

Supporting Information

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Two New Prenylated Stilbenes with an Irregular Sesquiterpenyl Side Chain from Propolis from Fiji Islands

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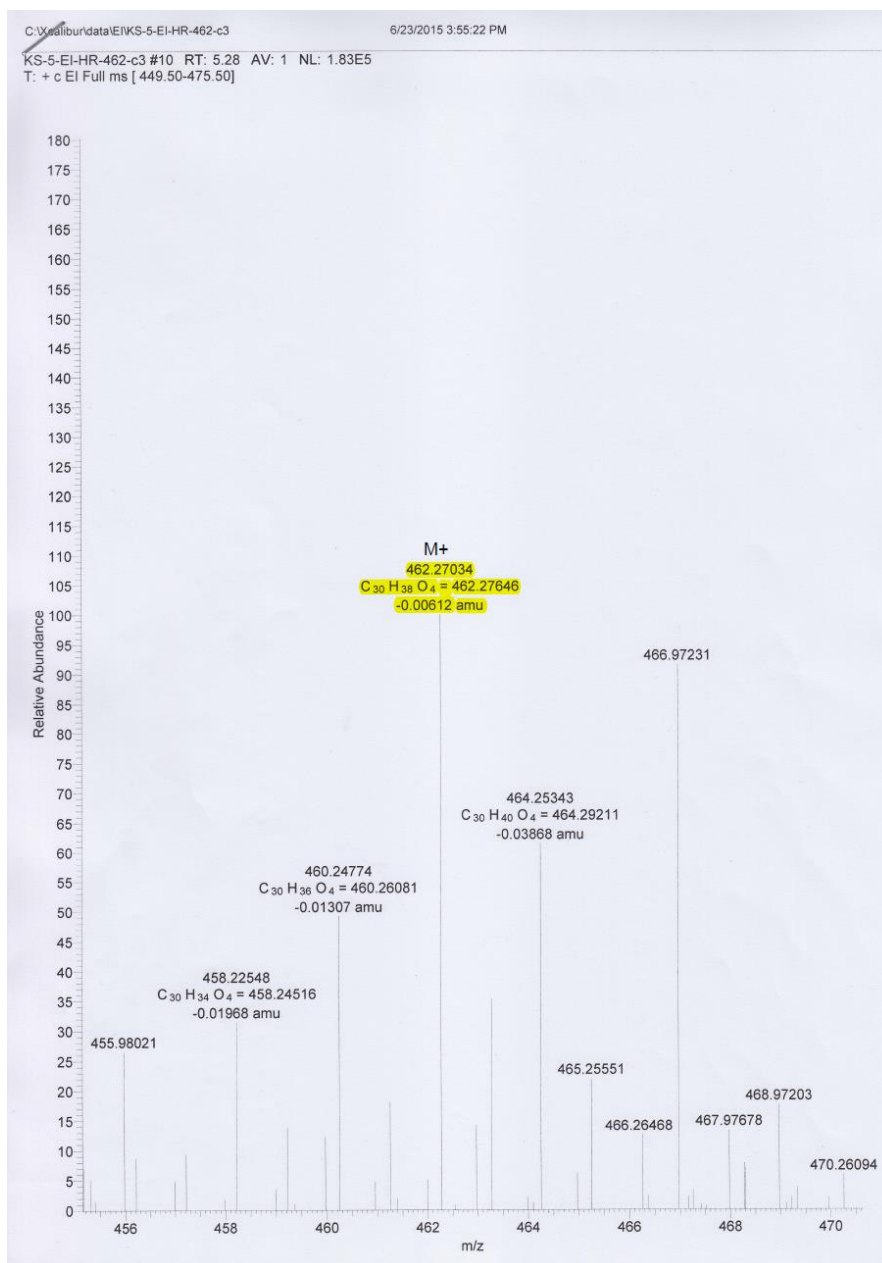
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²*Directorate of Medicinal and Aromatic Plants Research, Indian Council of Agricultural Research, 387 310 Boriavi, Anand, Gujarat, India*

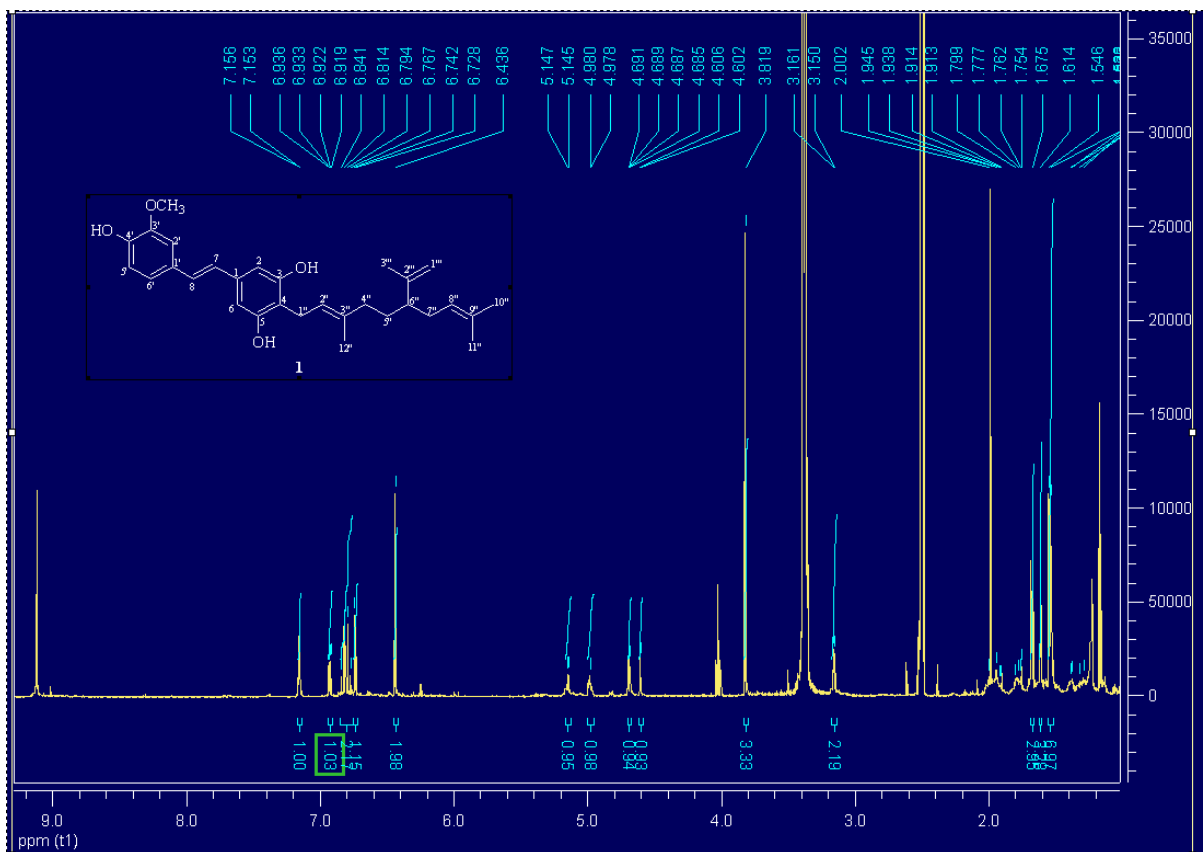
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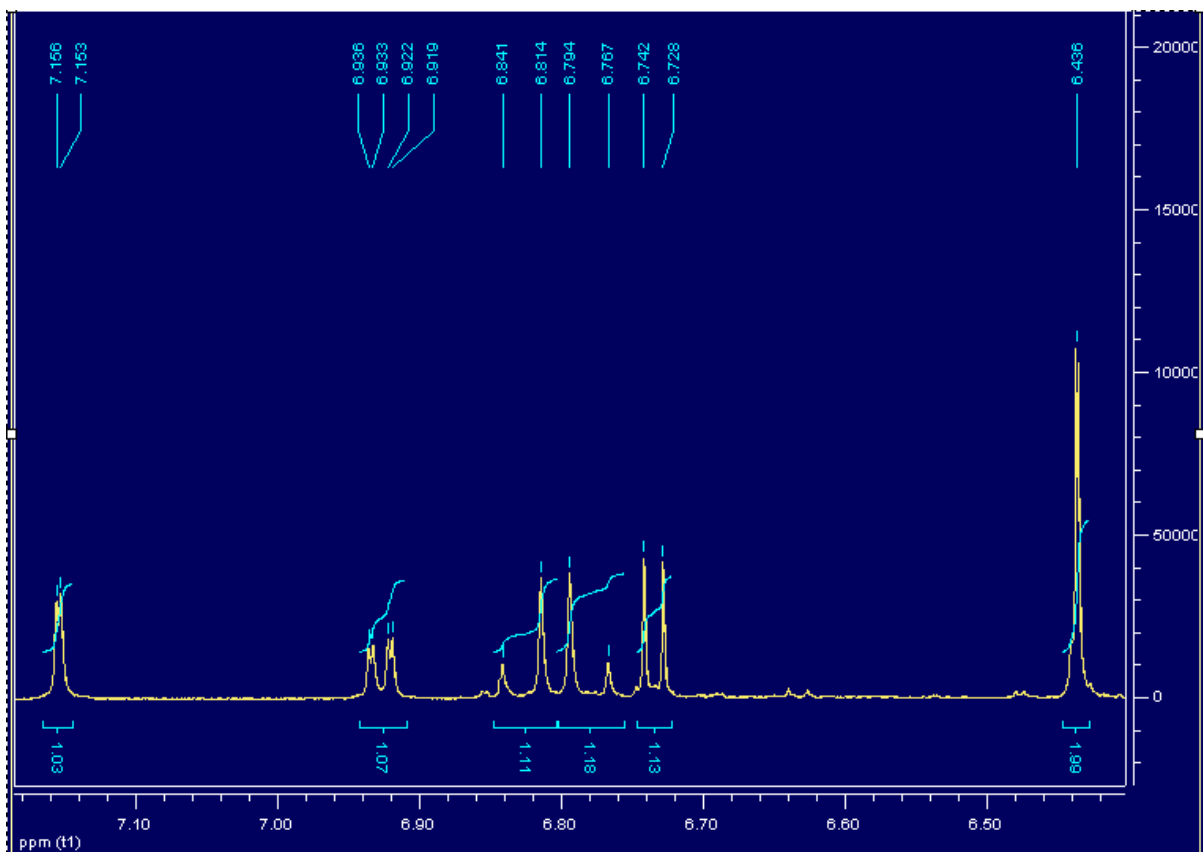


