molecules

MDPI

Supplementary Materials

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

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*Correspondence to: Prof. Gil-Saeng Jeong and Prof. Hyukjae Choi
#These two authors contributed equally to this work.

List of Figures

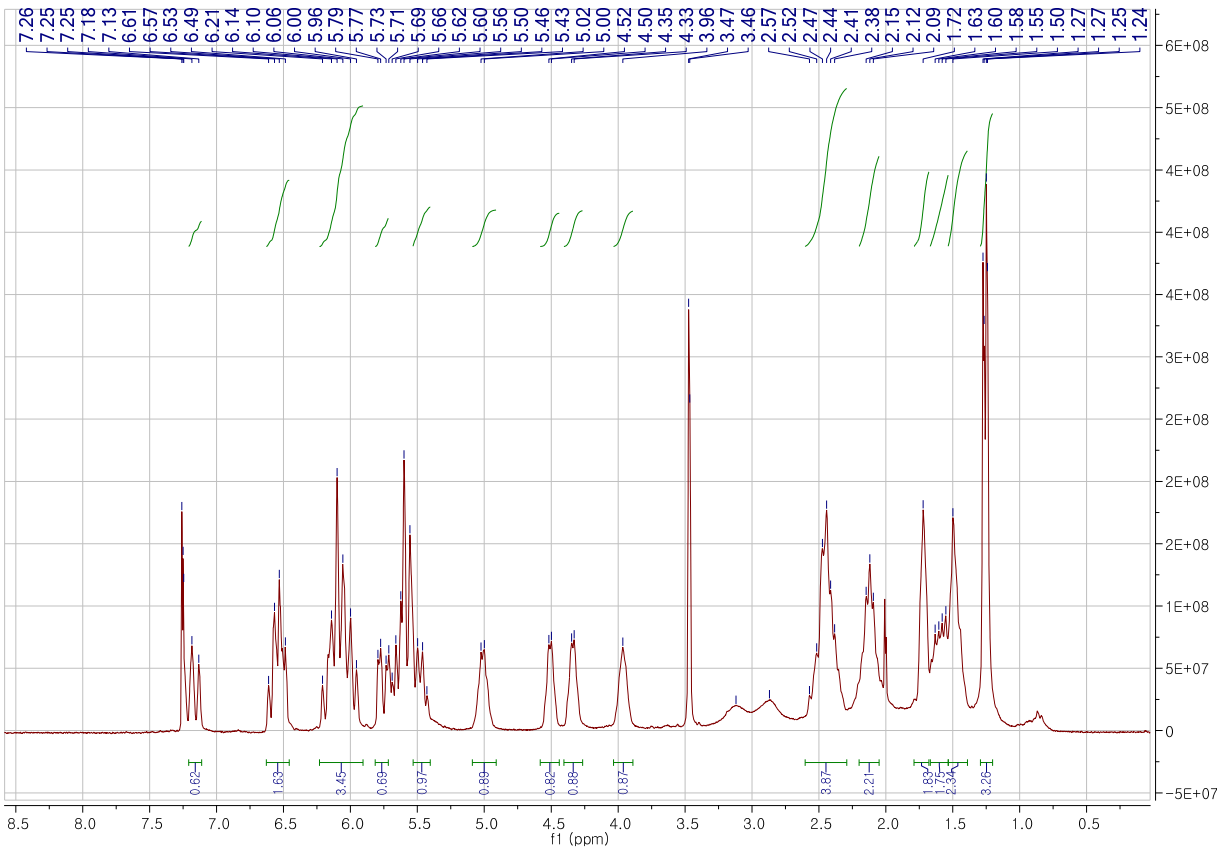


Figure S1: ^{1}H NMR (250 MHz, $CDCl_3$) spectrum of macrolactin A (**1**)

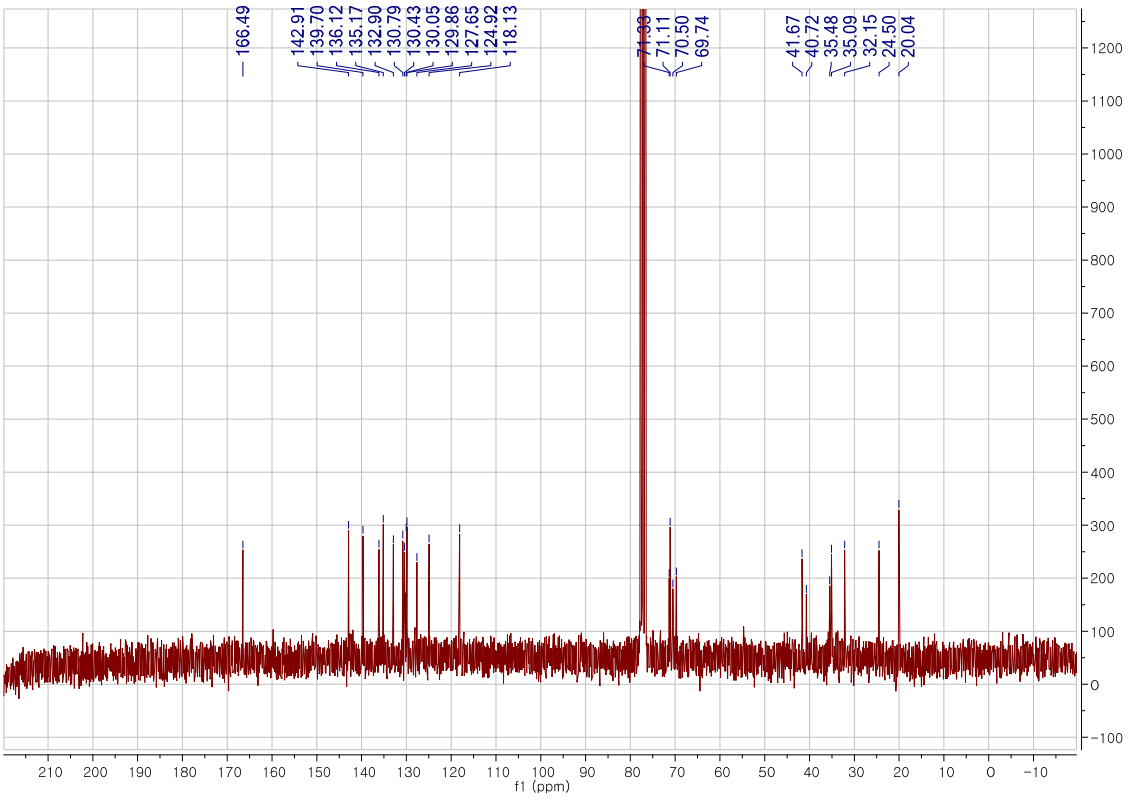


Figure S2. ^{13}C NMR (62.5 MHz, $CDCl_3$) spectrum of macrolactin A (**1**)

