

Supplemental Information for:

Tuaimenals B-H, Merosesquiterpenes from the Irish Deep-Sea Soft Coral *Duva florida* with Bioactivity Against Cervical Cancer Cell Lines

Joshua T. Welsch,[†] Tracess B. Smalley,[‡] Jenet K. Matlack,[‡] Nicole E. Avalon,[†] Jennifer M.

Binning,[‡] Mark P. Johnson,[§] A. Louise Allcock,[§] Bill J. Baker[†]

[†] Department of Chemistry, University of South Florida, Tampa, FL, USA.

[‡] Molecular Oncology, Moffitt Cancer Research Center, Tampa, FL, USA.

[§] Department of Zoology, National University of Ireland Galway, Galway, Ireland.

	Page
Figure S1: Tuaimenal B (1) ¹ H NMR spectrum (600 MHz, CDCl ₃).	4
Figure S2: Tuaimenal B (1) ¹³ C NMR spectrum (150 MHz, CDCl ₃).	5
Figure S3: Tuaimenal B (1) HSQC NMR spectrum (500 MHz, CDCl ₃).	5
Figure S4: Tuaimenal B (1) HMBC NMR spectrum (500 MHz, CDCl ₃).	6
Figure S5: Tuaimenal B (1) COSY NMR spectrum (500 MHz, CDCl ₃).	6
Figure S6: Tuaimenal B (1) NOESY NMR spectrum (500 MHz, CDCl ₃).	7
Figure S7: Tuaimenal B (1) zoomed NOESY NMR spectrum (500 MHz, CDCl ₃).	7
Figure S8: Tuaimenal B (1) HRESIMS (neg).	8
Figure S9: Tuaimenal B (1) UV λ _{max} (C ₂ H ₃ N).	8
Figure S10: Tuaimenal B (1) IR spectrum (thin film).	9
Figure S11: Tuaimenal C (2) ¹ H NMR spectrum (800 MHz, CDCl ₃).	9
Figure S12: Tuaimenal C (2) ¹³ C NMR spectrum (200 MHz, CDCl ₃).	10
Figure S13: Tuaimenal C (2) HSQC NMR spectrum (800 MHz, CDCl ₃).	10
Figure S14: Tuaimenal C (2) HMBC NMR spectrum (800 MHz, CDCl ₃).	11
Figure S15: Tuaimenal C (2) COSY NMR spectrum (800 MHz, CDCl ₃).	11
Figure S16: Tuaimenal C (2) NOESY NMR spectrum (800 MHz, CDCl ₃).	12

Figure S17: Tuaimenal C (2) zoomed NOESY NMR spectrum (800 MHz, CDCl ₃).	12
Figure S18: Tuaimenal C (2) HREIMS.	13
Figure S19: Tuaimenal C (2) UV λ_{\max} (C ₂ H ₃ N).	13
Figure S20: Tuaimenal C (2) IR spectrum (thin film).	14
Figure S21: Tuaimenal D (3) ¹ H NMR spectrum (600 MHz, CDCl ₃).	14
Figure S22: Tuaimenal D (3) ¹³ C NMR spectrum (150 MHz, CDCl ₃).	15
Figure S23: Tuaimenal D (3) ¹³ C NMR spectrum zoomed (150 MHz, CDCl ₃).	15
Figure S24: Tuaimenal D (3) HSCQ NMR spectrum (500 MHz, CDCl ₃).	16
Figure S25: Tuaimenal D (3) HMBC NMR spectrum (500 MHz, CDCl ₃).	16
Figure S26: Tuaimenal D (3) COSY NMR spectrum (500 MHz, CDCl ₃).	17
Figure S27: Tuaimenal D (3) NOESY NMR spectrum (500 MHz, CDCl ₃).	17
Figure S28: Tuaimenal D (3) zoomed NOESY NMR spectrum (500 MHz, CDCl ₃).	18
Figure S29: Tuaimenal D (3) HRESIMS (neg).	18
Figure S30: Tuaimenal D (3) UV λ_{\max} (C ₂ H ₃ N).	19
Figure S31: Tuaimenal D (3) IR spectrum (thin film).	19
Figure S32: Tuaimenal E (4) ¹ H NMR spectrum (600 MHz, CDCl ₃).	20
Figure S33: Tuaimenal E (4) ¹³ C NMR spectrum (150 MHz, CDCl ₃).	20
Figure S34: Tuaimenal E (4) HSCQ NMR spectrum (500 MHz, CDCl ₃).	21
Figure S35: Tuaimenal E (4) HMBC NMR spectrum (500 MHz, CDCl ₃).	21
Figure S36: Tuaimenal E (4) COSY NMR spectrum (500 MHz, CDCl ₃).	22
Figure S37: Tuaimenal E (4) NOESY NMR spectrum (500 MHz, CDCl ₃).	22
Figure S38: Tuaimenal E (4) zoomed NOESY NMR spectrum (500 MHz, CDCl ₃).	23
Figure S39: Tuaimenal E (4) HRESIMS (neg).	23
Figure S40: Tuaimenal E (4) UV λ_{\max} (C ₂ H ₃ N).	24
Figure S41: Tuaimenal E (4) IR spectrum (thin film).	24
Figure S42: Tuaimenal F (5) ¹ H NMR spectrum (600 MHz, CDCl ₃).	25
Figure S43: Tuaimenal F (5) ¹³ C NMR spectrum (150 MHz, CDCl ₃).	25
Figure S44: Tuaimenal F (5) HSCQ NMR spectrum (500 MHz, CDCl ₃).	26
Figure S45: Tuaimenal F (5) HMBC NMR spectrum (500 MHz, CDCl ₃).	26
Figure S46: Tuaimenal F (5) COSY NMR spectrum (500 MHz, CDCl ₃).	27
Figure S47: Tuaimenal F (5) NOESY NMR spectrum (500 MHz, CDCl ₃).	27
Figure S48: Tuaimenal F (5) zoomed NOESY NMR spectrum (500 MHz, CDCl ₃).	28
Figure S49: Tuaimenal F (5) HRESIMS (neg).	28
Figure S50: Tuaimenal F (5) UV λ_{\max} (C ₂ H ₃ N).	29
Figure S51: Tuaimenal F (5) IR spectrum (thin film).	29
Figure S52: Tuaimenal G (6) ¹ H NMR spectrum (600 MHz, CDCl ₃).	30
Figure S53: Tuaimenal G (6) ¹³ C NMR spectrum (150 MHz, CDCl ₃).	30
Figure S54: Tuaimenal G (6) HSCQ NMR spectrum (500 MHz, CDCl ₃).	31
Figure S55: Tuaimenal G (6) HMBC NMR spectrum (500 MHz, CDCl ₃).	31
Figure S56: Tuaimenal G (6) COSY NMR spectrum (500 MHz, CDCl ₃).	32
Figure S57: Tuaimenal G (6) NOESY NMR spectrum (500 MHz, CDCl ₃).	32
Figure S58: Tuaimenal G (6) zoomed NOESY NMR spectrum (500 MHz, CDCl ₃).	33
Figure S59: Tuaimenal G (6) HRESIMS (pos).	33
Figure S60: Tuaimenal G (6) UV λ_{\max} (C ₂ H ₃ N).	34
Figure S61: Tuaimenal G (6) IR spectrum (thin film).	34
Figure S62: Tuaimenal H (7) ¹ H NMR spectrum (600 MHz, CDCl ₃).	35

Figure S63: Tuaimenal H (7) ^{13}C NMR spectrum (150 MHz, CDCl_3).	35
Figure S64: Tuaimenal H (7) HSCQ NMR spectrum (500 MHz, CDCl_3).	36
Figure S65: Tuaimenal H (7) HMBC NMR spectrum (500 MHz, CDCl_3).	36
Figure S66: Tuaimenal H (7) COSY NMR spectrum (500 MHz, CDCl_3).	37
Figure S67: Tuaimenal H (7) NOESY NMR spectrum (500 MHz, CDCl_3).	37
Figure S68: Tuaimenal H (7) zoomed NOESY NMR spectrum (500 MHz, CDCl_3).	38
Figure S69: Tuaimenal H (7) HRESIMS (neg).	38
Figure S70: Tuaimenal H (7) UV λ_{max} ($\text{C}_2\text{H}_3\text{N}$).	39
Figure S71: Tuaimenal H (7) IR spectrum (thin film).	39
Figure S72: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (8) ^1H NMR spectrum (600 MHz, MeOD).	40
Figure S73: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (8) ^{13}C NMR spectrum (150 MHz, MeOD).	40
Figure S74: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (8) HSCQ NMR spectrum (500 MHz, MeOD).	41
Figure S75: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (8) HMBC NMR spectrum (500 MHz, MeOD).	41
Figure S76: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (8) COSY NMR spectrum (500 MHz, MeOD).	42
Figure S77: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (8) NOESY NMR spectrum (500 MHz, MeOD).	42
Figure S78: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (8) HRESIMS (neg).	43
Figure S79: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (8) UV λ_{max} ($\text{C}_2\text{H}_3\text{N}$).	43
Figure S80: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (8) IR spectrum (thin film).	44
Figure S81: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (8) X-ray crystal structure.	44
Figure S82: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (8) X-ray crystallography metadata and ellipsoid plot with anisotropic displacement parameters drawn at 50% probability.	45
Figure S83: Methyl 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (9) ^1H NMR spectrum (600 MHz, CDCl_3).	46
Figure S84: Methyl 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (9) ^{13}C NMR spectrum (150 MHz, CDCl_3).	46
Figure S85: Methyl 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (9) HSCQ NMR spectrum (500 MHz, CDCl_3).	47
Figure S86: Methyl 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (9) HMBC NMR spectrum (500 MHz, CDCl_3).	47
Figure S87: Methyl 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (9) COSY NMR spectrum (500 MHz, CDCl_3).	48
Figure S88: Methyl 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (9) NOESY NMR spectrum (500 MHz, CDCl_3).	48
Figure S89: Methyl 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (9) HRESIMS (pos).	49

Figure S90: 19-norchola-1,3,5(10)-trien-24-oic acid, 3-hydroxy-, methyl ester (9) UV λ_{\max} (C ₂ H ₃ N).	49
Figure S91: 19-norchola-1,3,5(10)-trien-24-oic acid, 3-hydroxy-, methyl ester (9) IR spectrum (thin film).	50
Figure S92: Tuaimenal A (10) ¹ H NMR spectrum (600 MHz, CDCl ₃).	50
Figure S93: Tuaimenal A (10) ¹³ C NMR spectrum (150 MHz, CDCl ₃).	51
Figure S94: Tuaimenal A (10) HSCQ NMR spectrum (500 MHz, CDCl ₃).	51
Figure S95: Tuaimenal A (10) HMBC NMR spectrum (500 MHz, CDCl ₃).	52
Figure S96: Tuaimenal A (10) COSY NMR spectrum (500 MHz, CDCl ₃).	52
Figure S97: Tuaimenal A (10) NOESY NMR spectrum (500 MHz, CDCl ₃).	53
Figure S98: Tuaimenal A (10) zoomed NOESY NMR spectrum (500 MHz, CDCl ₃).	53
Figure S99: Tuaimenal A (10) HRESIMS (neg).	54
Figure S100: Tuaimenal A (10) UV λ_{\max} (C ₂ H ₃ N).	54
Figure S101: Tuaimenal A (10) IR spectrum (thin film).	55
Table S1: Comparison of tuaimenal A (10) ¹ H and ¹³ C spectra to literature.	56
Table S2: Comparison of <i>Duva florida</i> steroids (8 and 9) ¹³ C NMR spectra to literature.	57
Figure S102: Integrated chromatogram displaying relative abundance of <i>R</i> and <i>S</i> enantiomers of tuaimenal E (4) separated utilizing a chiral HPLC column.	58

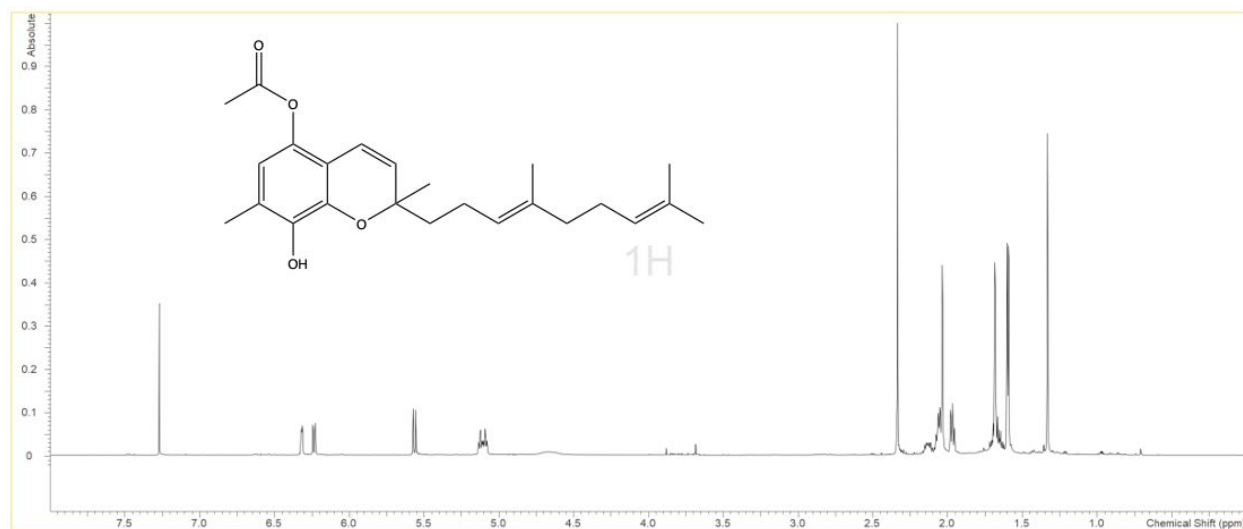


Figure S1: Tuaimenal B (**1**) ¹H NMR spectrum (600 MHz, CDCl₃).



Figure S2: Tuaimenal B (1) ¹³C NMR spectrum (150 MHz, CDCl₃).

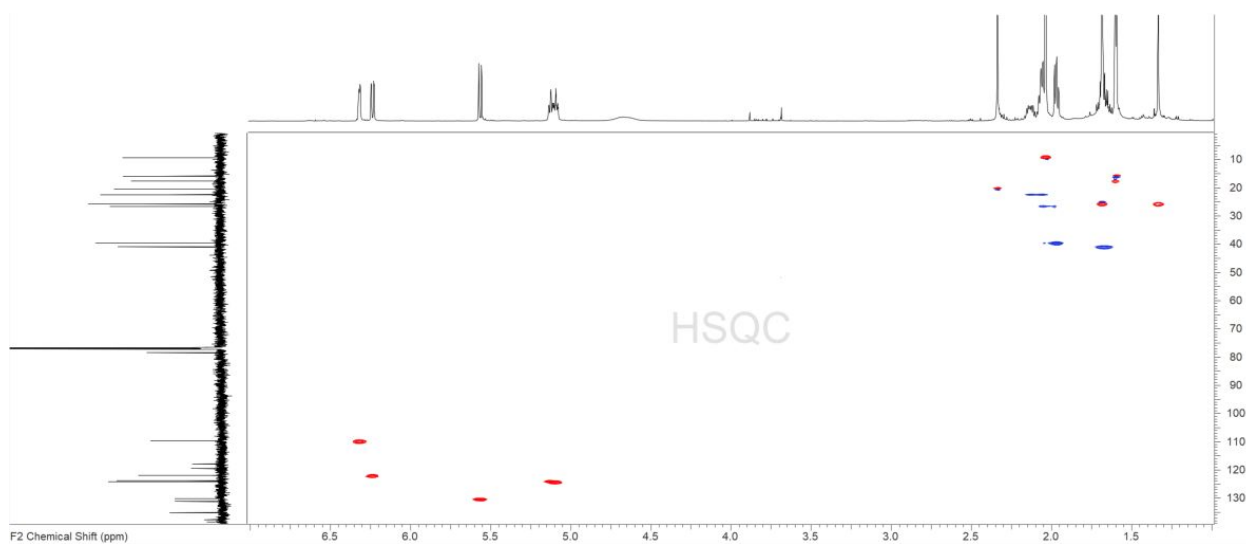


Figure S3: Tuaimenal B (1) HSQC NMR spectrum (500 MHz, CDCl₃).

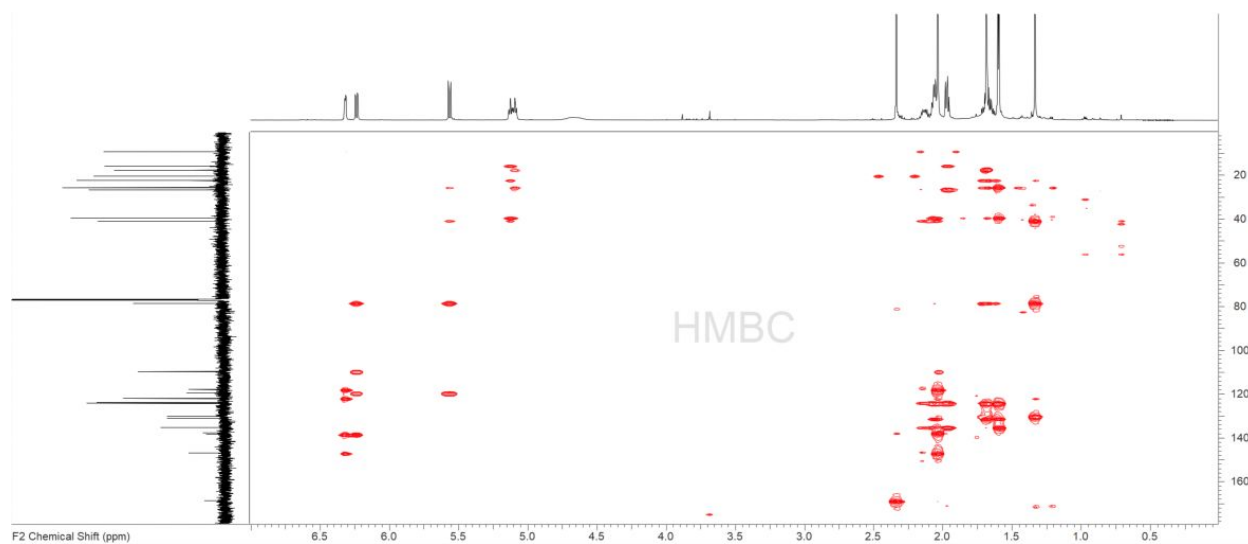


Figure S4: Tuaimenal B (1) HMBC NMR spectrum (500 MHz, CDCl₃).

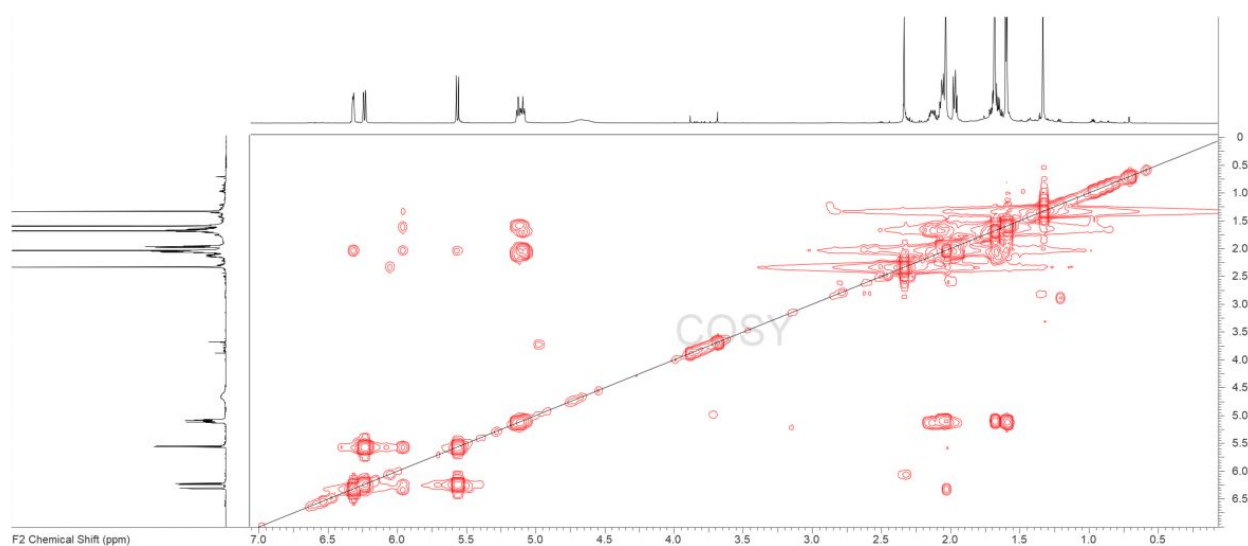


Figure S5: Tuaimenal B (1) COSY NMR spectrum (500 MHz, CDCl₃).

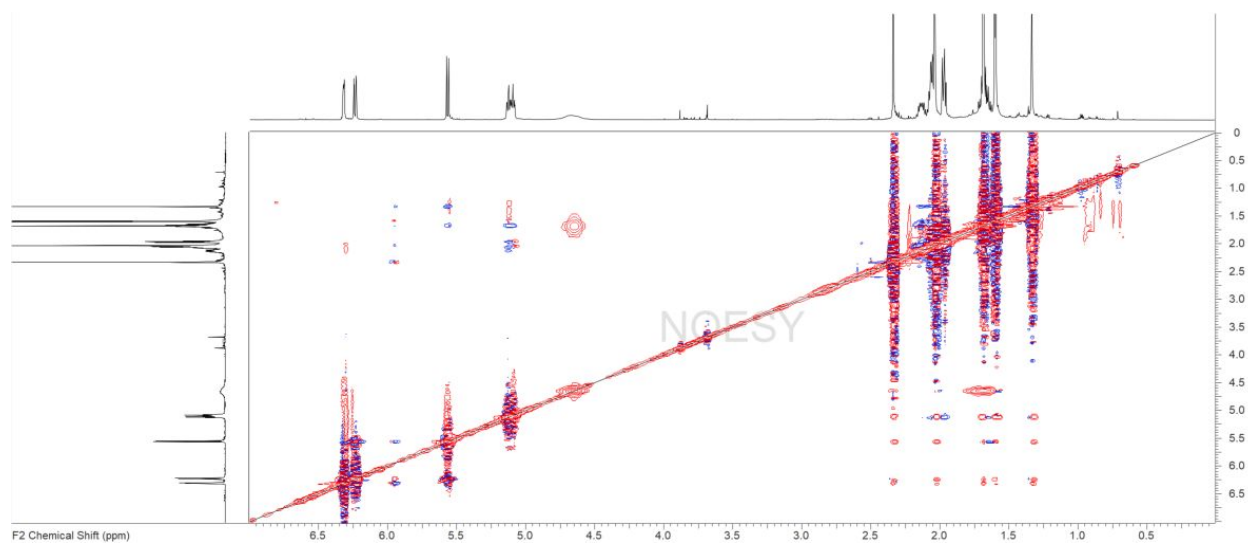


Figure S6: Tuaimenal B (**1**) NOESY NMR spectrum (500 MHz, CDCl₃).

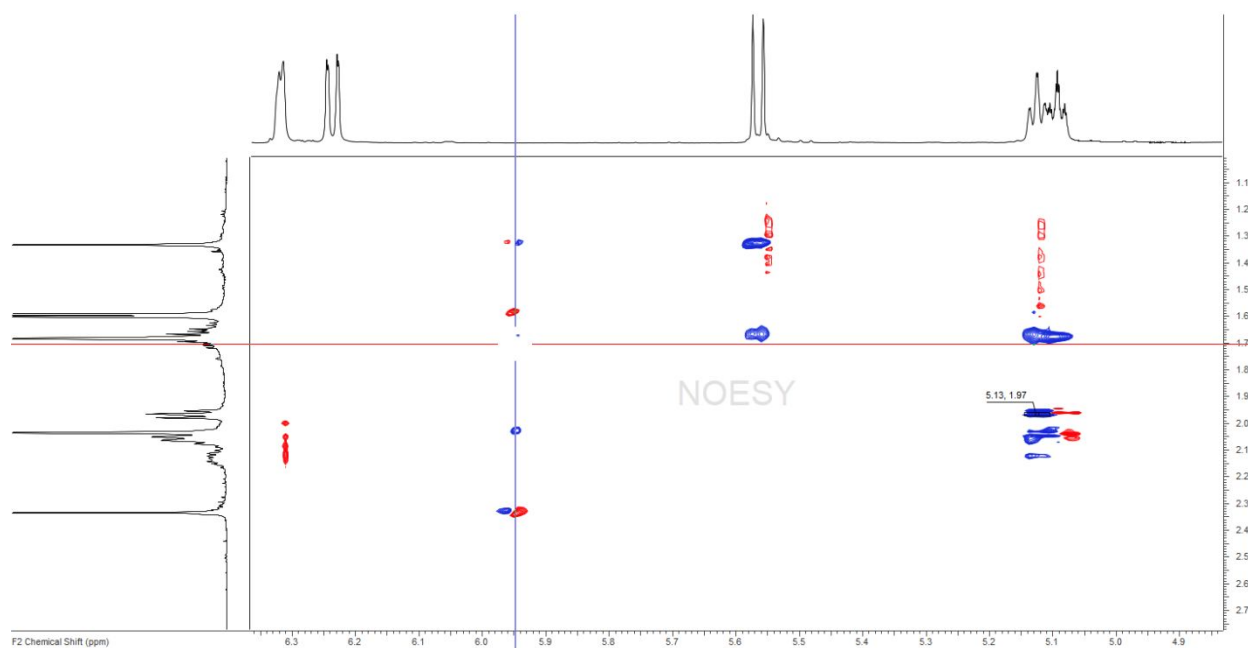


Figure S7: Tuaimenal B (**1**) zoomed NOESY NMR spectrum (500 MHz, CDCl₃).

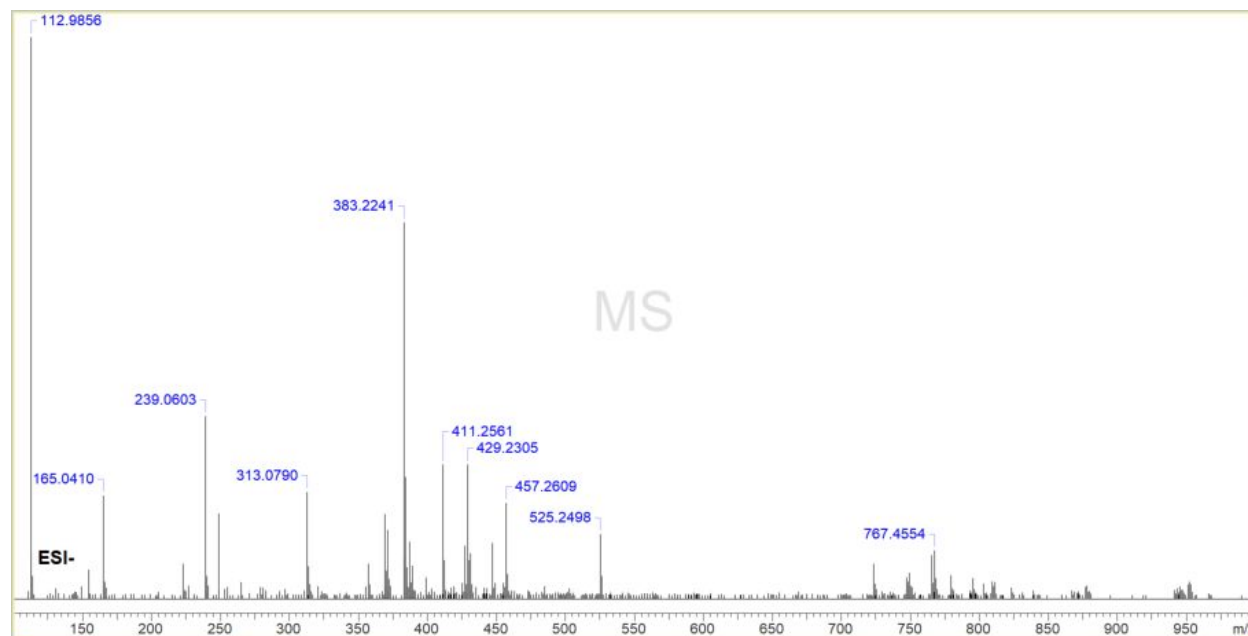


Figure S8: Tuaimenal B (1) HRESIMS (neg).

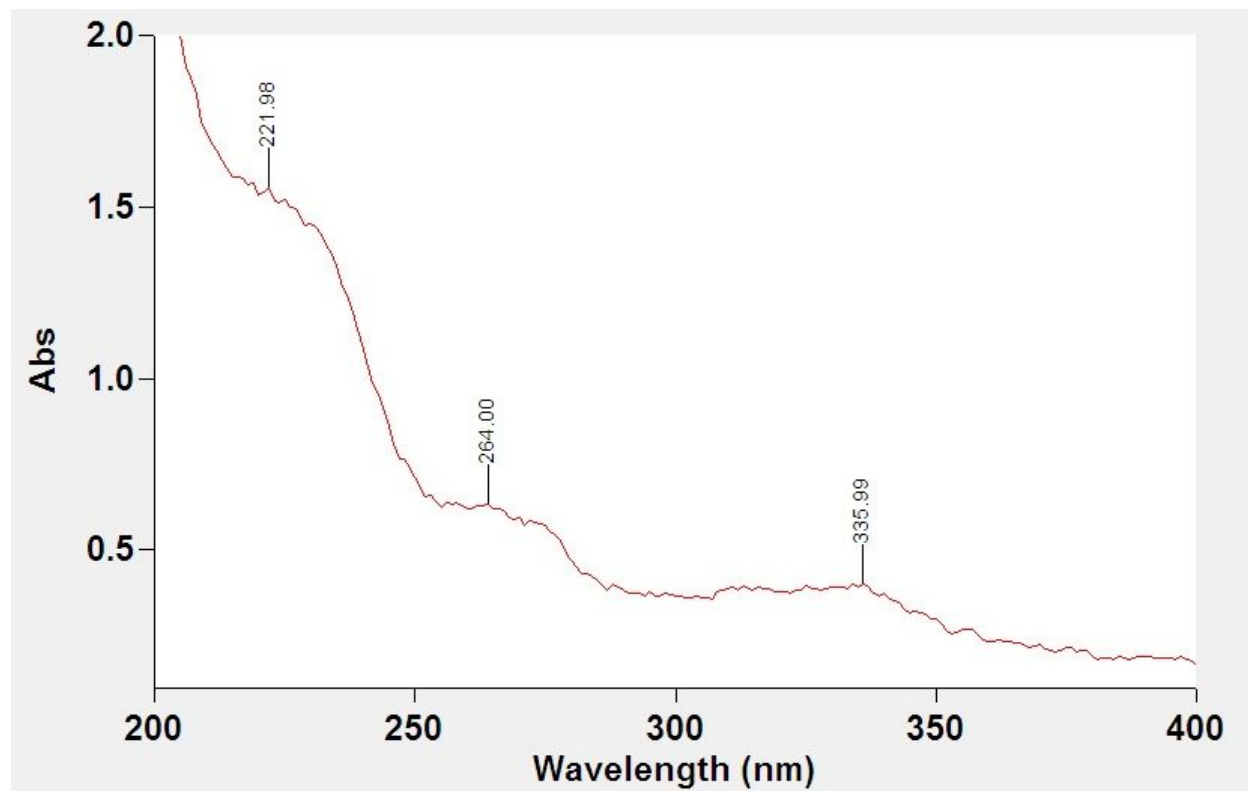


Figure S9: Tuaimenal B (1) UV λ_{\max} (C_2H_3N).

