

Supplementary Material

Six New Diterpene Glycosides from the Soft Coral *Lemnalia bournei*

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1. Experimental ECD spectrum of 1 and the calculated one

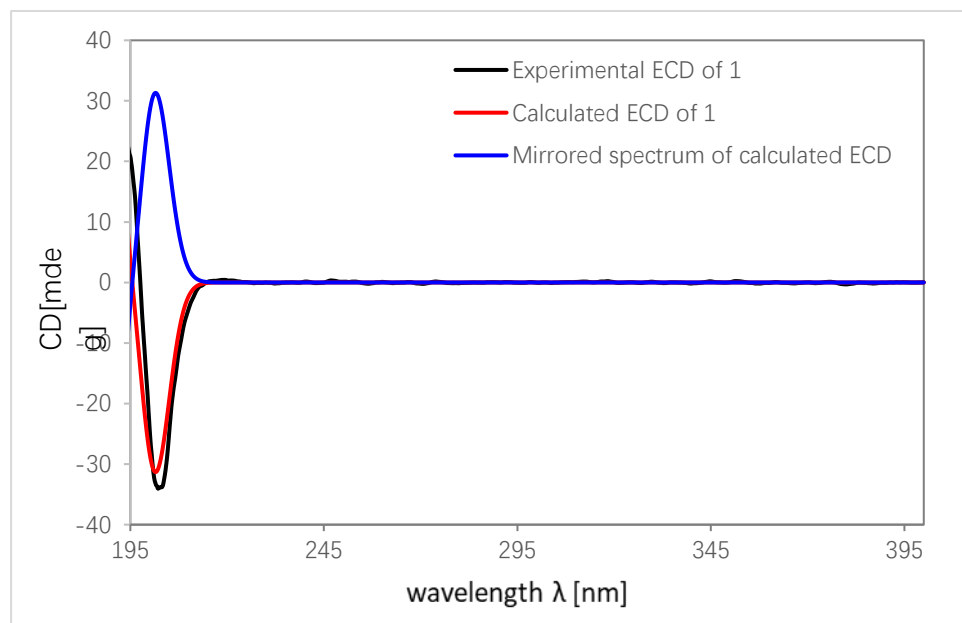
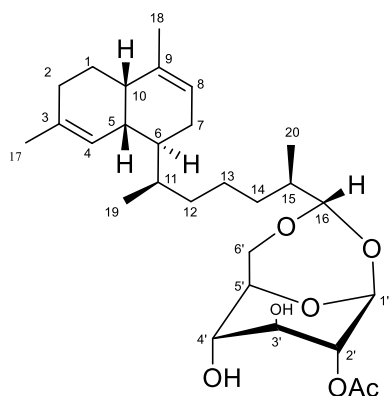


Figure S1 Experimental ECD spectrum of 1 and the calculated ECD spectra of (5R,6S,10S,11S)-1 (red) and (5S,6R,10R,11R)-1 (blue)

2. 1D, 2D NMR and HRMS spectra of the new isolated compounds

2.1 Spectroscopic data for Lemnabourside E (1)



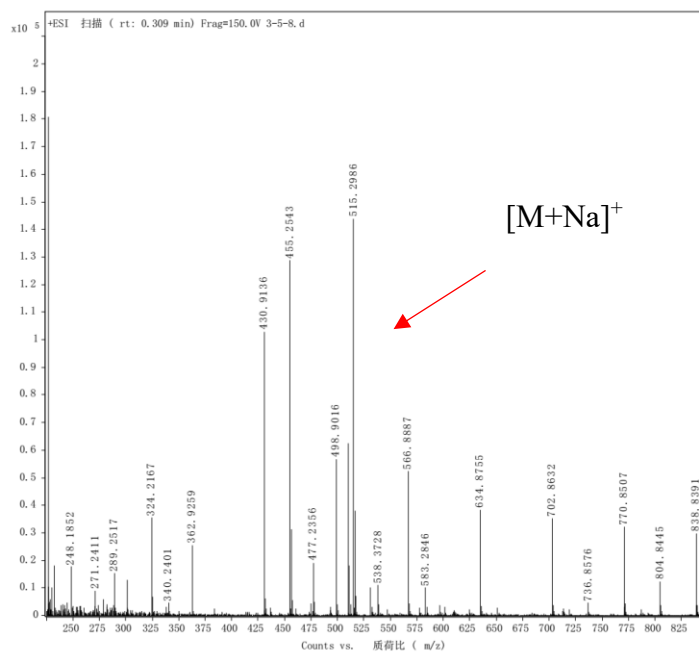


Figure S2 HRESIMS Spectrum of Lemnabourside E (1)

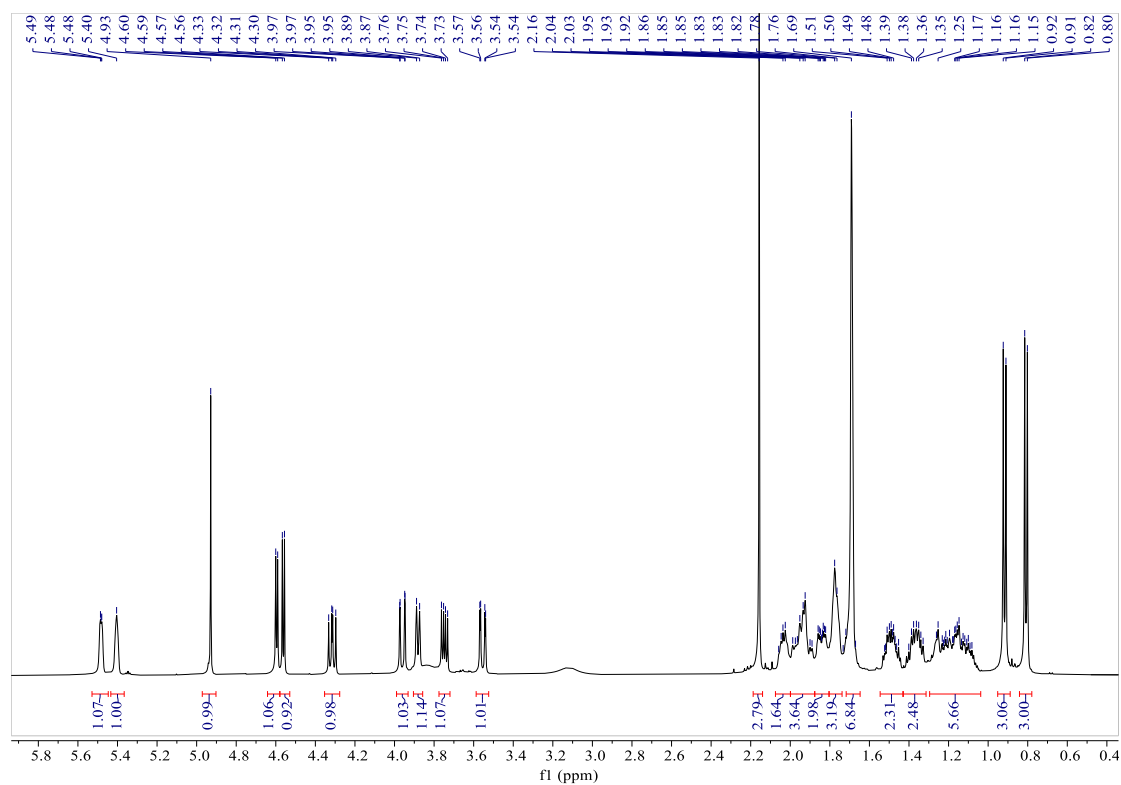


Figure S3 ^1H NMR Spectrum of Lemnabourside E (1) (600 MHz; CDCl_3)

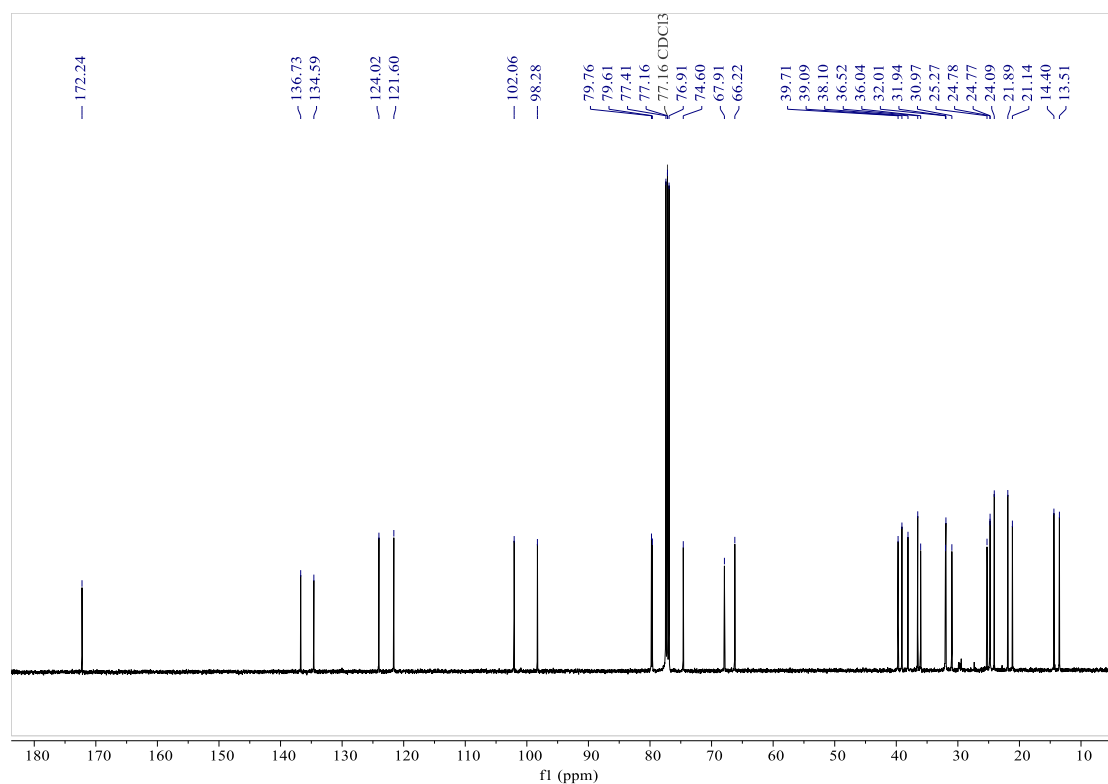


Figure S4 ^{13}C NMR Spectrum of Lemnabourside E (1) (150 MHz; CDCl_3)

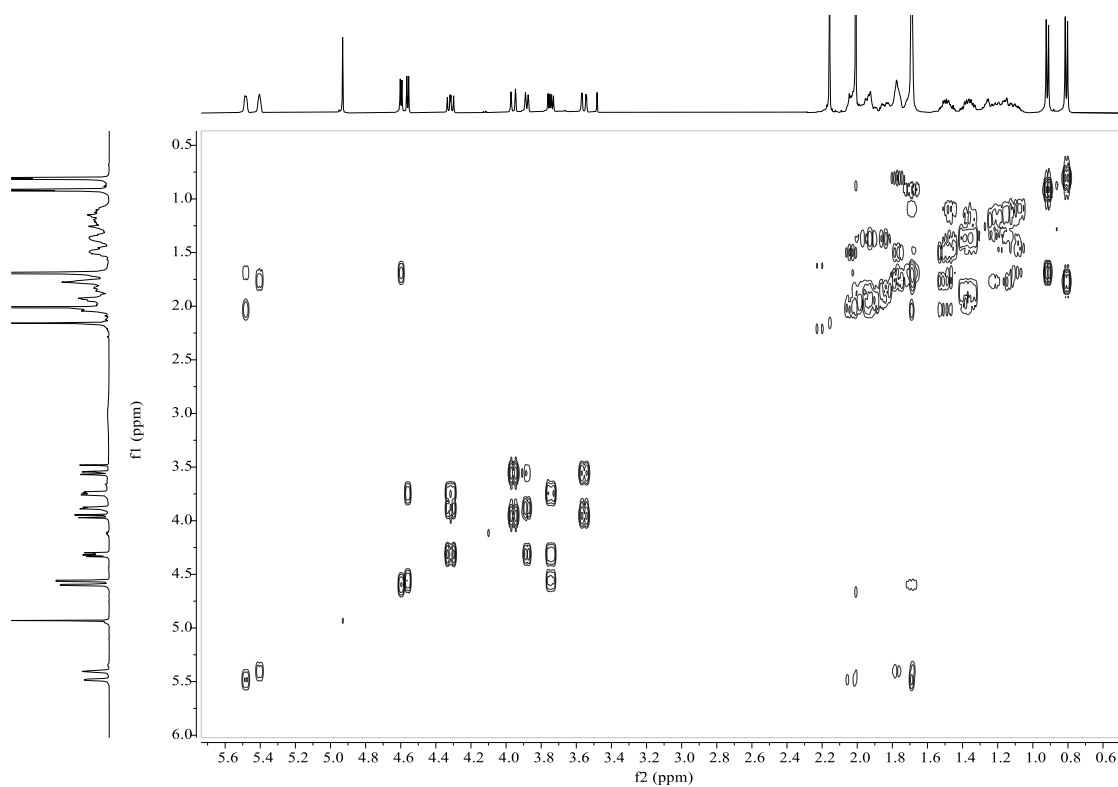


Figure S5 ^1H - ^1H COSY spectrum of Lemnabourside E (1) (600 MHz; CDCl_3)

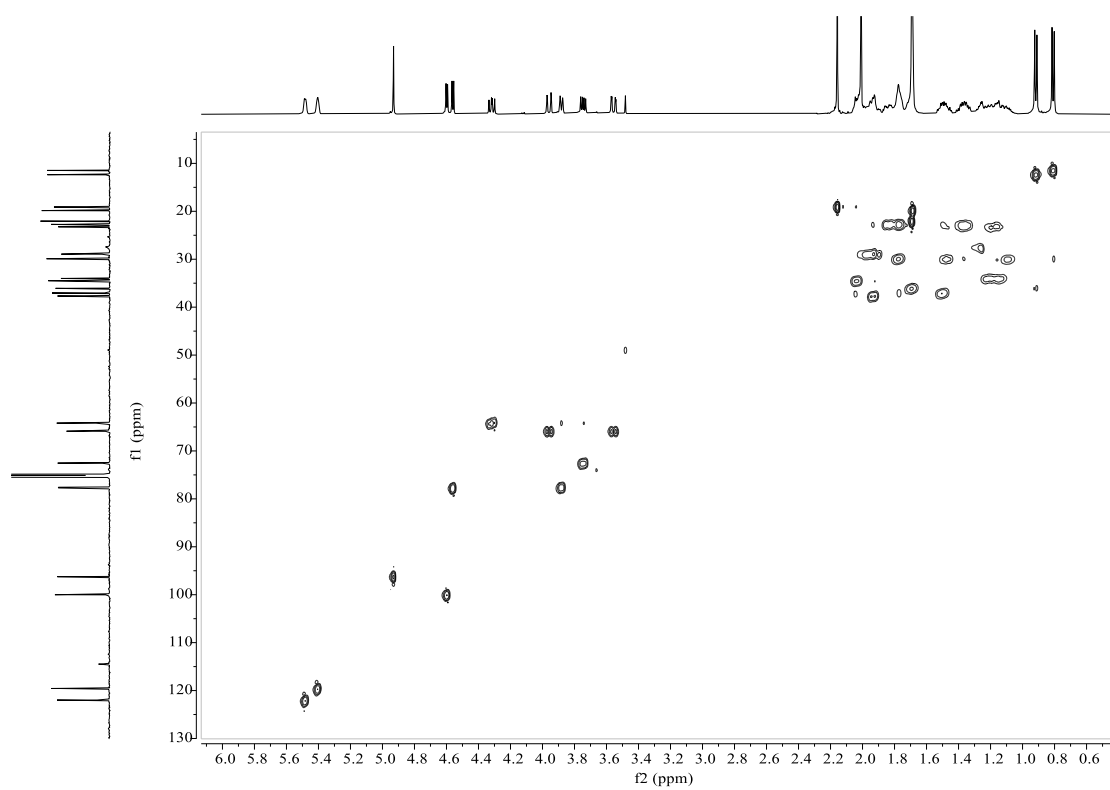


Figure S6 HSQC spectrum of Lemnabourside E (1) (600 MHz; CDCl₃)

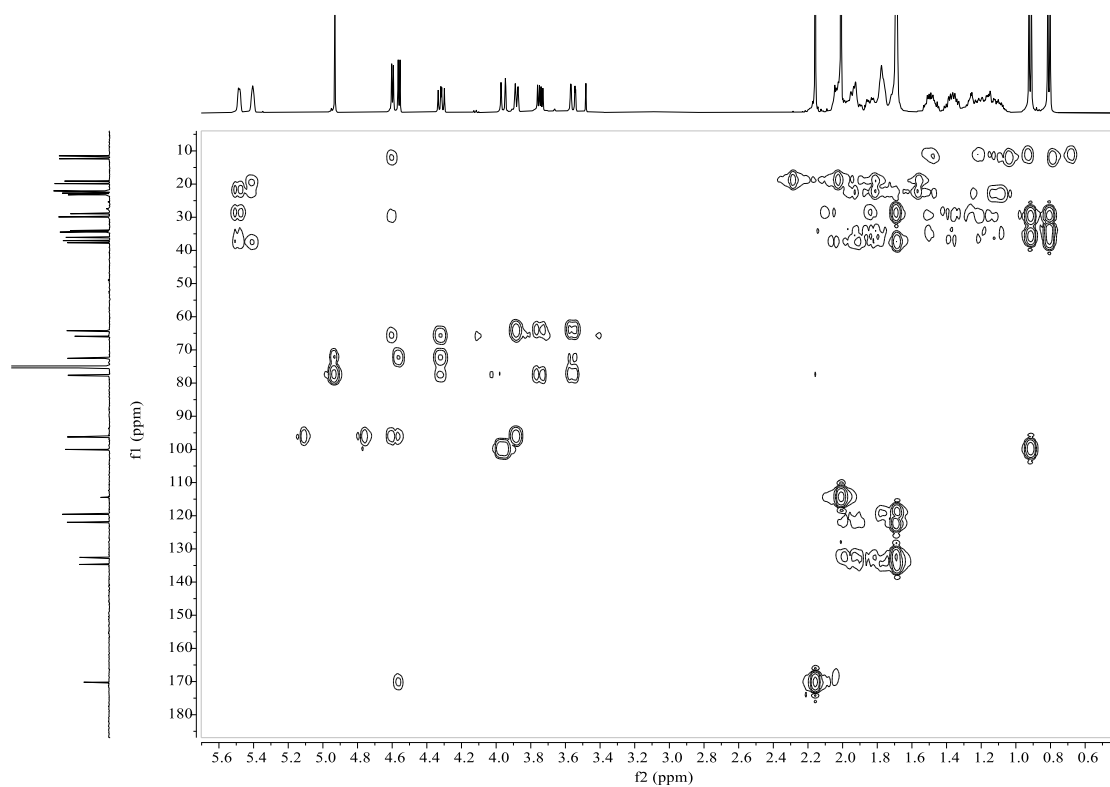
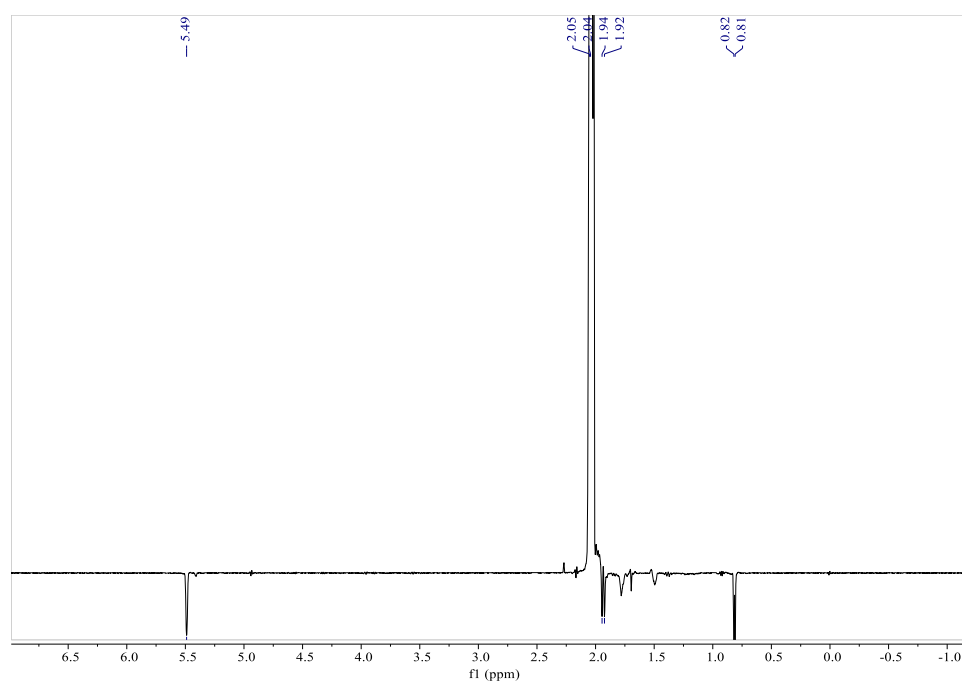
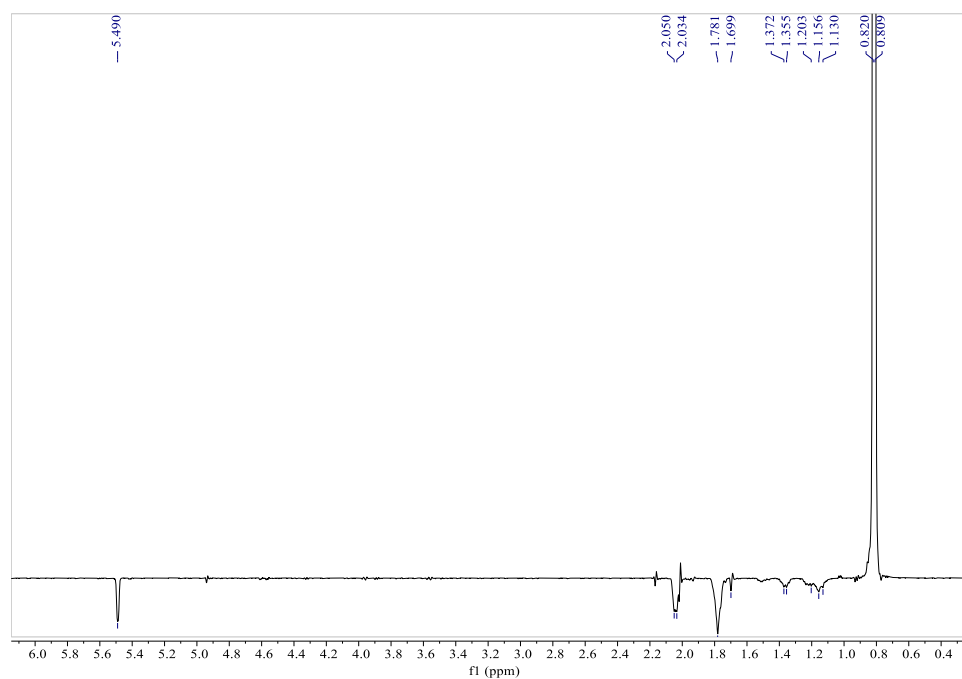
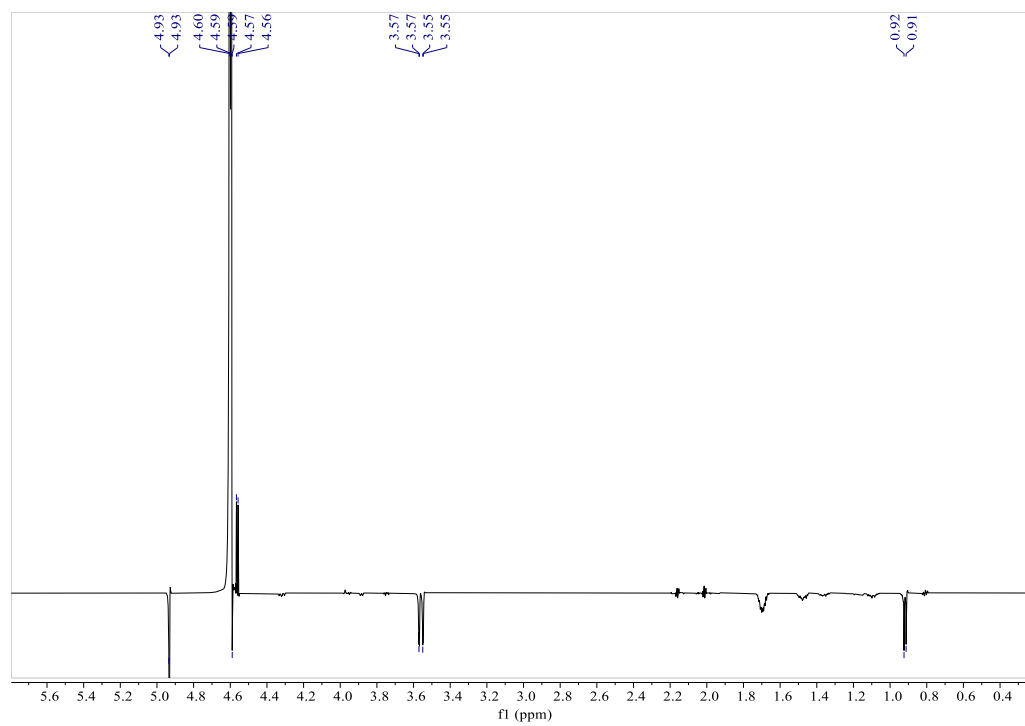
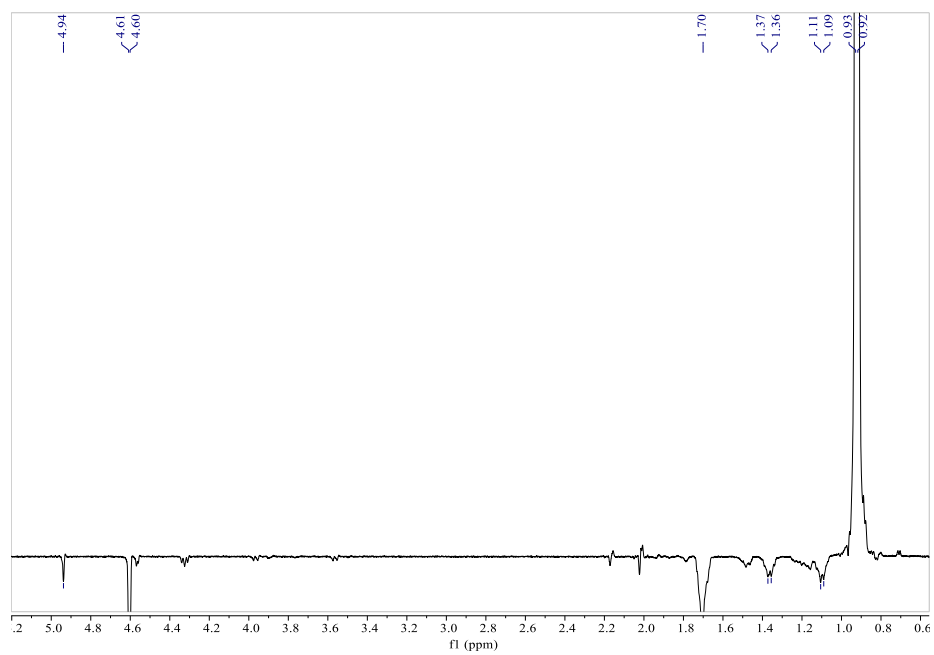