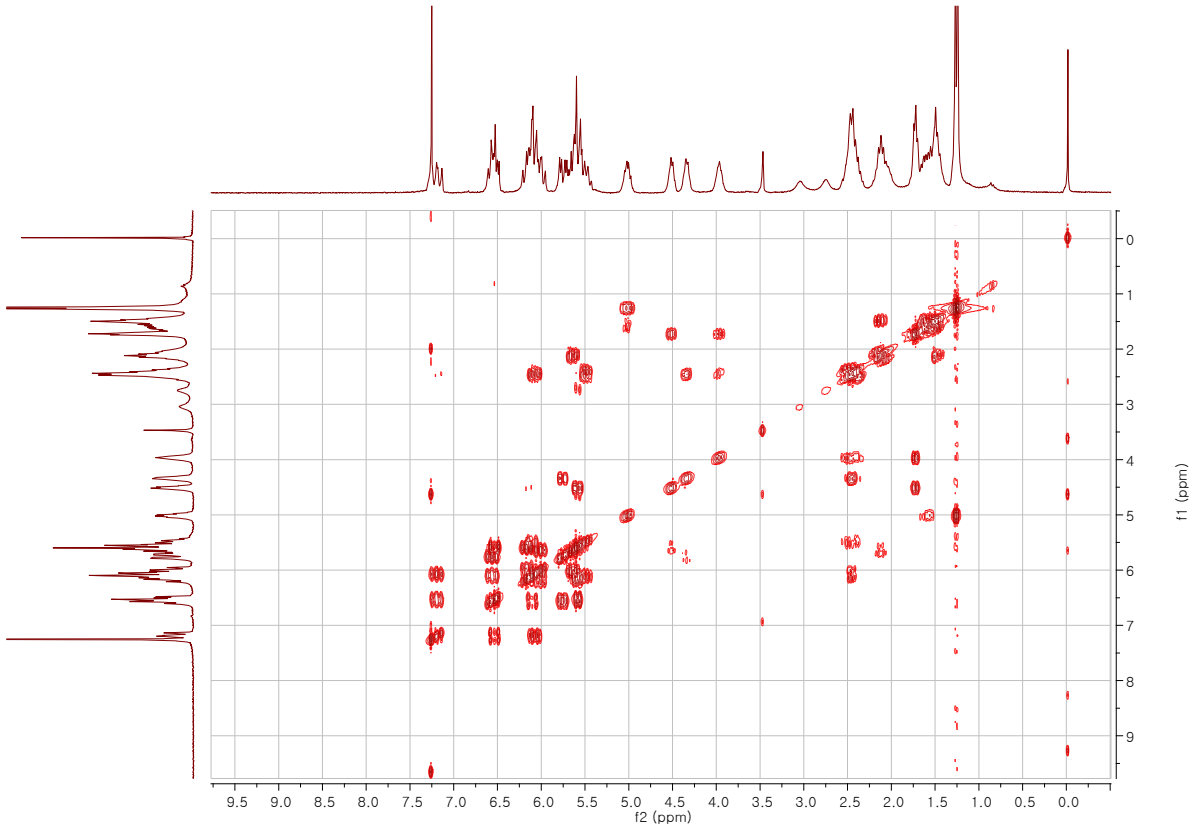


Figure S3. ^{1}H-^{1}H COSY (250 MHz, $CDCl_3$) spectrum of macrolactin A (**1**)

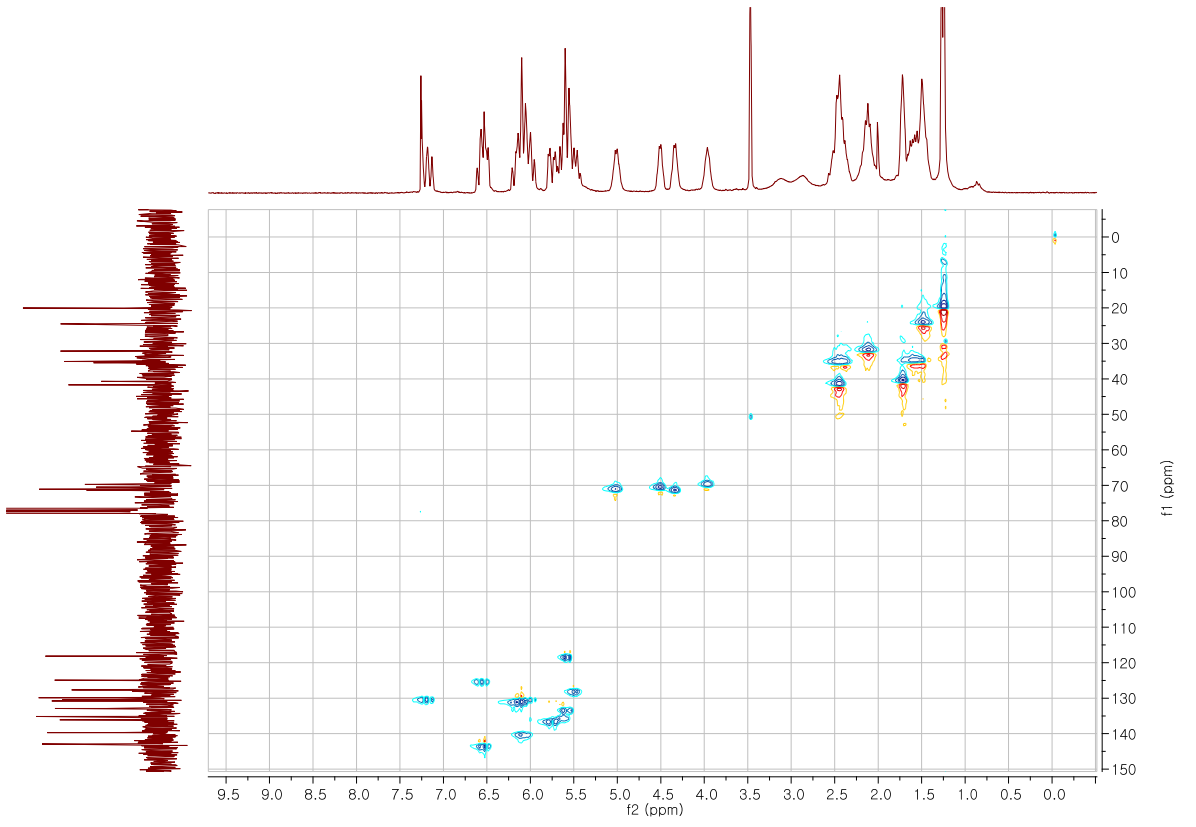


Figure S4. HMQC (250 MHz, $CDCl_3$) spectrum of macrolactin A (**1**)

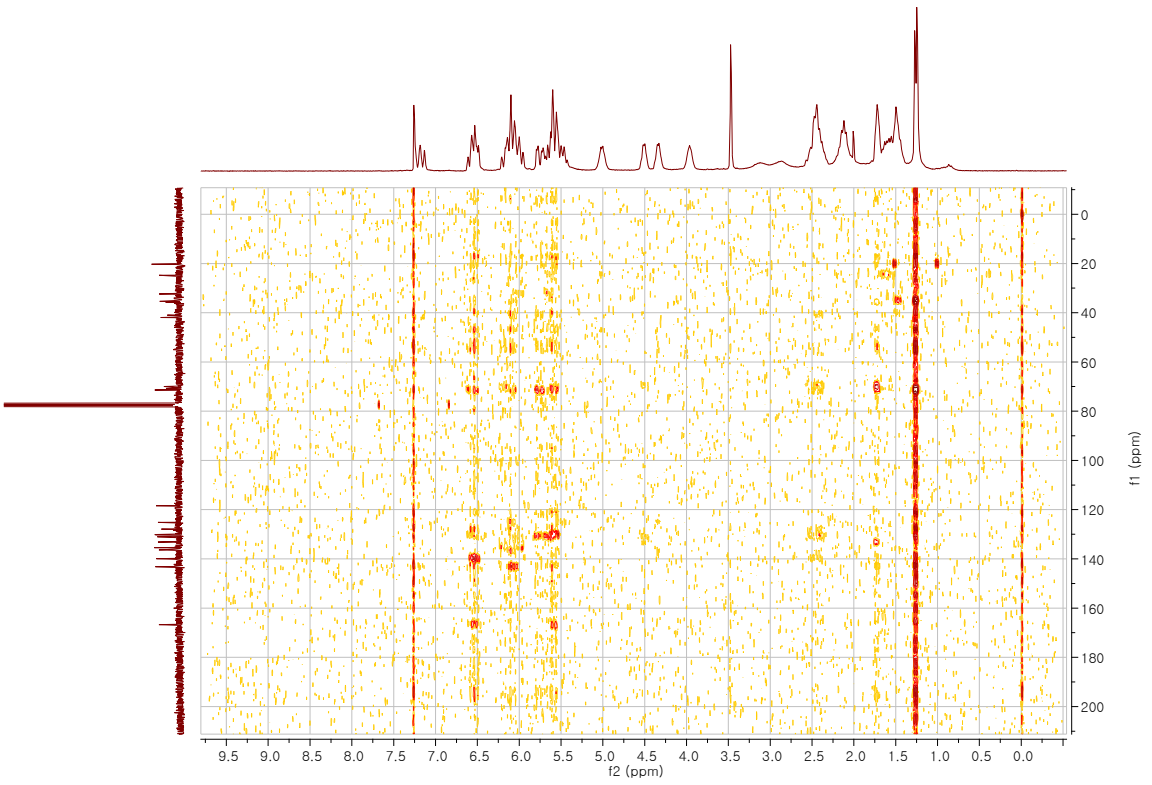


Figure S5. HMBC (250 MHz, $CDCl_3$) spectrum of macrolactin A (**1**)

