

Supporting Information

Bioactive Polyketides and Benzene Derivatives from Two Mangrove Sediment-Derived Fungi in the Beibu Gulf

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The physicochemical data of the known compounds 2, 3, 6–9, and 13–23.

Cordyanhydride A methyl ester (**2**): Yellow oil; ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ_{H} 7.30 (1H, dt, $J = 16.0, 6.5$ Hz, H-12), 6.65 (1H, dt, $J = 16.0, 1.5$ Hz, H-11), 3.81 (3H, s, OCH_3 -1), 2.91 (2H, t, $J = 7.0$ Hz, H-3), 2.82 (2H, dd, $J = 7.5, 6.5$ Hz, H₂-2), 2.71 (2H, ddd, $J = 12.5, 7.5, 2.5$ Hz, H-6), 2.63 (1H, dt, $J = 14.0, 7.0$ Hz, α 8-H), 2.50 (2H, pd, $J = 7.5, 1.5$ Hz, H-13), 2.28 (1H, hept, $J = 6.5$ Hz, β H-8), 1.52 (2H, p, $J = 7.0$ Hz, H-19), 1.27 (3H, t, $J = 7.5$ Hz, H-14), 1.10 (3H, t, $J = 7.5$ Hz, H-20); ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) δ_{C} 171.9 (C-1), 166.1 (C-17), 166.0 (C-16), 165.5 (C-15), 164.5 (C-18), 147.7 (C-12), 144.0 (C-5), 143.1 (C-4), 138.1 (C-10), 137.6 (C-9), 116.9 (C-11), 51.6 ($-\text{OCH}_3$), 37.6 (C-7), 30.6 (C-2), 27.9 (C-6), 27.3 (C-8), 26.6 (C-13), 25.7 (C-19), 19.4 (C-3), 12.4 (C-14), 10.5 (C-20).

Cordyanhydride A (**3**): Yellow oil; ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ_{H} 7.08 (1H, dt, $J = 15.4, 6.3$ Hz, H-12), 6.43 (1H, dt, $J = 15.4, 1.4$ Hz, H-11), 2.65 (2H, t, $J = 7.7$ Hz, H₂-3), 2.52 (4H, m, H-2/ α H-6/ α H-8), 2.41 (1H, dt, $J = 14.0, 6.3$ Hz, β H-6), 2.28 (2H, pd, $J = 7.7, 1.4$ Hz, H-13), 2.06 (1H, p, $J = 7.0$ Hz, β H-8), 1.30 (2H, p, $J = 7.0$ Hz, H-19), 1.05 (3H, t, $J = 7.7$ Hz, H-14), 0.88 (3H, t, $J = 7.7$ Hz, H-20); ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) δ_{C} 173.0 (C-1), 166.2 (C-17), 166.1 (C-16), 165.6 (C-15), 164.5 (C-18), 147.8 (C-12), 144.4 (C-5), 143.0 (C-4), 138.1 (C-10), 137.7 (C-9), 117.0 (C-11), 37.7 (C-7), 31.0 (C-2), 28.0 (C-6), 27.5 (C-8), 26.7 (C-13), 25.8 (C-19), 19.6 (C-3), 12.5 (C-14), 10.6 (C-20).

Austdiol (**5**): Yellow powder, $[\alpha]_{\text{D}}^{25} +23$ (c 0.05, CH_3OH); UV (CH_3OH) λ_{max} (log ϵ) 200 (3.61), 256 (3.71), 380 (3.93) nm; IR (film) ν_{max} 3392, 2920, 1681, 1471, 1199, 1138, 1045 cm^{-1} ; ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ_{H} 10.00 (1H, s, H-12), 8.20 (1H, s, H-1), 8.19 (1H, s, H-4), 5.93 (1H, brs, 8-OH), 5.23 (1H, brs, 7-OH), 4.39 (1H, s, H-8), 2.42 (3H, s, H-11), 1.09 (3H, s, H-13); ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) δ_{C} 198.3 (C-6), 189.4 (CHO-12), 166.3 (C-3), 151.9 (C-1), 148.7 (C-10), 122.2 (C-9), 108.2 (C-5), 106.4 (C-4), 74.3 (C-7), 70.6 (C-8), 18.8 (C-13), 19.9 (C-11); HRESIMS m/z 237.0765 $[\text{M} + \text{H}]^+$ (calcd for $\text{C}_{12}\text{H}_{13}\text{O}_5^+$, 237.0757), 259.0581 $[\text{M} + \text{Na}]^+$ (calcd for $\text{C}_{12}\text{H}_{12}\text{NaO}_5^+$, 259.0577).

7-epiaustdiol (**6**): Yellow powder, $[\alpha]_{\text{D}}^{25} +172$ (c 0.05, CH₃OH); ¹H NMR (700 MHz, DMSO-*d*₆) δ_{H} 9.98 (1H, s, H-12), 8.29 (1H, s, H-1), 8.20 (1H, s, H-4), 4.31 (1H, s, H-8), 2.42 (3H, s, H-11), 1.14 (3H, s, H-13); ¹³C NMR (175 MHz, DMSO-*d*₆) δ_{C} 198.3 (C-6), 189.2 (CHO-12), 166.0 (C-3), 152.7 (C-1), 148.0 (C-10), 121.5 (C-9), 108.2 (C-5), 106.7 (C-4), 74.5 (C-7), 71.5 (C-8), 21.9 (C-13), 20.0 (C-11).

8-*O*-methylepiaustdiol (**7**): Yellow powder, $[\alpha]_{\text{D}}^{25} +160$ (c 0.05, CH₃OH); ¹H NMR (500 MHz, DMSO-*d*₆) δ_{H} 9.96 (1H, s, H-12), 8.44 (1H, s, H-4), 8.18 (1H, s, H-1), 3.96 (1H, s, H-1), 3.18 (3H, s, H-14), 2.41 (3H, s, H-11), 1.11 (3H, s, H-13); ¹³C NMR (125 MHz, DMSO-*d*₆) δ_{C} 198.5 (C-6), 189.1 (CHO-12), 166.2 (C-3), 152.7 (C-1), 147.5 (C-10), 117.2 (C-9), 108.4 (C-5), 106.8 (C-4), 81.1 (C-8), 74.2 (C-7), 56.8 (C-14), 23.2 (C-13), 20.0 (C-11).

4-Hydroxy-3,6-dimethyl-2*H*-pyran-2-one (**8**): White powder, ¹H NMR (500 MHz, DMSO-*d*₆) δ_{H} 11.08 (1H, s, 3-OH), 5.98 (1H, s, H-4), 2.13 (3H, s, H-6), 1.73 (3H, s, H-7); ¹³C NMR (125 MHz, DMSO-*d*₆) δ_{C} 165.2 (C-1), 165.0 (C-3), 159.4 (C-5), 99.8 (C-4), 96.4 (C-2), 19.3 (C-6), 8.4 (C-7).

2,4-Dihydroxy-3,6-dimethylbenzoic acid (**9**): Red powder, ¹H NMR (700 MHz, DMSO-*d*₆) δ_{H} 13.44 (1H, s, 1-COOH), 12.62 (1H, s, 2-OH), 10.04 (1H, s, 4-OH), 6.25 (1H, s, H-5), 2.39 (3H, s, H-9), 1.93 (3H, s, H-8); ¹³C NMR (175 MHz, DMSO-*d*₆) δ_{C} 174.2 (C-7), 163.1 (C-2), 160.0 (C-4), 139.6 (C-6), 110.3 (C-5), 107.9 (C-1), 103.5 (C-3), 23.8 (C-9), 8.0 (C-8).

Stachyline G (**13**): Colorless oil; ¹H NMR (700 MHz, DMSO-*d*₆) δ_{H} 7.12 (2H, d, J = 8.0 Hz, H-2, 6), 6.80 (2H, d, J = 8.1 Hz, H-3, 5), 5.42 (1H, m, H-2'), 4.55 (2H, d, J = 6.4 Hz, H-1), 3.99 (2H, s, H-4'), 3.31 (2H, s, H-7), 1.75 (3H, s, H-5'); ¹³C NMR (175 MHz, DMSO-*d*₆) δ_{C} 174.2 (C-8), 156.58 (C-4), 140.24 (C-3'), 130.21 (C-2), 130.21 (C-6), 129.27 (C-1), 121.31 (C-2'), 114.05 (C-3), 114.05 (C-5), 63.57 (C-1'), 59.83 (C-4'), 42.24 (C-7), 20.99 (C-5).

Stachyline F (**14**): White powder; ¹H NMR (500 MHz, DMSO-*d*₆) δ_{H} 7.15 (2H, d, J = 8.5 Hz, H-2, 6), 6.87 (2H, d, J = 8.5 Hz, H-3, 5), 5.64 (1H, q, J = 5.4 Hz, H-2'), 4.57

(2H, d, $J = 6.5$ Hz, H-1'), 3.85 (2H, s, H-4'), 3.47 (2H, s, H-7), 1.65 (3H, s, H-5'); ^{13}C NMR (125 MHz, DMSO- d_6) δ_{C} 173.1 (C-8), 157.2 (C-4), 140.5 (C-3'), 130.4 (C-2), 130.4 (C-6), 127.0 (C-1), 118.2 (C-2'), 114.4 (C-3), 114.4 (C-5), 65.5 (C-1'), 64.0 (C-4'), 40.0 (C-7), 13.8 (C-5').

(*E*)-4-(4-Hydroxy-3-methylbut-2-enyloxy)benzaldehyde (**15**): Colorless oil; ^1H NMR (700 MHz, DMSO- d_6) δ_{H} 9.86 (1H, s, 1-CHO), 7.86 (2H, d, $J = 8.7$ Hz, H-2, 6), 7.13 (2H, d, $J = 8.7$ Hz, H-3, 5), 5.66 (1H, td, $J=6.6, 1.4$ Hz, H-2'), 4.72 (2H, d, $J = 6.7$ Hz, H-1'), 3.85 (2H, s, H-4'), 1.67 (3H, s, H-5'); ^{13}C NMR (175 MHz, DMSO- d_6) δ_{C} 191.3 (1-CHO), 163.5 (C-4), 141.5 (C-3'), 131.8 (C-2), 131.8 (C-6), 129.6 (C-1), 117.1 (C-2'), 115.1 (C-3), 115.1 (C-5), 65.3 (C-4'), 64.7 (C-1'), 13.8 (C-5').

Stachyline E (**16**): Colorless oil; ^1H NMR (500 MHz, DMSO- d_6) δ_{H} 7.14 (2H, d, $J = 8.3$ Hz, H-2, 6), 6.86 (2H, d, $J = 8.5$ Hz, H-3, 5), 4.19 (1H, dd, $J = 10.1, 2.2$ Hz, H-1'a), 3.76 (1H, dd, $J = 10.0, 8.1$ Hz, H-1'b), 3.52 (1H, dd, $J = 8.1, 2.2$ Hz, H-2'), 3.45 (2H, s, H-7), 1.13 (3H, s, H-4'), 1.07 (3H, s, H-5'); ^{13}C NMR (125 MHz, DMSO- d_6) δ_{C} 173.2 (C-8), 157.6 (C-4), 130.3 (C-2, 6), 127.1 (C-1), 114.3 (C-3, 5), 75.8 (C-2'), 70.8 (C-3'), 69.8 (C-1'a), 40.1 (C-7), 27.4 (C-4'), 24.3 (C-5').

Penialidins C (**17**): Yellow powder; ^1H NMR (500 MHz, DMSO- d_6) δ_{H} 6.86 (1H, s, H-13), 5.69 (1H, s, H-3), 5.15 (2H, s, H-6), 2.00 (3H, s, H-1); ^{13}C NMR (125 MHz, DMSO- d_6) δ_{C} 171.0 (C-7), 169.0 (C-14), 167.3 (C-2), 158.3 (C-4), 150.0 (C-12), 144.9 (C-9), 144.1 (C-11), 117.3 (C-10), 112.2 (C-8), 103.1 (C-13), 101.1 (C-5), 94.4 (C-3), 64.1 (C-6), 19.9 (C-1).

Dibutylphthalate (**18**): Colorless oil; ^1H NMR (500 MHz, DMSO- d_6) δ_{H} 7.73 (2H, dt, $J=7.3, 3.7$ Hz, H-2, 5), 7.68 (2H, dd, $J=5.7, 3.3$ Hz, H-3, 4); dibutyl protons: 4.24 (4H, t, $J=6.5$ Hz), 1.65 (4H, m), 1.39 (4H, m), 0.93 (6H, t, $J=7.4$ Hz, 2CH₃); ^{13}C NMR (125 MHz, DMSO) δ_{C} 167.5 (C-1), 132.2 (C-2), 132.1 (C-3), 129.2 (C-4), 65.6 (C-5), 30.5 (C-6), 19.2 (C-7), 14.1 (C-8).

Brefeldin G (**19**): White powder; ^1H NMR (500 MHz, DMSO- d_6) δ_{H} 6.73 (1H, dd, $J=15.5, 4.5$ Hz, H-3), 5.84 (1H, d, $J=15.4$ Hz, H-2), 5.32 (2H, m, H-10, 11), 4.07 (1H, d, $J=4.7$ Hz, H-4), 4.01 (1H, dd, $J=6.4, 4.4$ Hz, H-7), 2.39 (2H, t, $J=7.3$ Hz, H-14), 2.33 (1H, d, $J=8.4$ Hz, H-9), 2.06 (3H, s, H-16), 1.99 (1H, m, H-5), 1.90 (2H, m, H-12), 1.84 (1H, m, H-6a), 1.64 (1H, m, H-13a), 1.50 (2H, m, H-6b, 13b), 1.27-1.35 (2H, m, H-8). ^{13}C NMR (125 MHz, DMSO- d_6) δ_{C} 208.5 (C-15), 167.8 (C-1), 150.9 (C-3), 135.1 (C-11), 128.8 (C-10), 120.7 (C-2), 70.4 (C-7), 69.0 (C-4), 48.5 (C-5), 42.6 (C-9), 42.5 (C-8), 42.0 (C-14), 35.1 (C-6), 31.3 (C-12), 29.8 (C-16), 23.1 (C-13).

9,12-octadecadieonic acid (**20**): ^1H NMR (500 MHz, Chloroform- d) δ_{H} 5.36 (4H, m, H-9, 10, 12, 13), 2.77 (2H, t, $J=6.6$ Hz, H-11), 2.35 (2H, t, $J=7.5$ Hz, H-2), 2.05 (4H, q, $J=6.9$ Hz, H-8, 14), 1.63 (2H, m, H-3), 1.33 (14H, m, H-4, 5, 6, 7, 15, 16, 17), 0.89 (3H, t, $J=6.5$ Hz, H-18); ^{13}C NMR (125 MHz, Chloroform- d) δ_{C} 178.7 (C-1), 130.4 (C-9), 130.2 (C-10), 128.2 (C-12), 128.1 (C-13), 33.9, 31.7, 29.7, 29.5, 29.3, 29.2, 29.2, 27.4, 27.3, 25.8, 24.8, 22.7, 14.2.

α -linolenic acid (**21**): ^1H NMR (500 MHz, Chloroform- d) δ_{H} 5.45 (6H, m, H-9, 10, 12, 13, 15, 16), 2.81 (4H, t, $J=6.0$ Hz, H-11, 14), 2.34 (2H, t, $J=7.5$ Hz, H-2), 2.07 (4H, m, H-8, 17), 1.63 (2H, m, H-3), 1.33 (10H, d, $J=9.4$ Hz, H-4, 5, 6, 7), 0.97 (3H, t, $J=7.5$ Hz, H-18); ^{13}C NMR (125 MHz, Chloroform- d) δ_{C} 180.1 (C-1), 132.1 (C-9), 130.4 (C-10), 128.4 (C-12), 128.4 (C-13), 127.9 (C-15), 127.3 (C-16), 34.2 (C-2), 29.7 (C-4), 29.3 (C-5), 29.2 (C-6), 29.2 (C-7), 27.3 (C-3), 25.8 (C-8), 25.7 (C-11), 24.8 (C-14), 20.7 (C-17), 14.4 (C-18).