Figure S7 HMBC spectrum of Lemnabourside E (1) (600 MHz; CDCl₃)





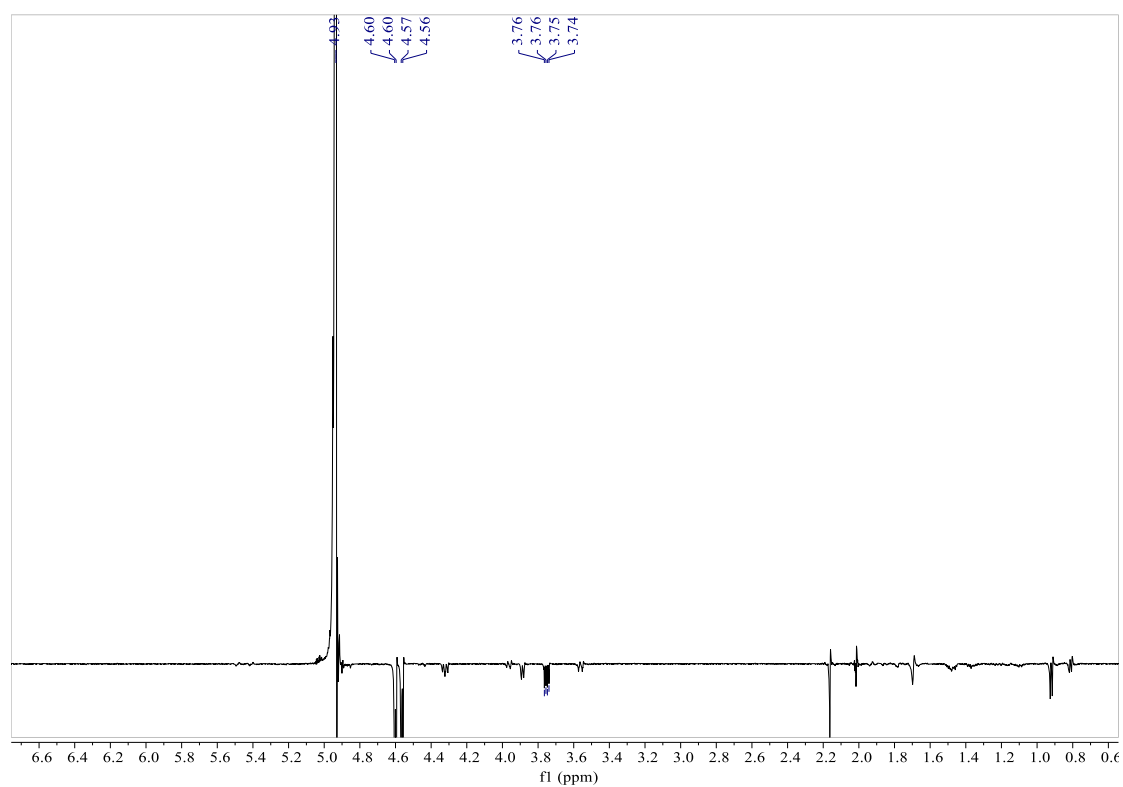
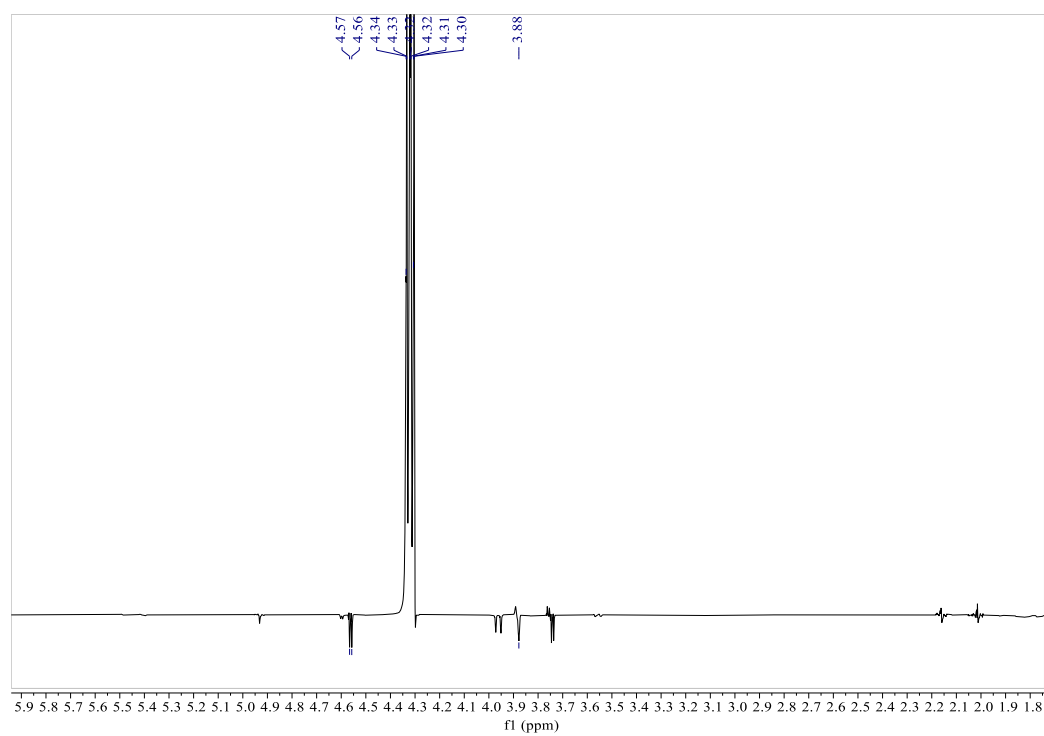


Figure S8 1D-NOE spectrum of Lemnabourside E (1) (600 MHz; CDCl₃)

3.2 Spectroscopic data for Lemnabourside F (2)

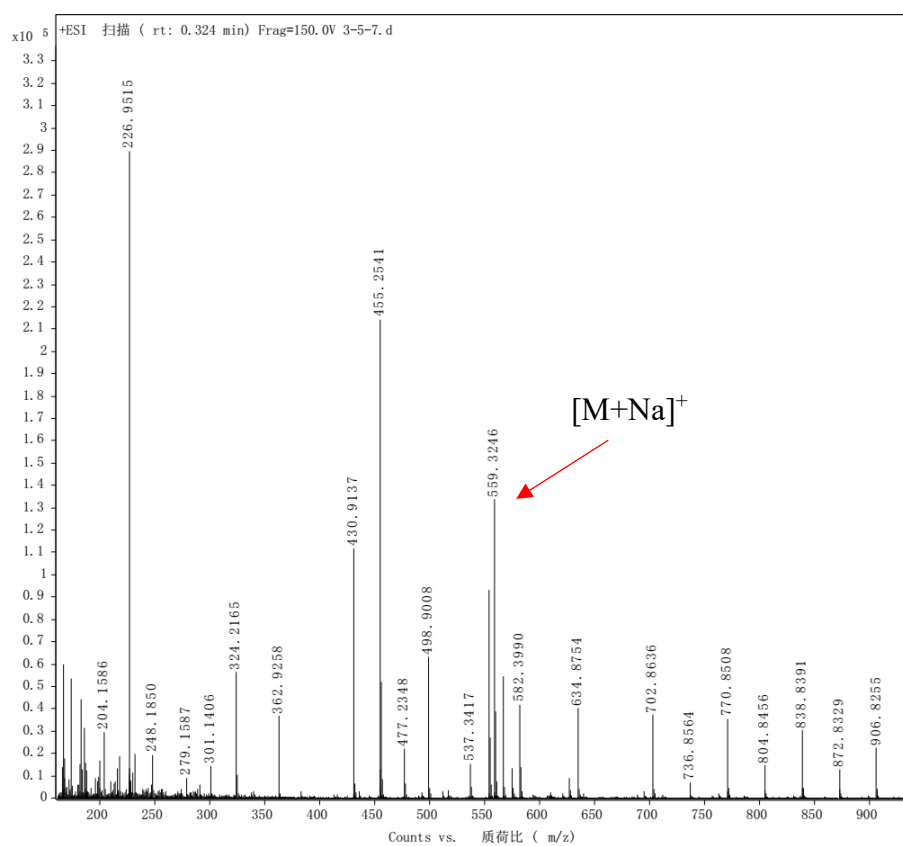
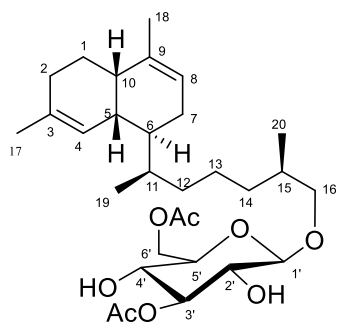


Figure S9 HRESIMS Spectrum of Lemnabourside F (2)

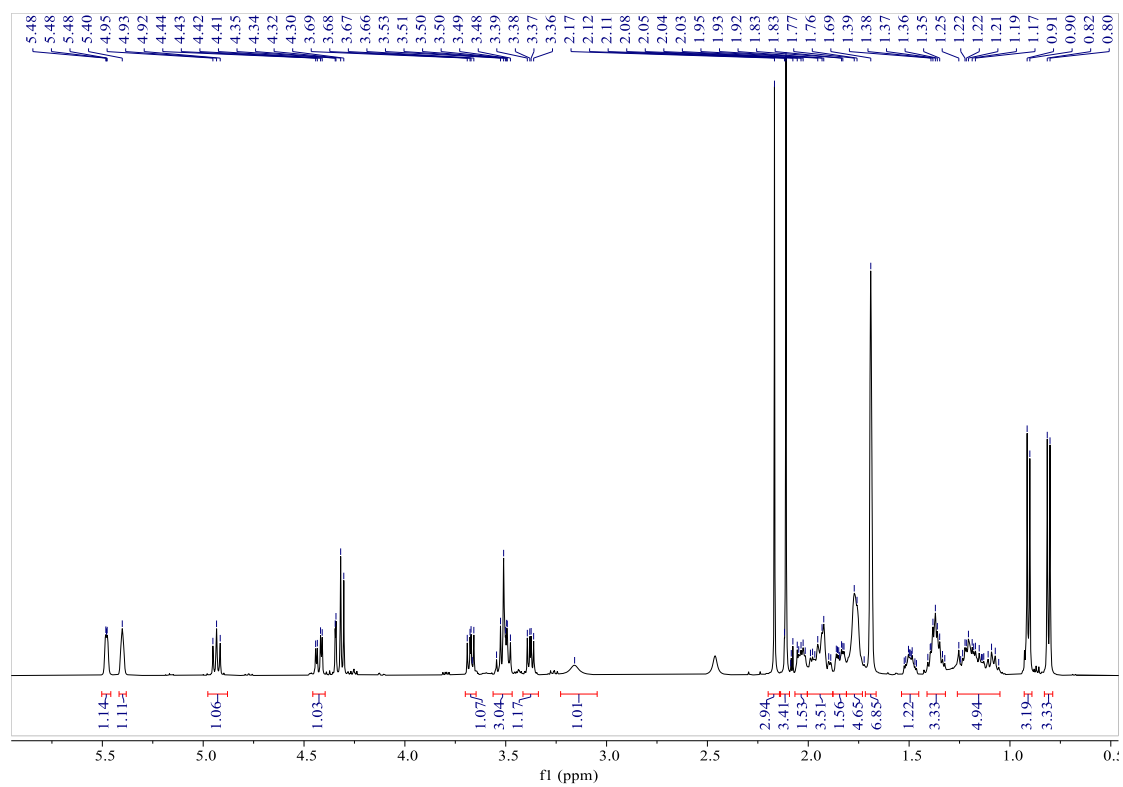


Figure S10 ¹H NMR Spectrum of Lemnabourside F (2) (600 MHz; CDCl₃)

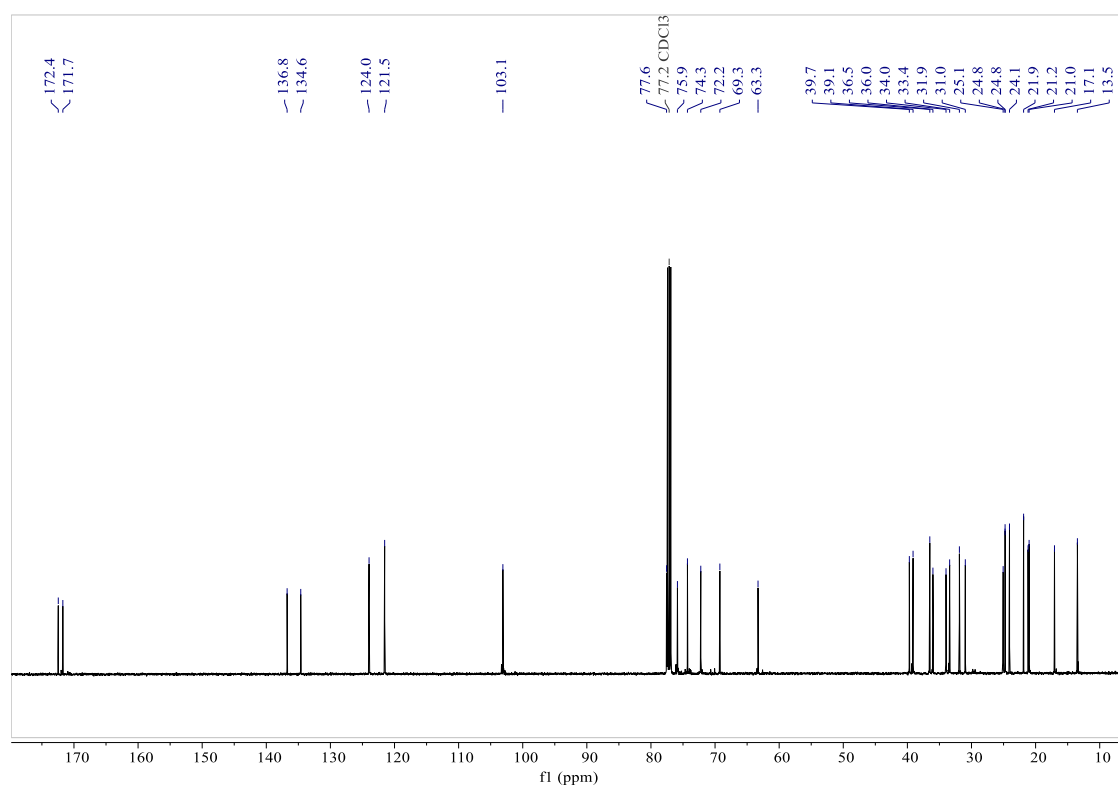


Figure S11 ¹³C NMR Spectrum of Lemnabourside F (2) (150 MHz; CDCl₃)

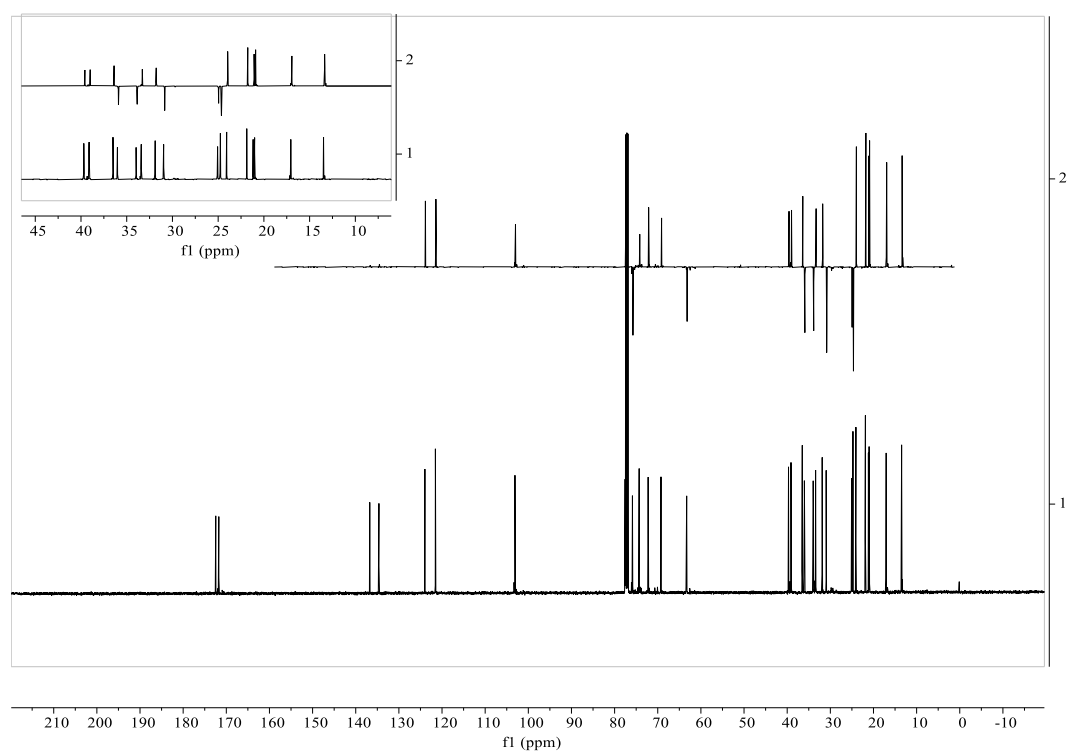


Figure S12 DEPT 135° NMR Spectrum of Lemnabourside F (2) (150 MHz; CDCl₃)

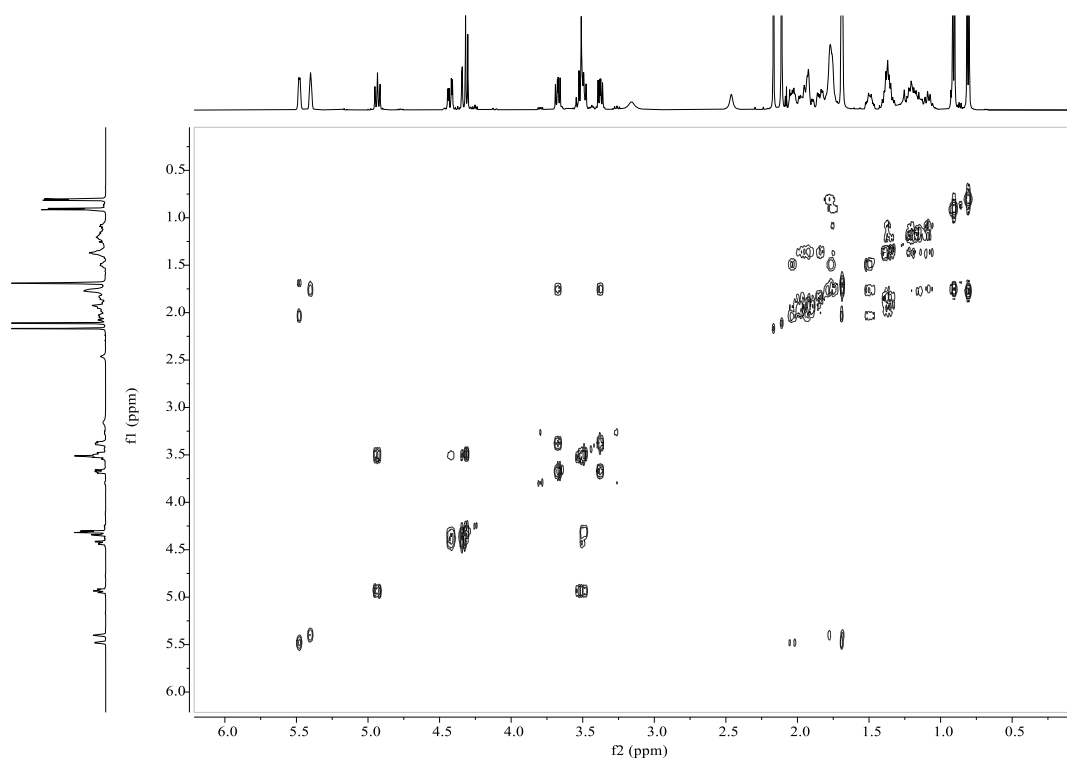


Figure S13 ¹H-¹H COSY spectrum of Lemnabourside F (2) (600 MHz; CDCl₃)

