Supporting Information

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Two new sesquiterpenes from a kind of TCM Pieces, Curcumae Radix

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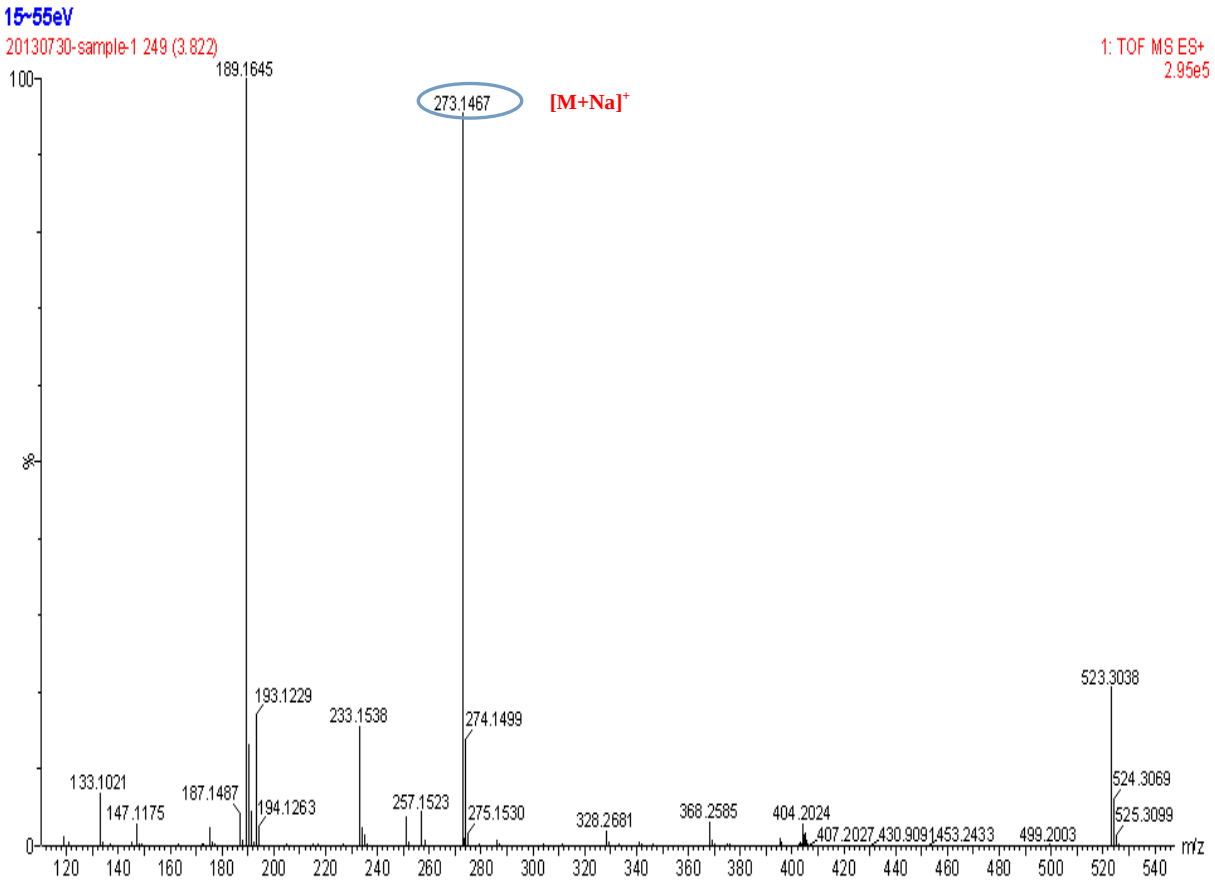
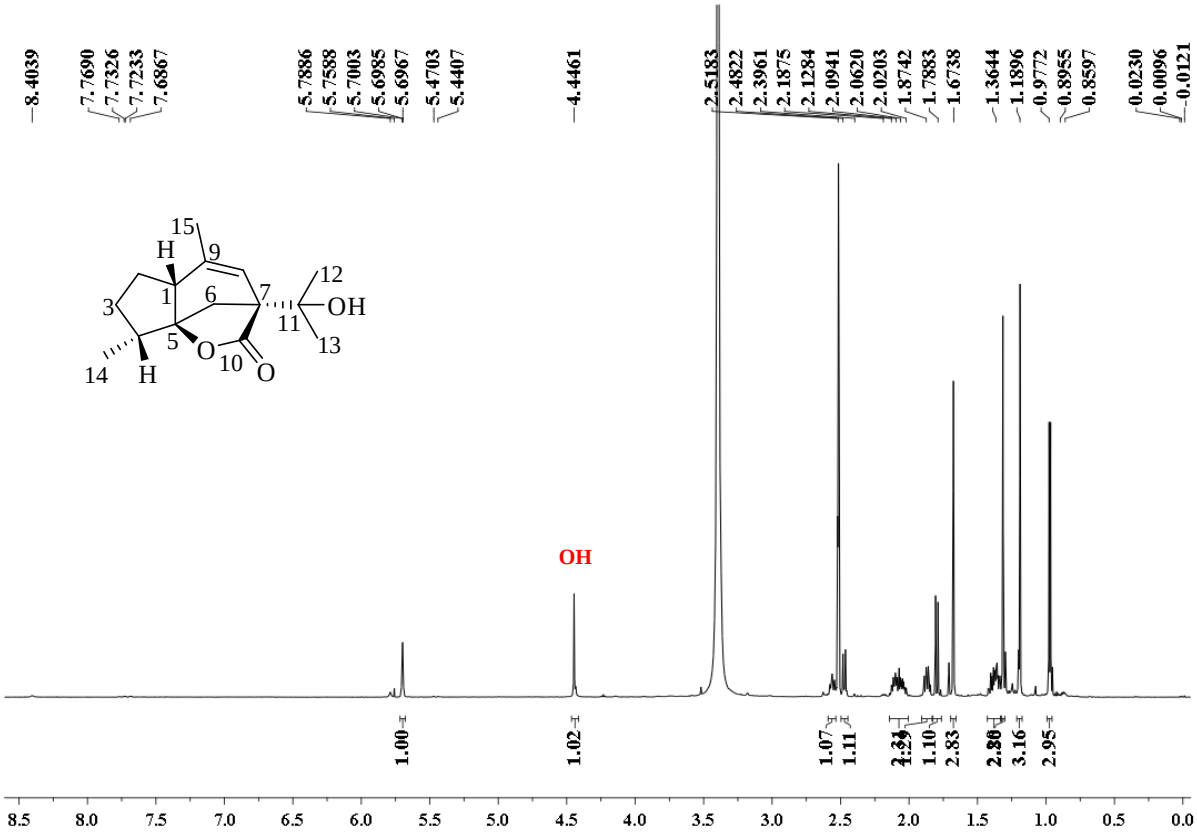
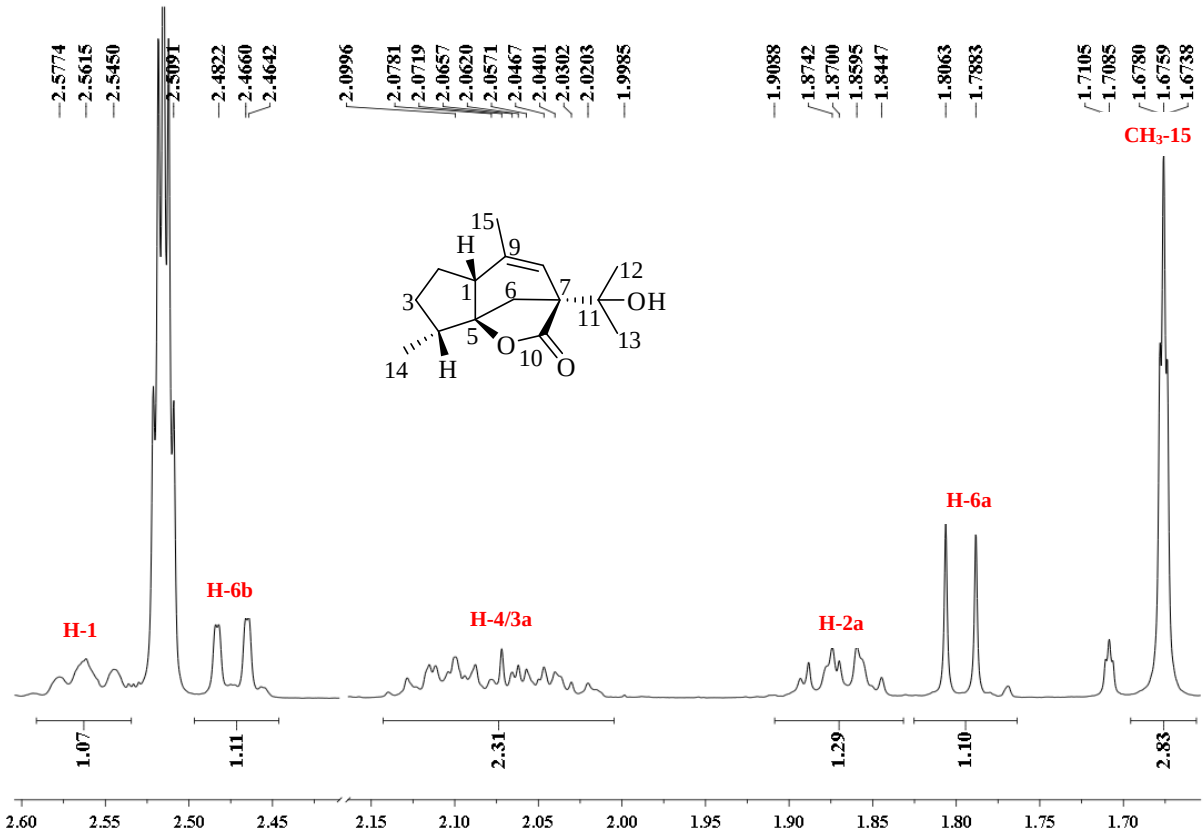


S1: HRESI-MS Spectrum of Compound **1 (**(1*R*,4*R*,5*S*,7*S*)-curwenyujinone)



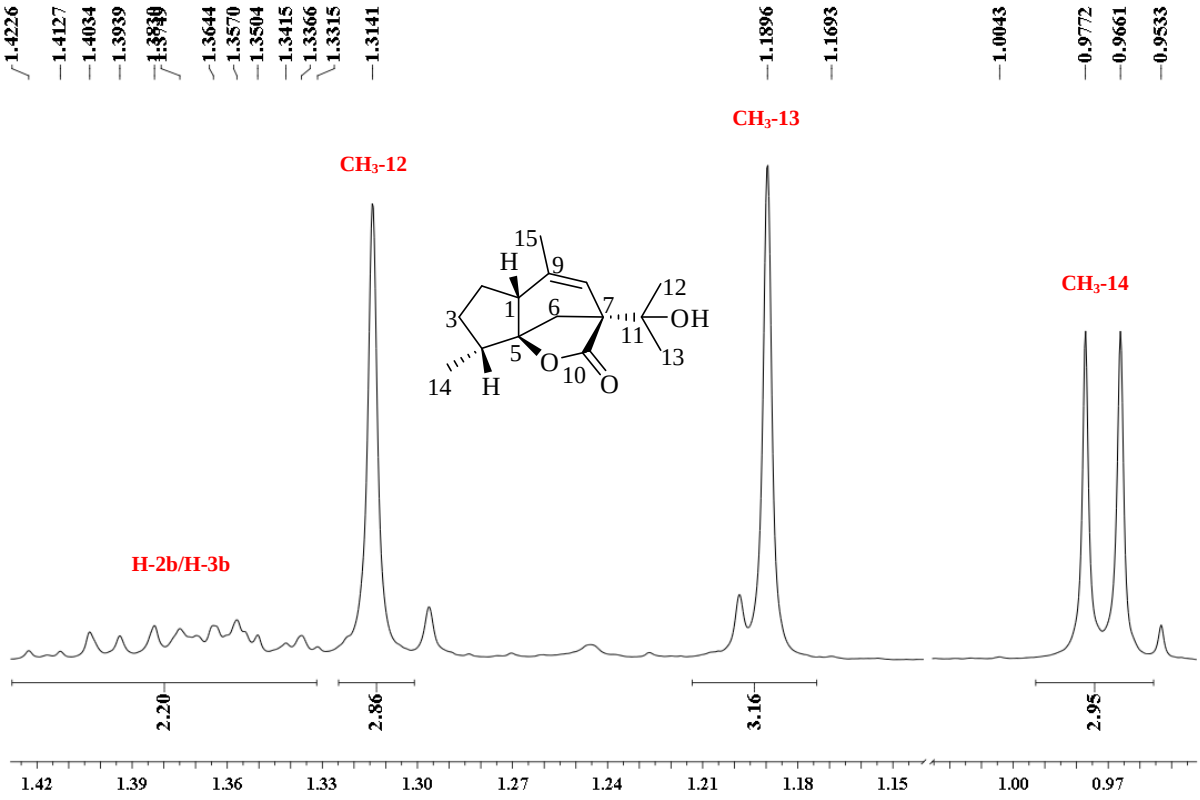
S2:[1]H-NMR(600MHz,DMSO-d_6) Spectrum of Compound **1 (**(1*R*,4*R*,5*S*,7*S*)-curwenyujinone)

*(1R,4R,5S,7S)-curwenyujinone (**1**)*: colorless oil. [1]H NMR (DMSO-d_6,600 MHz), δ: 0.97 (3H, d, 6.6, H-14), 1.19 (3H, s, H-13), 1.31 (3H, s, H-12), 1.35 (1H, m, H-3b), 1.38 (1H, m, H-2b), 1.68 (3H, br s, H-15), 1.79 (1H, d, 10.8, H-6a), 1.86 (1H, m, H-2a), 2.05 (1H, m, H-3a), 2.11 (1H, m, H-4), 2.47 (1H, dd, 10.8, 1.2, H-6b), 2.52 (1H, dd, 8.4, 9.6, H-1), 4.45 (1H, s, OH), 5.70 (1H, br s, H-8). [13]C NMR (DMSO-d_6, 150 MHz): 50.7 (C-1), 23.5 (C-2), 30.1 (C-3), 37.8 (C-4), 90.5 (C-5), 35.9 (C-6), 57.0(C-7), 122.3 (C-8), 139.3 (C-9), 176.3(C-10), 69.7(C-11), 25.4(C-12), 27.0 (C-13), 12.9(C-14), 20.7 (C-15).



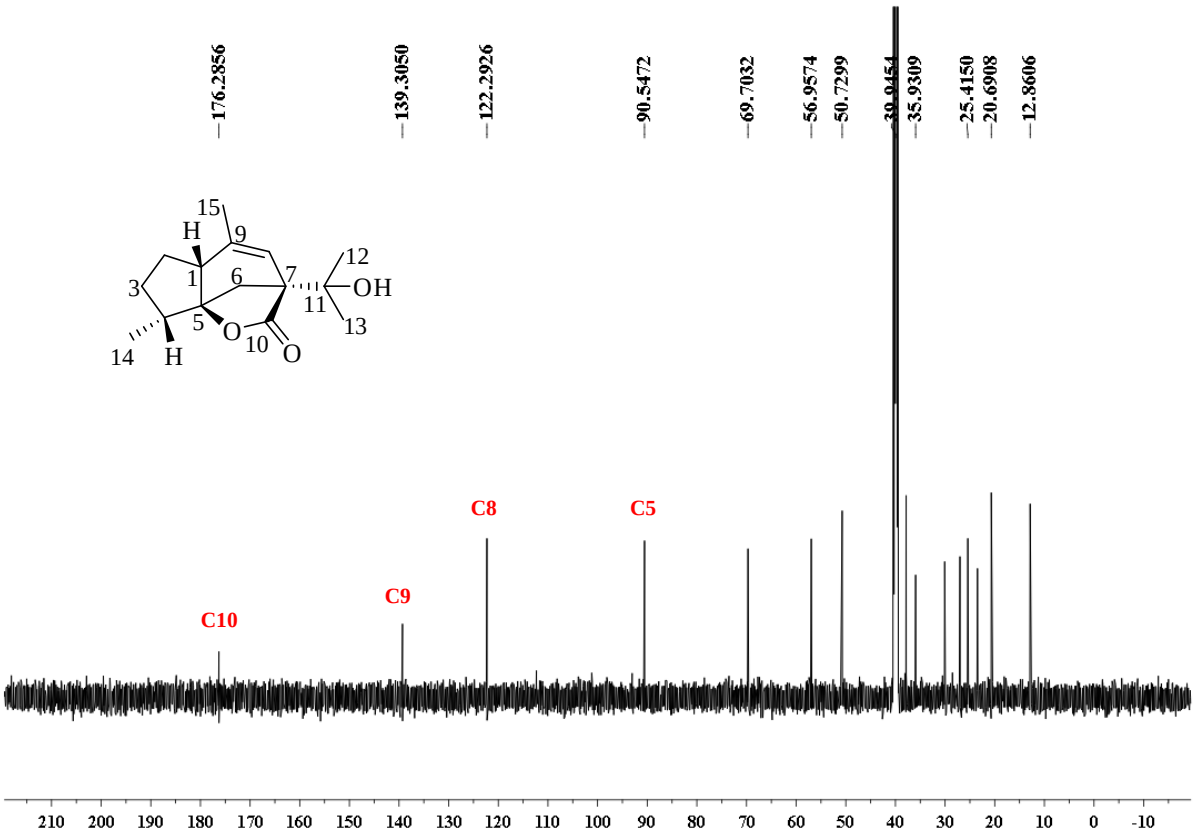
S3: ^{1}H-NMR Spectrum of Compound **1 (**(1*R*,4*R*,5*S*,7*S*)-curwenyujinone)