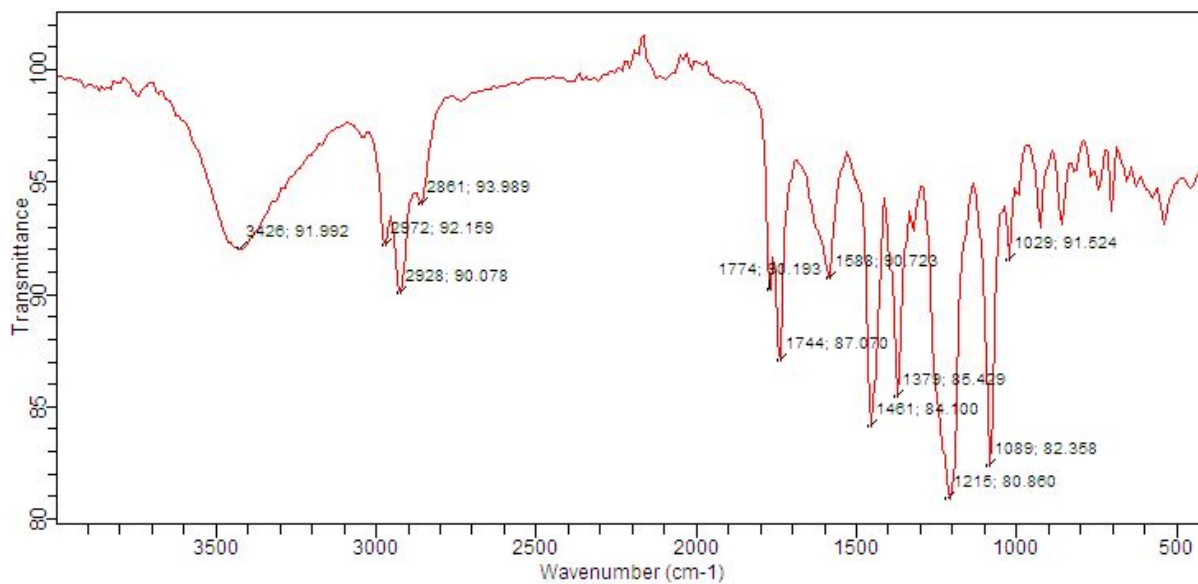


Figure S10: Tuaimenal B (**1**) IR spectrum (thin film).

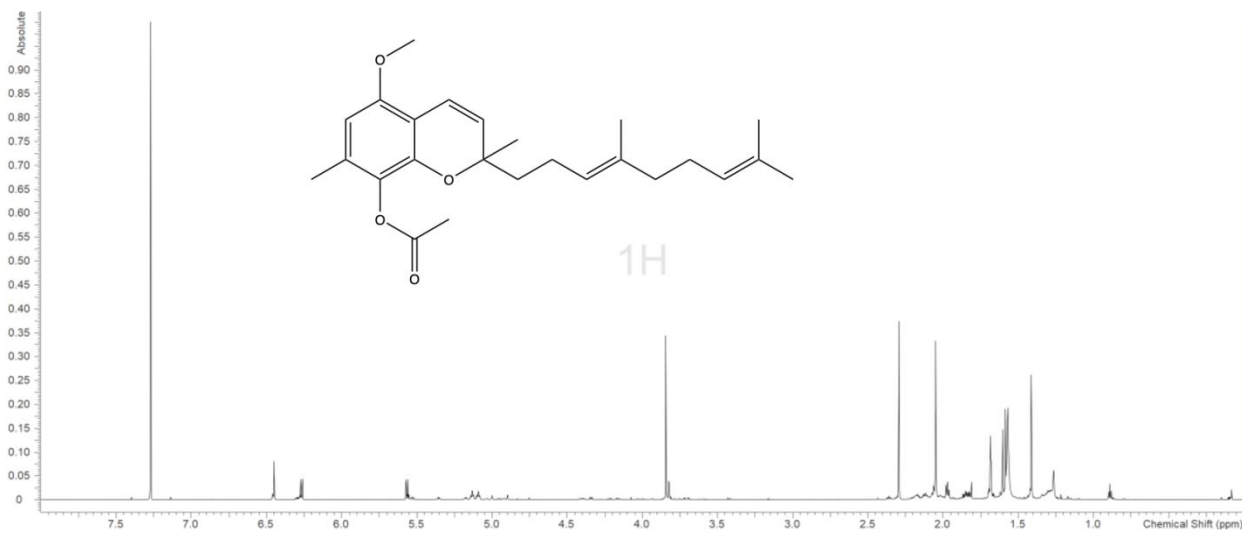


Figure S11: Tuaimenal C (**2**) ¹H NMR spectrum (800 MHz, CDCl₃).

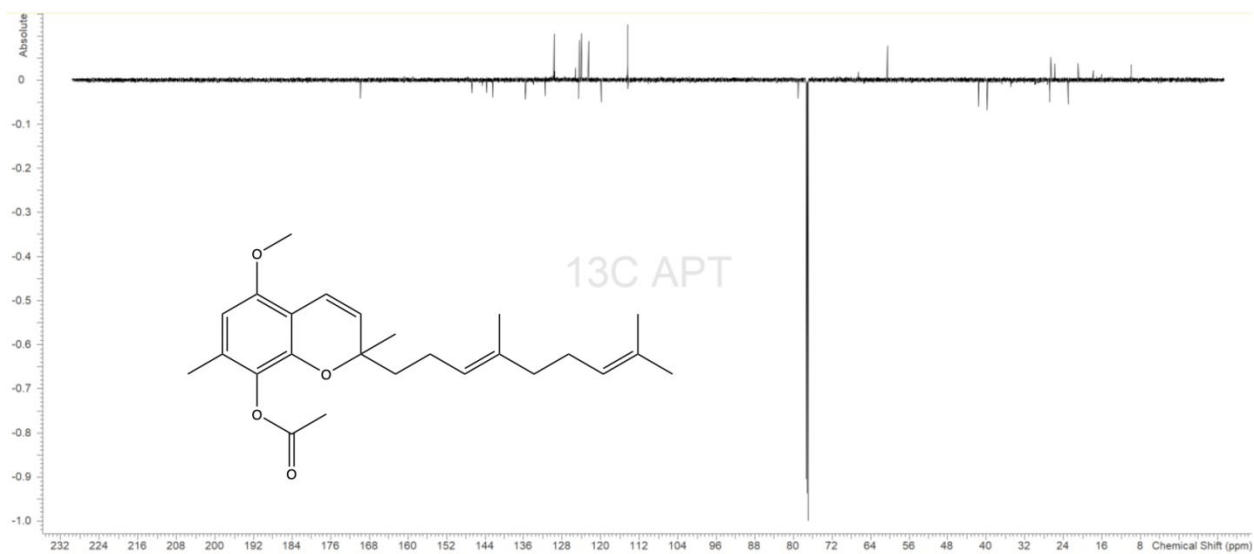


Figure S12: Tuaimenal C (**2**) ^{13}C NMR spectrum (200 MHz, CDCl_3).

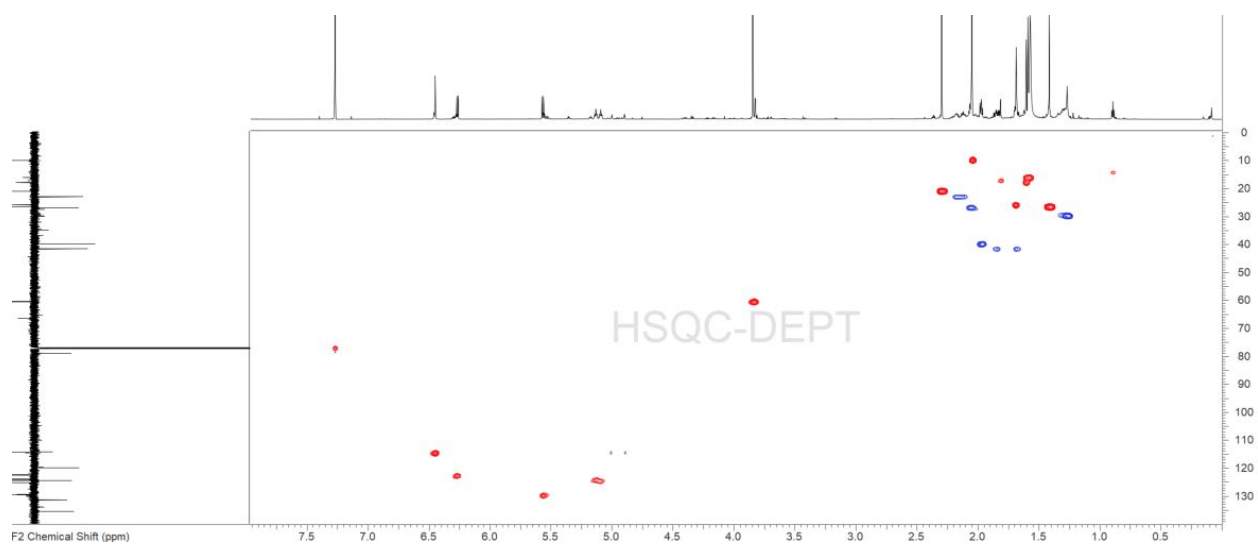


Figure S13: Tuaimenal C (**2**) HSQC NMR spectrum (800 MHz, CDCl_3).

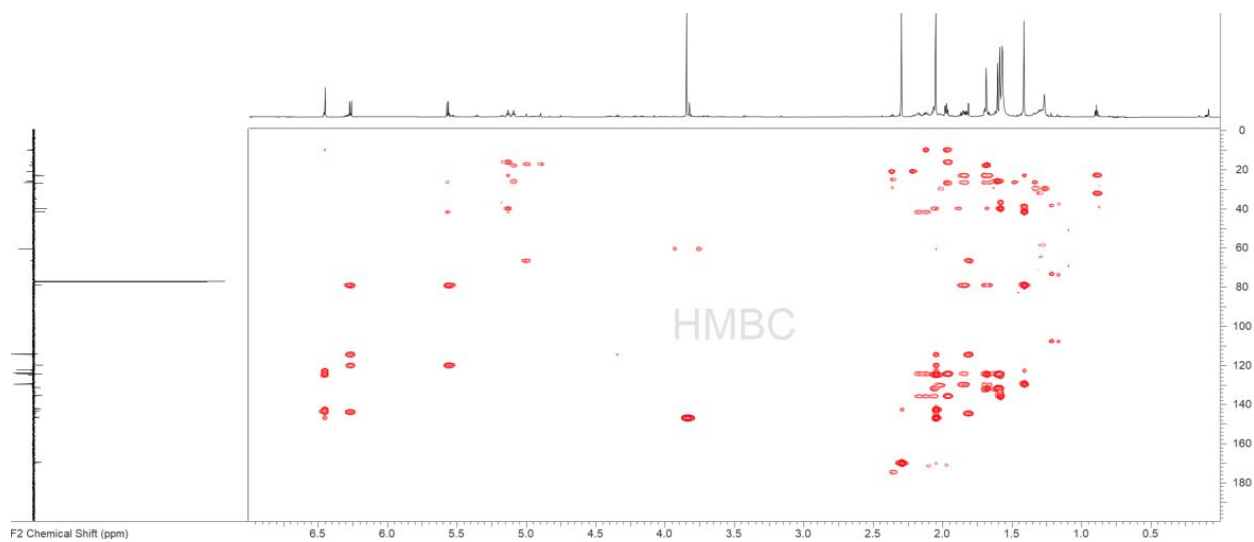


Figure S14: Tuaimenal C (**2**) HMBC NMR spectrum (800 MHz, CDCl₃).

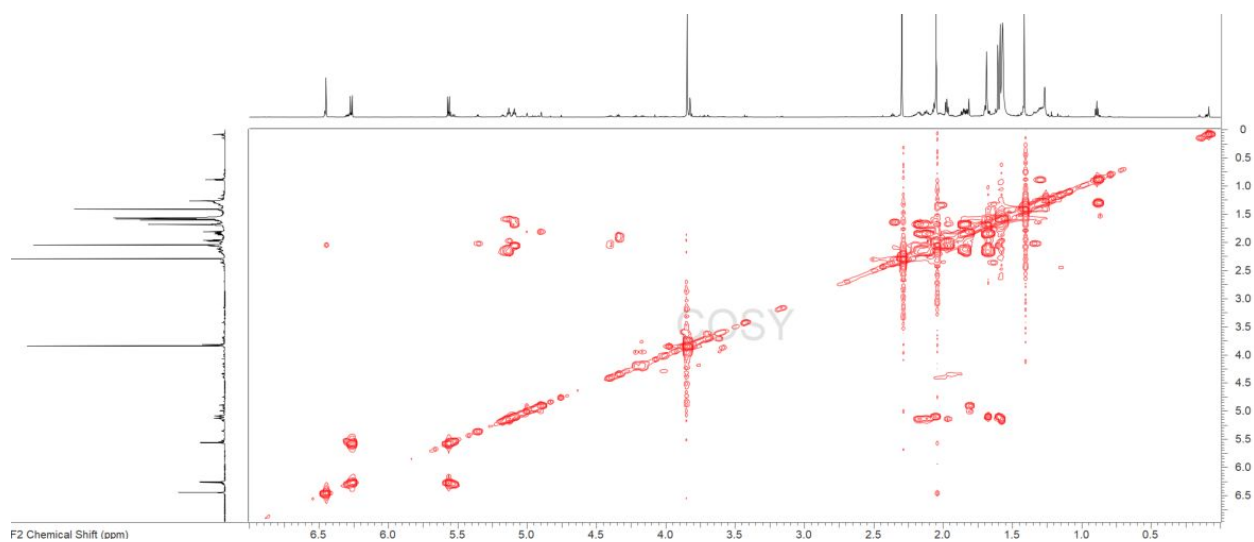


Figure S15: Tuaimenal C (**2**) COSY NMR spectrum (800 MHz, CDCl₃).

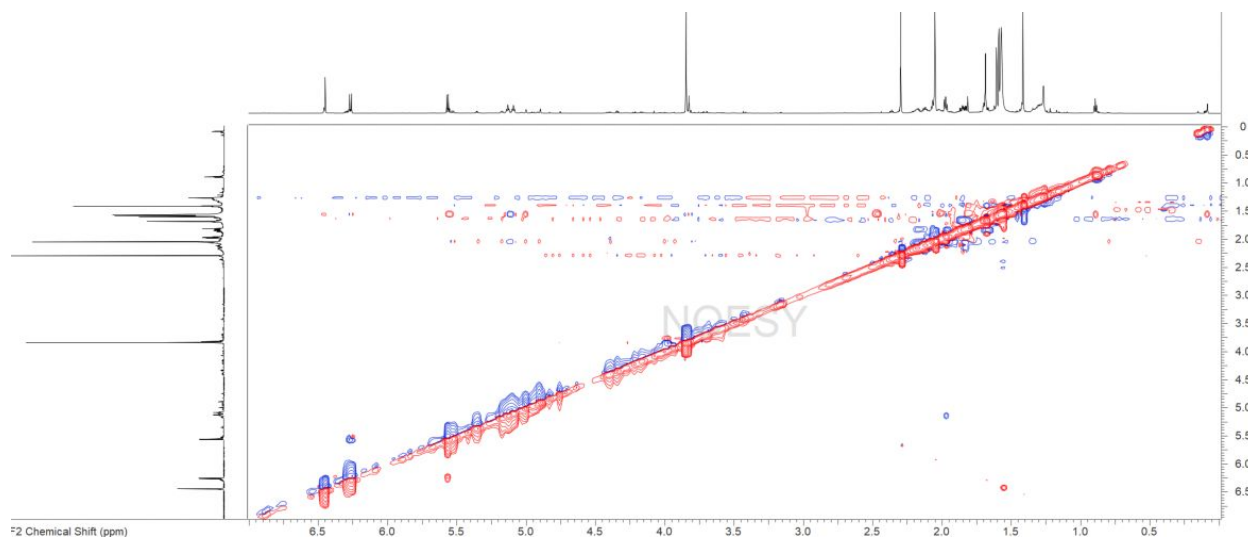


Figure S16: Tuaimenal C (**2**) NOESY NMR spectrum (800 MHz, CDCl₃).

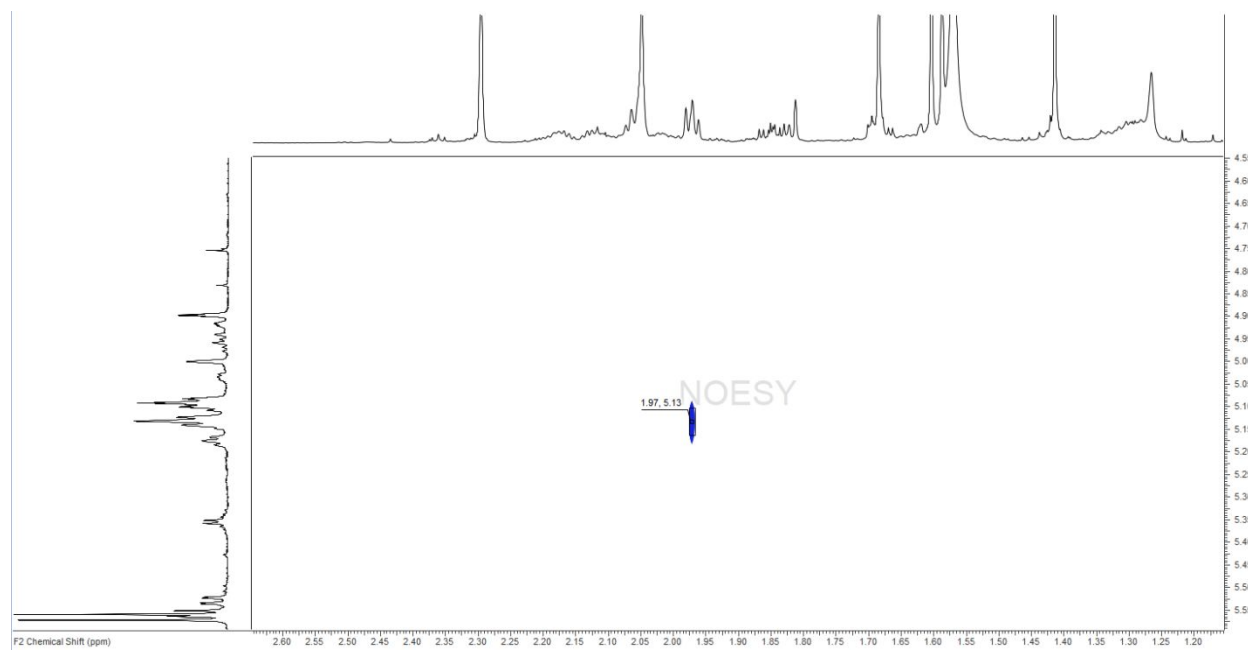


Figure S17: Tuaimenal C (**2**) zoomed NOESY NMR spectrum (800 MHz, CDCl₃).

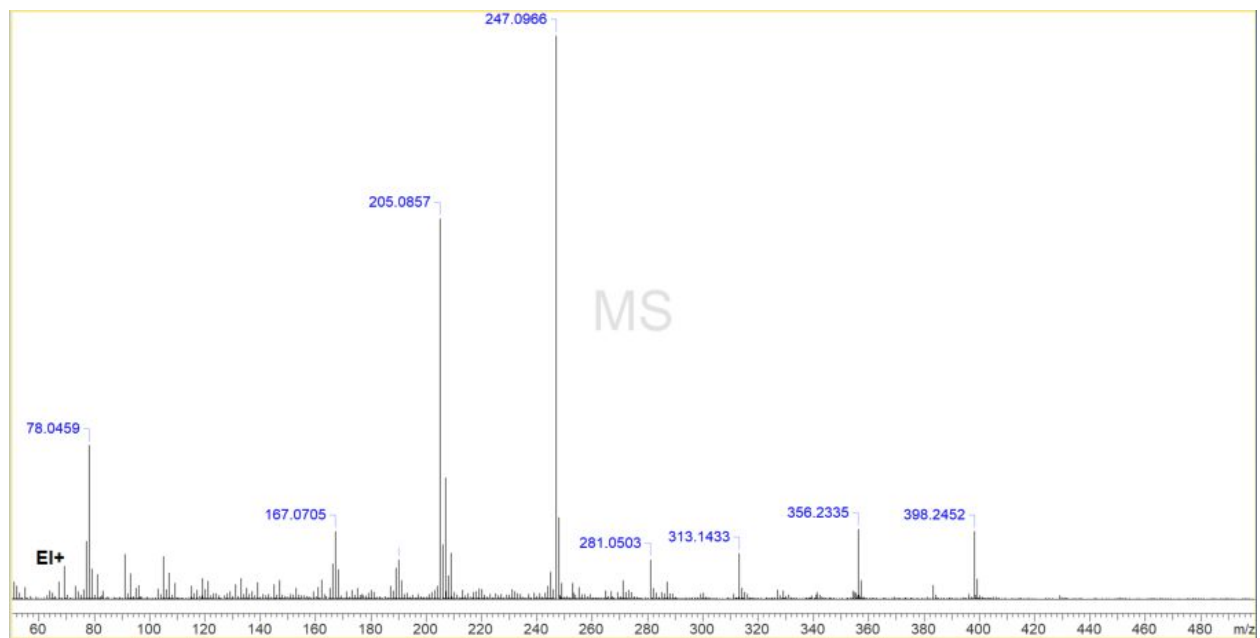


Figure S18: Tuaimenal C (2) HREIMS.

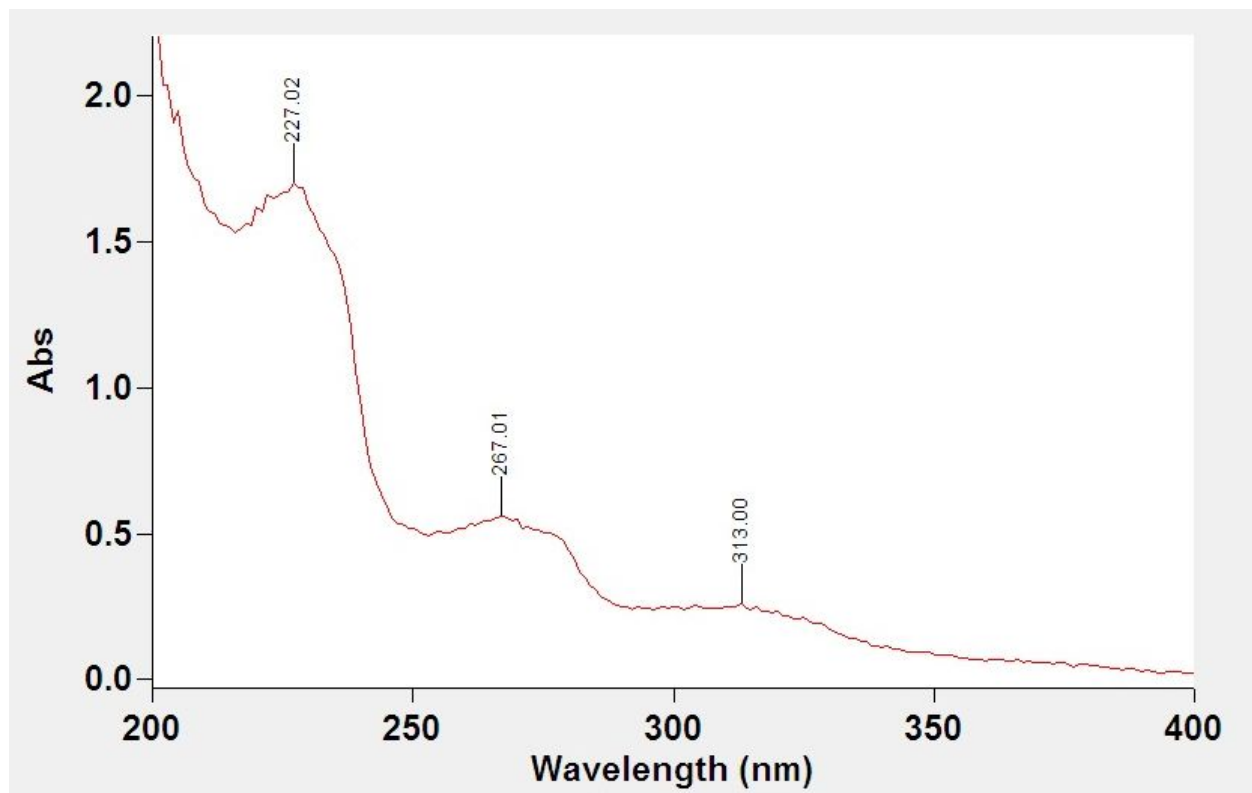


Figure S19: Tuaimenal C (2) UV λ_{\max} (C_2H_3N).

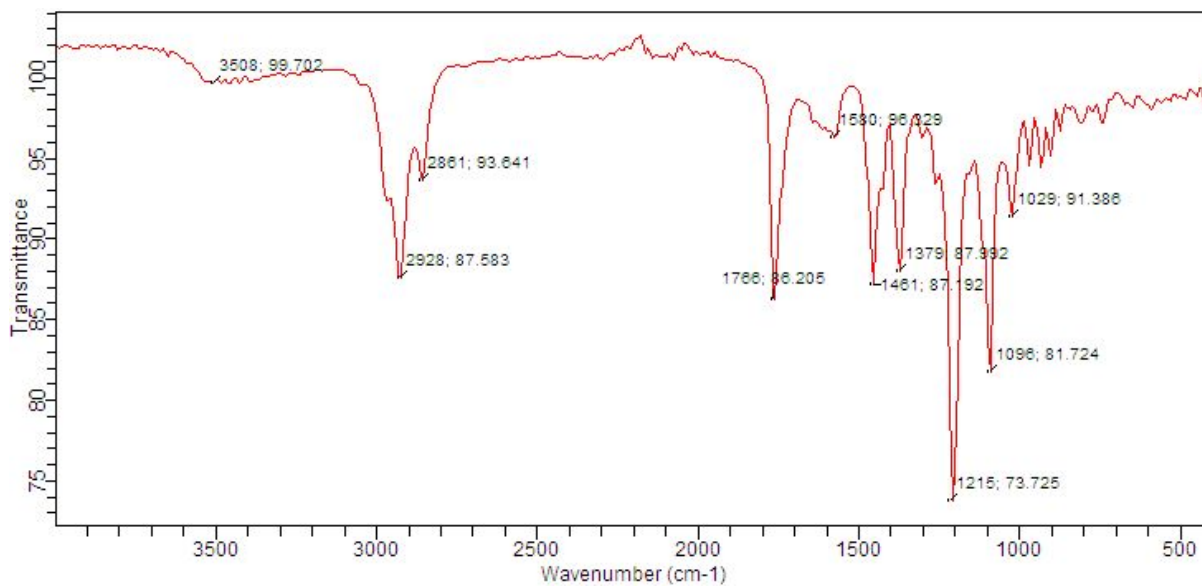


Figure S20: Tuaimenal C (**2**) IR spectrum (thin film).

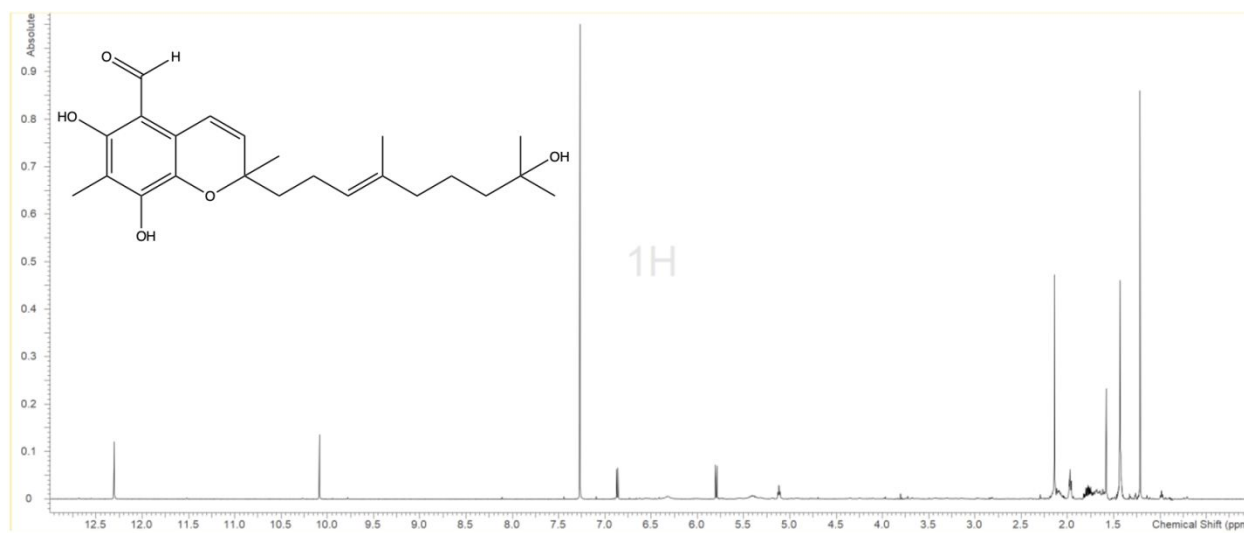


Figure S21: Tuaimenal D (**3**) ¹H NMR spectrum (600 MHz, CDCl₃).

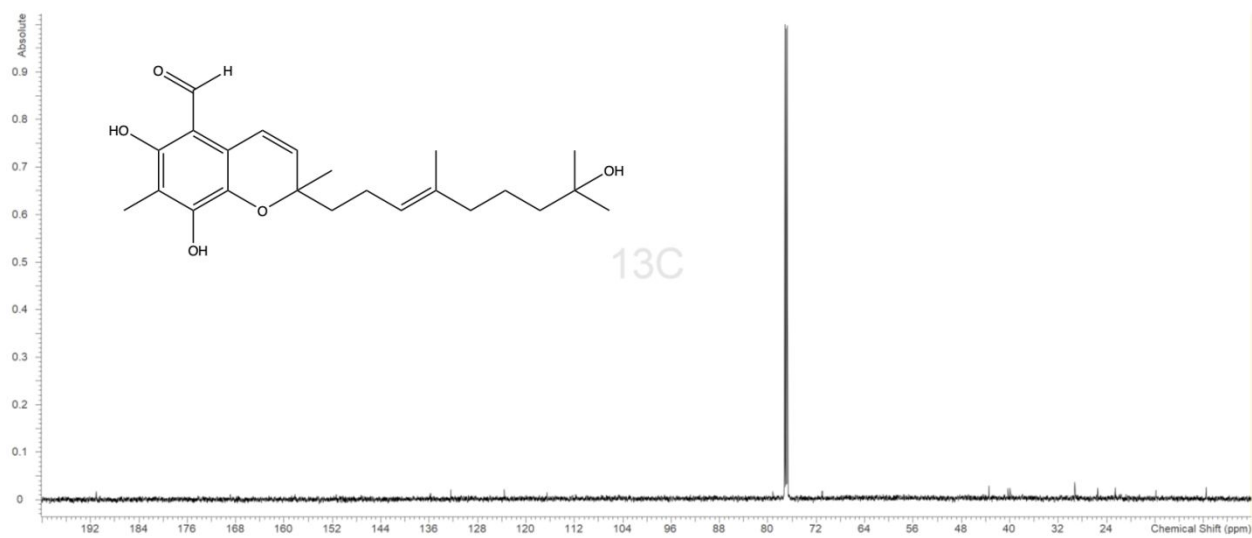


Figure S22: Tuaimenal D (**3**) ^{13}C NMR spectrum (150 MHz, CDCl_3).

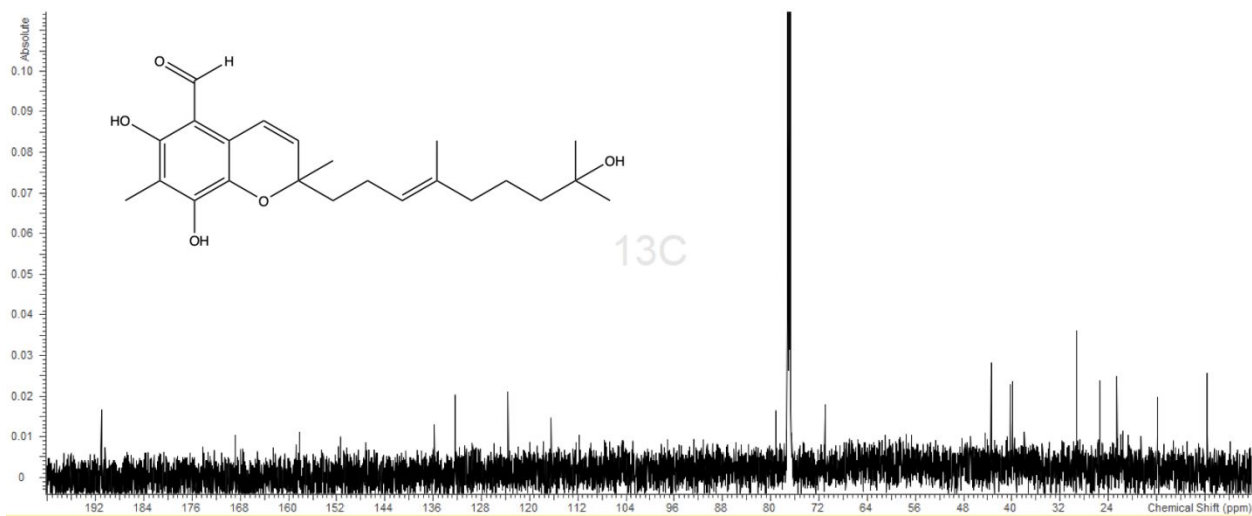


Figure S23: Tuaimenal D (**3**) ^{13}C NMR spectrum zoomed (150 MHz, CDCl_3).