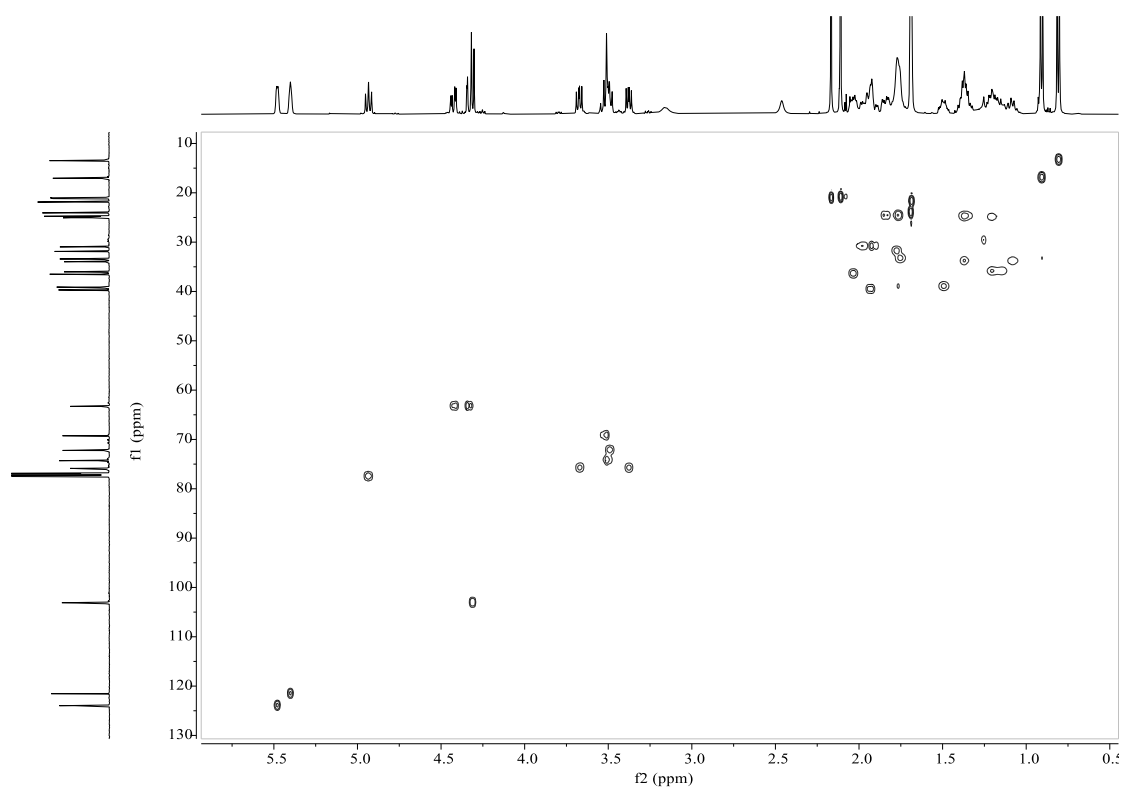


Figure S14 HSQC spectrum of Lemnabourside F (2) (600 MHz; CDCl₃)

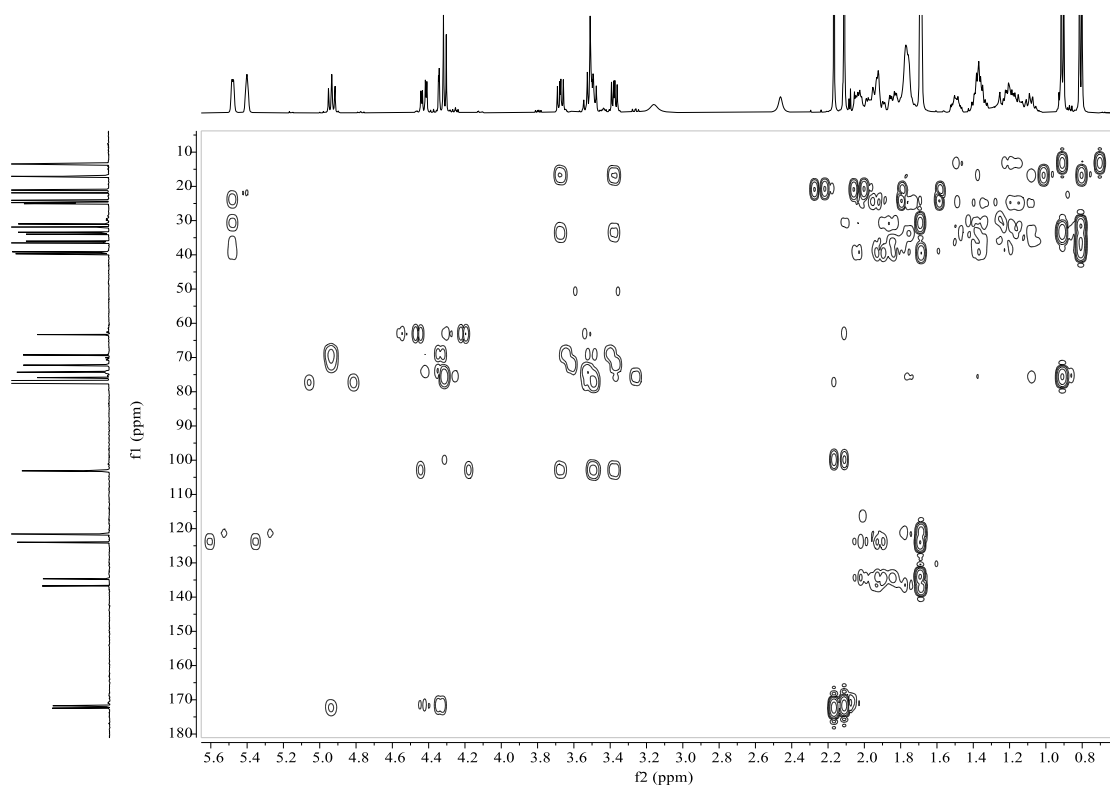


Figure S15 HMBC spectrum of Lemnabourside F (2) (600 MHz; CDCl₃)

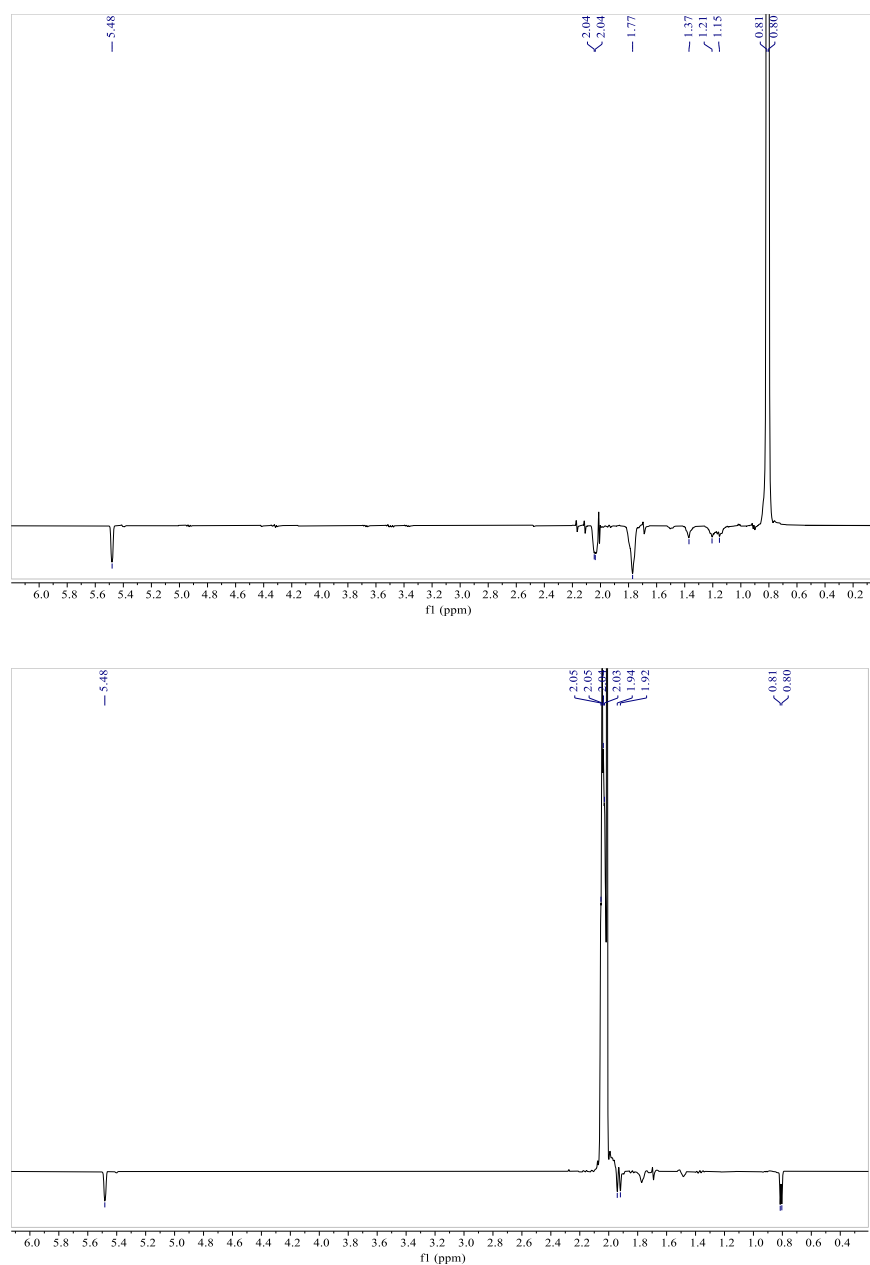
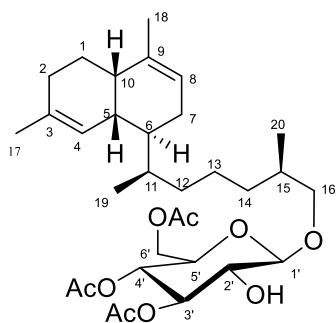


Figure S16 1D-NOE spectrum of Lemnabourside F (2) (600 MHz; CDCl₃)

3.3 Spectroscopic data for Lemnabourside G (3)



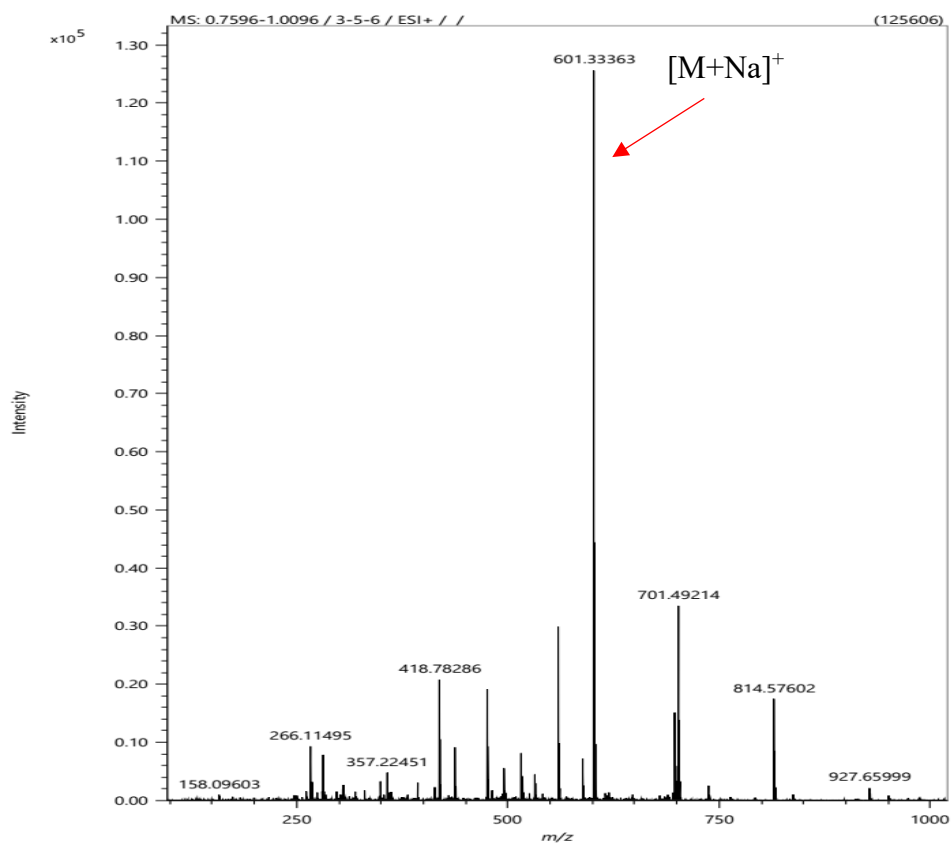


Figure S17 HRESIMS Spectrum of Lemnabourside G (3)

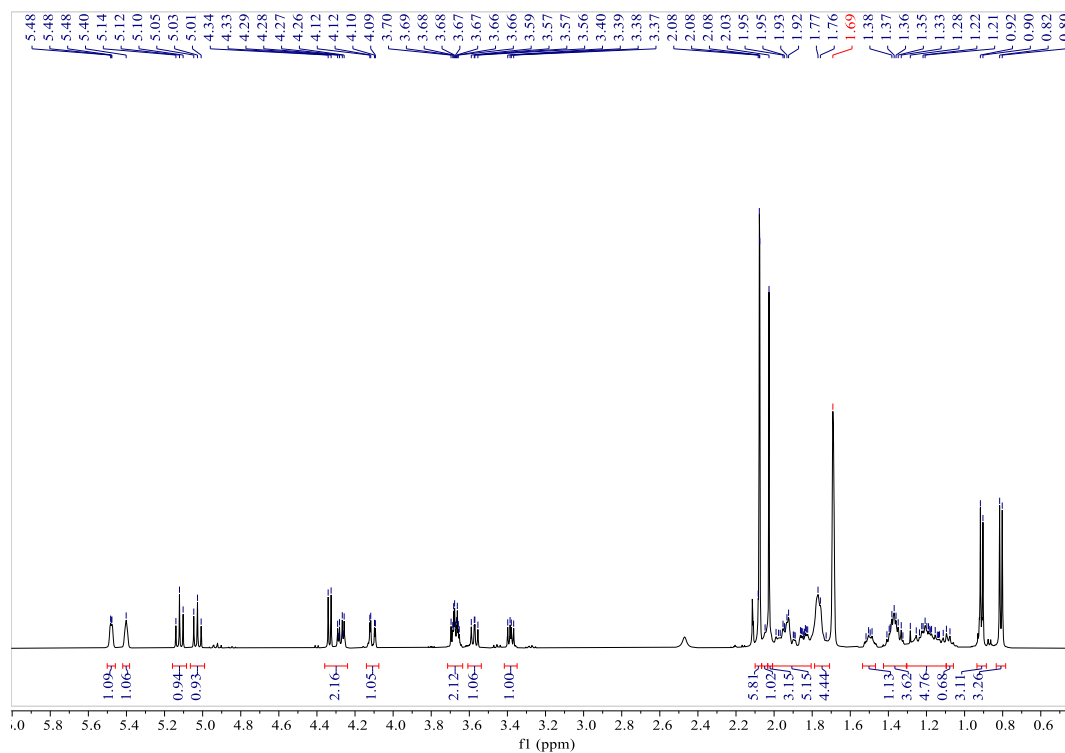


Figure S18 ^1H NMR Spectrum of Lemnabourside G (3) (600 MHz; CDCl_3)

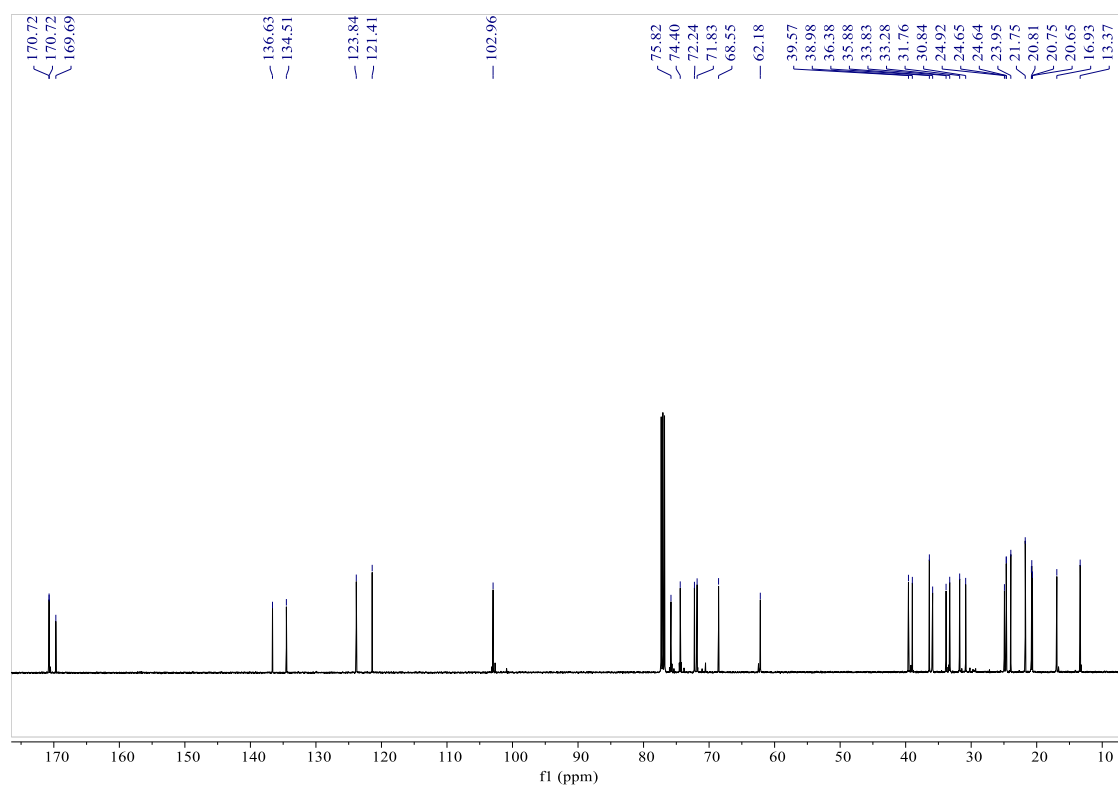


Figure S19 ^{13}C NMR Spectrum of Lemnabourside G (3) (150 MHz; CDCl_3)

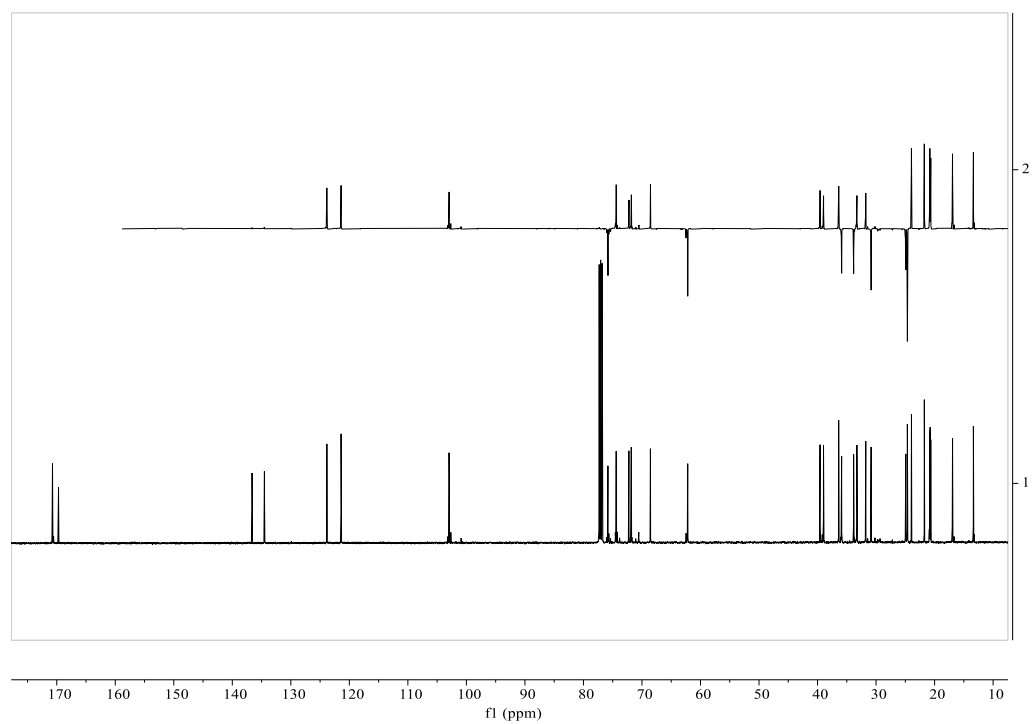


Figure S20 Dept 135° NMR Spectrum of Lemnabourside G (3) (150 MHz; CDCl_3)

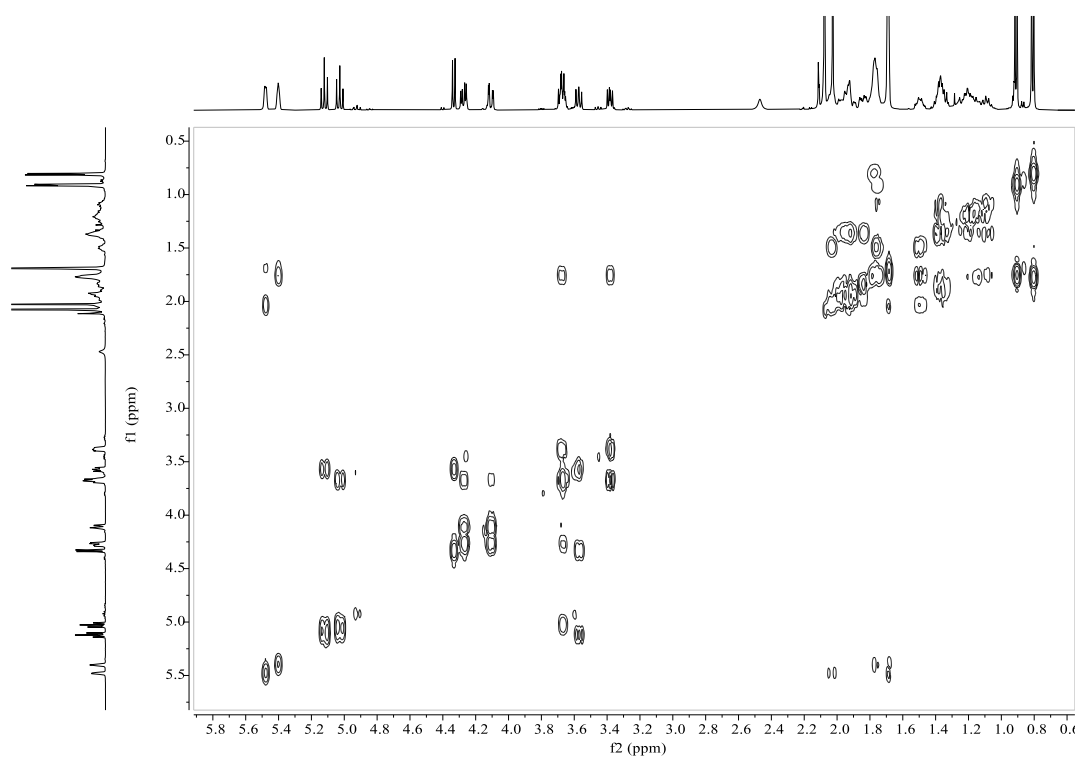


Figure S21 ^1H - ^1H COSY spectrum of Lemnabourside G (3) (600 MHz; CDCl_3)