(From 1.65 to 2.60 ppm)

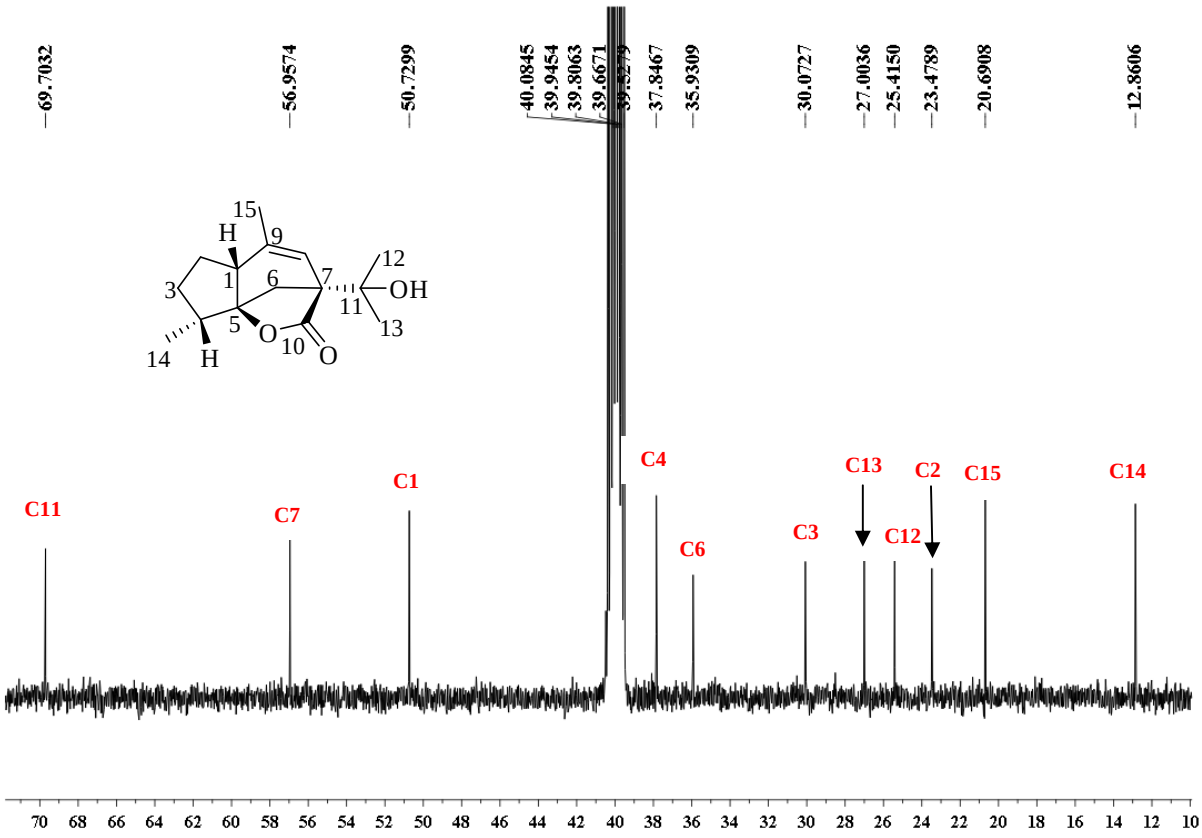


S4: ^{1}H-NMR Spectrum of Compound **1 (**(1*R*,4*R*,5*S*,7*S*)-curwenyujinone)

(From 0.95 to 1.42 ppm)

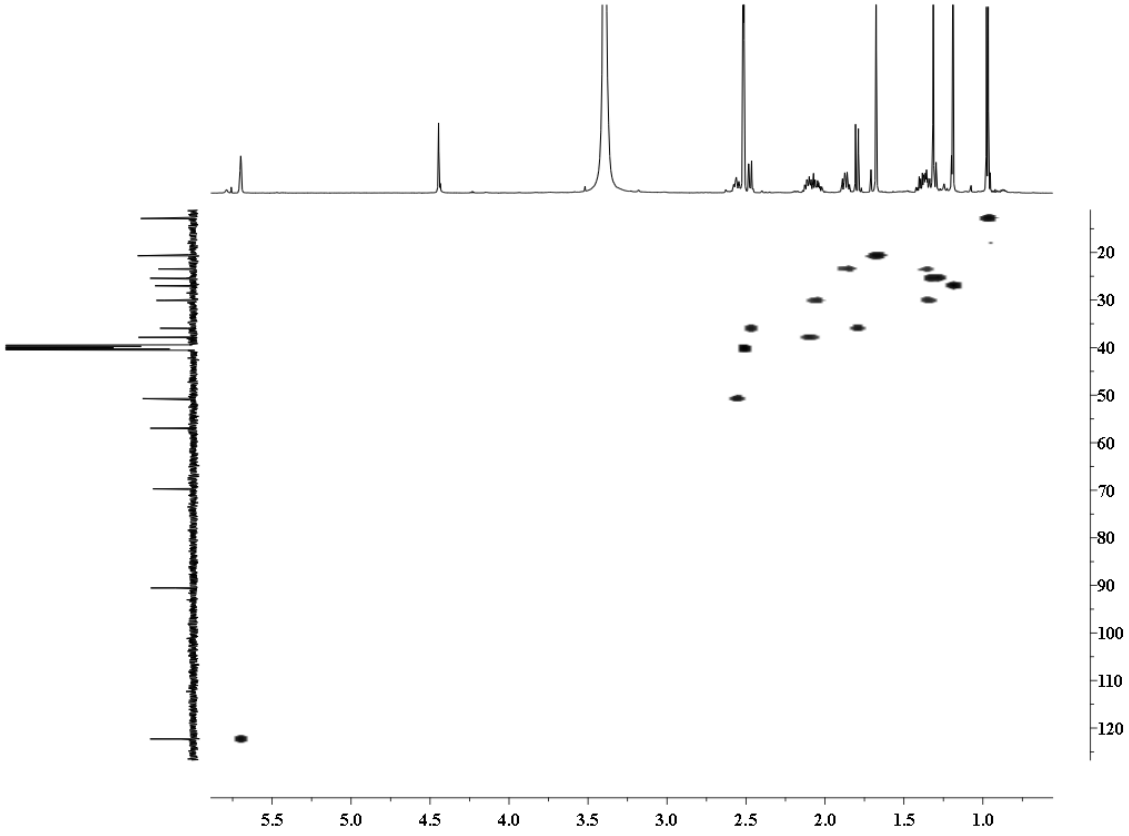


S5: ^{13}C-NMR (150MHz, DMSO-d_6) Spectrum of Compound **1 (**(1*R*,4*R*,5*S*,7*S*)-curwenyujinone)

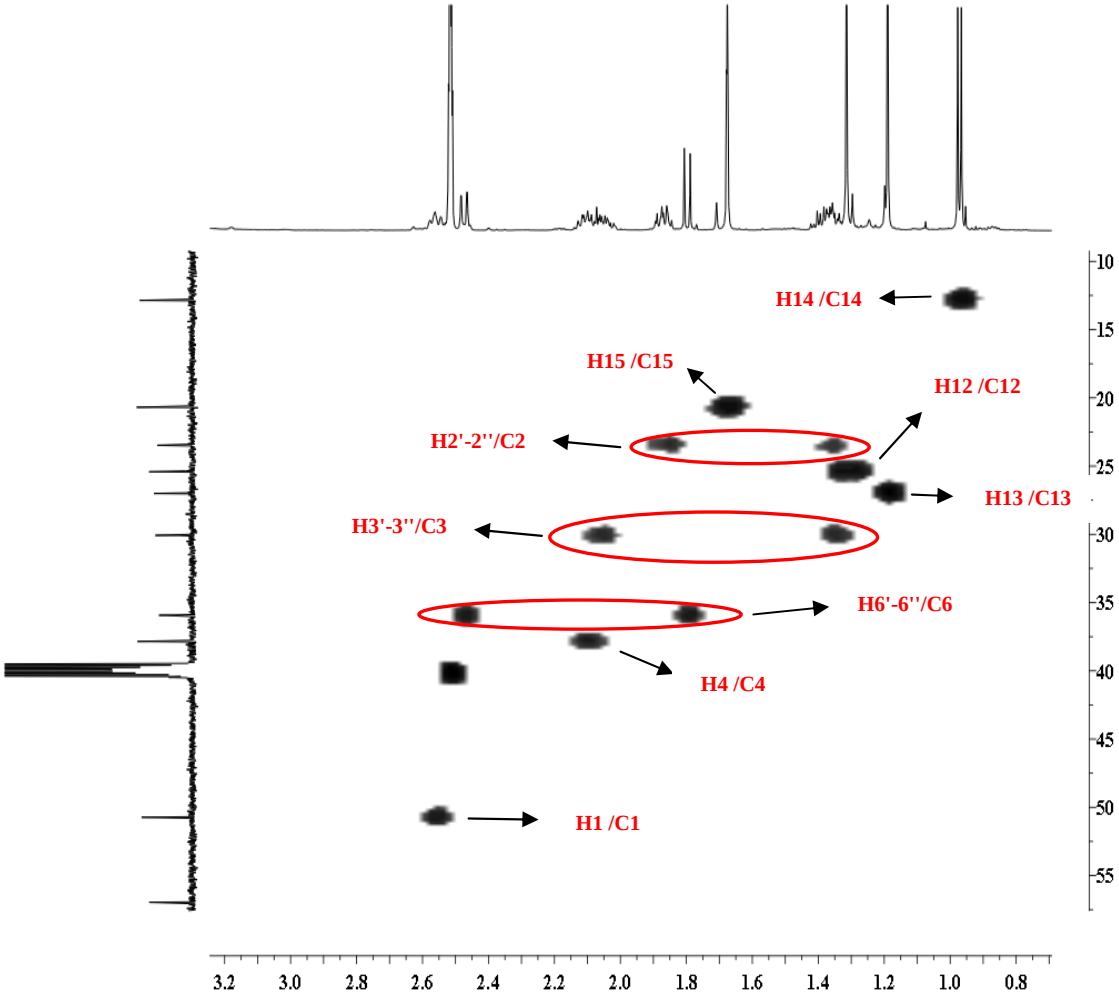


S6: ^{13}C-NMR Spectrum of Compound **1 (**(1*R*,4*R*,5*S*,7*S*)-curwenyujinone)

(From 10 to 70 ppm)

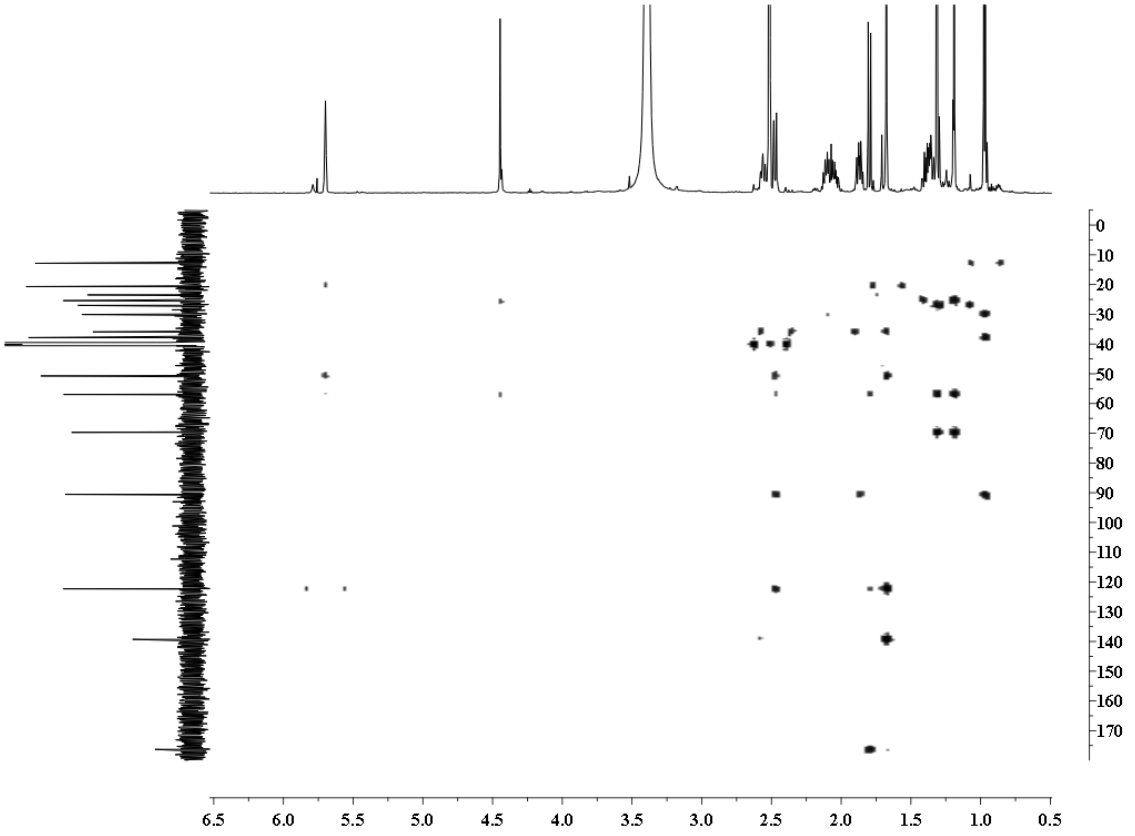


S7: HSQC (600 MHz) Spectrum of Compound **1 (**(1*R*,4*R*,5*S*,7*S*)-curwenyujinone)

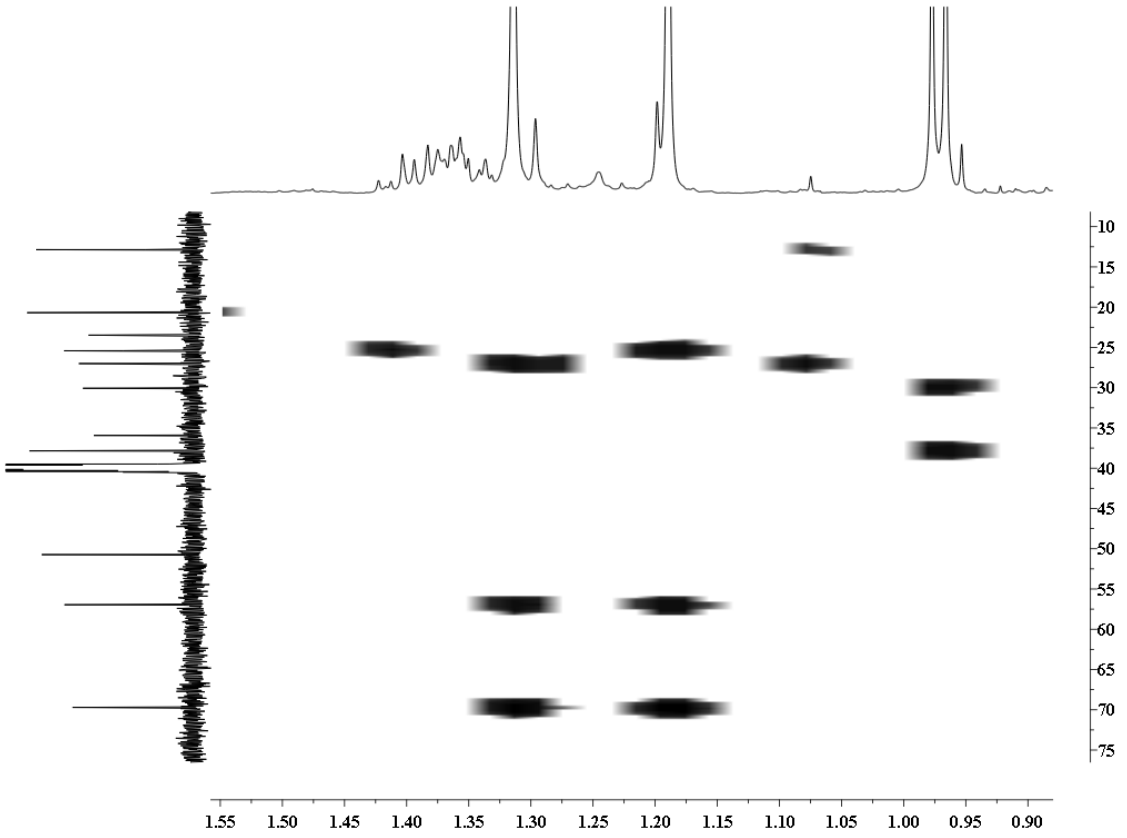


S8: HSQC (600 MHz) Spectrum of Compound **1 (**(1*R*,4*R*,5*S*,7*S*)-curwenyujinone)