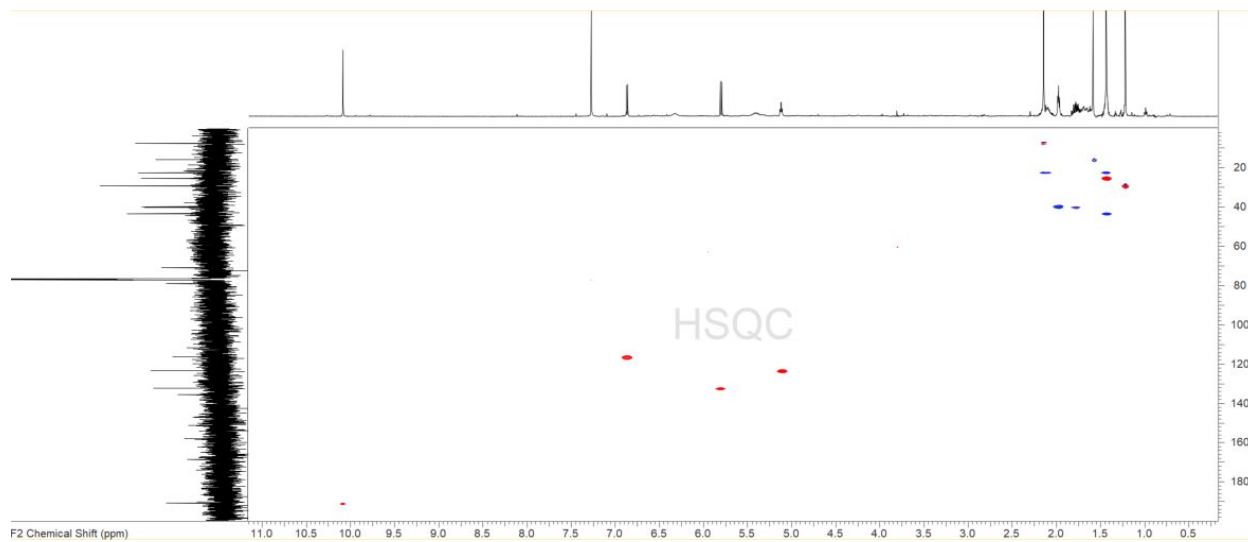


Figure S24: Tuaimenal D (**3**) HSCQ NMR spectrum (500 MHz, CDCl₃).

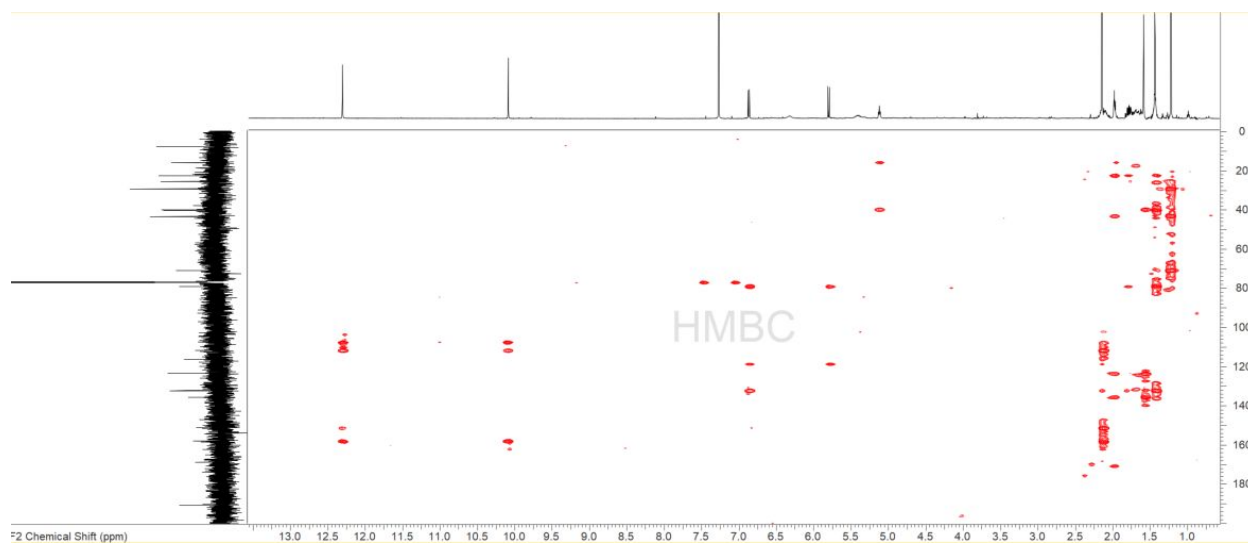


Figure S25: Tuaimenal D (**3**) HMBC NMR spectrum (500 MHz, CDCl₃).

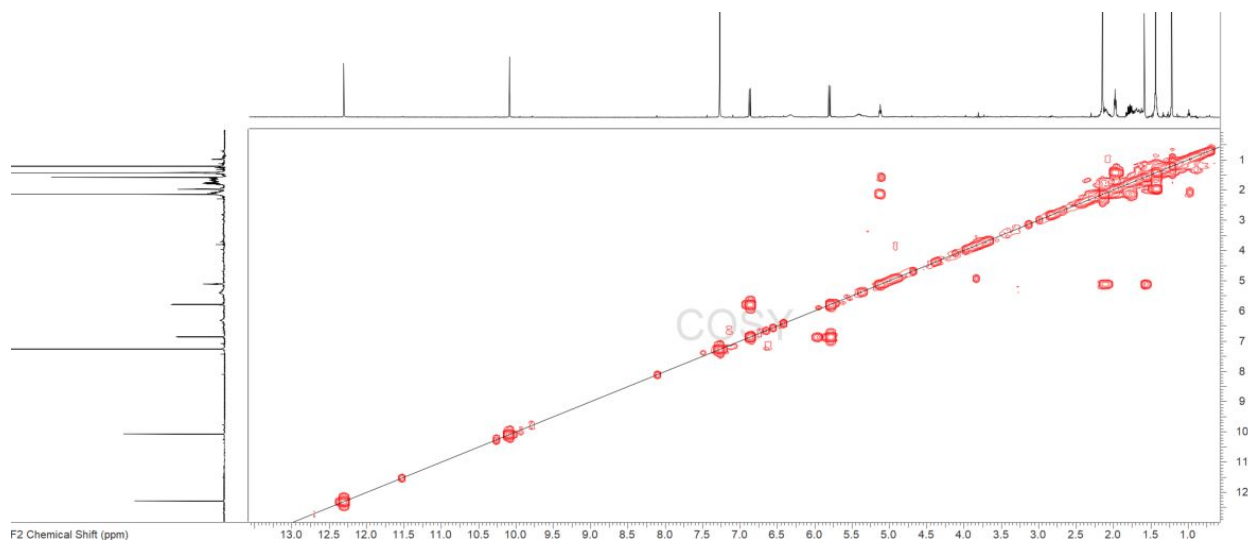


Figure S26: Tuaimenal D (**3**) COSY NMR spectrum (500 MHz, CDCl₃).

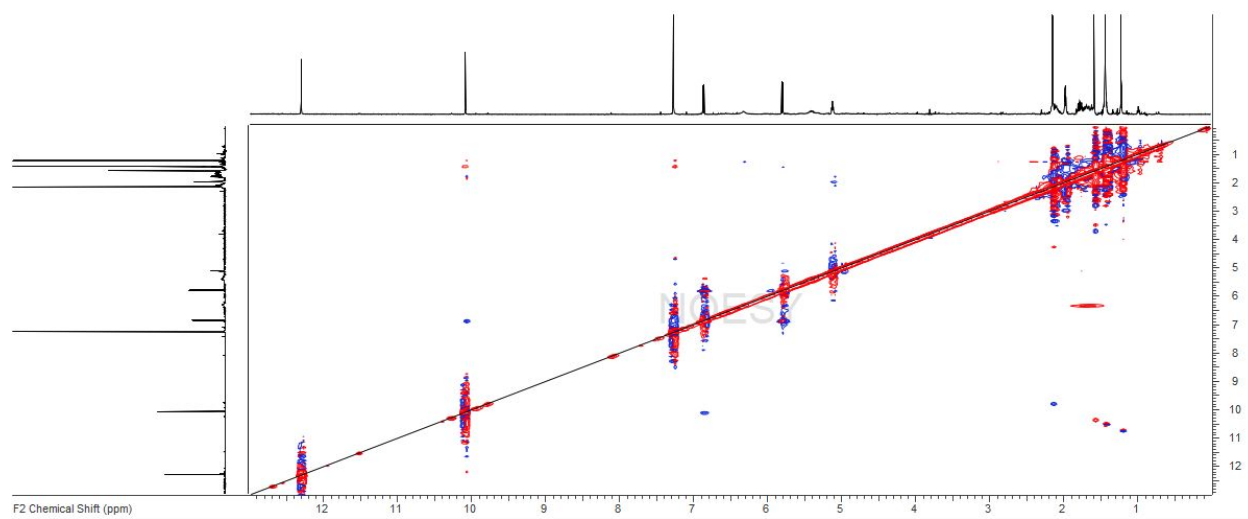


Figure S27: Tuaimenal D (**3**) NOESY NMR spectrum (500 MHz, CDCl₃).

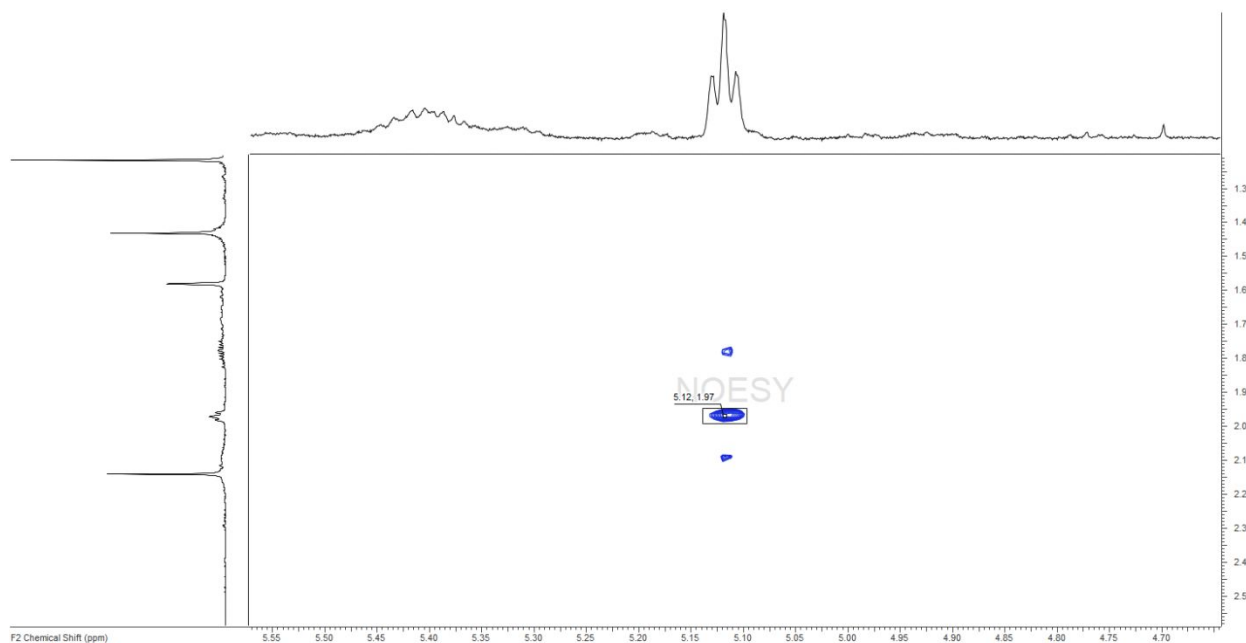


Figure S28: Tuaimenal D (**3**) zoomed NOESY NMR spectrum (500 MHz, CDCl₃).

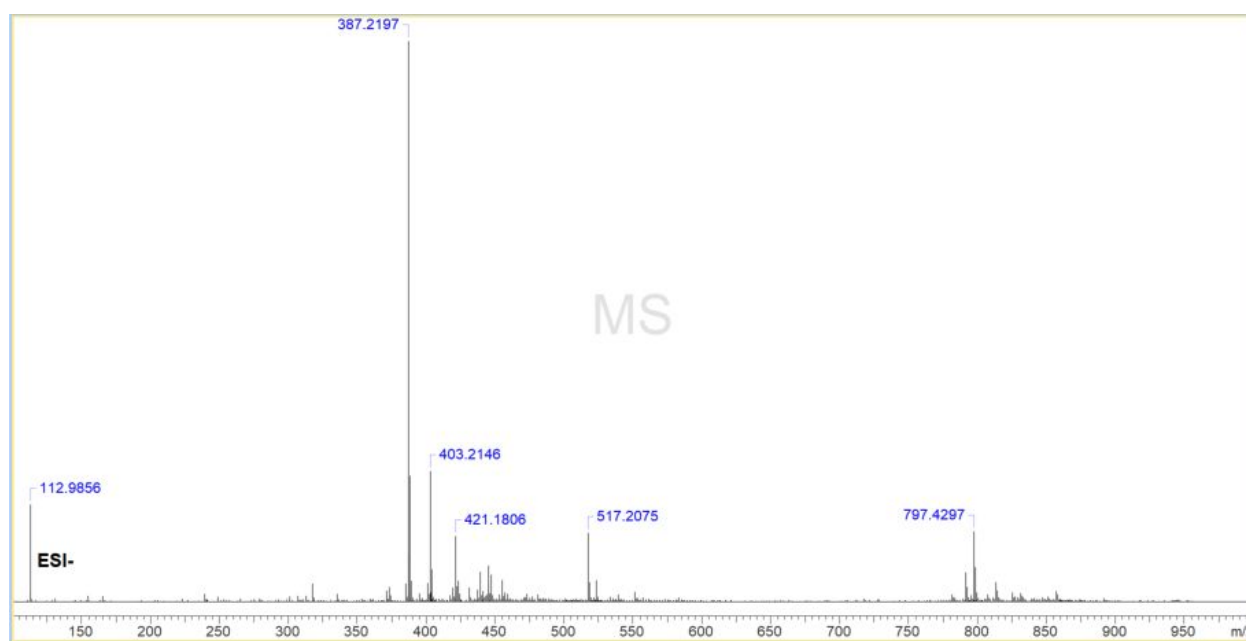


Figure S29: Tuaimenal D (**3**) HRESIMS (neg).

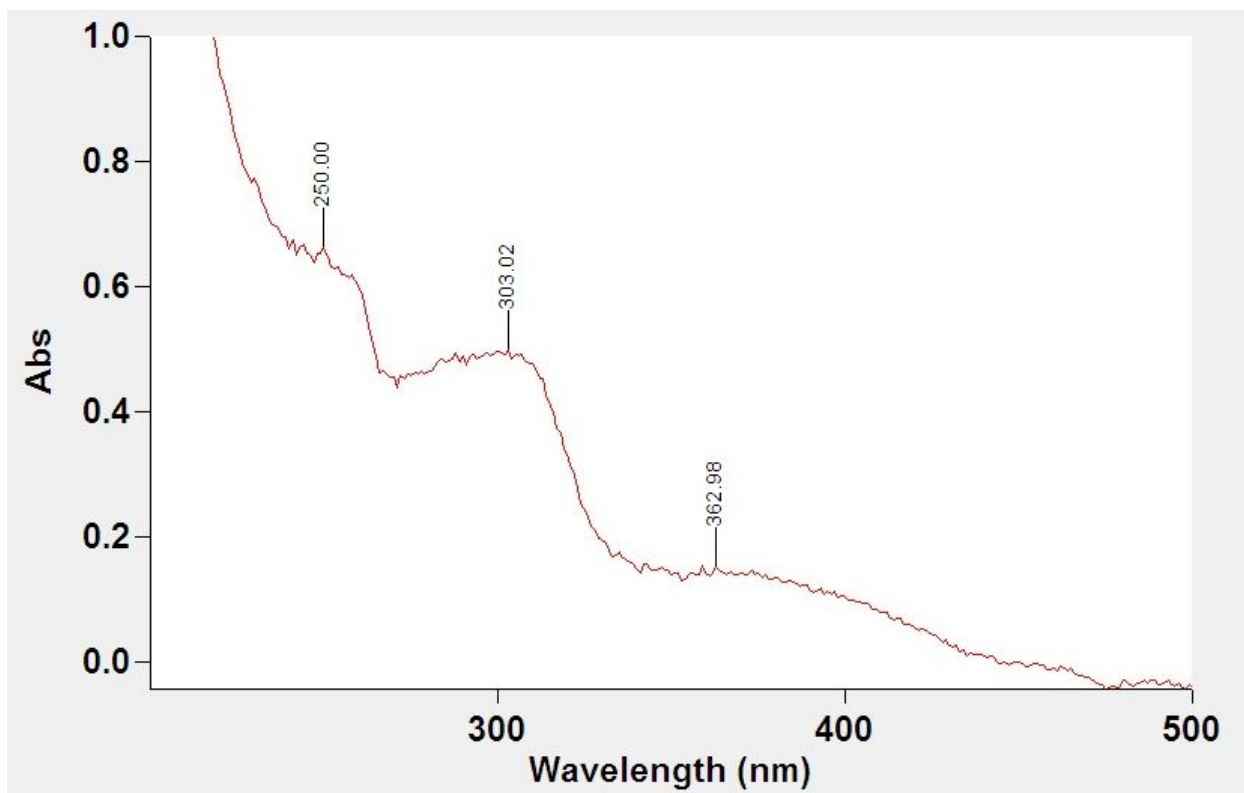


Figure S30: Tuaimenal D (**3**) UV λ_{max} (C_2H_3N).

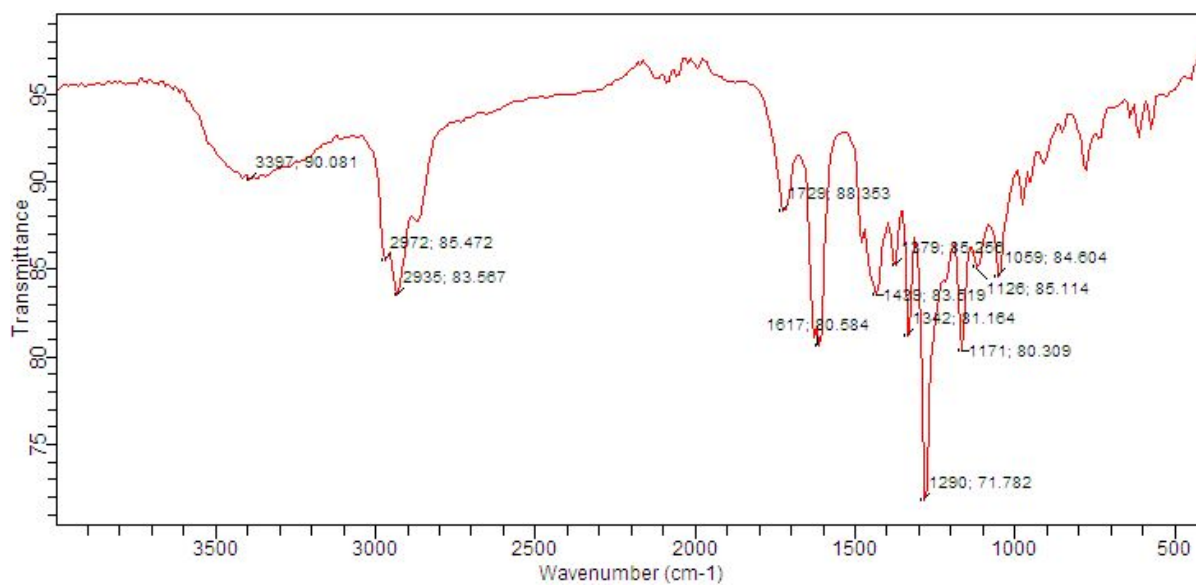


Figure S31: Tuaimenal D (**3**) IR spectrum (thin film).

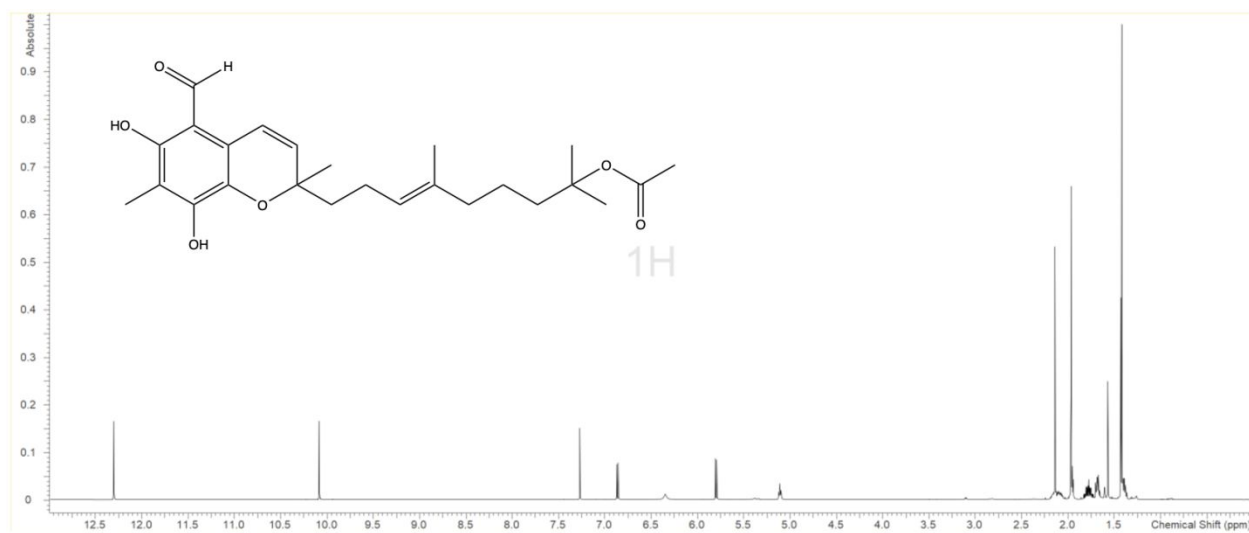


Figure S32: Tuaimenal E (**4**) ¹H NMR spectrum (600 MHz, CDCl₃).

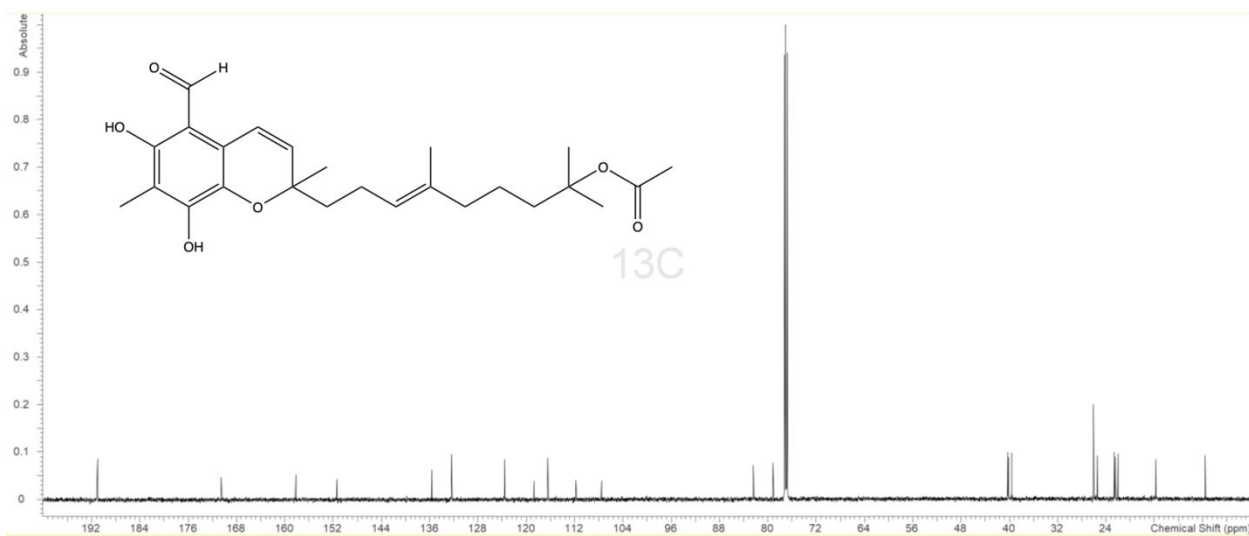


Figure S33: Tuaimenal E (**4**) ¹³C NMR spectrum (150 MHz, CDCl₃).

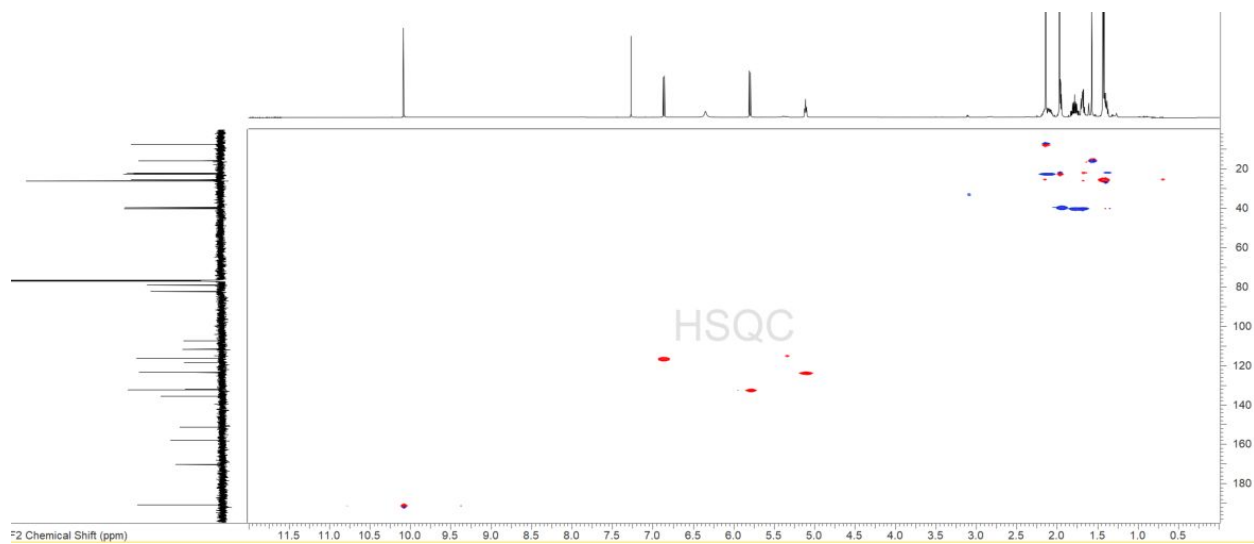


Figure S34: Tuaimenal E (**4**) HSCQ NMR spectrum (500 MHz, CDCl₃).

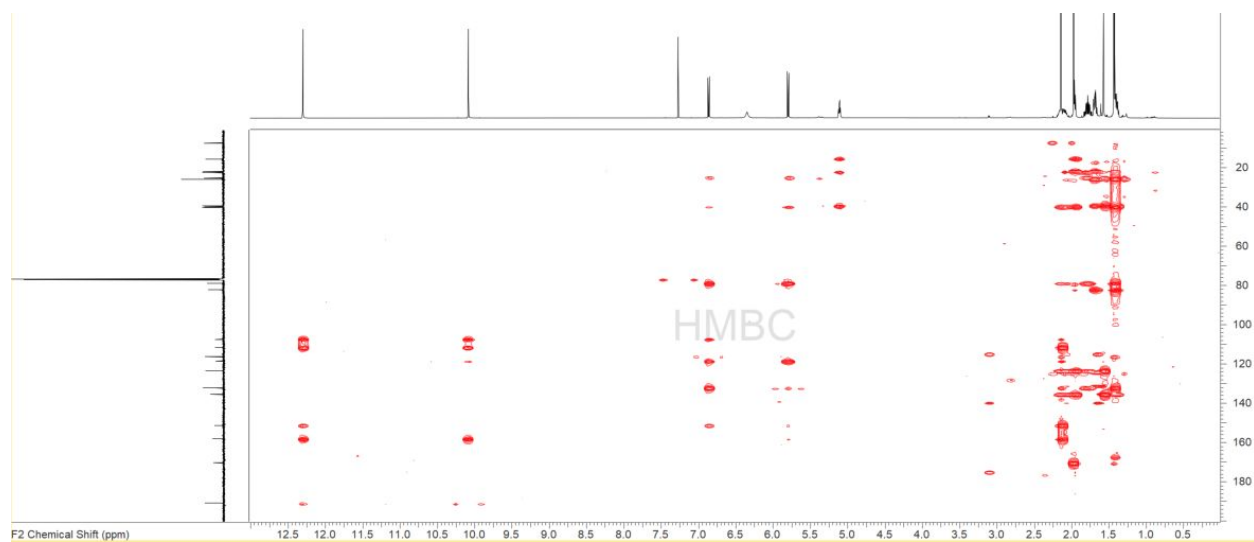


Figure S35: Tuaimenal E (**4**) HMBC NMR spectrum (500 MHz, CDCl₃).

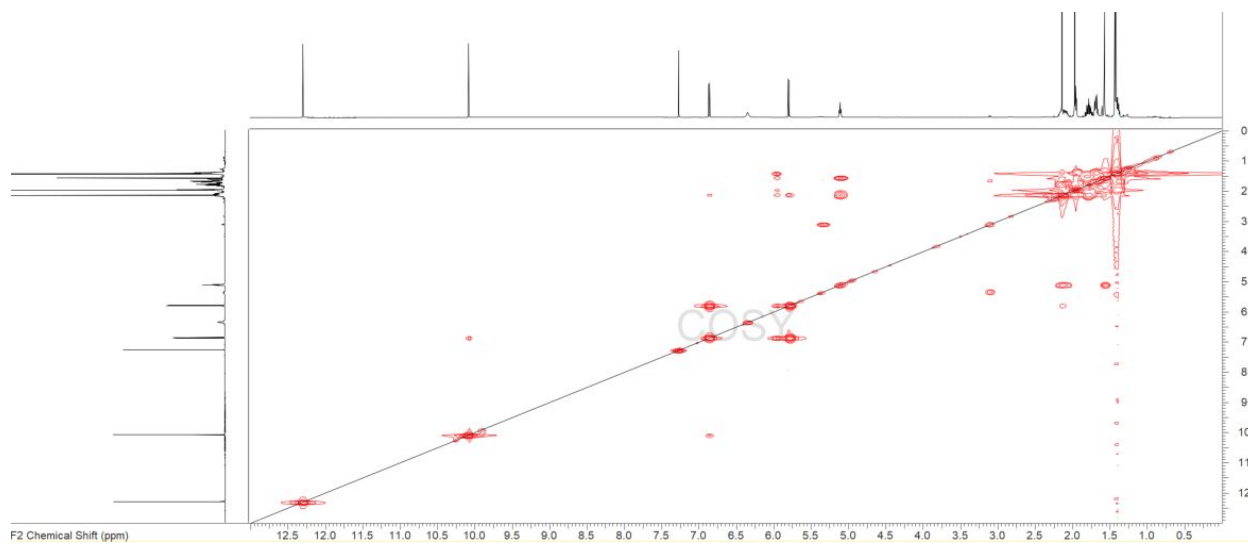


Figure S36: Tuaimenal E (**4**) COSY NMR spectrum (500 MHz, CDCl₃).