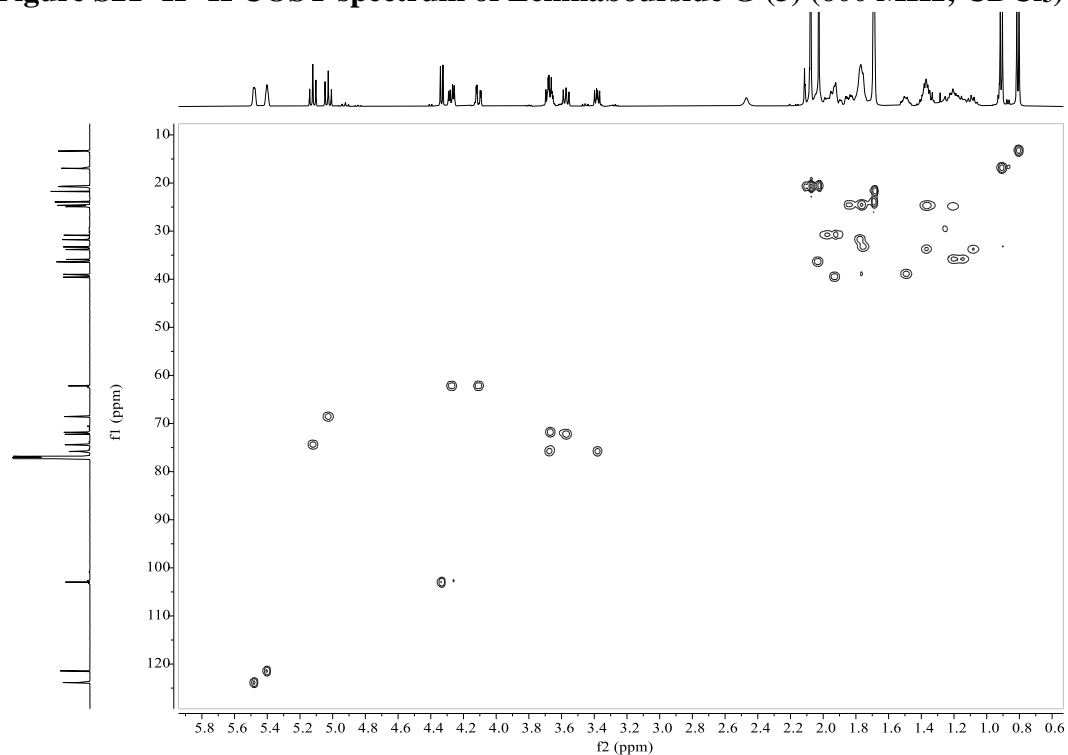


Figure S22 HSQC spectrum of Lemnabourside G (3) (600 MHz; CDCl_3)

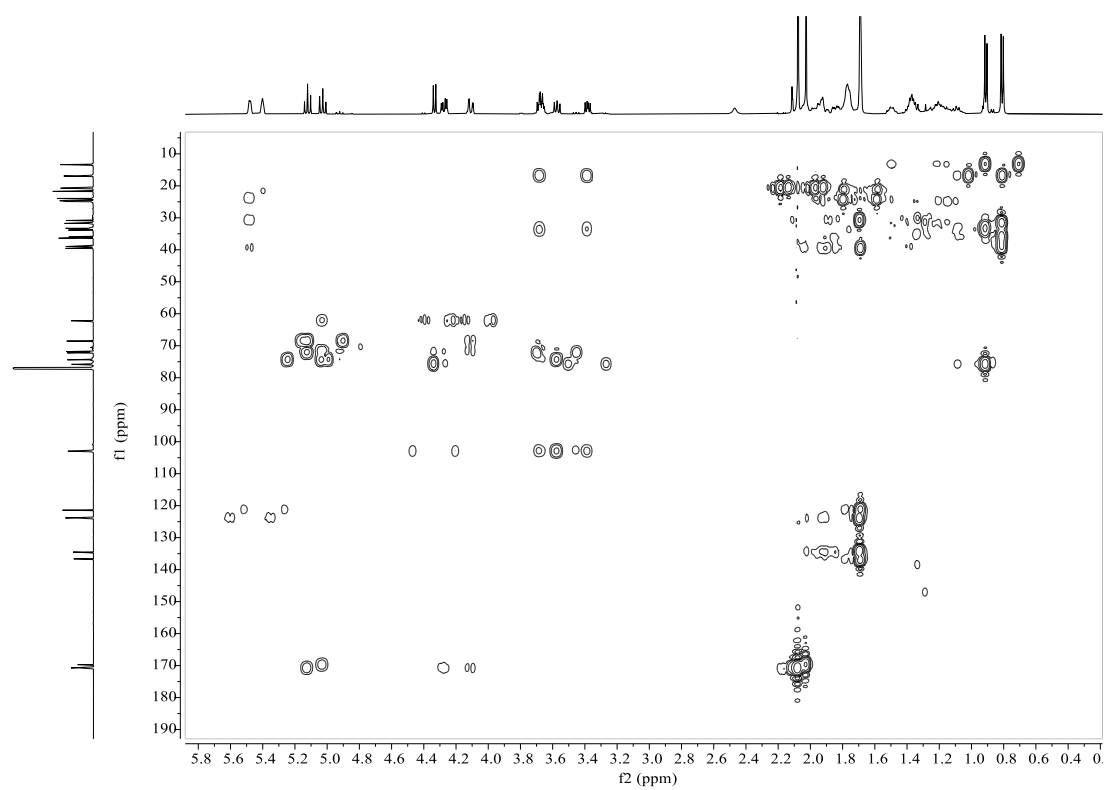


Figure S23 HMBC spectrum of Lemnabourside G (3) (600 MHz; CDCl₃)

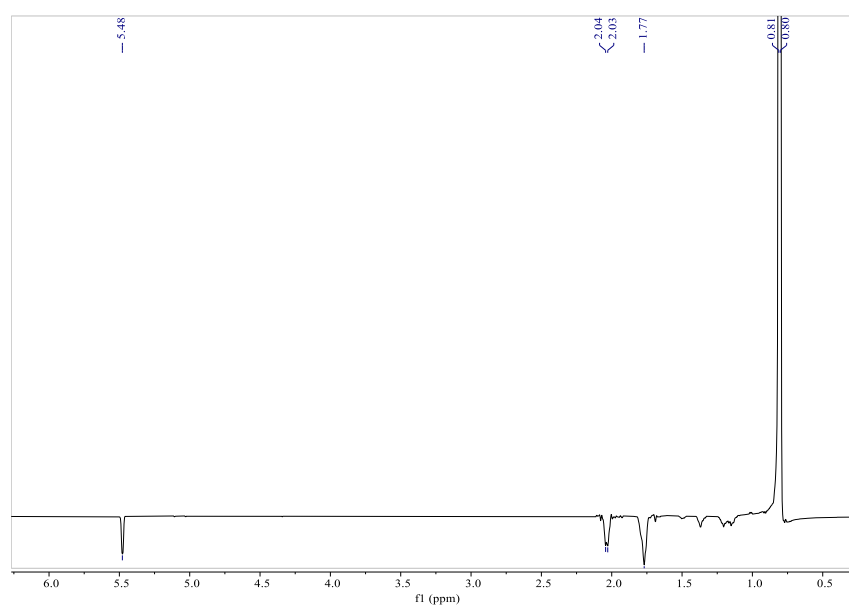


Figure S24 1D-NOE spectrum of Lemnabourside G (3) (600 MHz; CDCl₃)

3.4 Spectroscopic data for Lemnadiolbourside H (4)

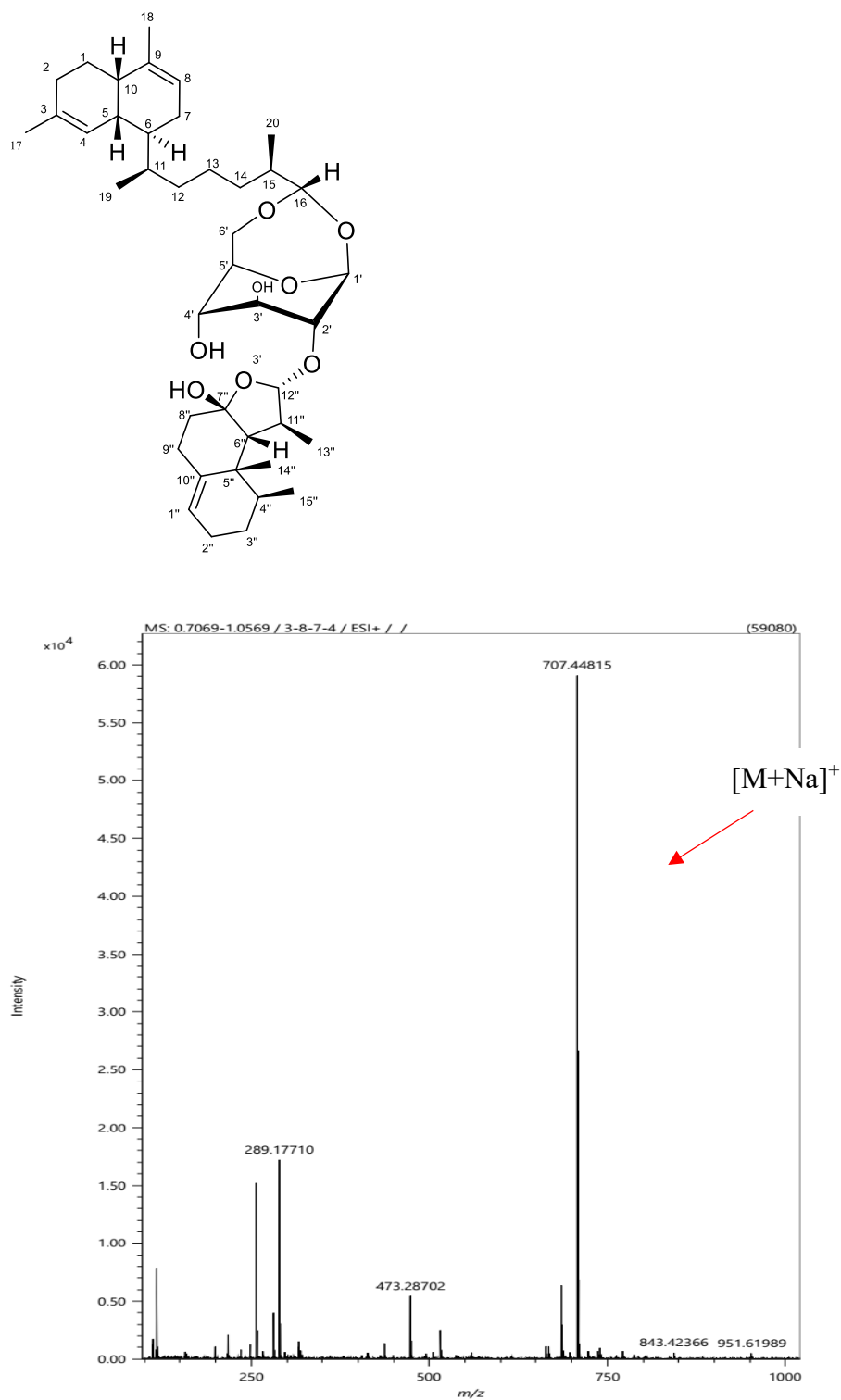


Figure S25 HRESIMS Spectrum of Lemnadiolbourside A (4)

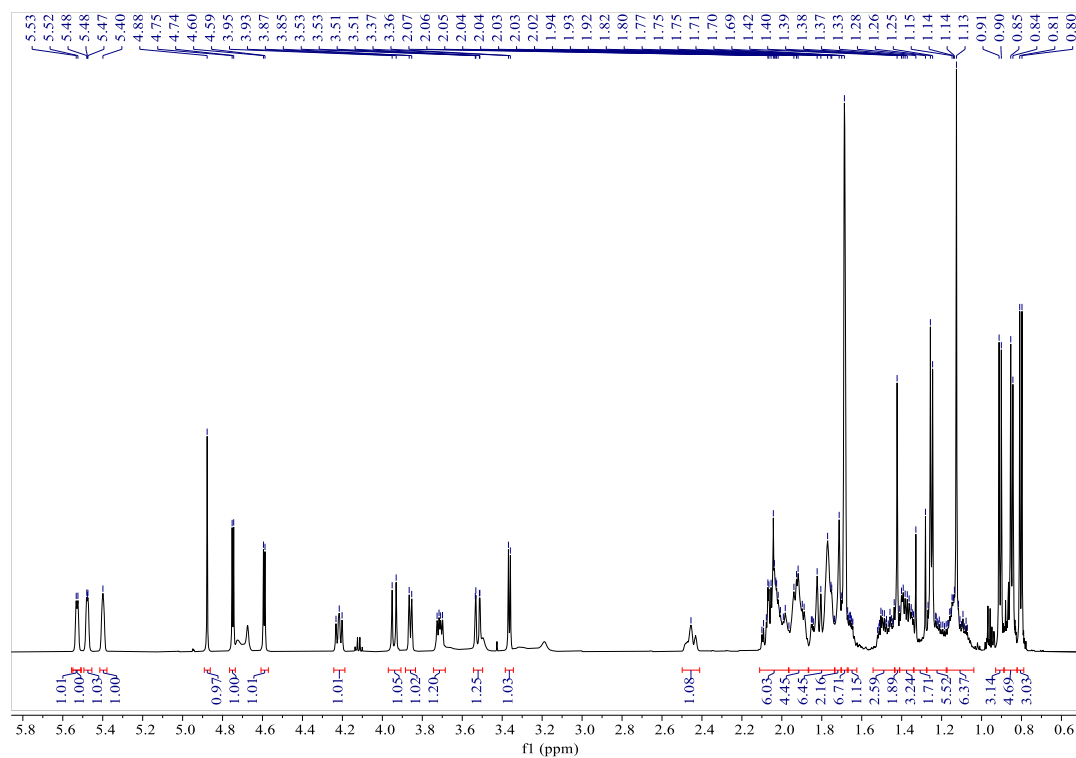


Figure S26 ¹H NMR Spectrum of Lemnadiolbourside A (4) (600 MHz; CDCl₃)

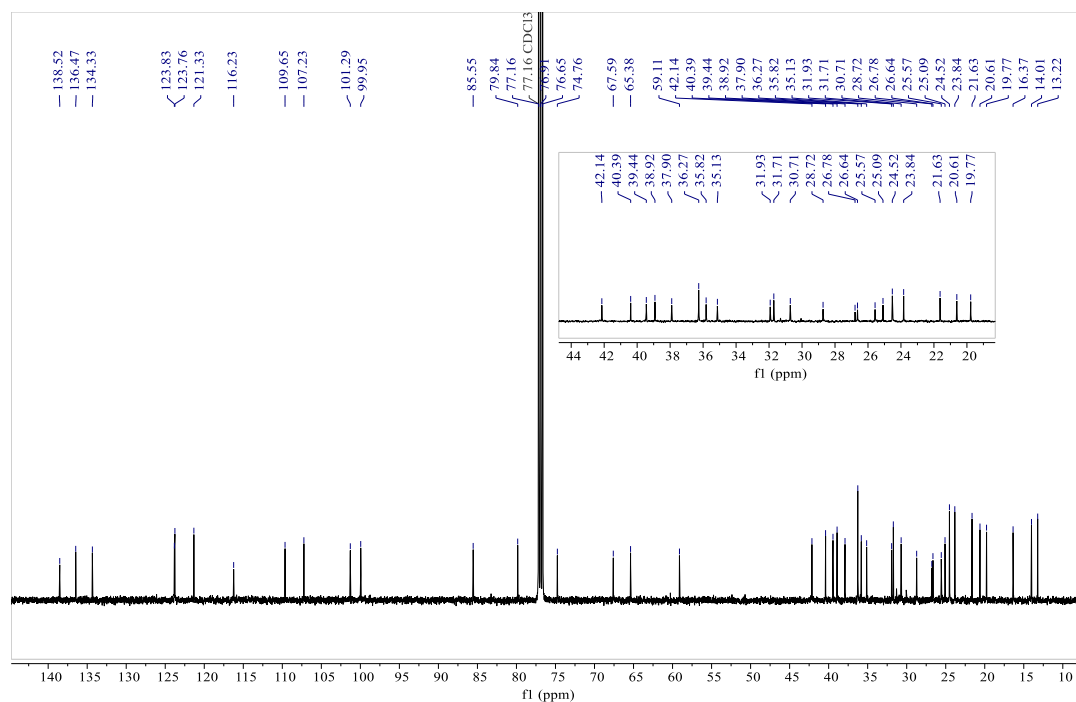


Figure S27 ¹³C NMR Spectrum of Lemnadiolbourside A (4) (150 MHz; CDCl₃)

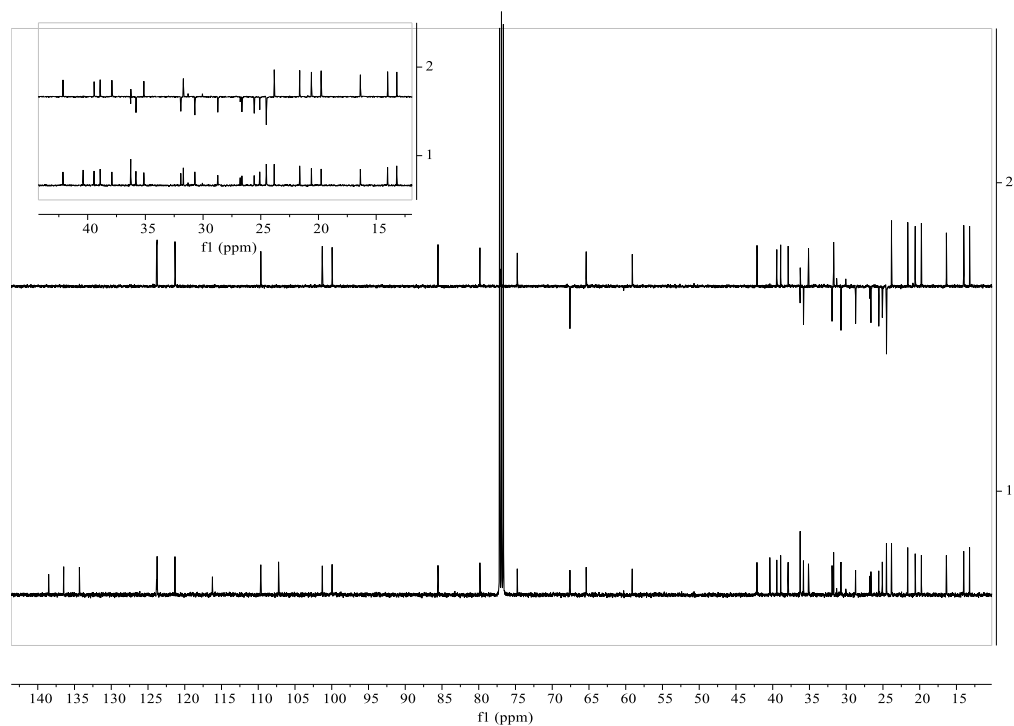


Figure S28 Dept 135° NMR Spectrum of Lemnadiolbourside A (4) (150 MHz; CDCl_3)

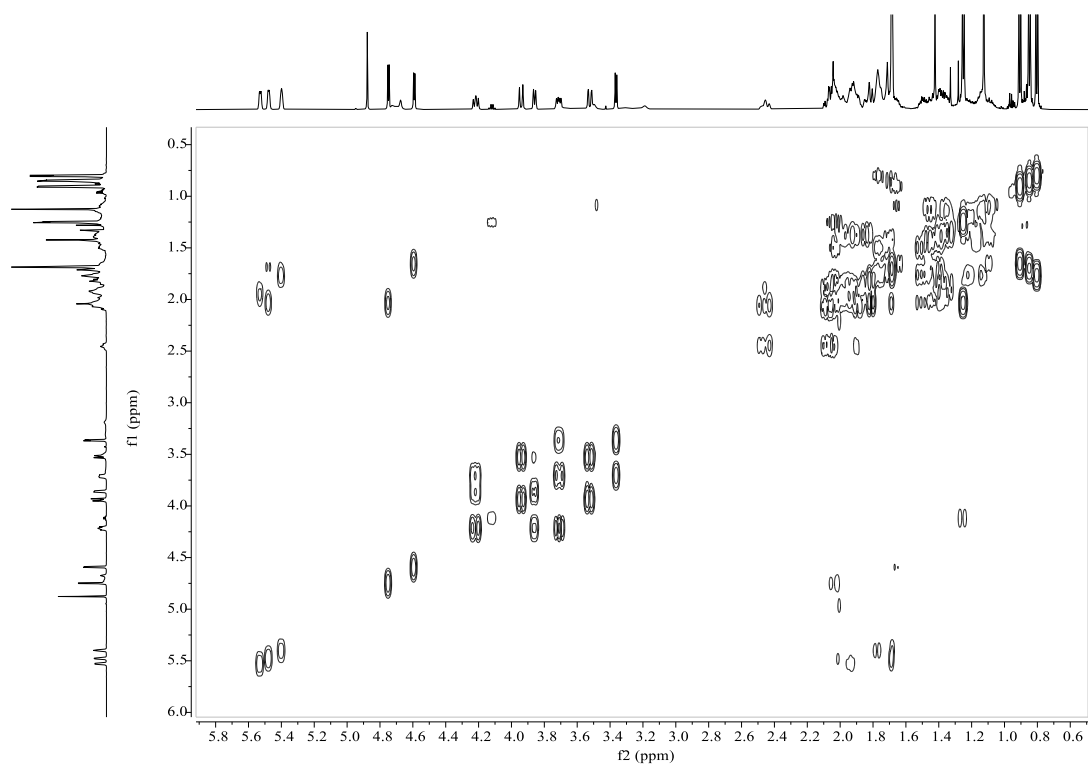


Figure S29 ^1H - ^1H COSY spectrum of Lemnadiolbourside A (4) (600 MHz; CDCl_3)

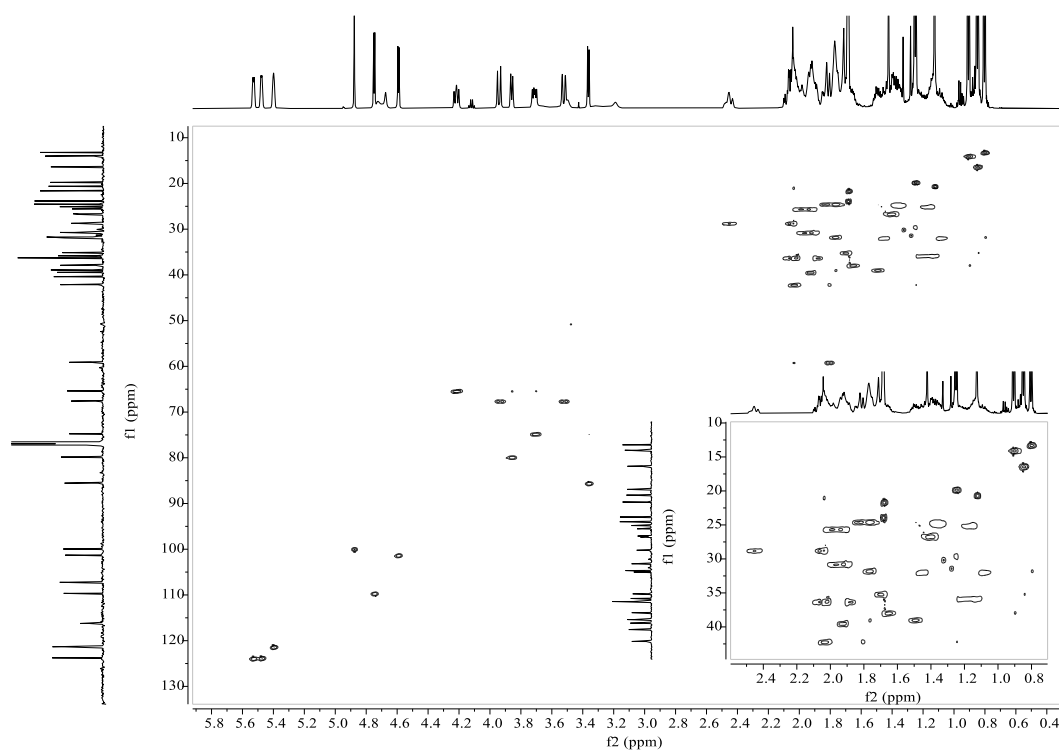


Figure S30 HSQC spectrum of Lemnadiolbourside A (4) (600 MHz; CDCl₃)

