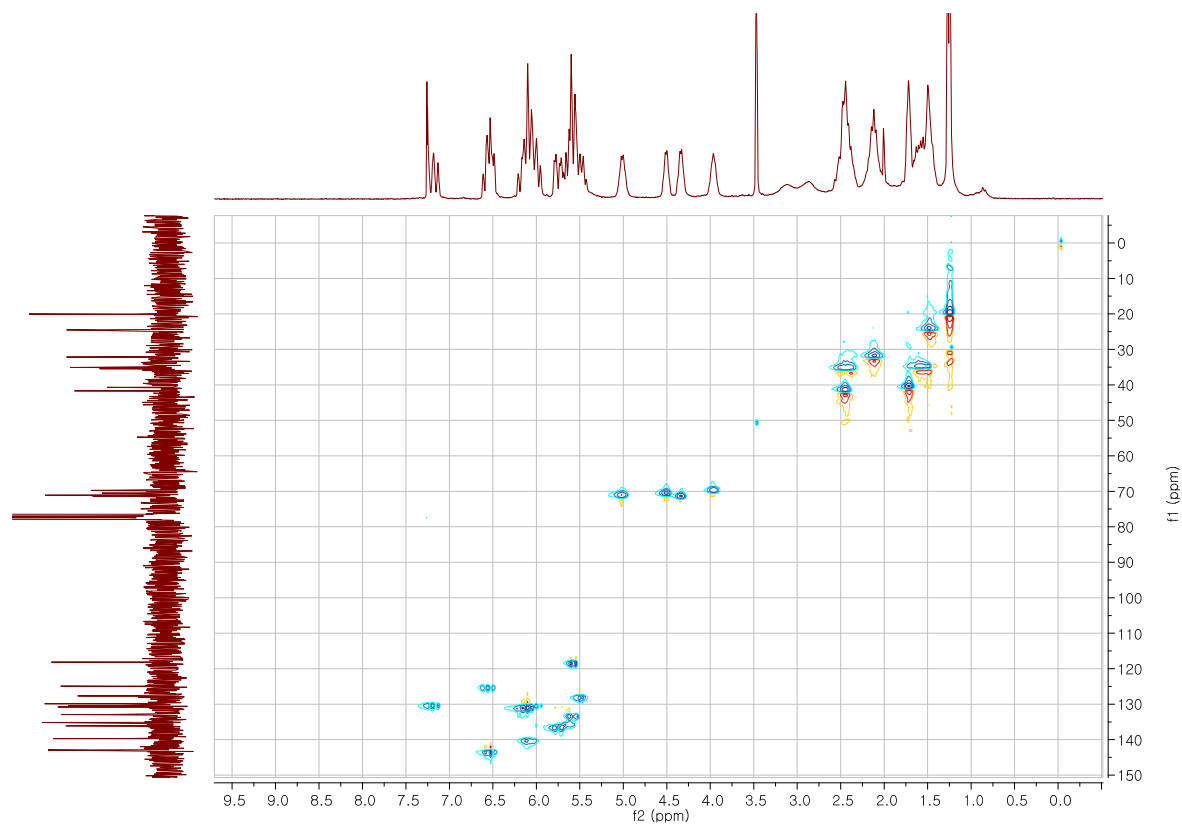
20 **Figure S1.**  $^1\text{H}$  NMR (250 MHz,  $\text{CDCl}_3$ ) spectrum of macrolactin A (1)

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22 **Figure S2.**  $^{13}\text{C}$  NMR (62.5 MHz,  $\text{CDCl}_3$ ) spectrum of macrolactin A (1)

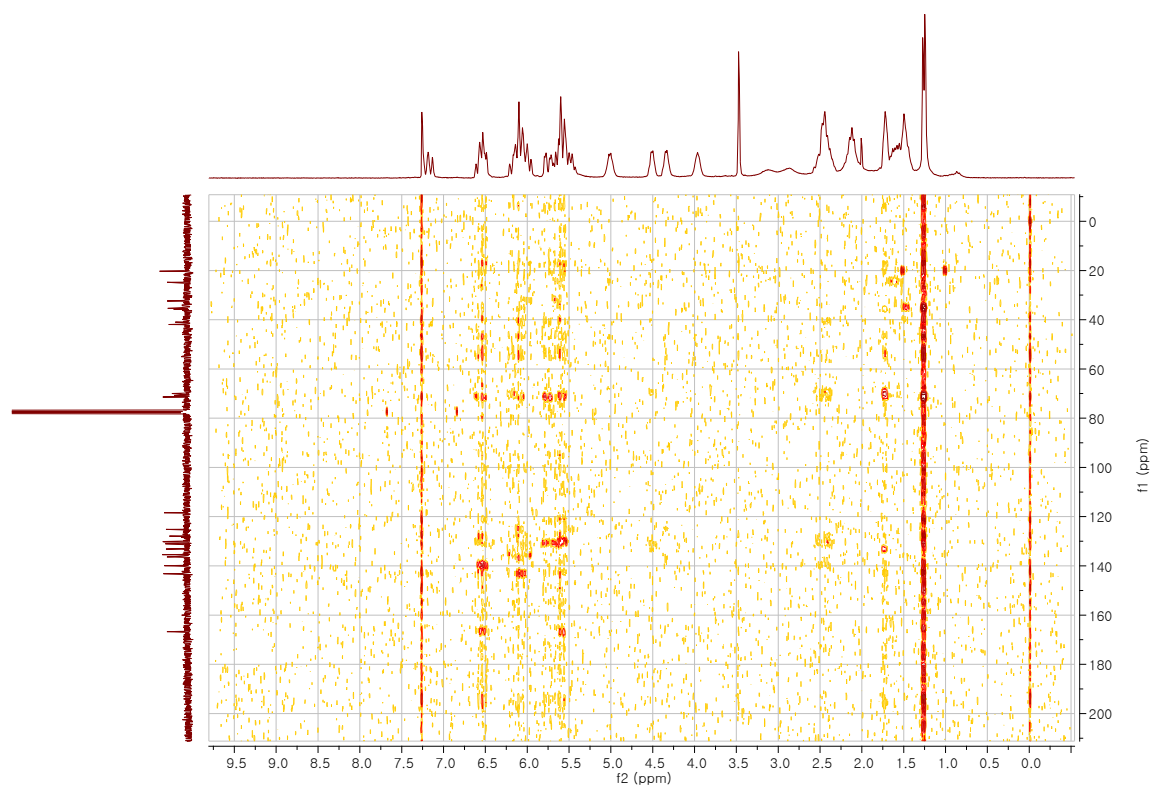


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24 **Figure S3.**  $^1\text{H}$ - $^1\text{H}$  COSY (250 MHz,  $\text{CDCl}_3$ ) spectrum of macrolactin A (**1**)