S1: Expansion of HREIMS Spectrum of Compound **1** (Solomonin B)

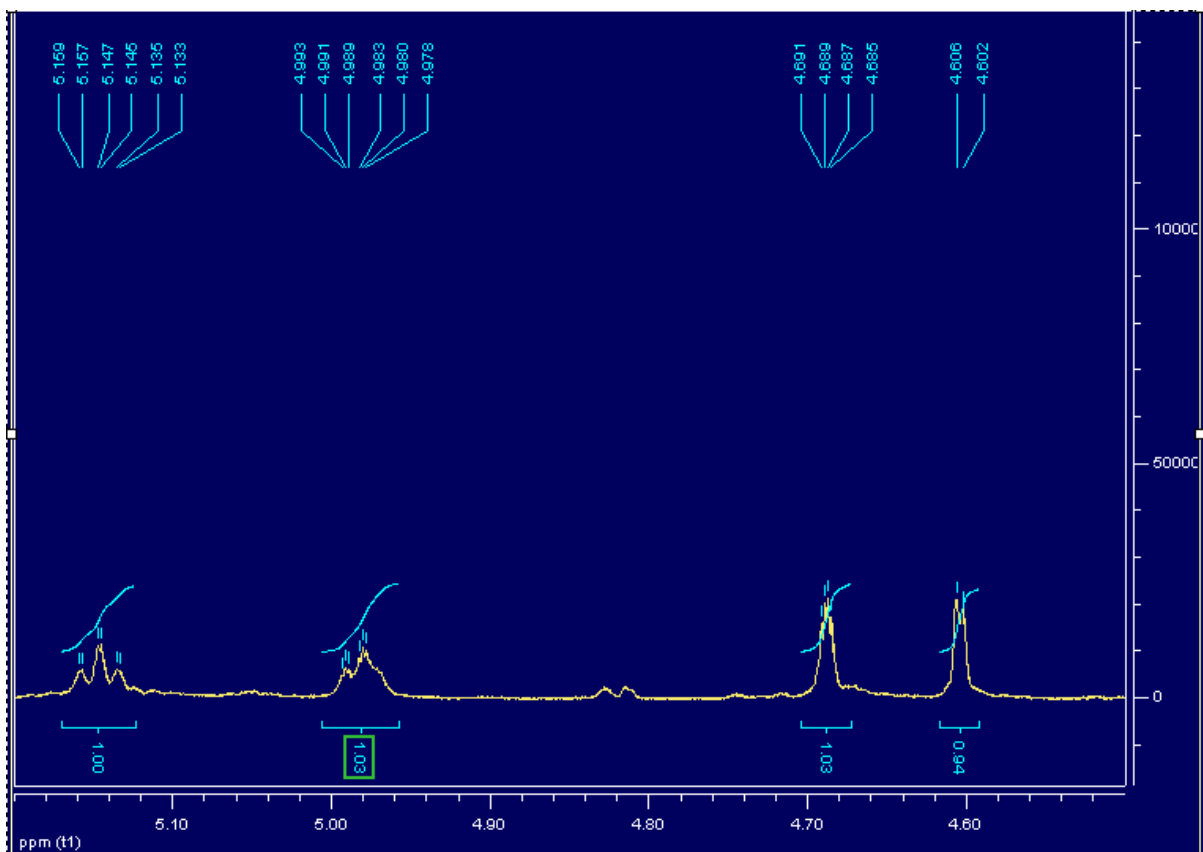


S2: ¹H-NMR (600 MHz, DMSO-*d*₆) Spectrum of Compound **1** (Solomonin B)

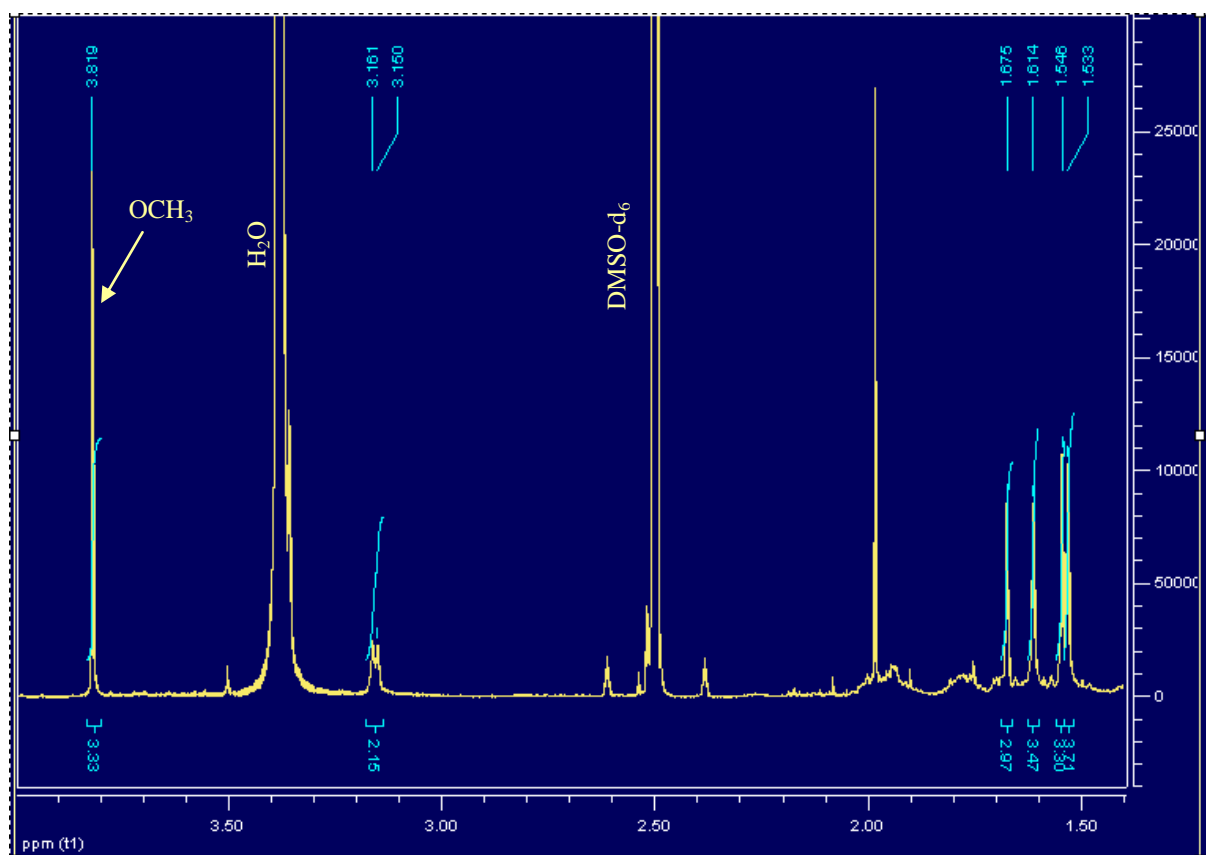
Solomonin B (**1**): yellow resin. ¹H-NMR (DMSO-*d*₆, 600 MHz), δ : 1.35 (m, H-5''), 1.53 (3H, s, H-10''), 1.55 (3H, s, H-3'''), 1.61 (3H, s, H-11''), 1.67 (3H, s, H-12''), 1.78 (m, H-4''), 1.94 (m, H-6''), 1.97 (m, H-7''), 3.16 (2H, d, H-1''), 3.82 (3H, s, OCH₃), 4.60 (1H, d, H-1''a), 4.69 (1H, q, H-1''b), 4.98 (1H, m, H-8''), 5.15 (1H, m, H-2''), 6.44 (2H, s, H-2/6), 6.74 (1H, d, H-5'), 6.78 (1H, d, H-8), 6.83 (1H, d, H-7), 6.92 (1H, dd, H-6'), 7.15 (1H, d, H-2'). ¹³C-NMR (DMSO-*d*₆, 150 MHz), δ : 135.5 (C-1), 104.2 (C-2/6), 156.0 (C-3/5), 113.8 (C-4), 125.9 (C-7), 127.1 (C-8), 128.6 (C-1'), 109.6 (C-2'), 147.8 (C-3'), 146.4 (C-4'), 115.5 (C-5'), 120.0 (C-6'), 55.6 (OCH₃), 22.0 (C-1''), 123.0 (C-2''), 133.1 (C-3''), 37.0 (C-4''), 30.5 (C-5''), 46.5 (C-6''), 31.7 (C-7''), 123.0 (C-8''), 131.0 (C-9''), 17.7 (C-10''), 25.6 (C-11''), 16.0 (C-12''), 111.3 (C-1'''), 147.2 (C-2'''), 18.4 (C-3'''). HREIMS: *m/z* 462.27034 (calc. for C₃₀H₃₈O₄).