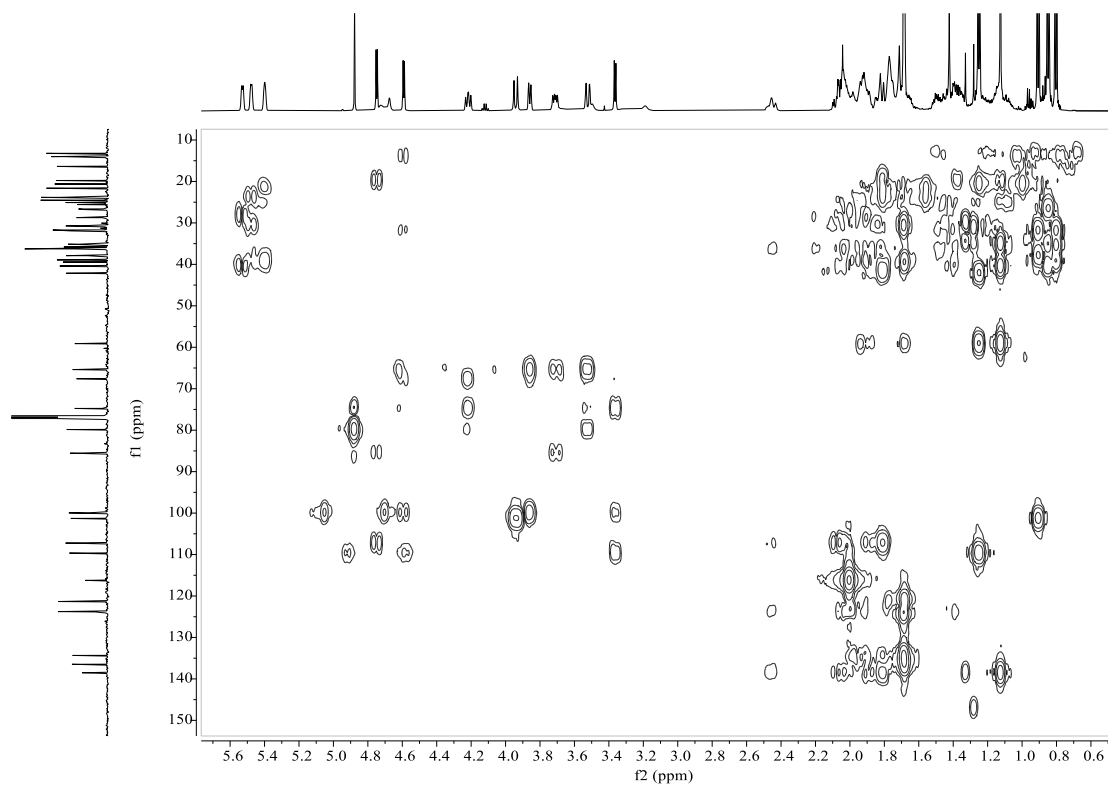
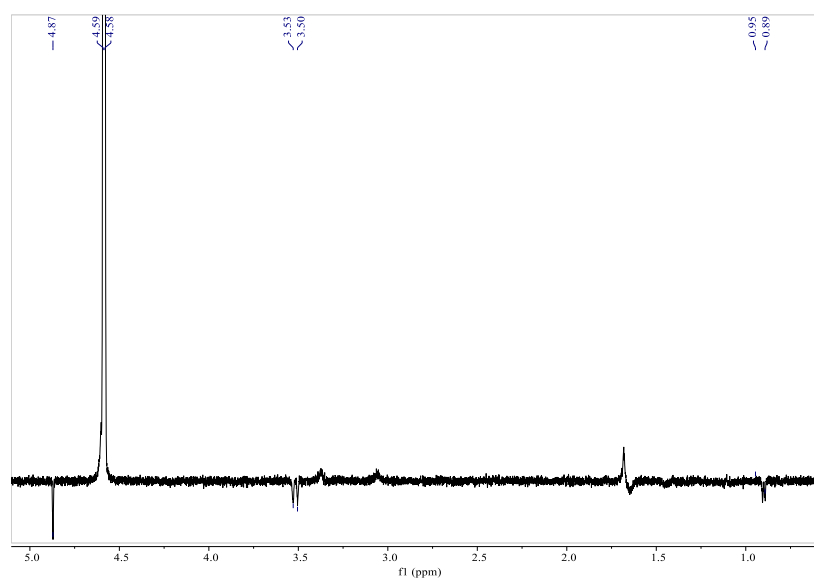
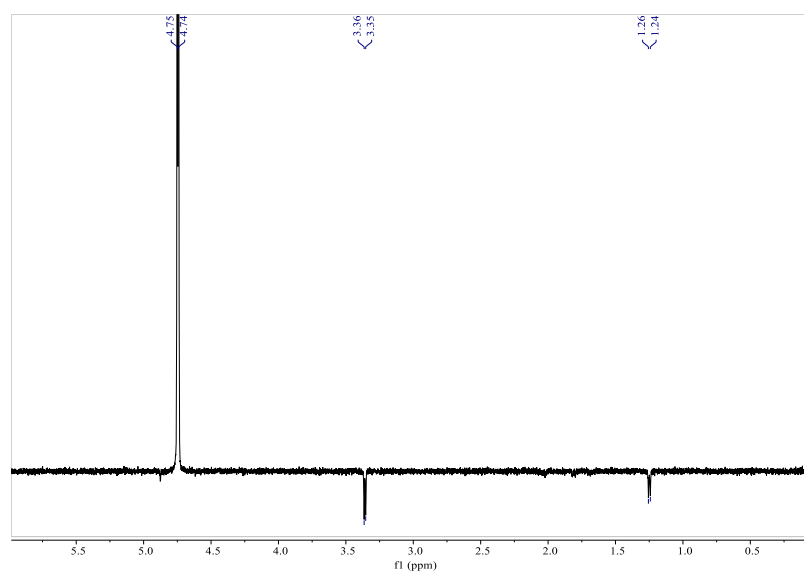
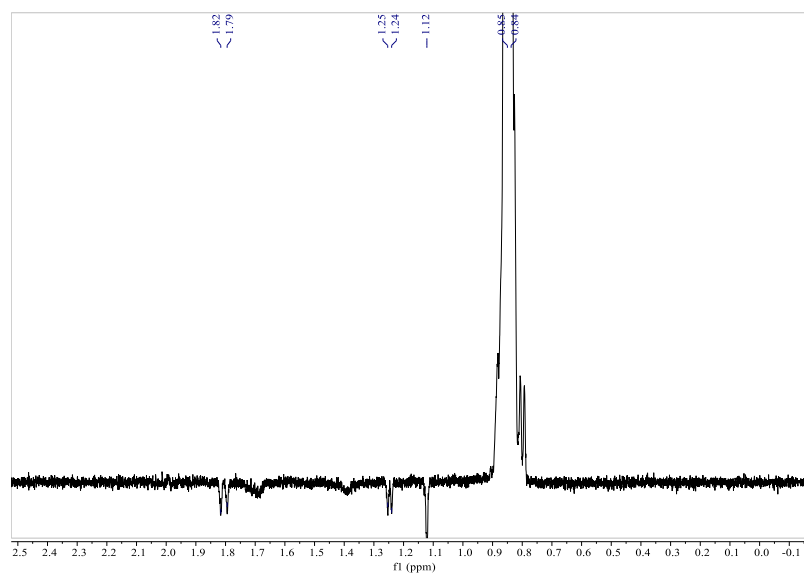


Figure S31 HMBC spectrum of Lemnadiolbourside A (4) (600 MHz; CDCl₃)



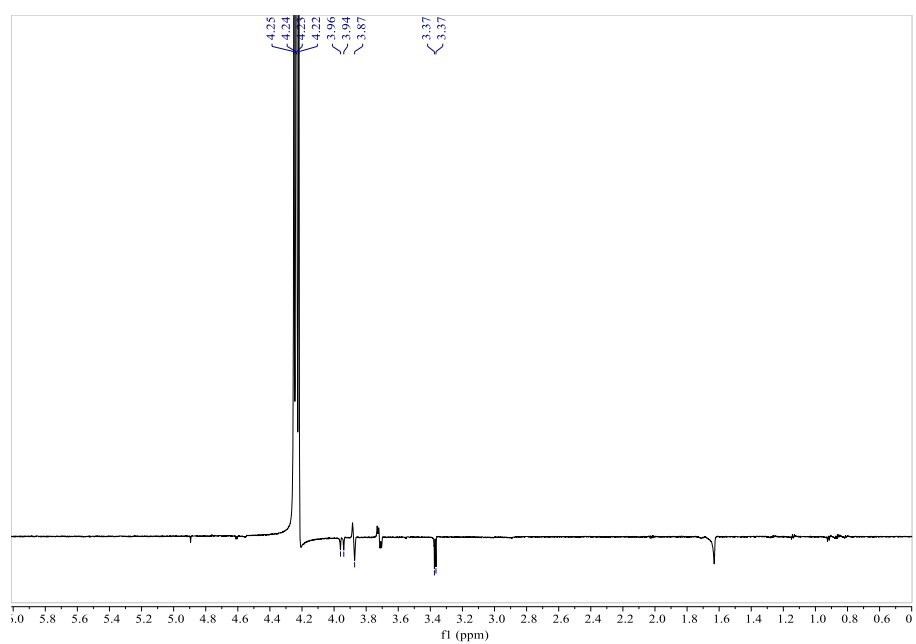
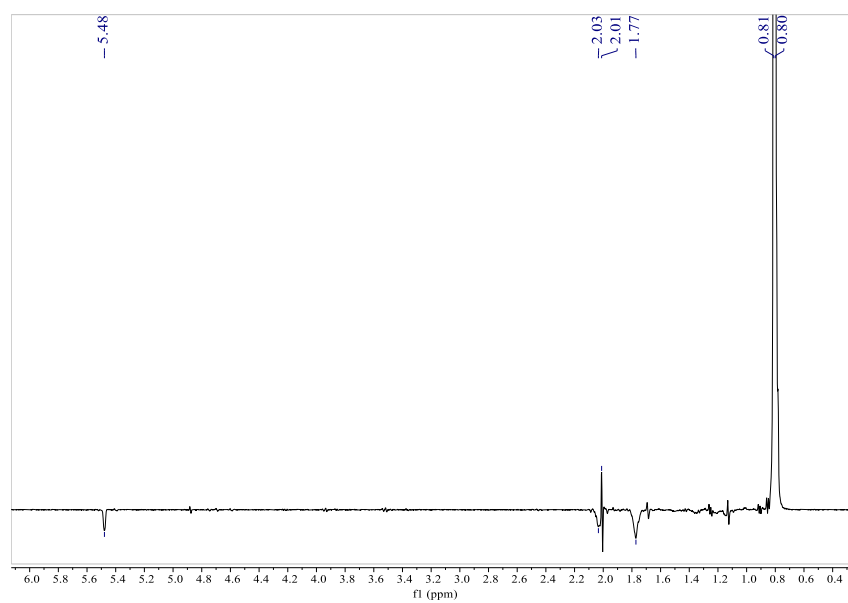


Figure S32 1D-NOE spectrum of Lemnadiolbourside A (4) (600 MHz; CDCl₃)

3.5 Spectroscopic data for Lemnadiolbourside B (5)

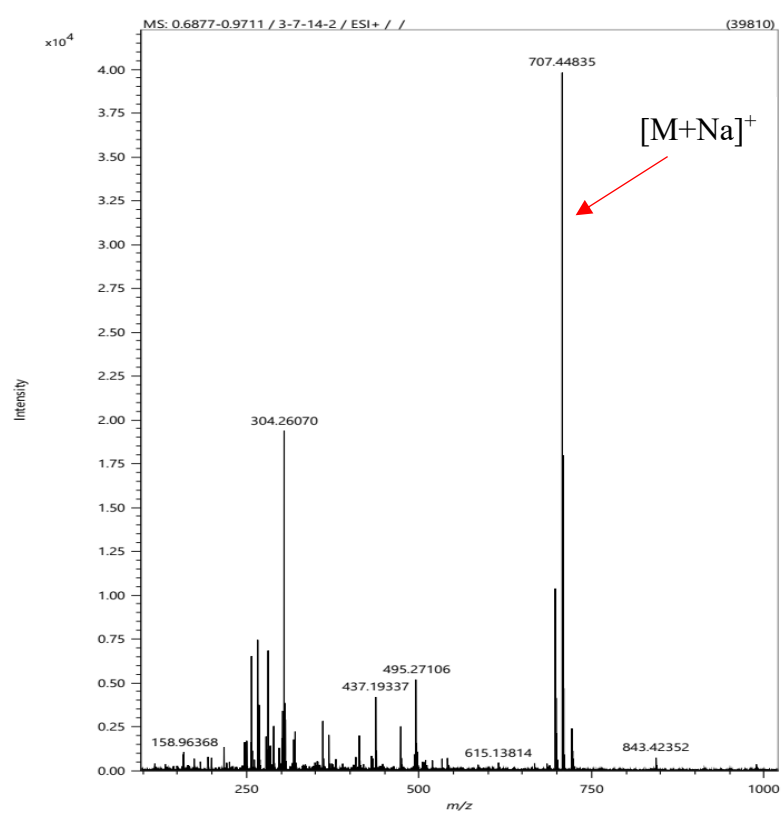
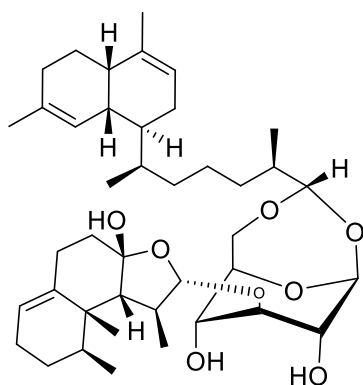


Figure S33 HRESIMS Spectrum of Lemnadiolbourside B (5)

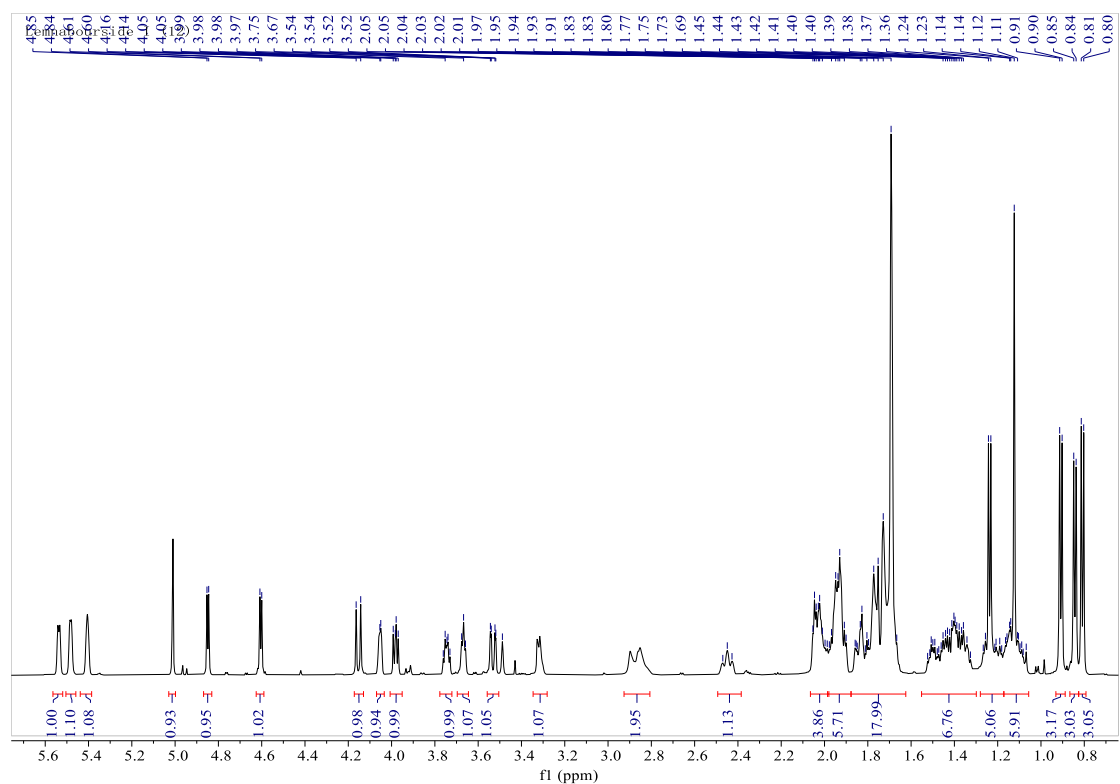


Figure S34 ^1H NMR Spectrum of Lemnadiolbourside B (5) (600 MHz; CDCl_3)

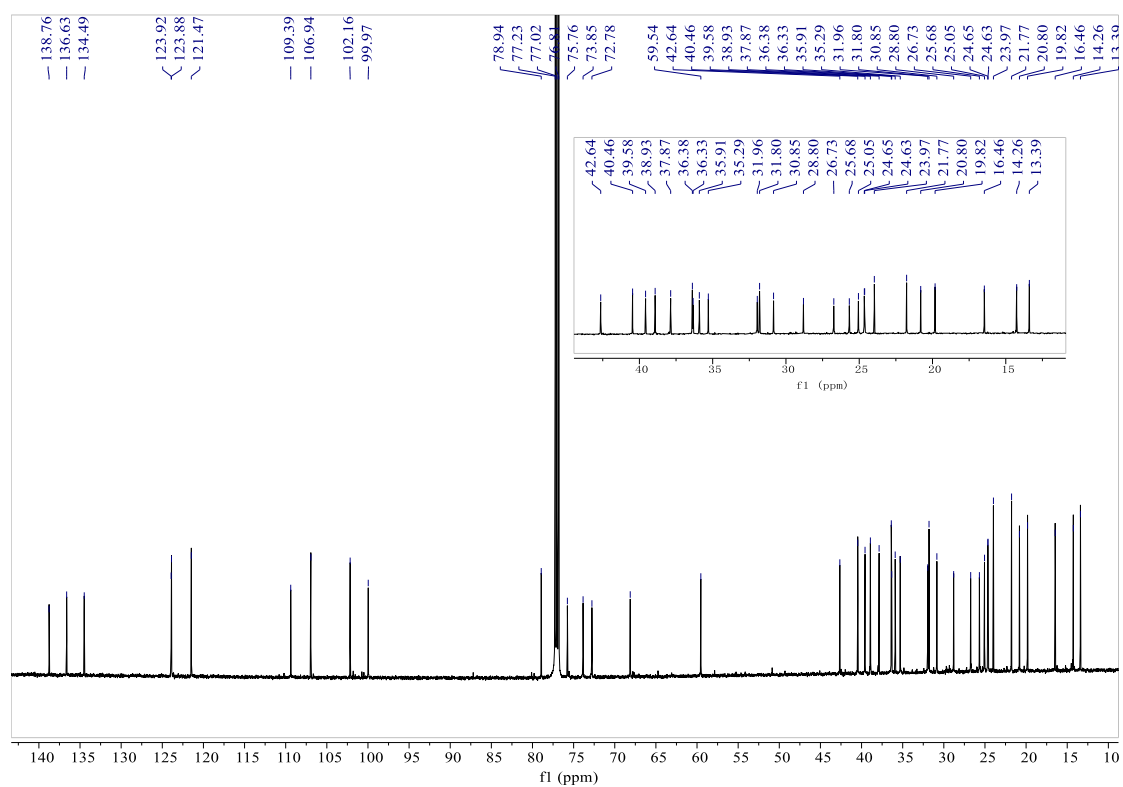


Figure S35 ^{13}C NMR Spectrum of Lemnadiolbourside B (5) (150 MHz; CDCl_3)

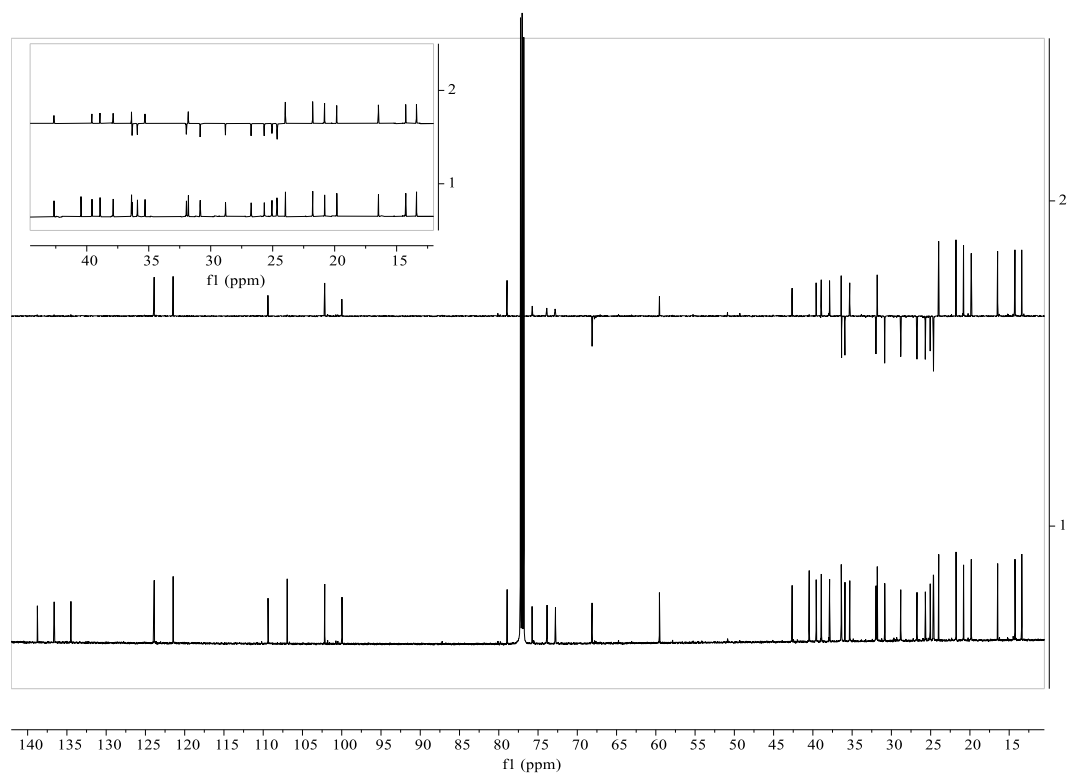


Figure S36 Dept 135° NMR Spectrum of Lemnadiolbourside B (5) (150 MHz; CDCl_3)

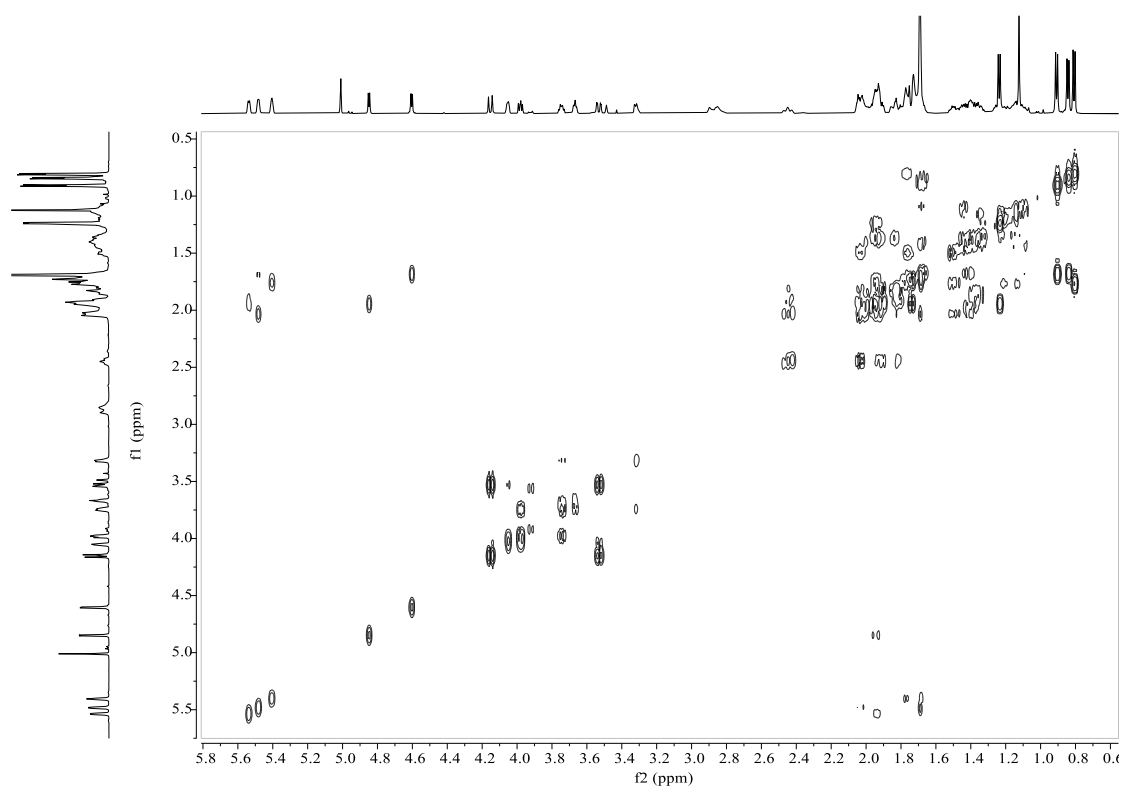


Figure S37 ^1H - ^1H COSY spectrum of Lemnadiolbourside B (5) (600 MHz; CDCl_3)