Linoleic acid (**22**): ^1H NMR (500 MHz, Chloroform- d) δ_{H} 11.30 (1H, s, -COOH), 5.35 (4H, ddq, $J=14.0, 7.1, 4.3, 3.4$ Hz, H-9, 10, 12, 13), 2.77 (2H, t, $J=6.5$ Hz, H-11), 2.34 (2H, t, $J=7.5$ Hz, H-2), 2.05 (4H, q, $J=6.8$ Hz, H-8, 14), 1.63 (2H, m, H-3), 1.32 (14H, m, H-4, 5, 6, 7, 15, 16, 17), 0.89 (3H, t, $J=6.8$ Hz, H-18); ^{13}C NMR (125 MHz, Chloroform- d) δ_{C} 180.7 (C-1), 130.3 (C-9), 130.1 (C-10), 128.2 (C-12), 128.0 (C-13), 34.3 (C-2), 31.7 (C-4), 29.7 (C-5), 29.5 (C-6), 29.3 (C-7), 29.2 (C-15), 29.2 (C-16), 27.3 (C-8), 27.3 (C-14), 25.8 (C-11), 24.8 (C-3), 22.7 (C-17), 14.2 (C-18).

Glycerol monlinoleate (**23**): ^1H NMR (500 MHz, Chloroform-*d*) δ_{H} 5.33 (4H, m, H-9', 10', 12', 13'), 4.12 (2H, m, H-1), 3.89 (1H, m, H-2), 3.66 (1H, dd, $J=11.6, 3.7$ Hz, H-3a), 3.56 (1H, dd, $J=11.6, 6.0$ Hz, H-3b), 2.75 (2H, t, $J=6.7$ Hz, H-11'), 2.32 (2H, t, $J=7.6$ Hz, H-2'), 2.03 (4H, q, $J=7.0$ Hz, H-8', 14'), 1.60 (2H, t, $J=7.3$ Hz, H-3'), 1.30 (14H, m, 4'~7', H-15'~17'), 0.87 (3H, t, $J=6.8$ Hz, H-18'); ^{13}C NMR (125 MHz, CDCl_3) δ_{C} 174.4 (C-1'), 130.3 (C-9'), 130.0 (C-13'), 128.1 (C-10'), 127.9 (C-12'), 70.3 (C-2), 65.1 (C-1), 63.4 (C-3), 34.2 (C-2'), 31.6 (C-14'), 29.6 (C-16'), 29.4 (C-7'), 29.2 (C-8'), 29.2 (C-2',15'), 27.2 (4', 5'), 25.7 (C-6'), 24.9 (C-8'), 22.6 (C-17'), 14.1 (C-18').

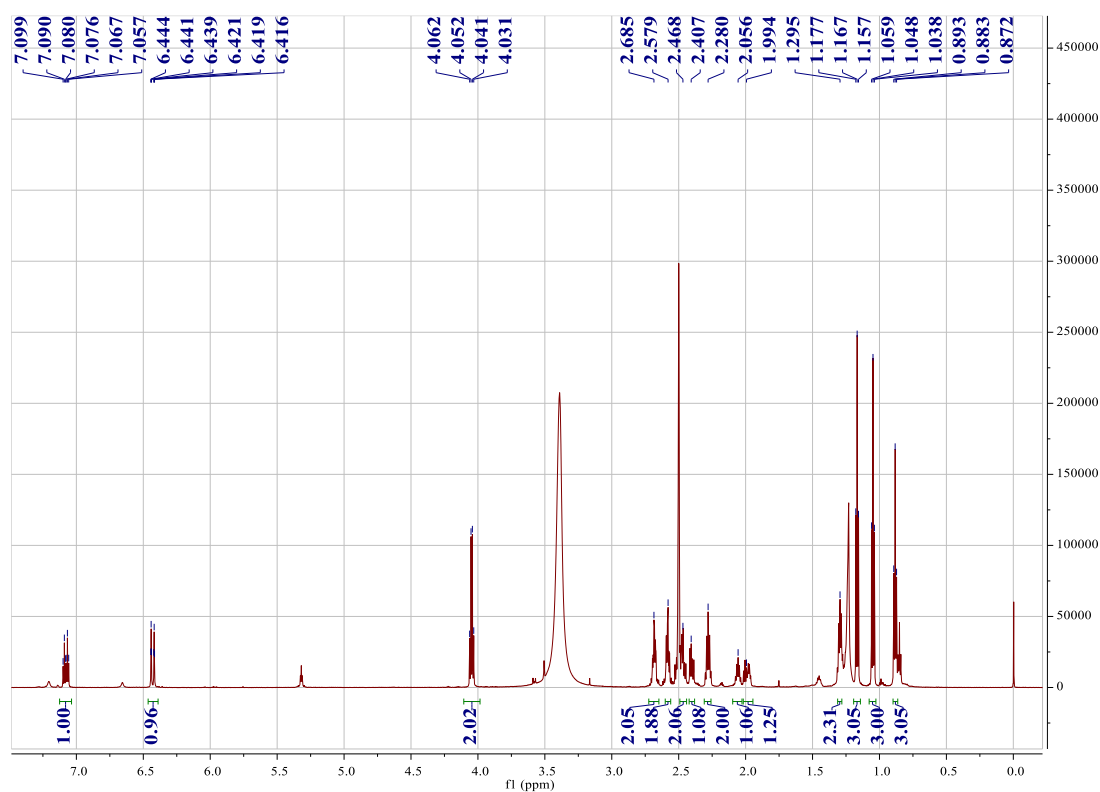


Figure S1. ^1H NMR spectrum of cordyanhydride A ethyl ester (**1**) in $\text{DMSO}-d_6$.

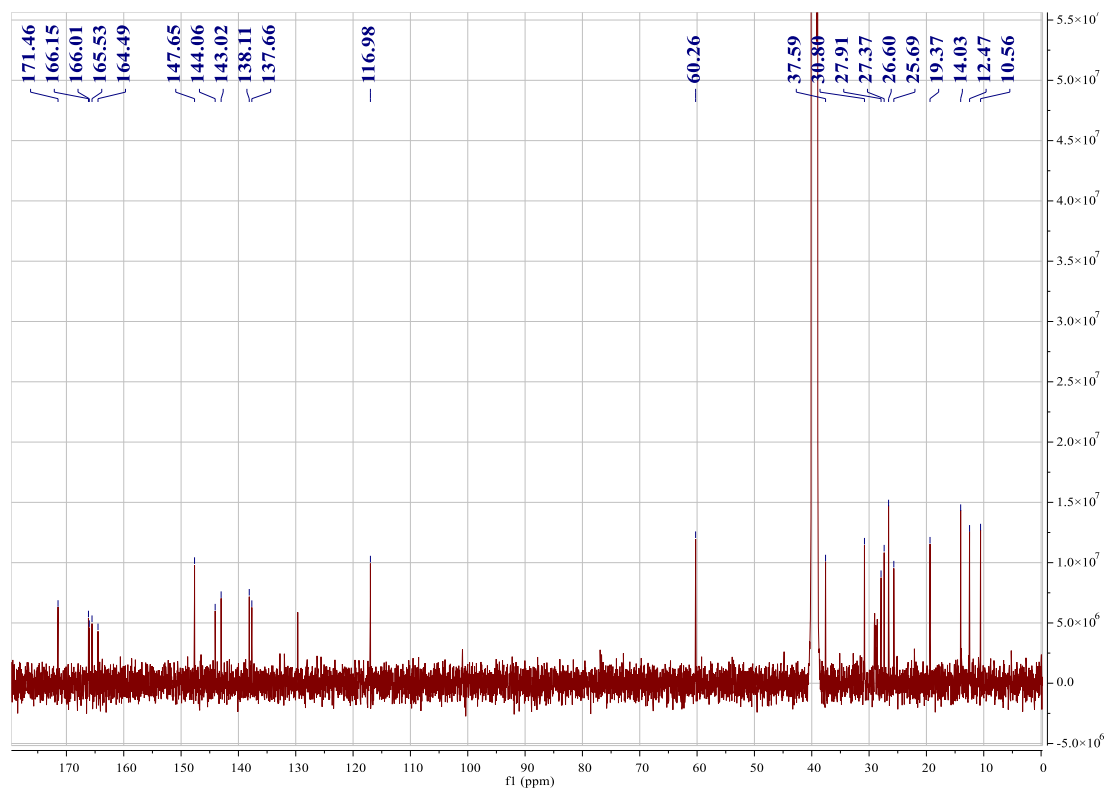


Figure S2. ^{13}C NMR spectrum of cordyanhydride A ethyl ester (**1**) in $\text{DMSO}-d_6$.

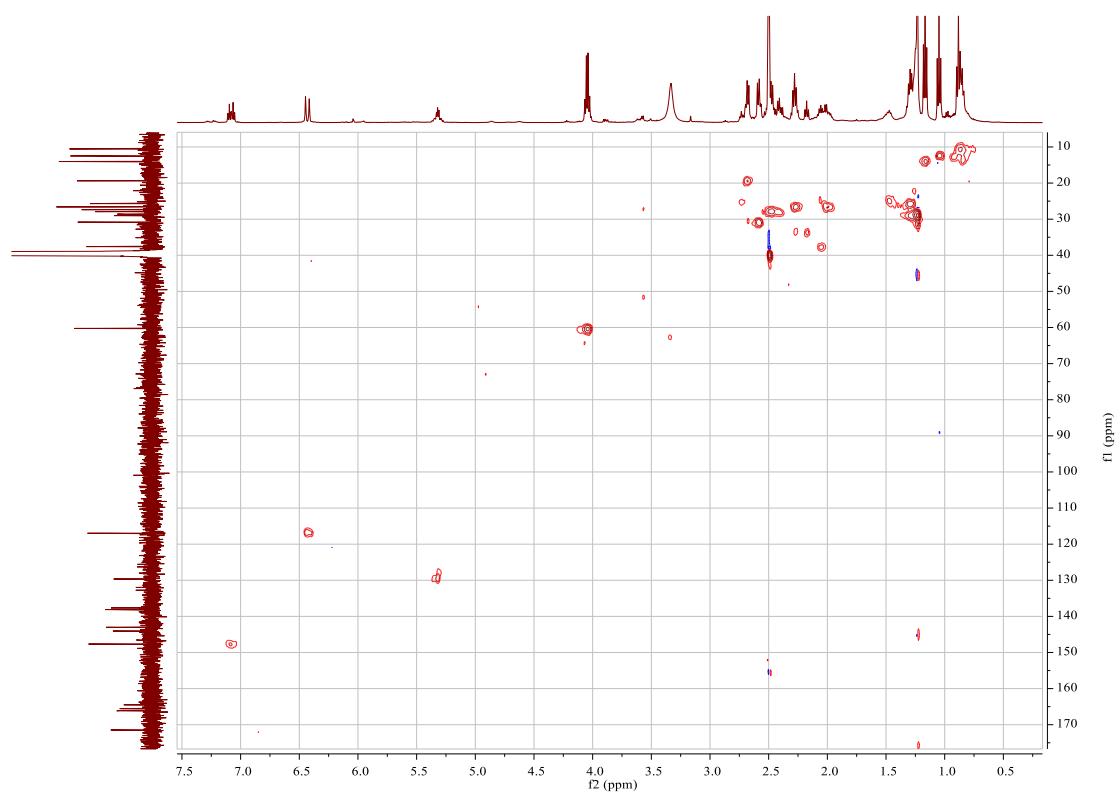


Figure S3. HSQC spectrum of cordyanhydride A ethyl ester (**1**) in DMSO- d_6 .

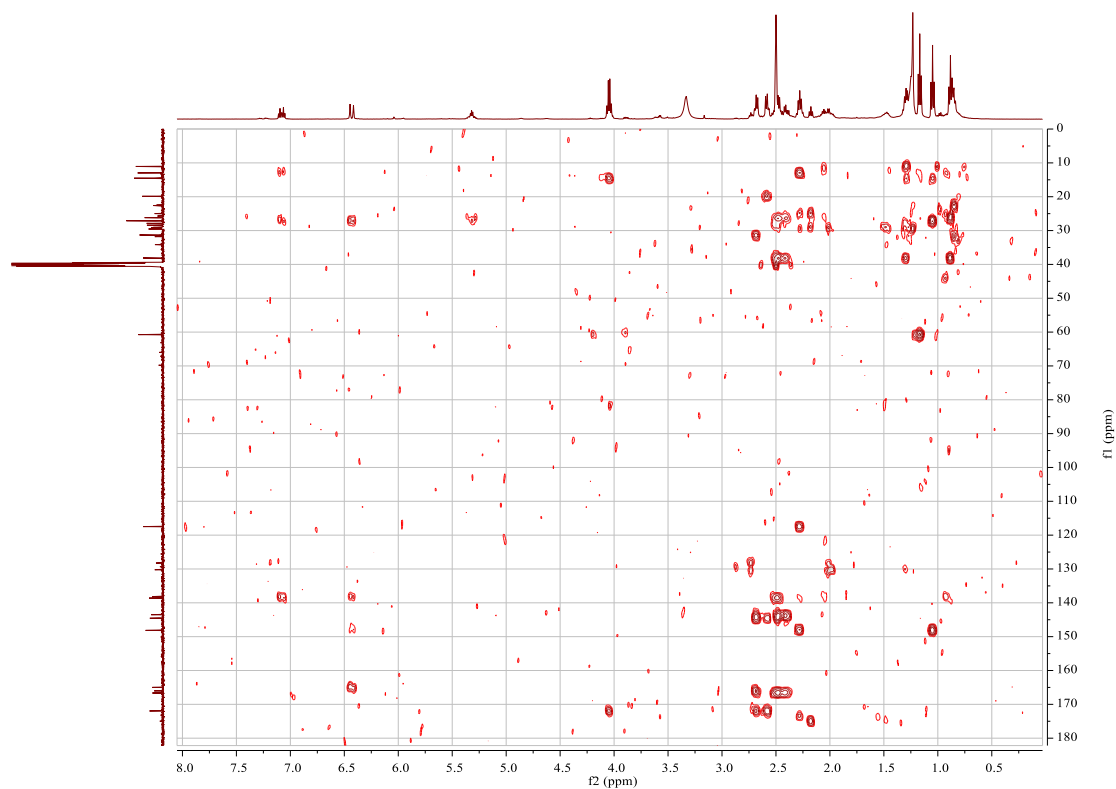


Figure S4. HMBC spectrum of cordyanhydride A ethyl ester (**1**) in DMSO- d_6 .