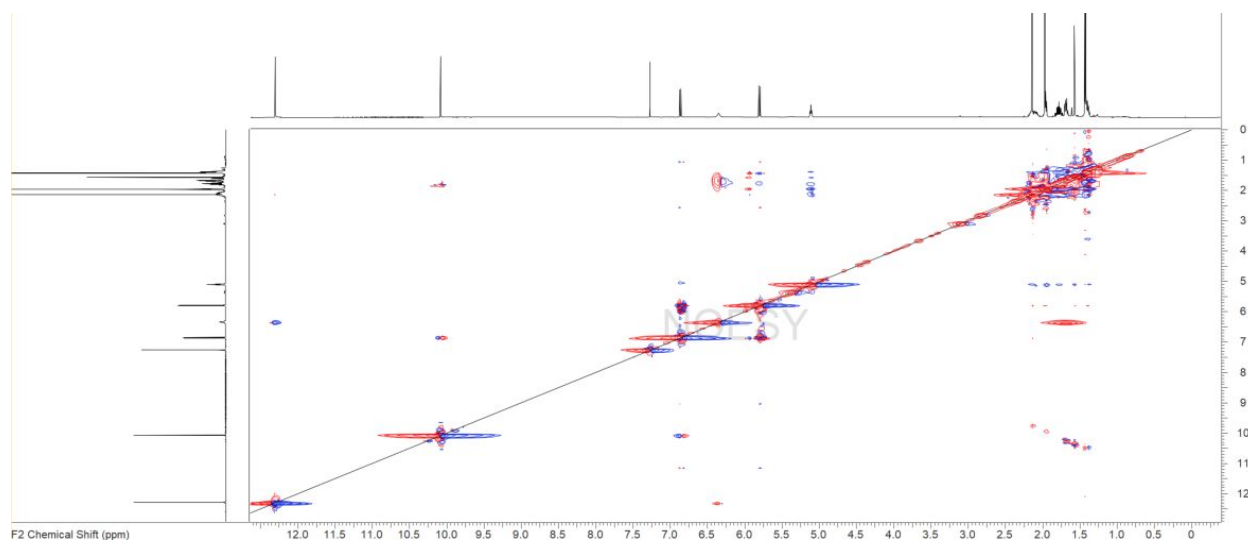


Figure S37: Tuaimenal E (**4**) NOESY NMR spectrum (500 MHz, CDCl₃).

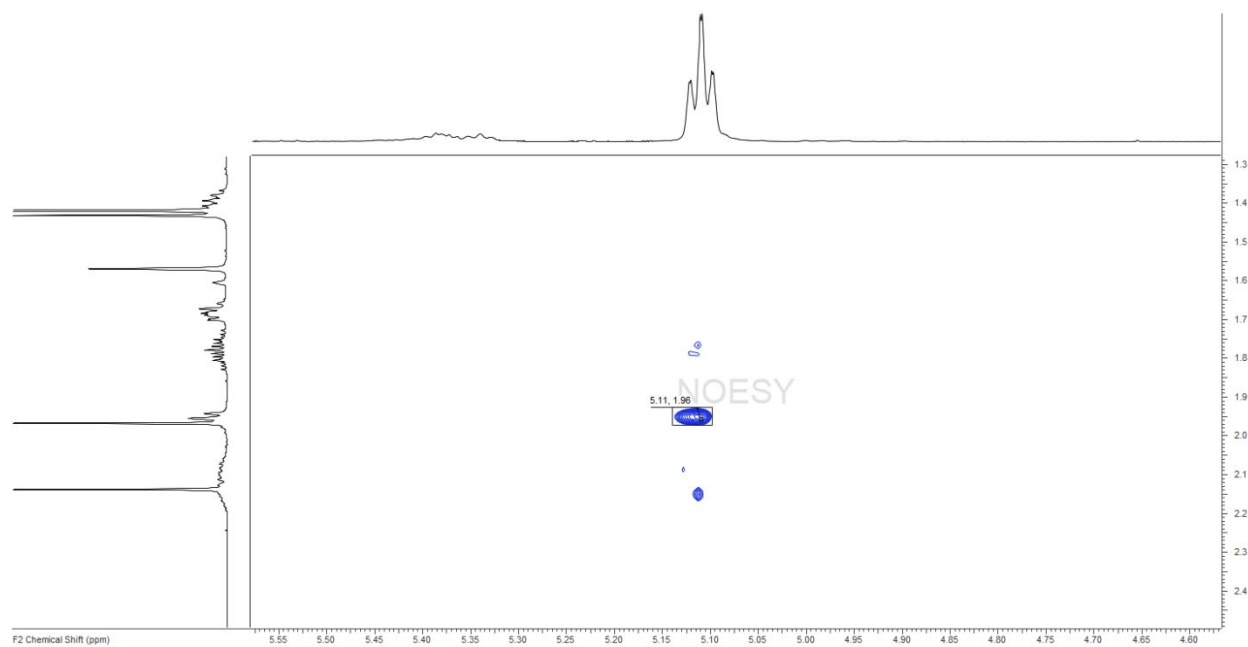


Figure S38: Tuaimenal E (**4**) zoomed NOESY NMR spectrum (500 MHz, CDCl_3).



Figure S39: Tuaimenal E (**4**) HRESIMS (neg).

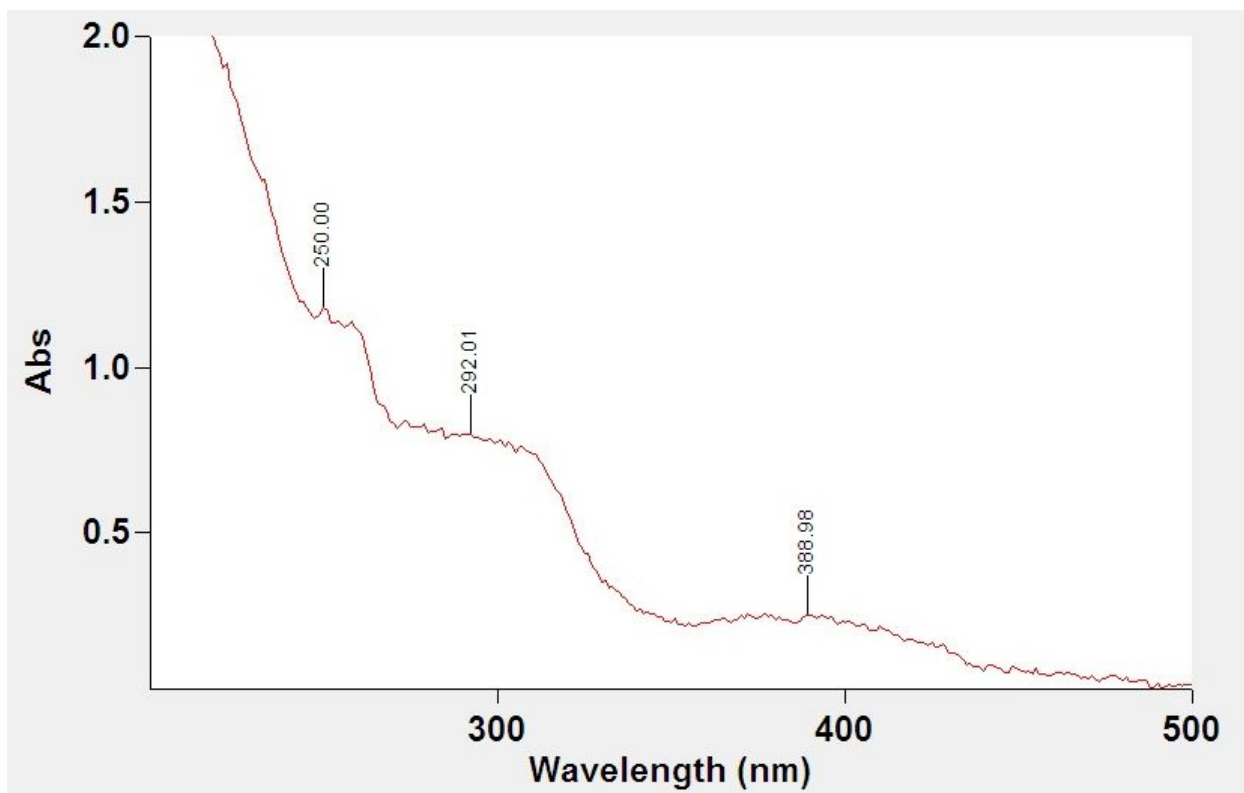


Figure S40: Tuaimenal E (**4**) UV λ_{\max} (C_2H_3N).

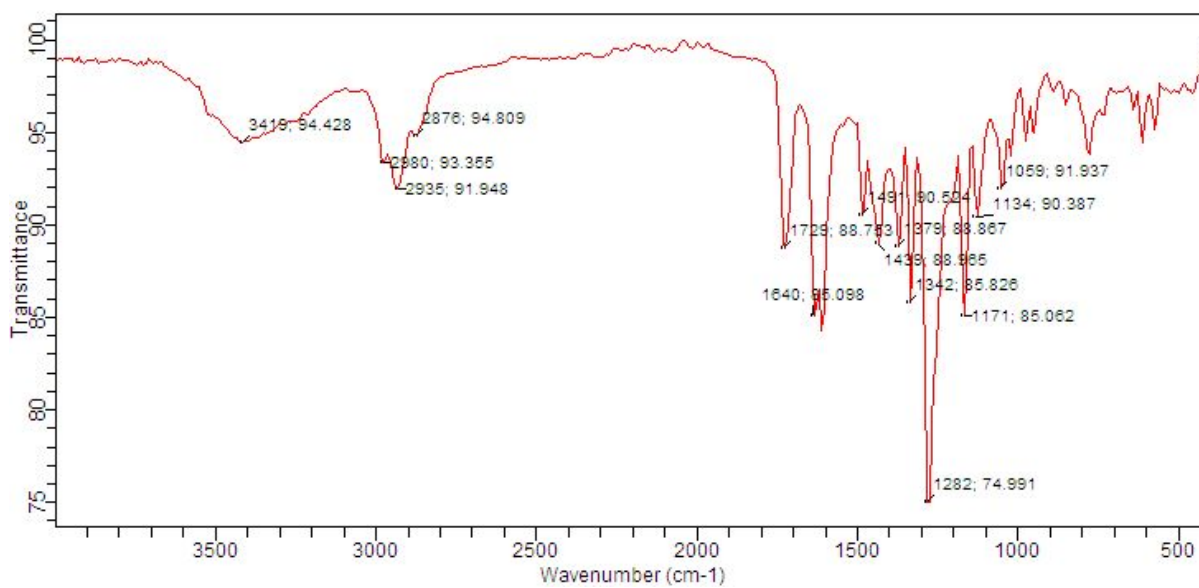


Figure S41: Tuaimenal E (**4**) IR spectrum (thin film).

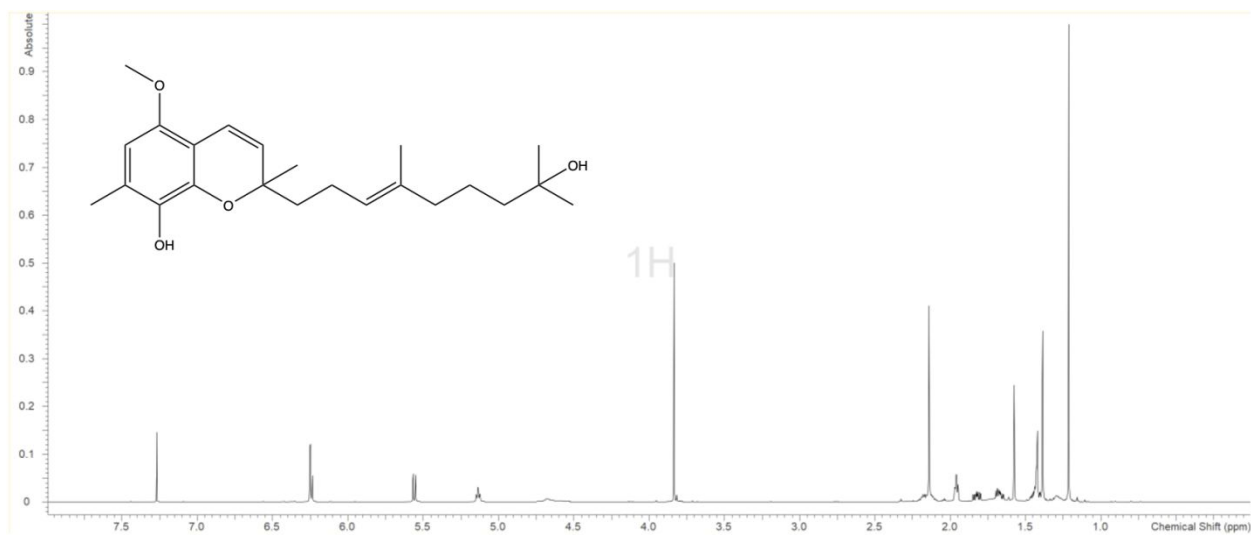


Figure S42: Tuaimenal F (**5**) ¹H NMR spectrum (600 MHz, CDCl₃).

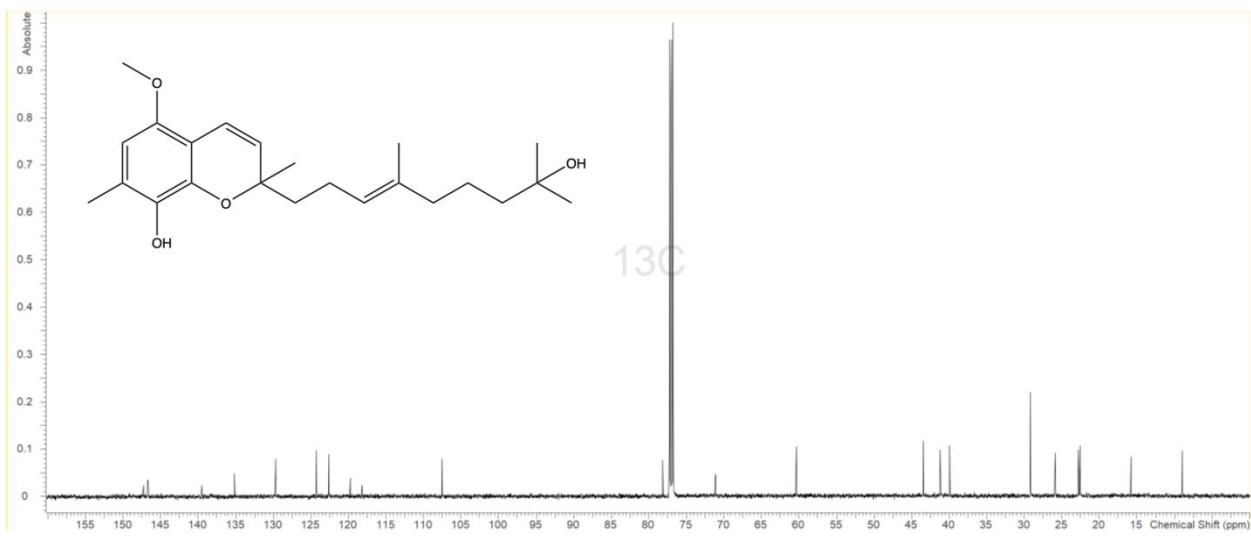


Figure S43: Tuaimenal F (**5**) ¹³C NMR spectrum (150 MHz, CDCl₃).

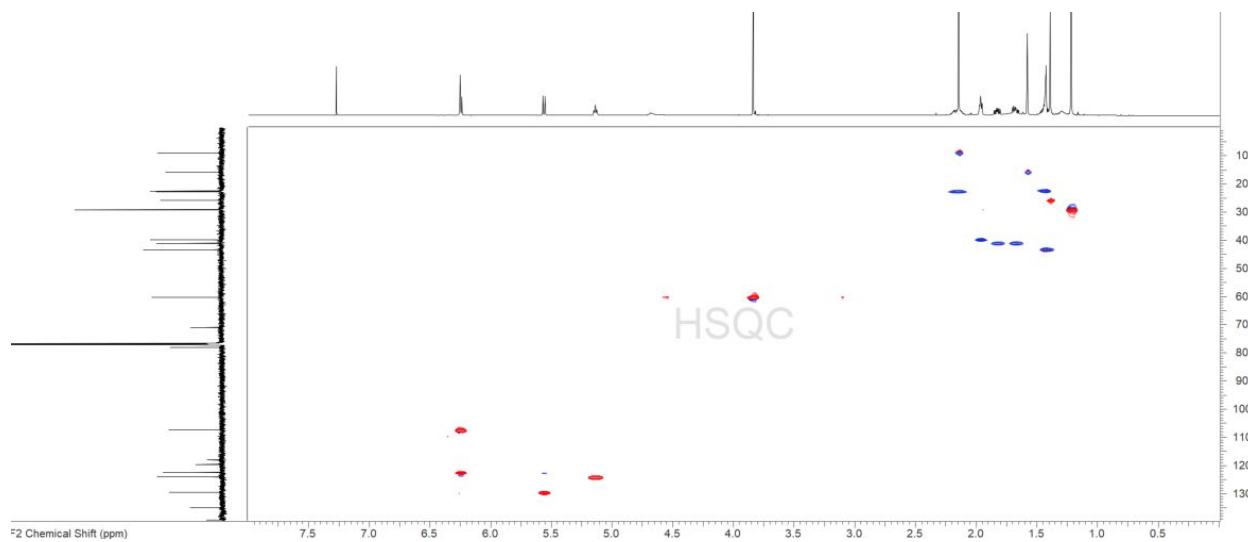


Figure S44: Tuaimenal F (**5**) HSCQ NMR spectrum (500 MHz, CDCl₃).

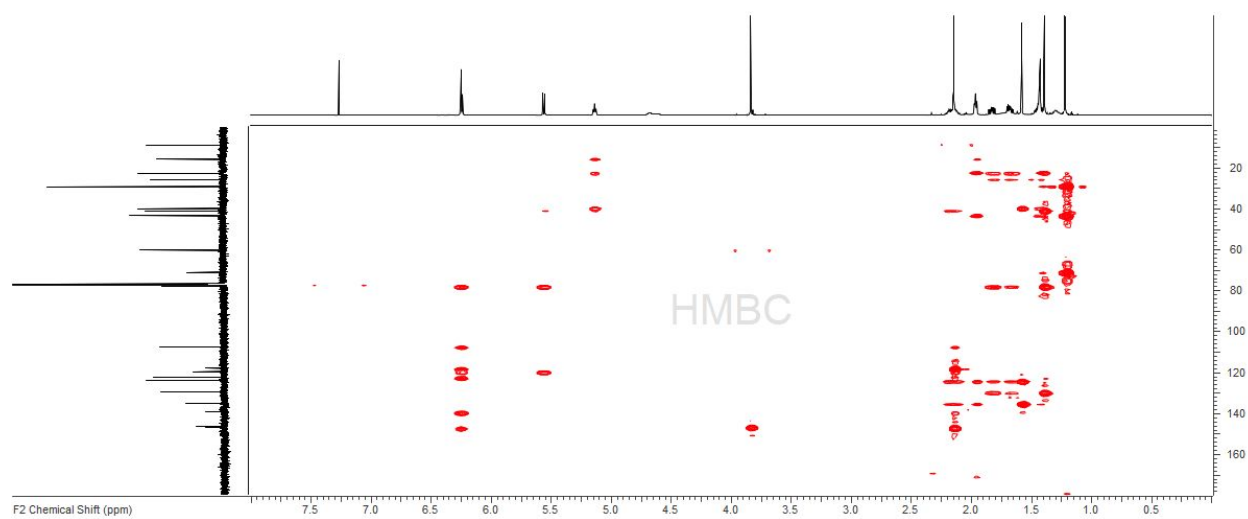


Figure S45: Tuaimenal F (**5**) HMBC NMR spectrum (500 MHz, CDCl₃).

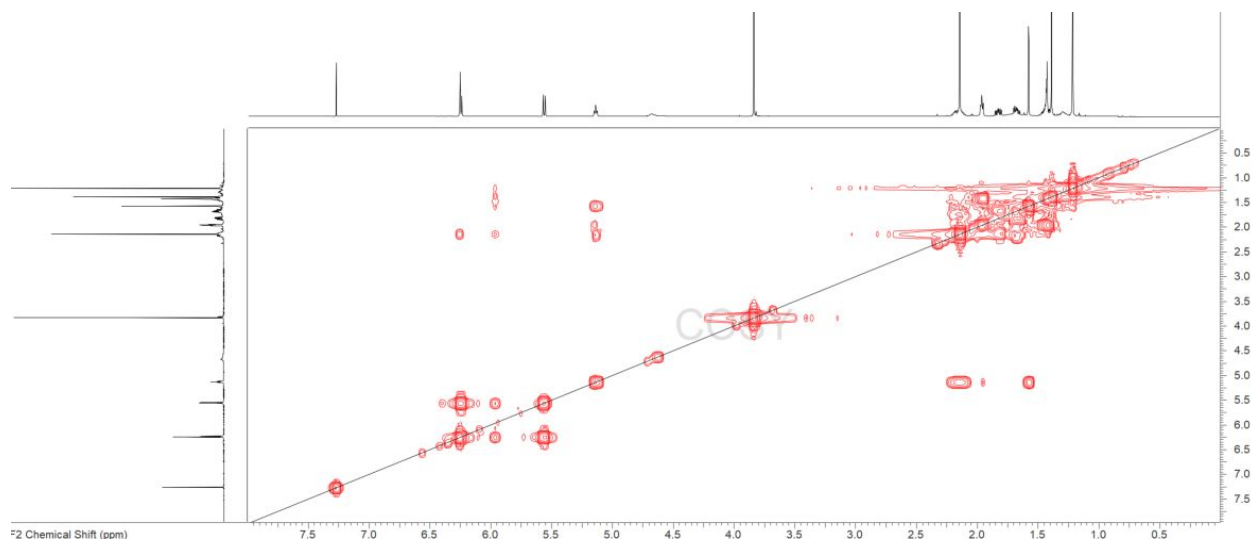


Figure S46: Tuaimenal F (**5**) COSY NMR spectrum (500 MHz, CDCl₃).

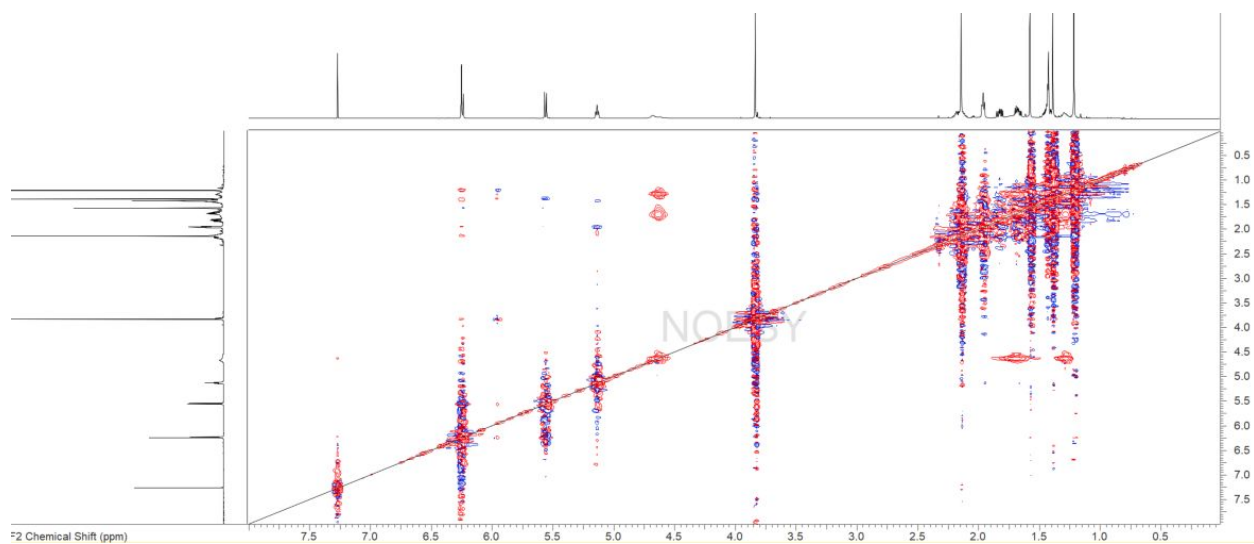


Figure S47: Tuaimenal F (**5**) NOESY NMR spectrum (500 MHz, CDCl₃).

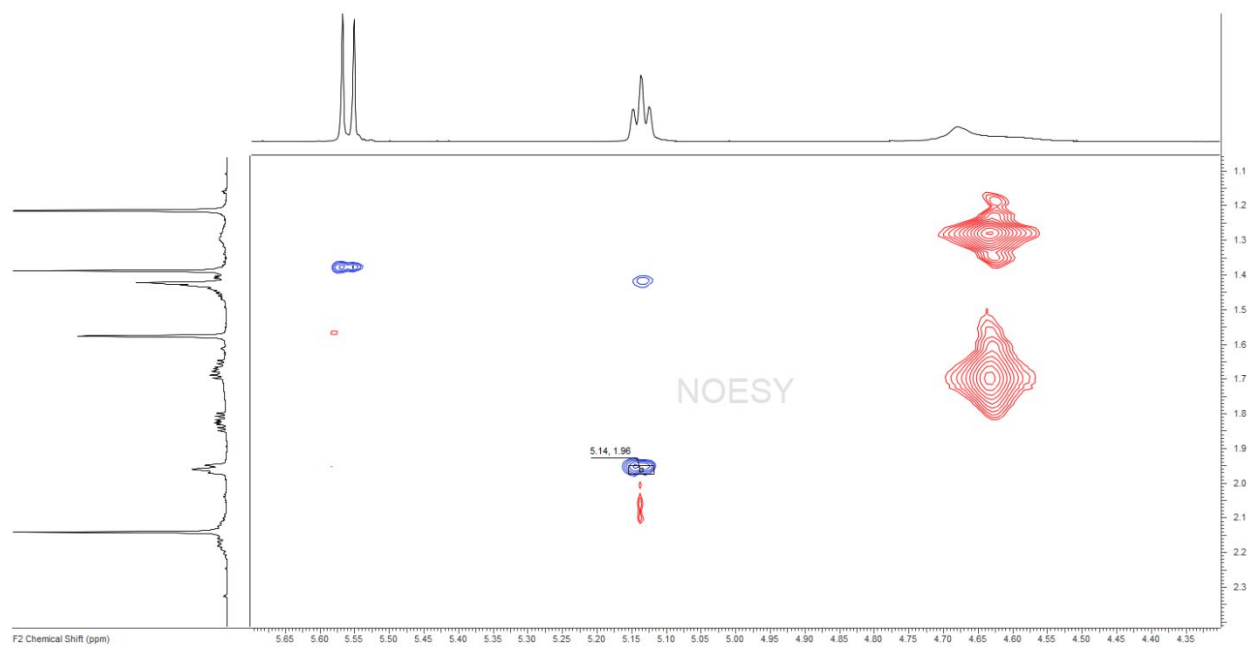


Figure S48: Tuaimenal F (**5**) zoomed NOESY NMR spectrum (500 MHz, CDCl_3).

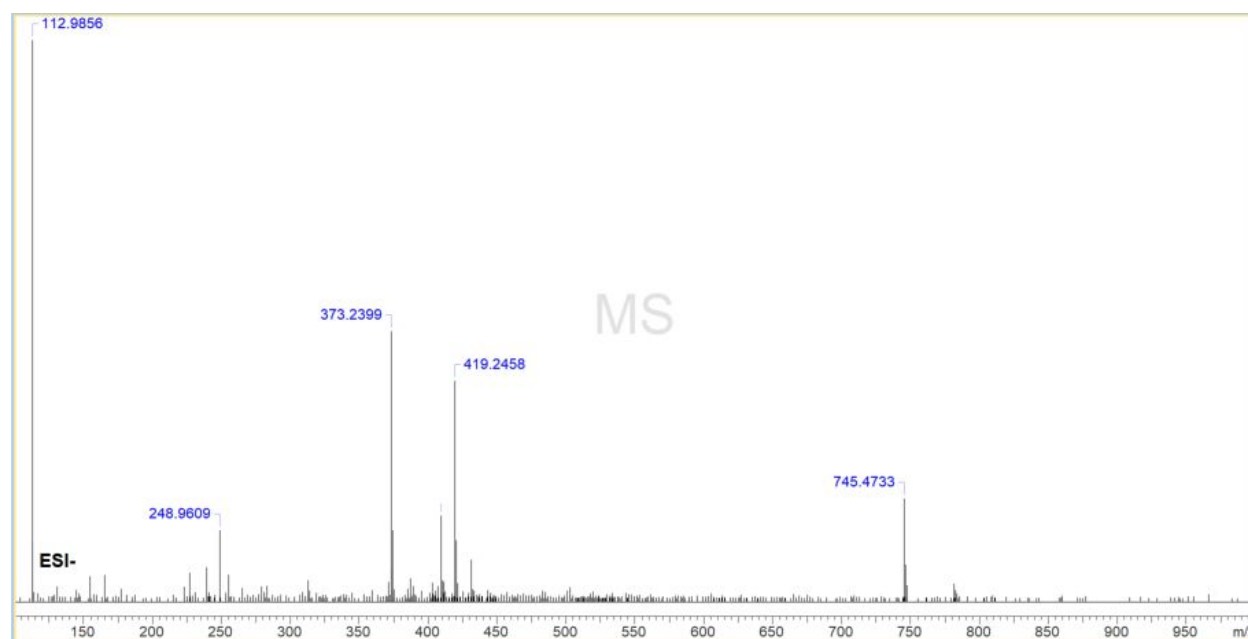


Figure S49: Tuaimenal F (**5**) HRESIMS (neg).

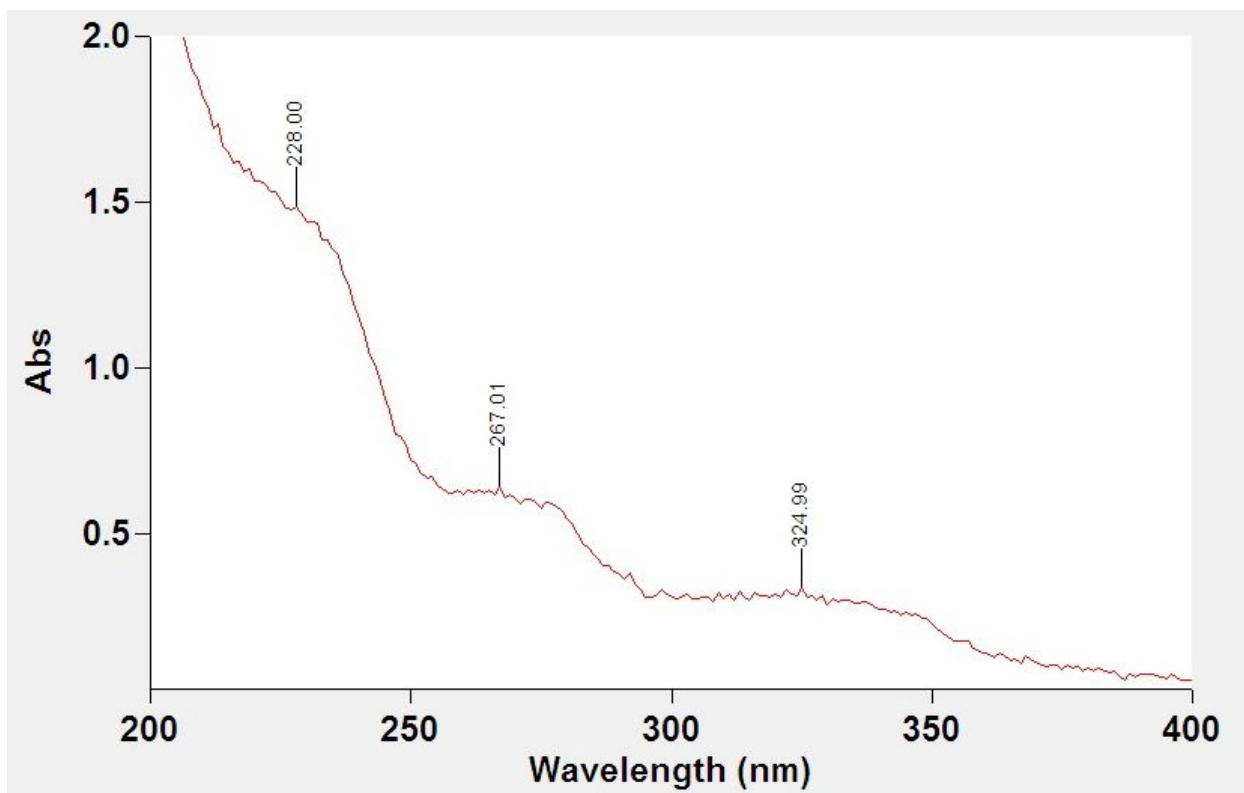


Figure S50: Tuaimenal F (**5**) UV λ_{\max} (C_2H_3N).