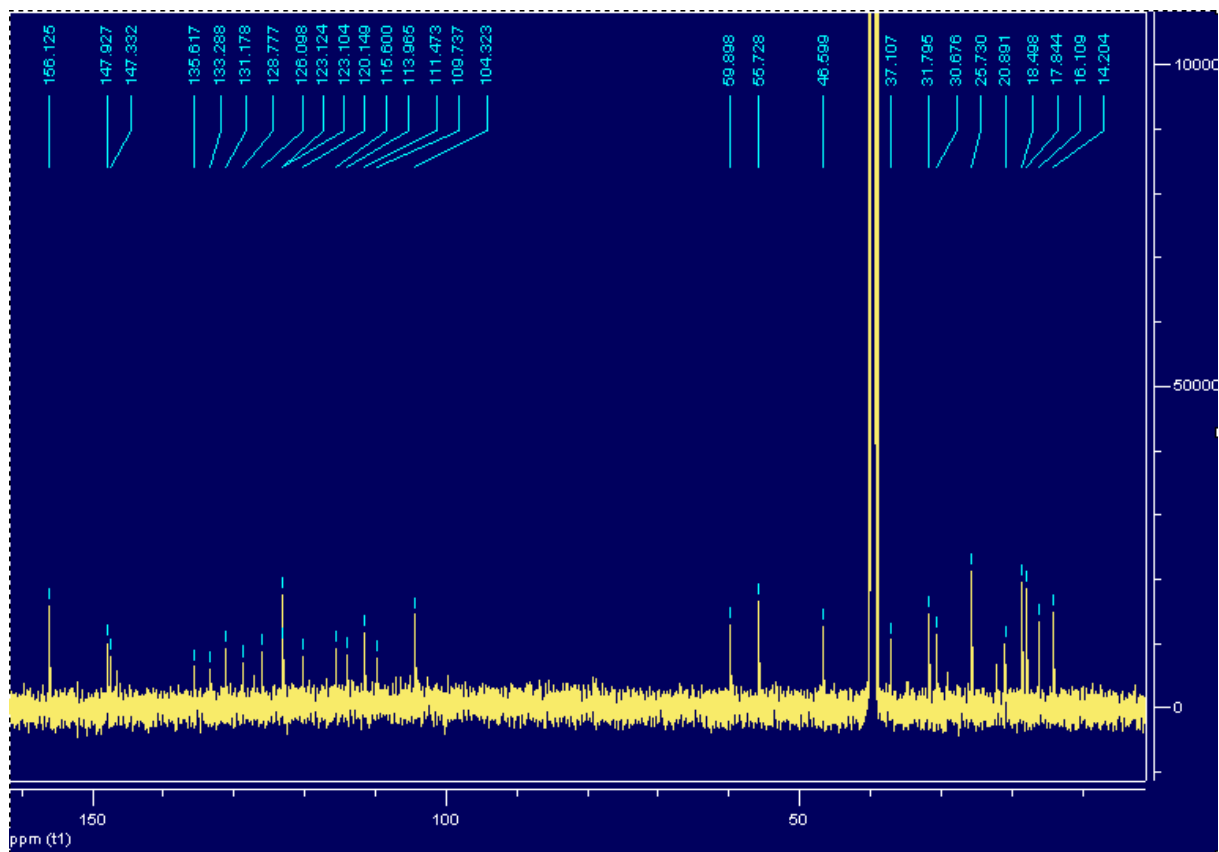
S3: ¹H-NMR Spectrum of Compound 1 (Solomonin B) (From 6.40 to 7.18 ppm)



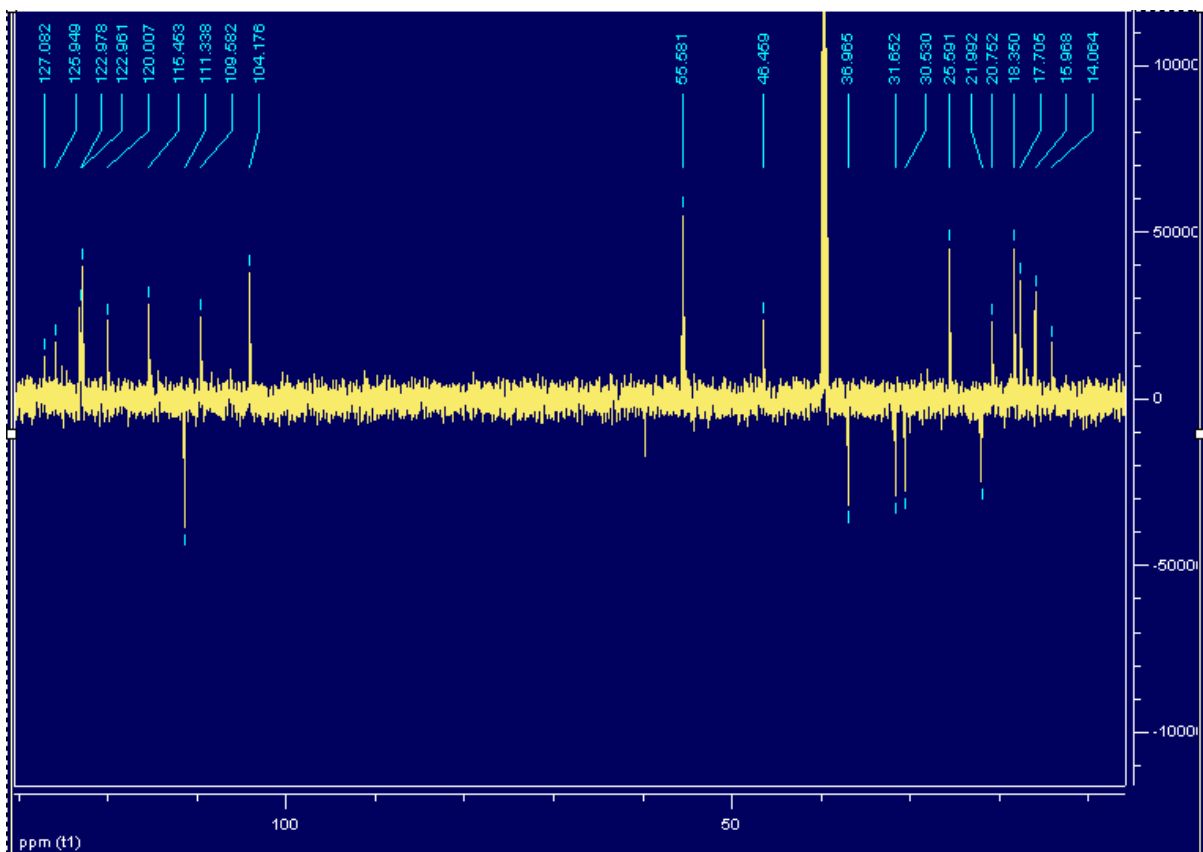
S4: ¹H-NMR Spectrum of Compound 1 (Solomonin B) (From 4.50 to 5.20 ppm)



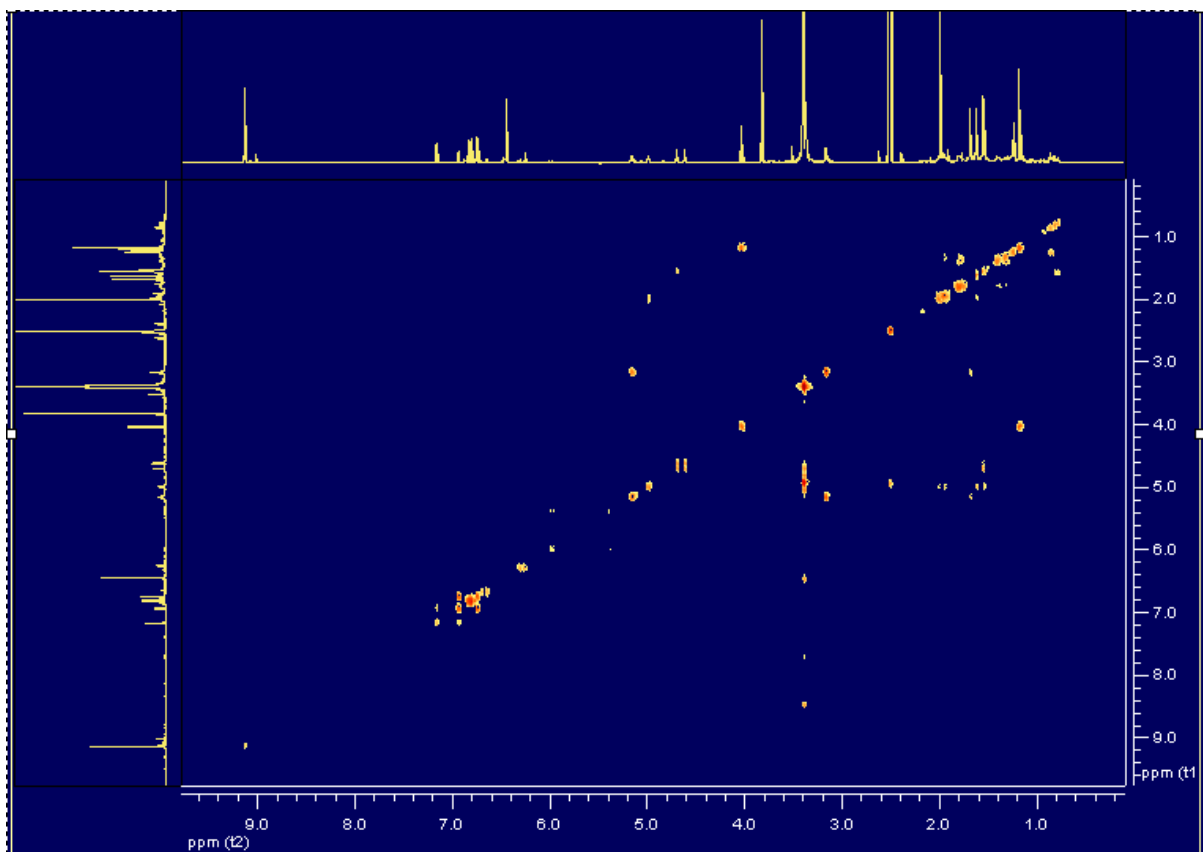
S5: ¹H-NMR Spectrum of Compound 1 (Solomonin B) (From 1.40 to 4.00 ppm)