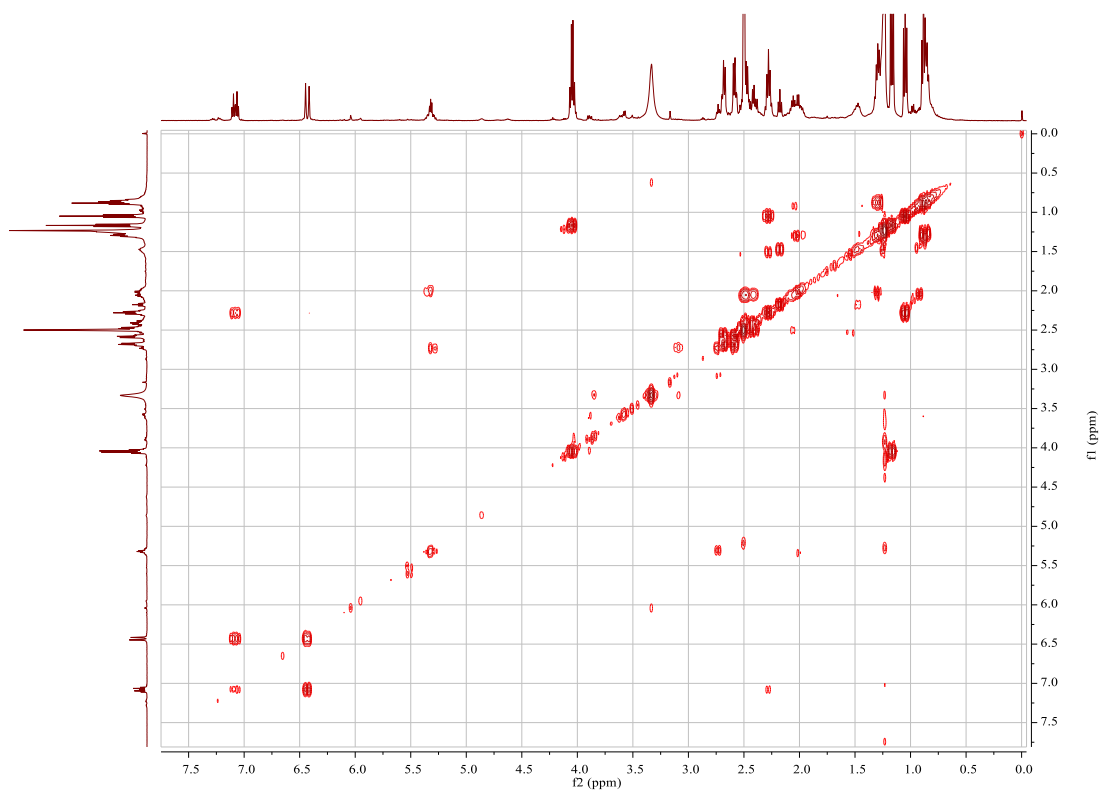
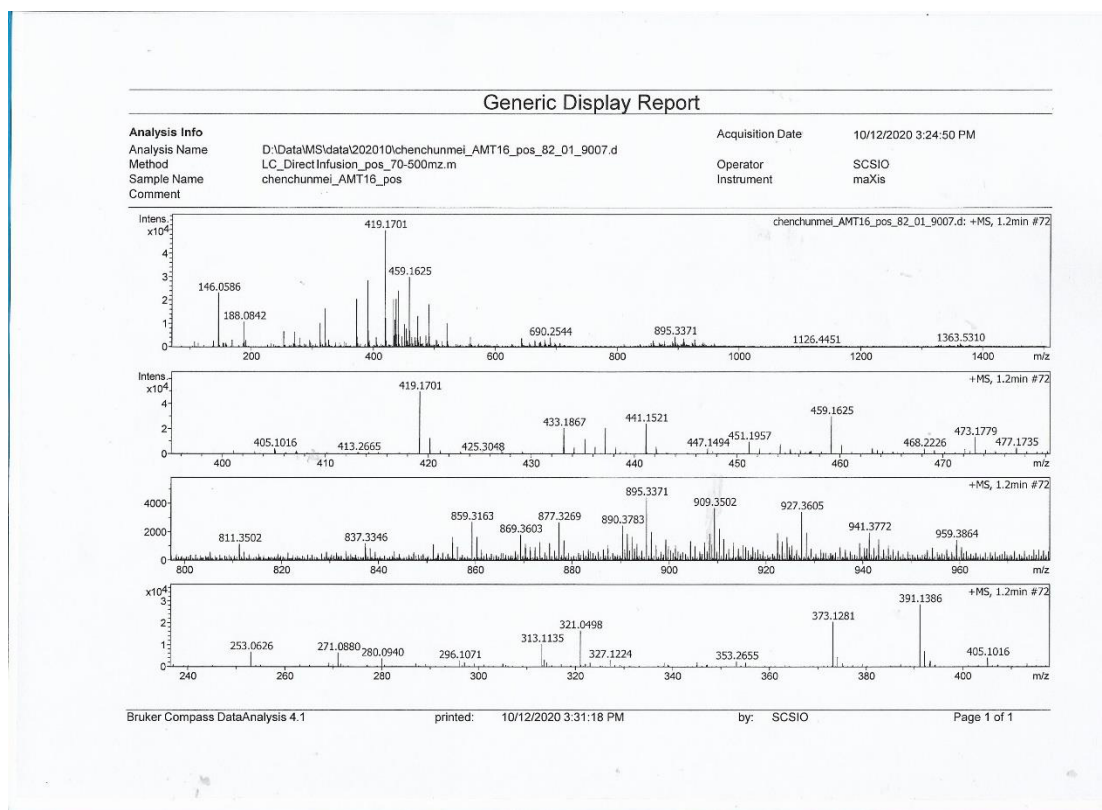


Figure S5. ^1H - ^1H COSY spectrum of cordyanhydride A ethyl ester (**1**) in $\text{DMSO-}d_6$.



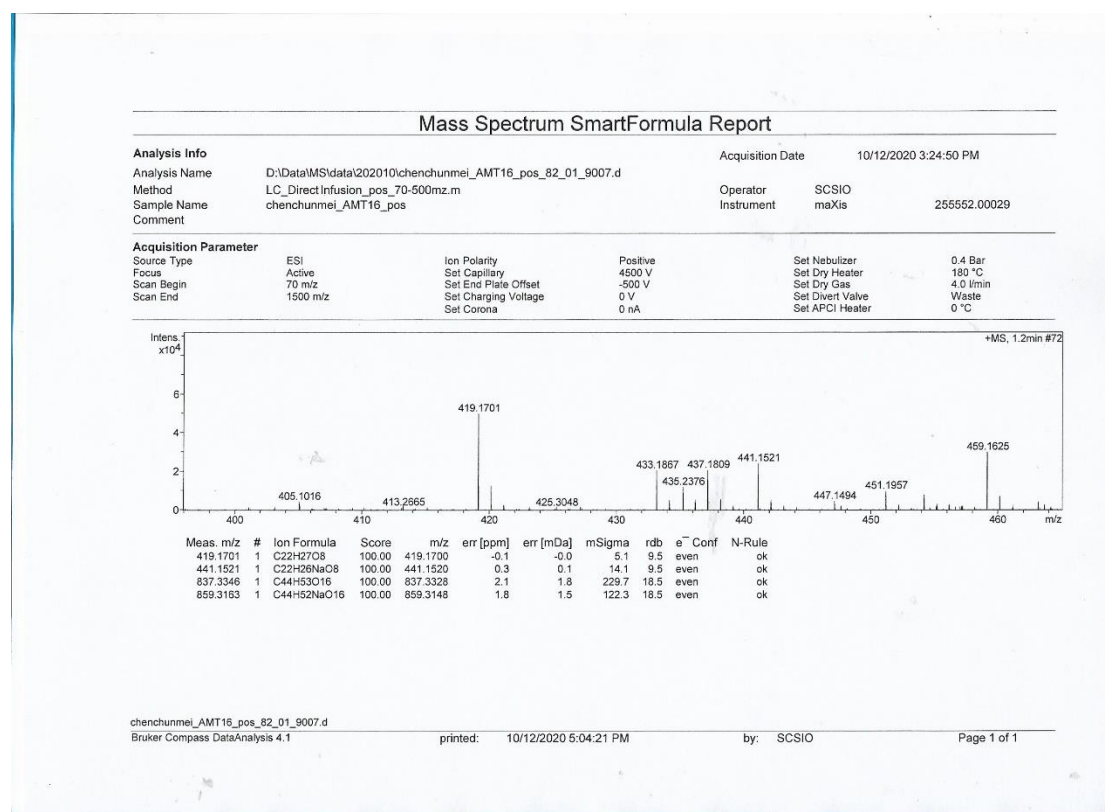


Figure S6. HRESIMS spectrum of cordyanhydride A ethyl ester (**1**).

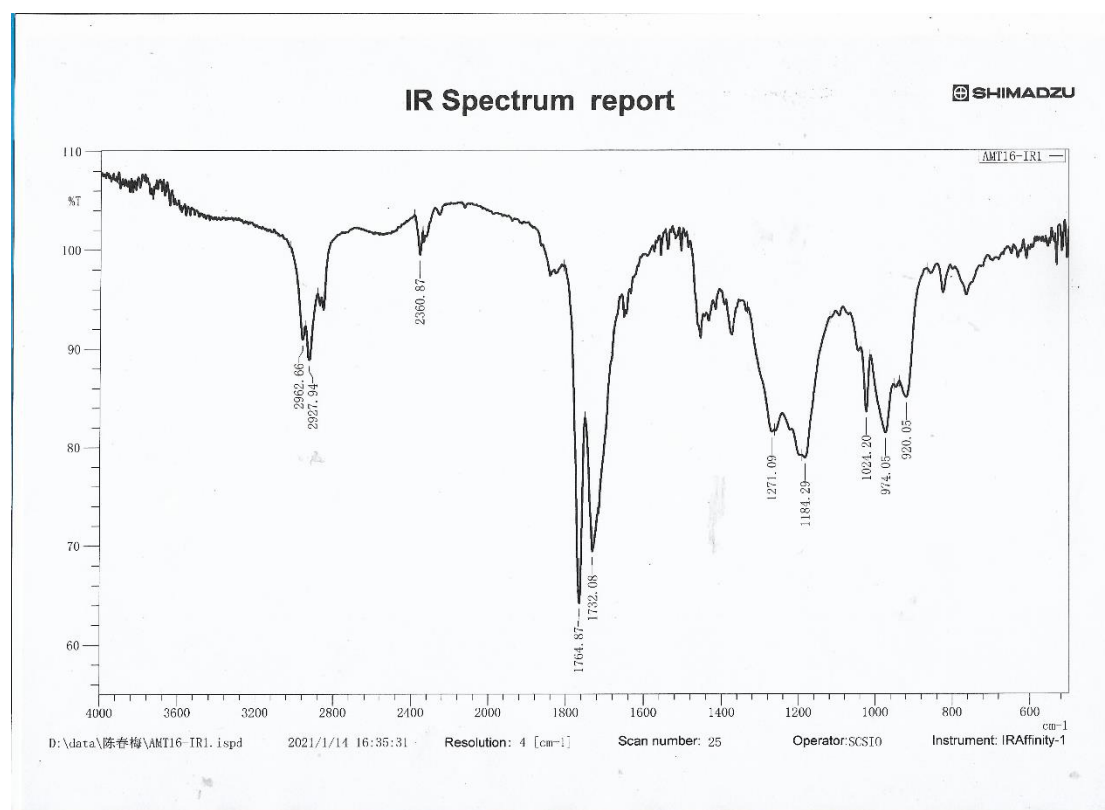


Figure S7. IR spectrum of cordyanhydride A ethyl ester (**1**).

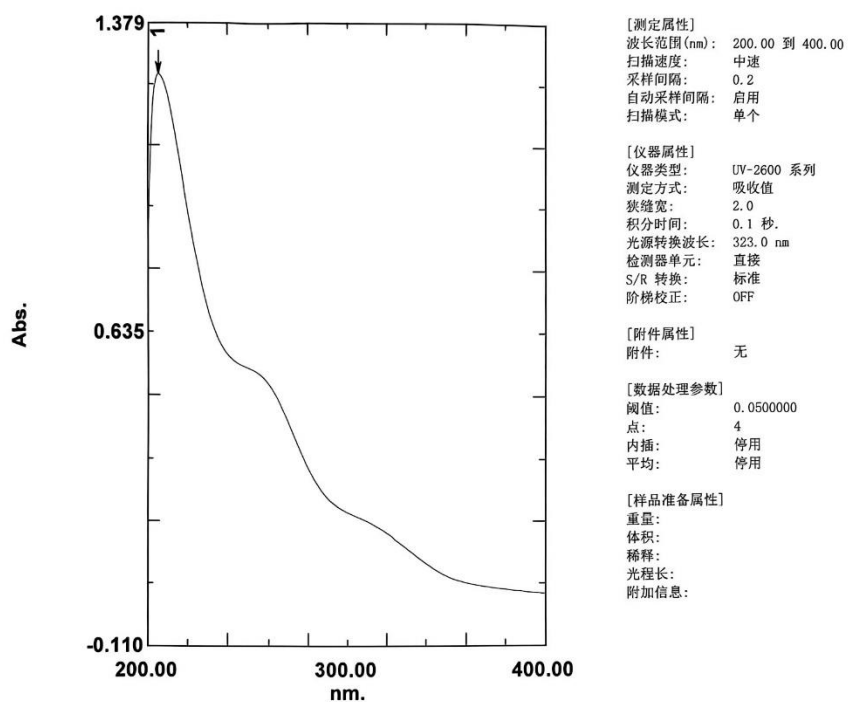


Figure S8. UV spectrum of cordyanhydride A ethyl ester (**1**) in MeOH.

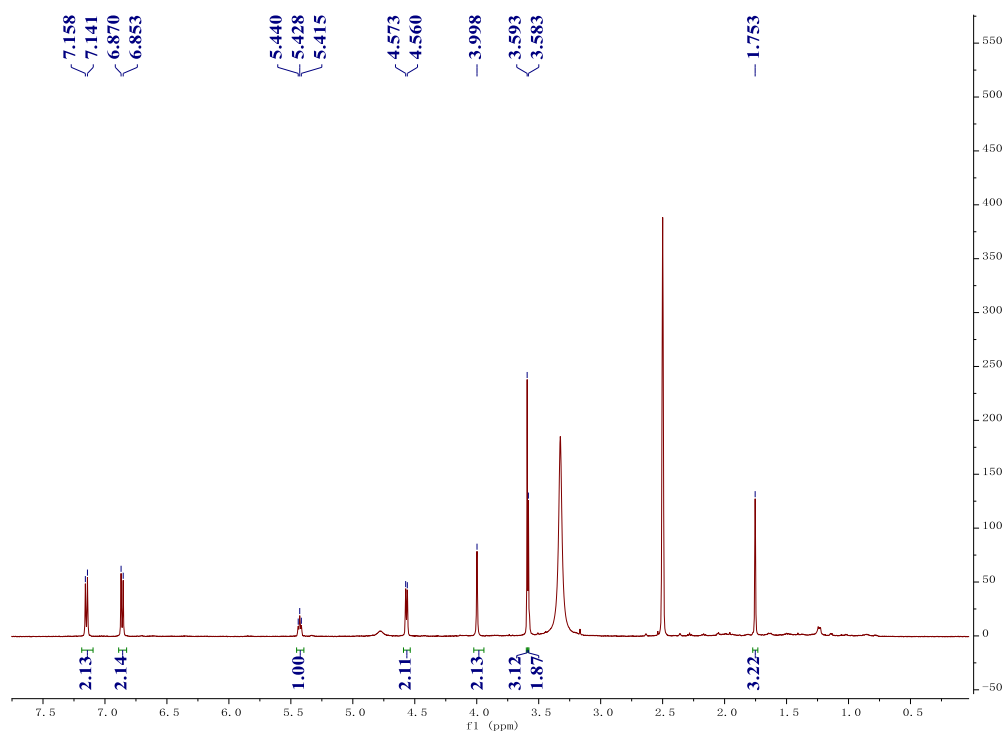


Figure S9. ^1H NMR spectrum of stachyline H (**10**) in $\text{DMSO}-d_6$.

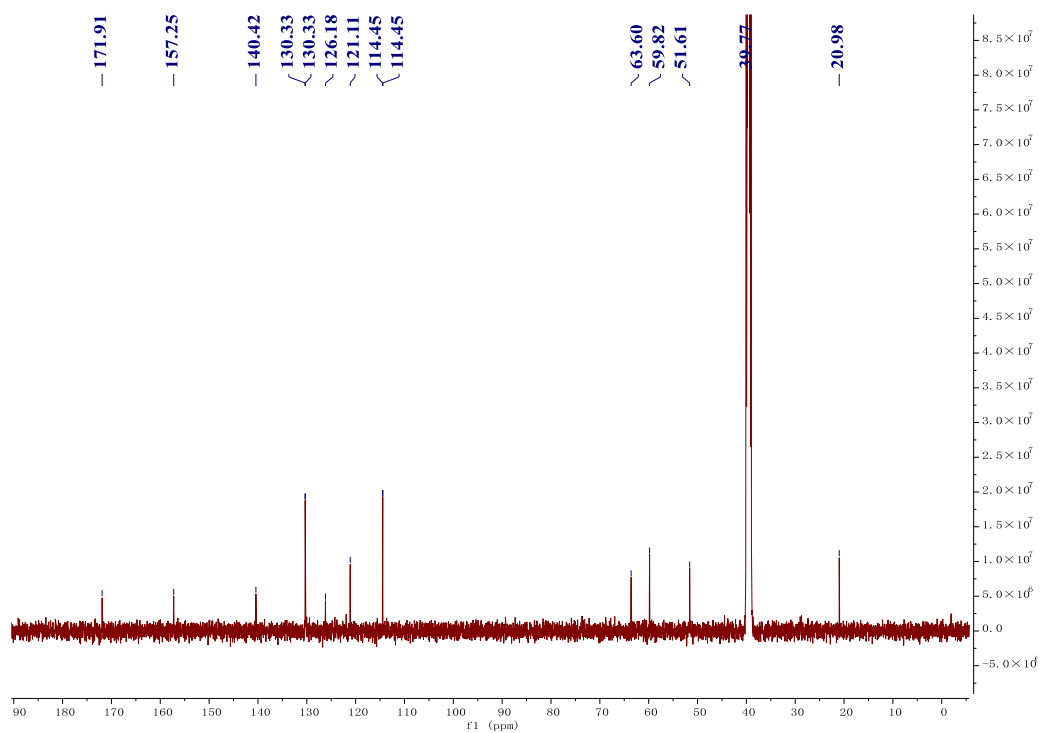


Figure S10. ^{13}C NMR spectrum of stachyline H (**10**) in $\text{DMSO-}d_6$.