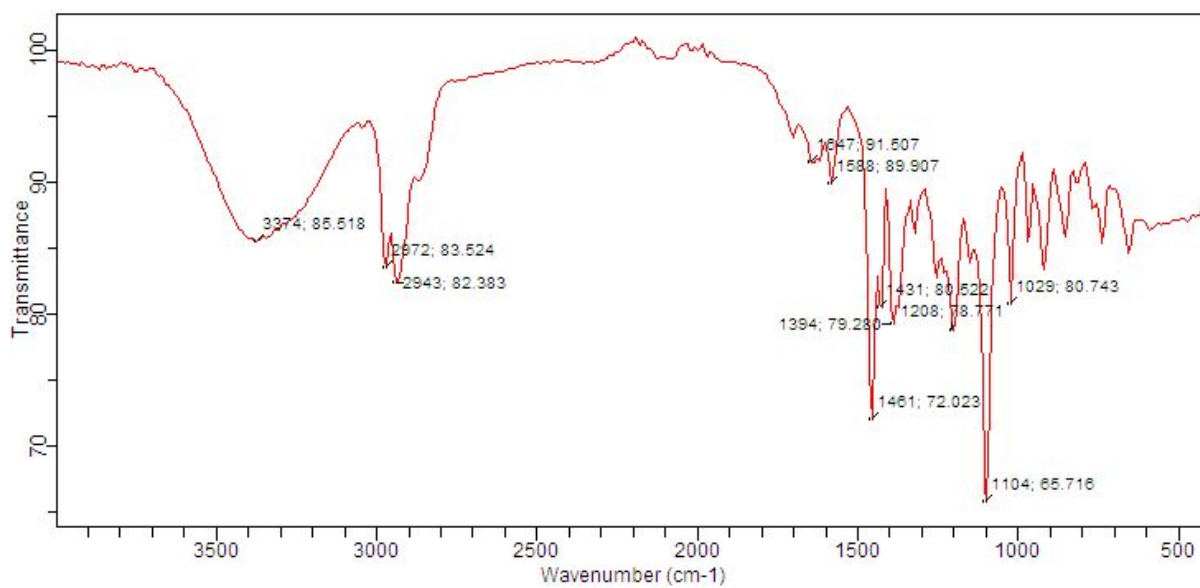


Figure S51: Tuaimenal F (**5**) IR spectrum (thin film).

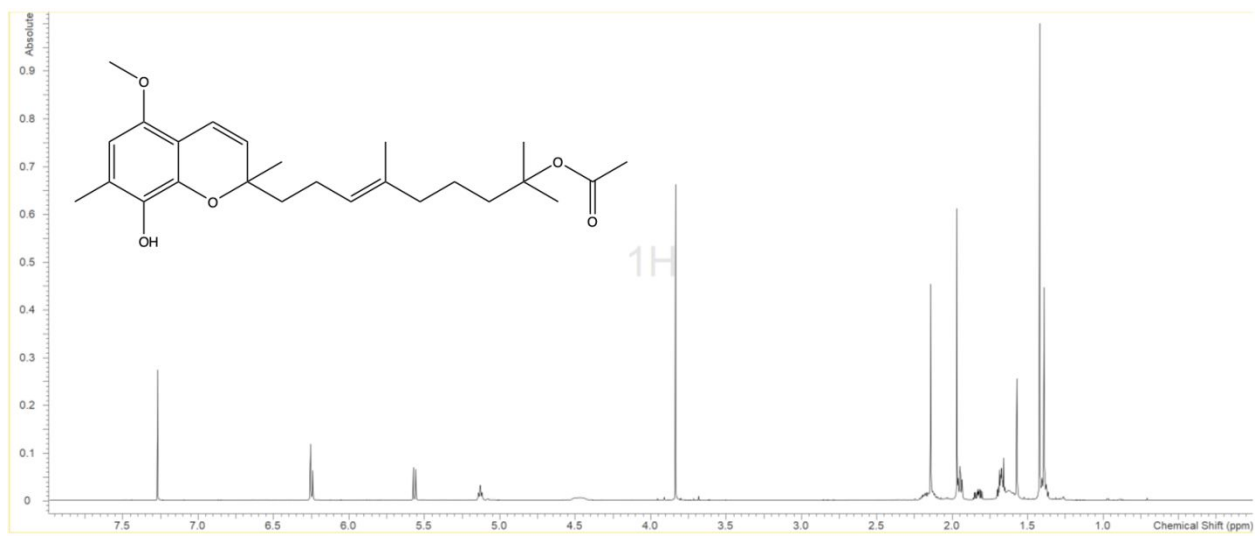


Figure S52: Tuaimenal G (**6**) ¹H NMR spectrum (600 MHz, CDCl₃).

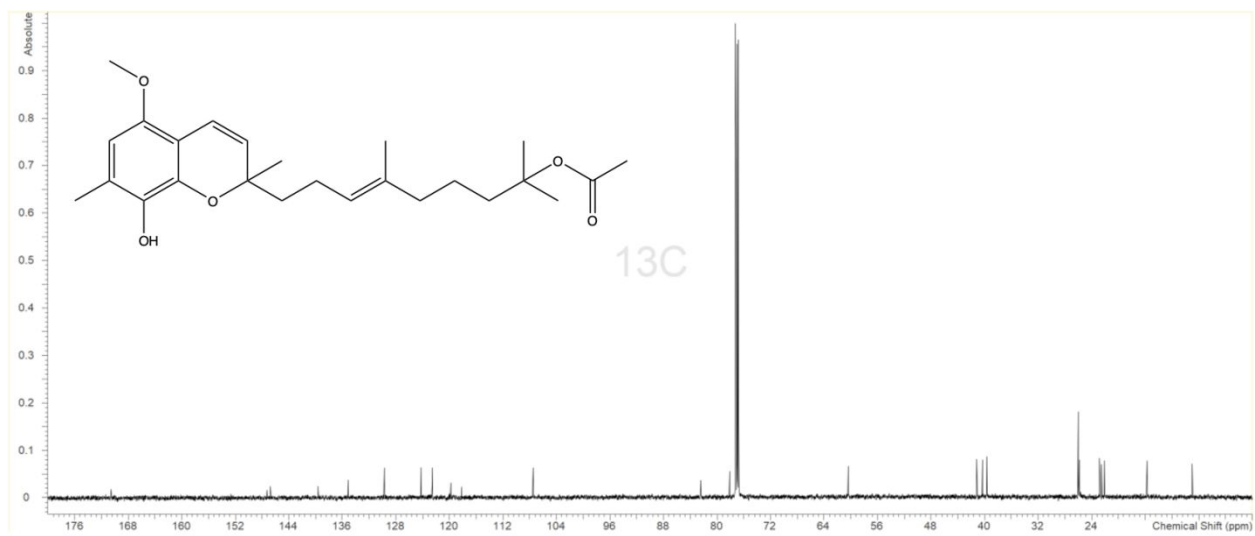


Figure S53: Tuaimenal G (**6**) ¹³C NMR spectrum (150 MHz, CDCl₃).

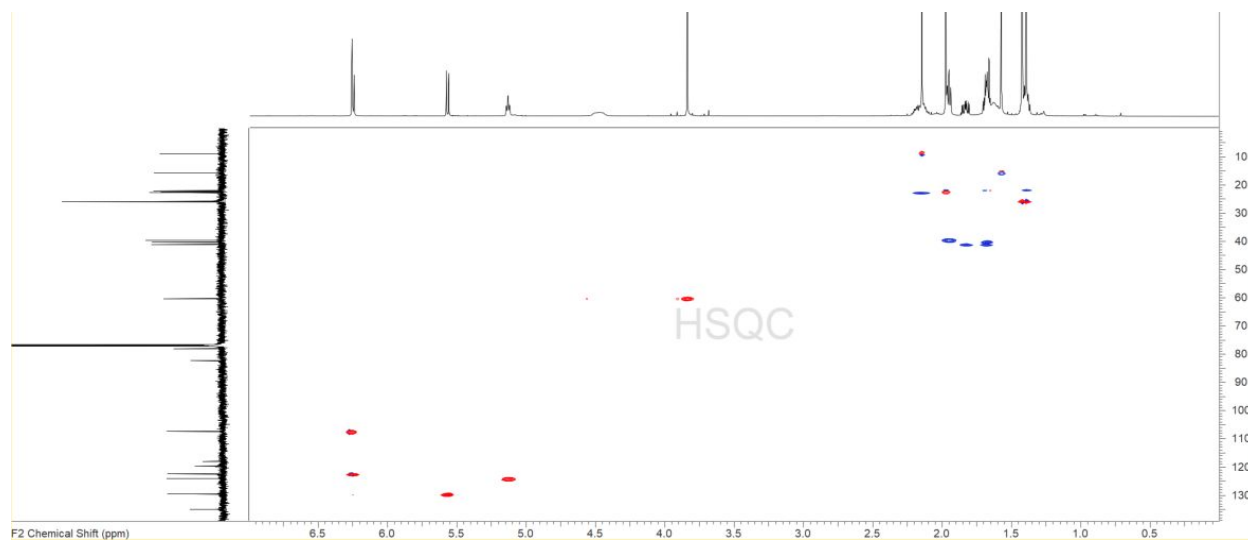


Figure S54: Tuaimenal G (**6**) HSCQ NMR spectrum (500 MHz, CDCl_3).

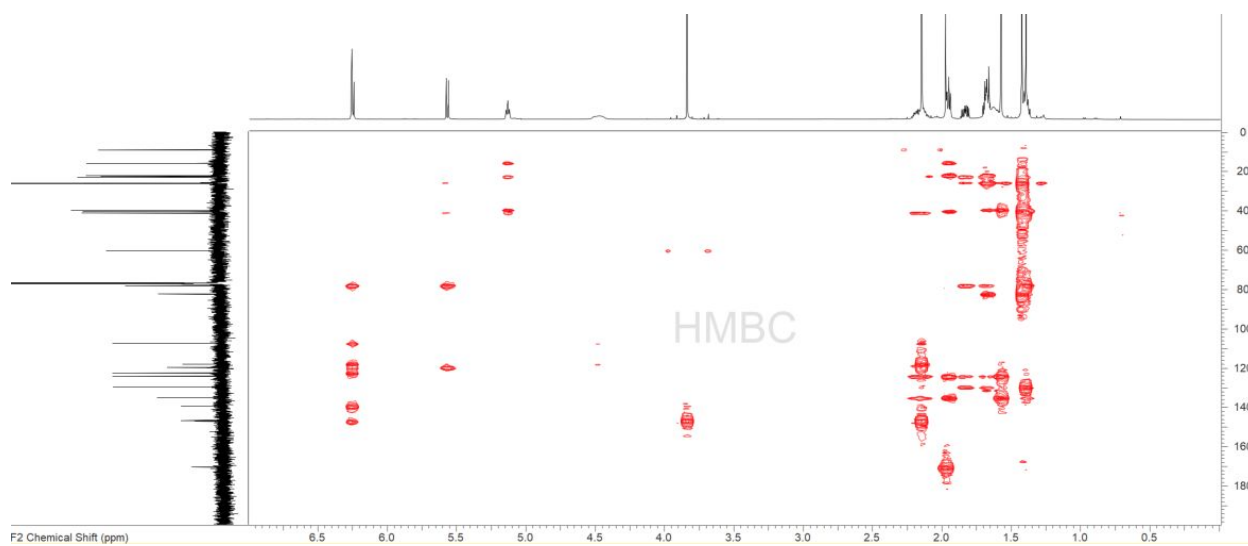


Figure S55: Tuaimenal G (**6**) HMBC NMR spectrum (500 MHz, CDCl_3).

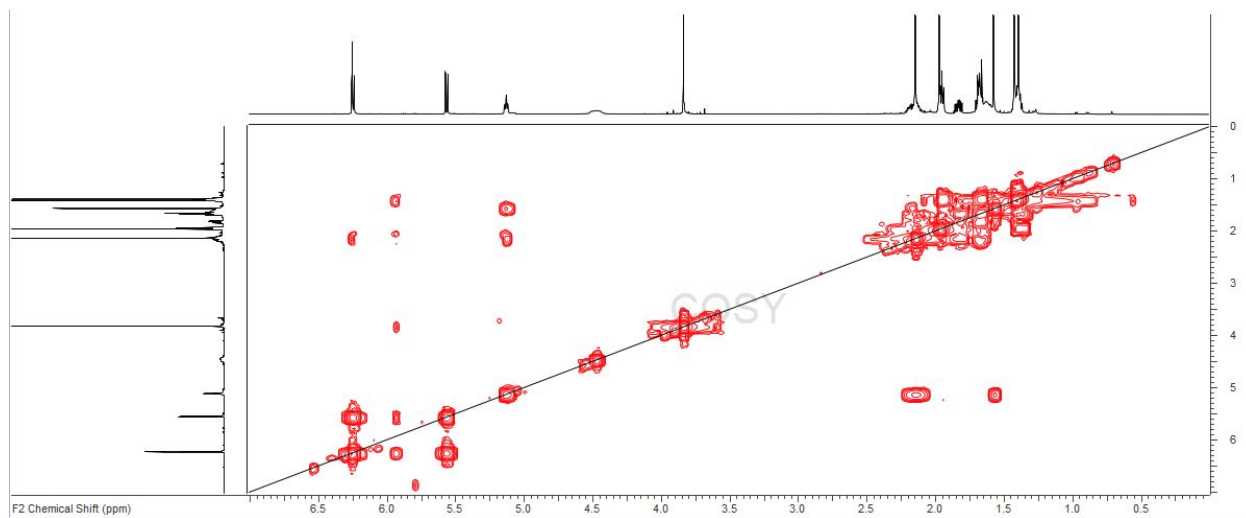


Figure S56: Tuaimenal G (**6**) COSY NMR spectrum (500 MHz, CDCl₃).

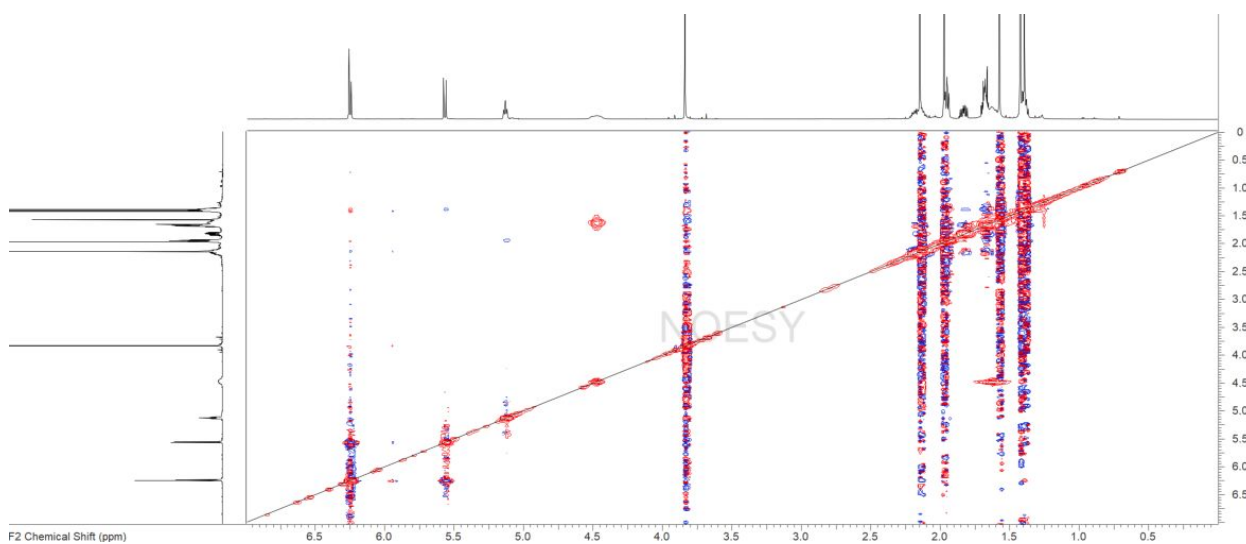


Figure S57: Tuaimenal G (**6**) NOESY NMR spectrum (500 MHz, CDCl₃).

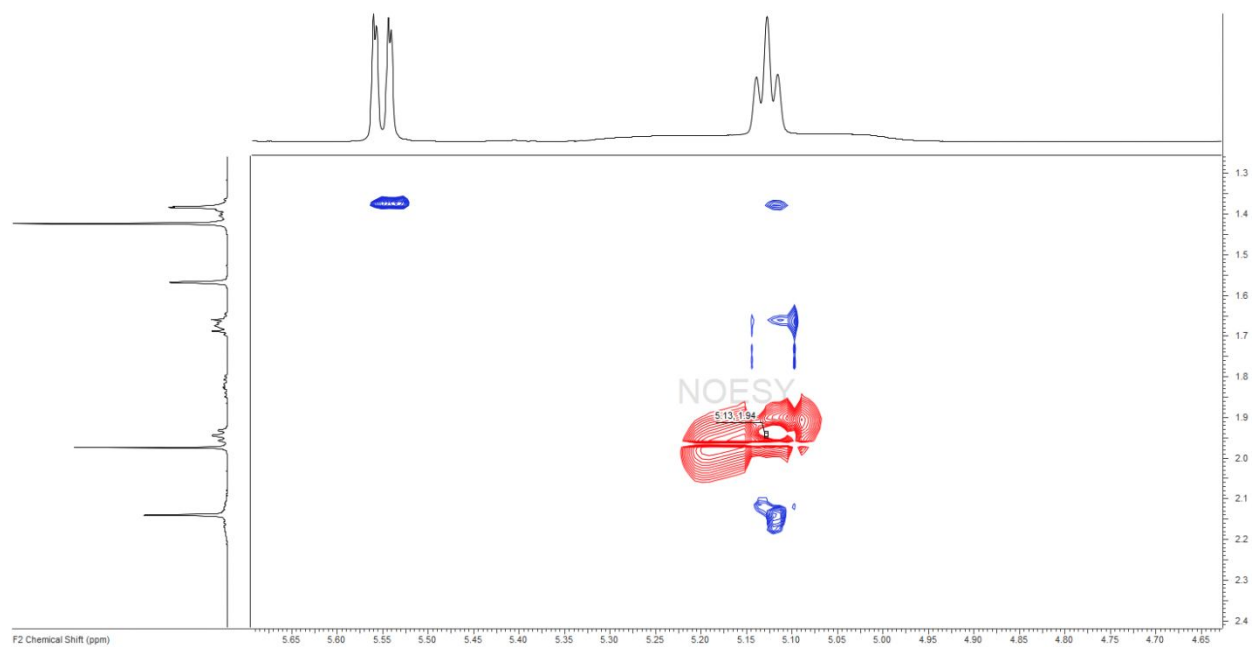


Figure S58: Tuaimenal G (**6**) zoomed NOESY NMR spectrum (500 MHz, CDCl₃).

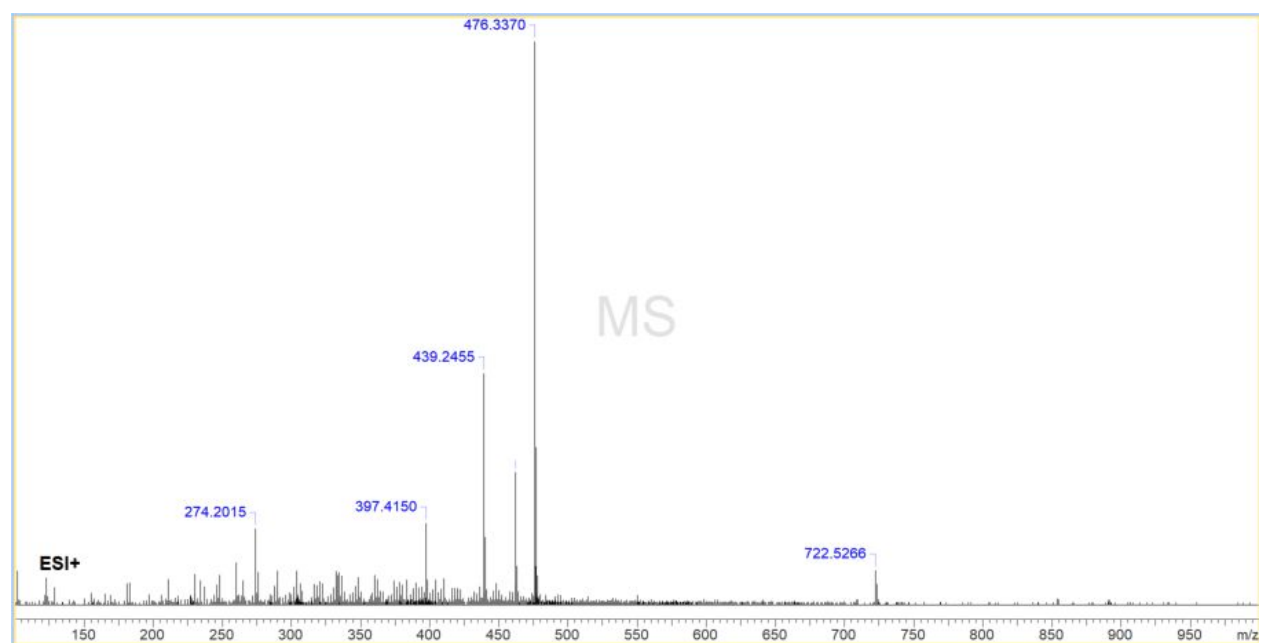


Figure S59: Tuaimenal G (**6**) HRESIMS (pos).

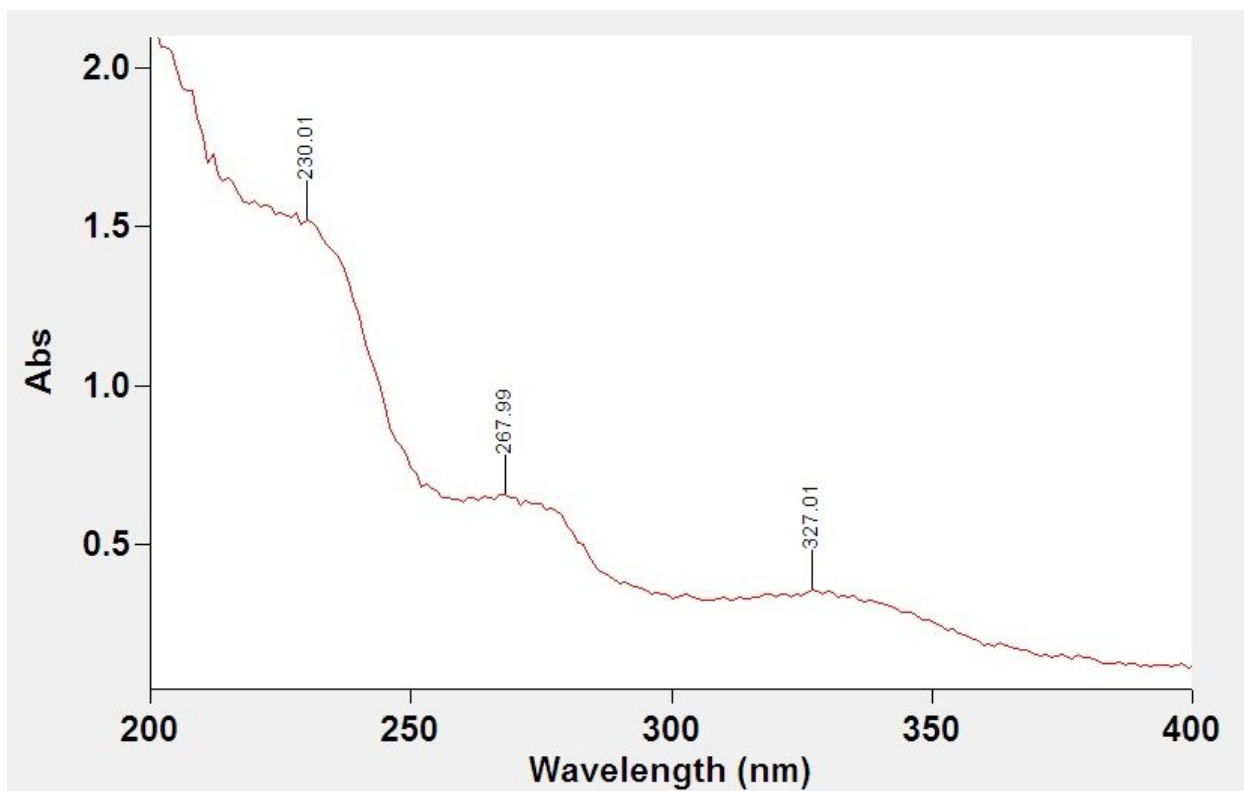


Figure S60: Tuaimenal G (6) UV λ_{\max} (C₂H₃N).

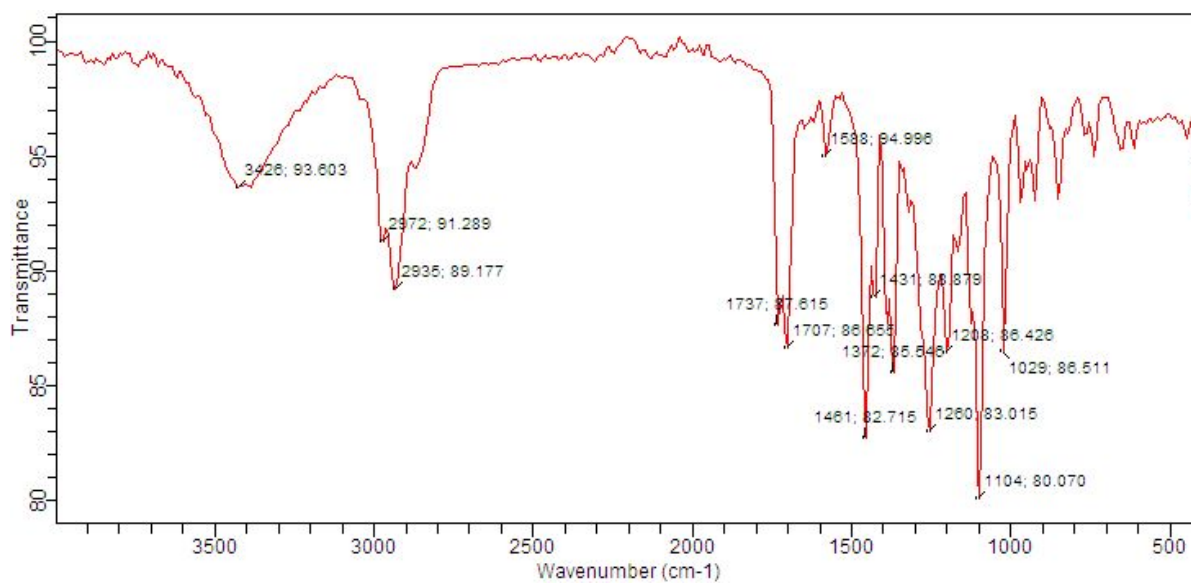


Figure S61: Tuaimenal G (6) IR spectrum (thin film).

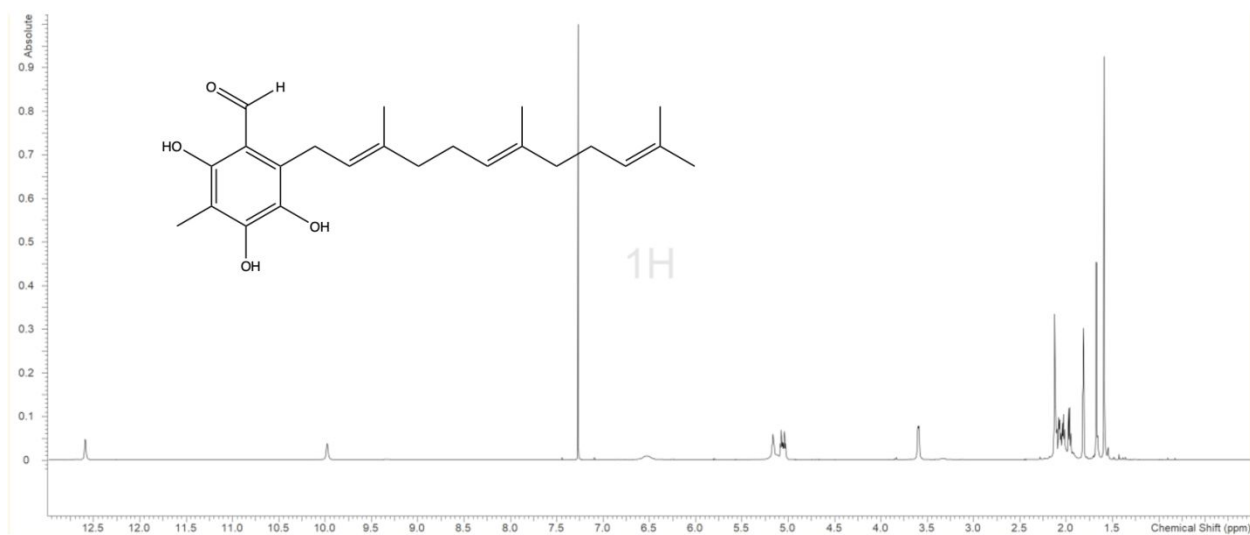


Figure S62: Tuaimenal H (7) ¹H NMR spectrum (600 MHz, CDCl₃).

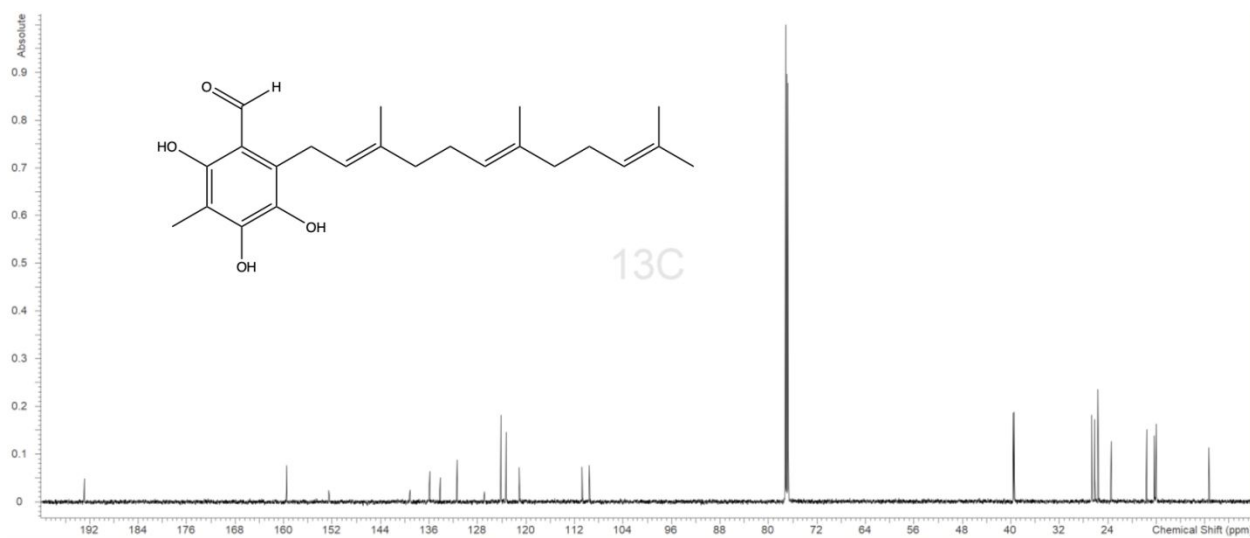


Figure S63: Tuaimenal H (7) ¹³C NMR spectrum (150 MHz, CDCl₃).

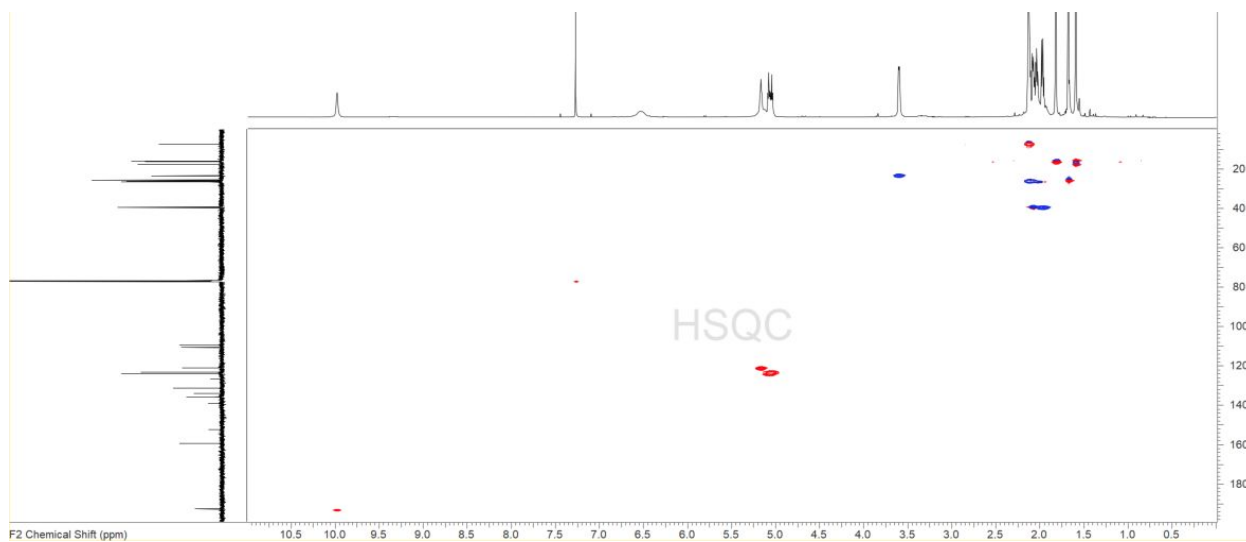


Figure S64: Tuaimenal H (7) HSCQ NMR spectrum (500 MHz, CDCl₃).