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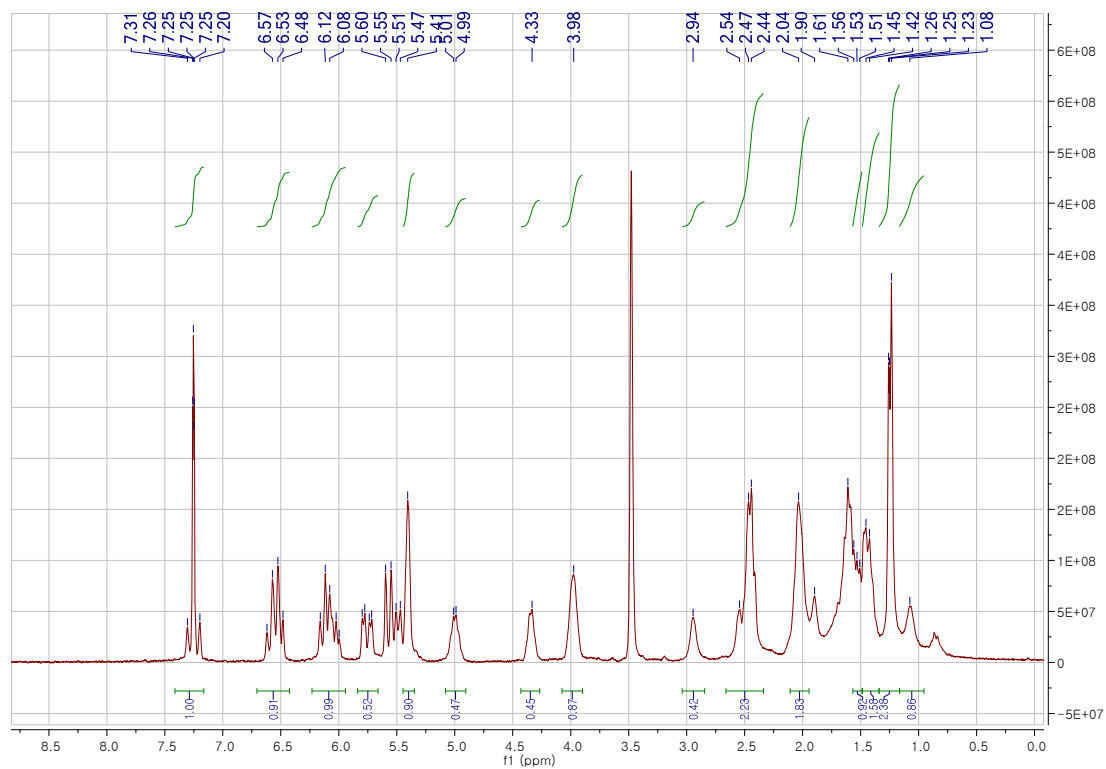
26 **Figure S4.** HMQC (250 MHz,  $\text{CDCl}_3$ ) spectrum of macrolactin A (**1**)



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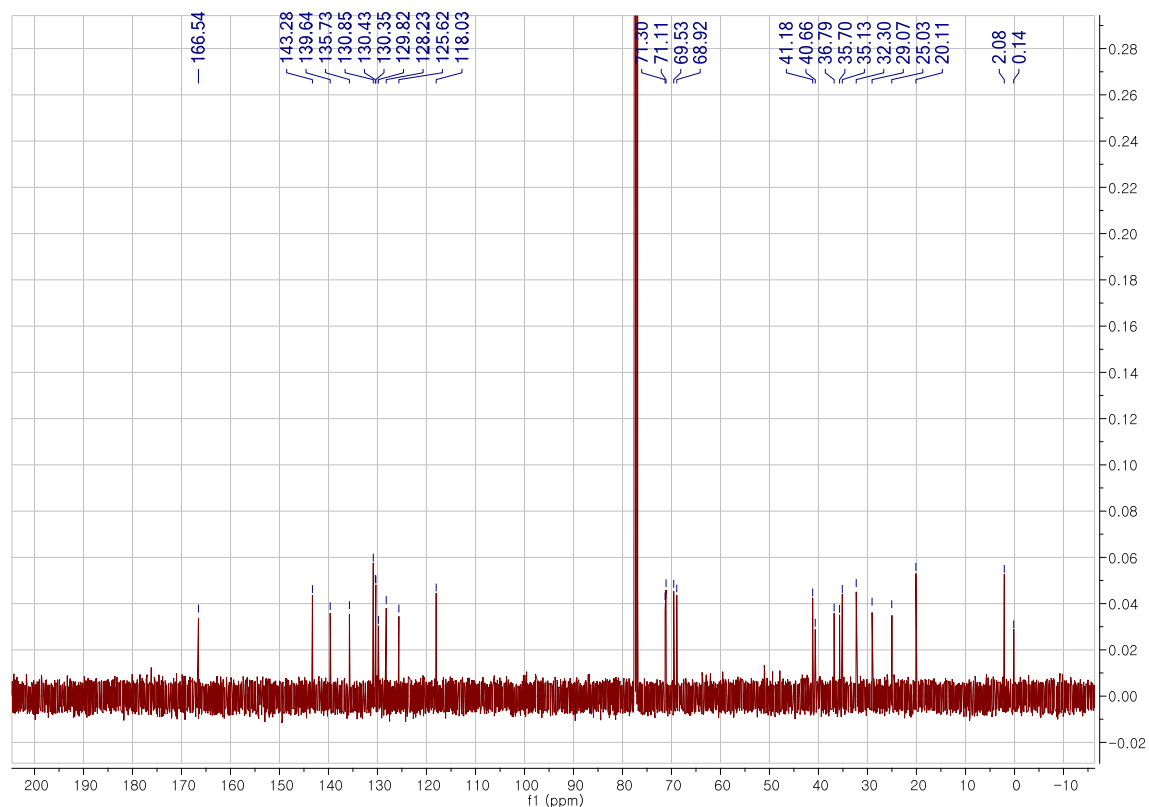
28 **Figure S5.** HMBC (250 MHz, CDCl<sub>3</sub>) spectrum of macrolactin A (**1**)