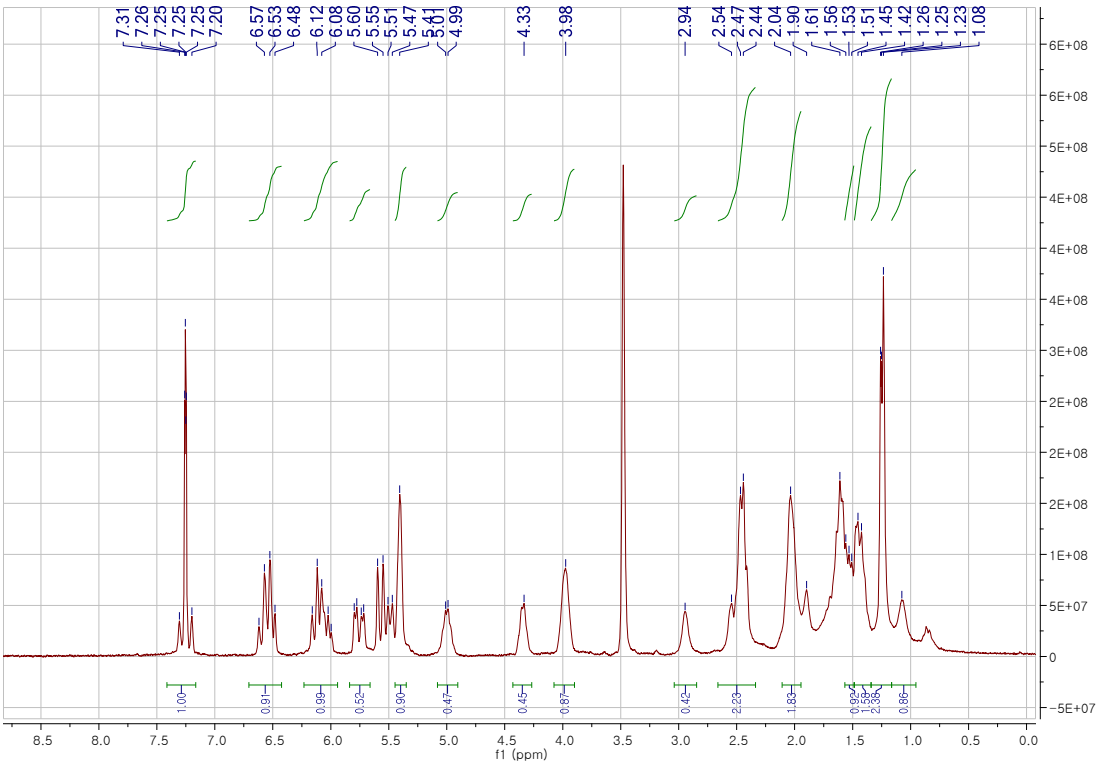


Figure S16. ^1H NMR (500 MHz, $CDCl_3$) spectrum of 15-*epi*-dihydromacrolactin F (**2**)

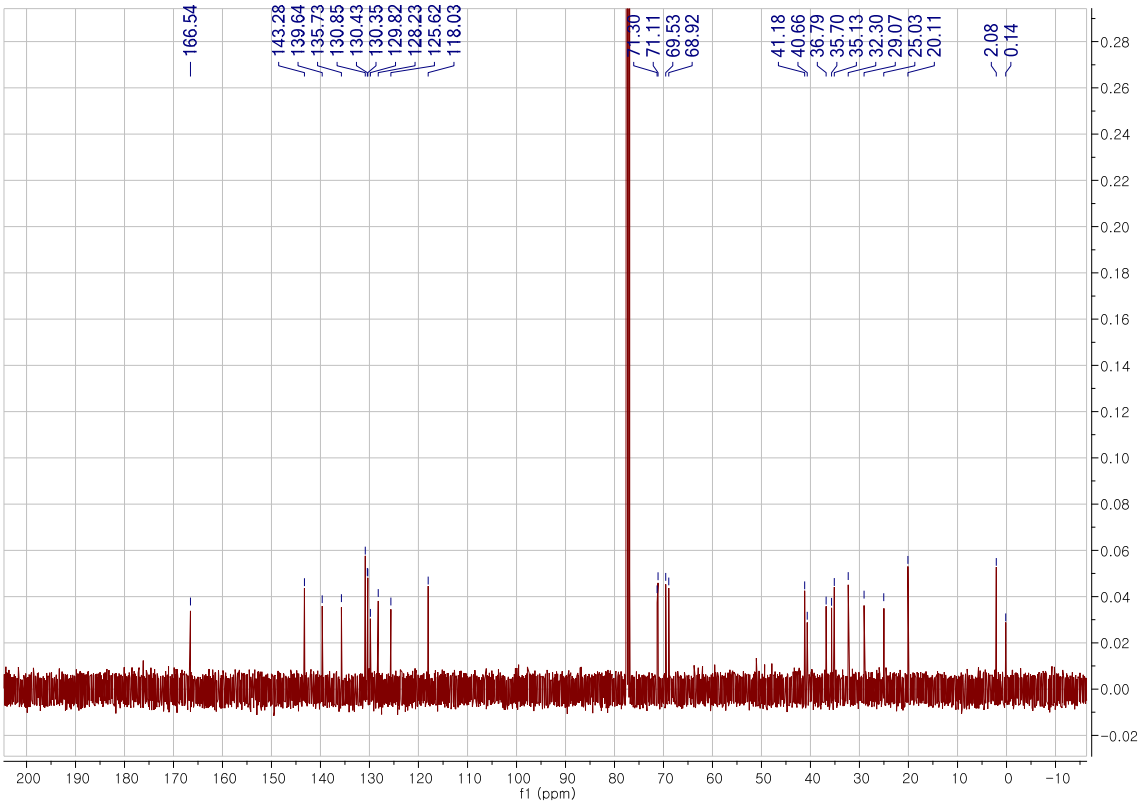


Figure S7. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of 15-*epi*-dihydromacrolactin F (**2**)