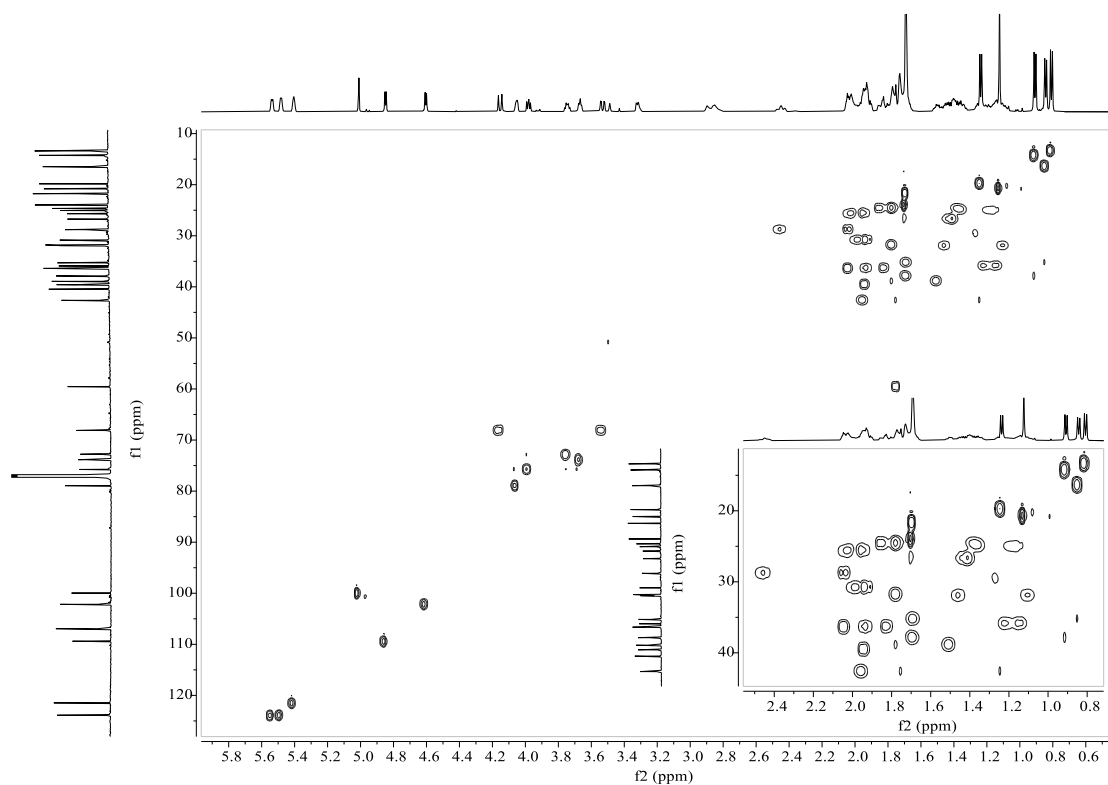


Figure S38 HSQC spectrum of Lemnadiolbourside B (5) (600 MHz; CDCl_3)

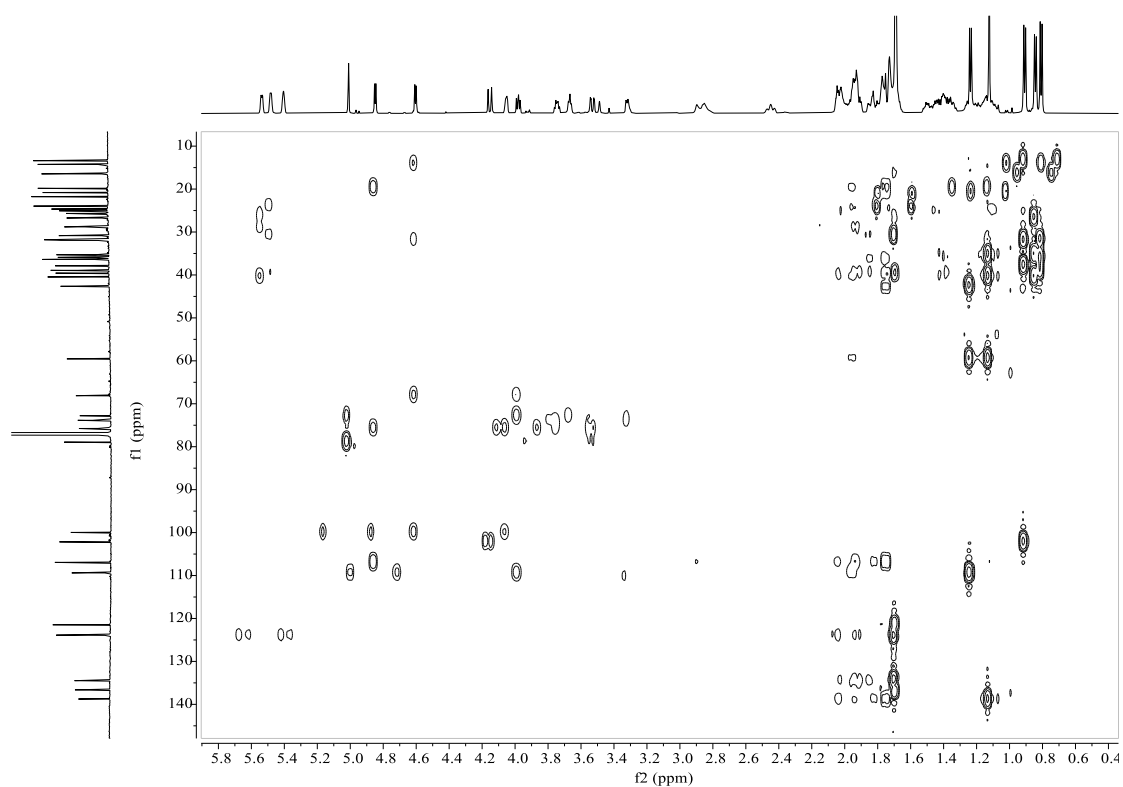
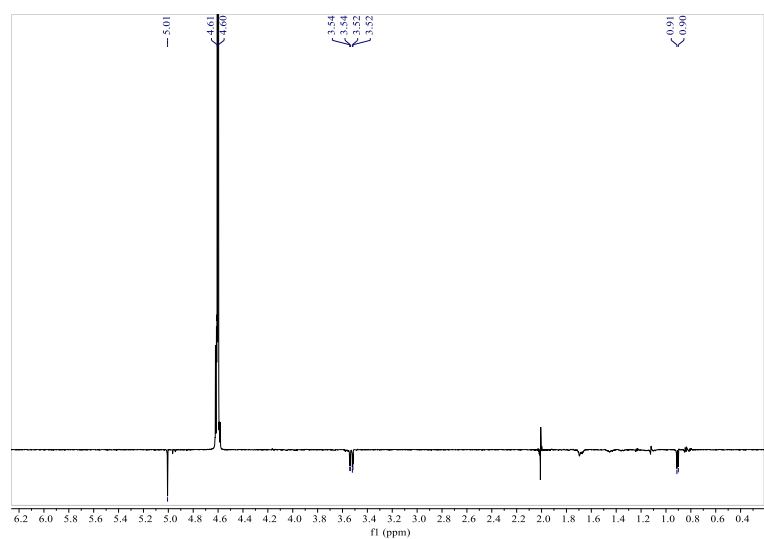
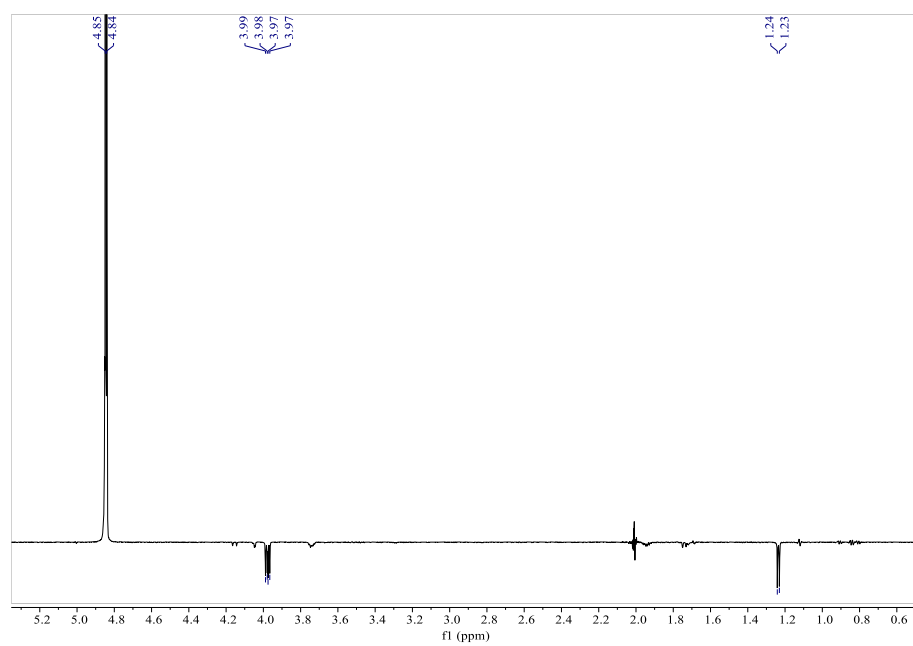


Figure S39 HMBC spectrum of Lemnadiolbourside B (**5**) (600 MHz; CDCl₃)



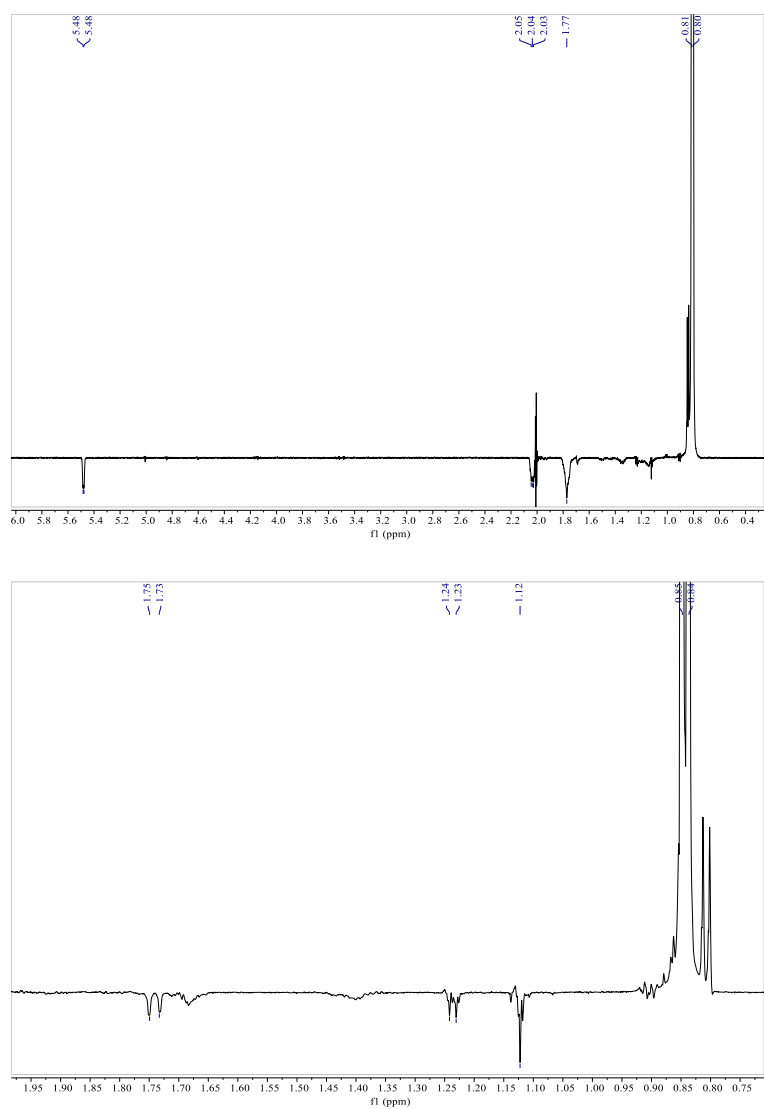
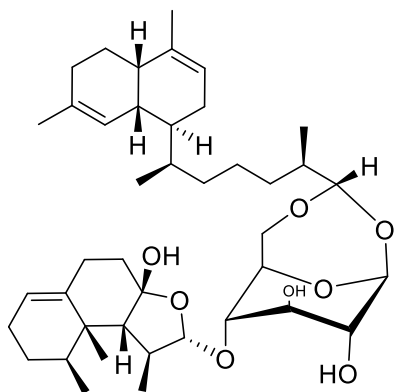


Figure S40 1D-NOE spectrum of Lemnadiolbourside B (5) (600 MHz; CDCl₃)

3.6 Spectroscopic data for Lemnadiolbourside C (6)



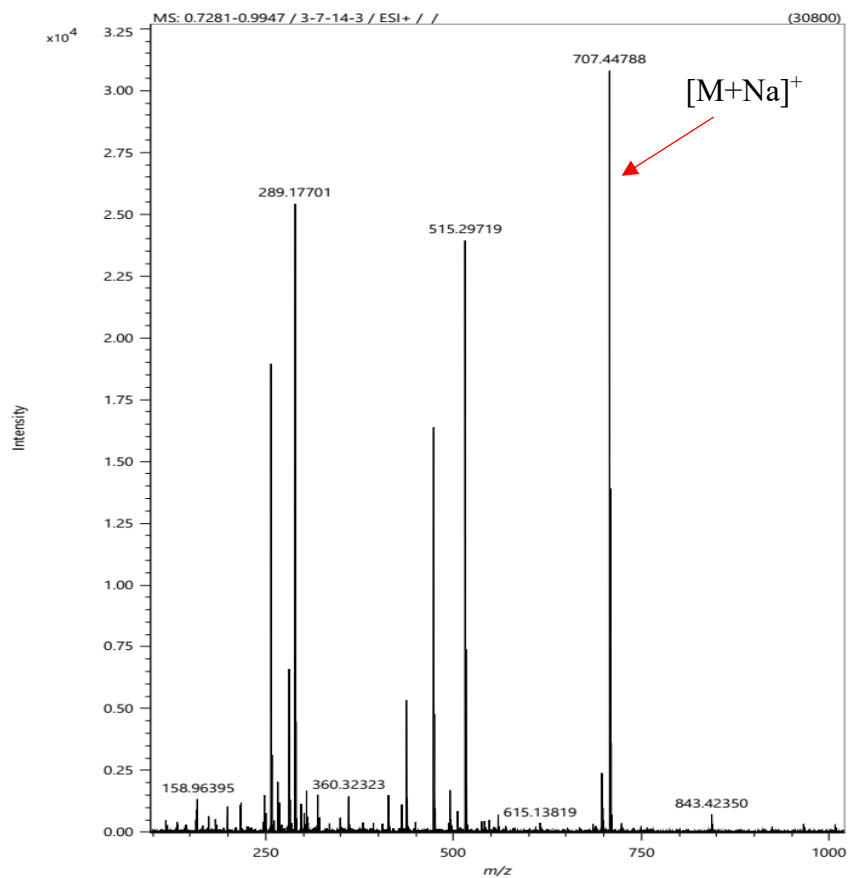


Figure S41 HRESIMS Spectrum of Lemnadiolbourside C (6)

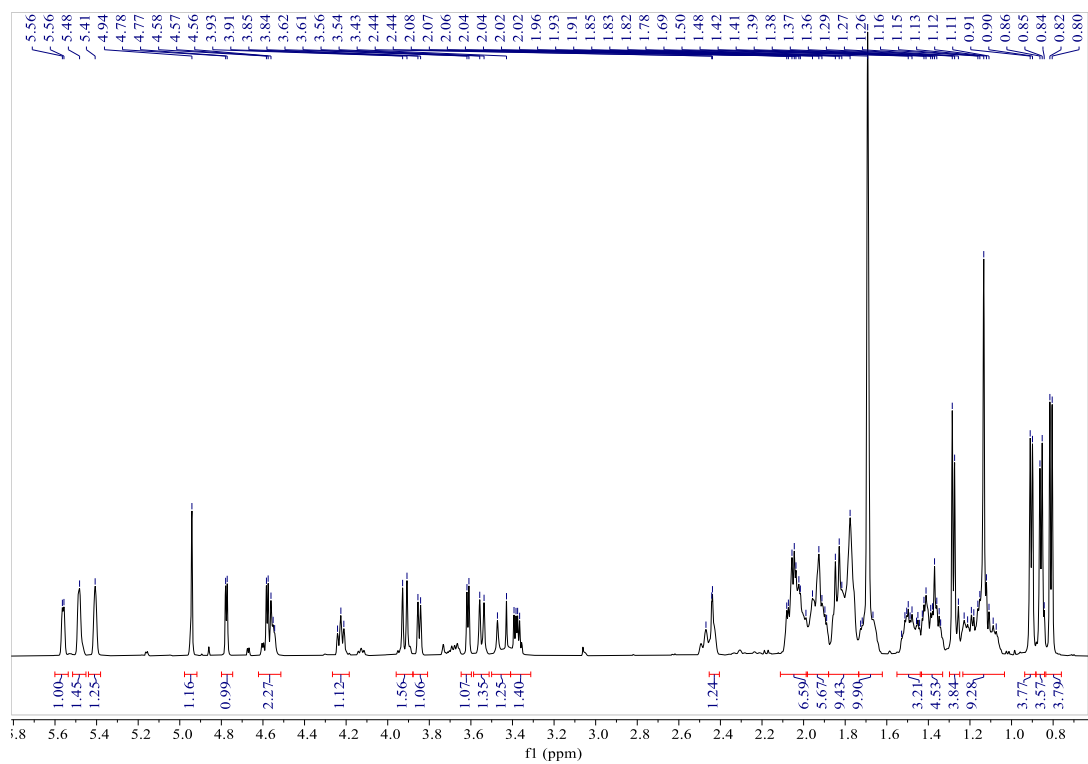


Figure S42 ^1H NMR Spectrum of Lemnadiolbourside C (6) (600 MHz; CDCl_3)

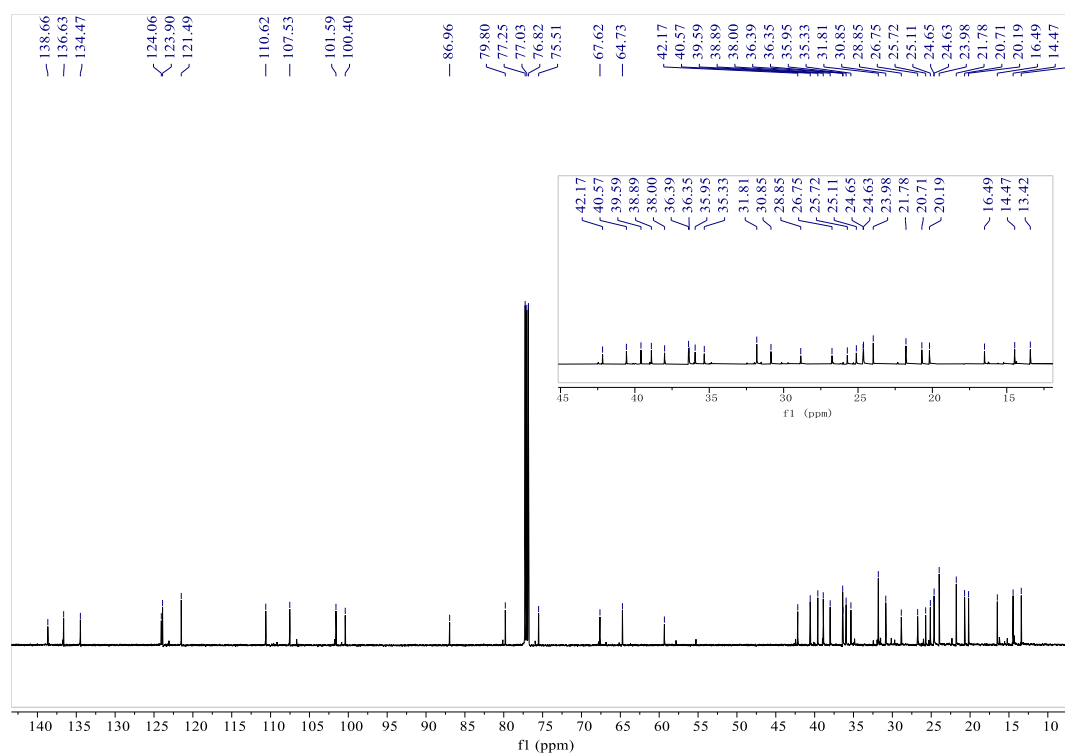


Figure S43 ^{13}C NMR Spectrum of Lemnadiolbourside C (6) (150 MHz; CDCl_3)

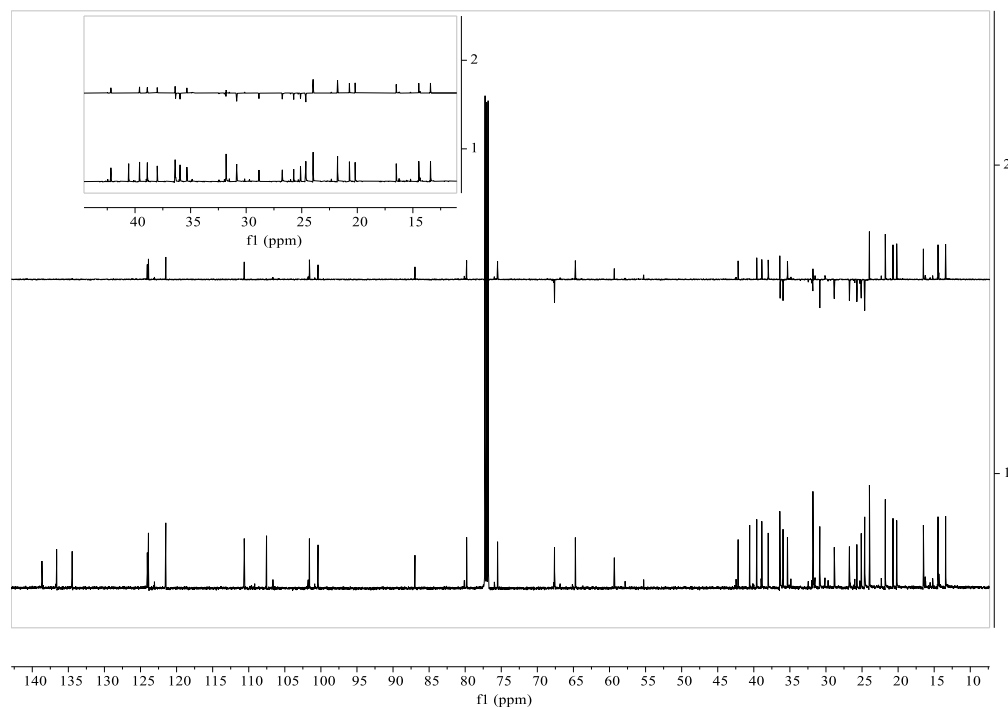


Figure S44 Dept $^{135}^\circ$ NMR Spectrum of Lemnadiolbourside C (6) (150 MHz; CDCl_3)