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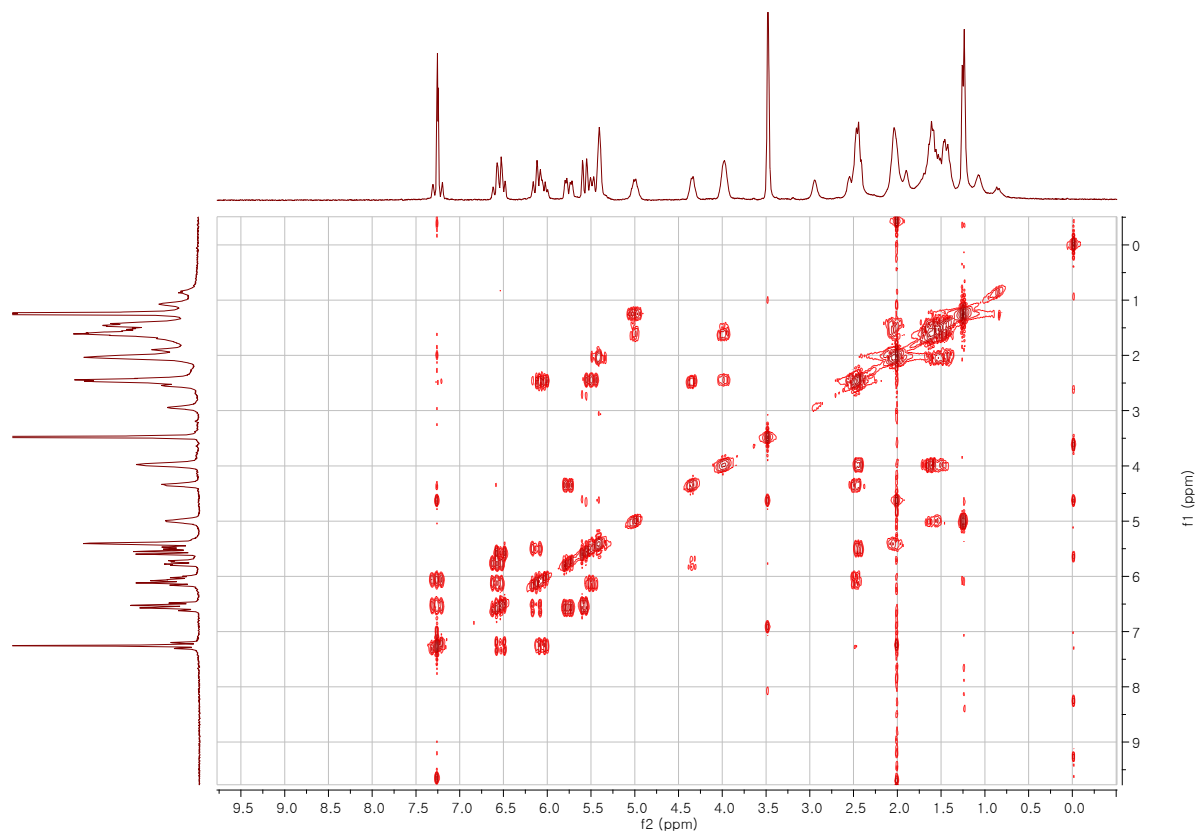


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31 **Figure S16.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of 15-*epi*-dihydromacrolactin F (**2**)

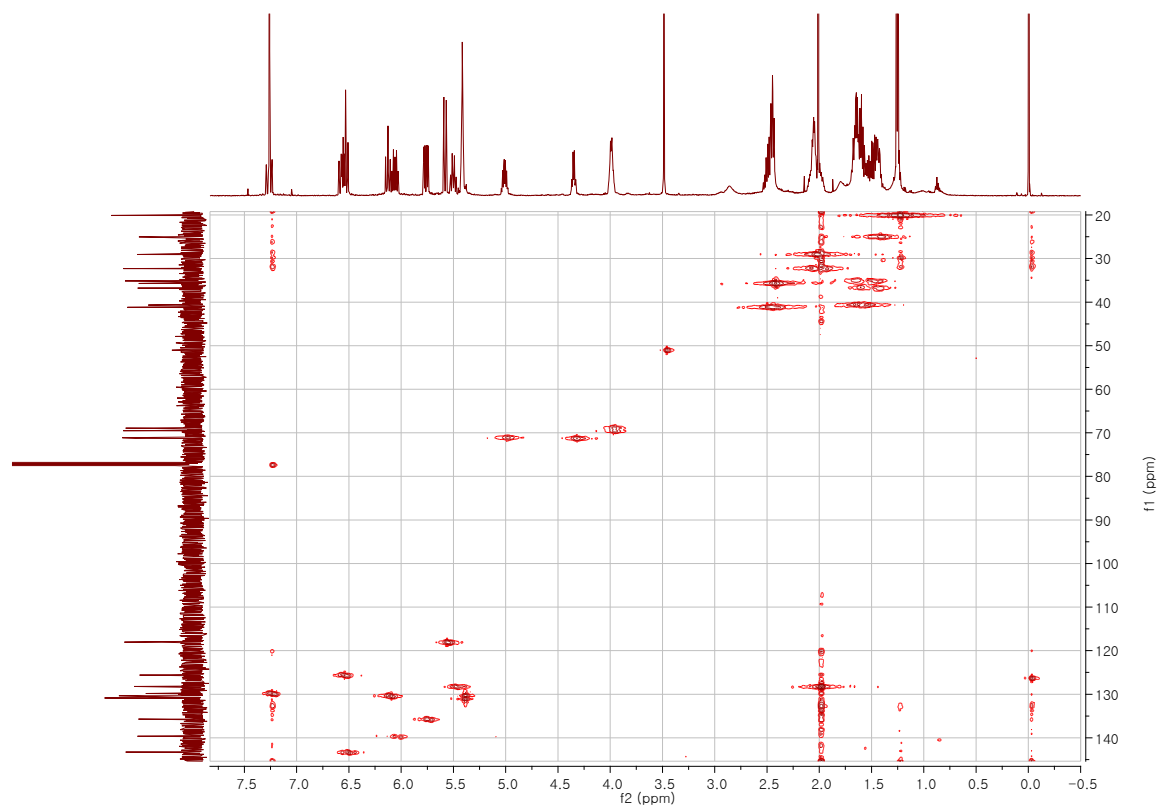


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33 **Figure S7.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of 15-*epi*-dihydromacrolactin F (2)

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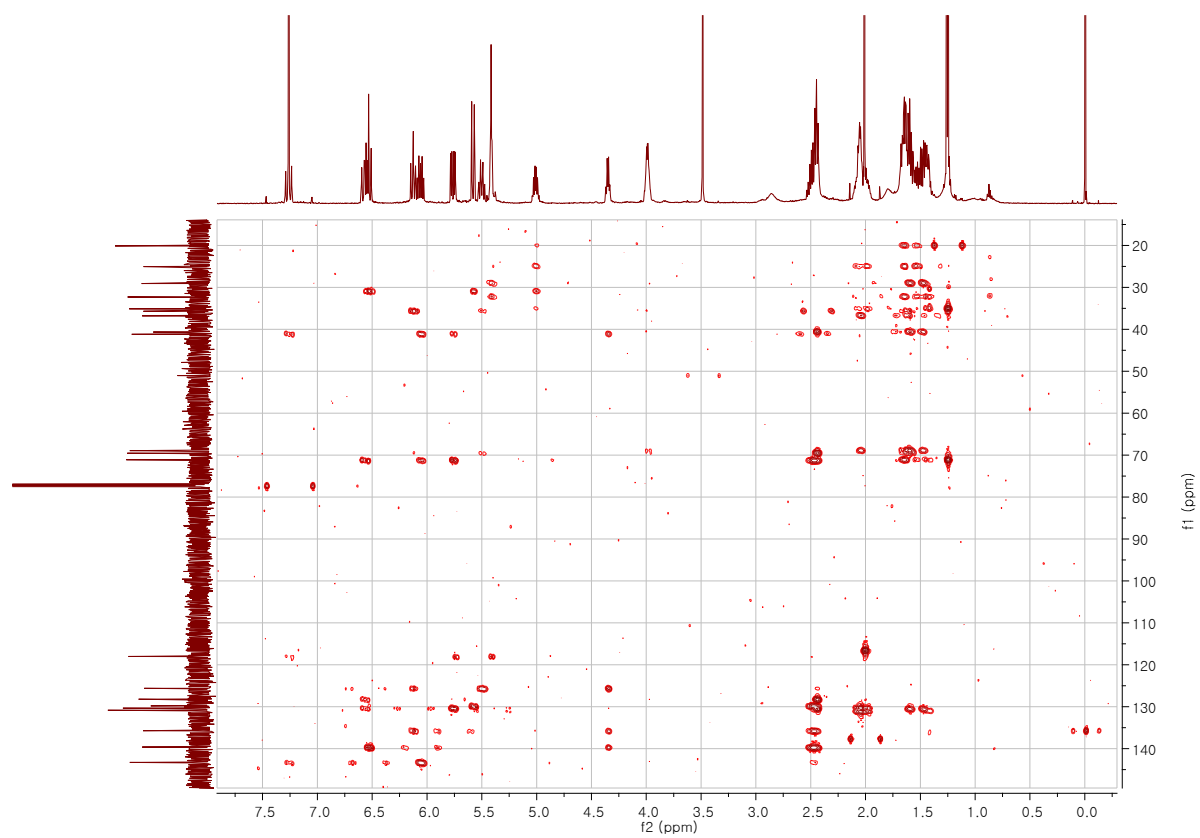
35 **Figure S8.**  $^1\text{H}$ - $^1\text{H}$  COSY (500 MHz,  $\text{CDCl}_3$ ) spectrum of 15-*epi*-dihydromacrolactin F (2)