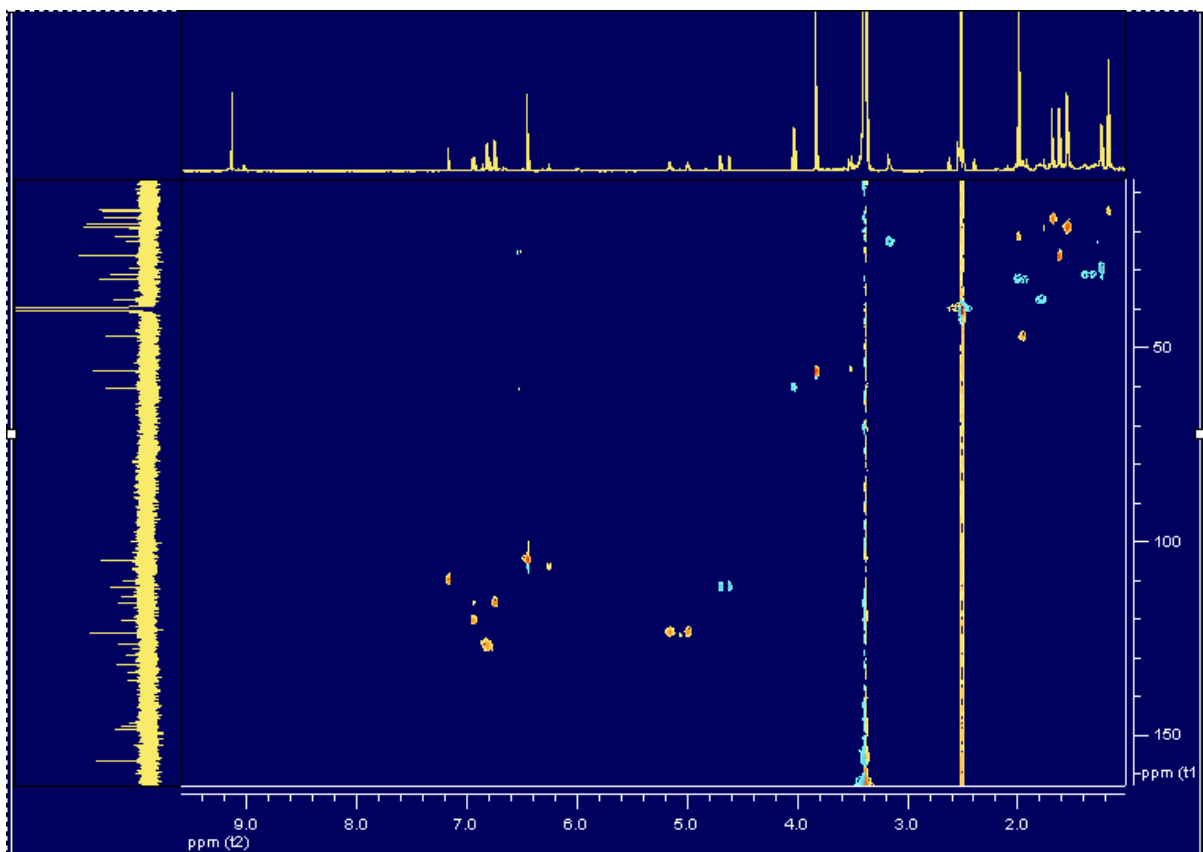
S6: ^{13}C -NMR (125 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **1** (Solomonin B)



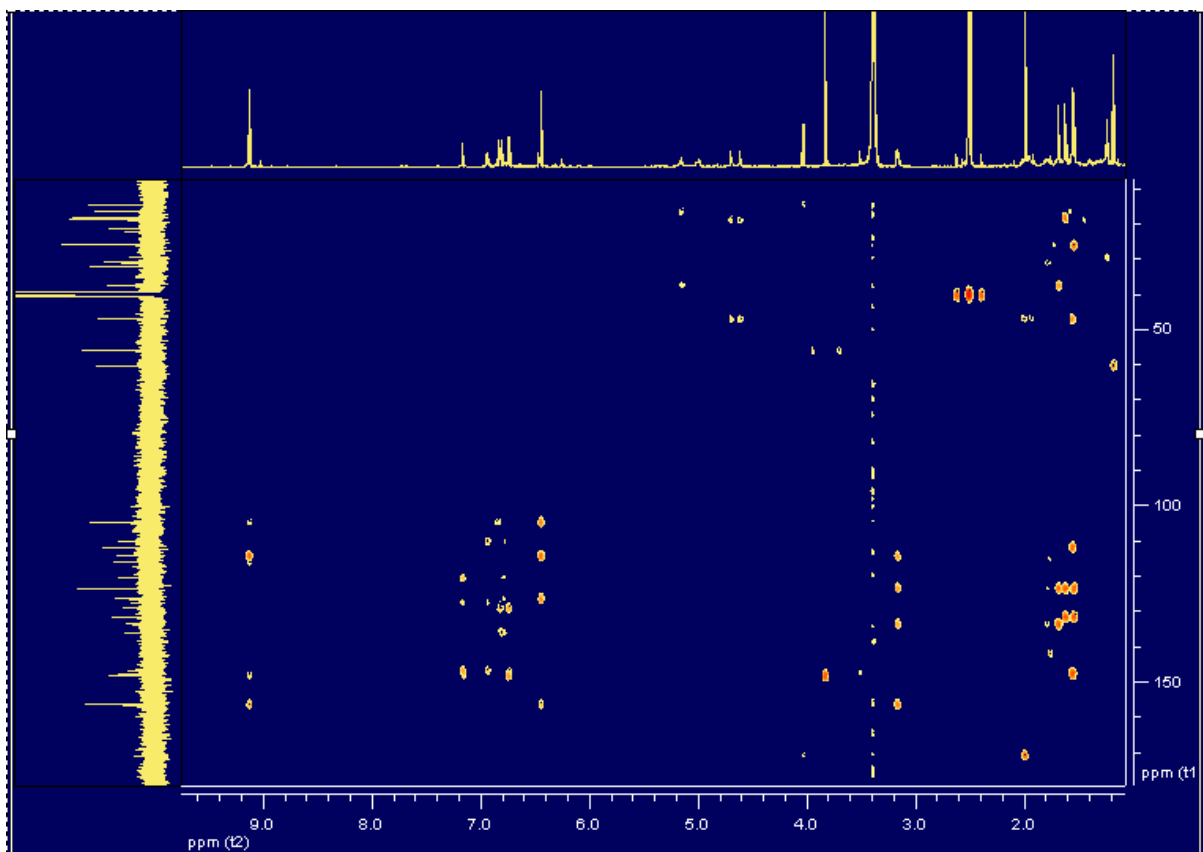
S7: DEPT (125 MHz, DMSO-*d*₆) Spectrum of Compound **1** (Solomonin B)



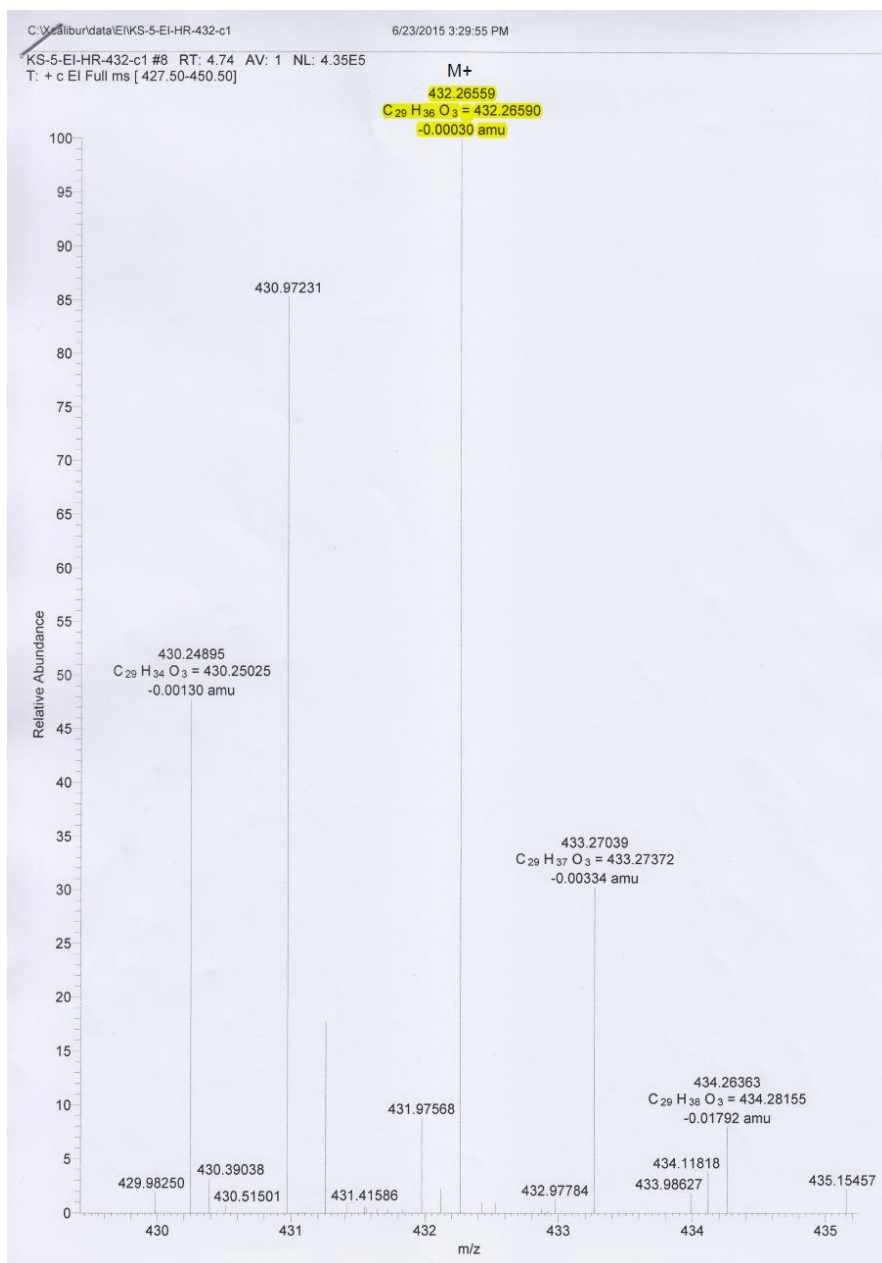
S8: COSY (600 MHz, DMSO-*d*₆) Spectrum of Compound **1** (Solomonin B)