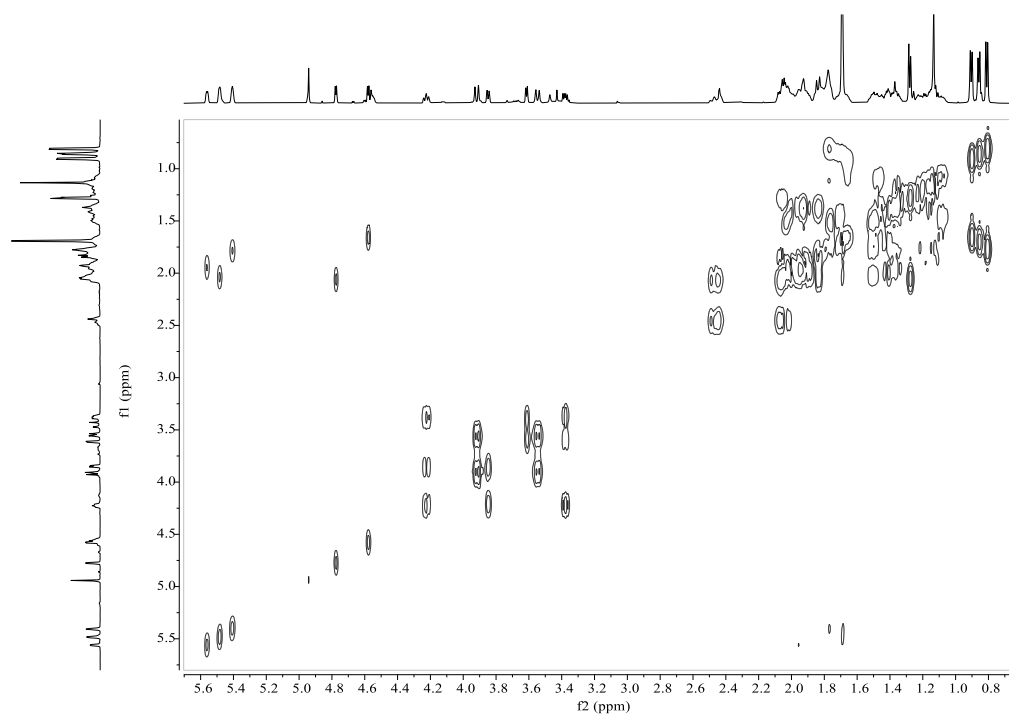


Figure S45 ^1H - ^1H COSY spectrum of Lemnadiolbourside C (6) (600 MHz; CDCl_3)

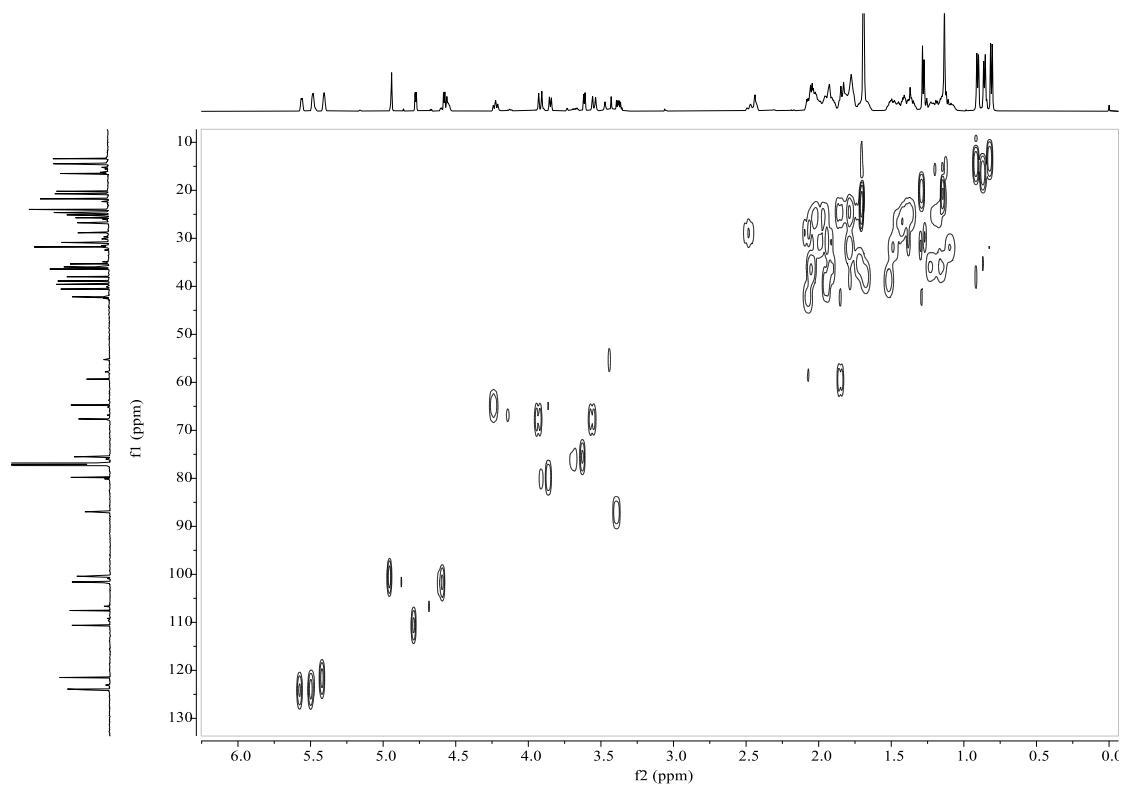


Figure S46 HSQC spectrum of Lemnadiolbourside C (6) (600 MHz; CDCl_3)

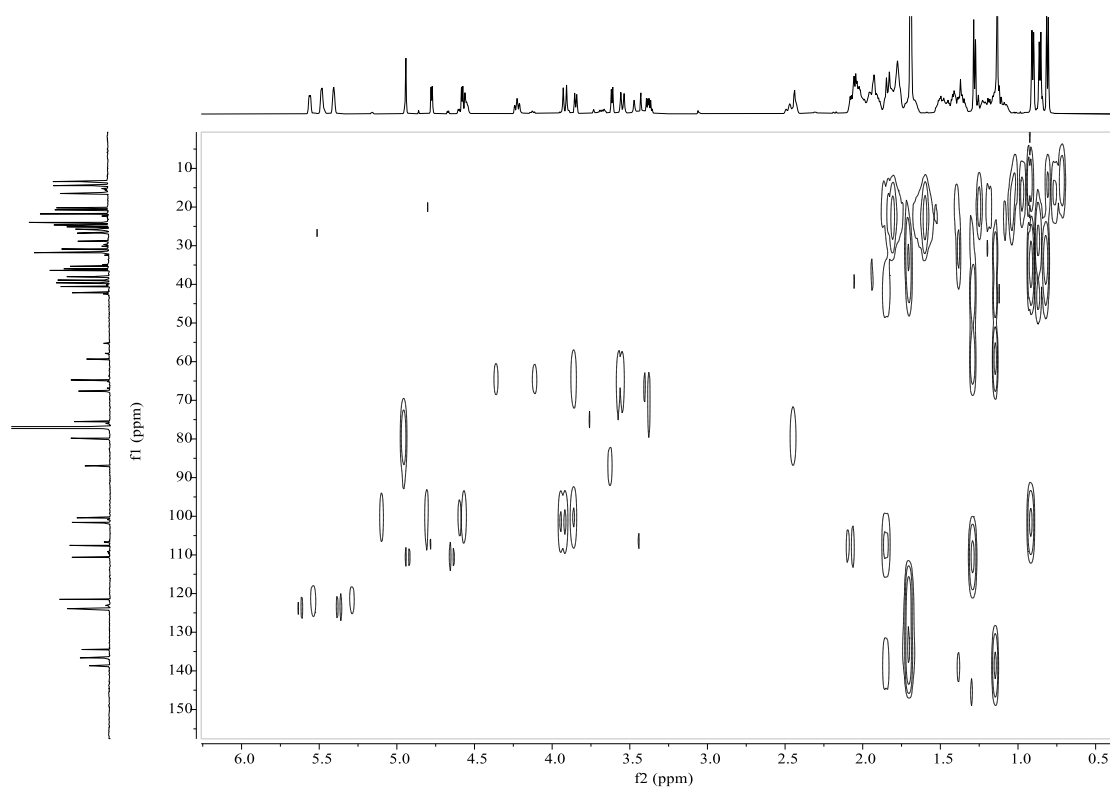
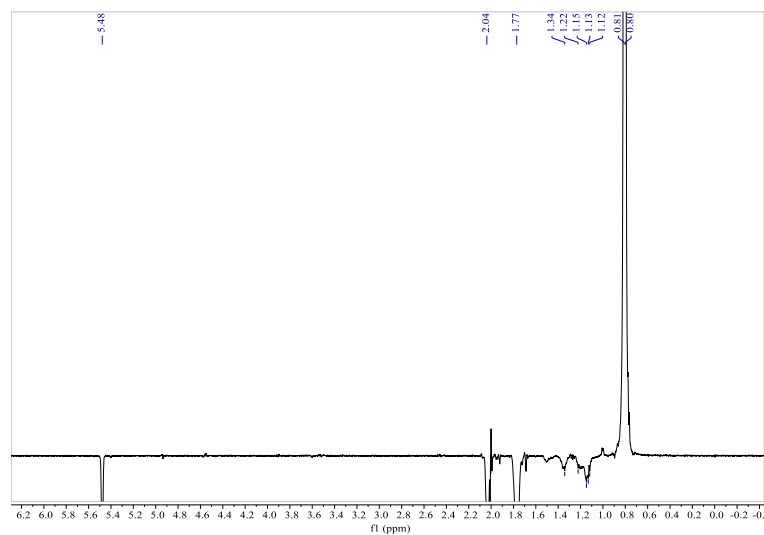


Figure S47 HMBC spectrum of Lemnadiolbourside C (6) (600 MHz; CDCl_3)



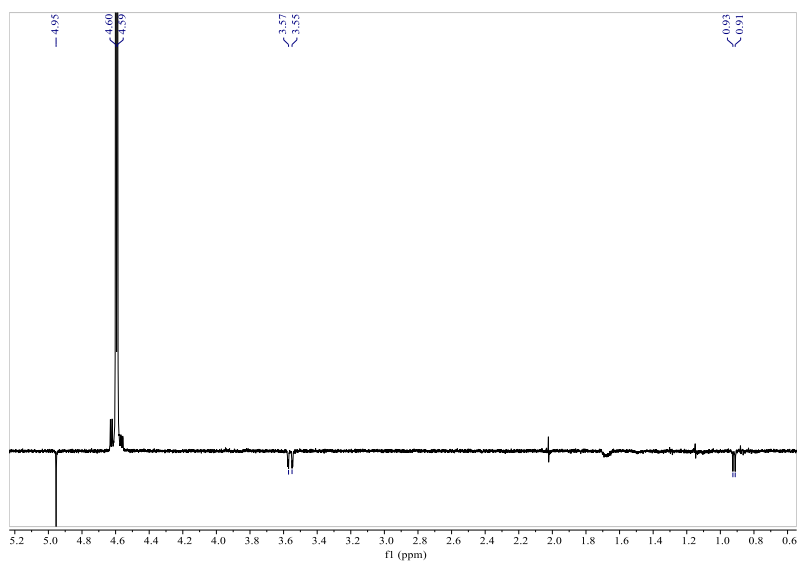
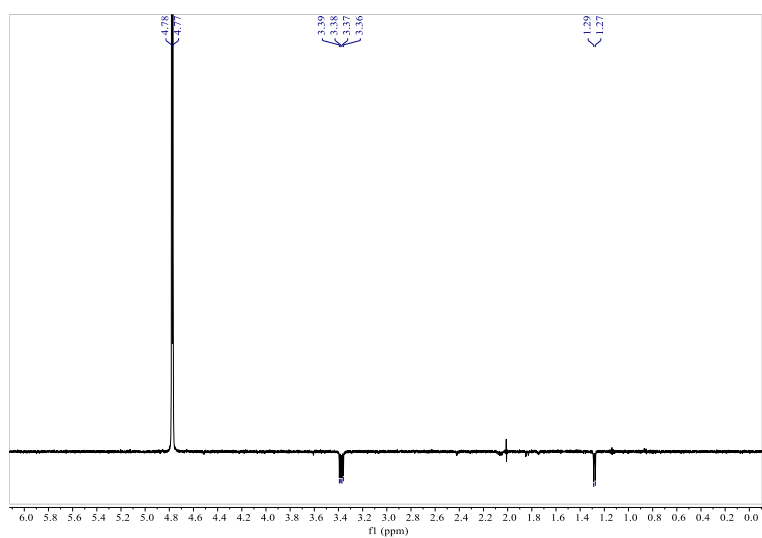
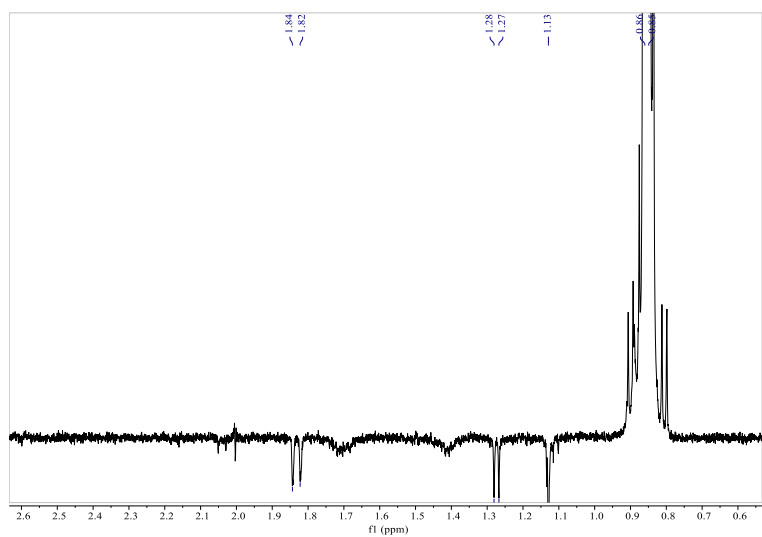


Figure S48 1D-NOE spectrum of Lemnadiolbourside C (6) (600 MHz; CDCl₃)

4. NMR spectra of the known isolated compounds

4.1 Spectroscopic data for compound 7

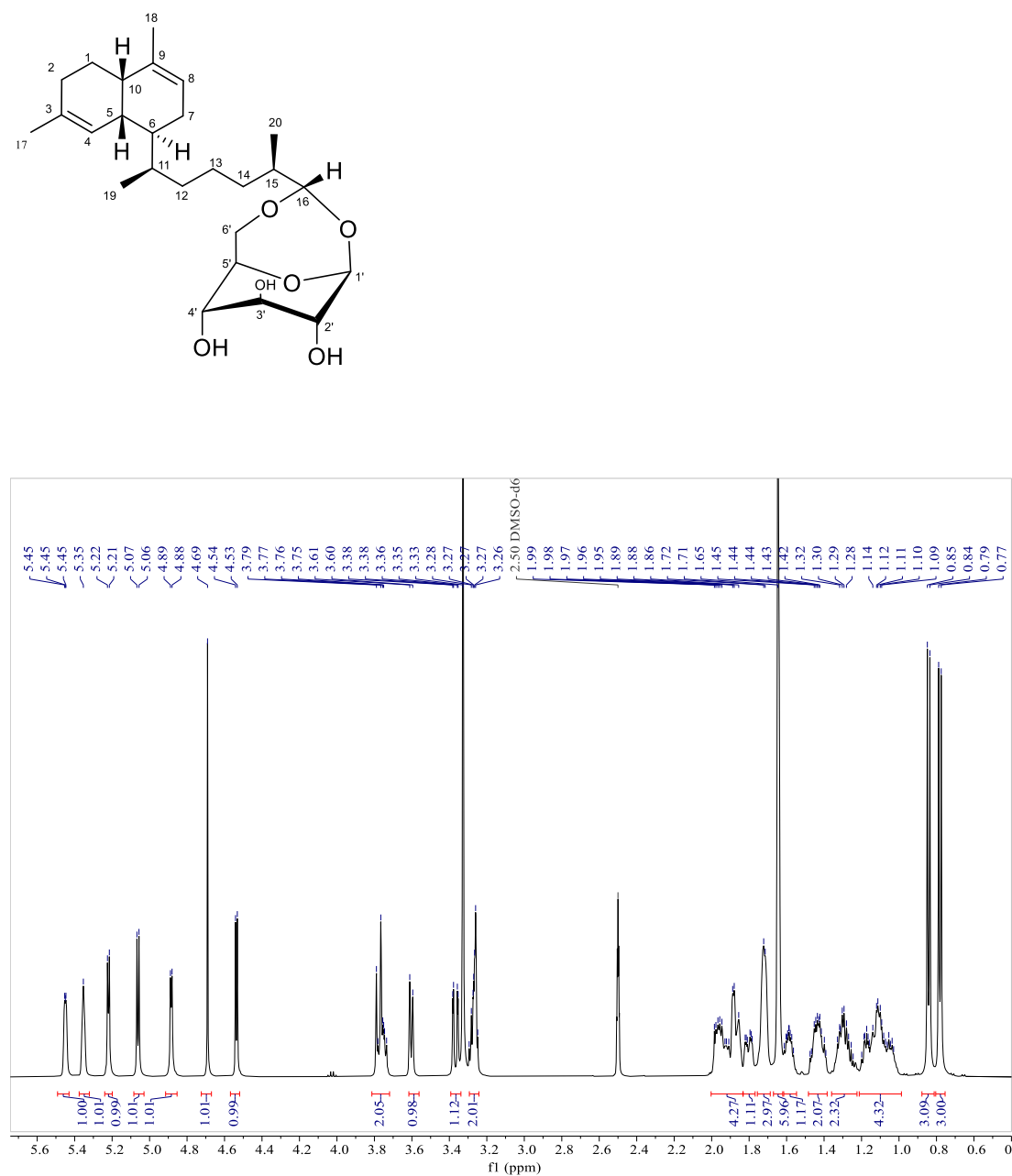


Figure S49 ¹H NMR Spectrum of compound 7 (600 MHz; DMSO-d₆)

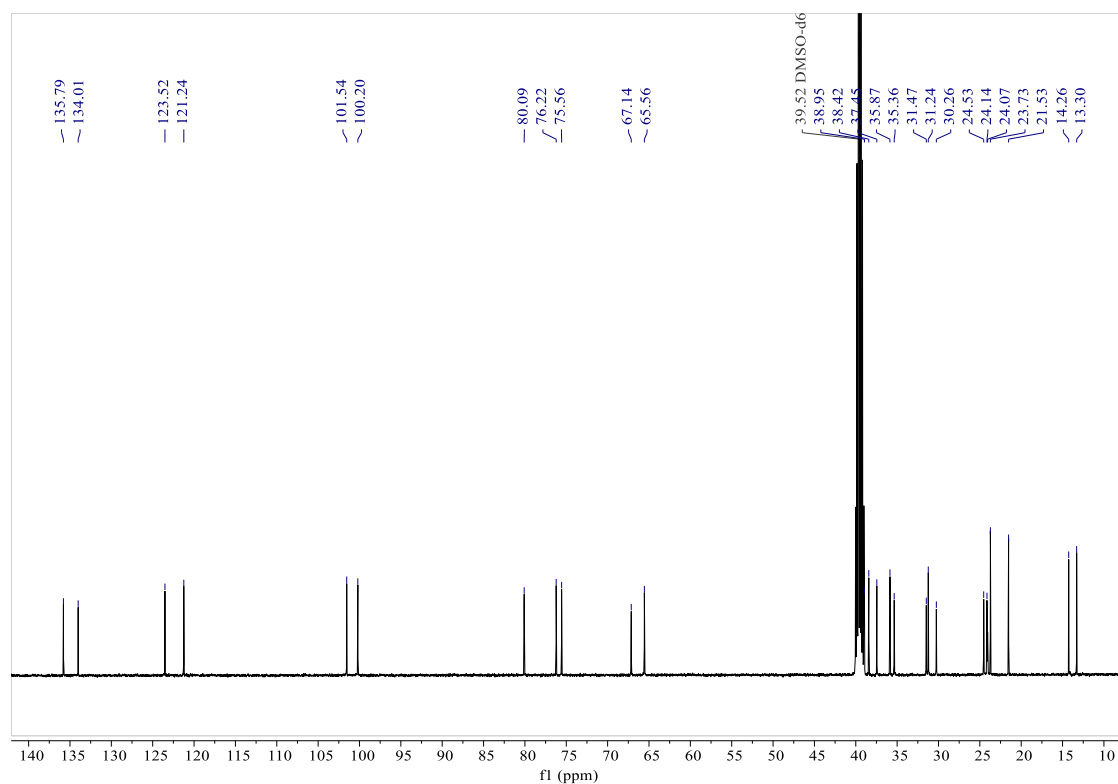
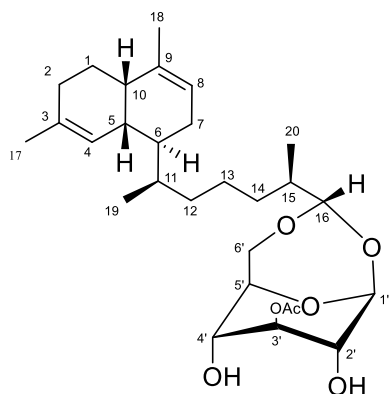


Figure S50 ^{13}C NMR Spectrum of compound **7** (150 MHz; DMSO-d_6)

4.2 Spectroscopic data for compound **8**



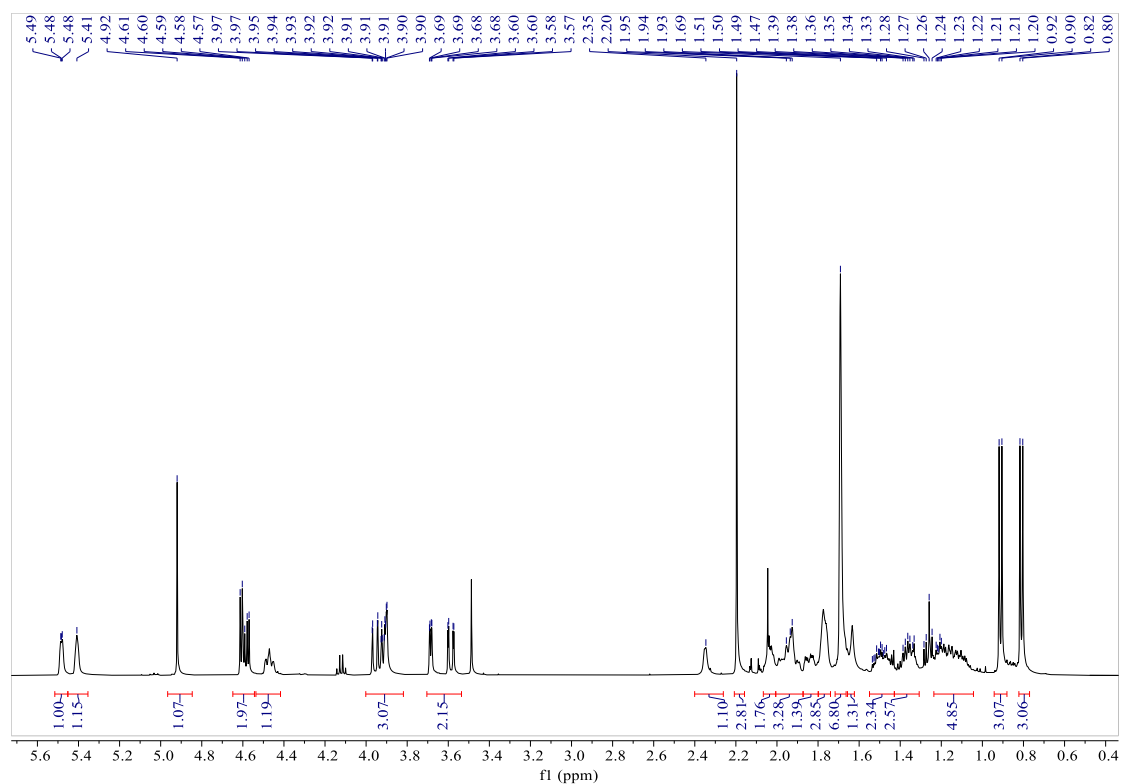


Figure S51 ¹H NMR Spectrum of compound 8 (600 MHz; CDCl₃)