(From 0.8 to 3.2 ppm)

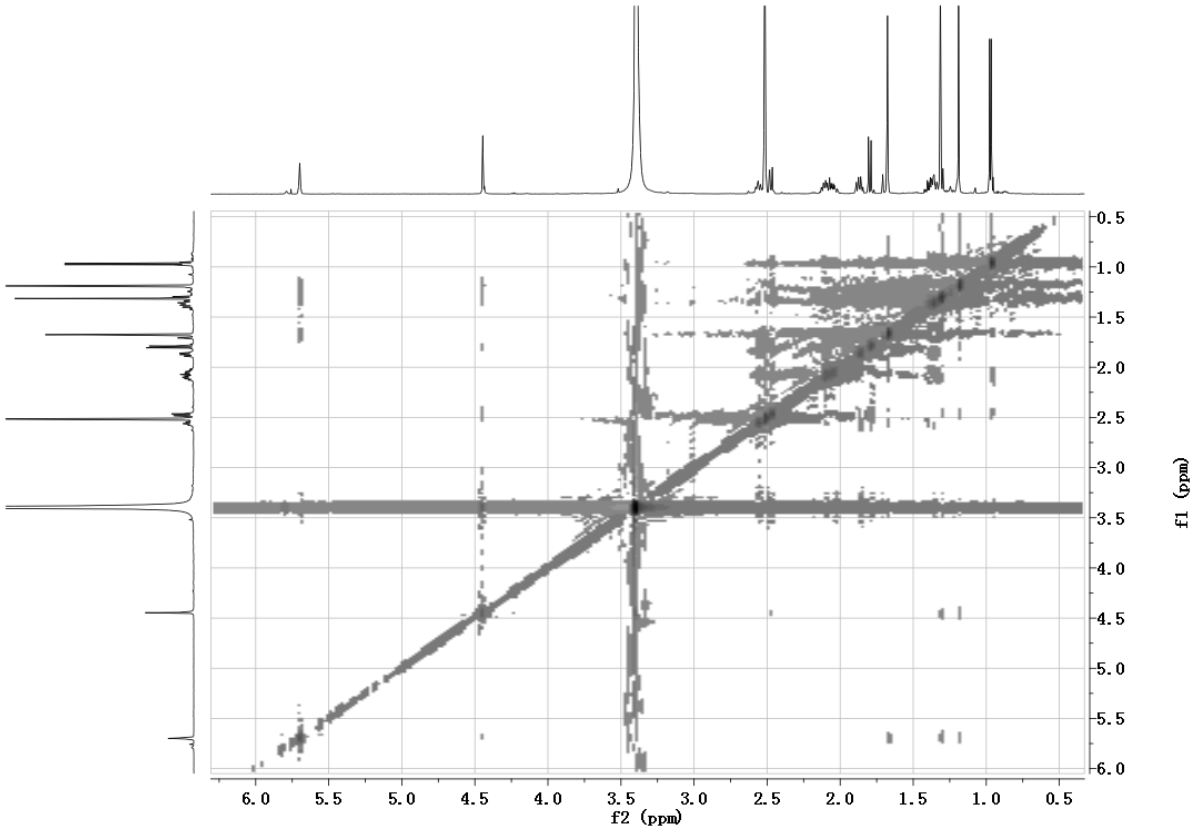


S9: HMBC (600MHz) Spectrum of Compound **1 (**(1*R*,4*R*,5*S*,7*S*)-curwenyujinone)

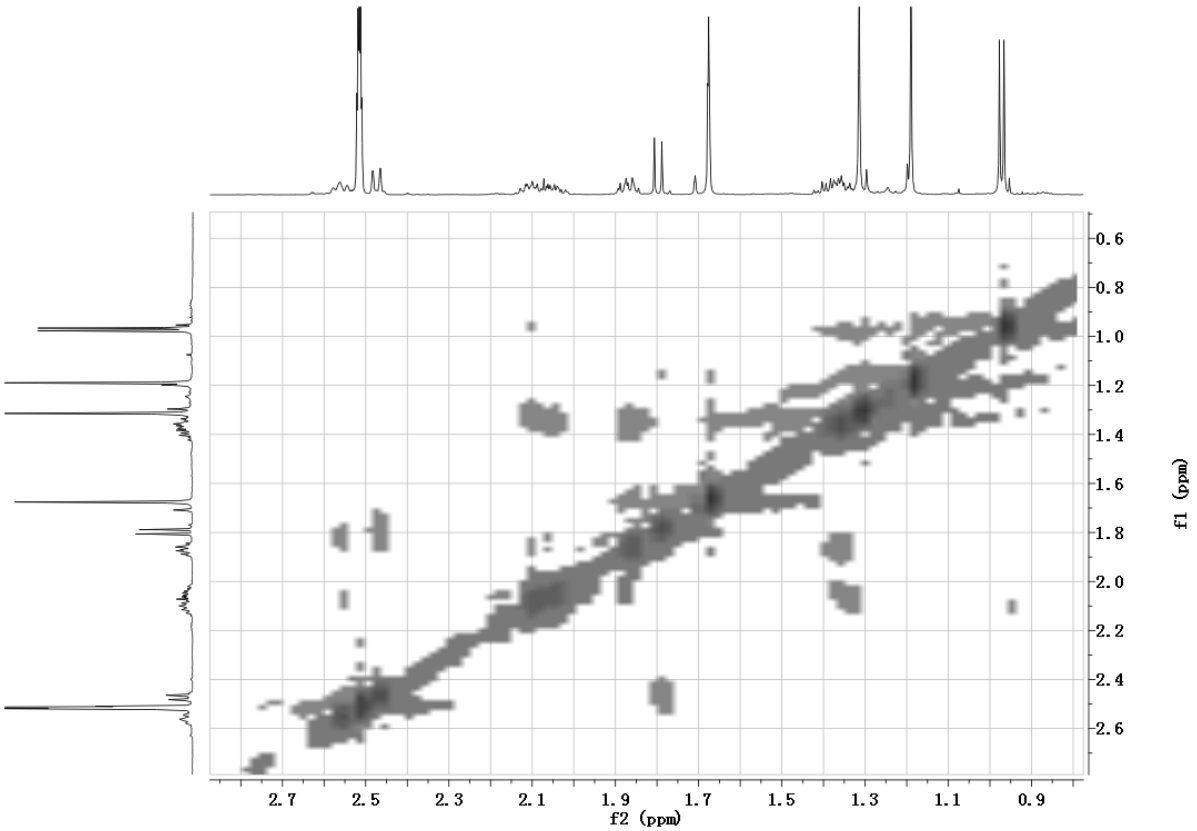


S10: HMBC Spectrum of Compound **1 (**(1*R*,4*R*,5*S*,7*S*)-curwenyujinone)

(From 10 to 75 ppm)

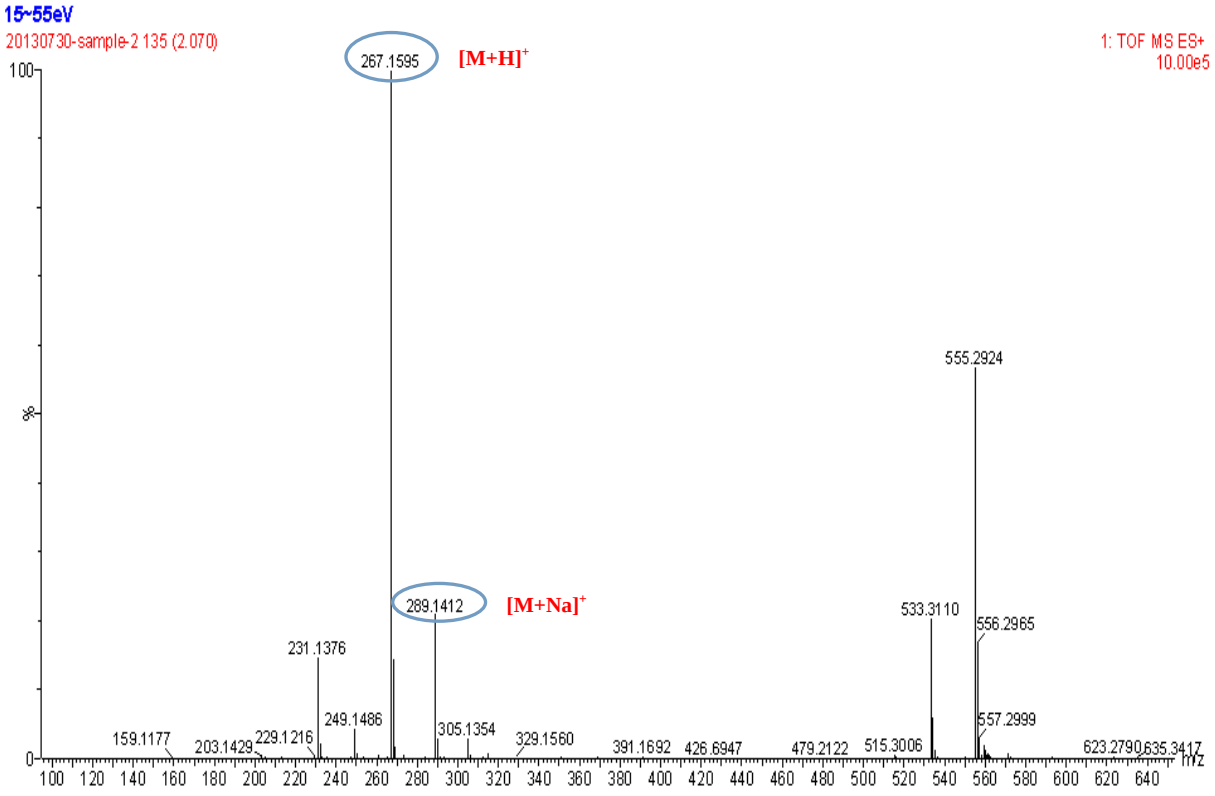


S11: NOESY (600MHz) Spectrum of Compound **1 (**(1*R*,4*R*,5*S*,7*S*)-curwenyujinone)

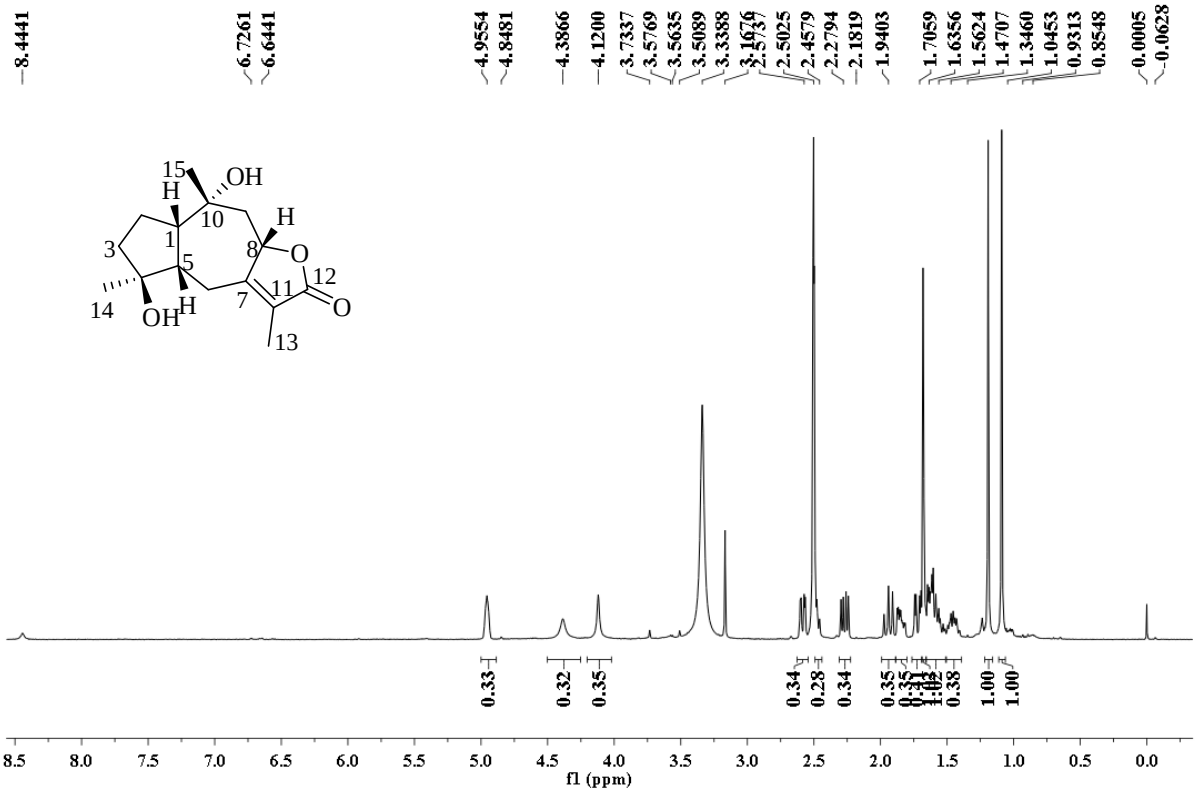


S12: NOESY (600MHz) Spectrum of Compound **1 (**(1*R*,4*R*,5*S*,7*S*)-curwenyujinone)

(From 0.9 to 2.8 ppm)