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37 **Figure S9.** HMQC (500 MHz, CDCl<sub>3</sub>) spectrum of 15-*epi*-dihydromacrolactin F (2)

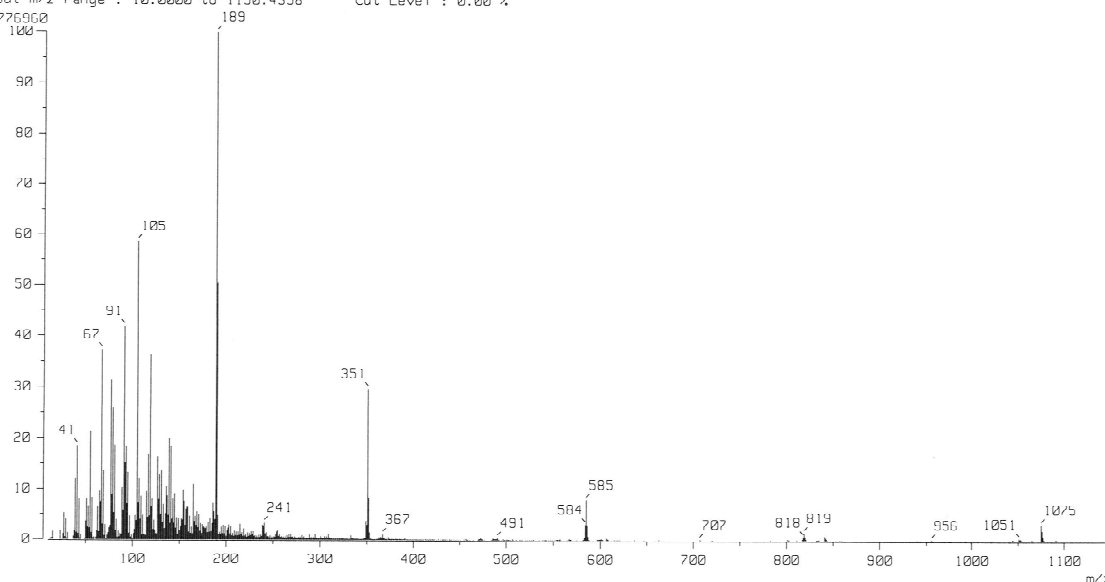
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40 **Figure S10.** HMBC (500 MHz, CDCl<sub>3</sub>) spectrum of 15-*epi*-dihydromacrolactin F (2)

[ Mass Spectrum ]  
 Data : FAB-M156 Date : 18-Jun-2015 16:04  
 Sample: (S)Irin-mosher ester HC001 E4  
 Note : m-NBA  
 Inlet : Direct Ion Mode : FAB+  
 Spectrum Type : Normal Ion [MF-Linear]  
 RT : 0.70 min Scan# : (3,5)  
 BP : m/z 189.0000 Int. : 1599.98  
 Output m/z range : 10.0000 to 1150.4358 Cut Level : 0.00 %



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[ Elemental Composition ]

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Data : FAB-M166 Date : 22-Jun-2015 17:41  
 Sample: HC001 E4  
 Note : m-NBA  
 Inlet : Direct Ion Mode : FAB+  
 RT : 0.90 min Scan# : (16,69)  
 Elements : C 150/0, H 200/0, O 10/0  
 Mass Tolerance : 10ppm, 5mmu if m/z < 500, 10mmu if m/z > 1000  
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
405.2642	4.6	+0.3 / +0.1	6.5 C 24 H 37 O 5

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[ Theoretical Ion Distribution ]

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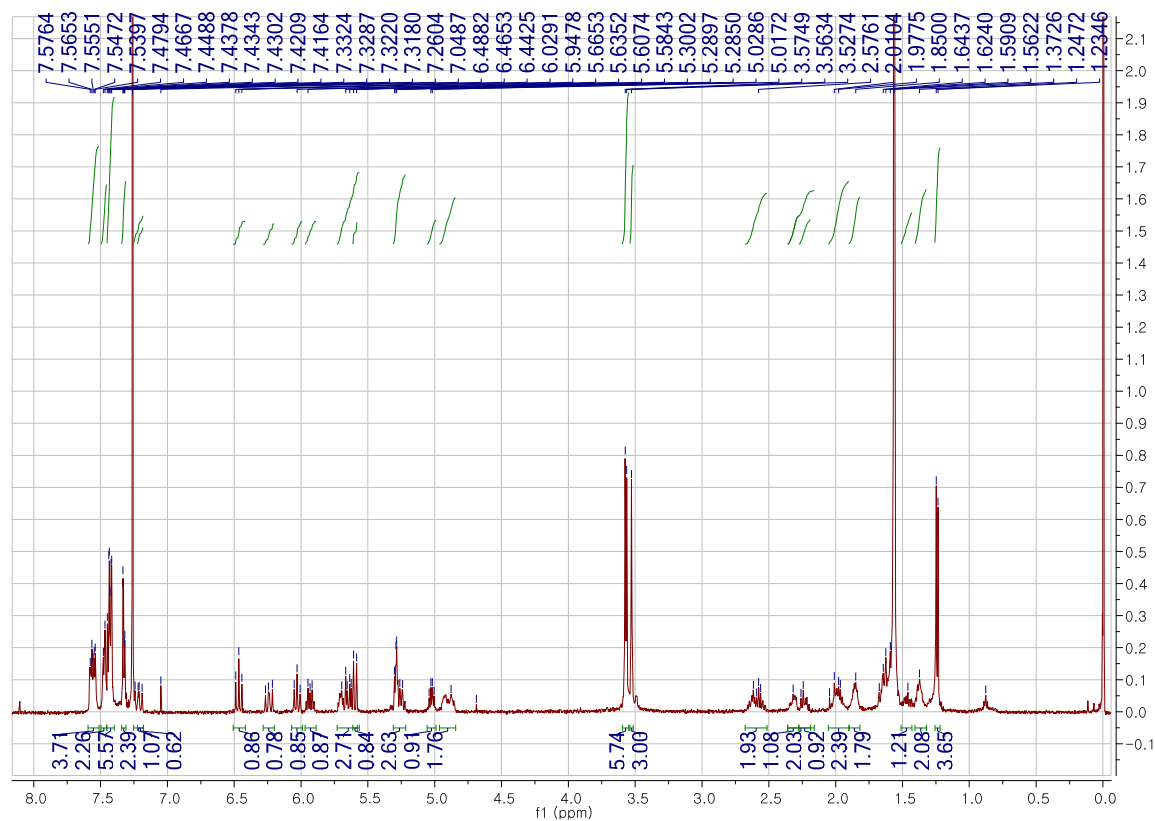
Molecular Formula : C<sub>24</sub>H<sub>37</sub>O<sub>5</sub>  
 (m/z 405.2641, MW 405.5548, U.S. 6.5)  
 Base Peak : 405.2641, Averaged MW : 405.5509(a), 405.5517(w)