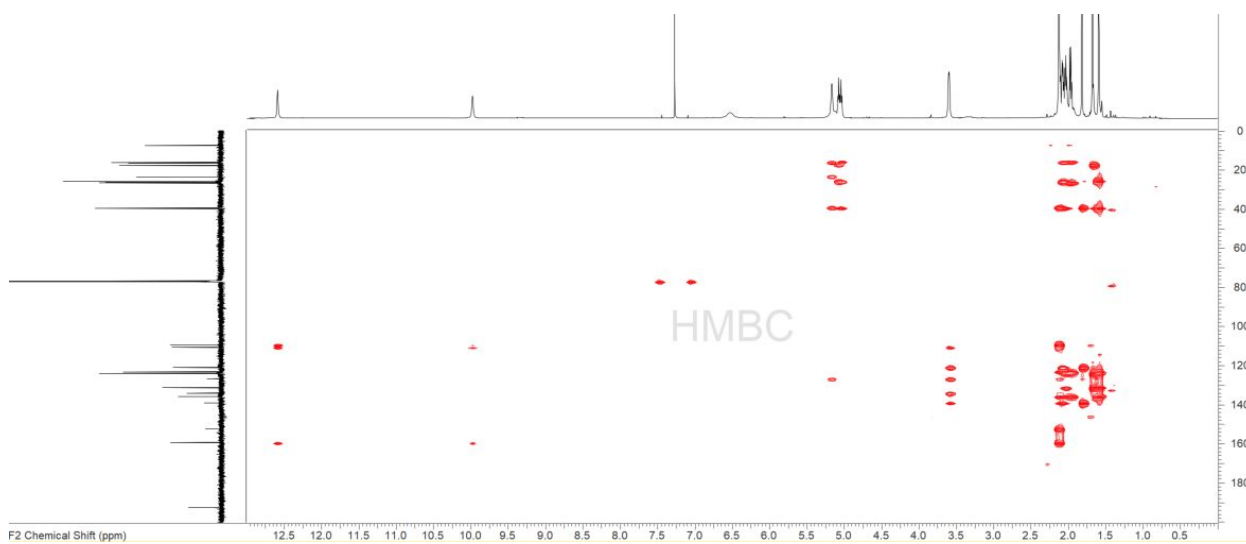


Figure S65: Tuaimenal H (7) HMBC NMR spectrum (500 MHz, CDCl₃).

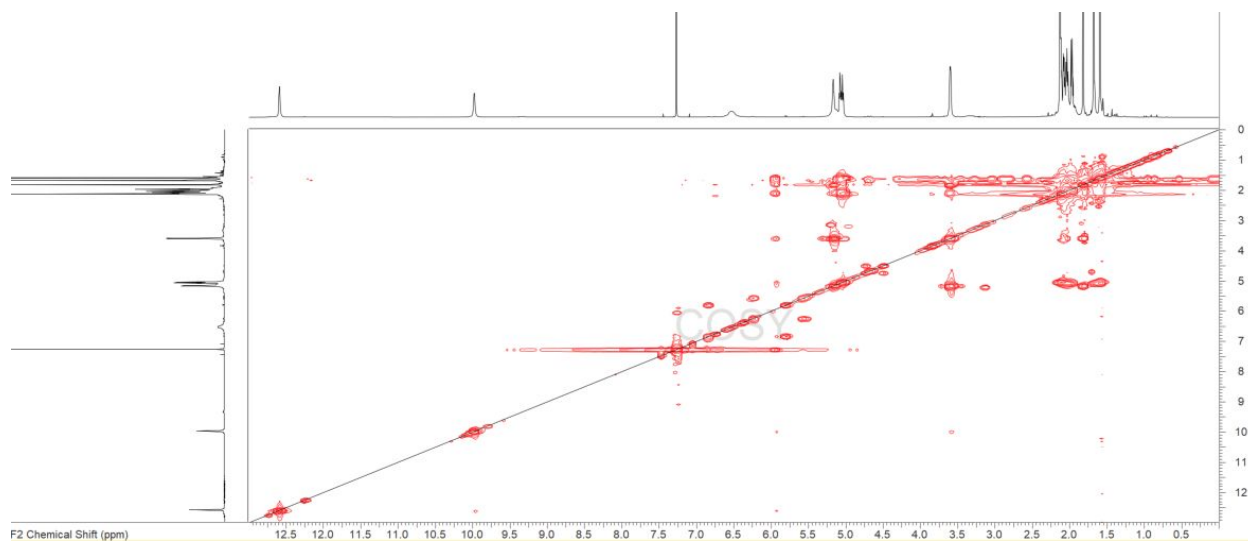


Figure S66: Tuaimenal H (7) COSY NMR spectrum (500 MHz, CDCl₃).

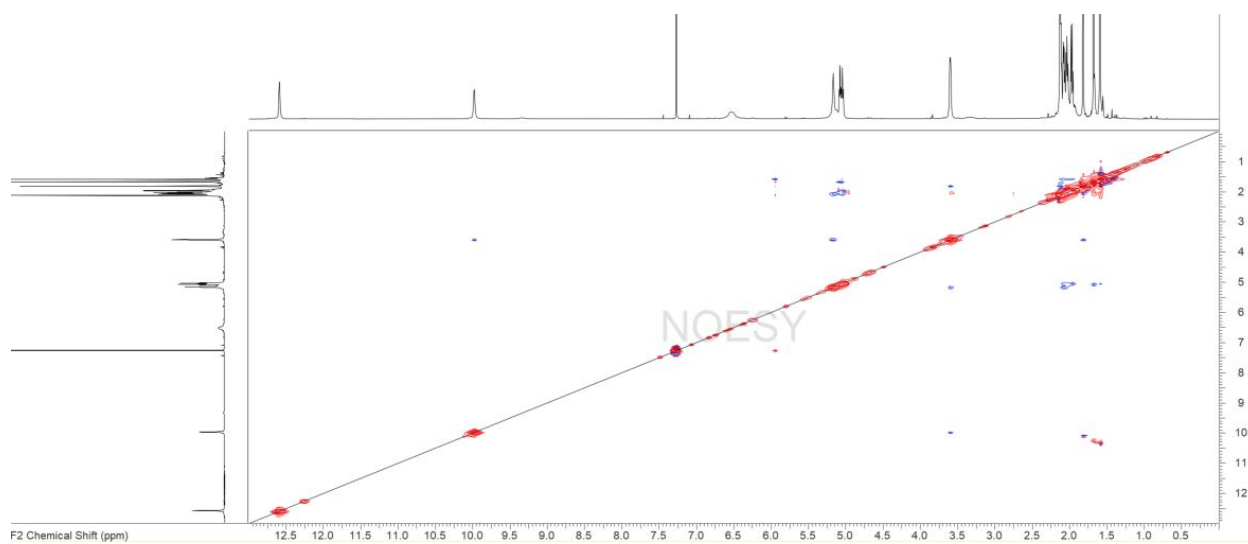


Figure S67: Tuaimenal H (7) NOESY NMR spectrum (500 MHz, CDCl₃).

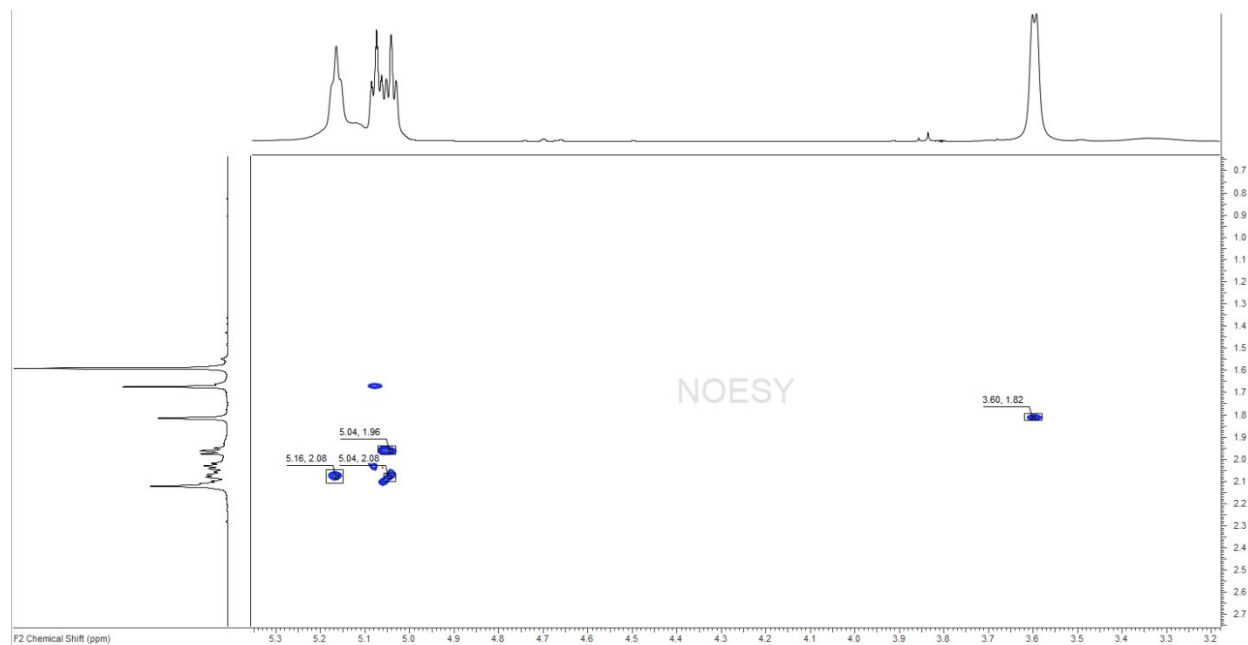


Figure S68: Tuaimenal H (**7**) zoomed NOESY NMR spectrum (500 MHz, CDCl_3).

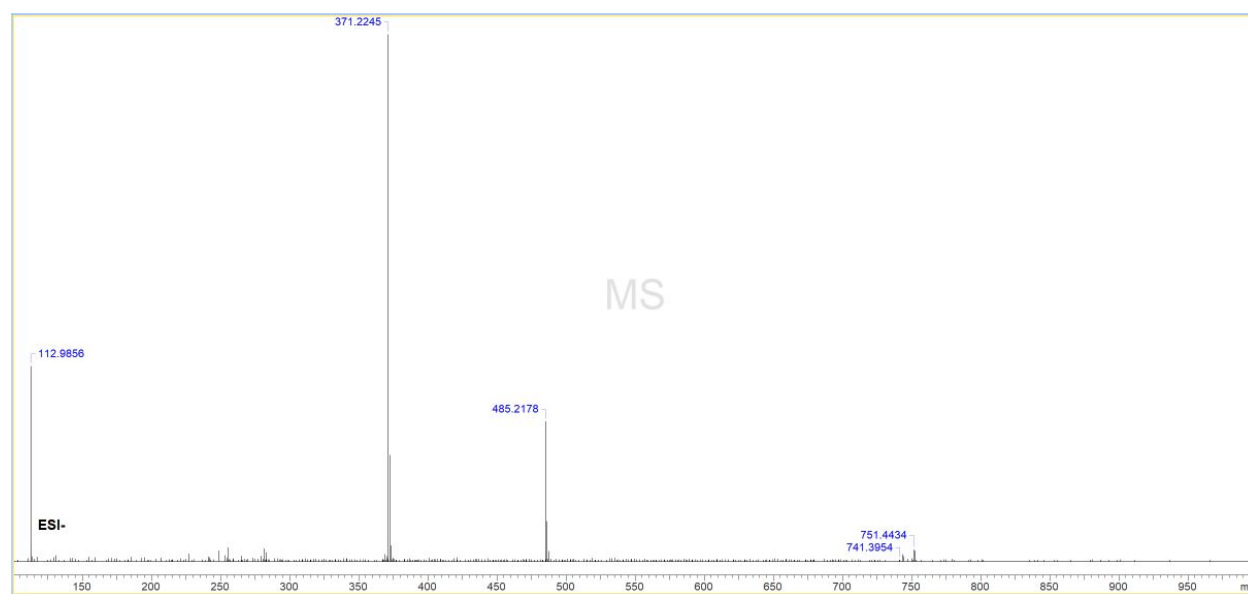


Figure S69: Tuaimenal H (**7**) HRESIMS (neg).

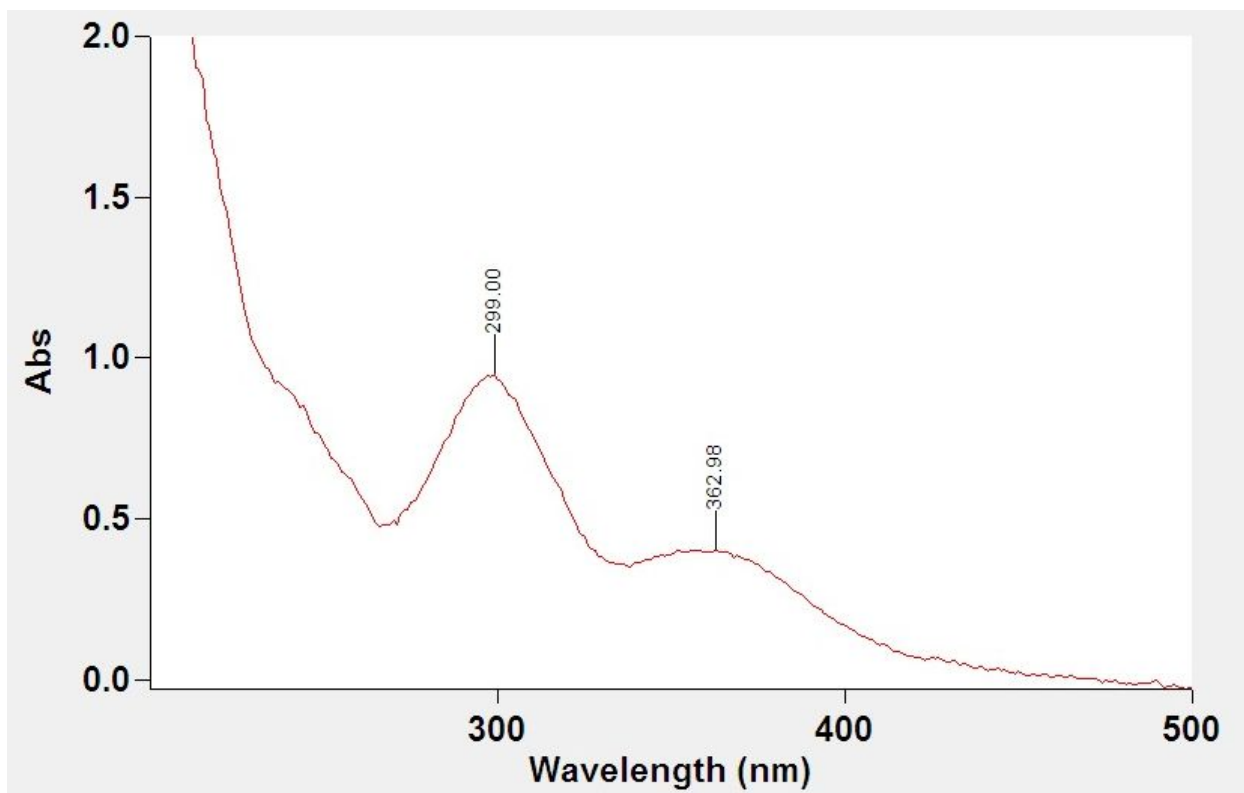


Figure S70: Tuaimenal H (7) UV λ_{max} (C_2H_3N).

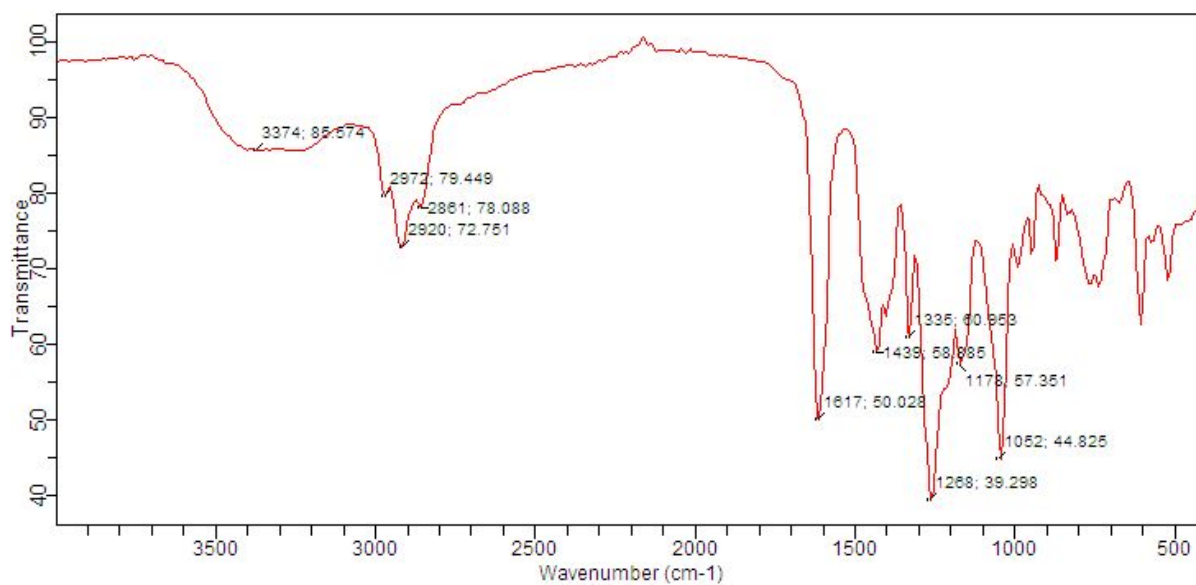


Figure S71: Tuaimenal H (7) IR spectrum (thin film).

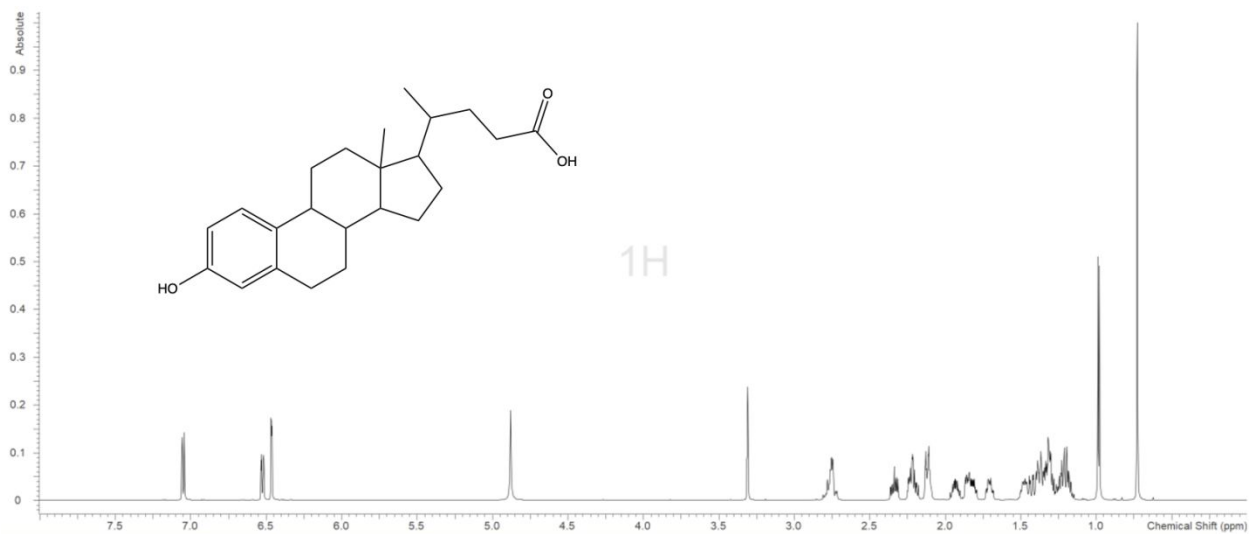


Figure S72: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**8**) ¹H NMR spectrum (600 MHz, MeOD).

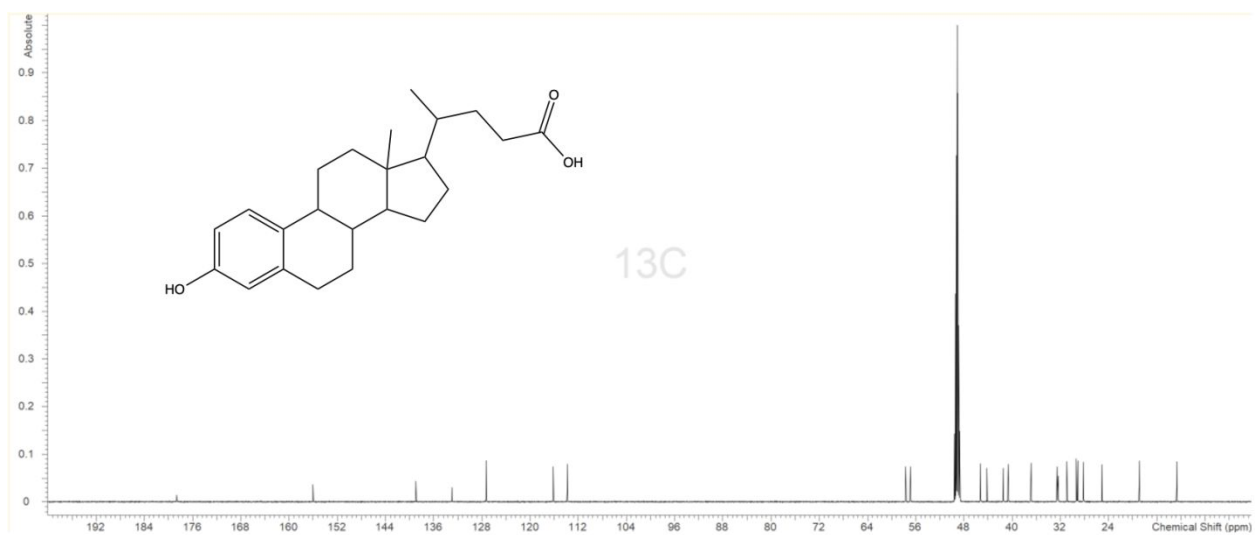


Figure S73: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**8**) ¹³C NMR spectrum (150 MHz, MeOD).

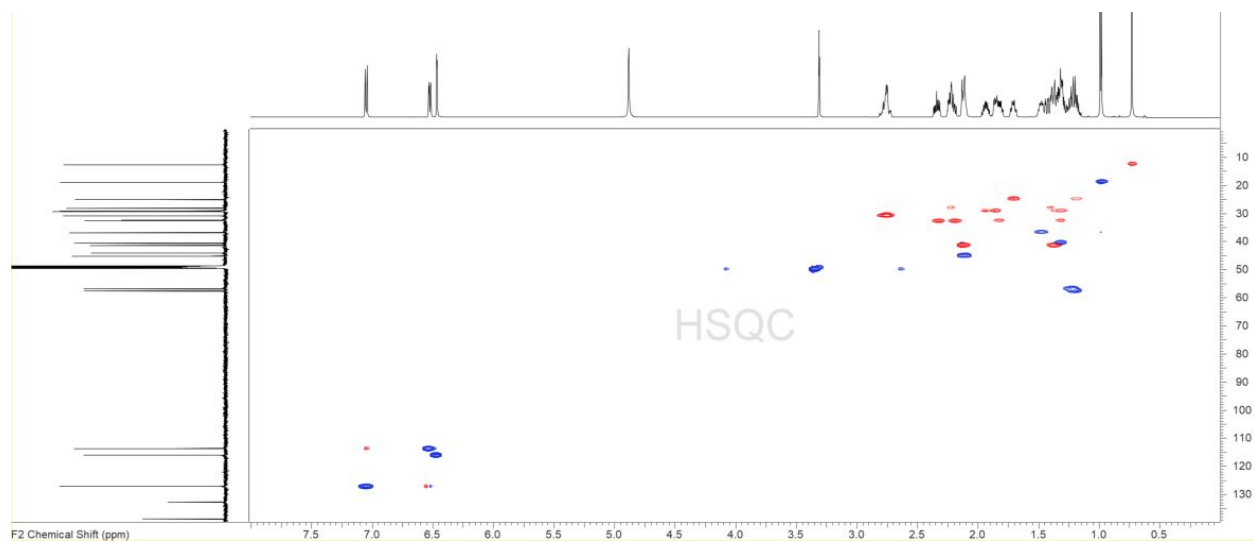


Figure S74: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**8**) HSCQ NMR spectrum (500 MHz, MeOD).

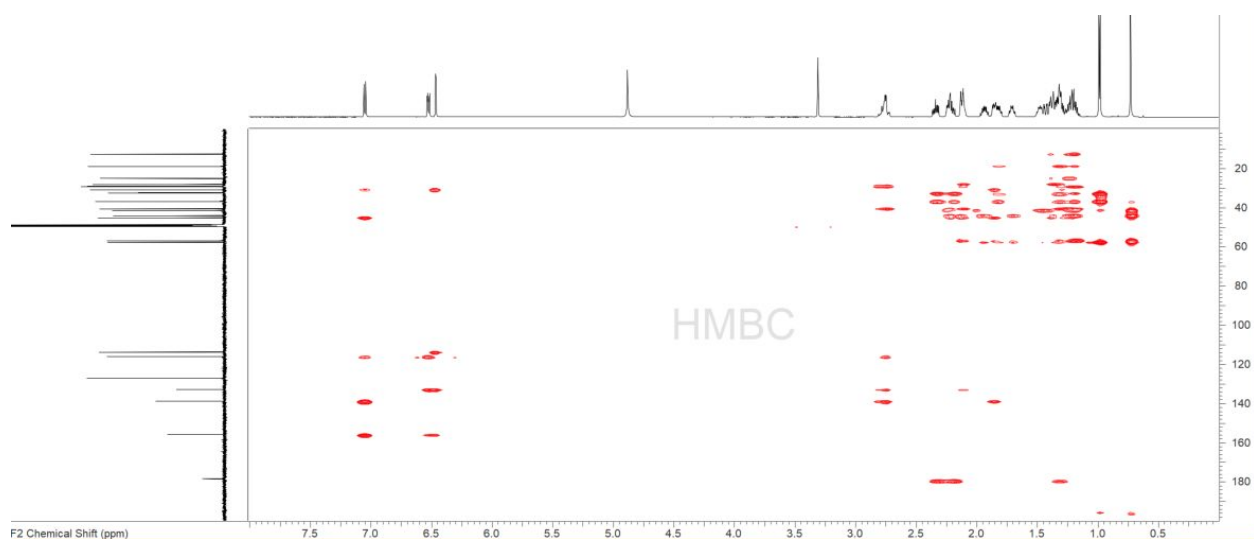


Figure S75: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**8**) HMBC NMR spectrum (500 MHz, MeOD).

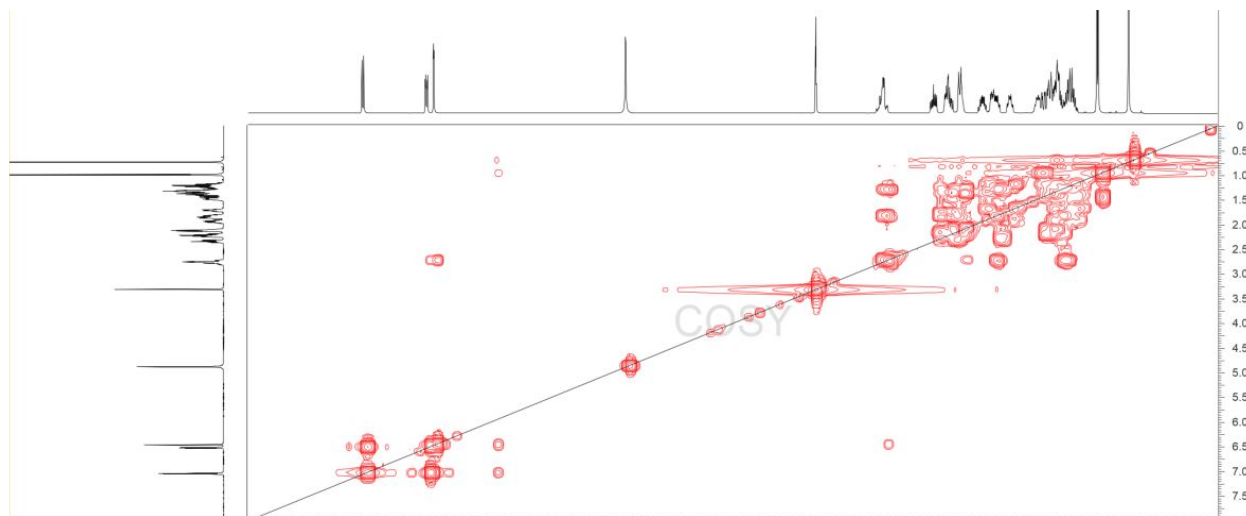


Figure S76: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**8**) COSY NMR spectrum (500 MHz, MeOD).

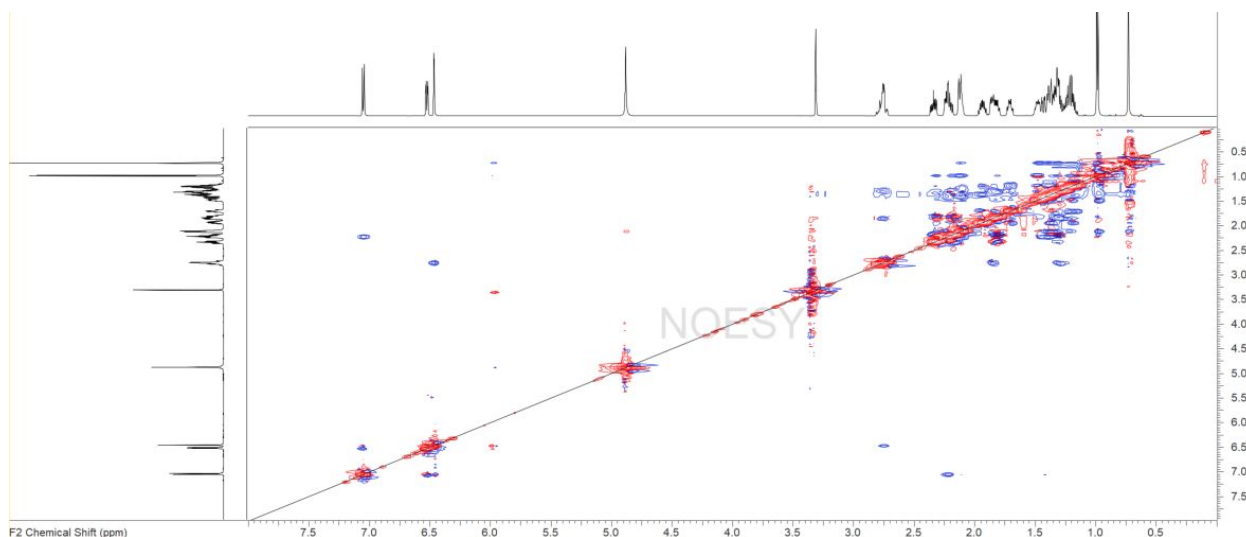


Figure S77: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**8**) NOESY NMR spectrum (500 MHz, MeOD).