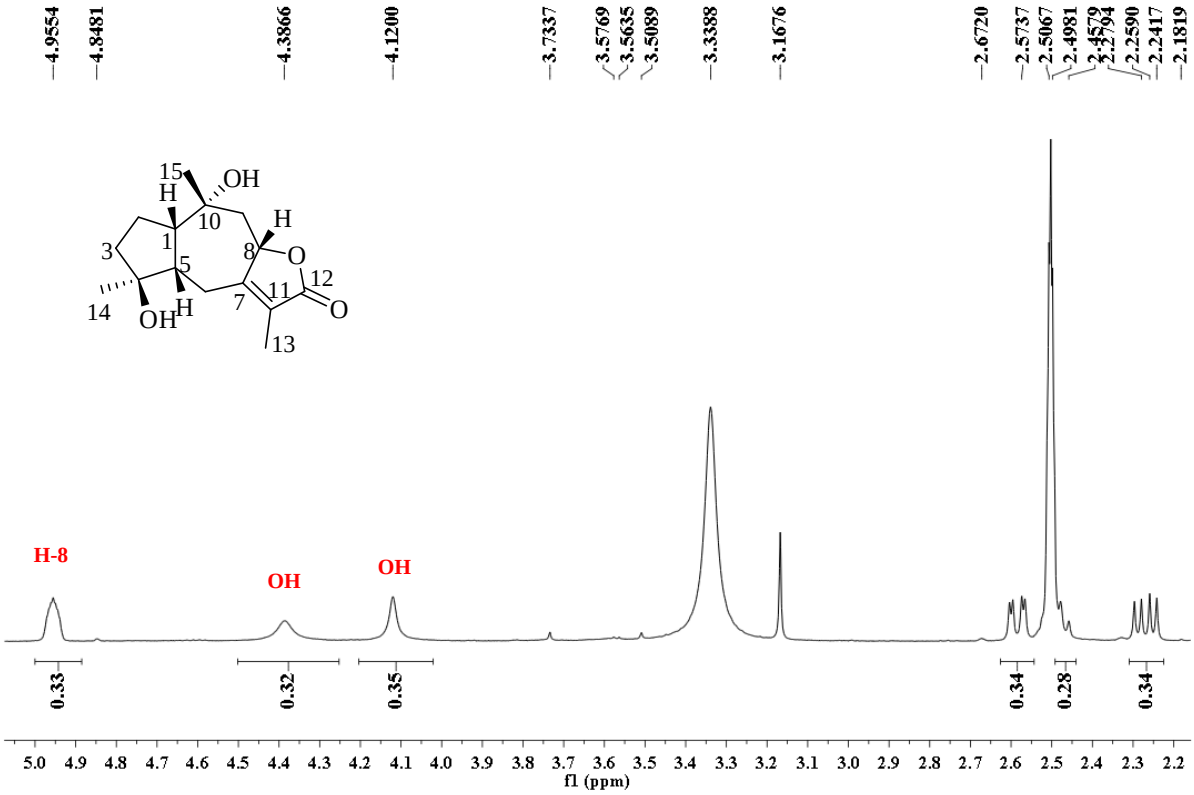


S13: HRESI-MS Spectrum of Compound **2 Z**edoalactone H

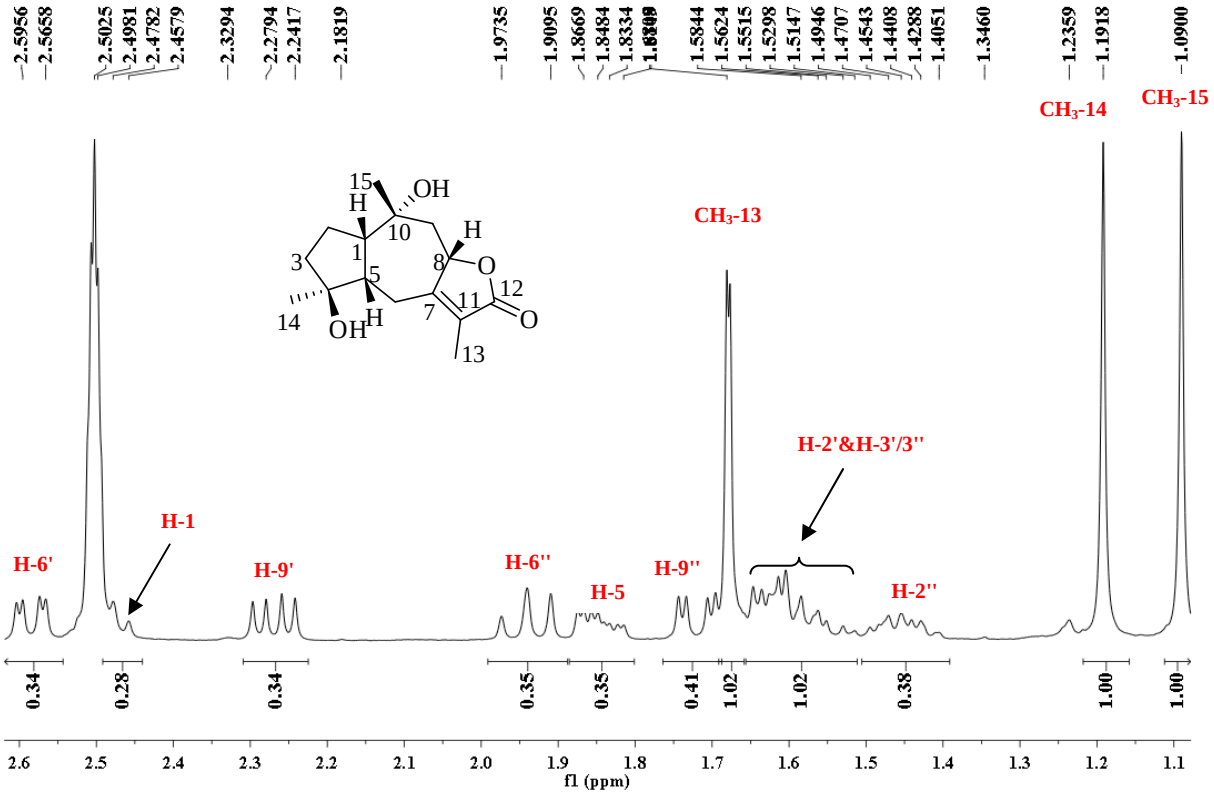


S14: ^{1}H-NMR (600MHz, DMSO-d_6) Spectrum of Compound **2** Zedoalactone H

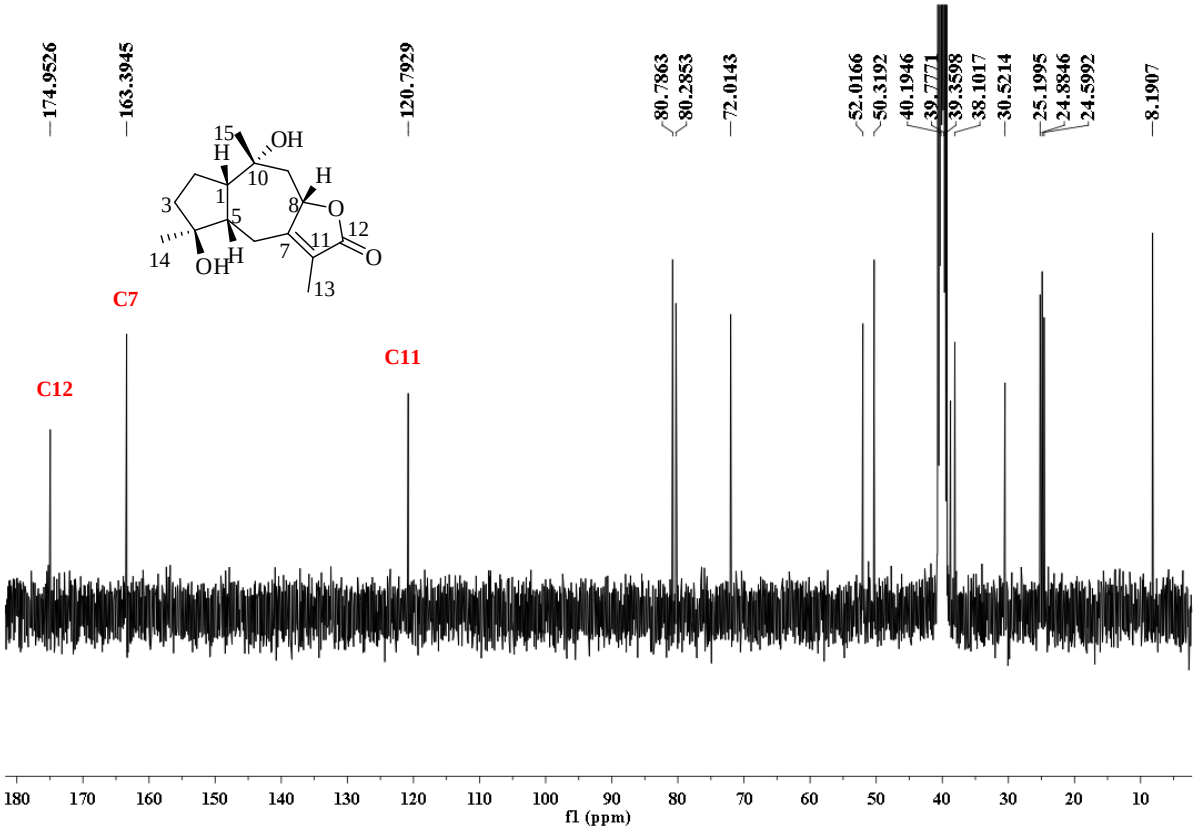
Zedoalactone H (2): colourless oil, ^{1}H-NMR (600 MHz, DMSO-d_6), δ: 4.97 (1H, m, H-8), 4.40 (1H, br s, OH), 4.13 (1H, br s, OH), 2.60 (1H, dd, 3.6, 12.0, H-6), 2.50 (1H, dd, 7.8, 10.4, H-1), 2.28 (1H, dd, 7.2, 15.0, H-9), 1.95 (1H, t, 12.6, H-6), 1.86 (1H, ddd, 3.6, 7.8, 13.8, H-5), 1.73 (1H, dd, 3.6, 15.6, H-9), 1.69 (3H, d, 1.8, H-13), 1.65 (1H, m, H-2), 1.65 (1H, m, H-3), 1.58 (1H, m, H-3), 1.47 (1H, m, H-2), 1.20 (3H, s, H-14), 1.10 (3H, s, H-15). ^{13}C NMR (DMSO-d_6, 150 MHz): 52.0 (C-1), 24.9 (C-2), 38.1 (C-3), 80.3(C-4), 50.3 (C-5), 24.6 (C-6), 163.4(C-7), 80.8 (C-8), 38.8 (C-9), 72.0(C-10), 120.8(C-11), 175.0(C-12), 8.2 (C-13), 25.2(C-14), 30.5 (C-15).



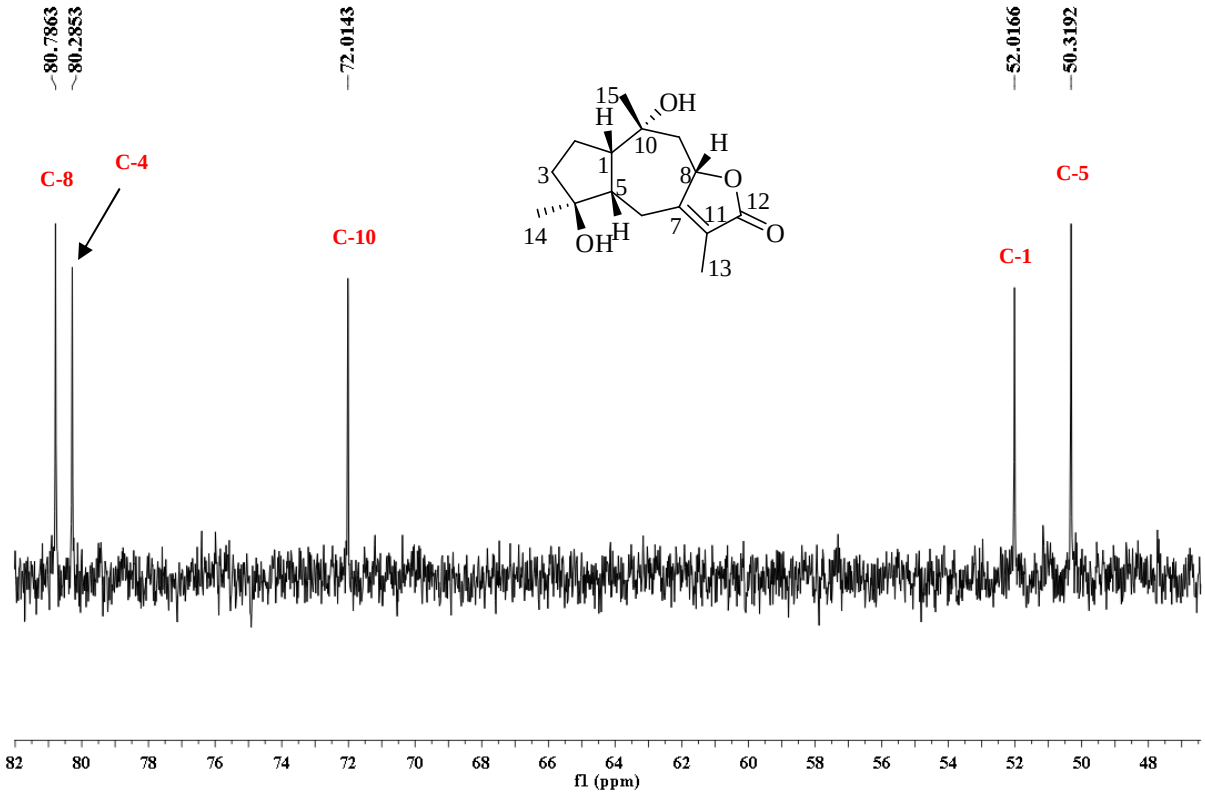
S15: ^{1}H-NMR Spectrum of Compound **2 Z**edoalactone H (From 2.20 to 5.00 ppm)



S16: [1]H-NMR Spectrum of Compound **2** Zedoalactone H (From 1.10 to 2.60 ppm)

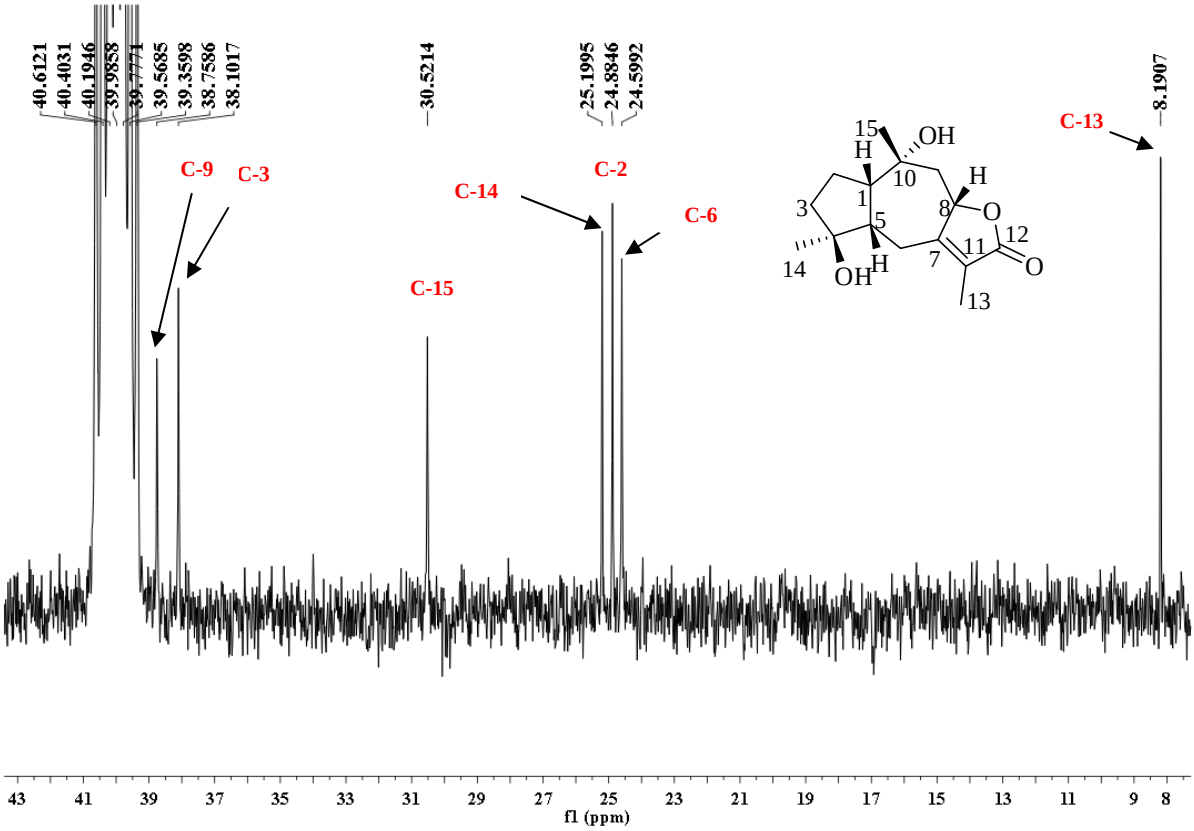


S17: ^{13}C-NMR (150MHz, DMSO-d_6) Spectrum of Compound **2** Zedoalactone H



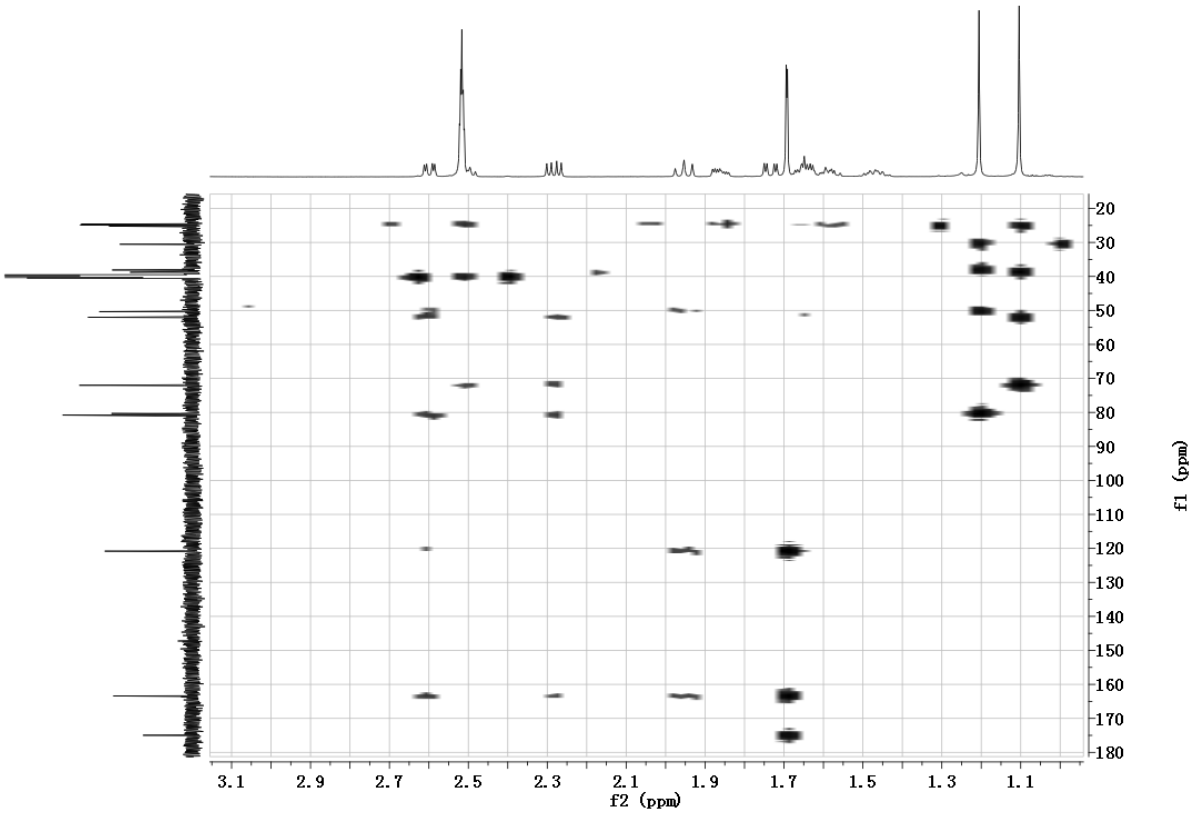
S18: ^{13}C-NMR (150MHz, DMSO-d_6) Spectrum of Compound **2** Zedoalactone H