m/z	INT.
405.2641	100.0000 *****
406.2675	26.8841 *****
407.2703	4.4677 ***
408.2730	0.5541
409.2756	0.0554
410.2783	0.0047
411.2809	0.0003

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44 **Figure S11.** HR-FAB-MS of 15-*epi*-dihydromacrolactin F (2)

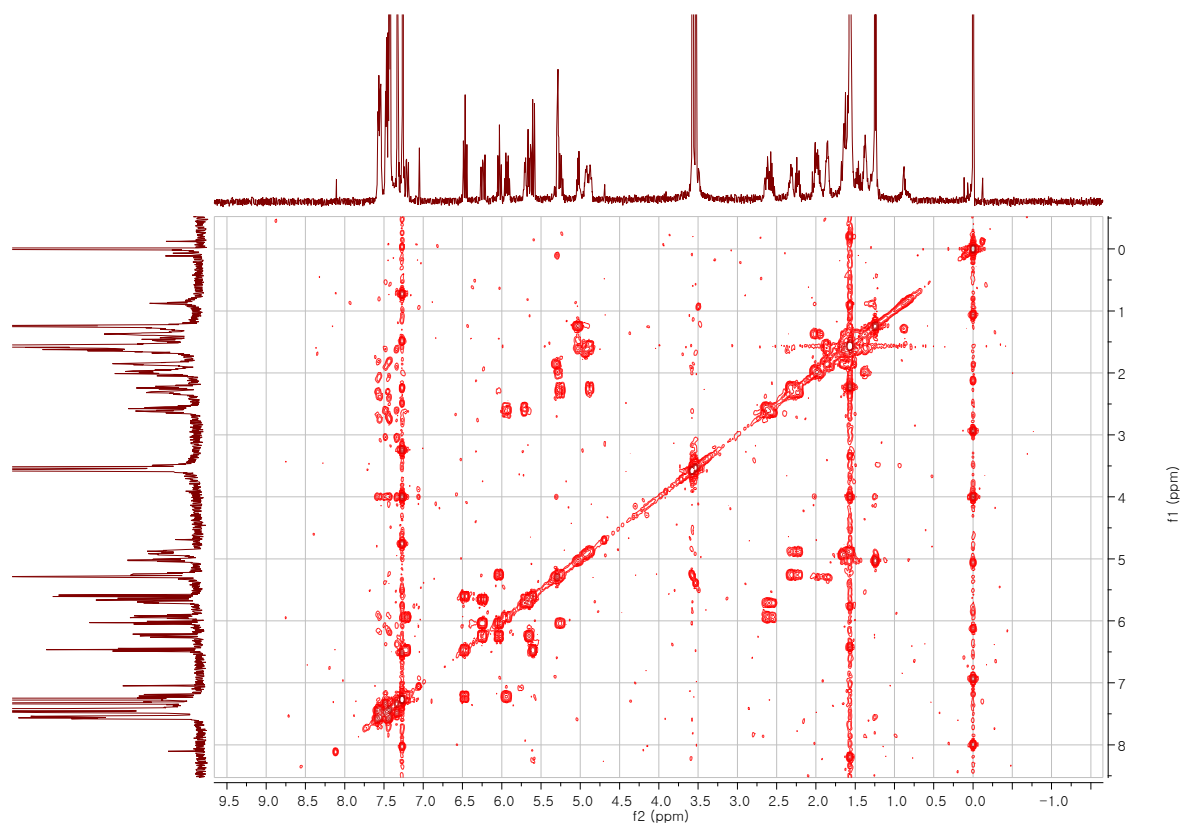
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47 **Figure S12.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of *tris*-(S)-MTPA ester of 2 (2a)

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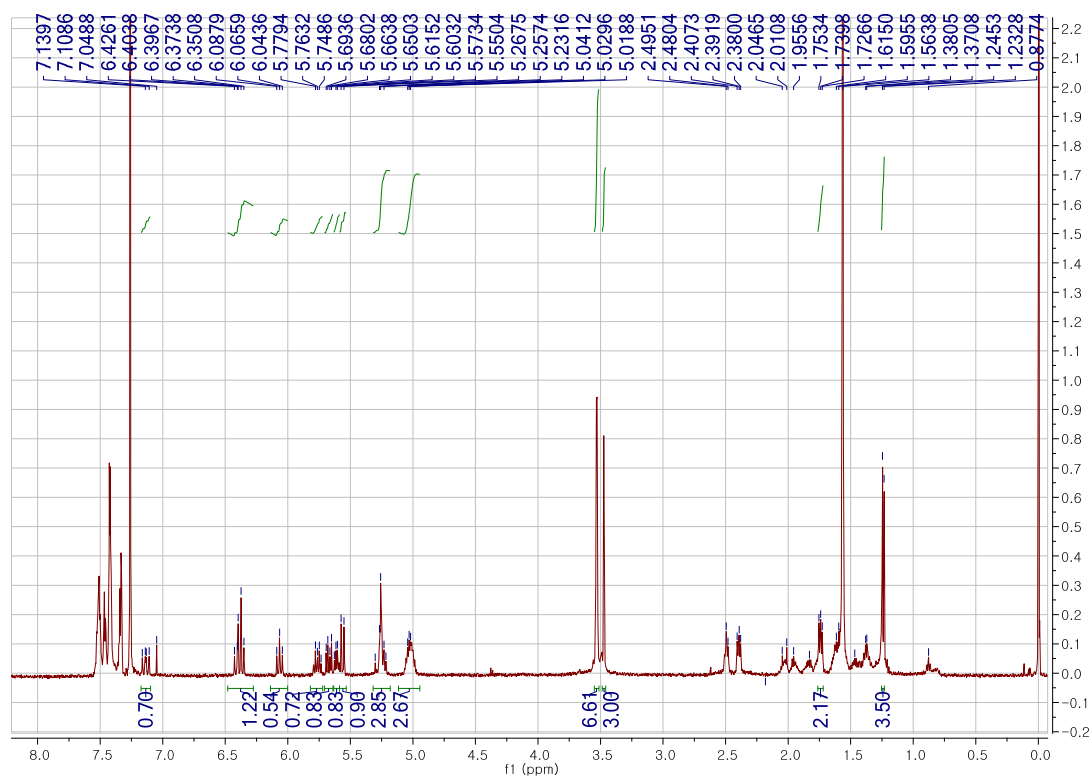