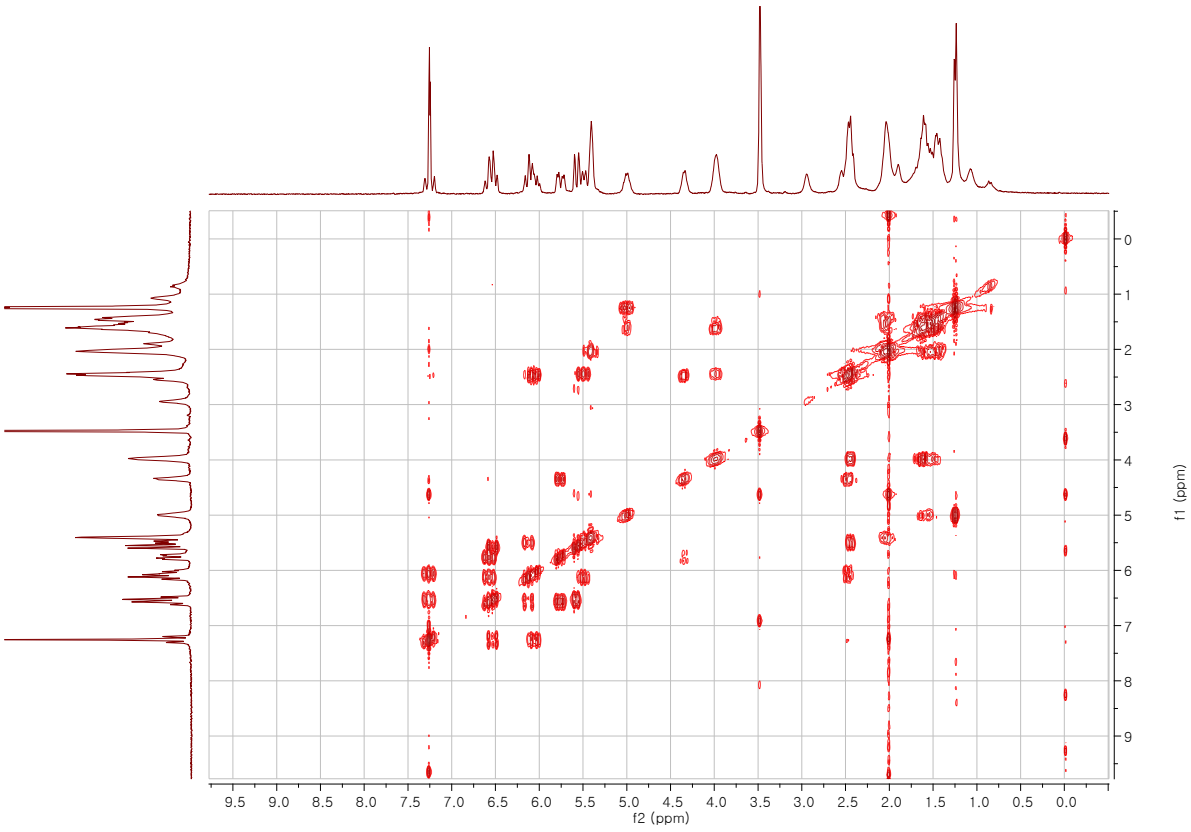


Figure S8. ^{1}H-^{1}H COSY (500 MHz, $CDCl_3$) spectrum of 15-*epi*-dihydromacrolactin F (**2**)

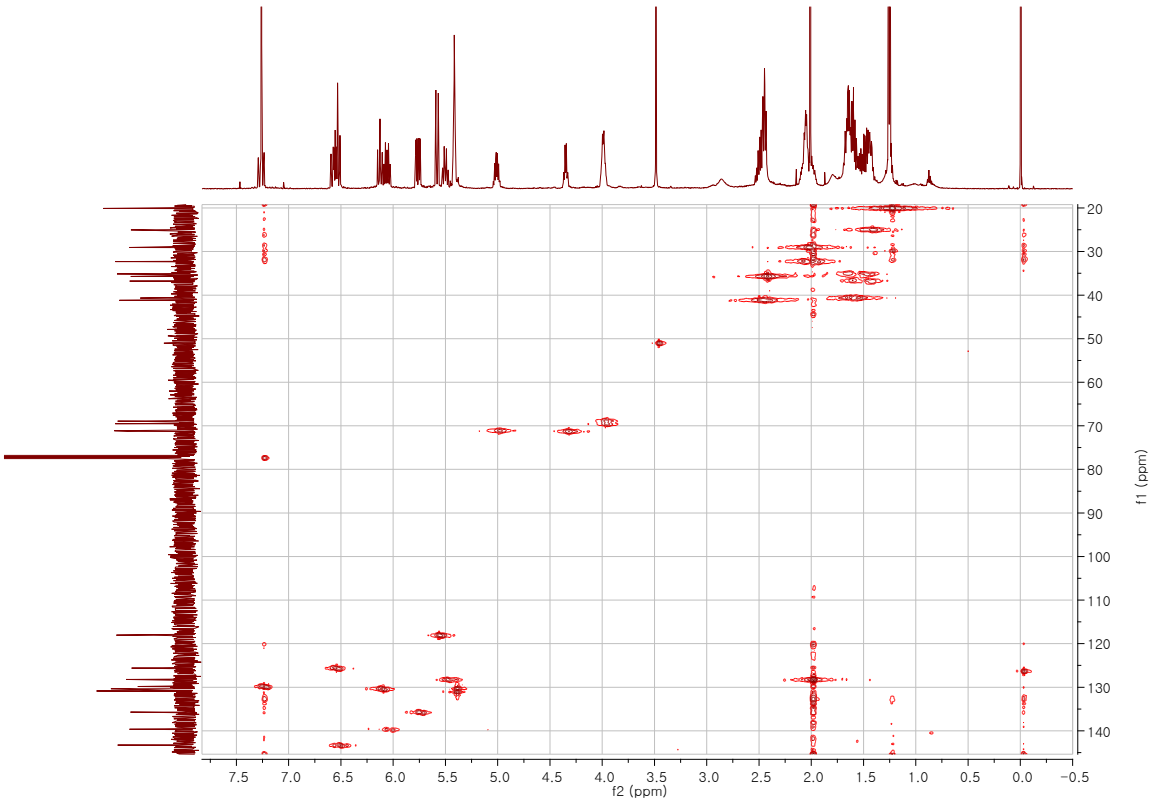


Figure S9. HMQC (500 MHz, $CDCl_3$) spectrum of 15-*epi*-dihydromacrolactin F (**2**)

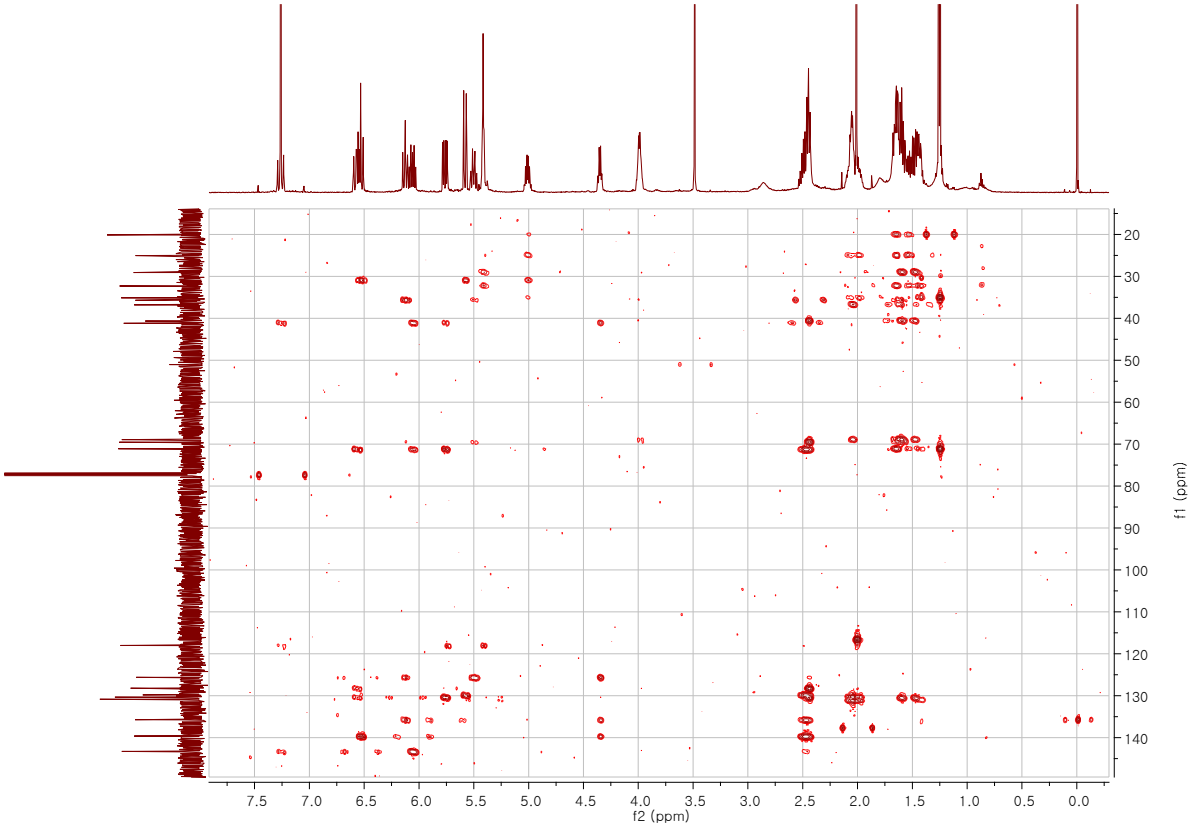
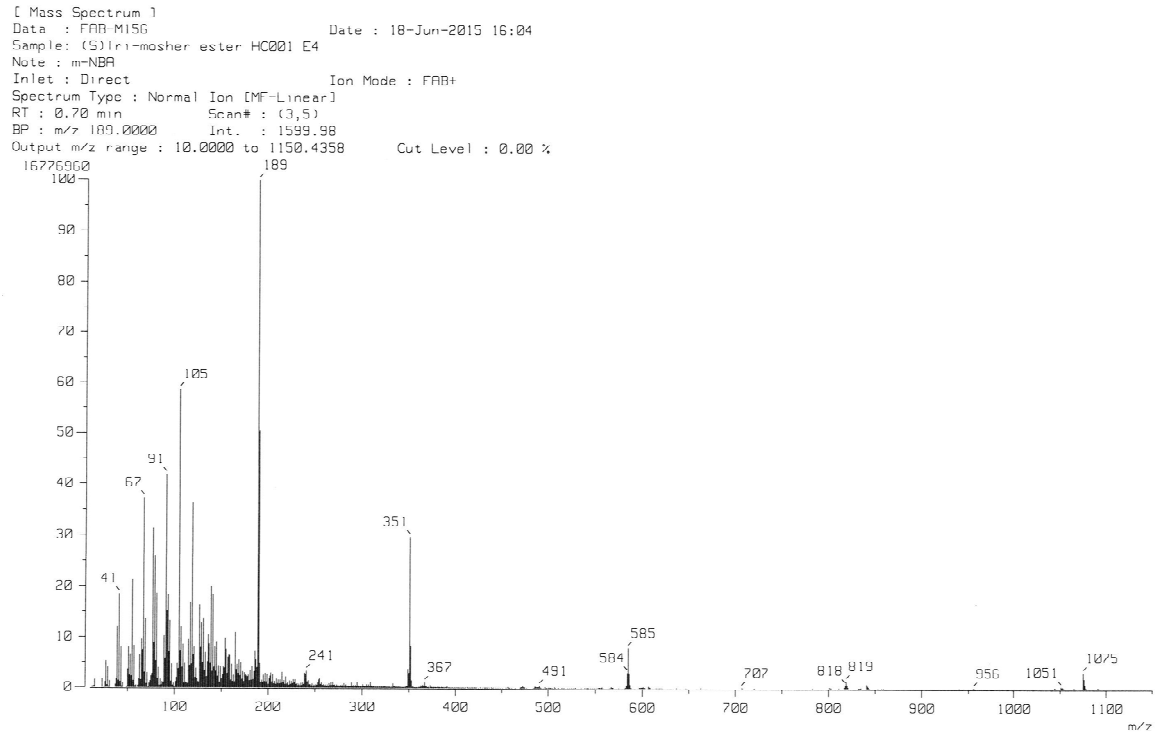