(From 47 to 82 ppm)

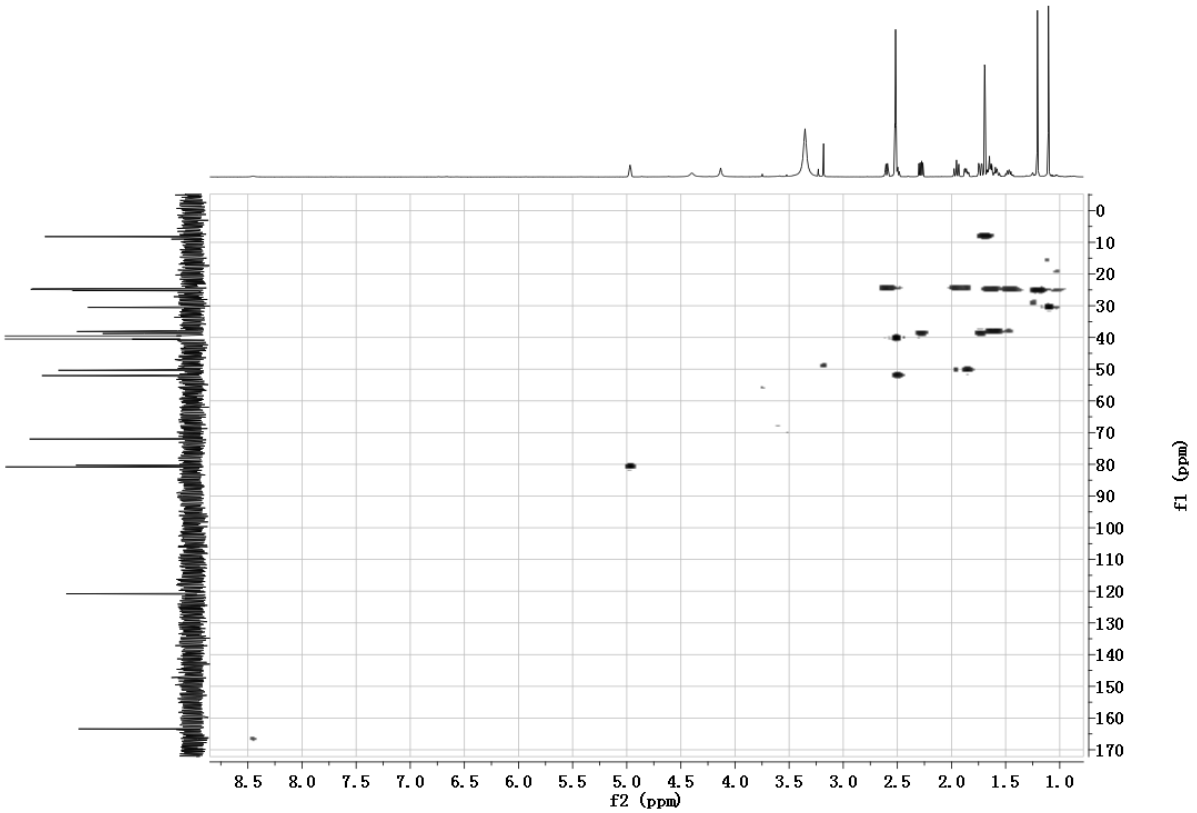


S19: ^{13}C-NMR (150MHz, DMSO-d_6) Spectrum of Compound **2** Zedoalactone H

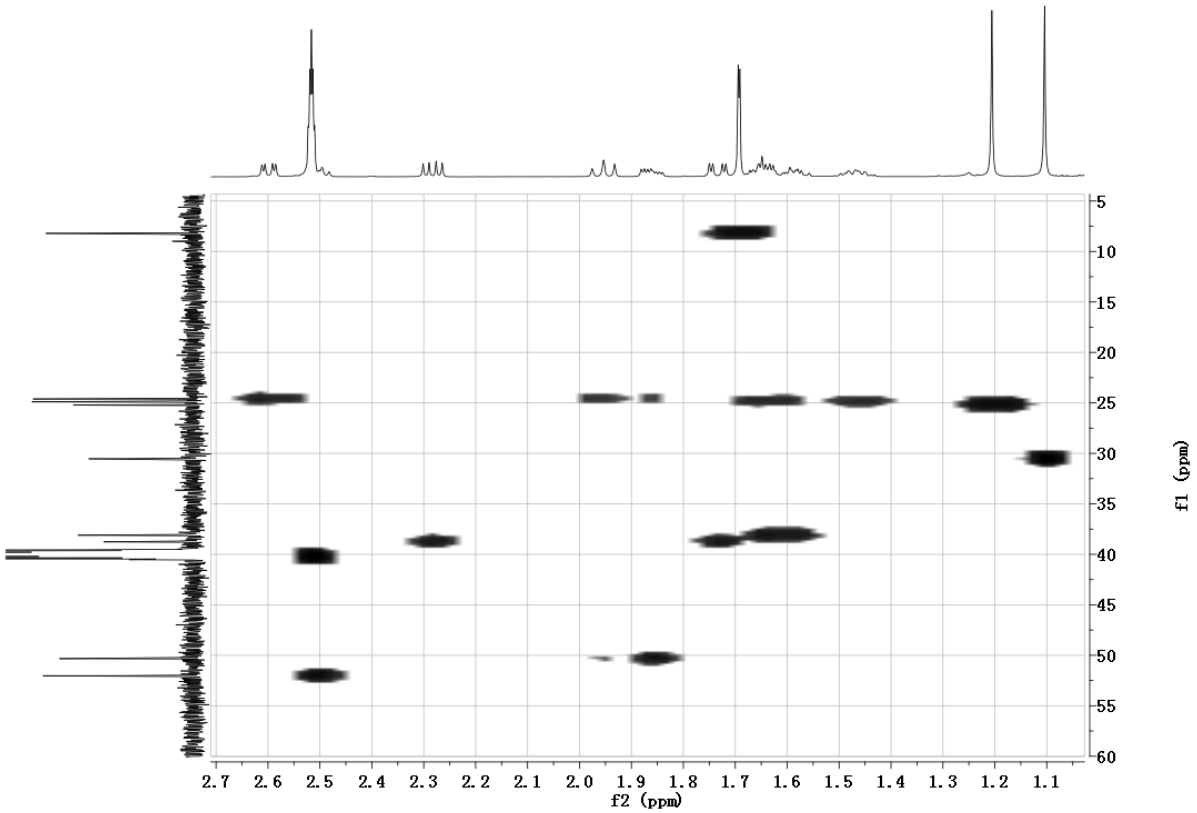
(From 8 to 43 ppm)



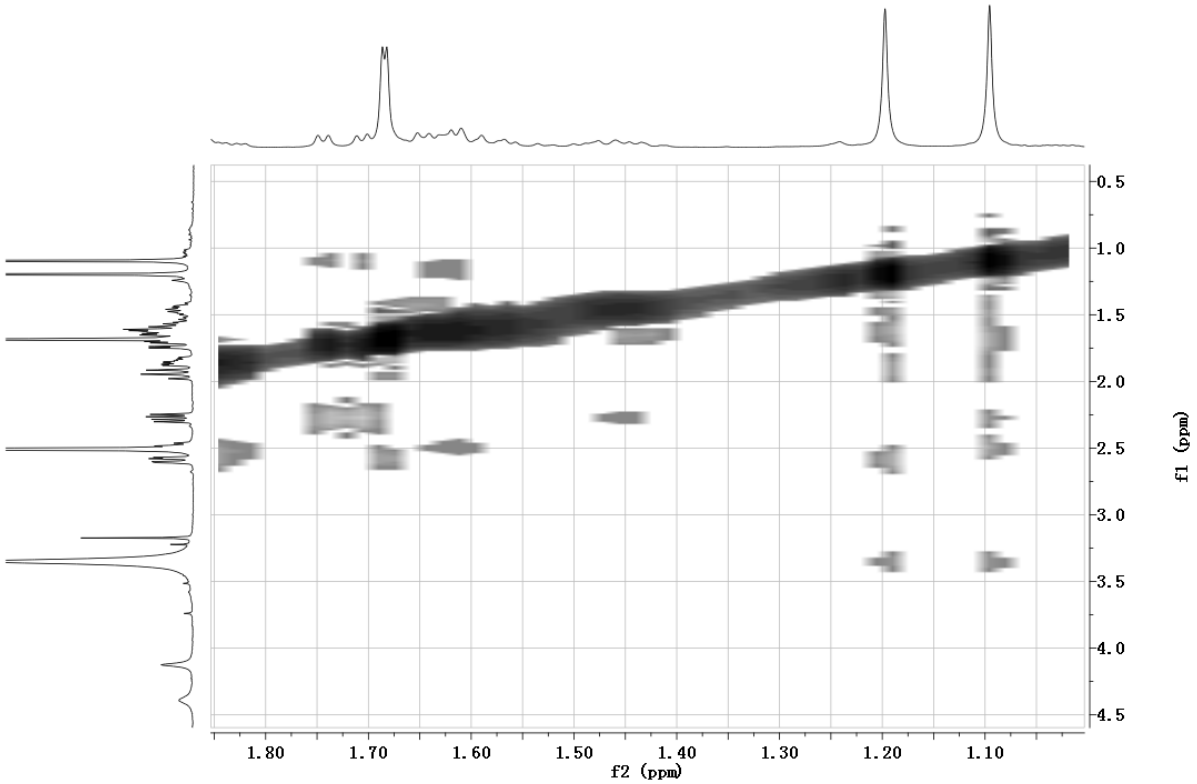
S20: HSQC (600 MHz) Spectrum of Compound **2** Zedoalactone H



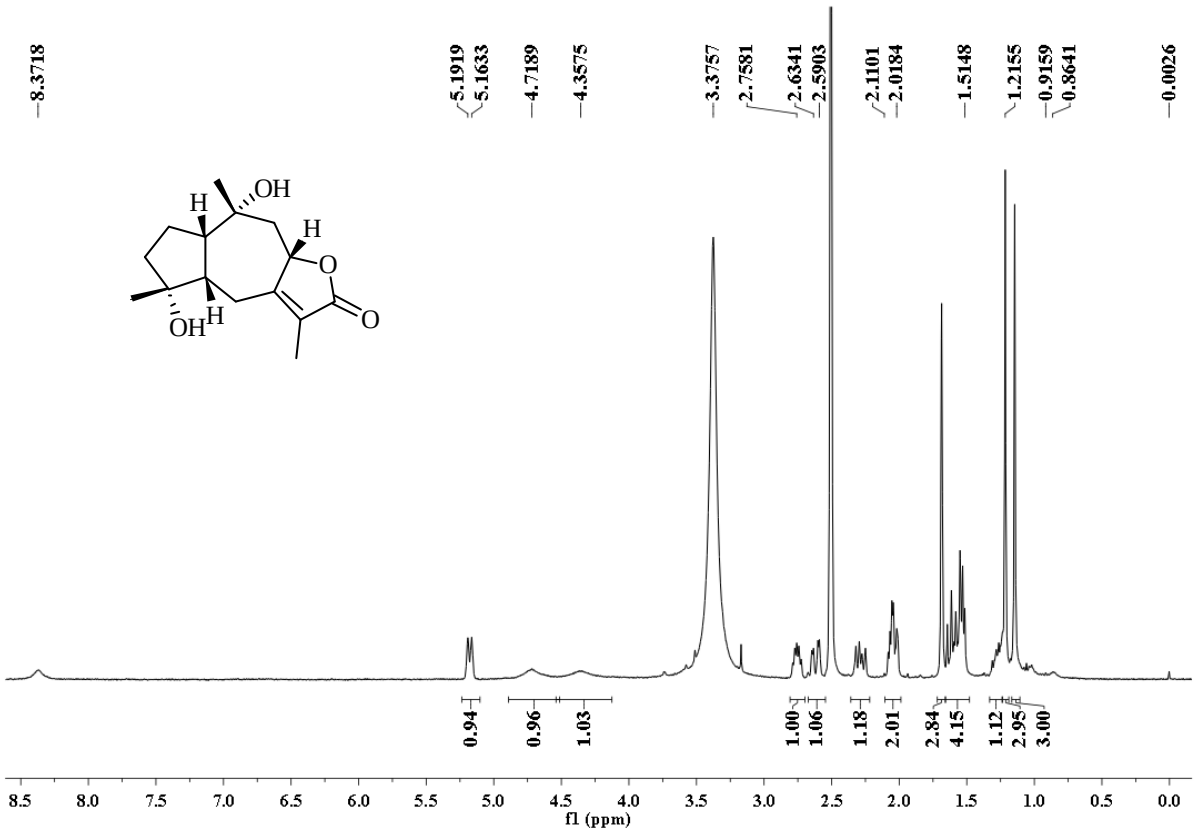
S21: HMBC (600 MHz) Spectrum of Compound **2** Zedoalactone H



S22: HMBC (600 MHz) Spectrum of Compound **2** Zedoalactone H (From 5 to 60 ppm)