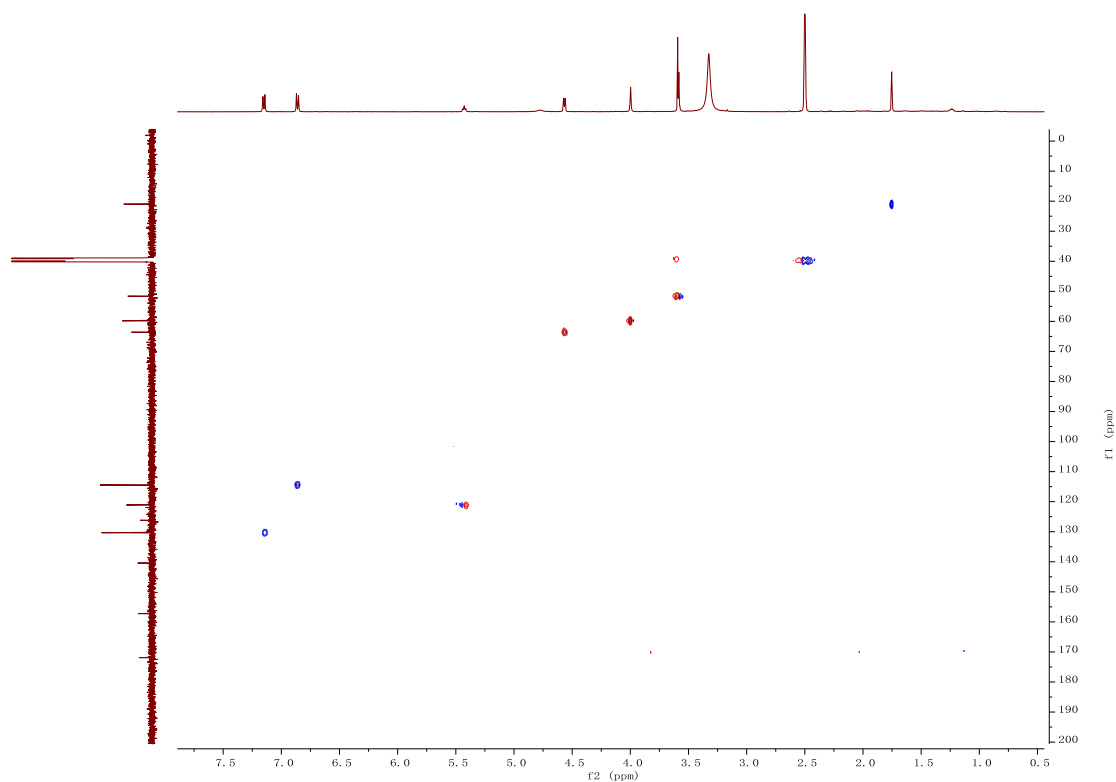


Figure S11. HSQC spectrum of stachyline H (**10**) in $\text{DMSO-}d_6$.

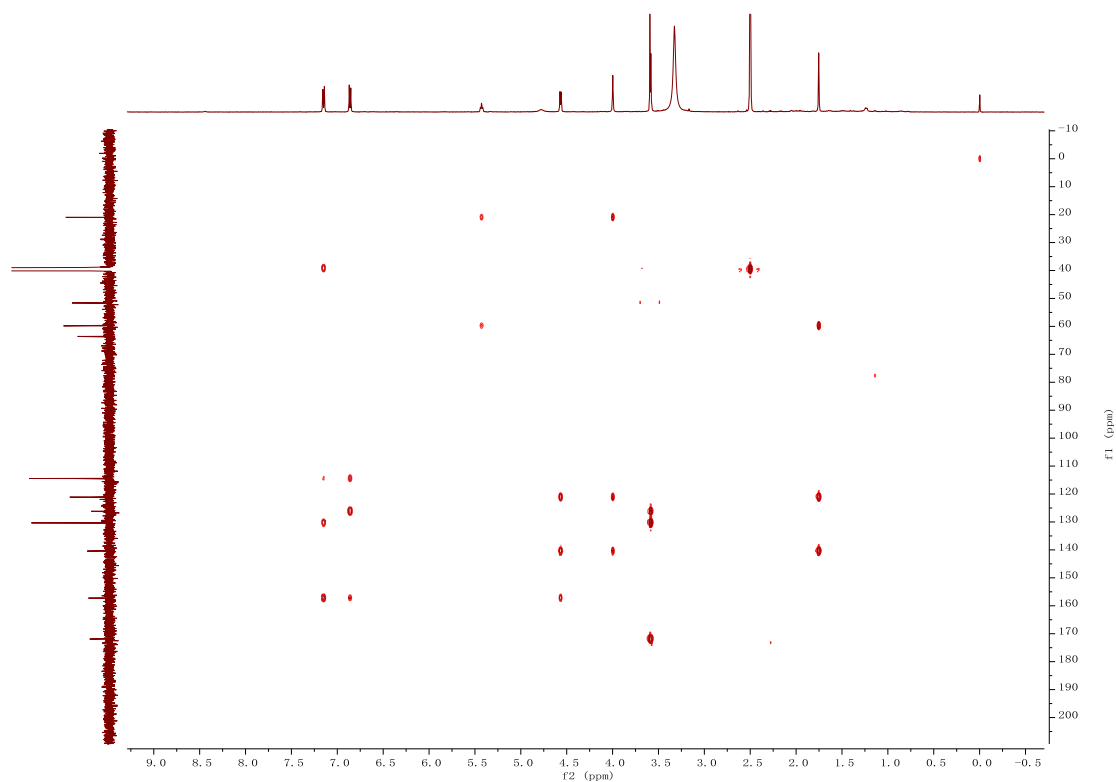


Figure S12. HMBC spectrum of stachyline H (**10**) in DMSO- d_6 .

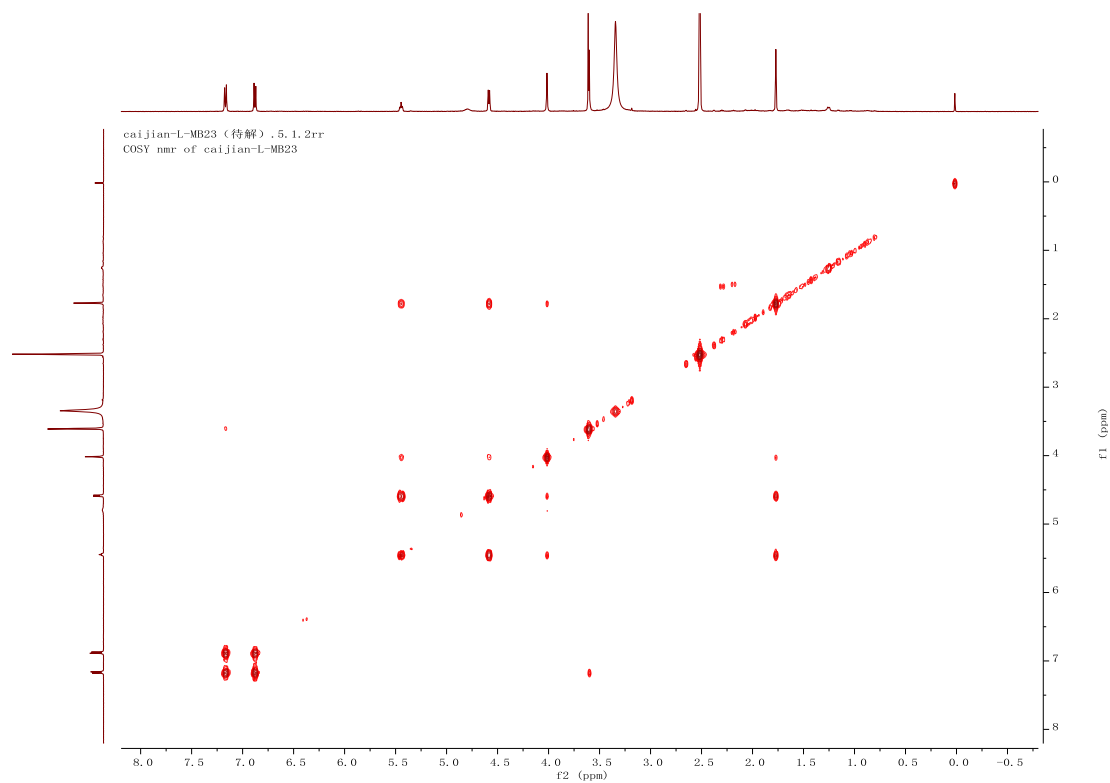


Figure S13. ^1H - ^1H COSY spectrum of stachyline H (**10**) in DMSO- d_6 .

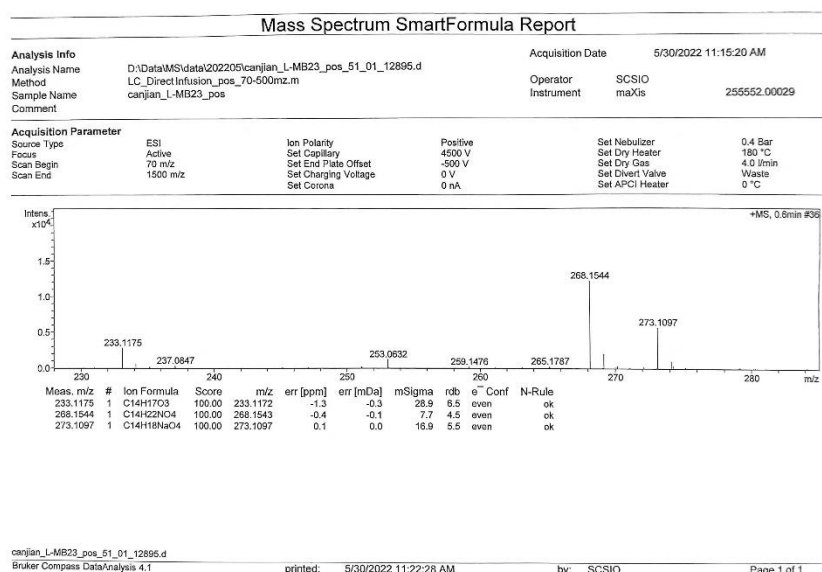


Figure S15. HRESIMS spectrum of stachyline H (**10**).

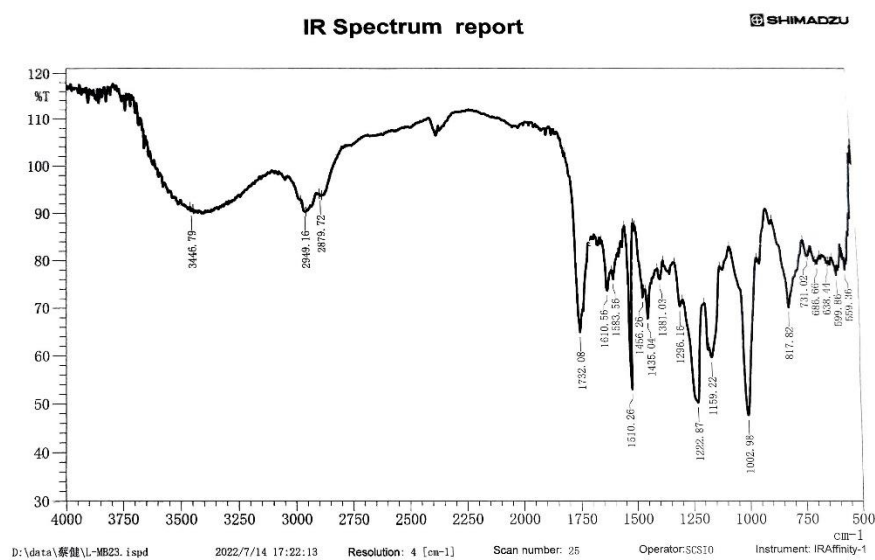
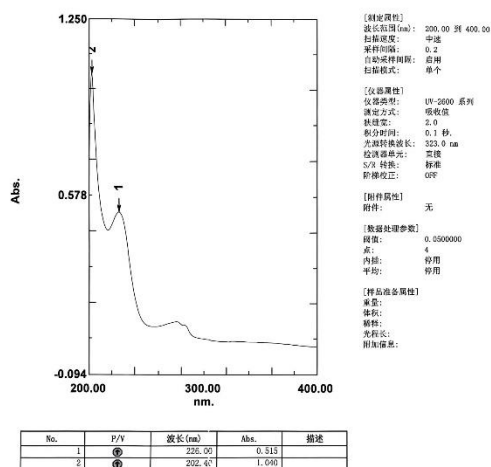
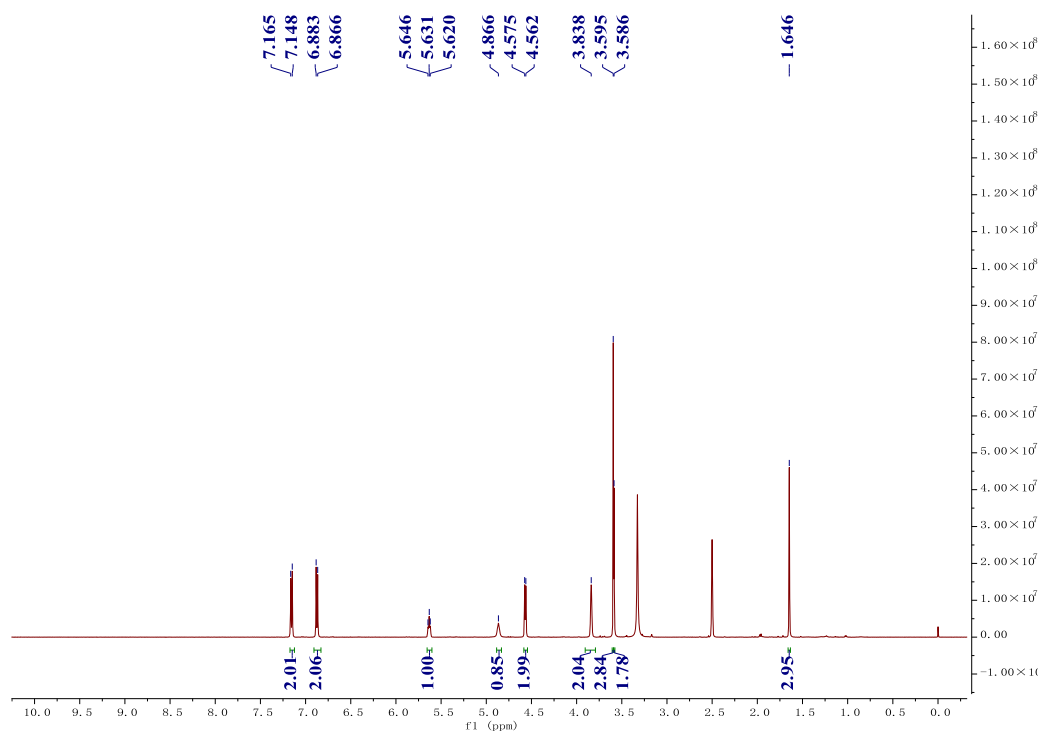


Figure S16. IR spectrum of stachyline H (**10**).

数据集: MB23 - RawData



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Figure S17. UV spectrum of stachyline H (**10**) in MeOH.Figure S18. ^1H NMR spectrum of stachyline I (**11**) in $\text{DMSO}-d_6$.