Figure S10. HMBC (500 MHz, $CDCl_3$) spectrum of 15-*epi*-dihydromacrolactin F (**2**)



41

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[ Elemental Composition ]                                        Page: 1
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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42

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[ Theoretical Ion Distribution ]                                 Page: 1
Molecular Formula : C24 H37 O5
                    (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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43

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

45

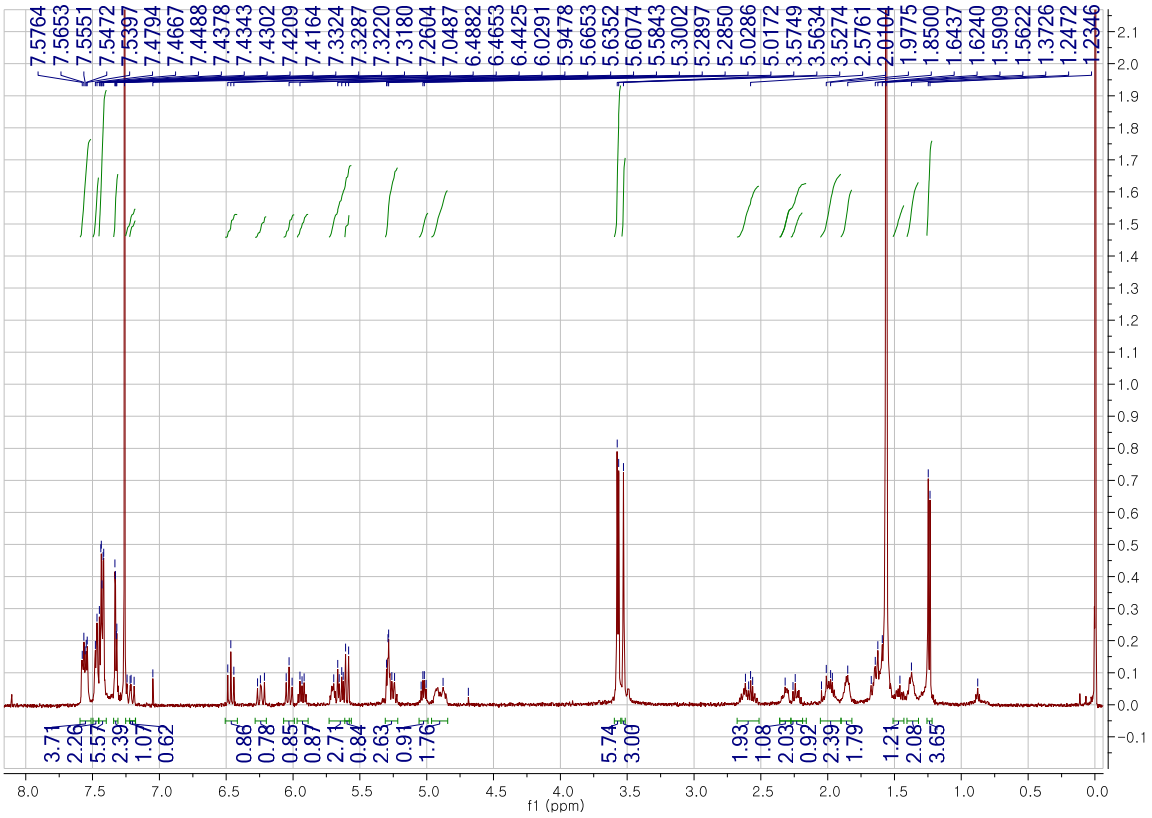

Figure S12. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of *tris*-(*S*)-MTPA *e*ster of **2** (**2a**)