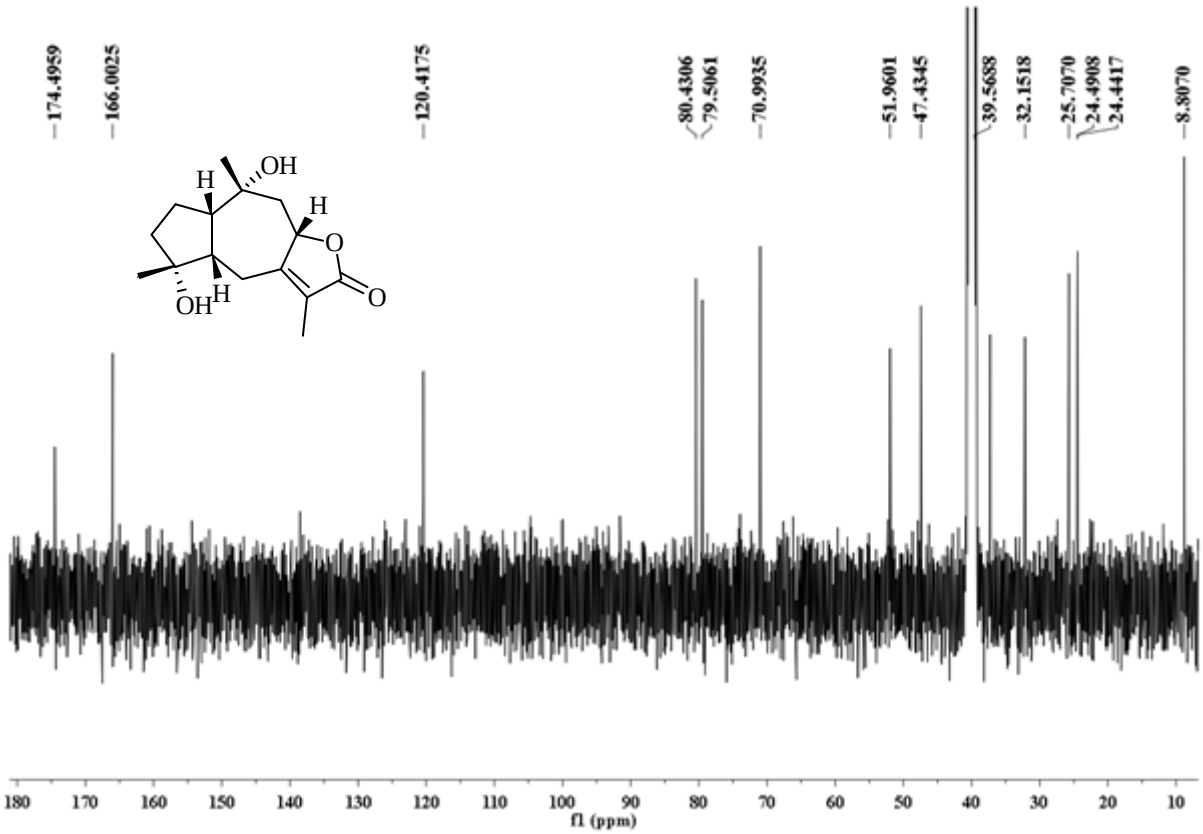


S23: NOESY (600MHz) Spectrum of Compound **2** Zedoalactone H

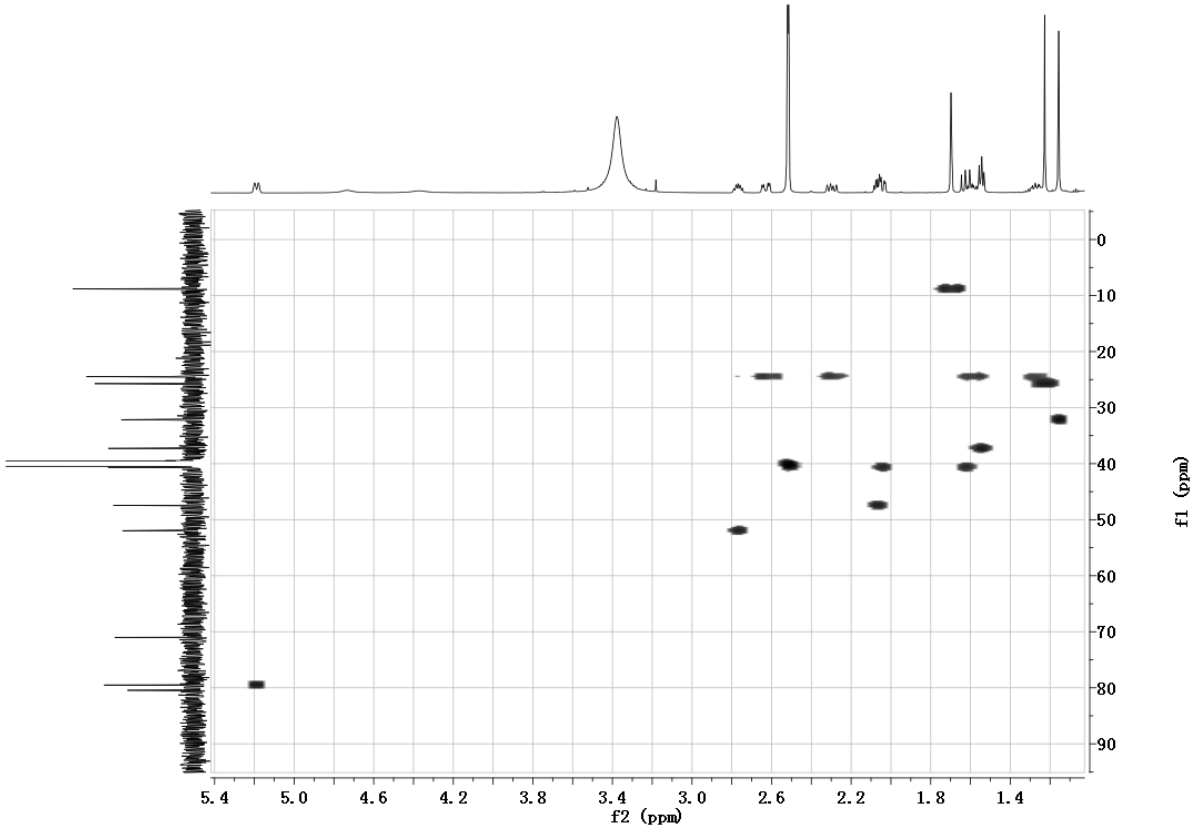


S24: ^{1}H-NMR (600MHz, DMSO-d_6) Spectrum of Compound **3** Zedoalactone E

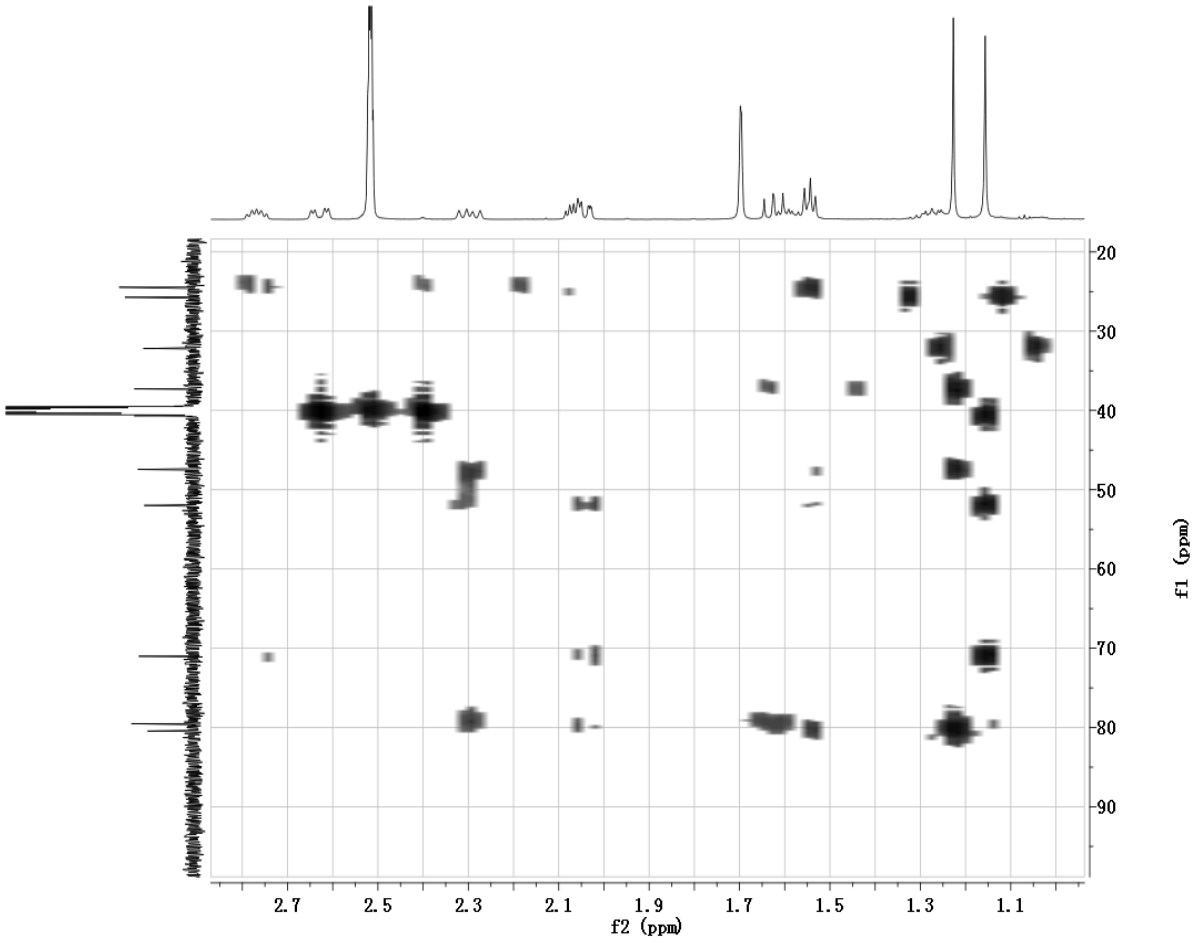
Zedoalactone E (3): colourless oil, ^{1}H-NMR (600 MHz, DMSO-d_6), δ: 5.19 (1H, d, 10.8, H-8), 4.73 (1H, br s, OH), 4.37 (1H, br s, OH), 2.77 (1H, m, H-1), 2.63 (1H, dd, 18.0, 4.8, H-6), 2.30 (1H, dd, 10.2, 18.0, H-6), 2.07 (1H, dd, 4.8, 10.2, H-5), 2.04 (1H, ddd, 1.8, 3.6, 10.2, H-9), 1.70 (3H, s, H-13), 1.62 (1H, dd, 11.4, 13.2, H-9), 1.59 (1H, m, H-2), 1.54 (2H, t, 7.8, 6.7, H-3), 1.27 (1H, m, H-2), 1.23 (3H, s, H-14), 1.16 (3H, s, H-15). ^{13}C NMR (DMSO-d_6, 150 MHz): 52.0 (C-1), 24.5 (C-2), 37.3(C-3), 80.4 (C-4), 47.4 (C-5), 24.5 (C-6), 166.0(C-7), 79.5 (C-8), 40.7 (C-9), 71.0(C-10), 120.4(C-11), 174.5(C-12), 8.8(C-13), 25.7(C-14), 32.2(C-15). [15]



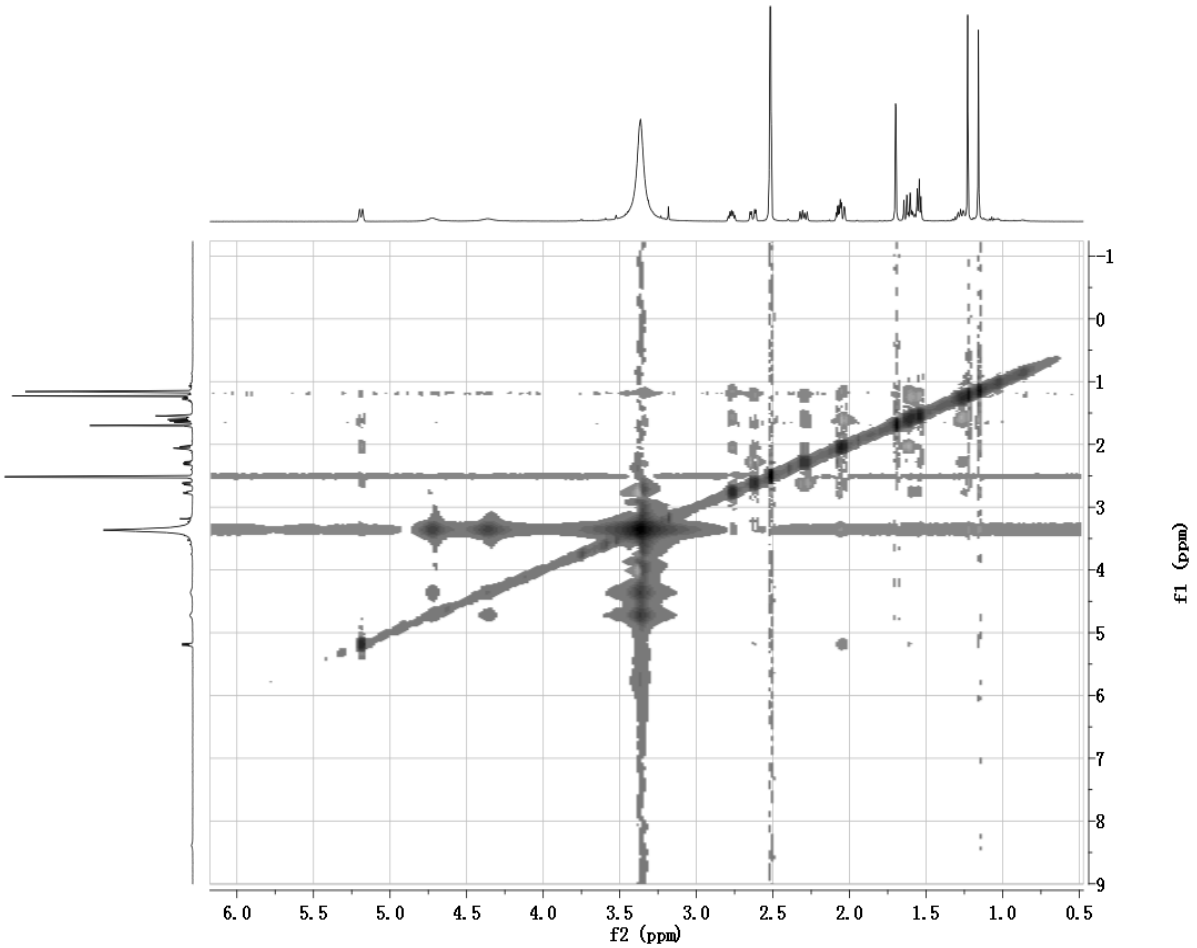
S25: ^{13}C-NMR (150MHz, DMSO-d_6) Spectrum of Compound **3 Z**edoalactone E



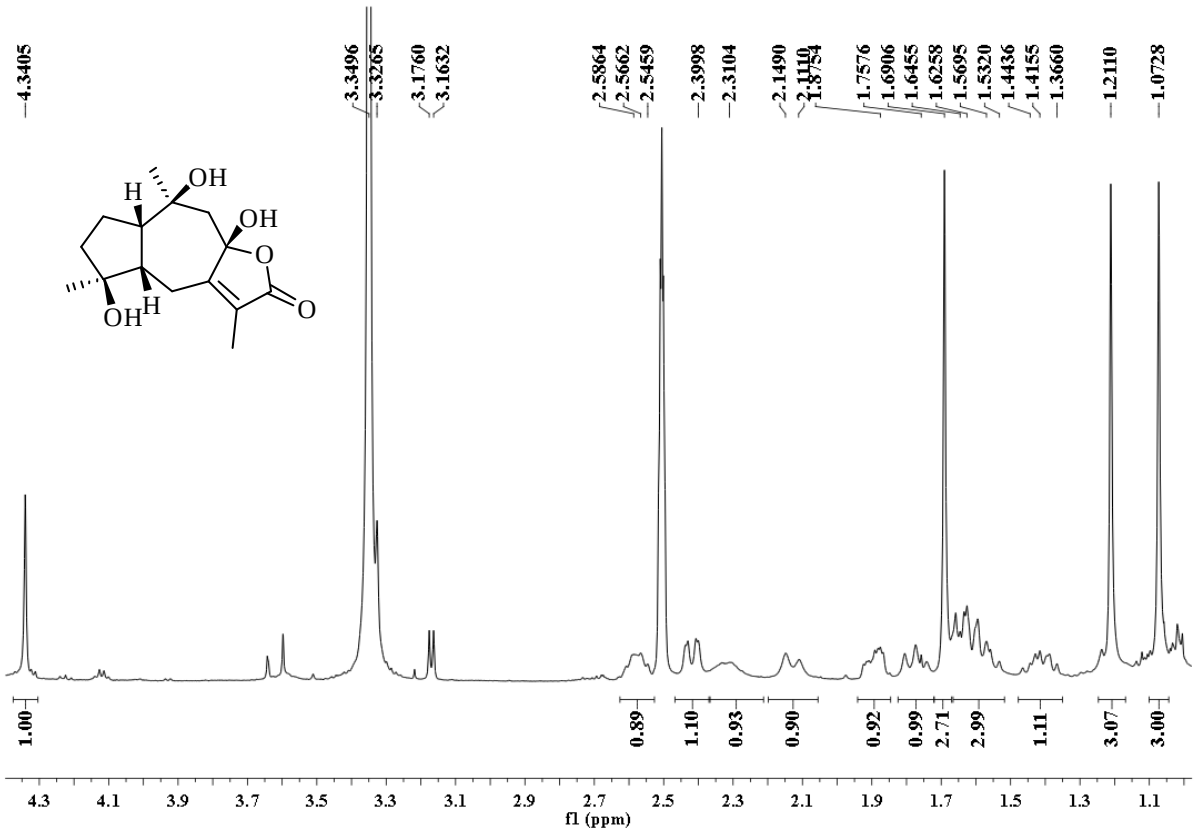
S26: HSQC (600 MHz) Spectrum of Compound **3** Zedoalactone E