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50 **Figure S13.**  $^1\text{H}$ - $^1\text{H}$  COSY (500 MHz,  $\text{CDCl}_3$ ) spectrum of *tris*-(S)-MTPA ester of 2 (2a)

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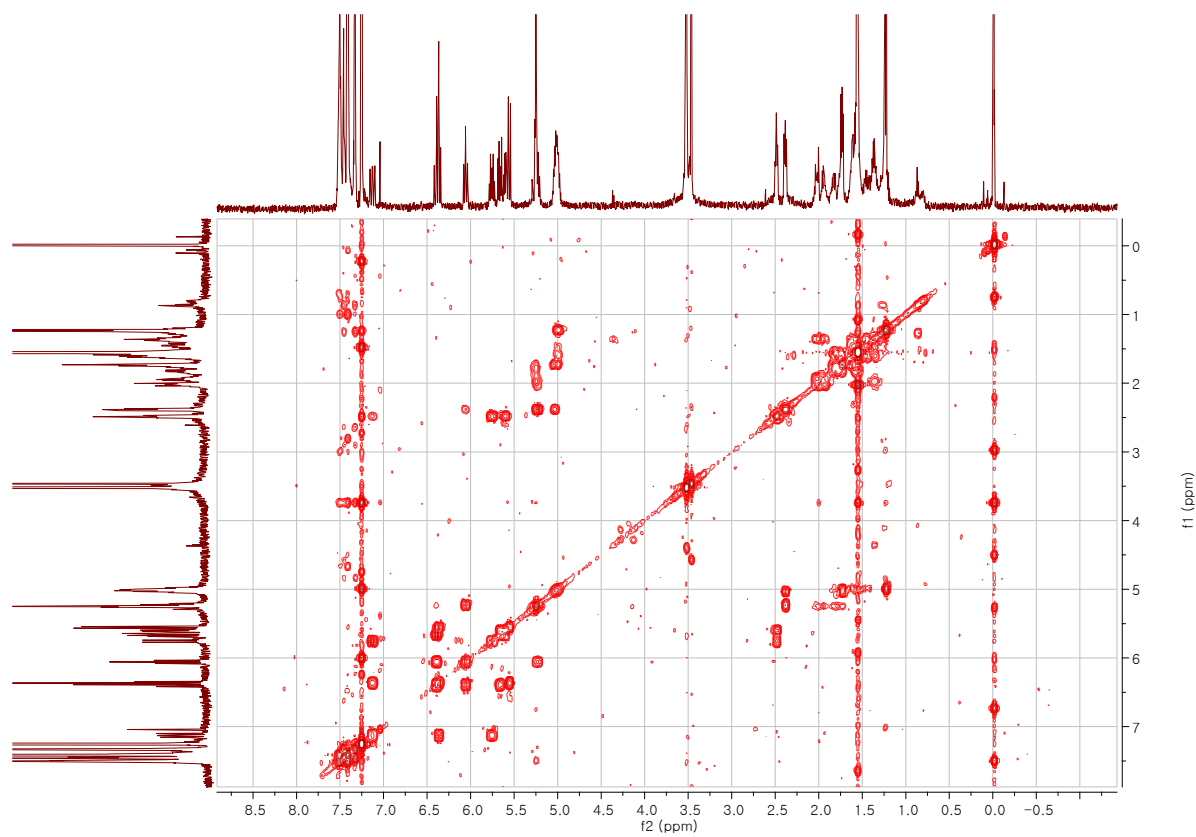




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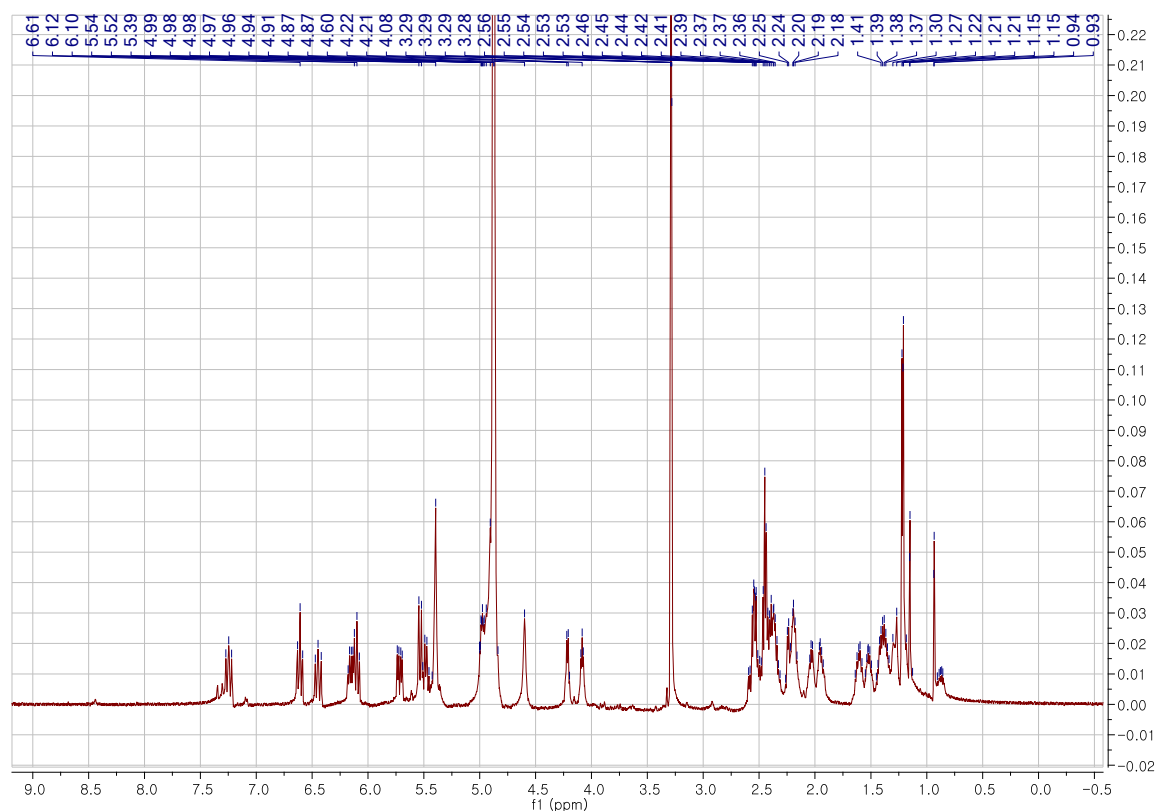
53 **Figure S14.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of *tris*-(*R*)-MTPA ester of **2** (**2b**)