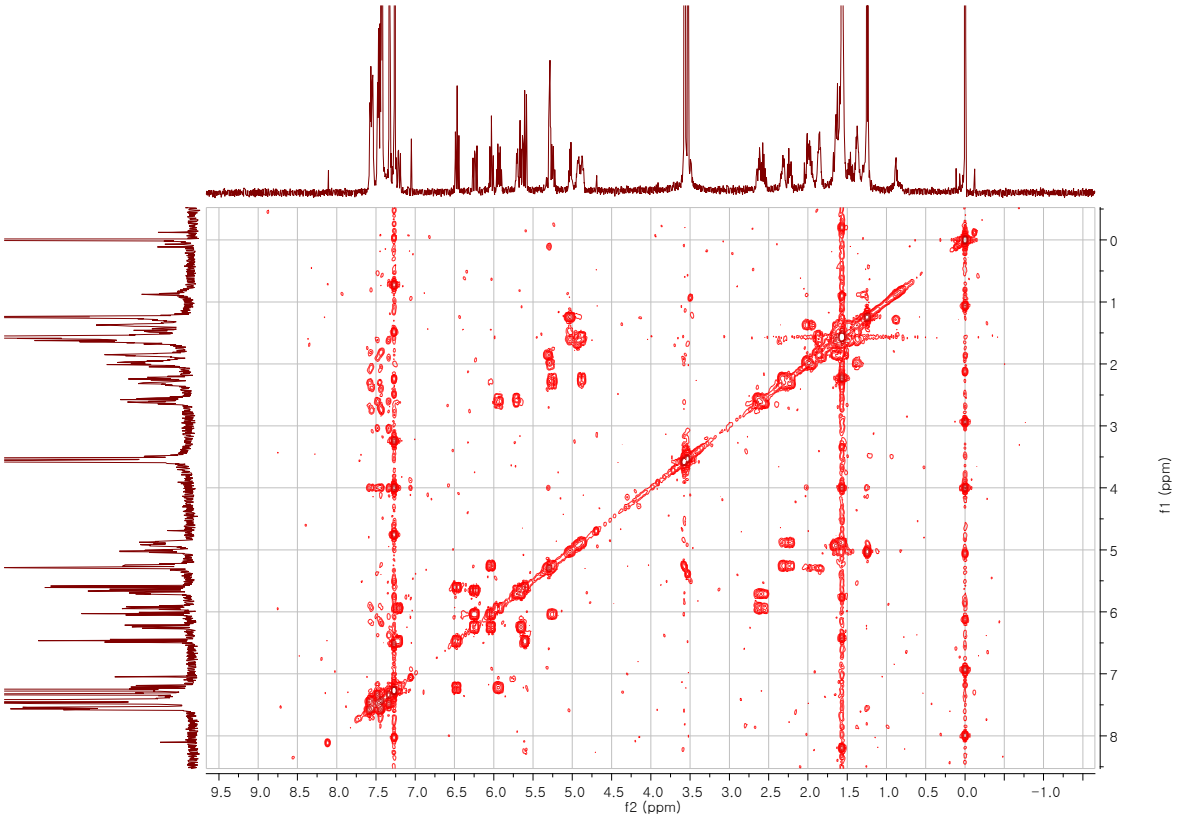

Figure S13. ^{1}H-^{1}H COSY (500 MHz, $CDCl_3$) spectrum of *tris*-(*S*)-MTPA *e*ster of **2** (**2a**)

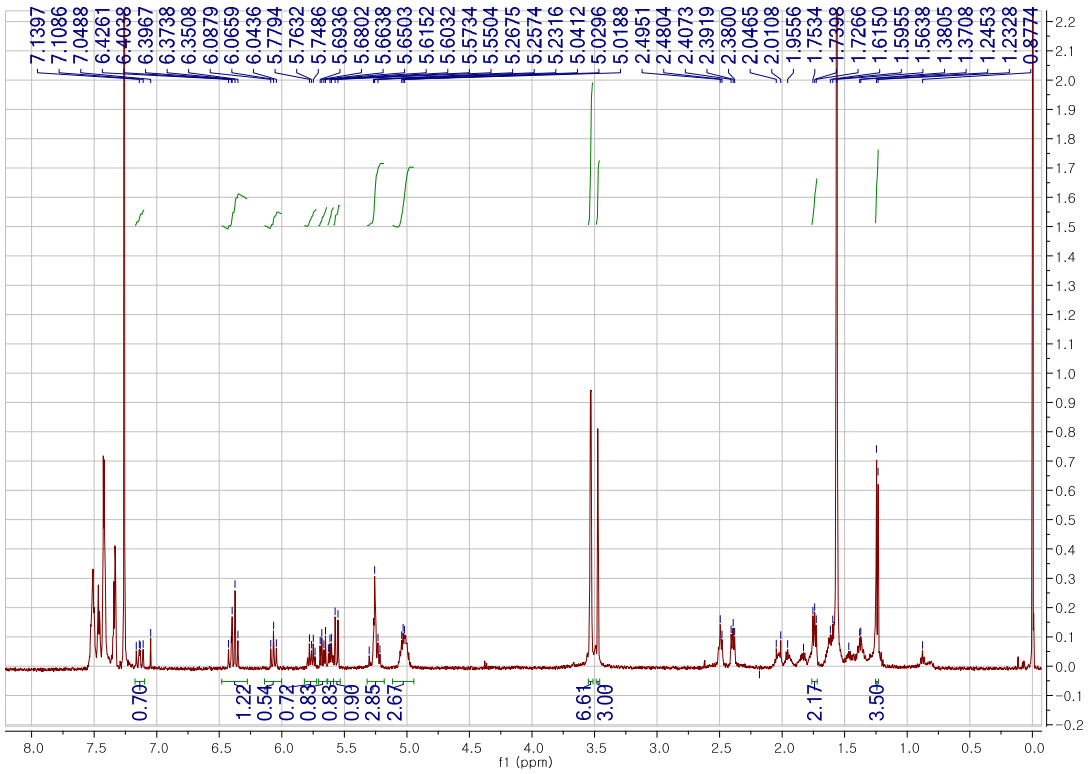

Figure S14. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of *tris*-(*R*)-MTPA *e*ster of **2** (**2b**)

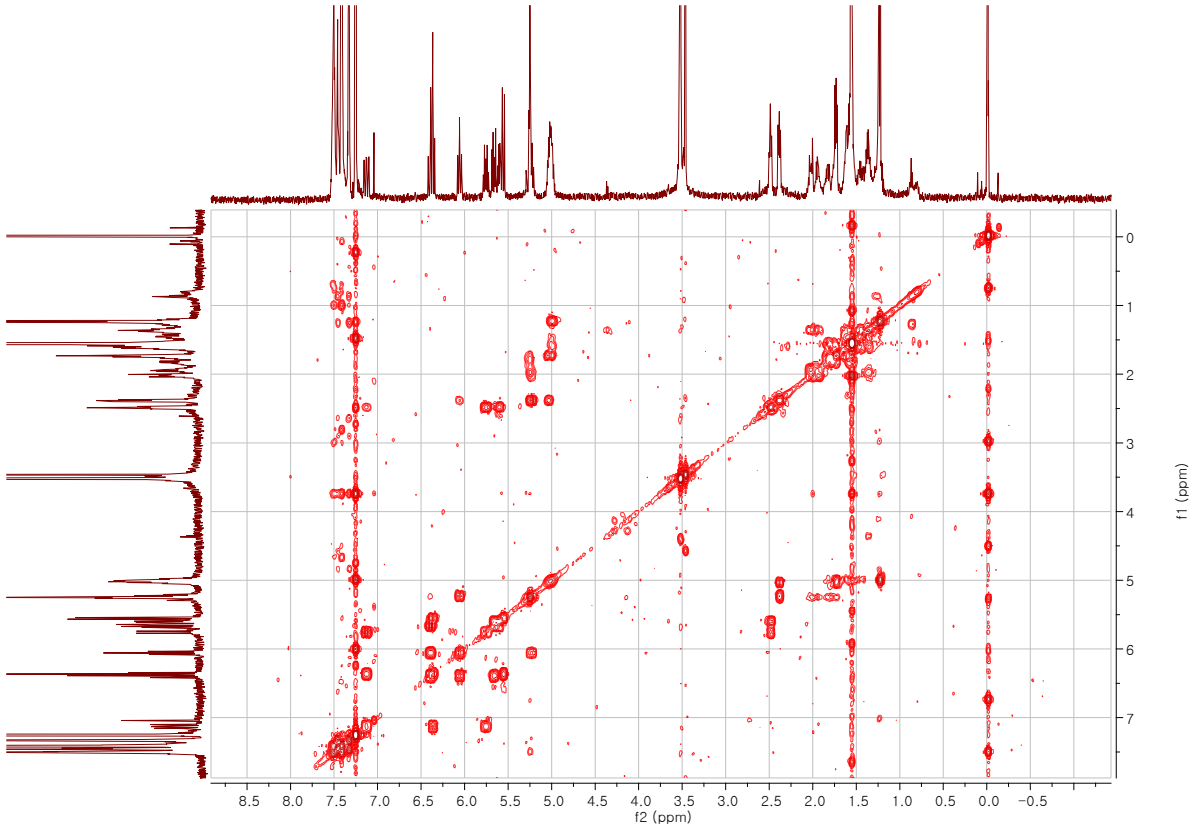

Figure S15. ^{1}H-^{1}H COSY (500 MHz, $CDCl_3$) spectrum of *tris*-(*R*)-MTPA *e*ster of **2** (**2b**)