S27: HMBC (600 MHz) Spectrum of Compound **3** Zedoalactone E

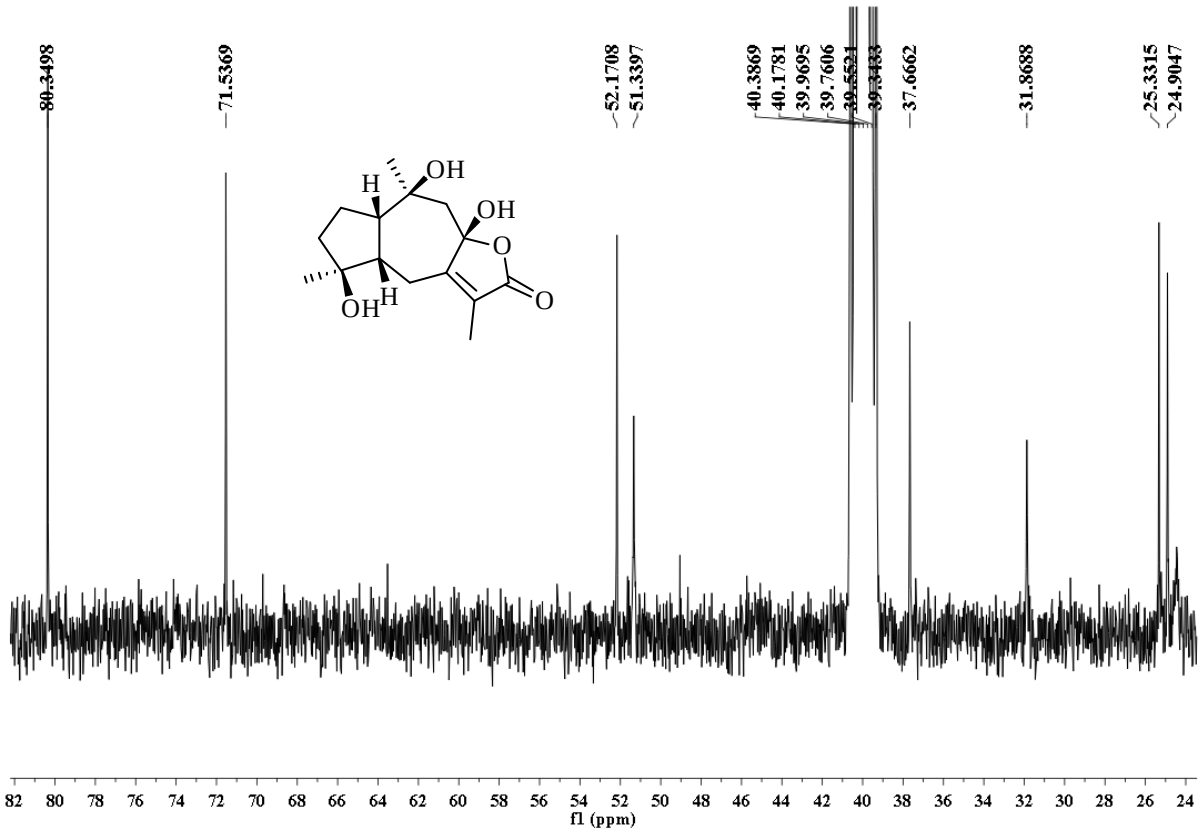


S28: NOESY (600 MHz) Spectrum of Compound **3** Zedoalactone E

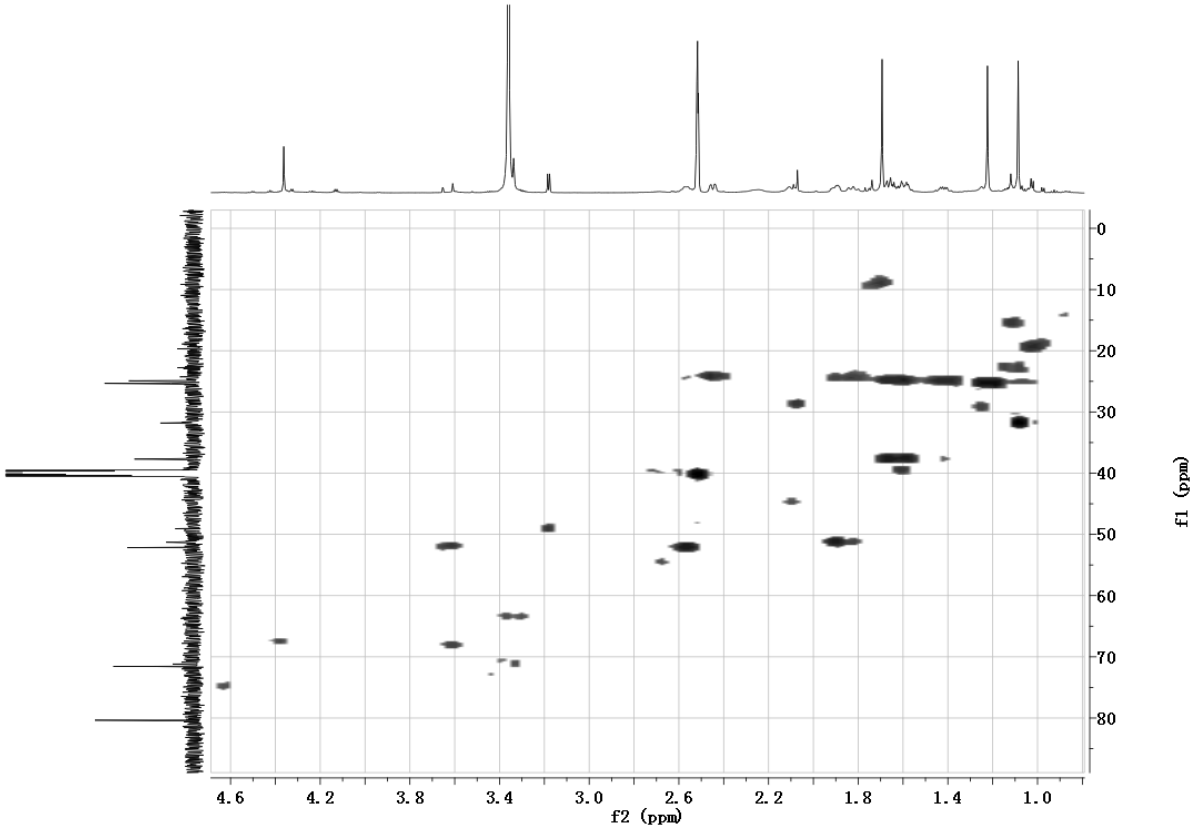


S29: ^{1}H-NMR (600MHz, DMSO-d_6) Spectrum of Compound **4** Zedoarolide B

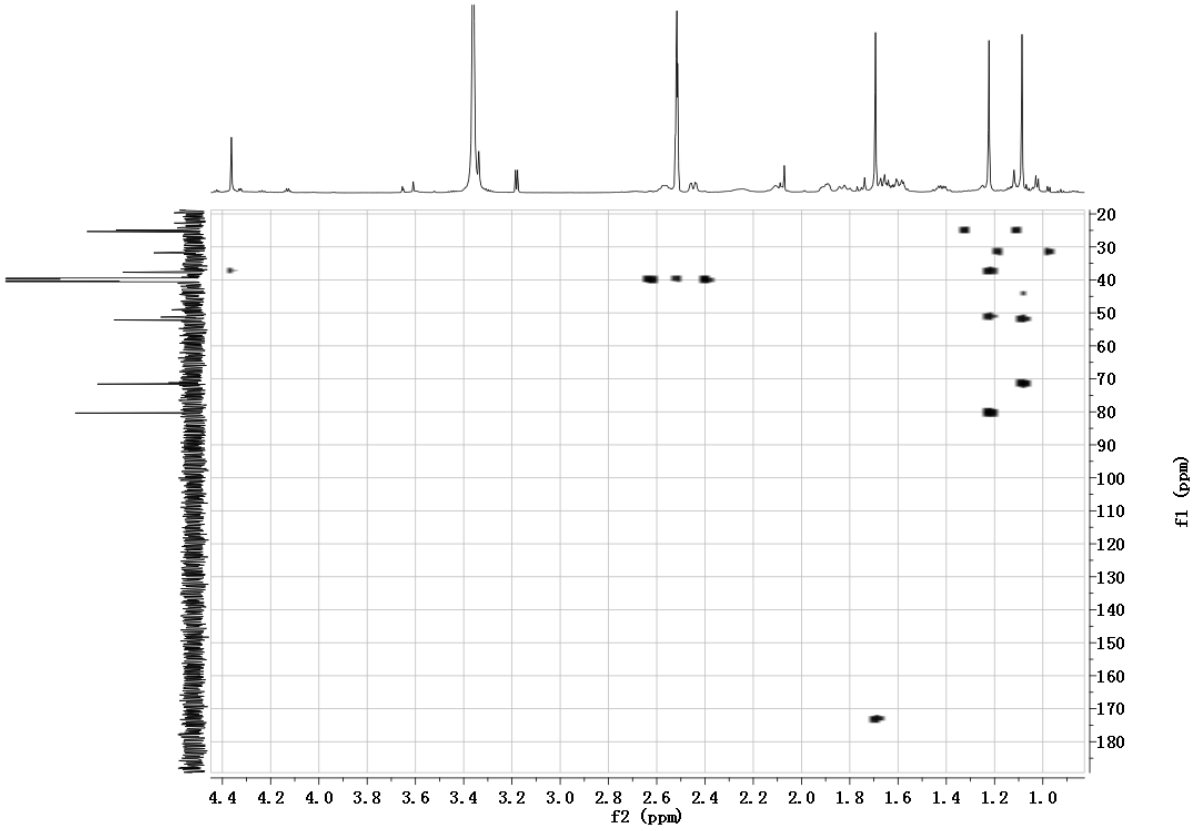
Zedoarolide B (4): colourless oil. ^{1}H-NMR (DMSO-d_6, 600 MHz): 4.34 (1H, s, OH-4); 2.52 (1H, m, H-1); 2.42 (1H, dd, 3.0, 12.0, H-6a); 1.75 (1H, m, H-6b); 1.88 (1H, m, H-5); 1.68 (3H, s, Me-13); 1.56~1.65 (2H, m, H-3); 1.40 (1H, m, H-2); 1.21 (3H, s, Me-14); 1.07 (3H, s, Me-15). ^{13}C-NMR (DMSO-d_6, 150MHz): 52.2 (C-1), 24.9 (C-2), 37.7 (C-3), 80.4 (C-4), 51.3 (C-5), 24.2 (C-6), 71.6 (C-10), 173.1 (C-12), 8.8 (C-13), 25.3 (C-14), 31.8 (C-15). [16]



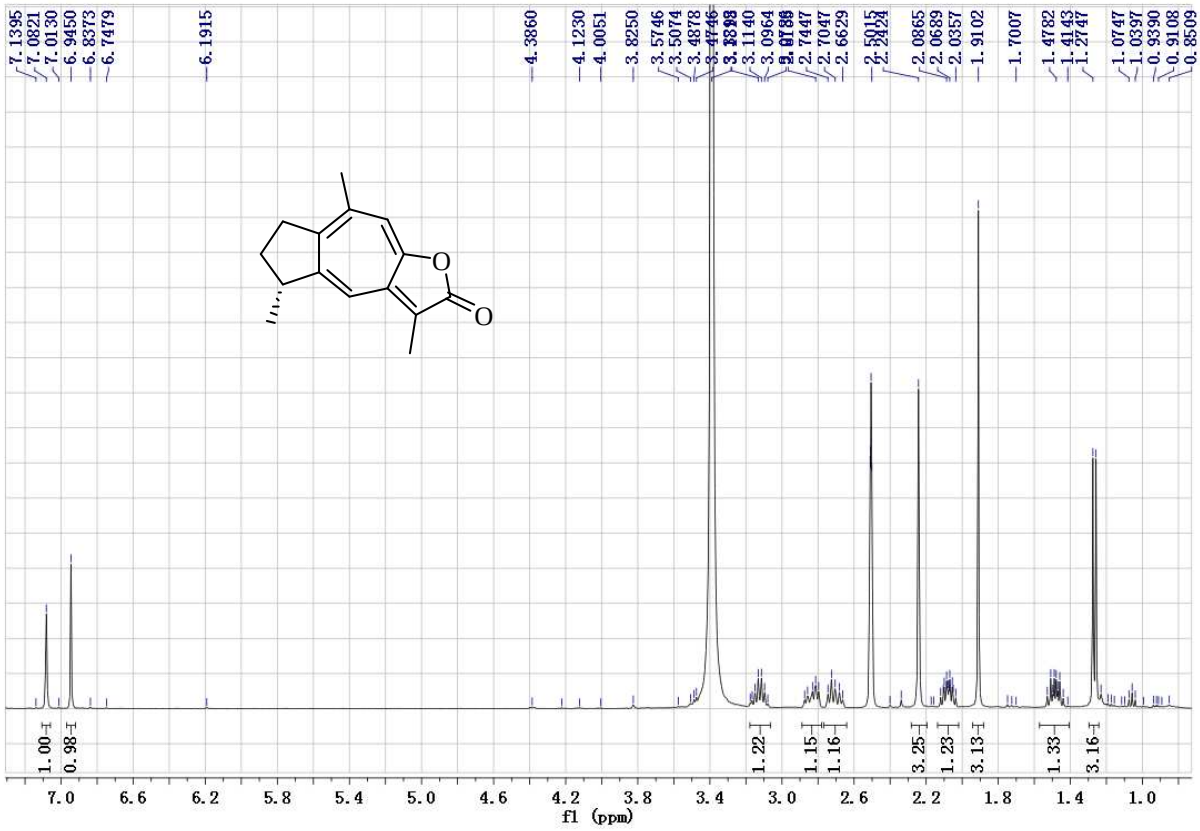
S30: ^{13}C-NMR (150MHz, DMSO-d_6) Spectrum of Compound **4** Zedoarolide B



S31: HSQC (600 MHz) Spectrum of Compound **4** Zedoarolide B

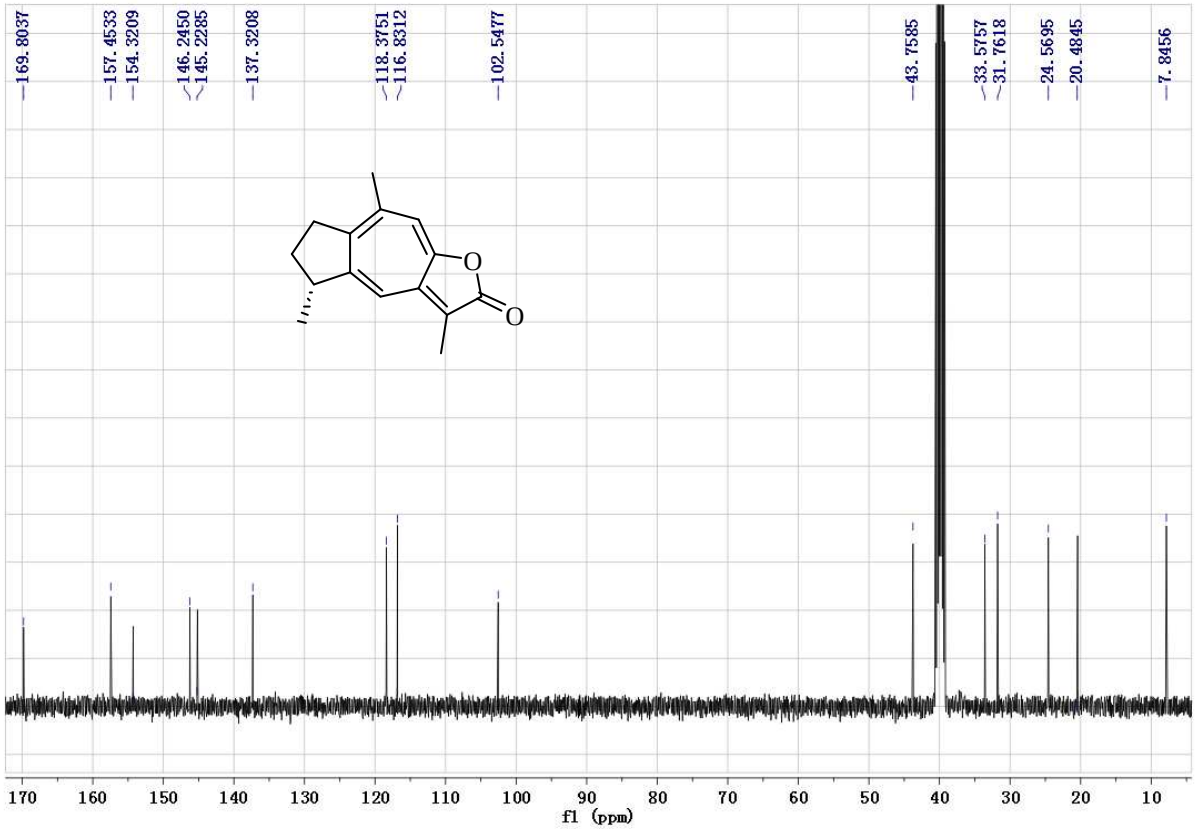


S32: HMBC (600 MHz) Spectrum of Compound **4** Zedoarolide B

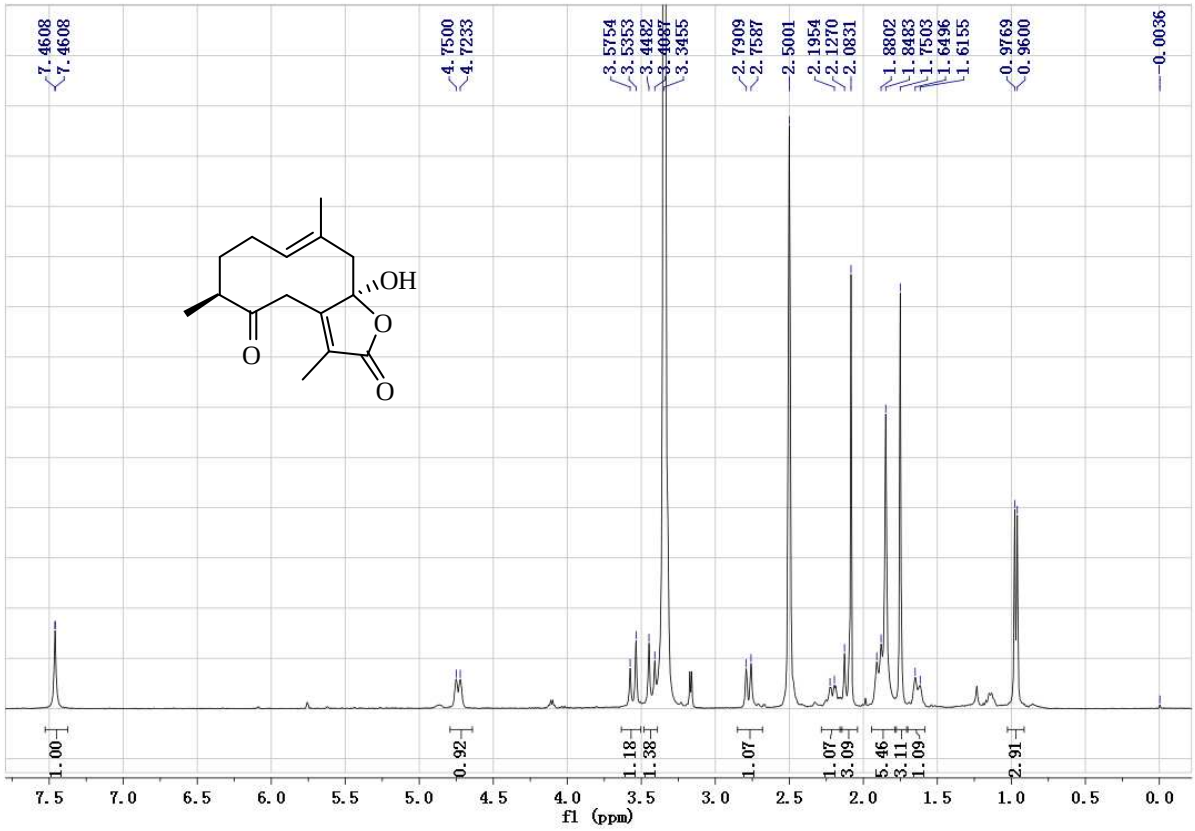


S33: ^{1}H-NMR (400MHz, DMSO-d_6) Spectrum of Compound 5 Gweicurculactone

Gweicurculactone (5): Orange red needle crystal. ^{1}H-NMR (DMSO-d_6, 400MHz): 7.09 (1H, s, H-6); 6.95 (1H, s, H-9); 3.14 (1H, m, H-4); 2.77 (2H, m, H-2); 2.08 (1H, m, H-3a); 2.25 (3H, s, Me-14); 1.92 (3H, s, Me-13); 1.49 (1H, m, H-3b); 1.27 (3H, d, 6.9, Me-15). ^{13}C-NMR (DMSO-d_6, 100 MHz): 145.2 (C-1), 33.6 (C-2), 31.8 (C-3), 43.8 (C-4), 157.5 (C-5), 118.4 (C-6), 146.2 (C-7), 154.3 (C-8), 116.8 (C-9), 137.3 (C-10),102.5 (C-11), 169.8 (C-12), 7.8 (C-13), 24.6 (C-14), 20.5 (C-15). [17]