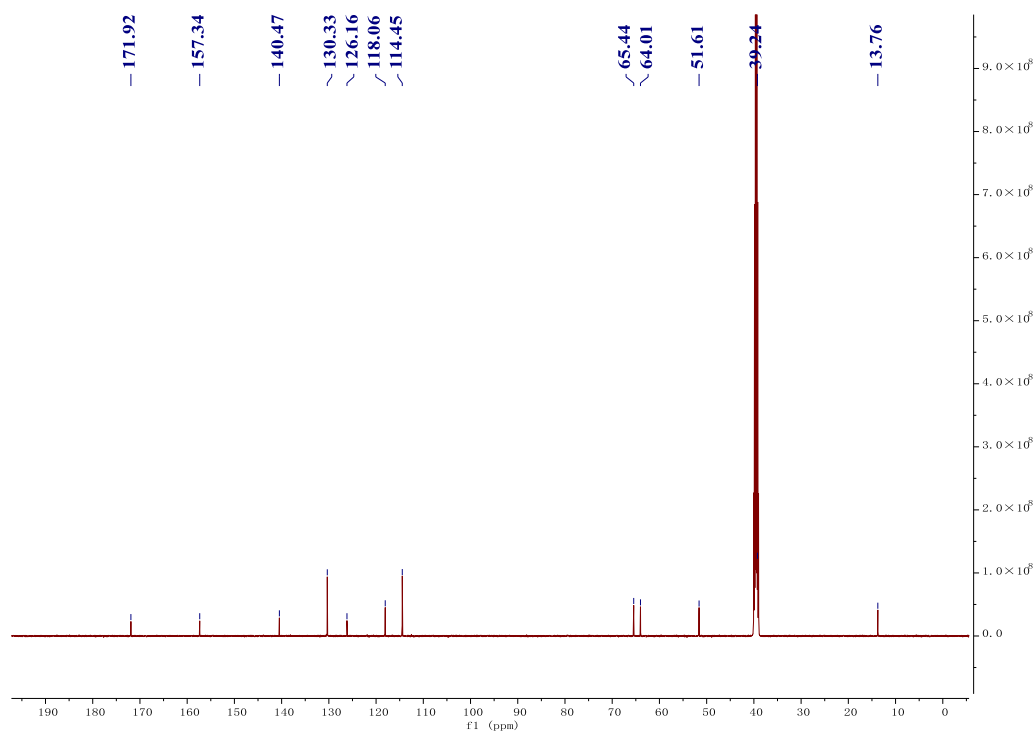


Figure S19. ^{13}C NMR spectrum of stachyline I (**11**) in $\text{DMSO-}d_6$.

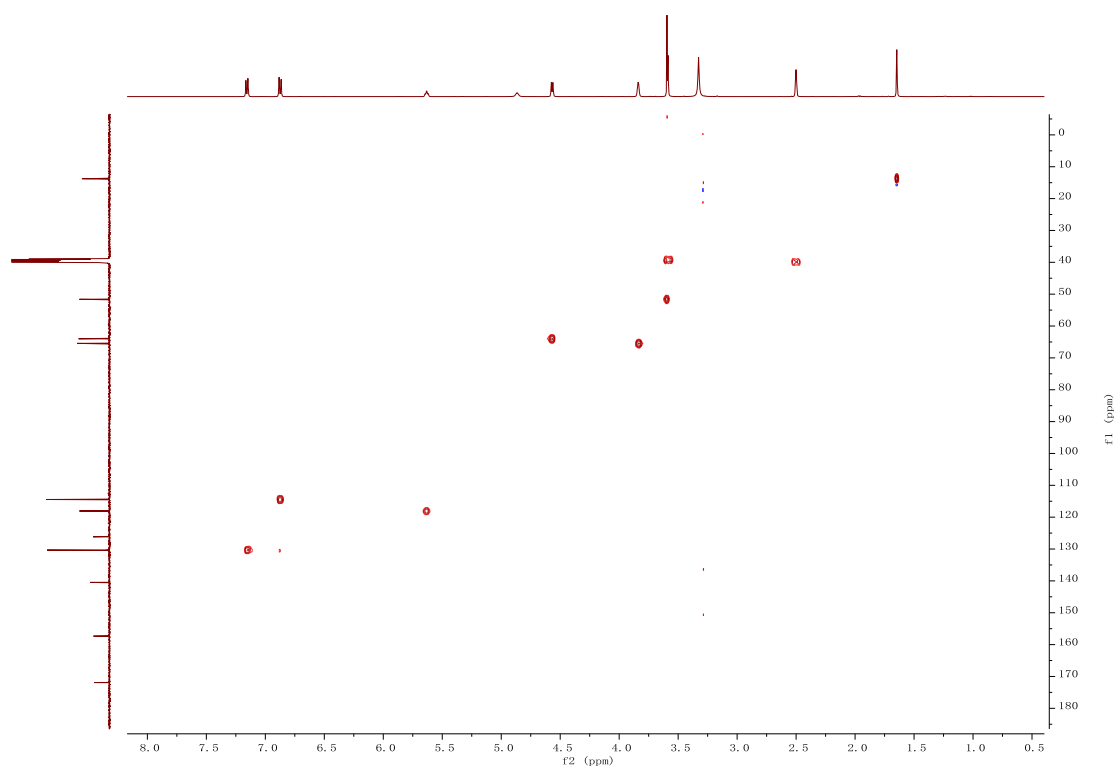


Figure S20. HSQC spectrum of stachyline I (**11**) in $\text{DMSO-}d_6$.

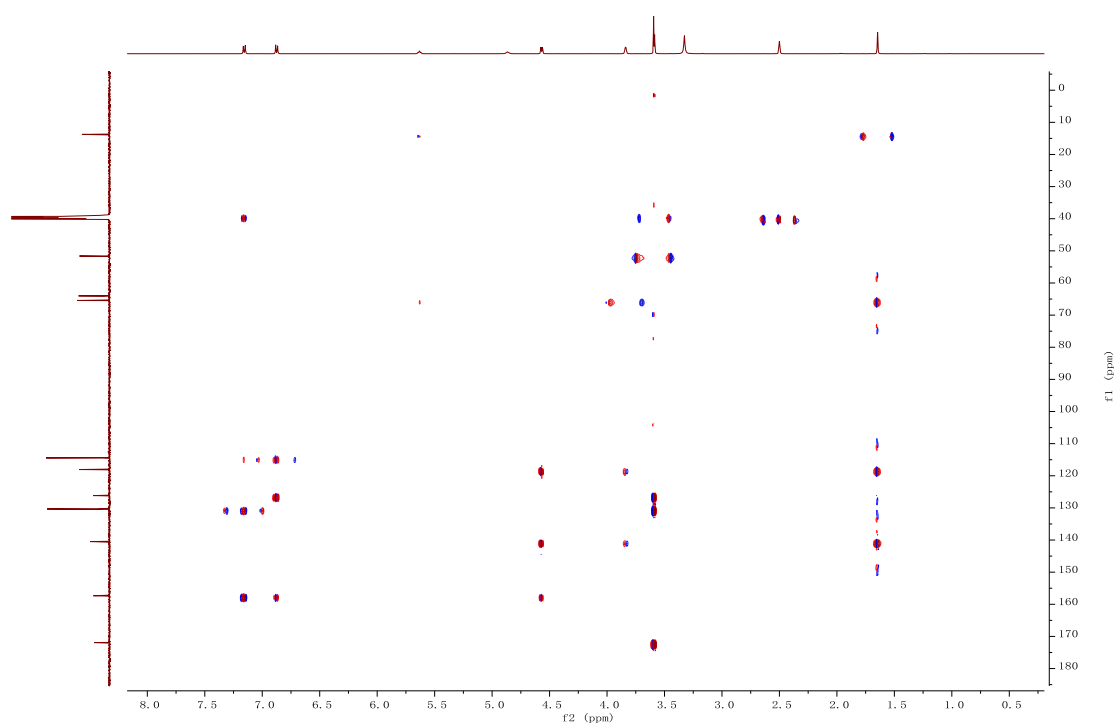


Figure S21. HMBC spectrum of stachyline I (**11**) in DMSO- d_6 .

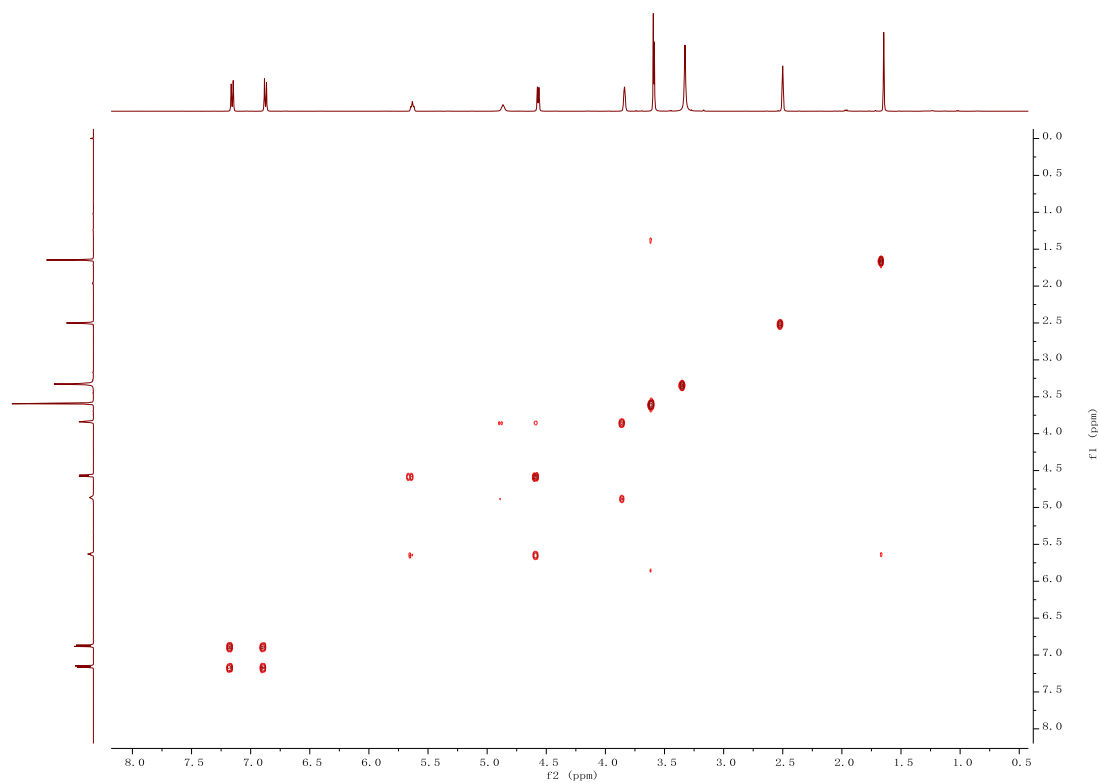


Figure S22. ^1H - ^1H COSY spectrum of stachyline I (**11**) in DMSO- d_6 .

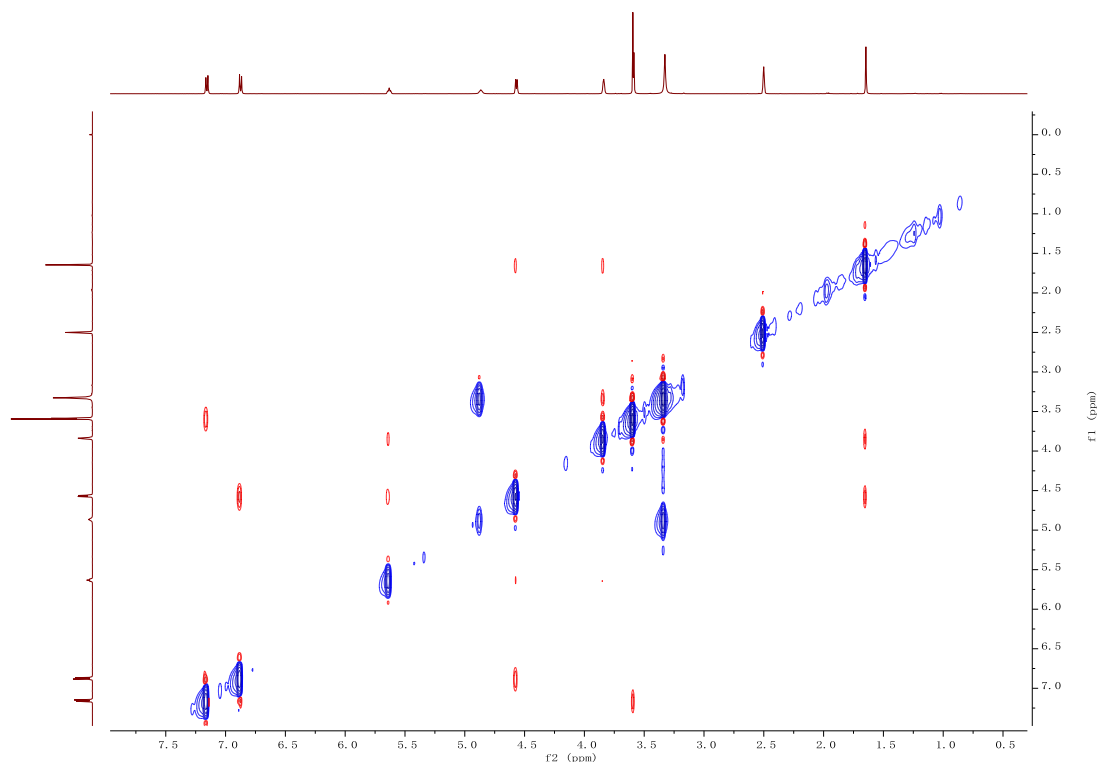
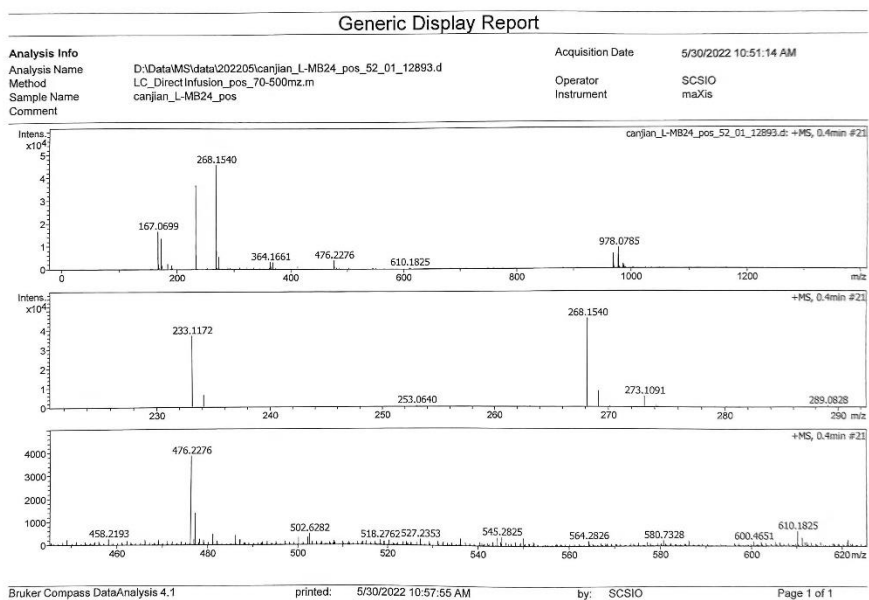


Figure S23. NOESY spectrum of stachyline I (**11**) in DMSO- d_6 .



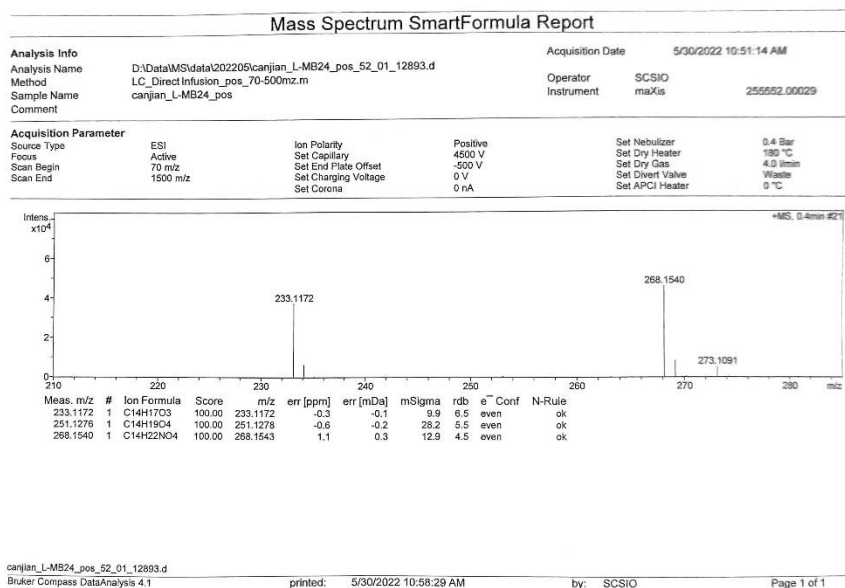


Figure S24. HRESIMS spectrum of stachyline I (11).