S9: HSQC (600 MHz, DMSO- d_6) Spectrum of Compound **1** (Solomonin B)

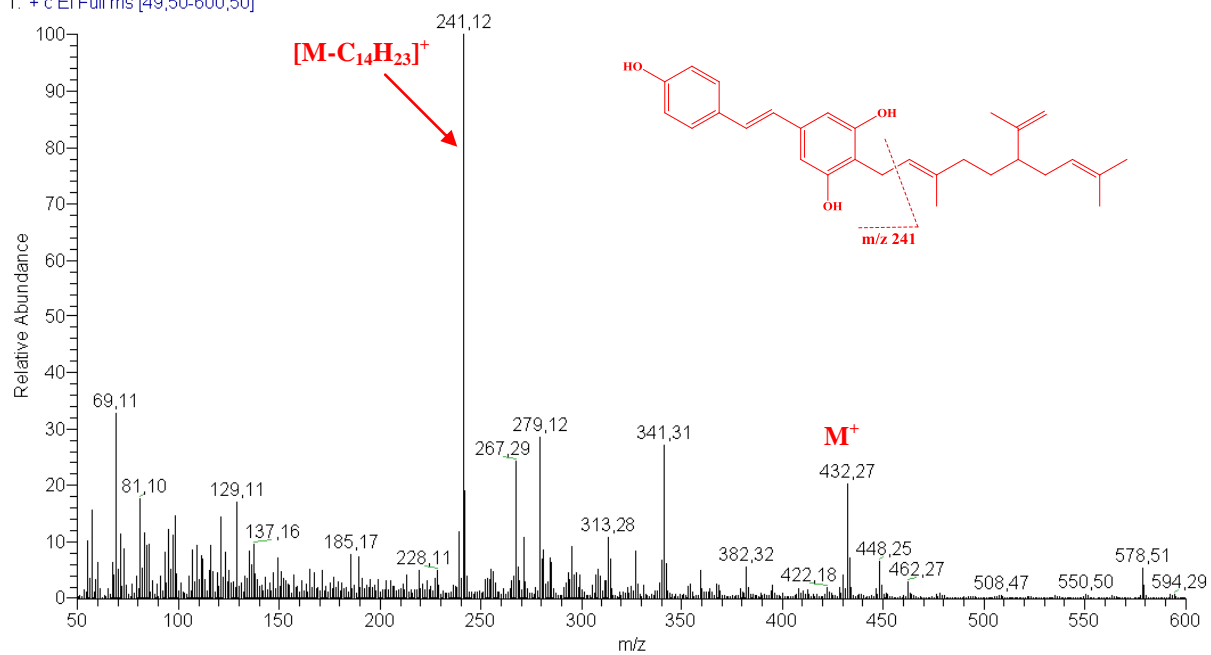


S10: HMBC (600 MHz, DMSO-*d*₆) Spectrum of Compound **1** (Solomonin B)

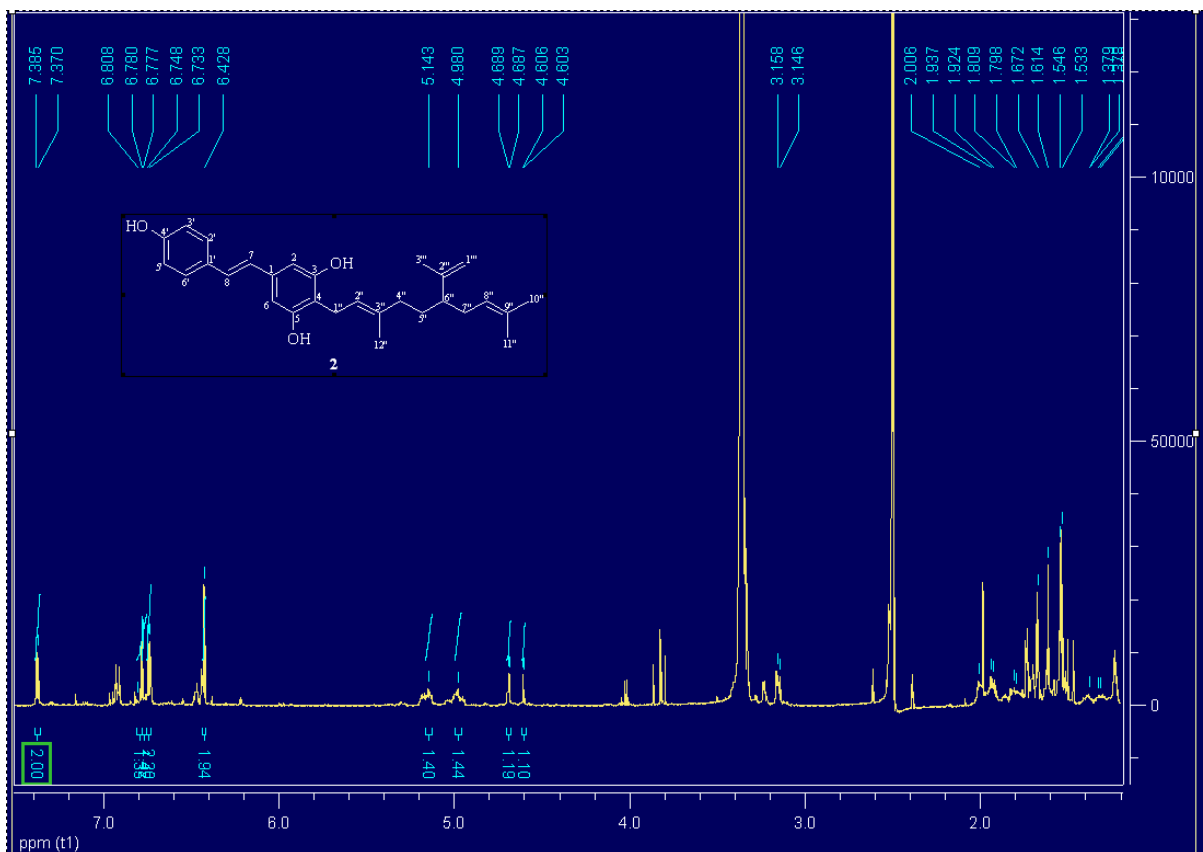


S11: Expansion of HREIMS Spectrum of Compound **2** (Solomonin C)

KS-5-b-ELLR #58 RT: 5,37 AV: 1 NL: 3,27E7
T: + c EI Full ms [49,50-600,50]

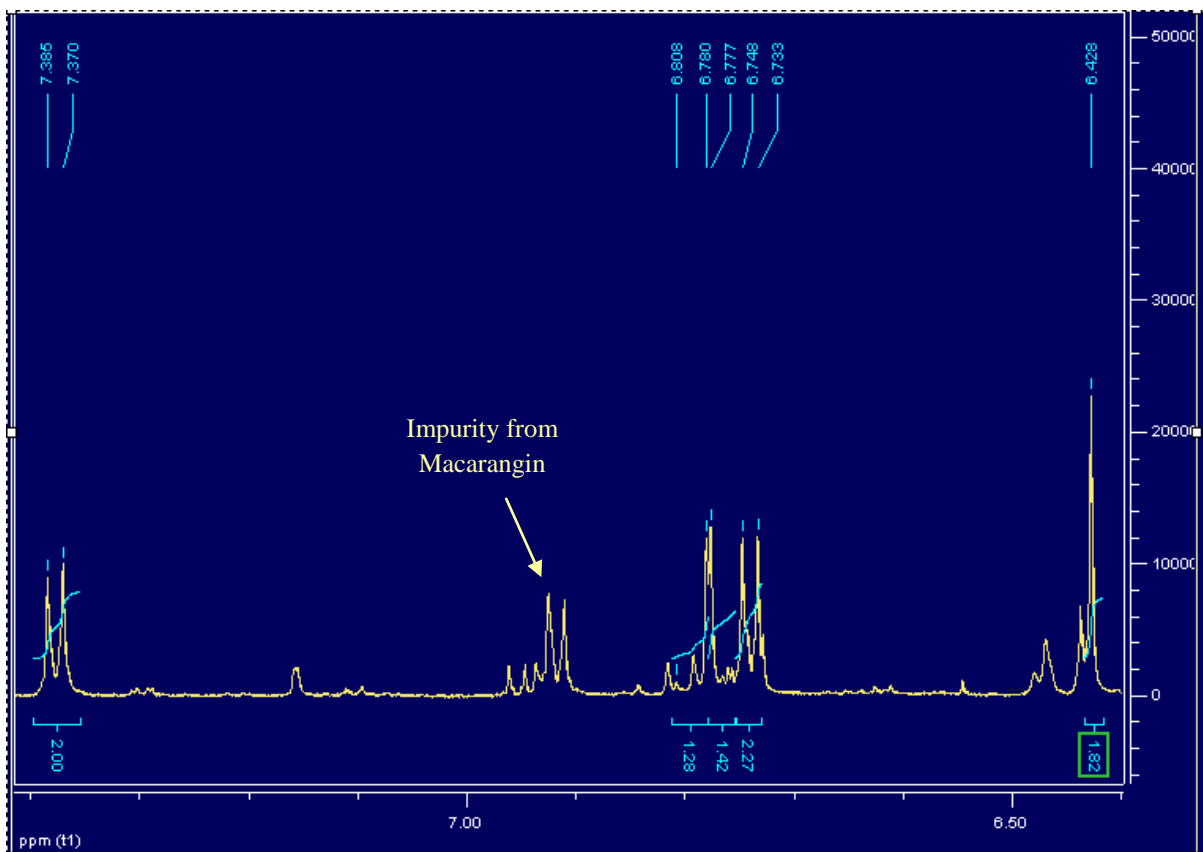


S12: EIMS Spectrum of Compound 2 (Solomonin C)