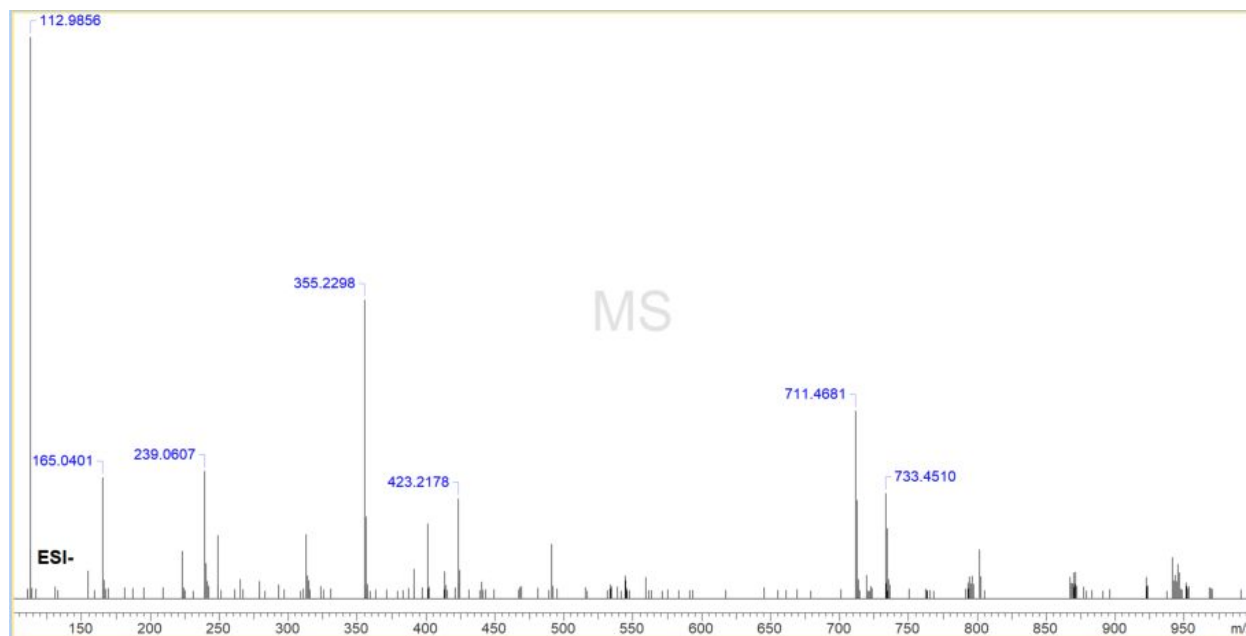


Figure S78: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**8**) HRESIMS (neg).

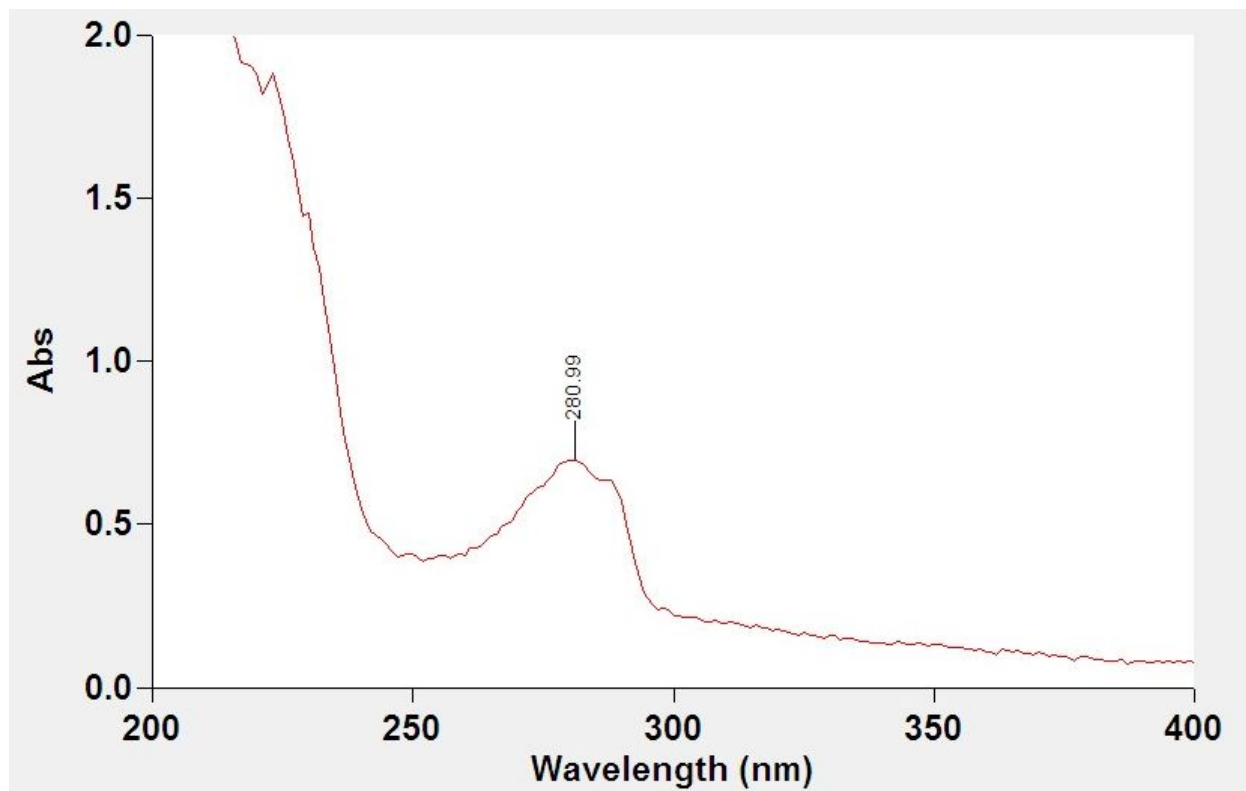


Figure S79: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**8**) UV λ_{max} ($\text{C}_2\text{H}_3\text{N}$).

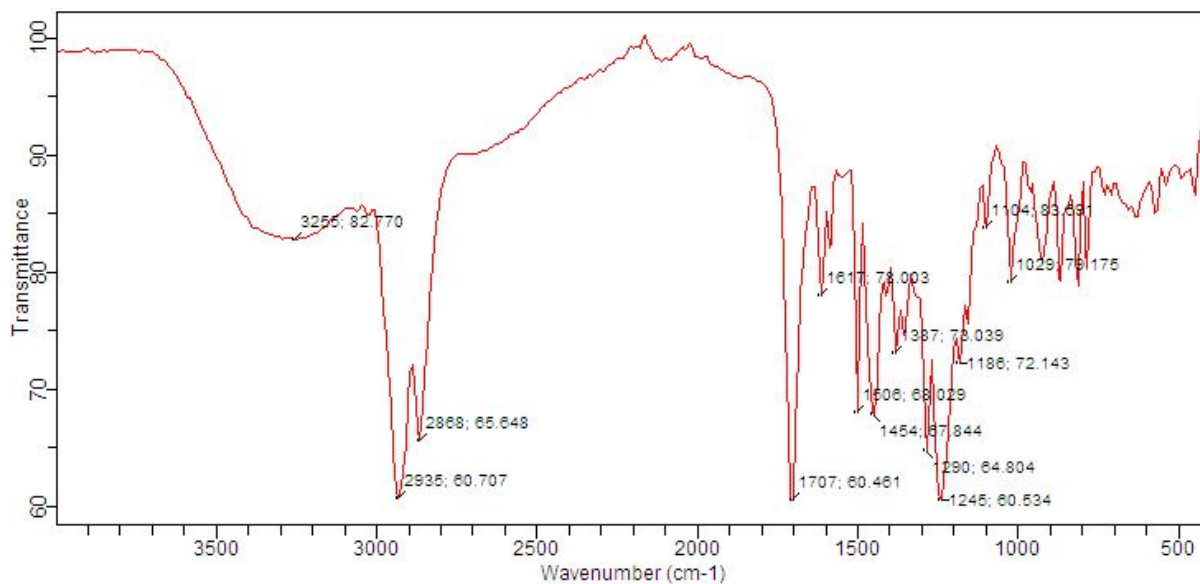


Figure S80: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**8**) IR spectrum (thin film).

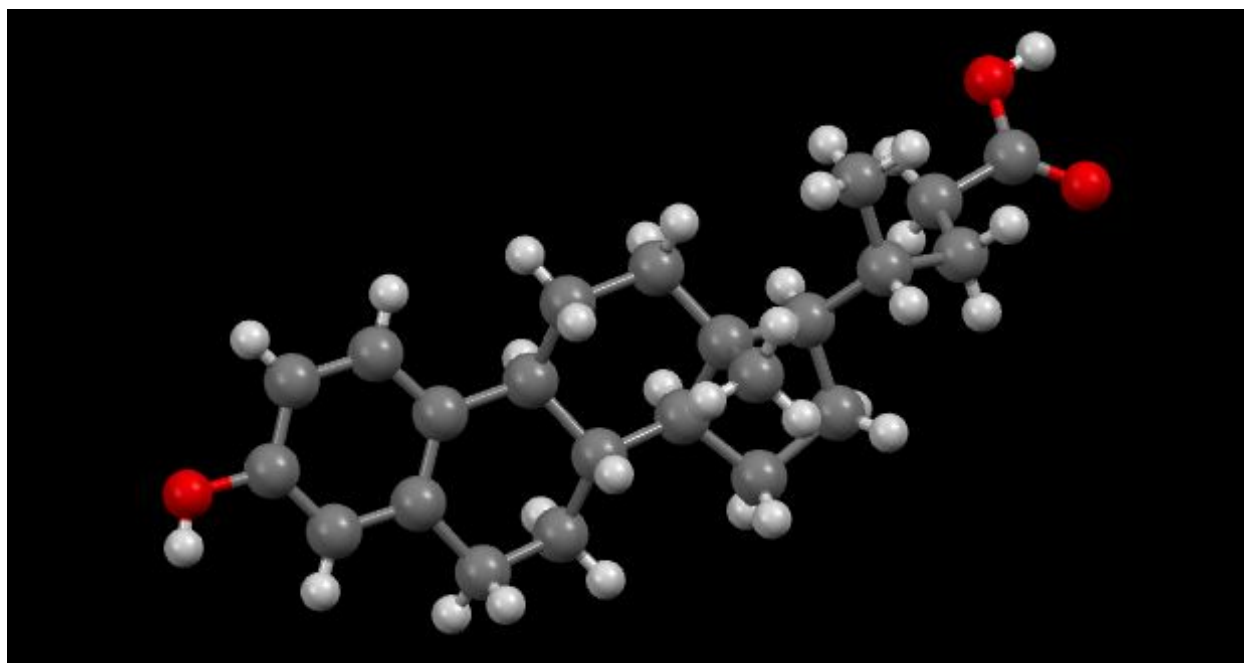


Figure S81: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**8**) X-ray crystal structure.

Identification code	JTW-045
Empirical formula	C ₂₃ H ₃₂ O ₃
Formula weight	356.48
Temperature/K	100
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	6.46790(10)
b/Å	9.6023(2)
c/Å	30.7076(5)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	1907.15(6)
Z	4
ρ _{calc} /g/cm ³	1.242
μ/mm ⁻¹	0.629
F(000)	776.0
Crystal size/mm ³	0.2 × 0.2 × 0.1
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	5.756 to 158.692
Index ranges	-8 ≤ h ≤ 8, -12 ≤ k ≤ 12, -38 ≤ l ≤ 38
Reflections collected	44886
Independent reflections	4106 [R _{int} = 0.0296, R _{sigma} = 0.0141]
Data/restraints/parameters	4106/0/245
Goodness-of-fit on F ²	1.080
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0344, wR ₂ = 0.0916
Final R indexes [all data]	R ₁ = 0.0347, wR ₂ = 0.0919
Largest diff. peak/hole / e Å ⁻³	0.16/-0.18
Flack parameter	0.00(3)

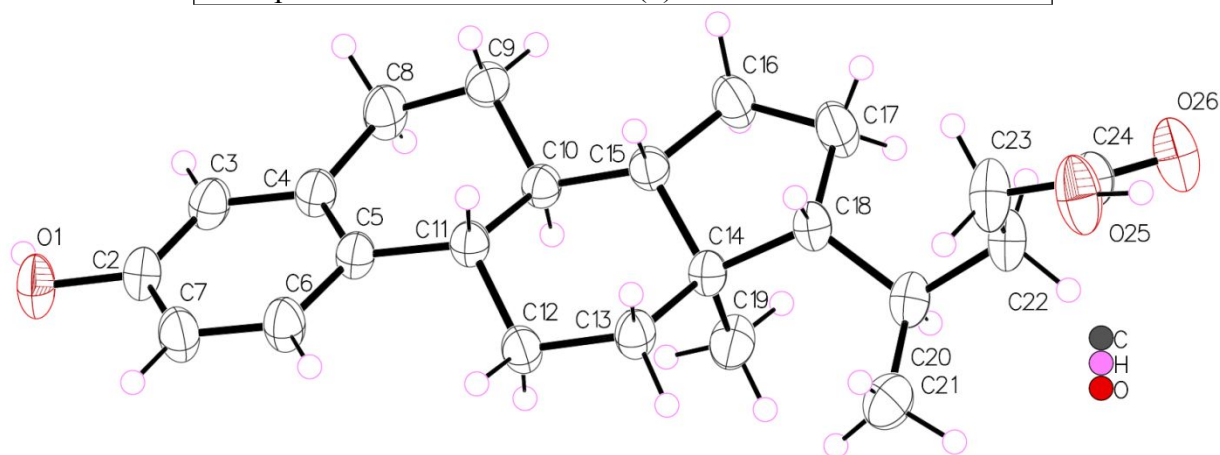


Figure S82: 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**8**) X-ray crystallography metadata and ellipsoid plot with anisotropic displacement parameters drawn at 50% probability.

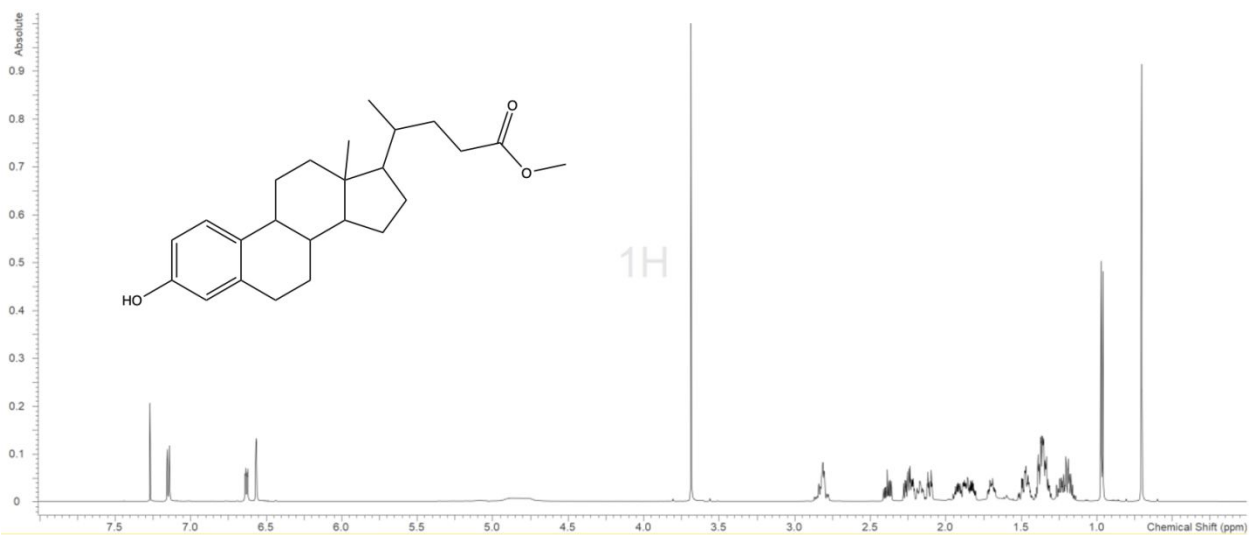


Figure S83: Methyl 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**9**) ^1H NMR spectrum (600 MHz, CDCl_3).

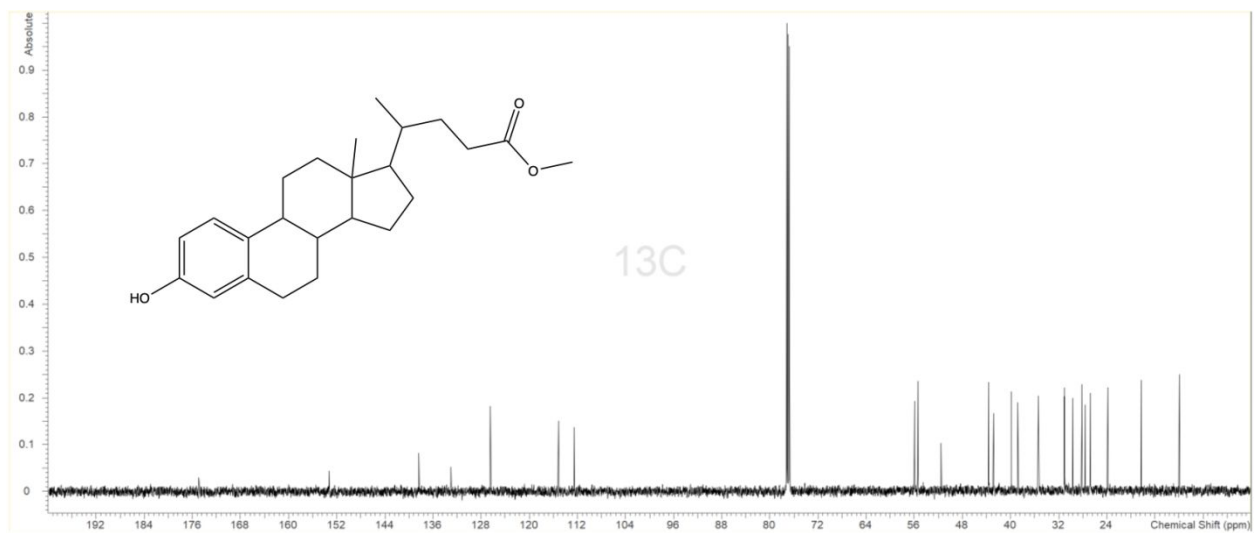


Figure S84: Methyl 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**9**) ^{13}C NMR spectrum (150 MHz, CDCl_3).

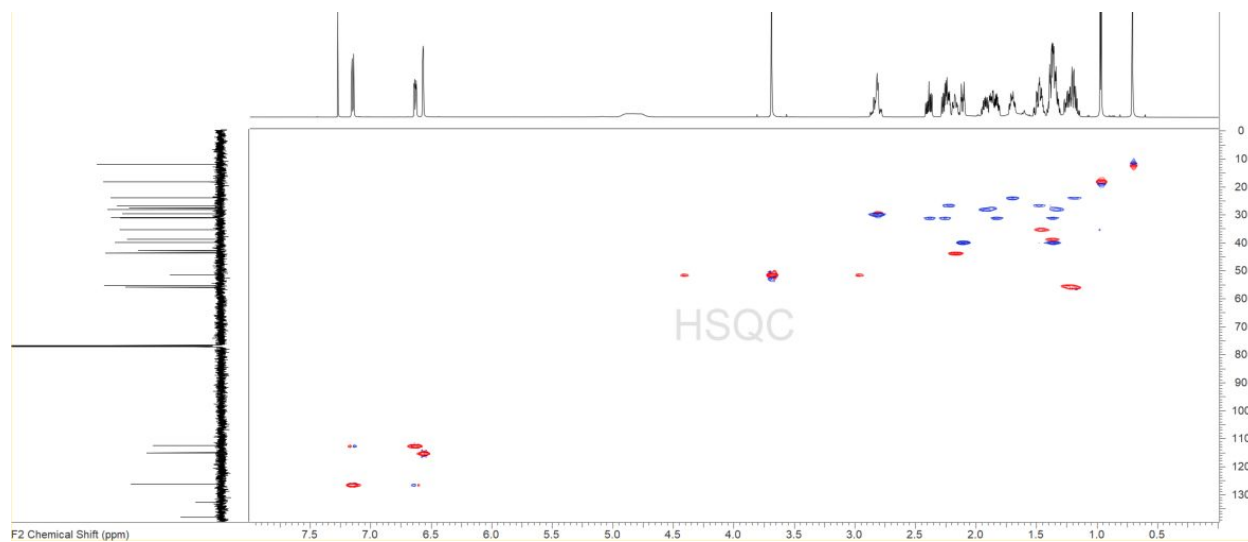


Figure S85: Methyl 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**9**) HSCQ NMR spectrum (500 MHz, CDCl₃).

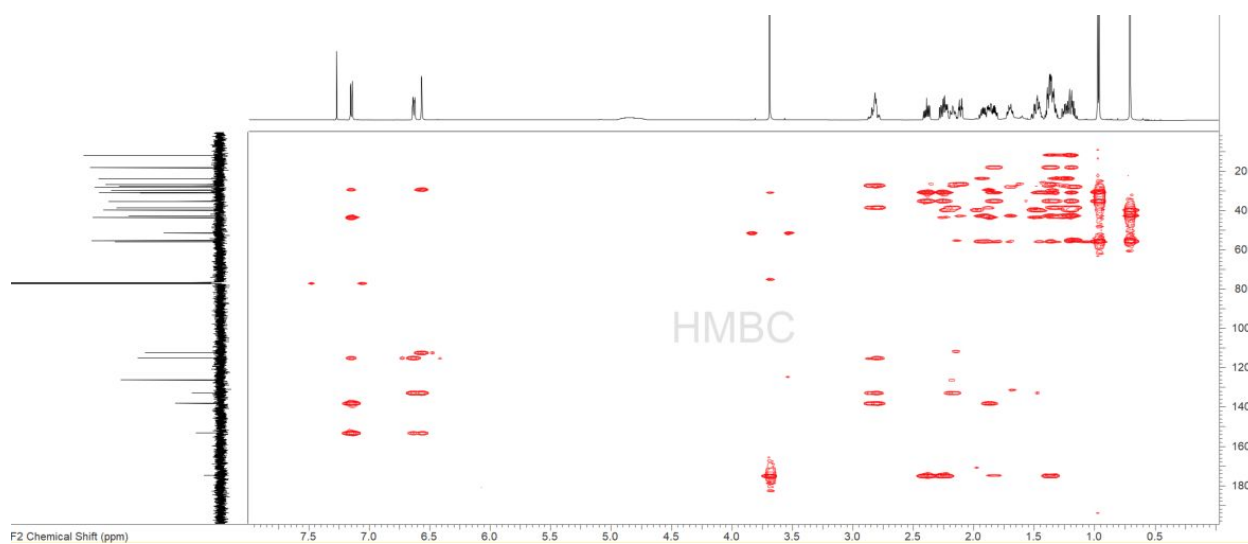


Figure S86: Methyl 30hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**9**) HMBC NMR spectrum (500 MHz, CDCl₃).

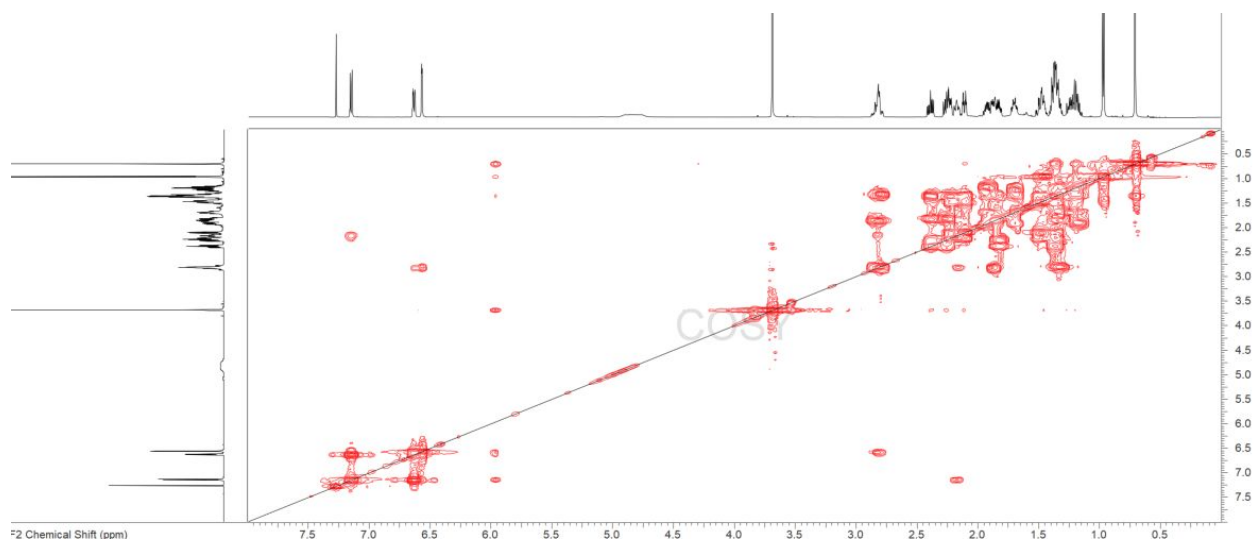


Figure S87: Methyl 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**9**) COSY NMR spectrum (500 MHz, CDCl₃).

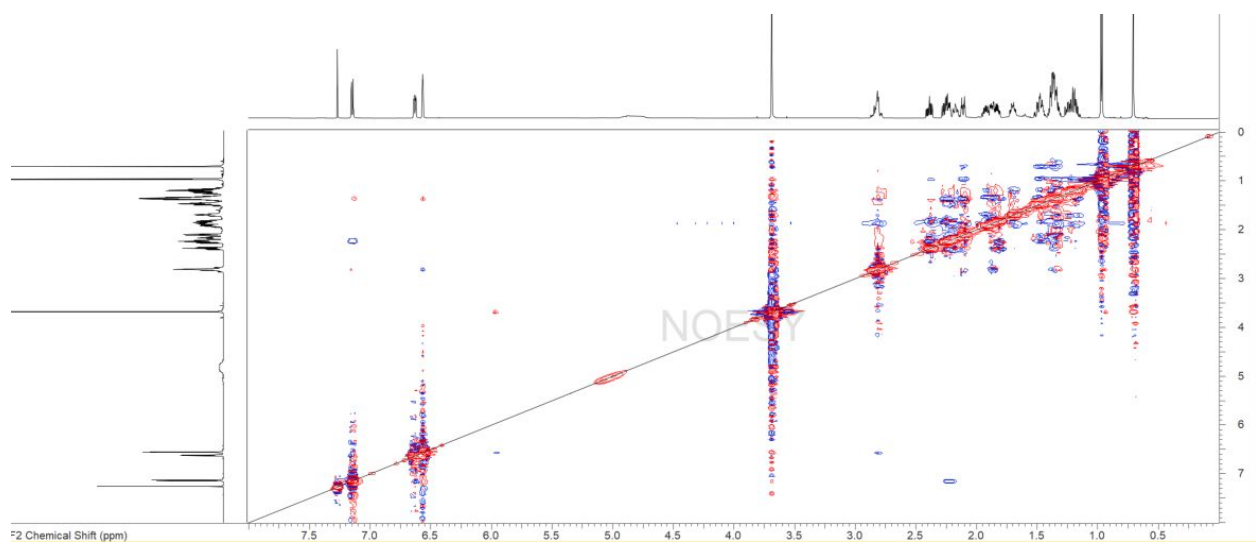


Figure S88: Methyl 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**9**) NOESY NMR spectrum (500 MHz, CDCl₃).

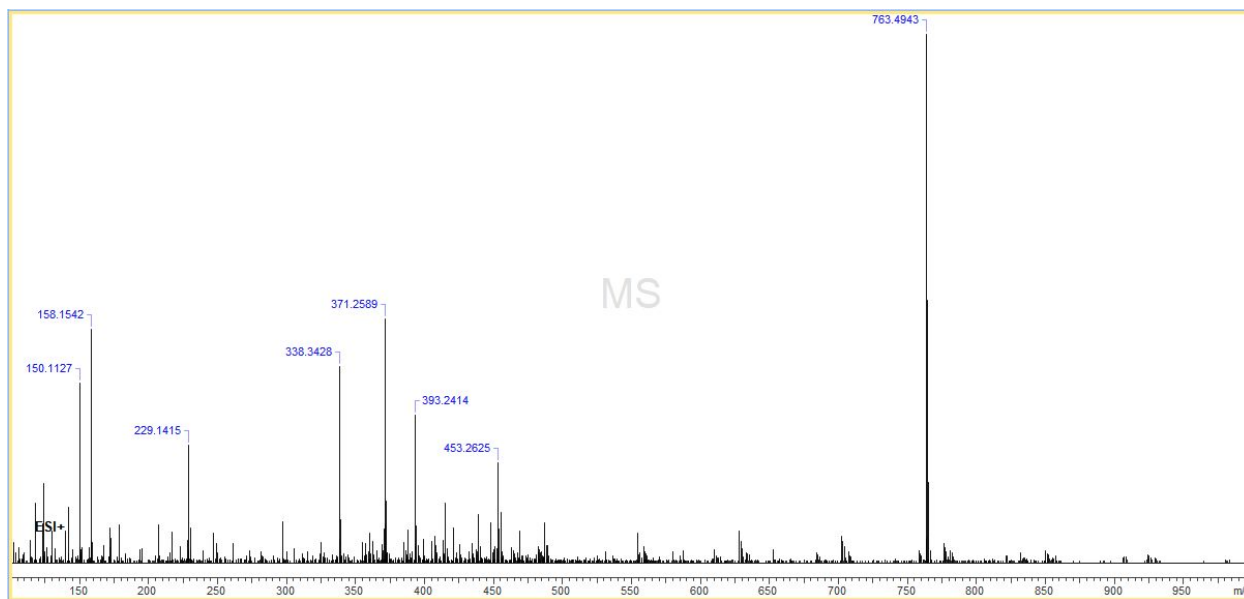


Figure S89: Methyl 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**9**) HRESIMS (pos).

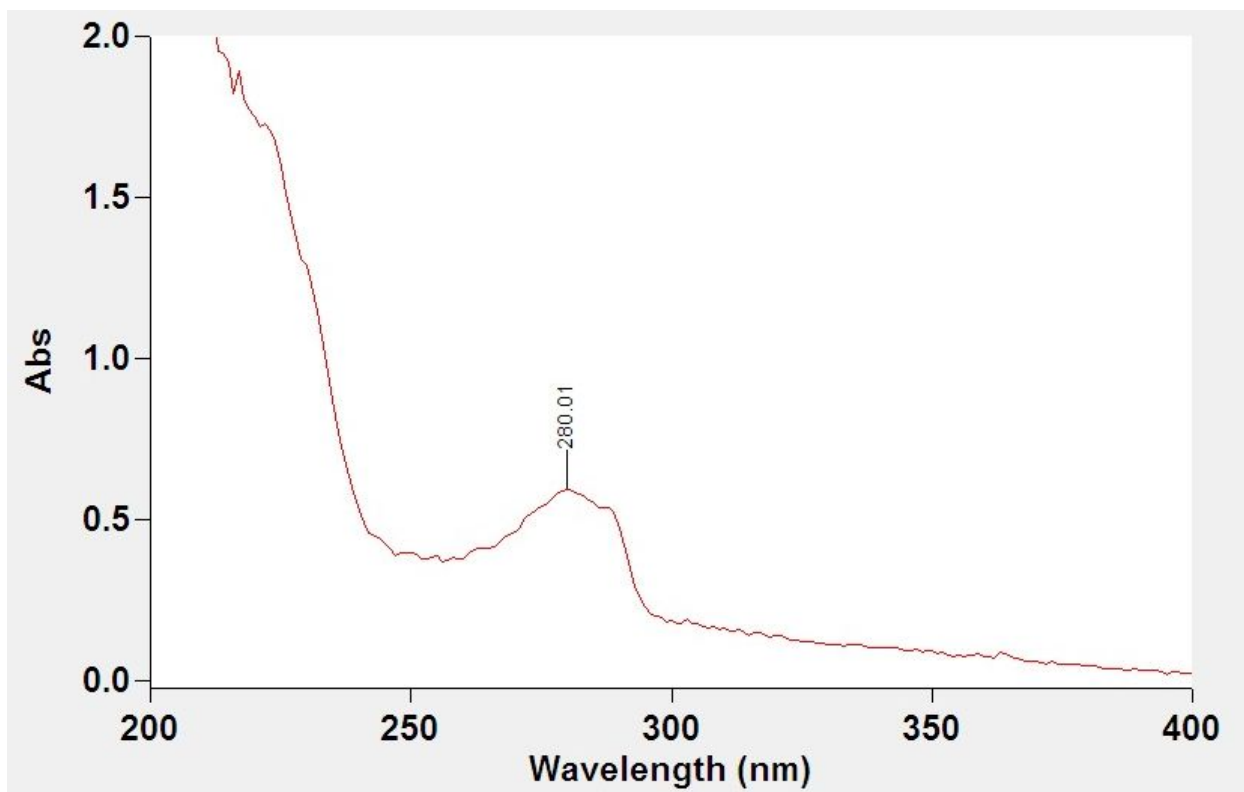


Figure S90: Methyl 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**9**) UV λ_{max} ($\text{C}_2\text{H}_3\text{N}$).