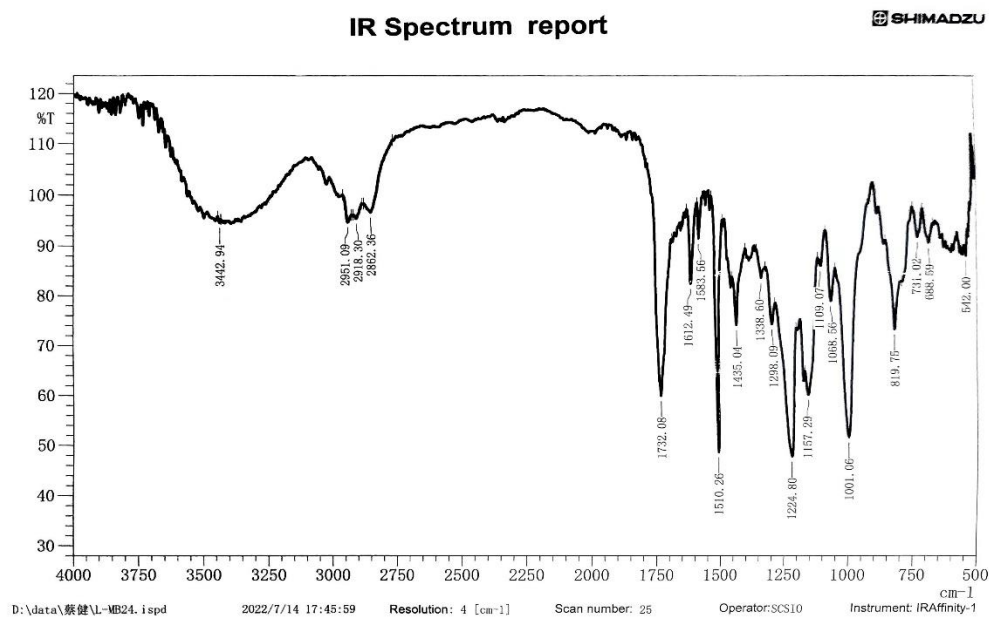
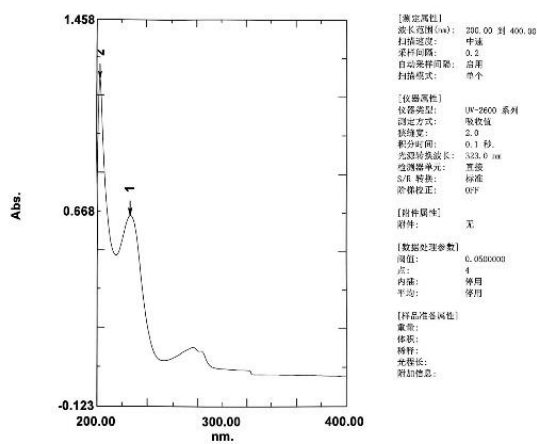


Figure S25. IR spectrum of stachyline I (11).

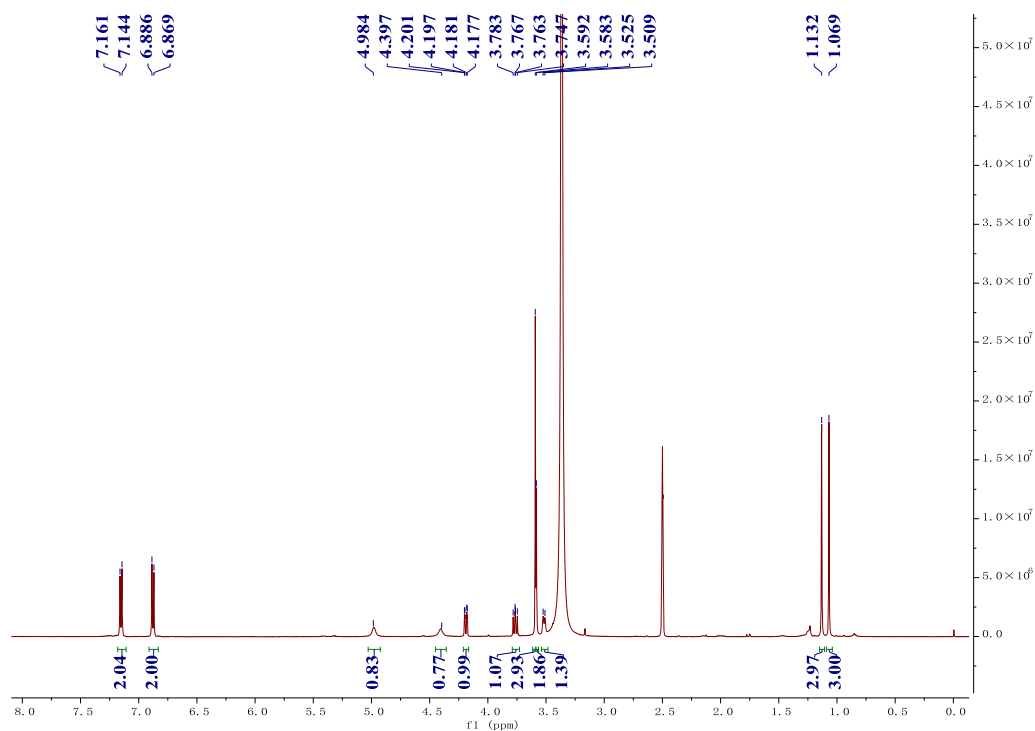
数据表: MB24 - RawData



No.	P/V	波长 (nm)	Abs.	描述
1	①	225.46	0.651	
2	②	202.46	1.210	

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Figure S26. UV spectrum of stachyline I (11) in MeOH.

Figure S27. ^1H NMR spectrum of stachyline J (12) in $\text{DMSO}-d_6$.

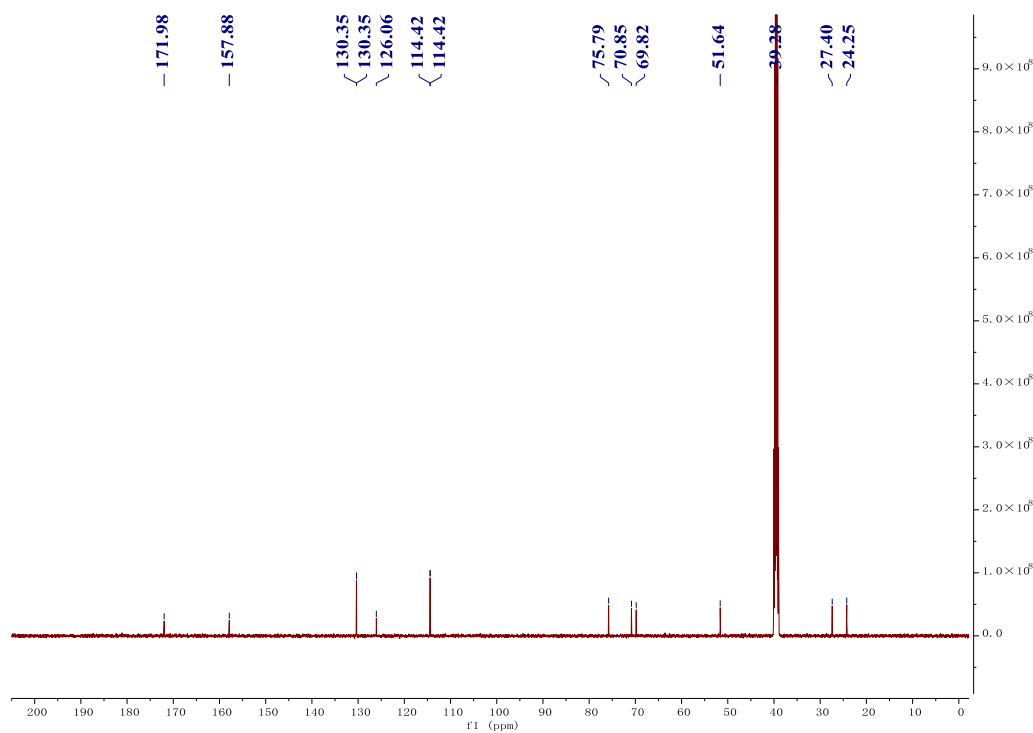


Figure S28. ¹³C NMR spectrum of stachyline J (**12**) in DMSO-*d*₆.

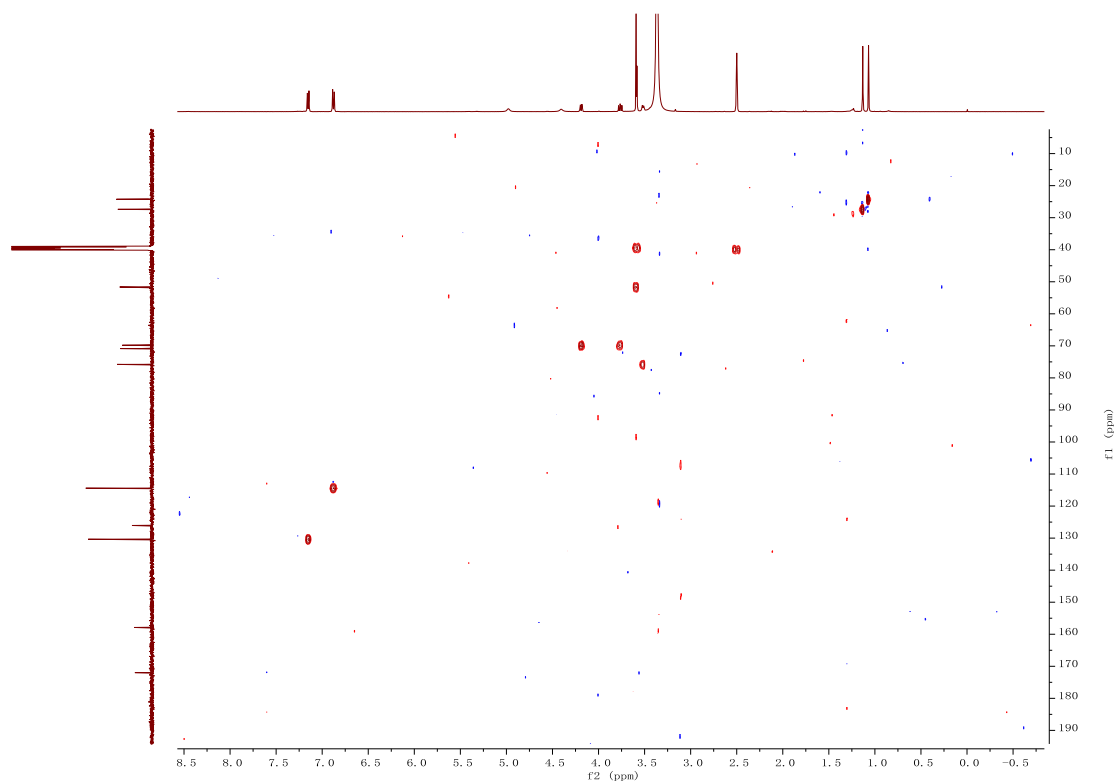


Figure S29. HSQC spectrum of stachyline J (**12**) in DMSO-*d*₆.

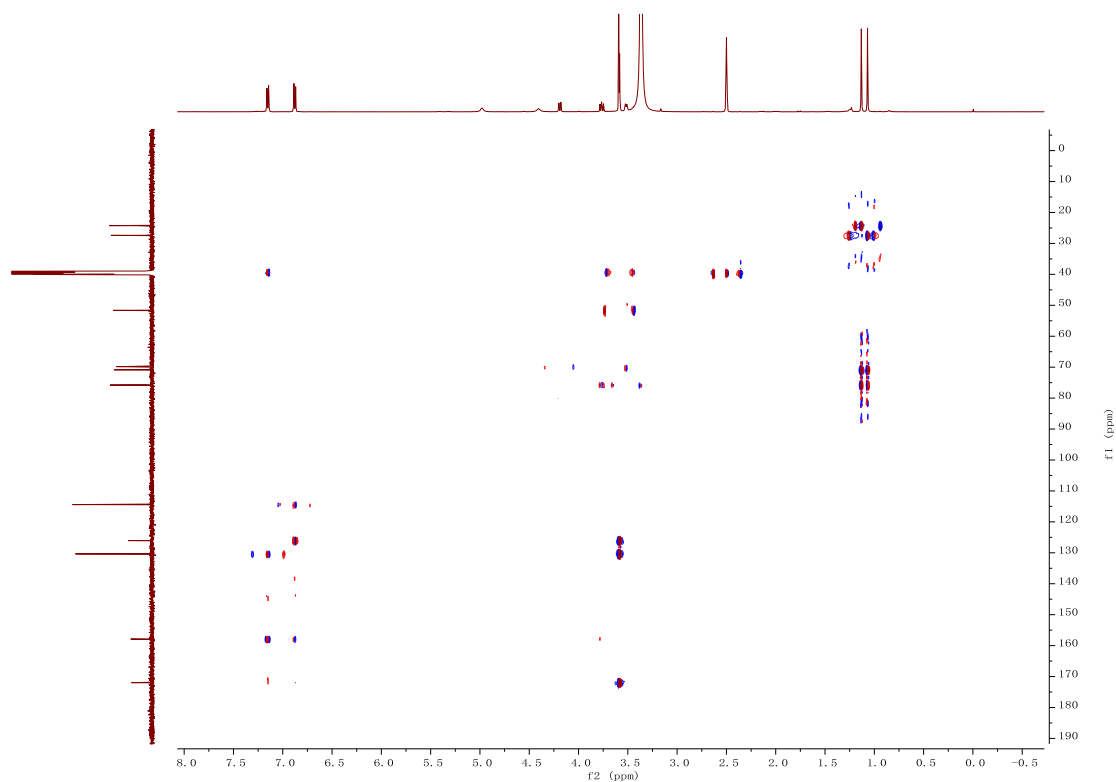


Figure S30. HMBC spectrum of stachyline J (**12**) in DMSO- d_6 .

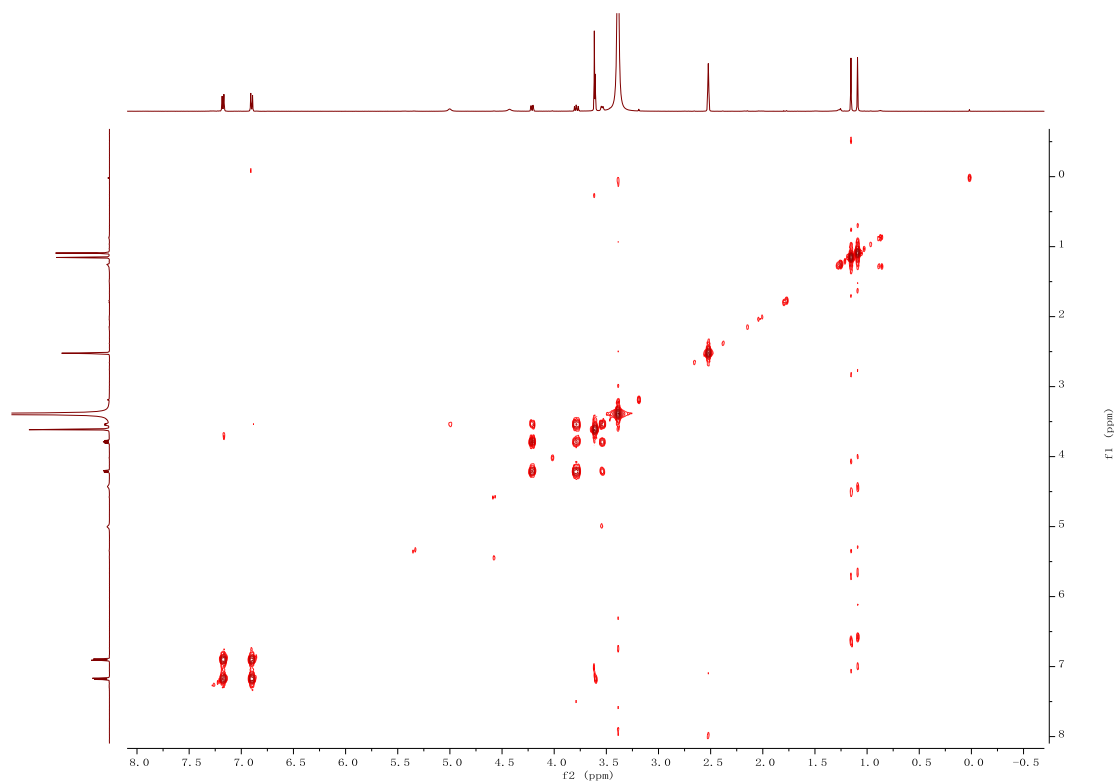


Figure S31. ^1H - ^1H COSY spectrum of stachyline J (**12**) in DMSO- d_6 .