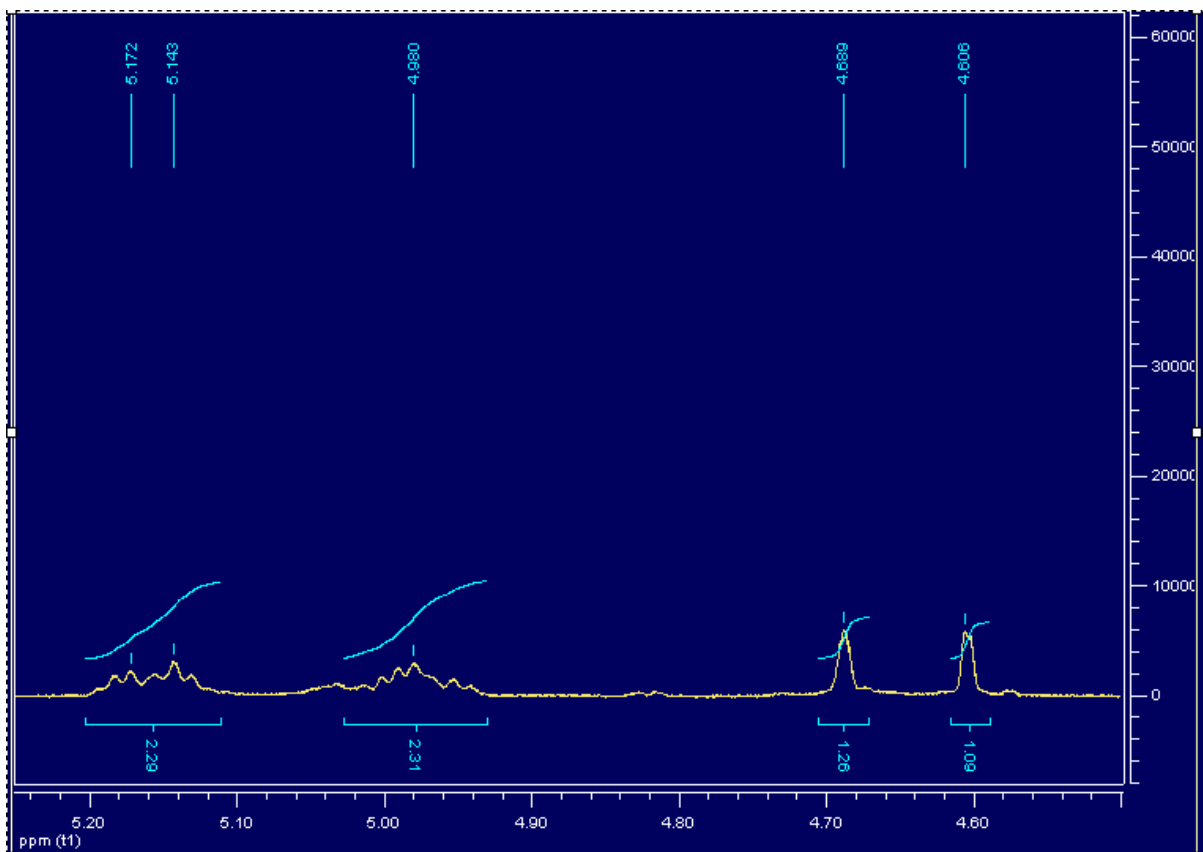


S13: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **2** (Solomonin C)

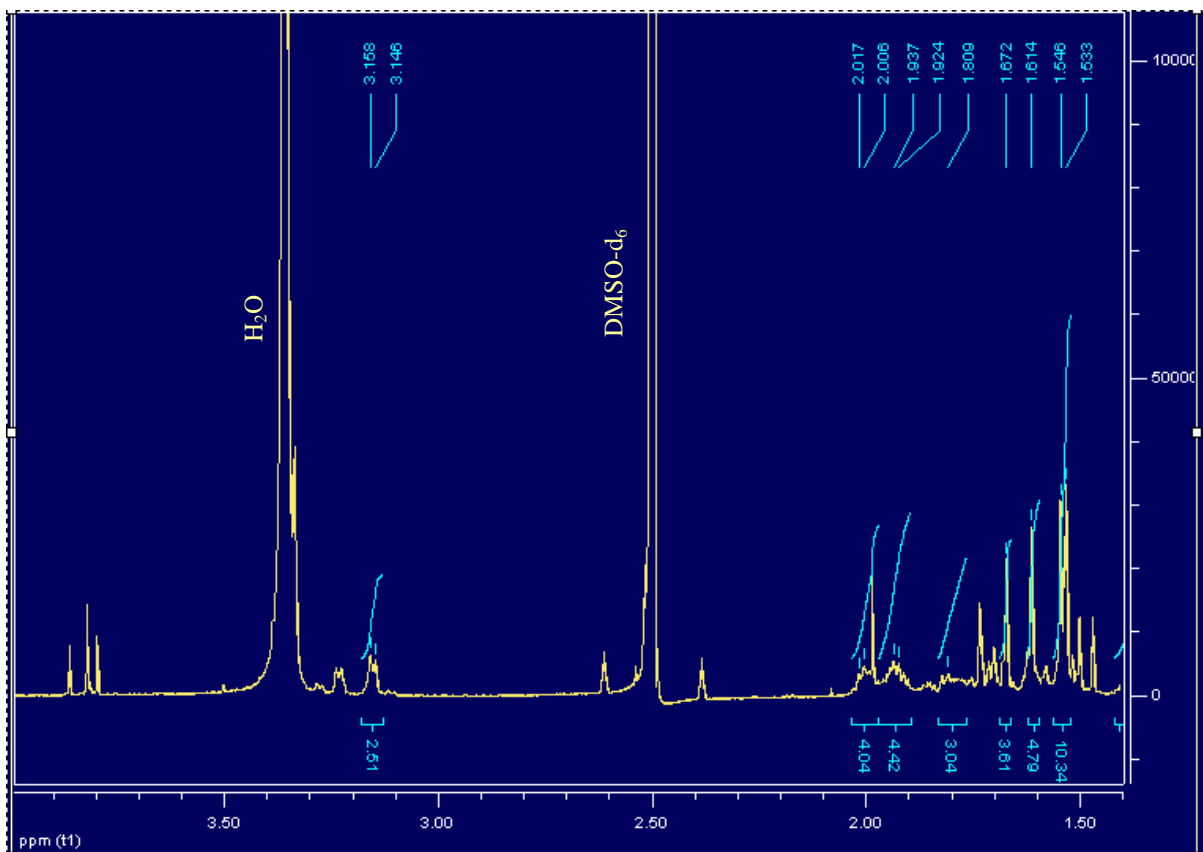
Solomonin C (**2**): yellow resin. $^1\text{H-NMR}$ ($\text{DMSO-}d_6$, 600 MHz), δ : 1.31 (m, H-5''a), 1.38 (m, H-5''b), 1.53 (3H, s, H-10''), 1.55 (3H, s, H-3'''), 1.61 (3H, s, H-11''), 1.67 (3H, s, H-12''), 1.79 (m, H-4''), 1.91 (m, H-6''), 1.93 (m, H-7''), 3.15 (2H, d, H-1''), 4.61 (1H, br. s, H-1'''a), 4.69 (1H, br. s, H-1'''b), 4.98 (1H, m, H-8''), 5.14 (1H, m, H-2''), 6.43 (2H, s, H-2/6), 6.74 (2H, d, H-3'/5'), 6.76 (1H, d, H-8), 6.79 (1H, d, H-7), 7.38 (2H, d, H-2'/6'). $^{13}\text{C-NMR}$ ($\text{DMSO-}d_6$, 150 MHz), δ : 135.7 (C-1), 104.4 (C-2/6), 156.3 (C-3/5), 114.0 (C-4), 126.0 (C-7), 127.3 (C-8), 128.5 (C-1'), 128.2 (C-2'/6'), 115.4 (C-3'/5'), 157.6 (C-4'), 22.4 (C-1''), 123.0 (C-2''), 133.4 (C-3''), 37.4 (C-4''), 30.4 (C-5''), 46.7 (C-6''), 32.1 (C-7''), 123.3 (C-8''), 131.3 (C-9''), 18.3 (C-10''), 26.2 (C-11''), 16.5 (C-12''), 111.6 (C-1'''), 147.3 (C-2'''), 18.6 (C-3'''). HREIMS: m/z 432.26559 (calc. for $\text{C}_{29}\text{H}_{36}\text{O}_3$).