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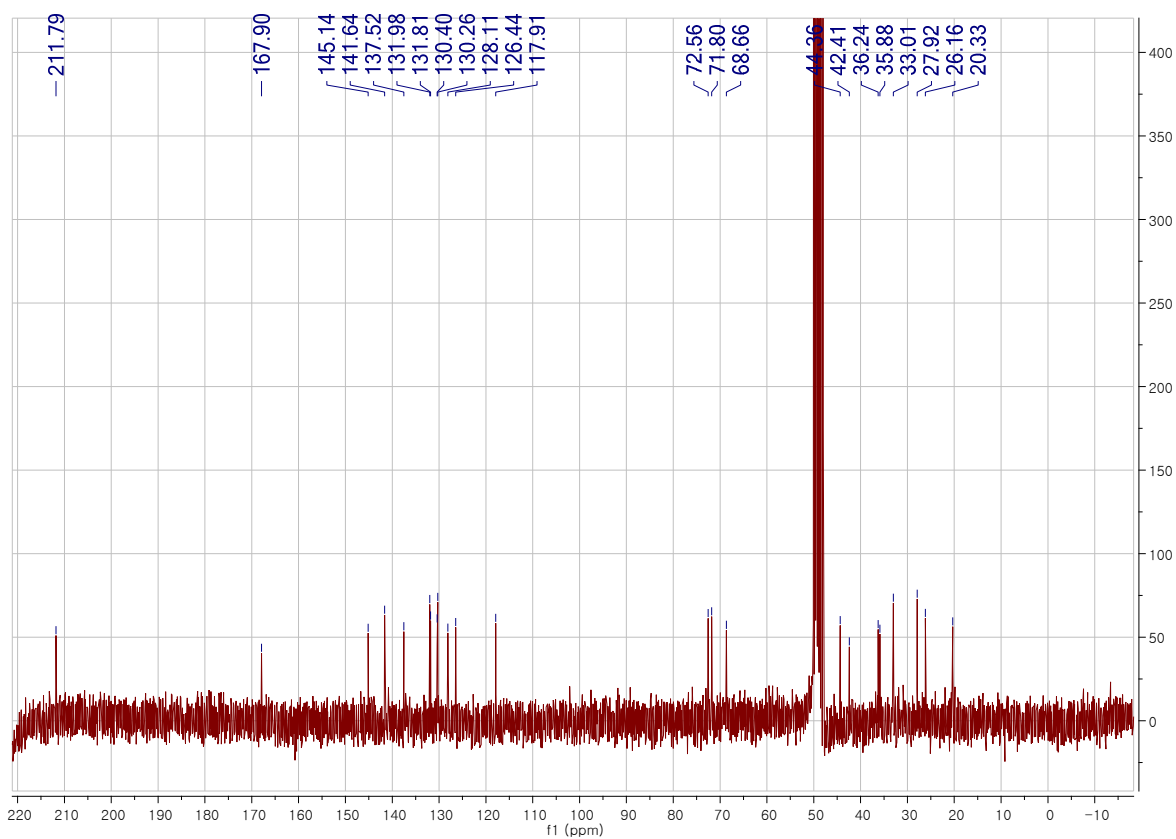
56 **Figure S15.**  $^1\text{H}$ - $^1\text{H}$  COSY (500 MHz,  $\text{CDCl}_3$ ) spectrum of *tris*-(*R*)-MTPA ester of **2** (**2b**)



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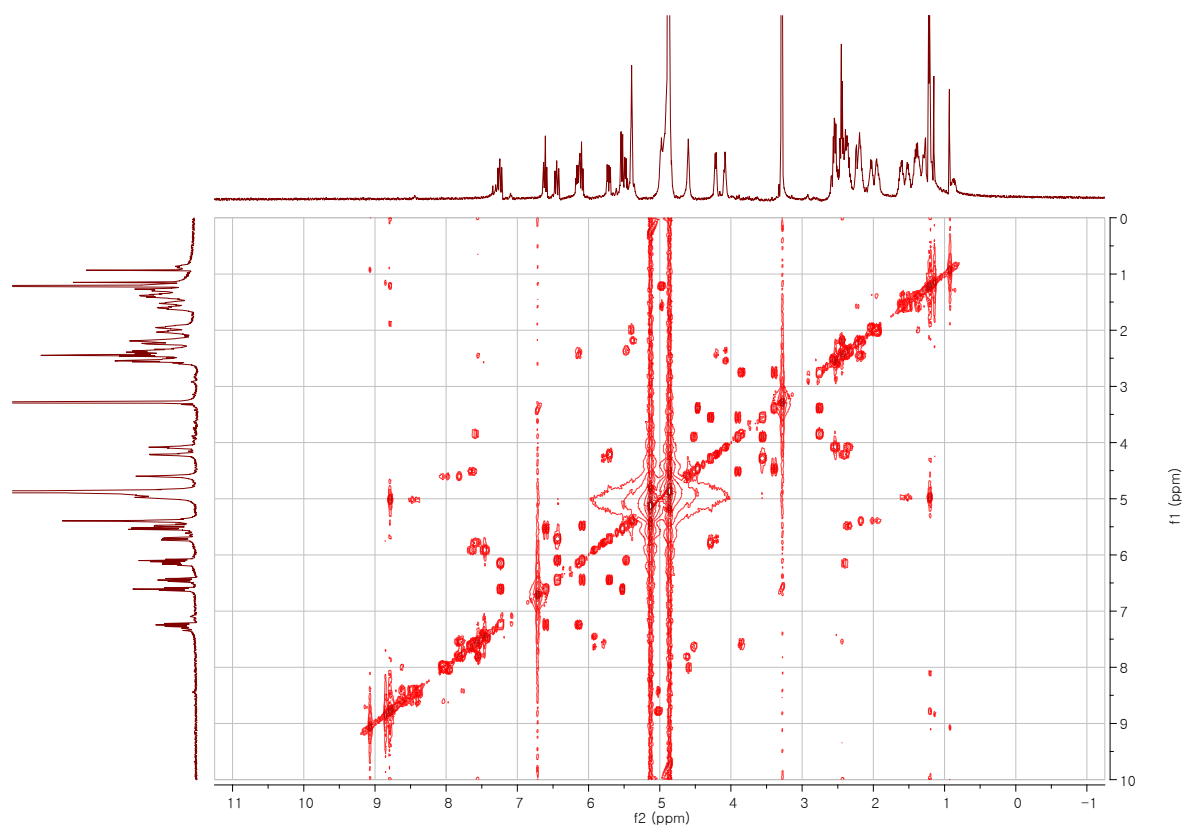
58 **Figure S16.** <sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD) spectrum of macrolactin F (3)