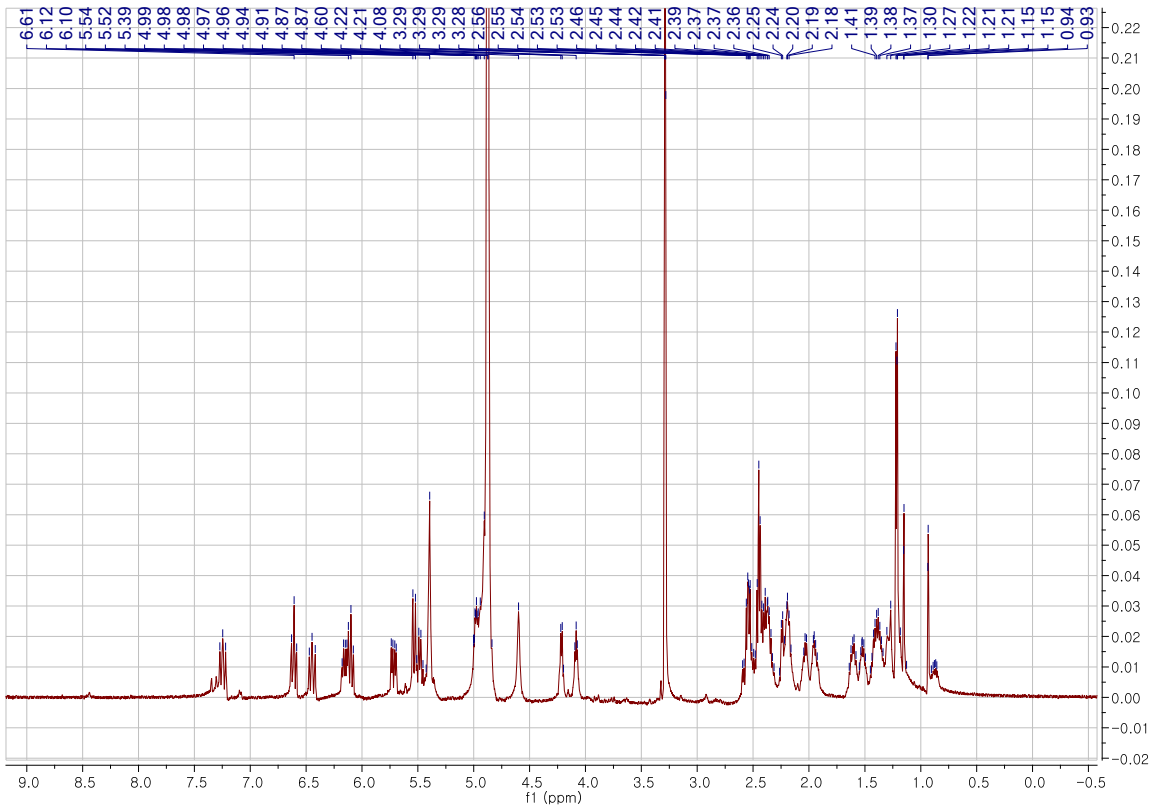

Figure S16. ^{1}H NMR (500 MHz, CD_3OD) spectrum of macrolactin F (**3**)

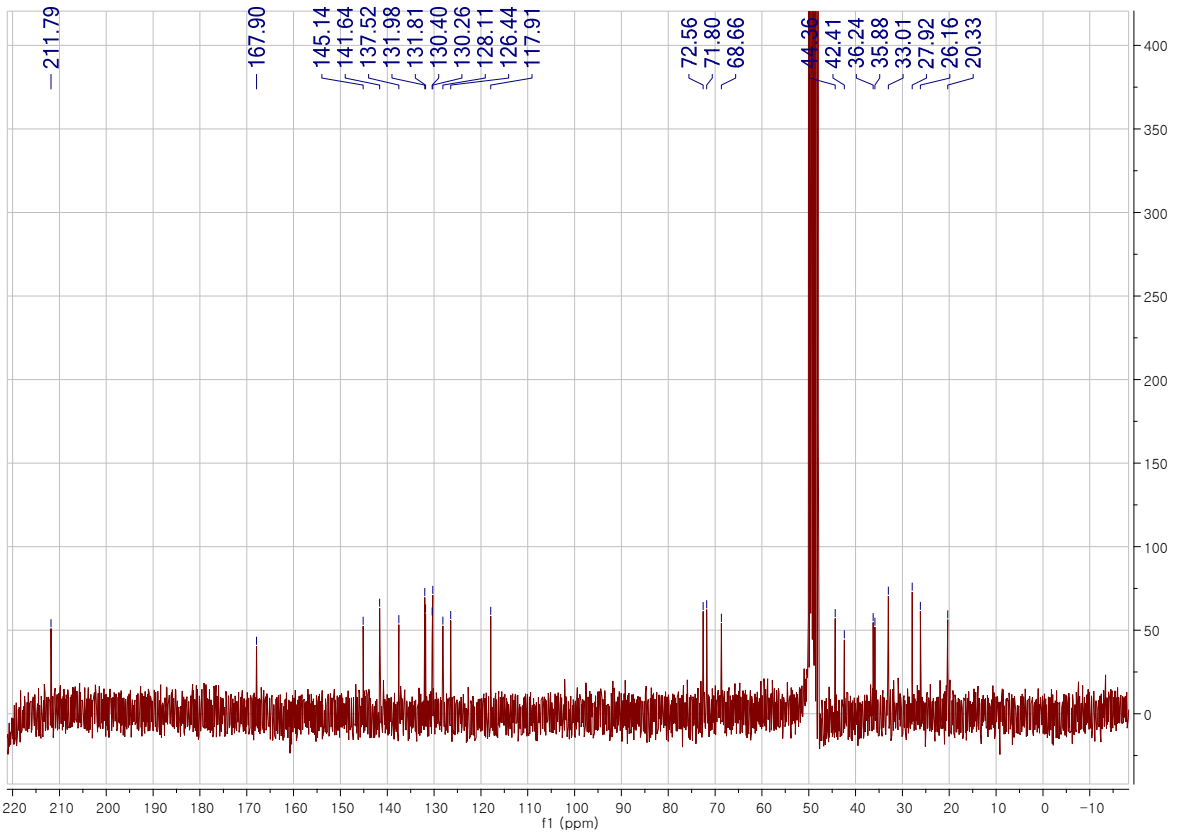

Figure S17. ^{13}C NMR (125 MHz, CD_3OD) spectrum of macrolactin F (**3**)