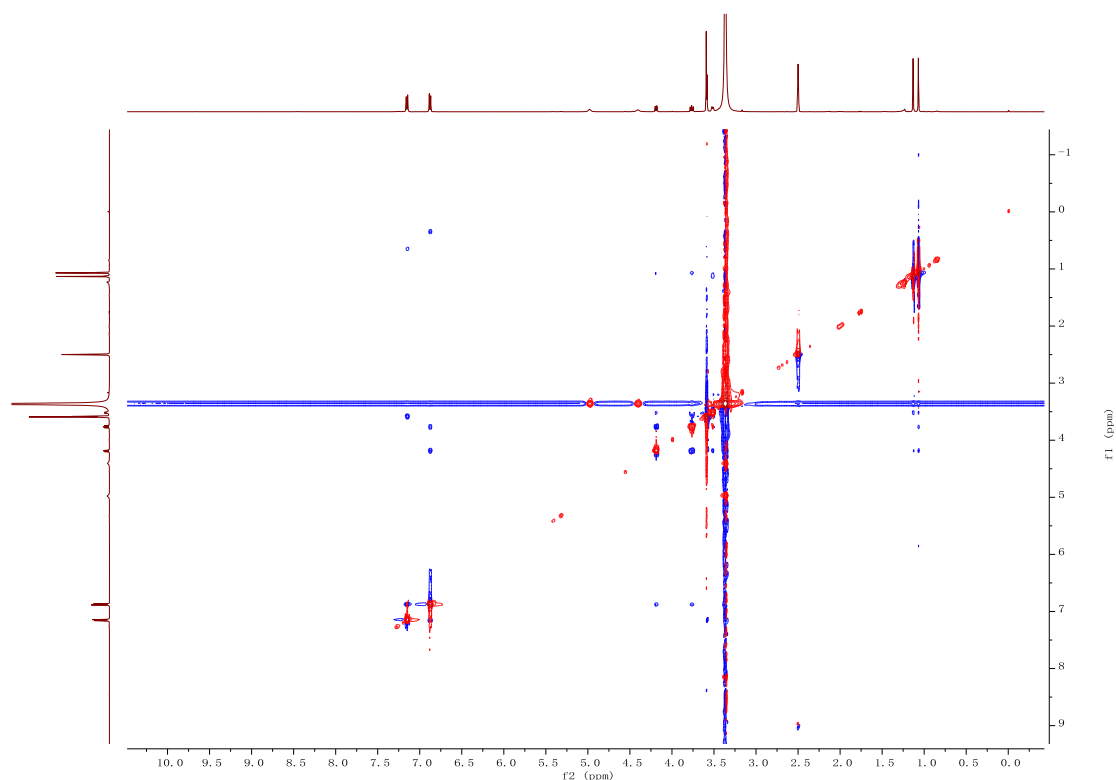
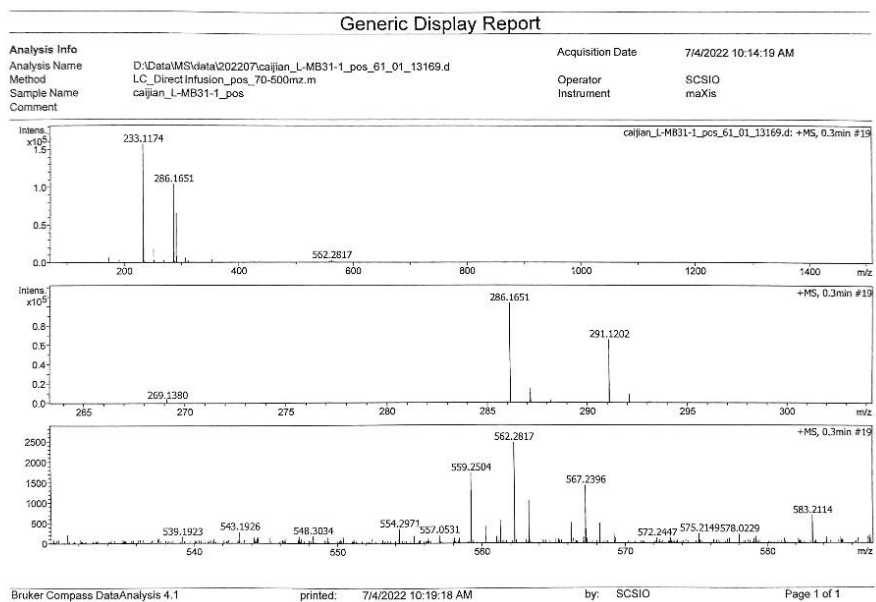


Figure S32. NOESY spectrum of stachyline J (**12**) in DMSO-d₆.



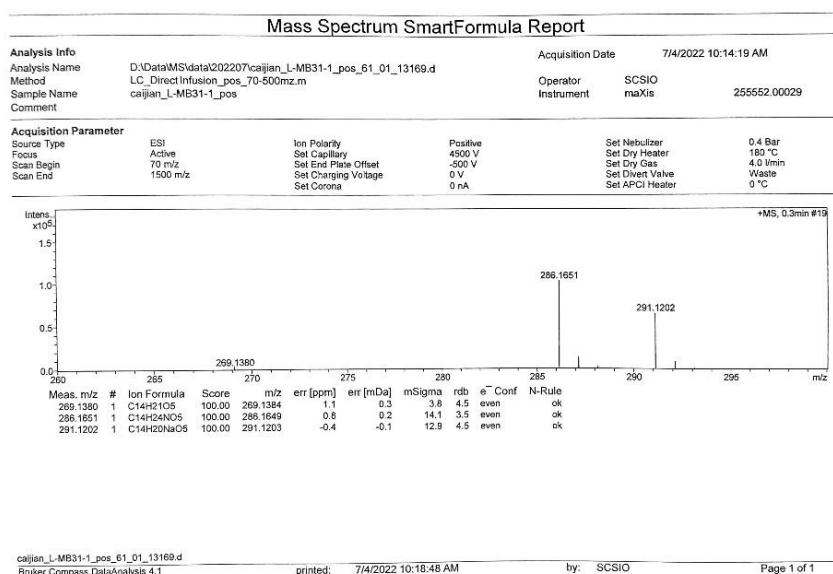


Figure S33. HRESIMS spectrum of stachyline J (12).

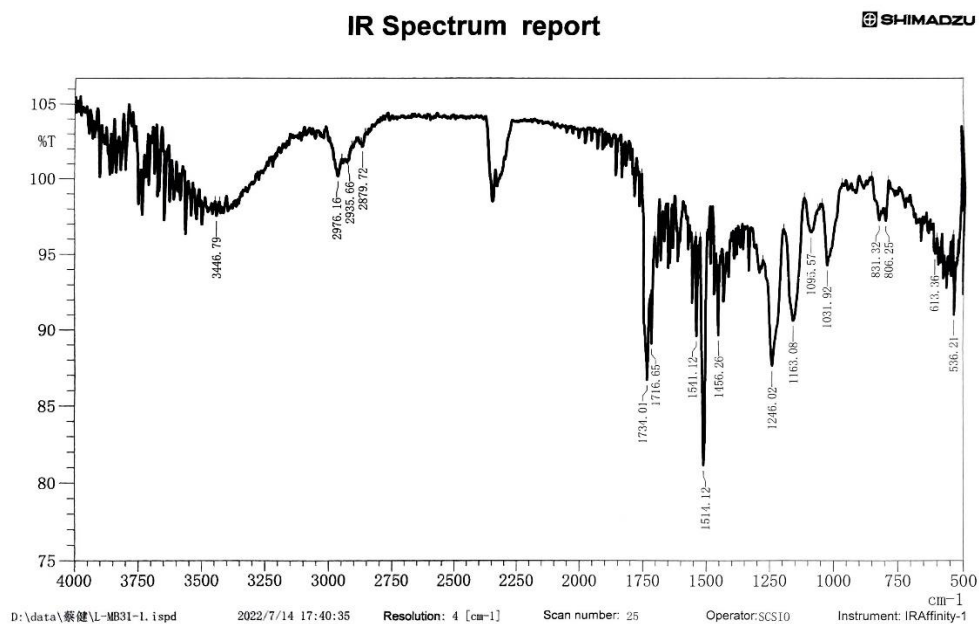


Figure S34. IR spectrum of stachyline J (12).

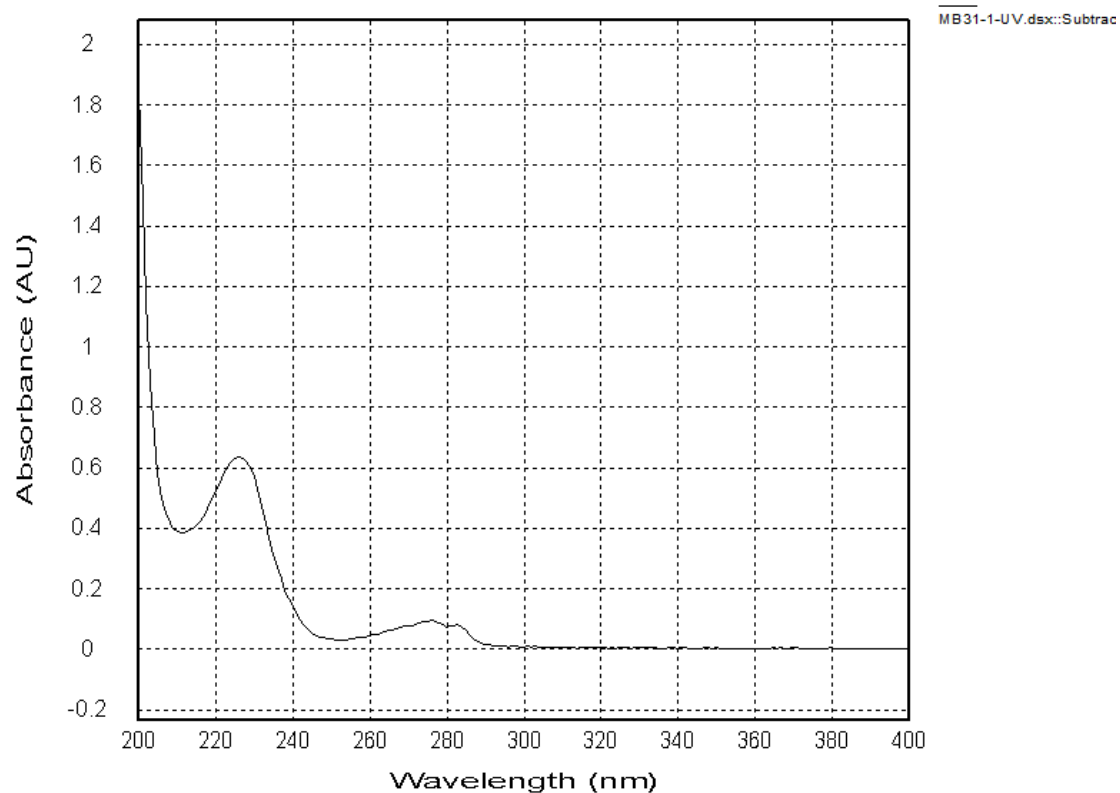


Figure S35. UV spectrum of stachyline J (**12**) in MeOH.

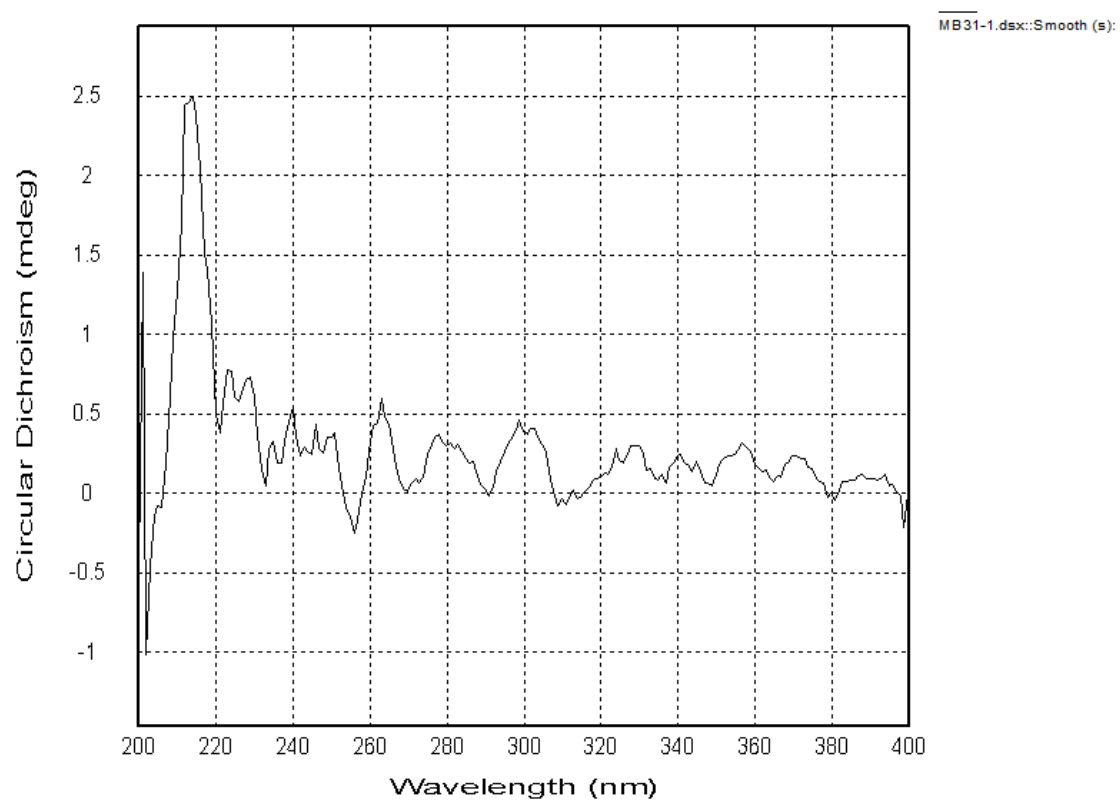


Figure S36. ECD spectrum of stachyline J (**12**) in MeOH.

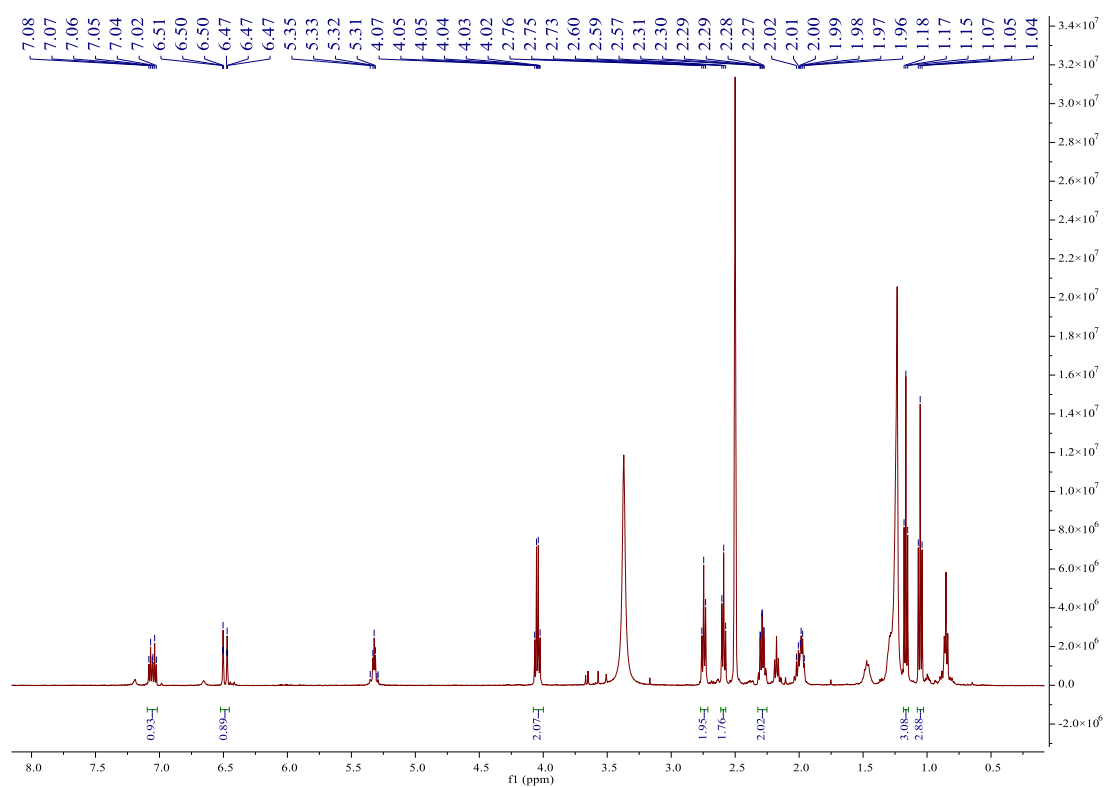


Figure S37. ^1H NMR spectrum of maleicanhydridane (**4**) in $\text{DMSO}-d_6$.