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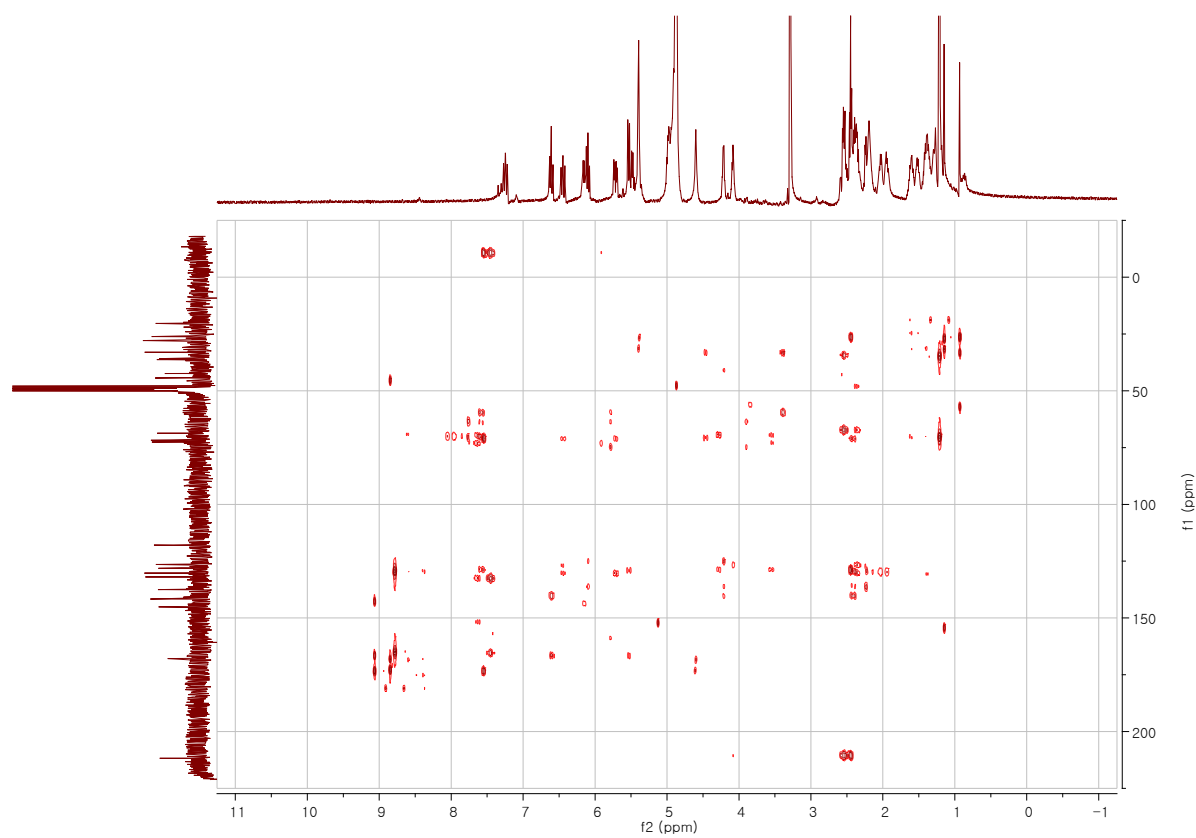


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61 **Figure S17.** <sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD) spectrum of macrolactin F (3)

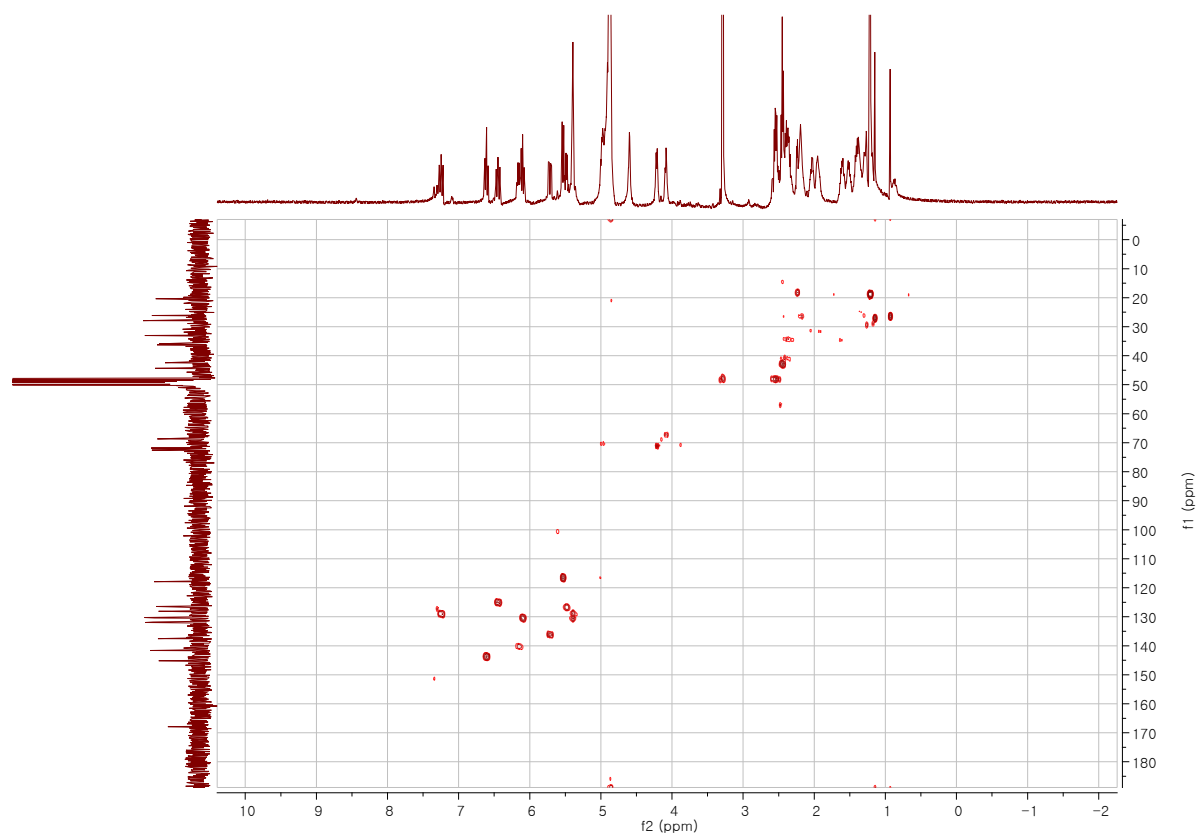


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63 **Figure S18.**  $^1\text{H}$ - $^1\text{H}$  COSY (500 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of macrolactin F (3)

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65 **Figure S19.** HMQC (500 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of macrolactin F (3)



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68 **Figure S20.** HMBC (500 MHz, CD<sub>3</sub>OD) spectrum of macrolactin F (**3**)

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