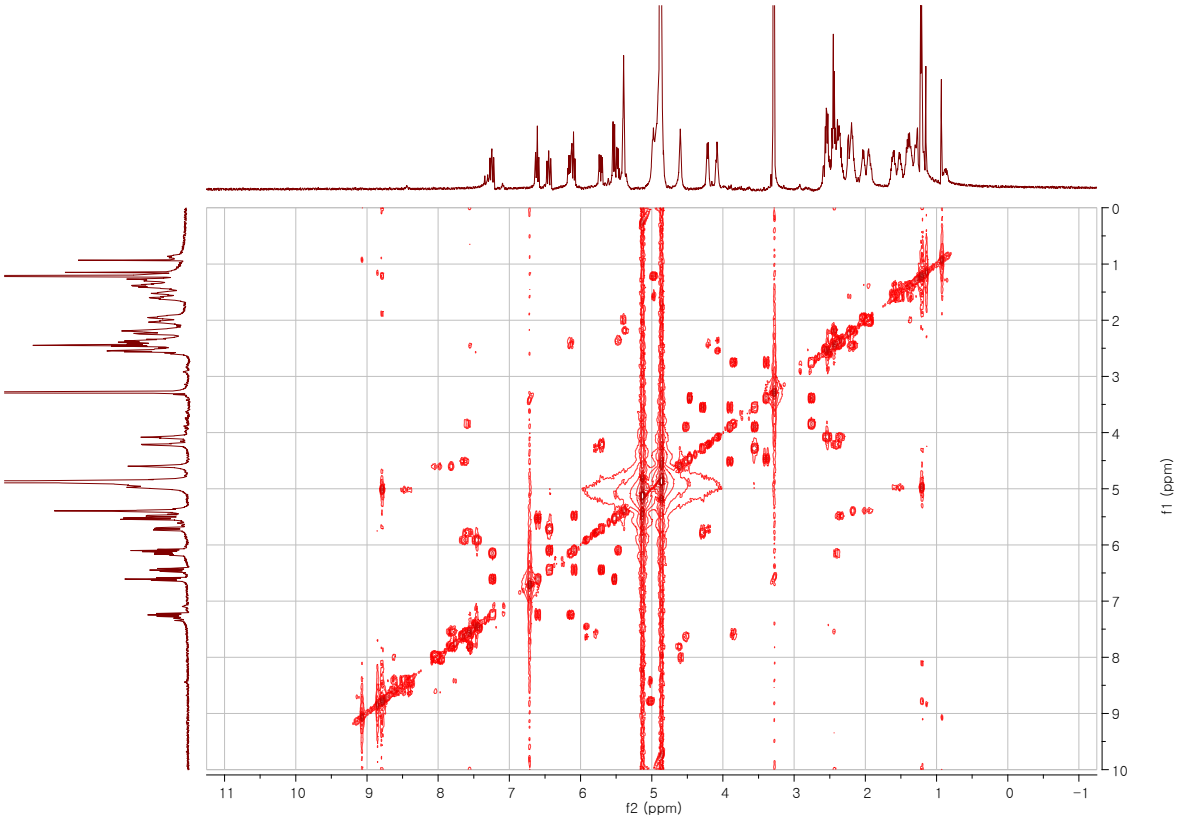

Figure S18. ^{1}H-^{1}H COSY (500 MHz, CD_3OD) spectrum of macrolactin F (**3**)

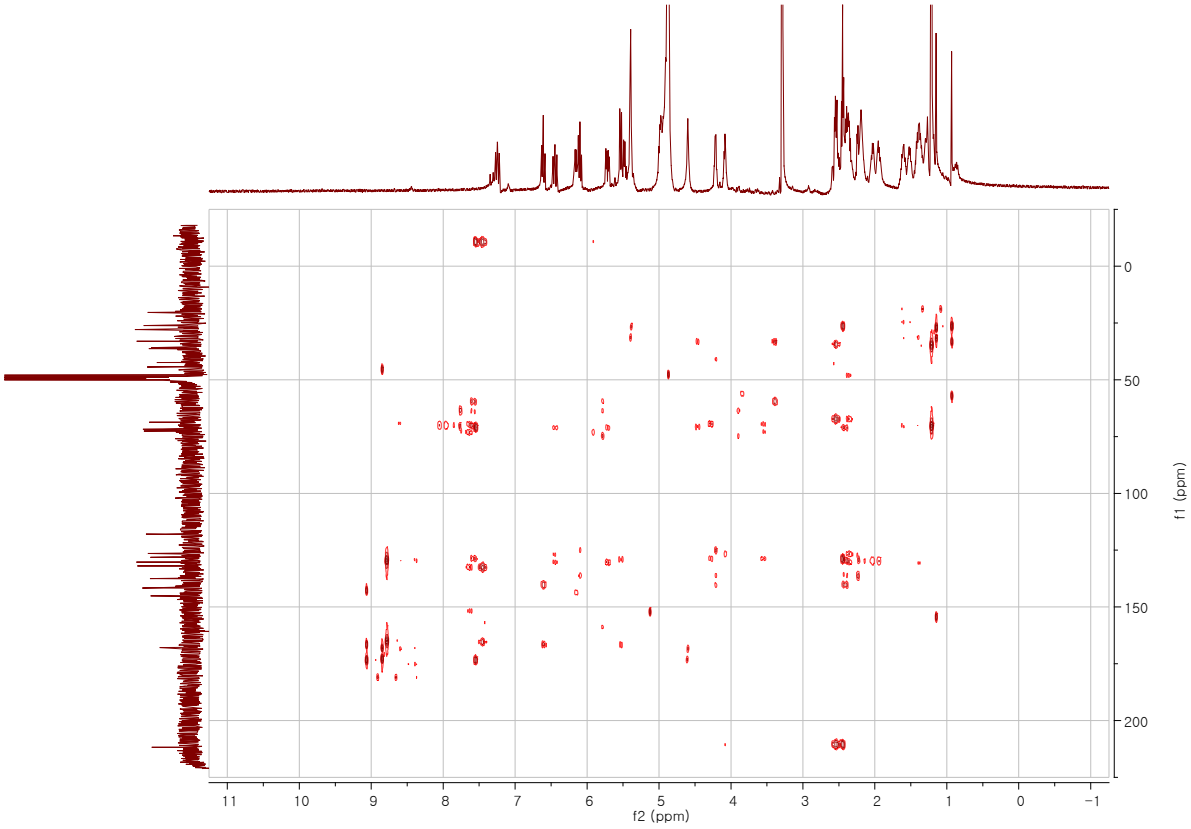

Figure S19. HMQC (500 MHz, CD_3OD) spectrum of macrolactin F (**3**)

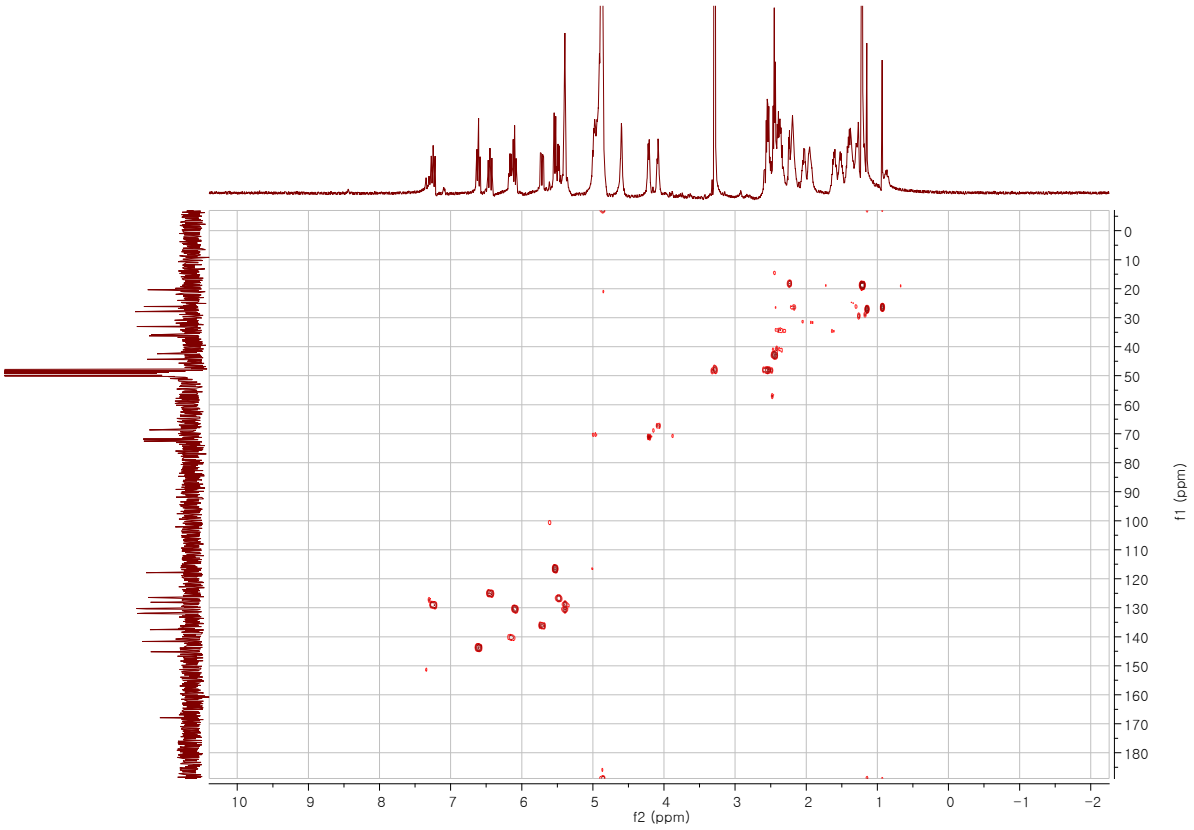

Figure S20. HMBC (500 MHz, CD_3OD) spectrum of macrolactin F (**3**)