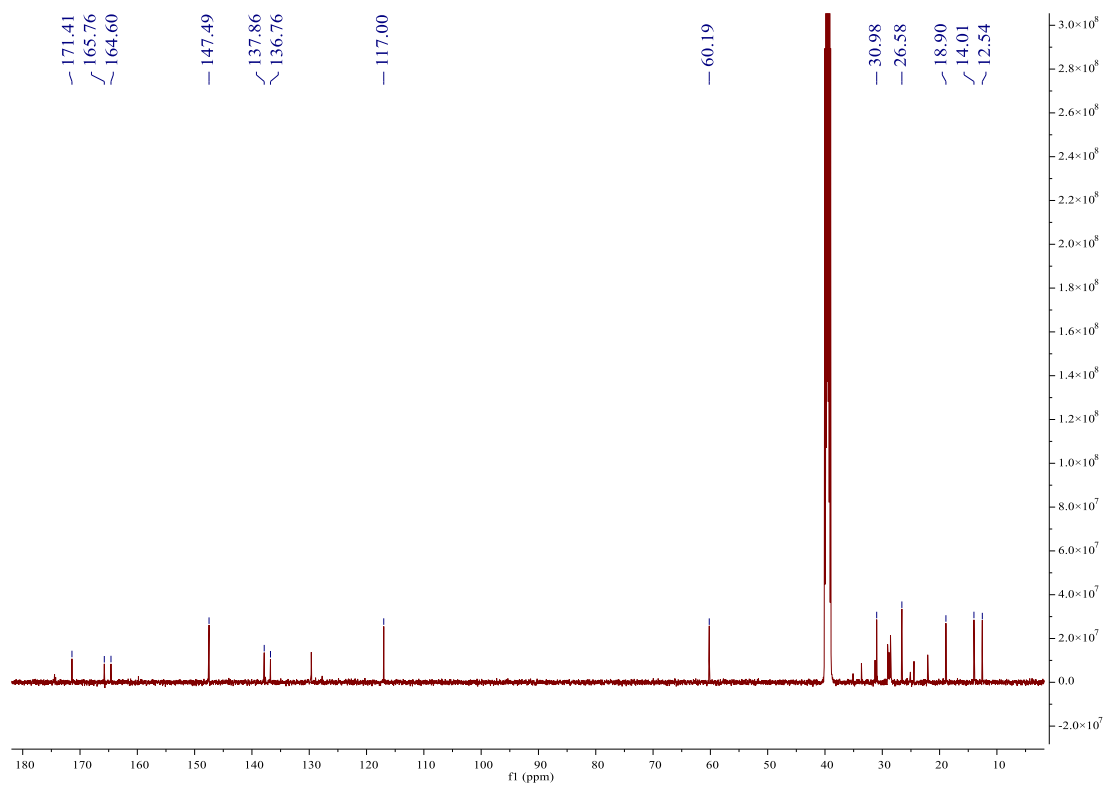


Figure S38. ^{13}C NMR spectrum of maleicanhydridane (**4**) in $\text{DMSO}-d_6$.

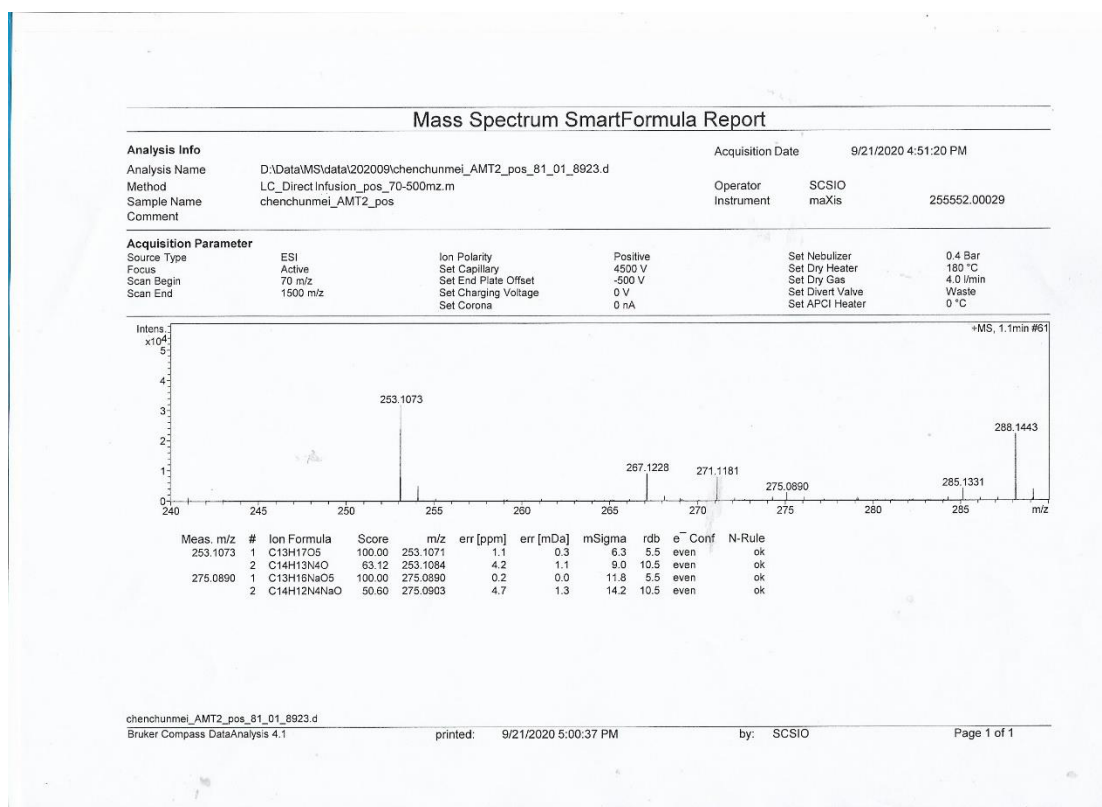
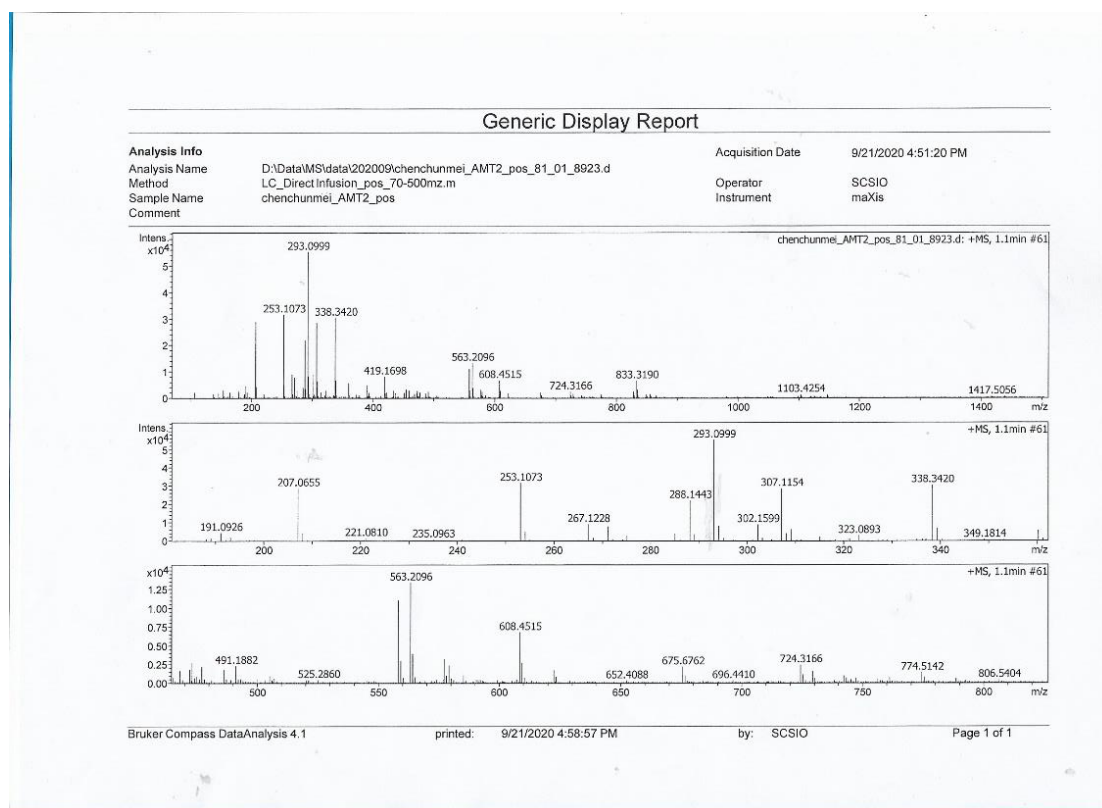


Figure S39. HRESIMS spectrum of maleicanhydridane (**4**).

ECD Calculation Details for **5**.

The ECD spectra were generated based on Boltzmann distribution theory by the SpecDis 1.71 under a half band width of 0.18 eV and shifted by 0 nm to facilitate comparison to the experimental data.

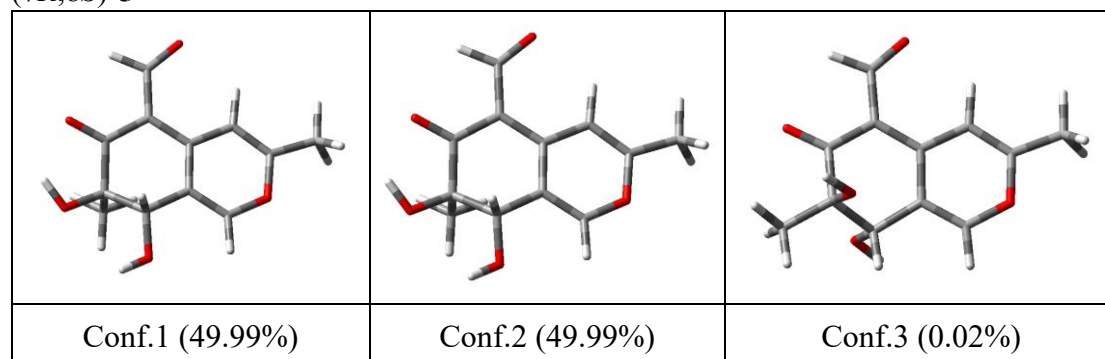
Table S1. Energies of **5** at MMFF94 force field.

Configuration	Conformer	Energy (kcal/mol)	Population (%)
(7 <i>R</i> ,8 <i>S</i>)- 5	1	252.95	51.6
(7 <i>R</i> ,8 <i>S</i>)- 5	2	253.12	48.1
(7 <i>R</i> ,8 <i>S</i>)- 5	3	266.20	0.2
(7 <i>S</i> ,8 <i>R</i>)- 5	1	252.95	51.6
(7 <i>S</i> ,8 <i>R</i>)- 5	2	253.12	48.1
(7 <i>S</i> ,8 <i>R</i>)- 5	3	266.20	0.2

Table S2. Energies of **5** at B3LYP/6–31+g(d) level in methanol.

Configuration	Conformer	E (Hartree)	E (kcal/mol)	Population (%)
(7 <i>R</i> ,8 <i>S</i>)- 5	1	–840.8541634	–527644.396075134	49.99
(7 <i>R</i> ,8 <i>S</i>)- 5	2	–840.8541634	–527644.396075134	49.99
(7 <i>R</i> ,8 <i>S</i>)- 5	3	–840.8465769	–527639.635470519	0.02
(7 <i>S</i> ,8 <i>R</i>)- 5	1	–840.8541634	–527644.396075134	49.99
(7 <i>S</i> ,8 <i>R</i>)- 5	2	–840.8541634	–527644.396075134	49.99
(7 <i>S</i> ,8 <i>R</i>)- 5	3	–840.8465769	–527639.635470519	0.02

(7*R*,8*S*)-**5**



(7*S*,8*R*)-**5**

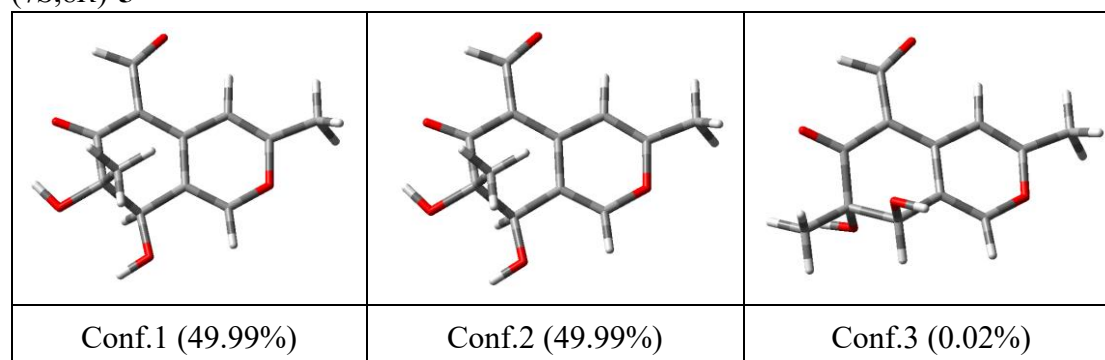


Figure S9. The optimized conformers and equilibrium populations of **5**.

The strain's (*Talaromyces* sp. SCSIO 41050) ITS sequence of the rDNA

TACTTCCGTAAGGGGGACCTGCGGAAGGATCATTACCGAGTGAGGGCCCTC
 GCGGCCCAACCTCCCACCCTTGTCTCATATACCTGTTGCTTCGGCGGGCCC
 ACCGGGGCCACCTGGTCGCCGGGGGACGTCTGTCCCCGGGCCCCGCGCCCCG
 CCGGAGCGCCCTTTGAACCCTGATGAAGATGGGCTGTCTGAGTGATATGAA
 AATTGTCAAACTTTCAACAACGAATCTCTTGGTTCCGGCATCGATGAAGA
 ACGCAGCGAAATGCGATAAGTAATGTGAATTGCAGAATTCCGTGAATCATC
 GAATCTTTGAACGCACATTGCGCCCCCTGGCATTCCGGGGGGCATGCCTGT
 CCGAGCGTCATTTCTGCCCTCAAGCACGGCTTGTGTGTTGGGTGTGGTCCC
 TCCGGGGACCTGCCCCGAAAGGCAGCGGCGACGTCCGTCTGGTCCTCGAGC
 GTATGGGGCTCTGTCACTCGCTCGGGAAGGACCTGCGGAGGTTGGTCACC
 ACCACATCTTTTTTACAAGGTTGACCTCGGATCAGGTAGGAGTTACCCGCT
 GAACTTAAGCATATCTAGACGCCGAGGAA

The strain's (*Penicillium* sp. SCSIO 41411) ITS sequence of the rDNA

TGATATGCTTAAGTTCAGCGGGTATCCCTACCTGATCCGAGGTCAACCTGAG
 AAAGATTGAGGGGGGTCGCCGGCGGGCGCCGGCCGGGCCTACAGAGCGG
 GTGACGAAGCCCCATACGCTCGAGGACCGGACGCGGTGCCGCCGCTGCCT
 TTCGGGGCCCGCCCCCGGTAGCCGGGGGGCGGGGGCCCAACACACAAGCCG
 TGCTTGAGGGCAGCAATGACGCTCGGACAGGCATGCCCCCGGAATACCA

GGGGGCGCAATGTGCGTTCAAAGACTCGATGATTCACTGAATTCTGCAATT
CACATTACTTATCGCATTTTCGCTGCGTTCTTCATCGATGCCGGAACCAAGAG
ATCCGTTGTTGAAAGTTTTAACTGATTTAGCTAATCGCTCAGACTGCATTCT
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CCGCA