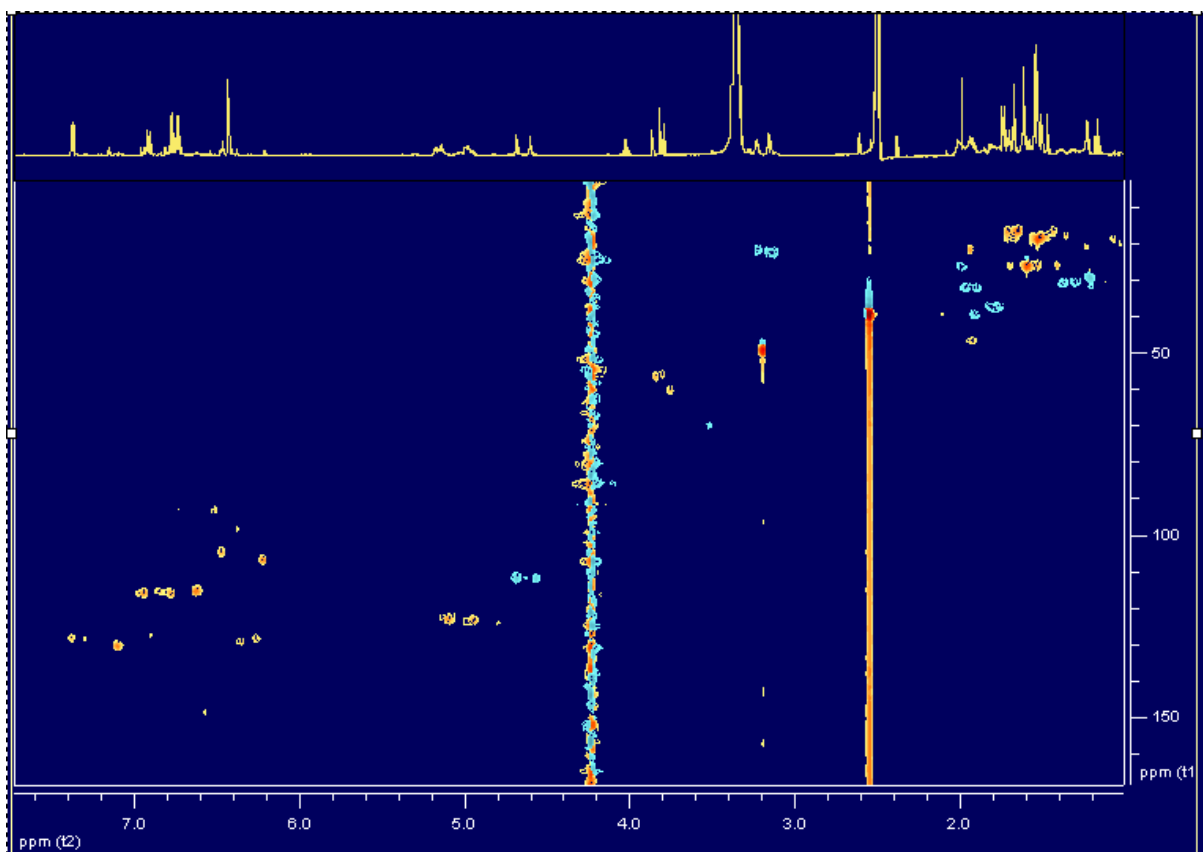
S14: ¹H-NMR Spectrum of Compound 2 (Solomonin C) (From 6.40 to 7.42 ppm)



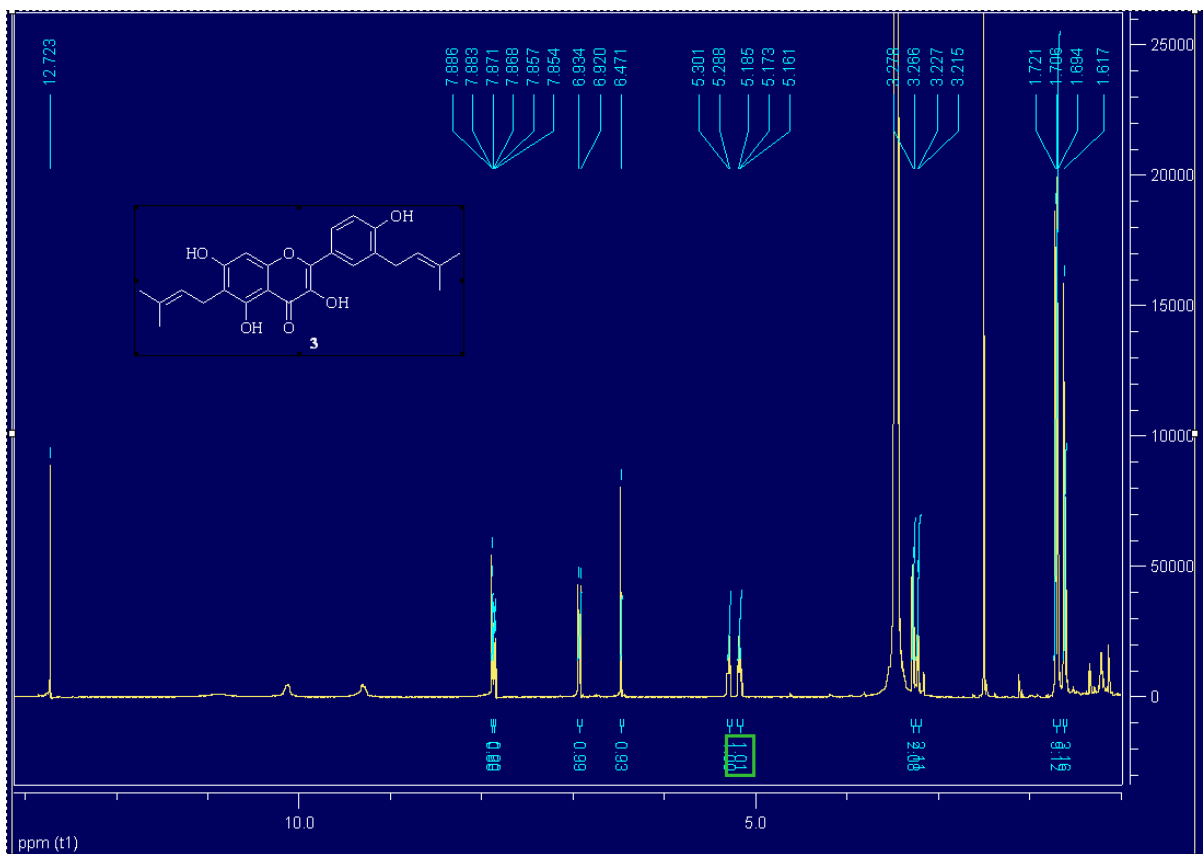
S15: ¹H-NMR Spectrum of Compound **2** (Solomonin C) (From 4.50 to 5.25 ppm)



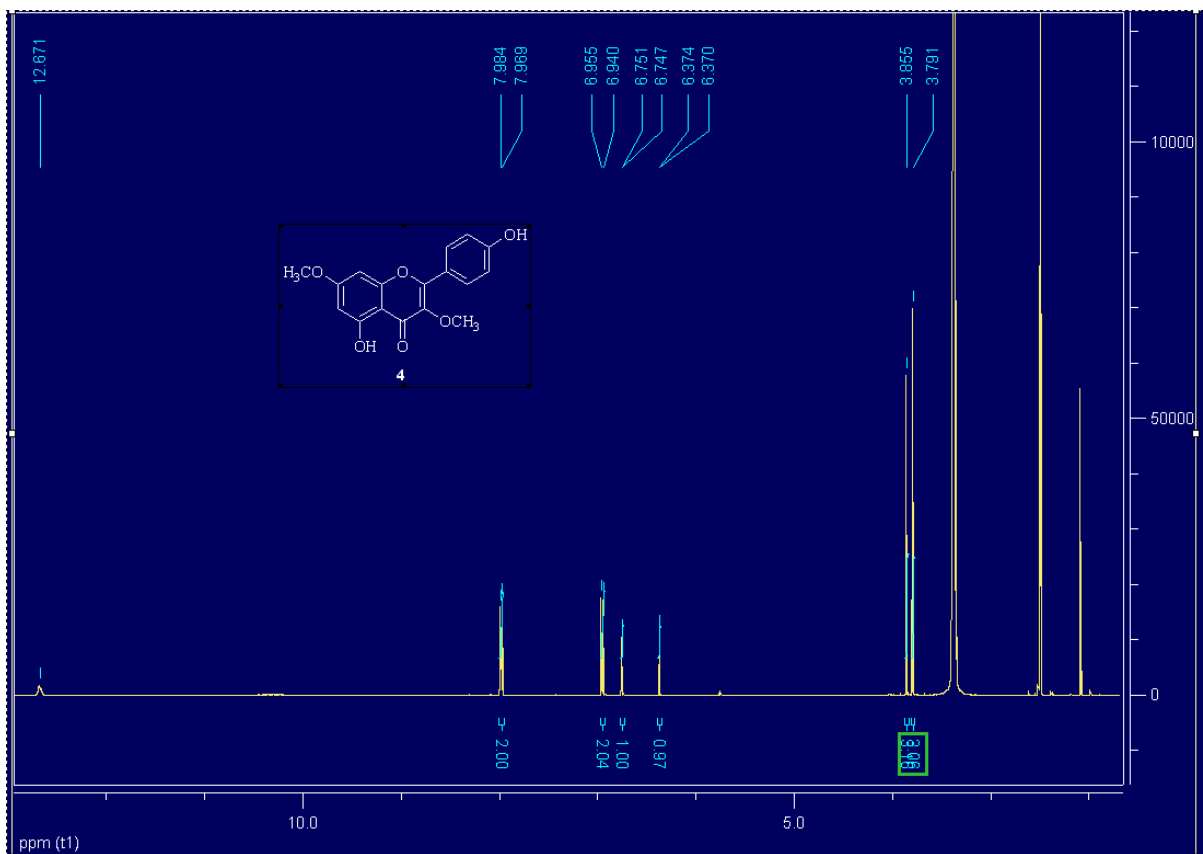
S16: $^1\text{H-NMR}$ Spectrum of Compound 2 (Solomonin C) (From 1.40 to 4.00 ppm)