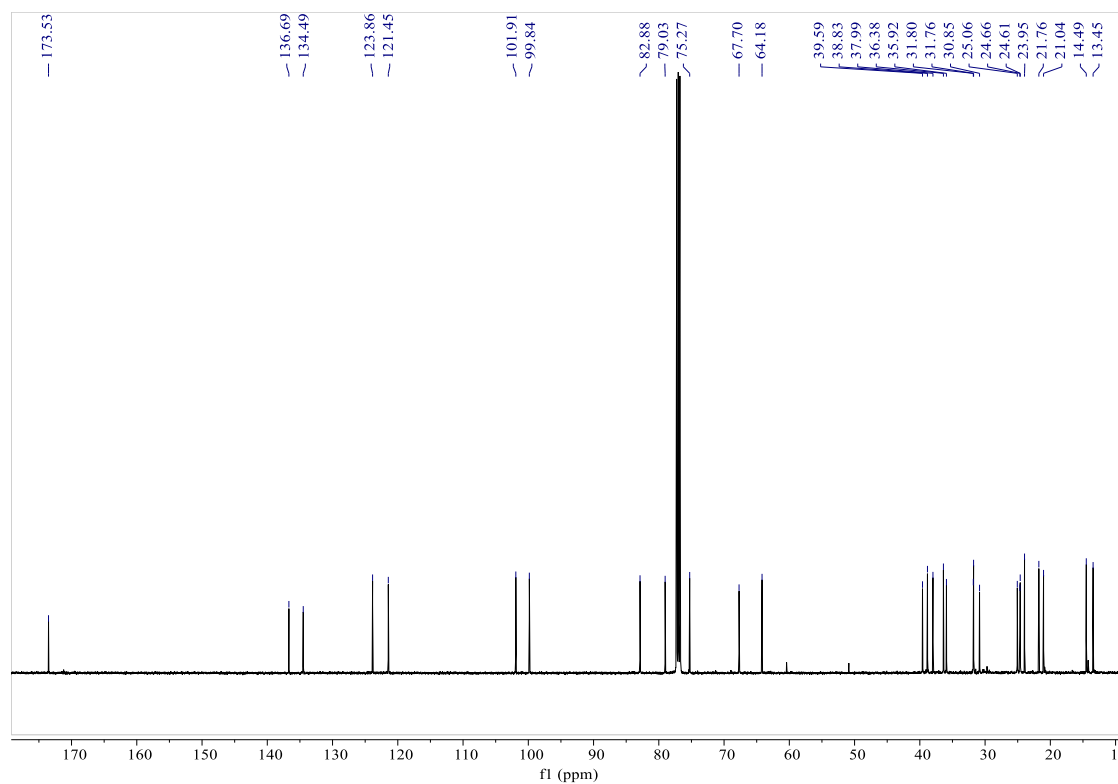


Figure S52 ¹³C NMR Spectrum of compound 8 (150 MHz; CDCl₃)

4.3 Spectroscopic data for compound 9

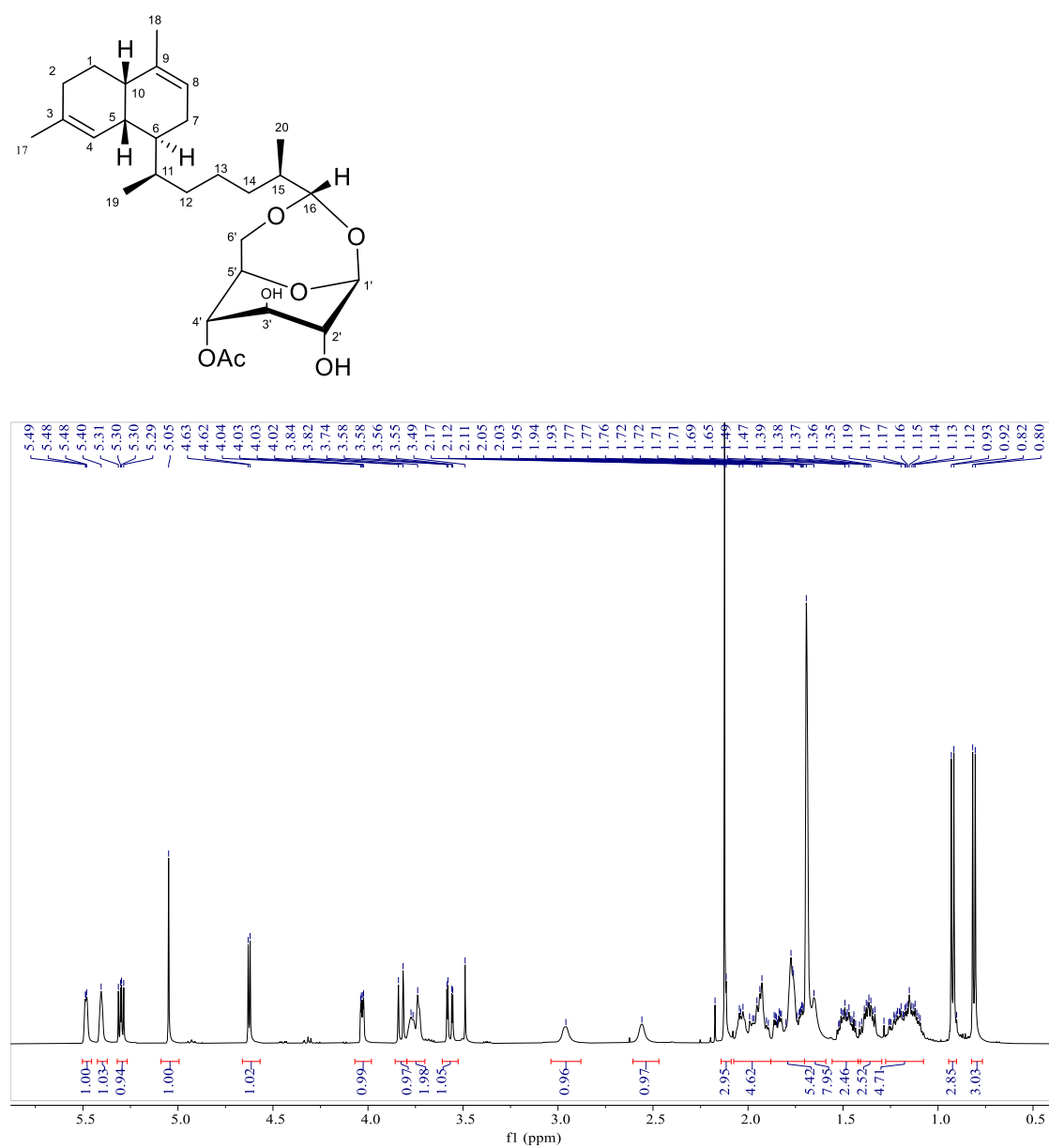


Figure S53 ^1H NMR Spectrum of compound 9 (600 MHz; CDCl_3)

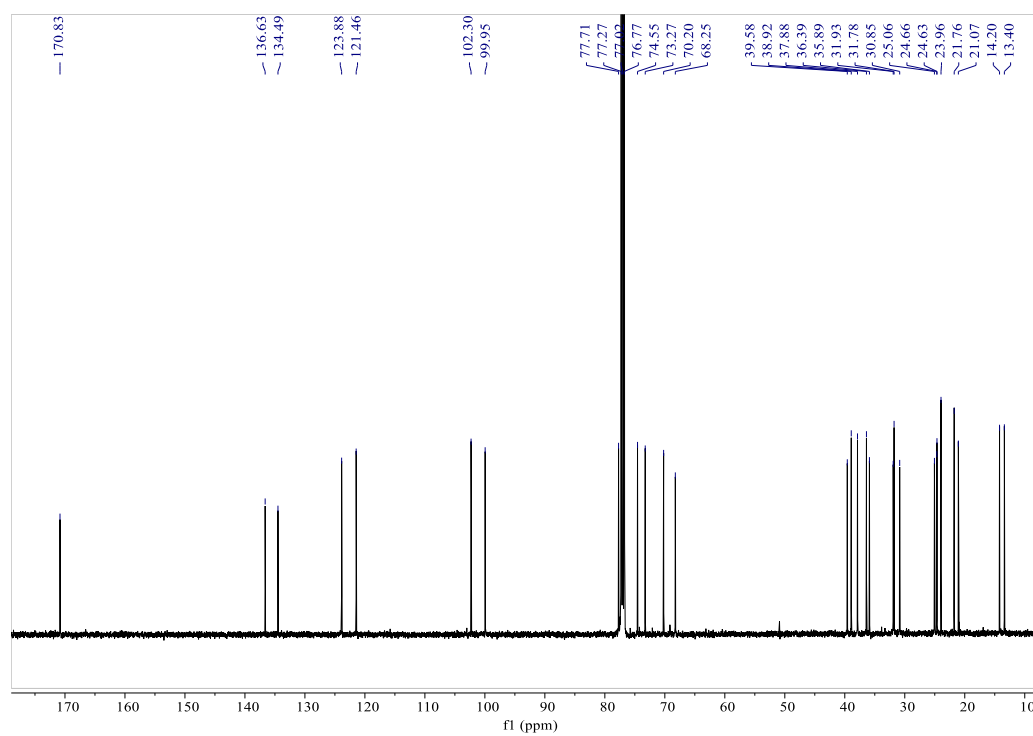
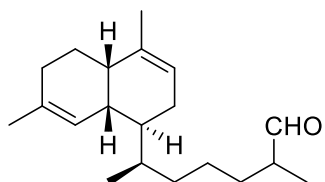


Figure S54 ^{13}C NMR Spectrum of compound 9 (150 MHz; CDCl_3)

2. ^1H NMR data for bicyclic diterpene aldehyde aglycon and bicyclic diterpene alcohol aglycon





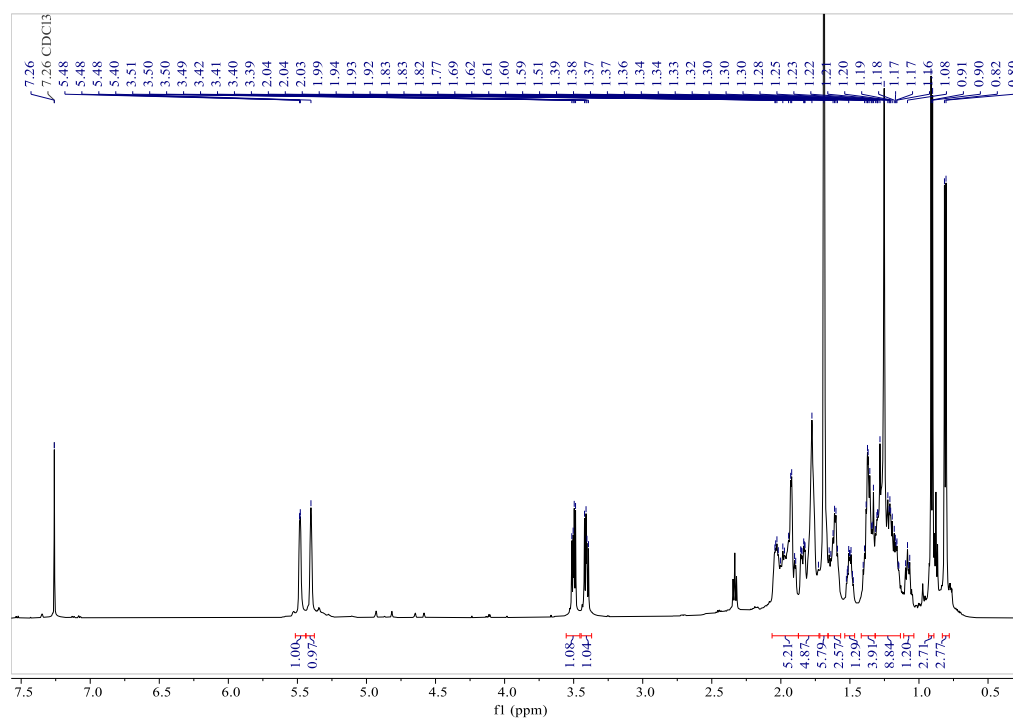
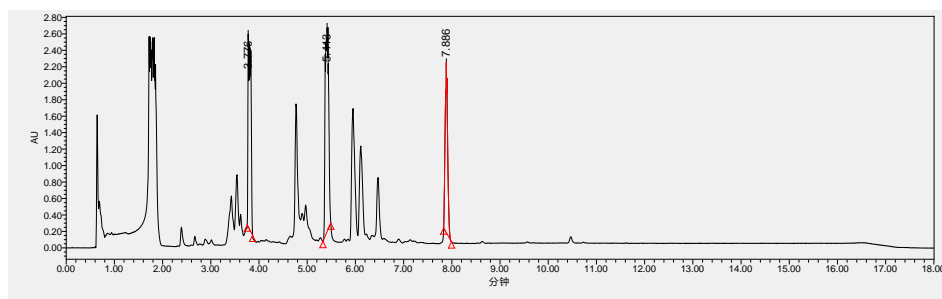


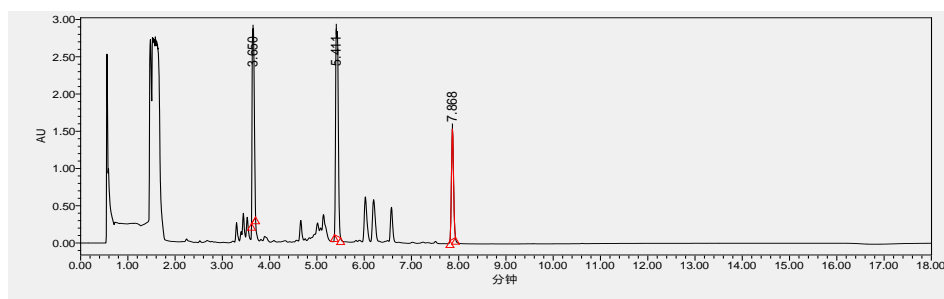
Figure S56 ^1H NMR Spectrum of aglycon of bicyclic diterpene alcohol aglycon (600 MHz; CDCl_3)

6. HPLC chromatograms of the sugar derivatives of compounds 1-6 and the standard D-glucose

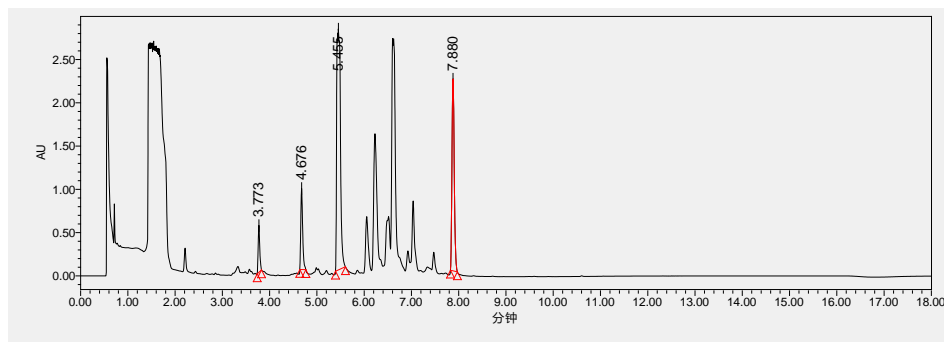
D-GLU



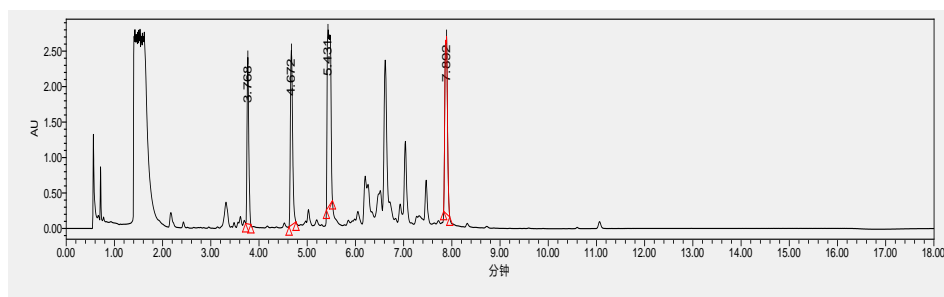
Compound 1



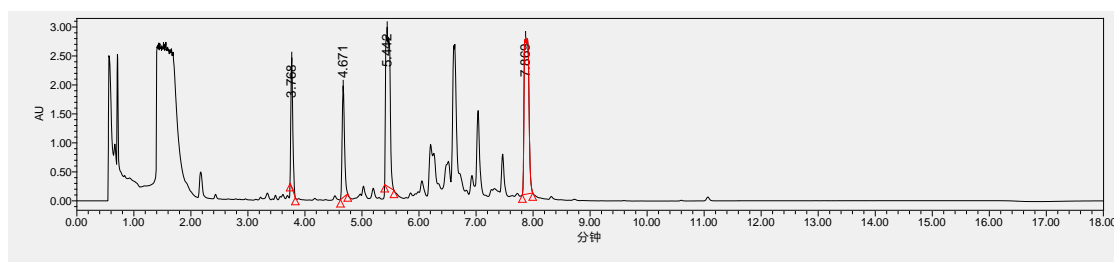
Compound 2



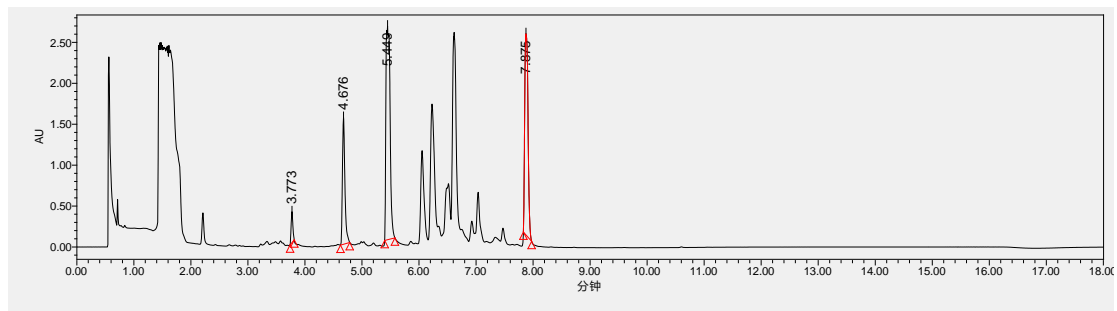
Compound 3



Compound 4



Compound 5



Compound 6

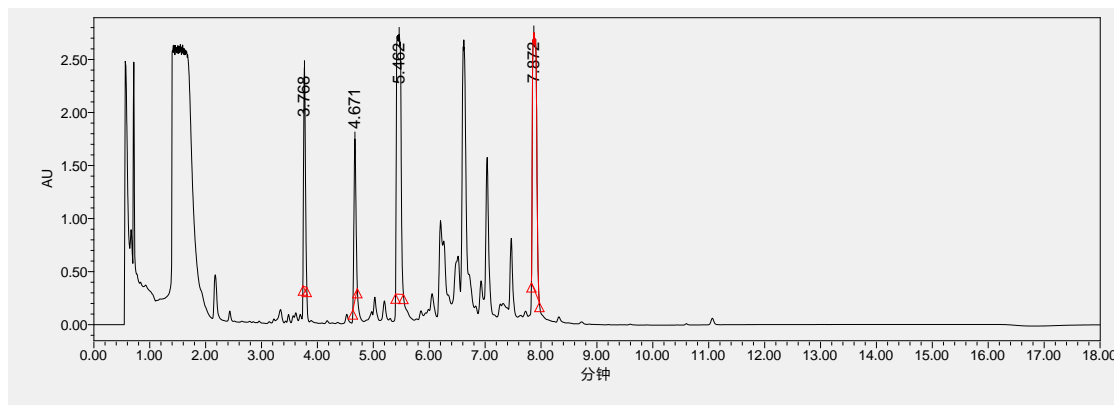


Figure S57 HPLC chromatograms of the sugar derivatives of compounds 1-6 and the standard D-glucose

7. Photos of *Lemnalia bournei* underwater and fresh sample after collected



Figure S58 Photos of *Lemnalia bournei* underwater and fresh sample after collected

8. Photomicrographs of the spicules extracted from *Lemnalia bournei*

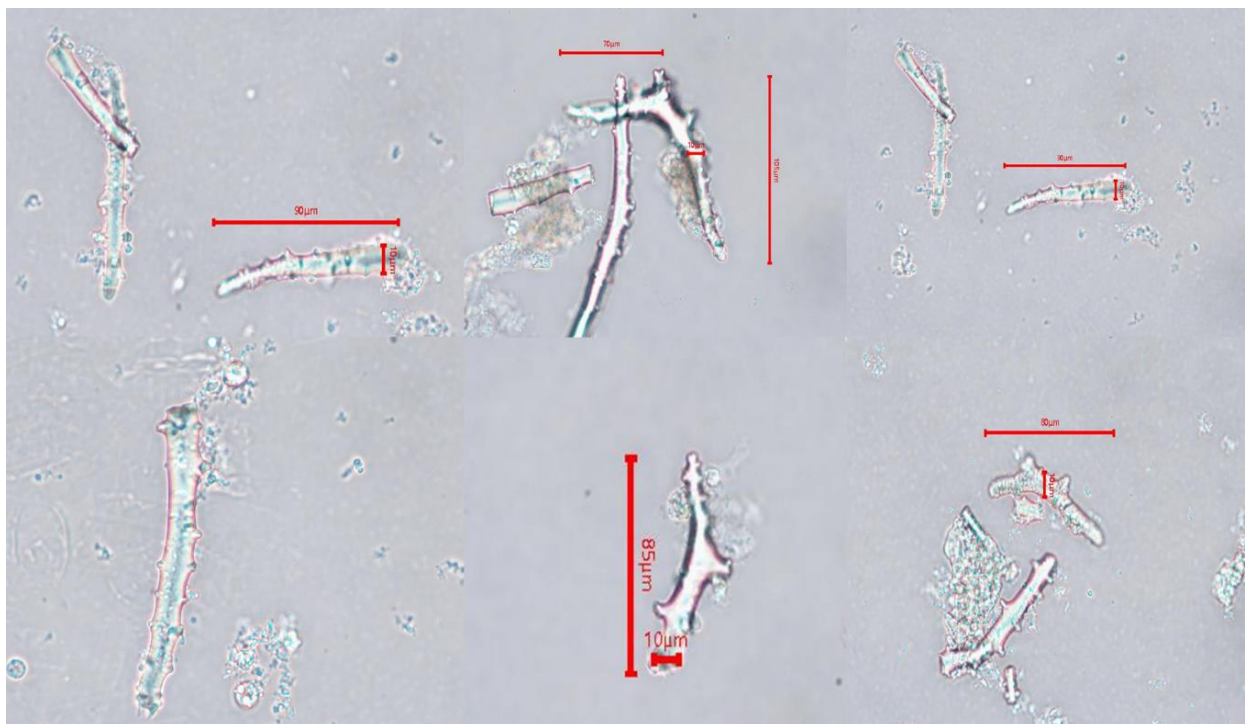


Figure S59 Photomicrographs of the spicules extracted from the soft coral. a) spicules from the tentacles; b) spicules from the cortex of the distal part of the stem; c) spicules from the cortex of the distal part of the stem