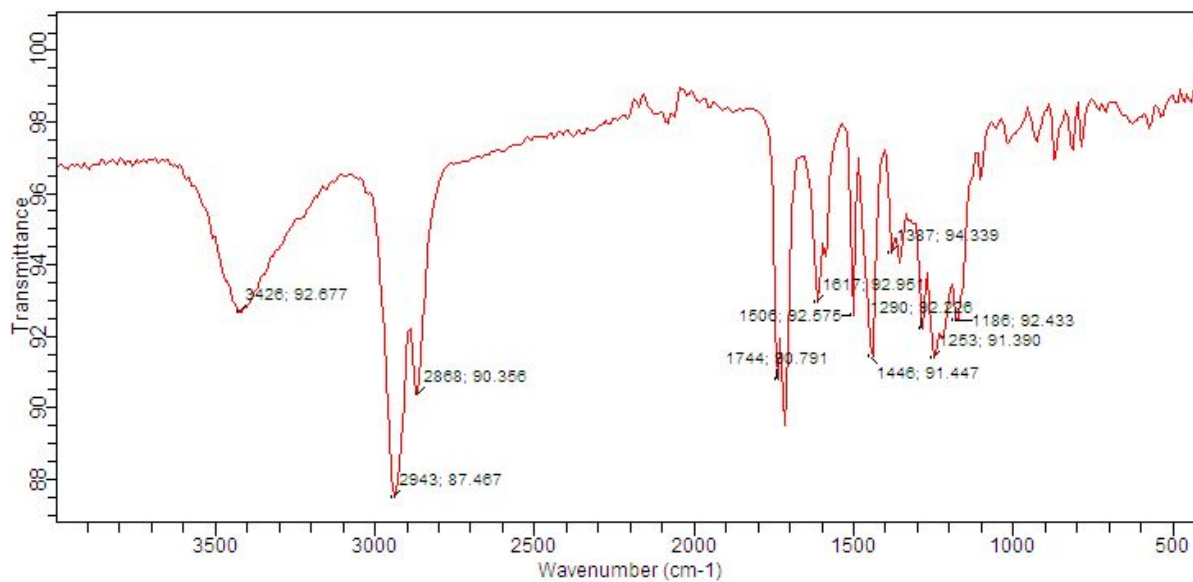


Figure S91: Methyl 3-hydroxy-19-norchola-1,3,5(10)-trien-24-oic acid (**9**) IR spectrum (thin film).

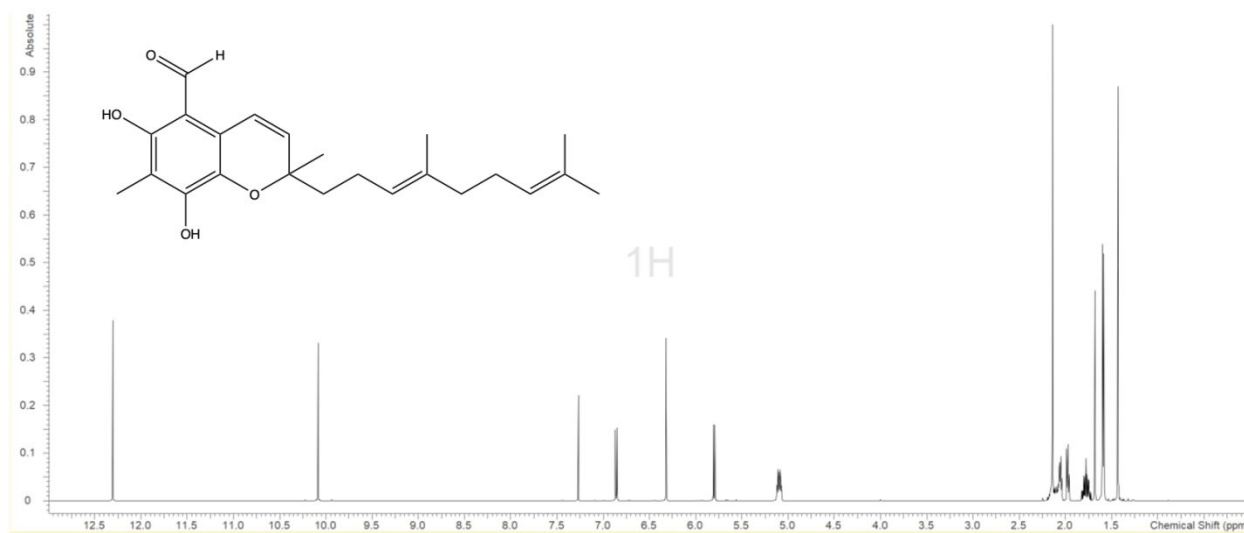


Figure S92: Tuaimenal A (**10**) ^1H NMR spectrum (600 MHz, CDCl_3).

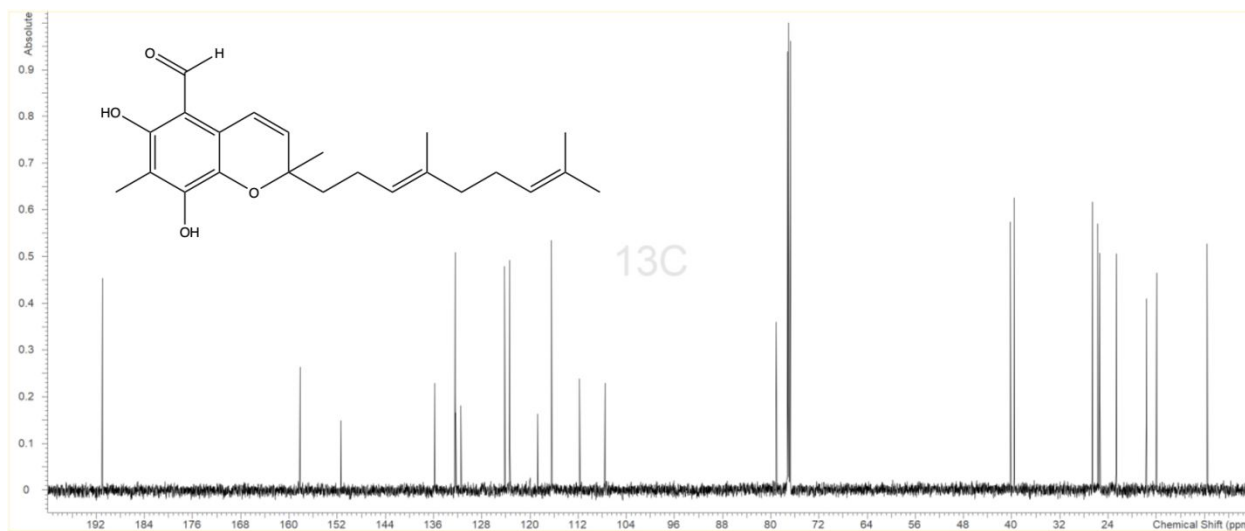


Figure S93: Tuaimenal A (**10**) ^{13}C NMR spectrum (150 MHz, CDCl_3).

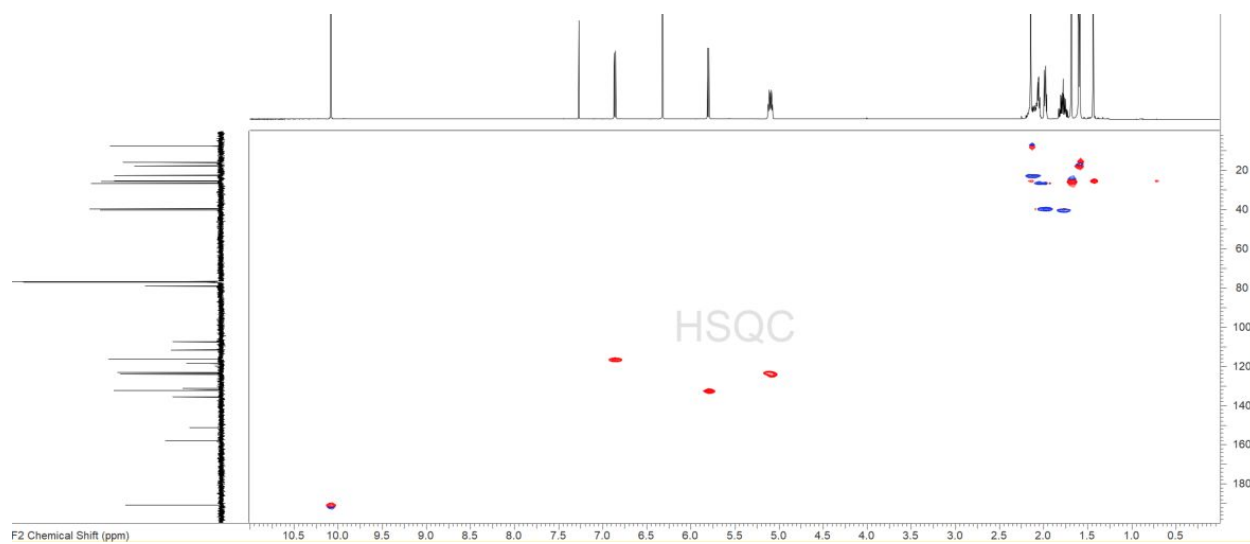


Figure S94: Tuaimenal A (**10**) HSQC NMR spectrum (500 MHz, CDCl_3).

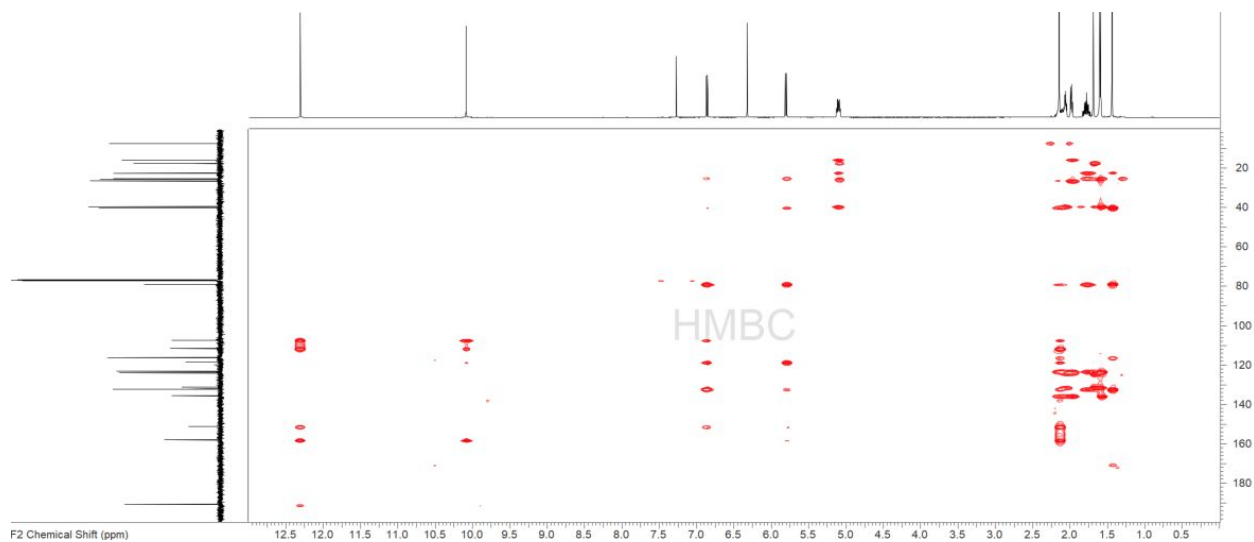


Figure S95: Tuaimenal A (**10**) HMBC NMR spectrum (500 MHz, CDCl₃).

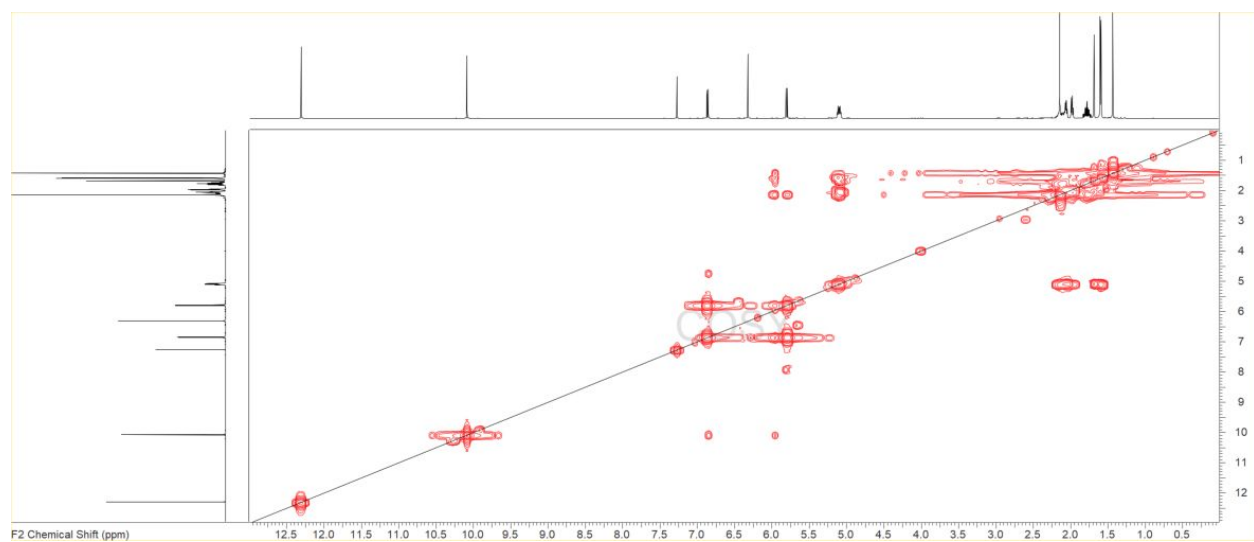


Figure S96: Tuaimenal A (**10**) COSY NMR spectrum (500 MHz, CDCl₃).

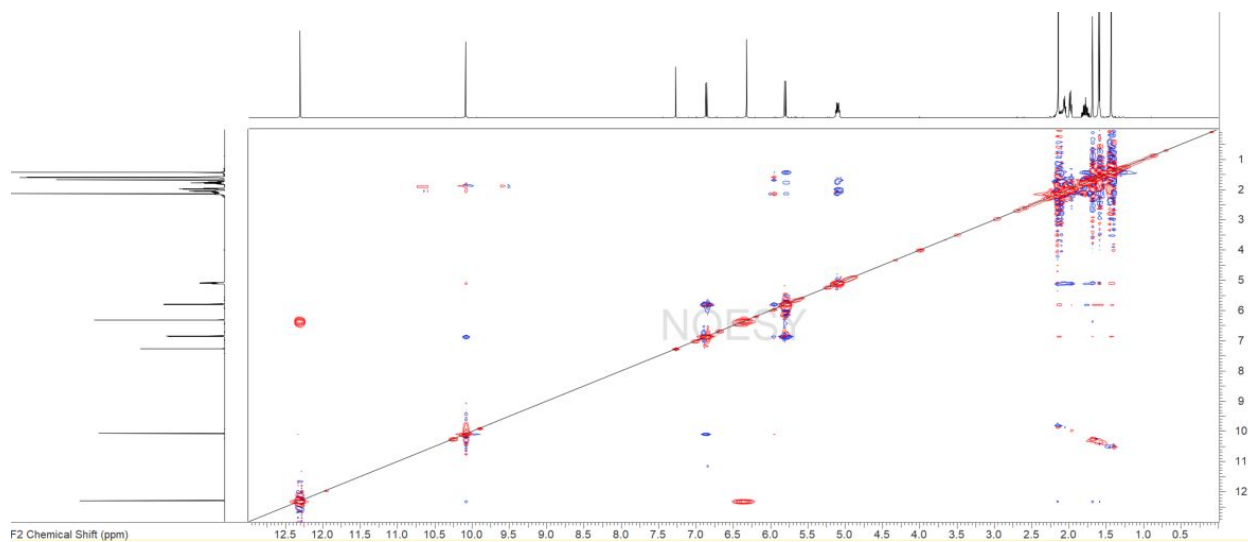


Figure S97: Tuaimenal A (**10**) NOESY NMR spectrum (500 MHz, CDCl₃).

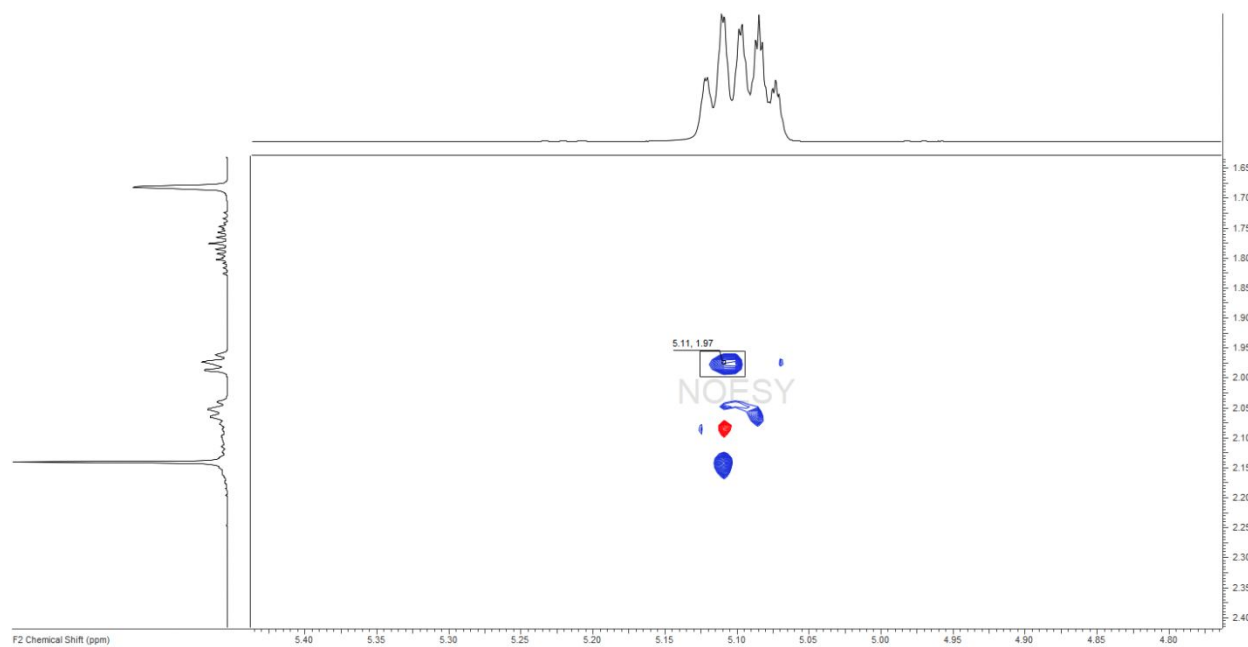


Figure S98: Tuaimenal A (**10**) zoomed NOESY NMR spectrum (500 MHz, CDCl₃).

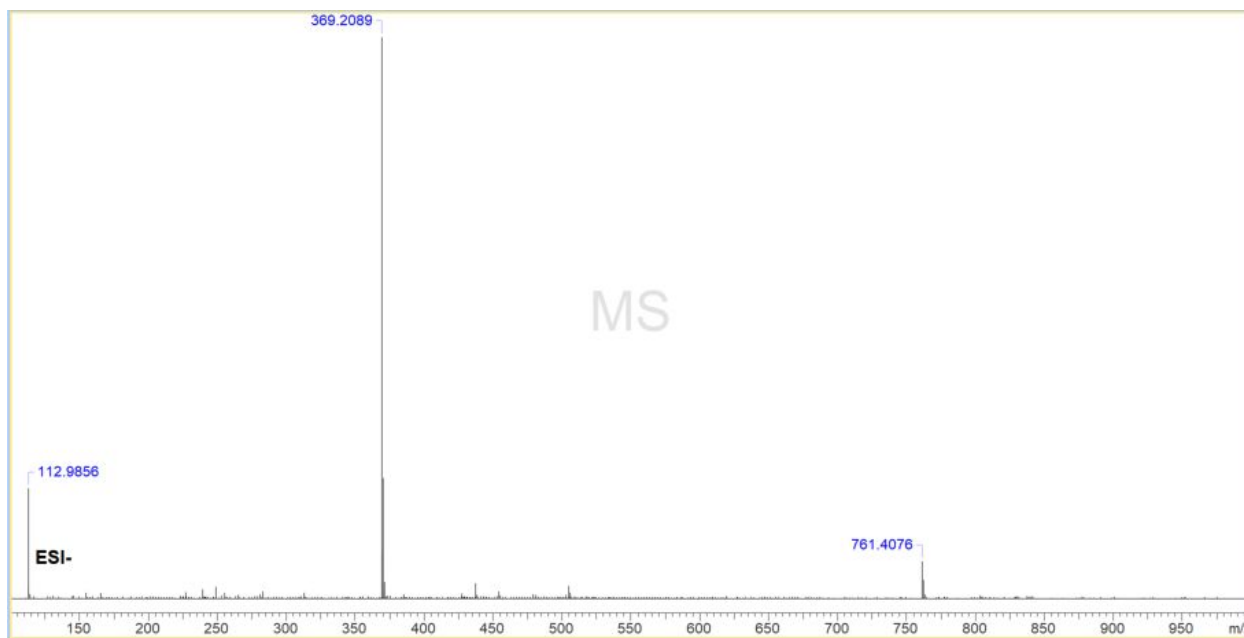


Figure S99: Tuaimenal A (**10**) HRESIMS (neg).

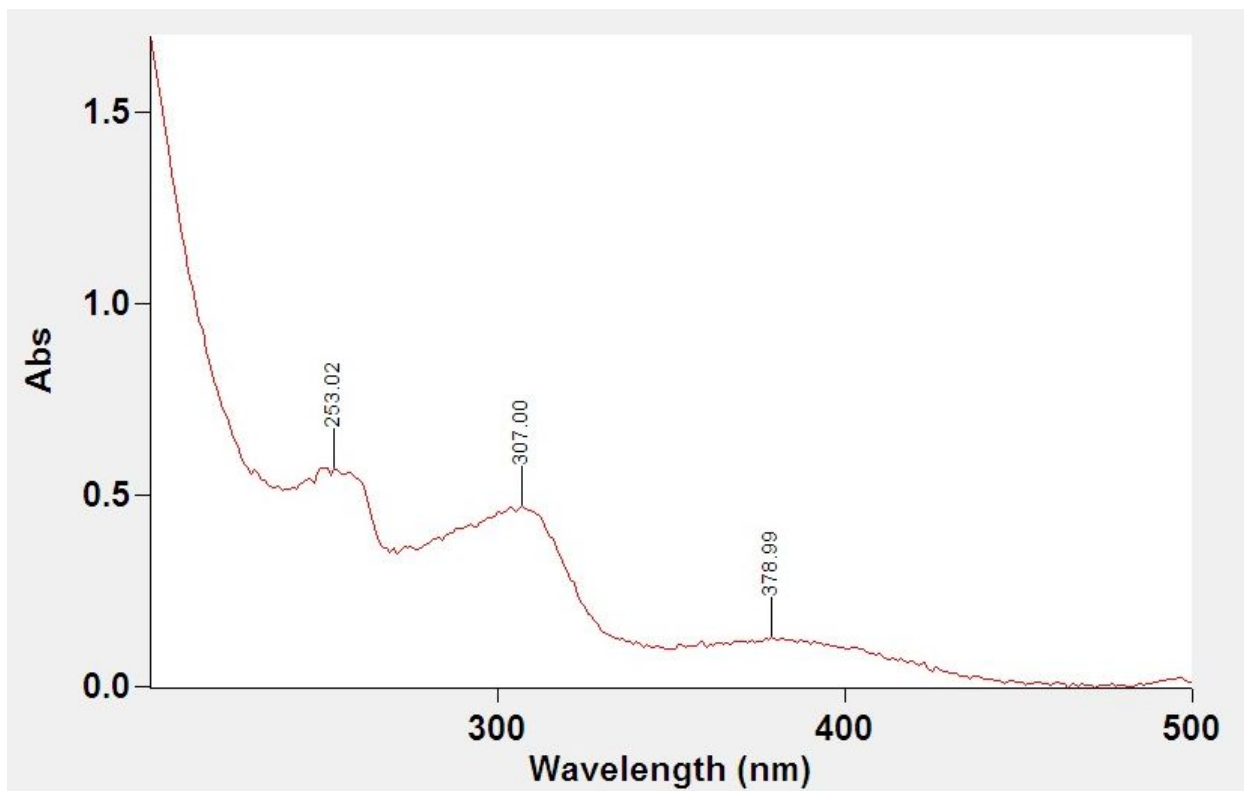


Figure S100: Tuaimenal A (**10**) UV λ_{max} ($\text{C}_2\text{H}_3\text{N}$).

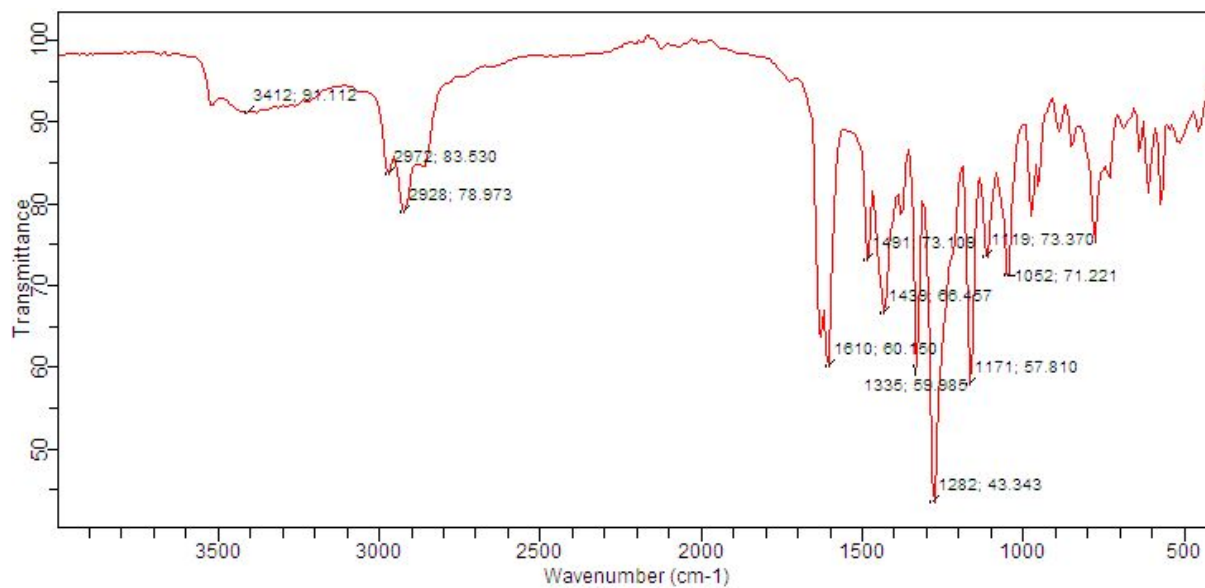


Figure S101: Tuaimenal A (**10**) IR spectrum (thin film).

Table S1: Comparison of tuaimenal A (**10**) ^1H and ^{13}C NMR spectra to literature.

Tuaimenal A^a				
Pos	Literature $\delta_{\text{C}}^{\text{b}}$, type	Literature $\delta_{\text{H}}^{\text{c}}$	Experimental $\delta_{\text{C}}^{\text{b}}$, type	Experimental $\delta_{\text{H}}^{\text{c}}$
1	132.3, C		132.3, C	
2	151.4, C		151.4, C	
3	111.7, C		111.7, C	
4	158.2, C		158.2, C	
5	107.5, C		107.6, C	
6	118.7, C		118.7, C	
7	116.4, CH	6.86, d (10.1)	116.4, CH	6.86, d (10.2)
8	132.4, CH	5.80, d (10.1)	132.4, CH	5.80, d (9.1)
9	79.1, C		79.1, C	
10	40.2, CH ₂	1.78, m	40.2, CH ₂	1.78, m
11	22.6, CH ₂	2.13, m	22.6, CH ₂	2.12, m
12	123.3, CH	5.11, t	123.3, CH	5.11, t
13	135.8, C		135.8, C	
14	39.6, CH ₂	1.99, t	39.6, CH ₂	1.97, t
15	26.6, CH ₂	2.05, m	26.6, CH ₂	2.05, m
16	124.1, CH	5.07, t	124.2, CH	5.08, t
17	131.4, CH		131.4, CH	
18	17.7, CH ₃	1.59, s	17.6, CH ₃	1.60, s
19	25.7, CH ₃	1.68, s	25.7, CH ₃	1.68, s
20	16.0, CH ₃	1.58, s	16.0, CH ₃	1.58, s
21	25.4, CH ₃	1.43, s	25.4, CH ₃	1.43, s
22	7.6, CH ₃	2.14, s	7.5, CH ₃	2.14, s
23	191.1, CH	10.08, s	191.0, CH	10.08, s
OH _a		12.31, s		12.31, s
OH _b		6.37, s		6.32, s

^a CDCl₃, ppm; ^b 150 MHz; ^c 600 MHz, multiplicity, (*J* (Hz))

Table S2: Comparison of *Duva florida* steroids (**8** and **9**) ¹³C NMR spectra to literature.

Pos	Cmpd 8 Literature δ_C^b , type	Cmpd 8 Experimental δ_C^c , type	Cmpd 9 Experimental δ_C^c , type
1	127.0	127.3	126.4
2	113.5	113.8	112.6
3	156.7	156.0	153.3
4	115.9	116.2	115.2
5	139.7	138.9	138.3
6	30.8	30.9	29.7
7	28.9	29.1	27.6
8	40.4	40.6	38.8
9	45.2	45.2	43.7
10	133.5	132.9	133.0
11	27.8	28.2	26.7
12	41.3	41.5	39.9
13	44.6	44.2	42.8
14	57.0	56.9	55.4
15	29.2	29.4	23.9
16	24.8	25.1	28.2
17	57.4	57.7	56.0
18	12.4	12.7	12.0
20	37.2	36.9	35.4
21	18.9	18.9	18.3
22	34.0	32.6	31.1
23	36.3	32.4	31.0
24	167.5	178.6	175.0
25			51.5

^a CDCl₃, ppm; ^b 125 MHz; ^c 150 MHz

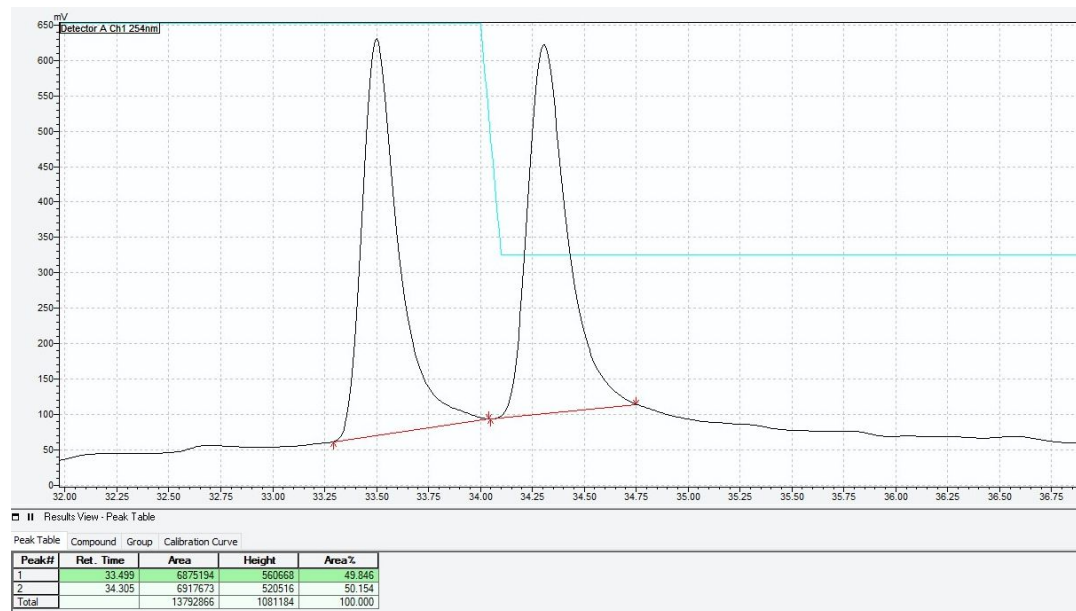


Figure S102: Integrated chromatogram displaying relative abundance of *R* and *S* enantiomers of tuaimenal E (4) separated utilizing a chiral HPLC column.