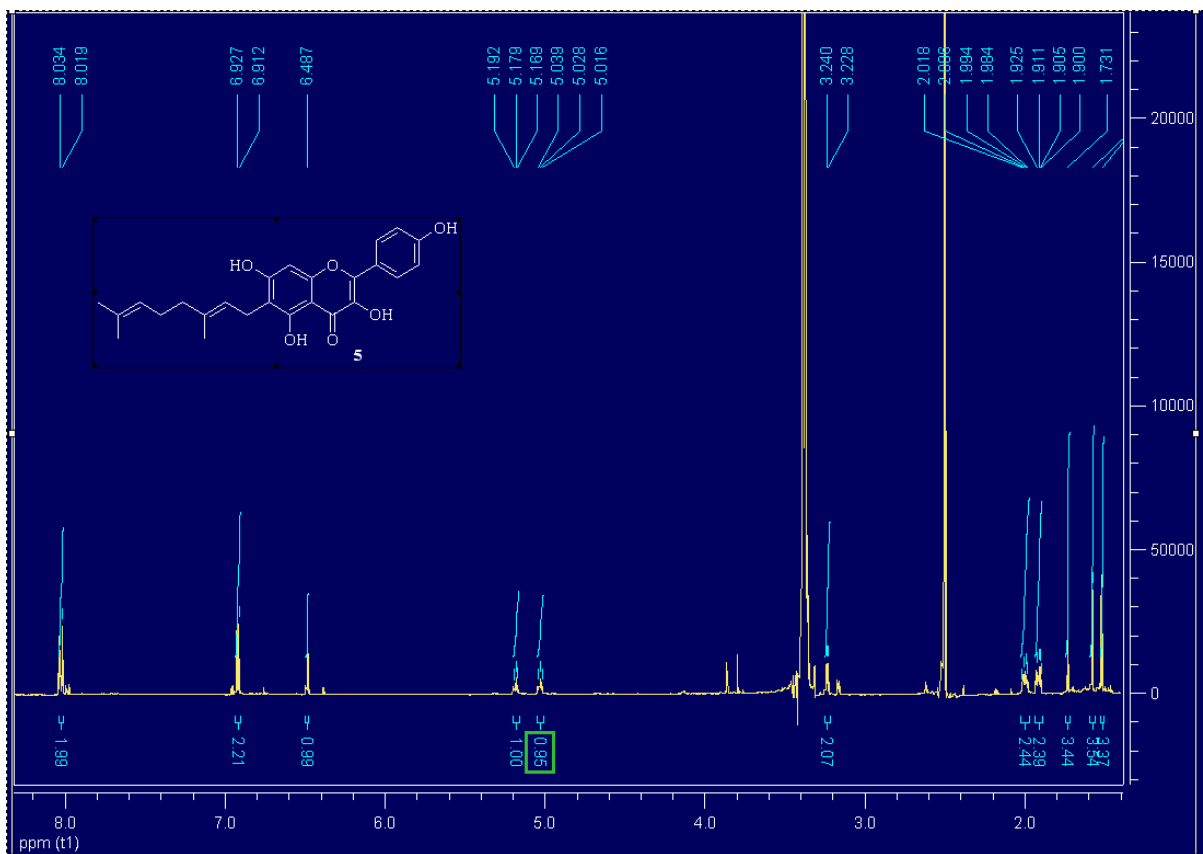
S17: HSQC (600 MHz, DMSO-*d*₆) Spectrum of Compound **2** (Solomonin C)



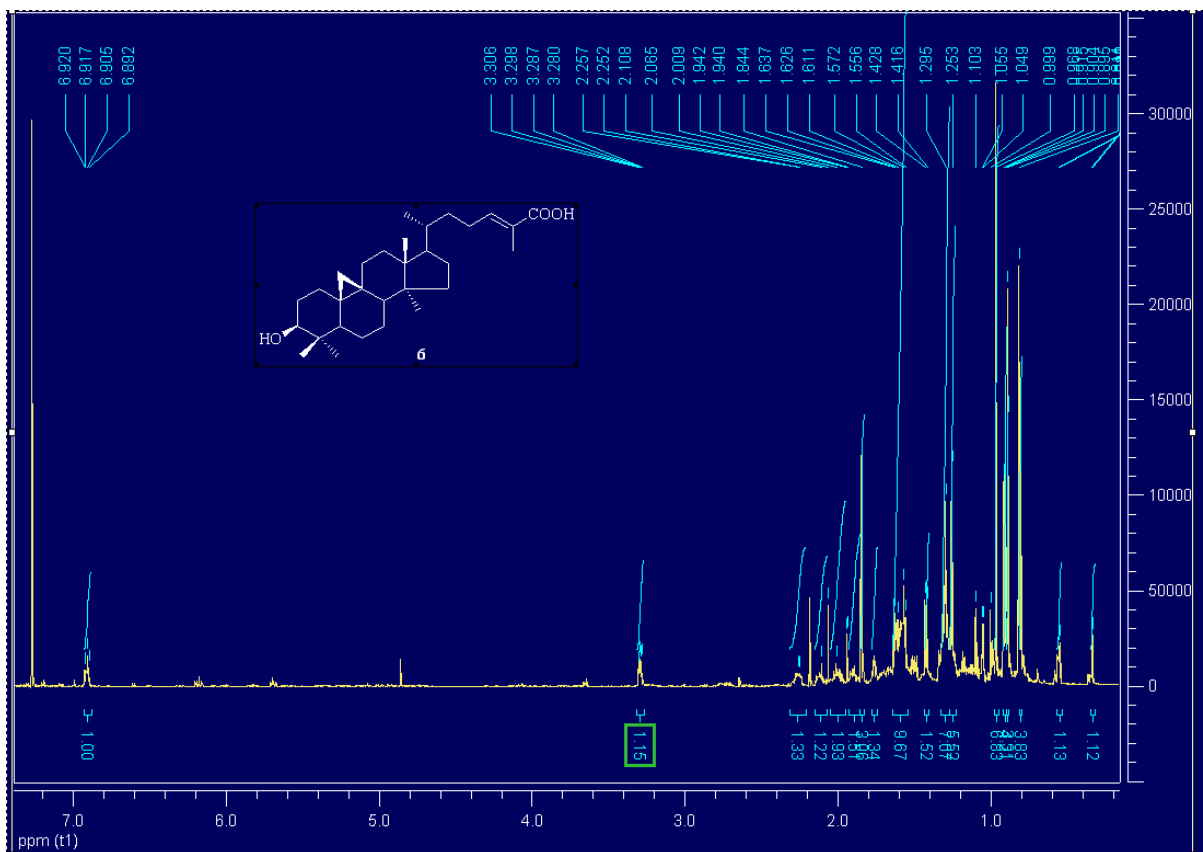
S18: ¹H-NMR (600 MHz, DMSO-*d*₆) Spectrum of Compound **3** (Glyasperin A)



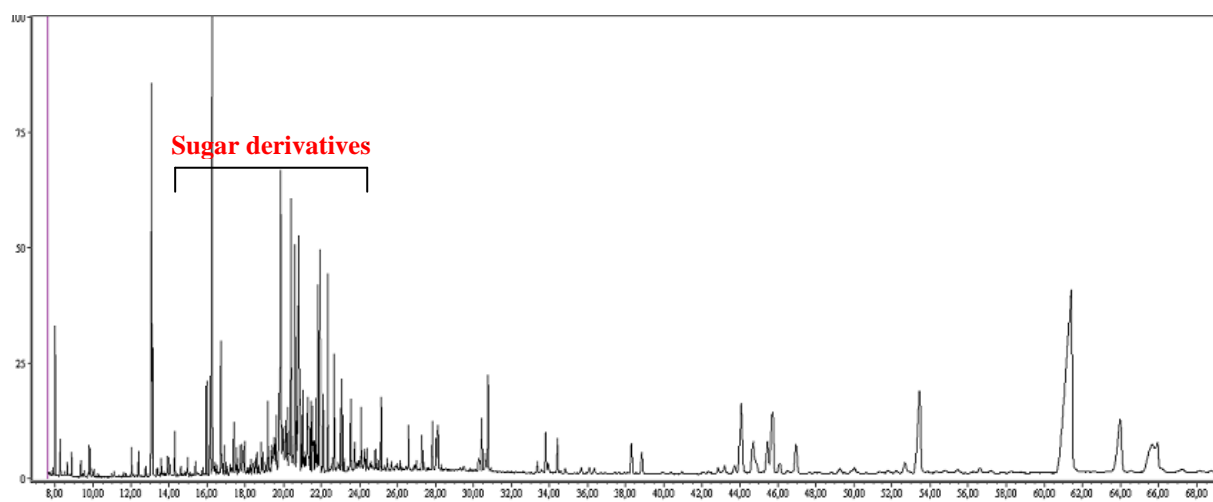
S19: ¹H-NMR (600 MHz, DMSO-*d*₆) Spectrum of Compound **4** (Kumatakenin)



S20: ¹H-NMR (600 MHz, DMSO-d₆) Spectrum of Compound 5 (Macarangin)



S21: $^1\text{H-NMR}$ (600 MHz, CDCl_3) Spectrum of Compound 6 (Mangiferolic acid)



S22: GC/MS fingerprint of ethanol extract of Fijian propolis (after silylation)