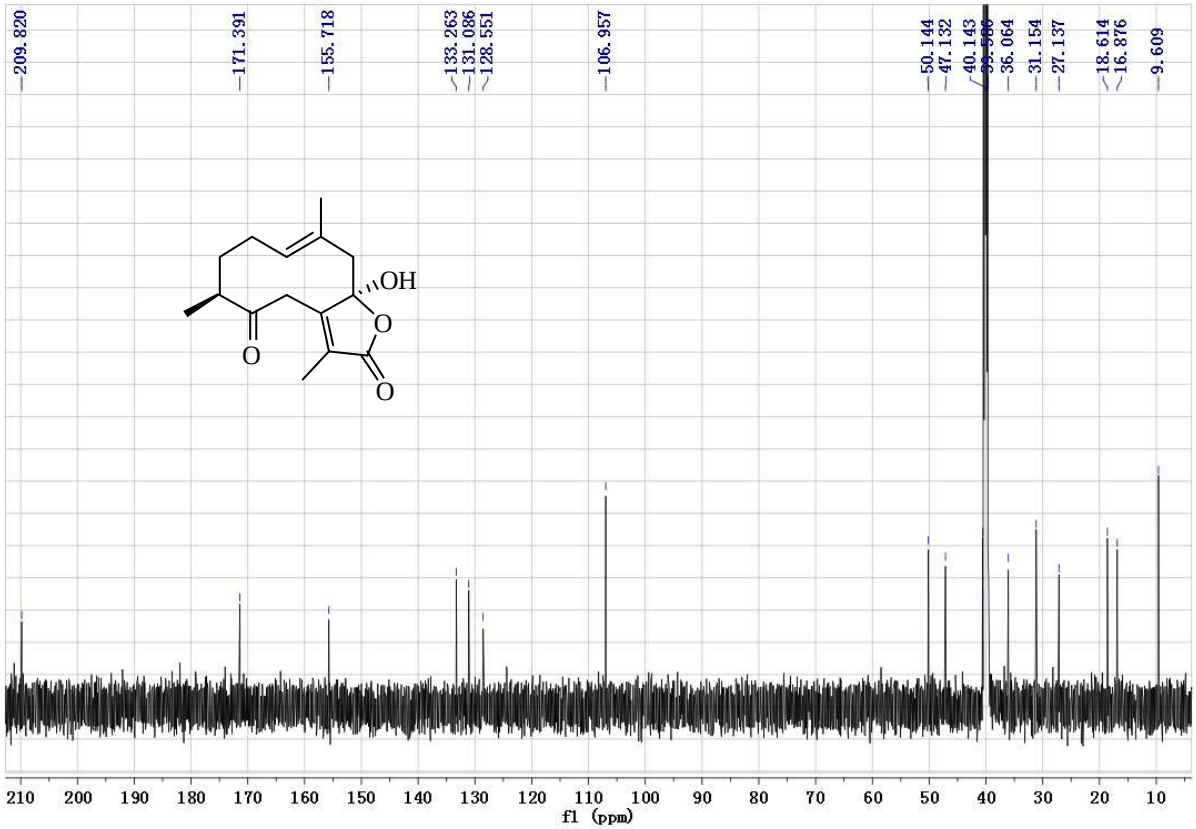


S34: ^{13}C-NMR (100MHz, DMSO-d_6) Spectrum of Compound **5** Gweicurculactone

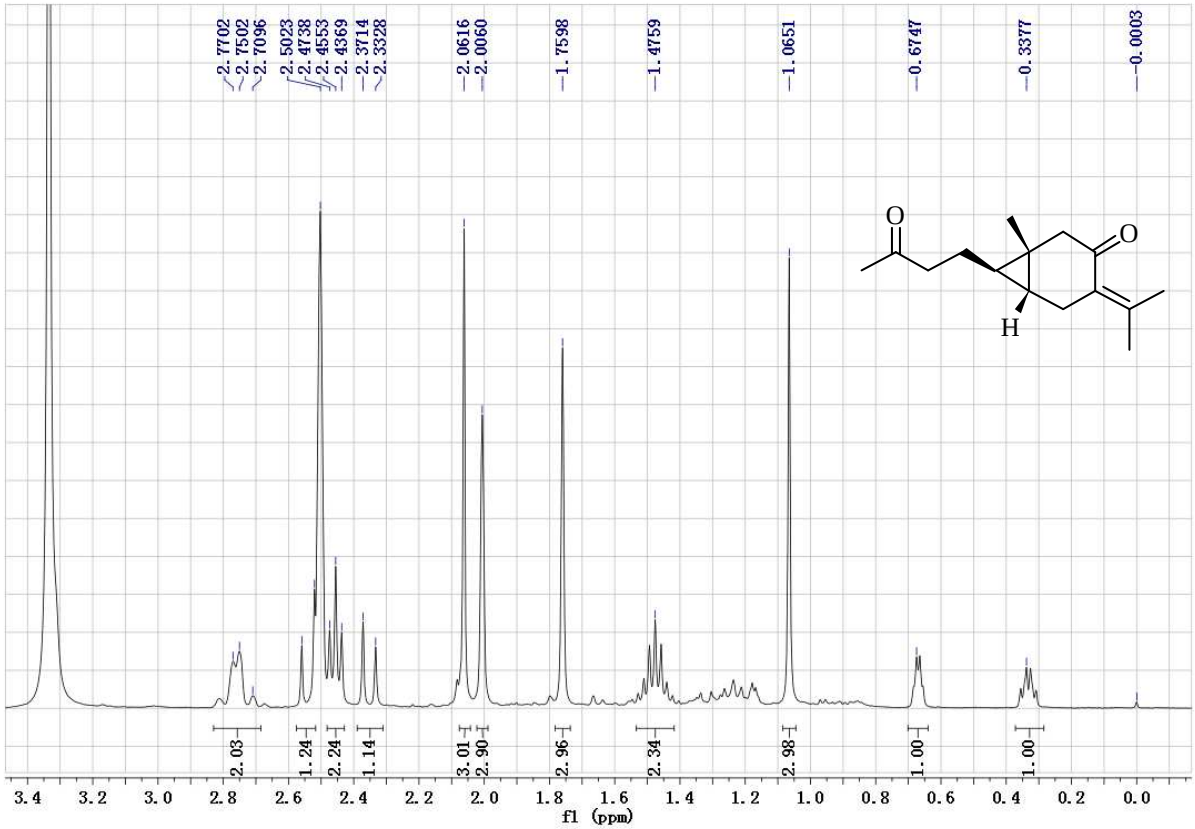


S35: ^{1}H-NMR (400 MHz, DMSO-d_6) Spectrum of Compound **6** Curdionolide A

Curdionolide A (6): colorless oil. ^{1}H-NMR(DMSO-d_6, 400 MHz): 7.49 (1H, br s, OH-8); 4.74 (1H, d, 10.8, H-1); 3.57 (1H, d, 15.6, H-6b); 3.44 (1H, d, 15.6, H-6a); 2.78 (1H, d, 13.2, H-9b); 2.49 (1H, m, H-4); 2.22 (1H, m, H-2b); 2.12 (1H, d, 13.2, H-9a); 1.90 (1H, m, H-2a); 1.87 (1H, m, H-3b); 1.86 (3H, s, Me-15); 1.77 (3H, s,Me-13); 1.64 (1H, m, H-3a); 0.98 (3H, d, J=6.6, Me-14). ^{13}C-NMR (DMSO-d_6, 100 MHz): 133.3 (C-1), 27.1 (C-2), 36.1 (C-3), 47.1 (C-4), 209.8 (C-5), 40.6 (C-6), 155.7 (C-7), 107.0 (C-8), 50.1 (C-9), 131.1 (C-10), 128.5 (C-11), 171.4 (C-12), 9.6 (C-13), 18.6 (C-14), 16.9 (C-15). [18]

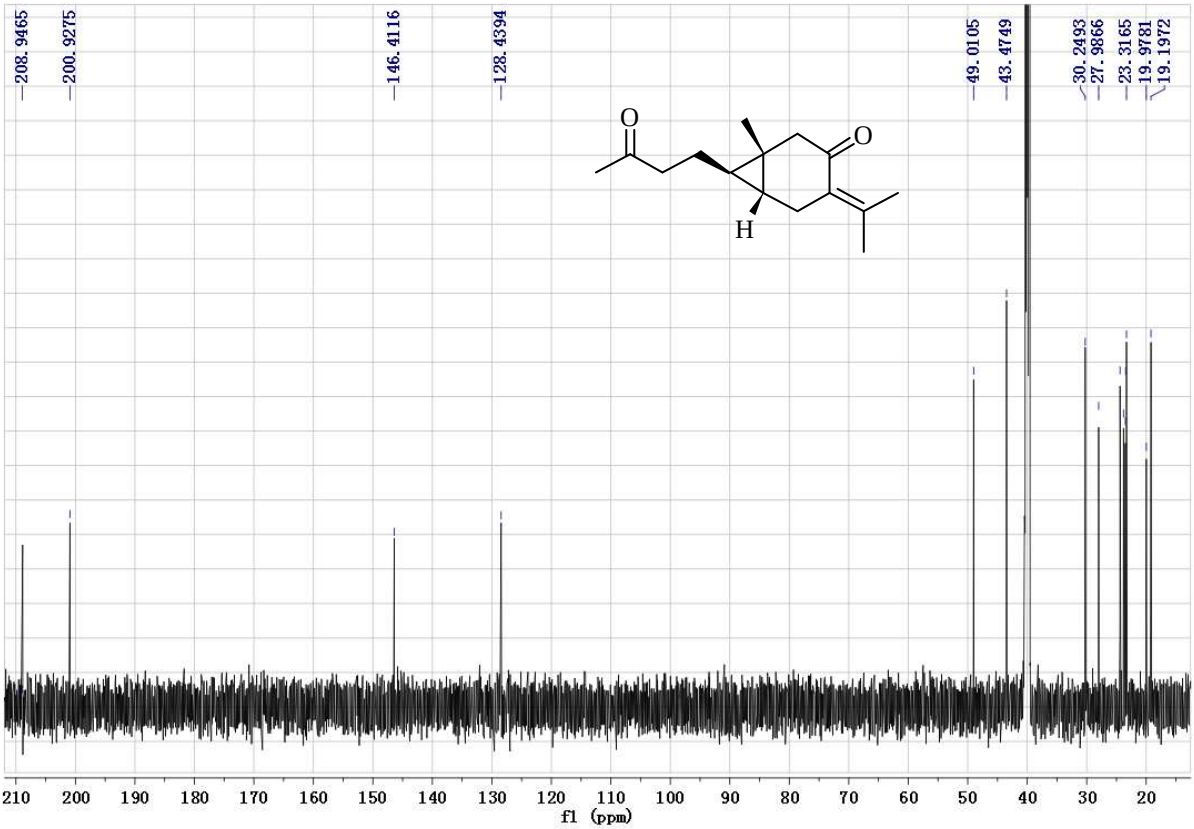


S36: ^{13}C-NMR (100MHz, DMSO-d_6) Spectrum of Compound **6** Curdionolide A

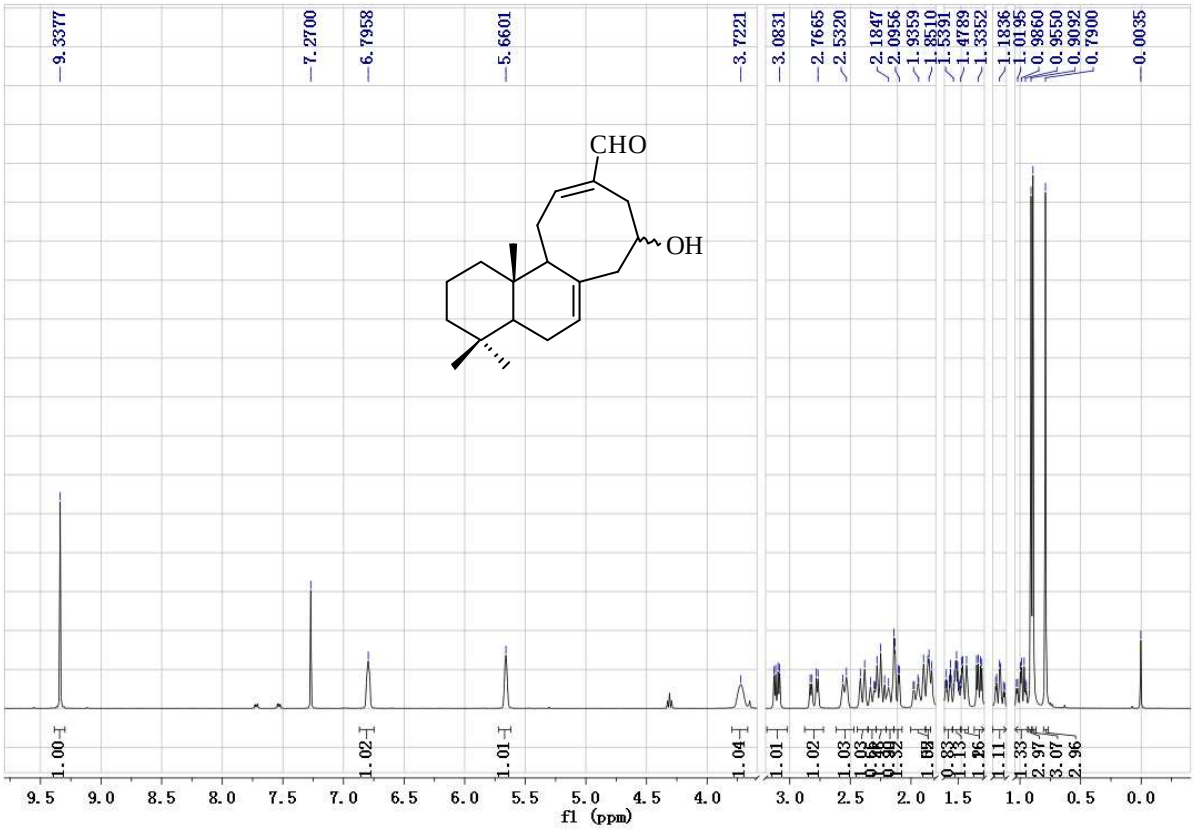


S37: ^{1}H-NMR (400 MHz, DMSO-d_6) Spectrum of Compound **7** Curcumenone

Curcumenone (7). colourless oil. ^{1}H-NMR (DMSO-d_6, 400 MHz): 0.34 (1H, m, H-1); 0.67 (1H, m, H-5); 1.07 (3H, s, Me-15); 1.48 (2H, m, H-2); 1.76 (3H, s, Me-13); 2.00 (3H, s, Me-12); 2.06 (3H, s, Me-14); 2.35 (1H, d, 15.4, H-9a); 2.48 (2H, t, 7.4, H-3); 2.54(1H, d, 15.4, H-9b); 2.74(2H, m, H-6). ^{13}C-NMR (DMSO-d_6, 100 MHz): 24.4 (C-1), 23.3 (C-2), 43.5 (C-3), 208.9 (C-4), 23.8 (C-5), 28.0 (C-6), 128.4 (C-7), 200.9 (C-8), 49.0 (C-9), 20.0 (C-10), 146.4 (C-11), 23.5 (C-12), 23.5 (C-13), 30.2 (C-14), 19.2 (C-15). [19]

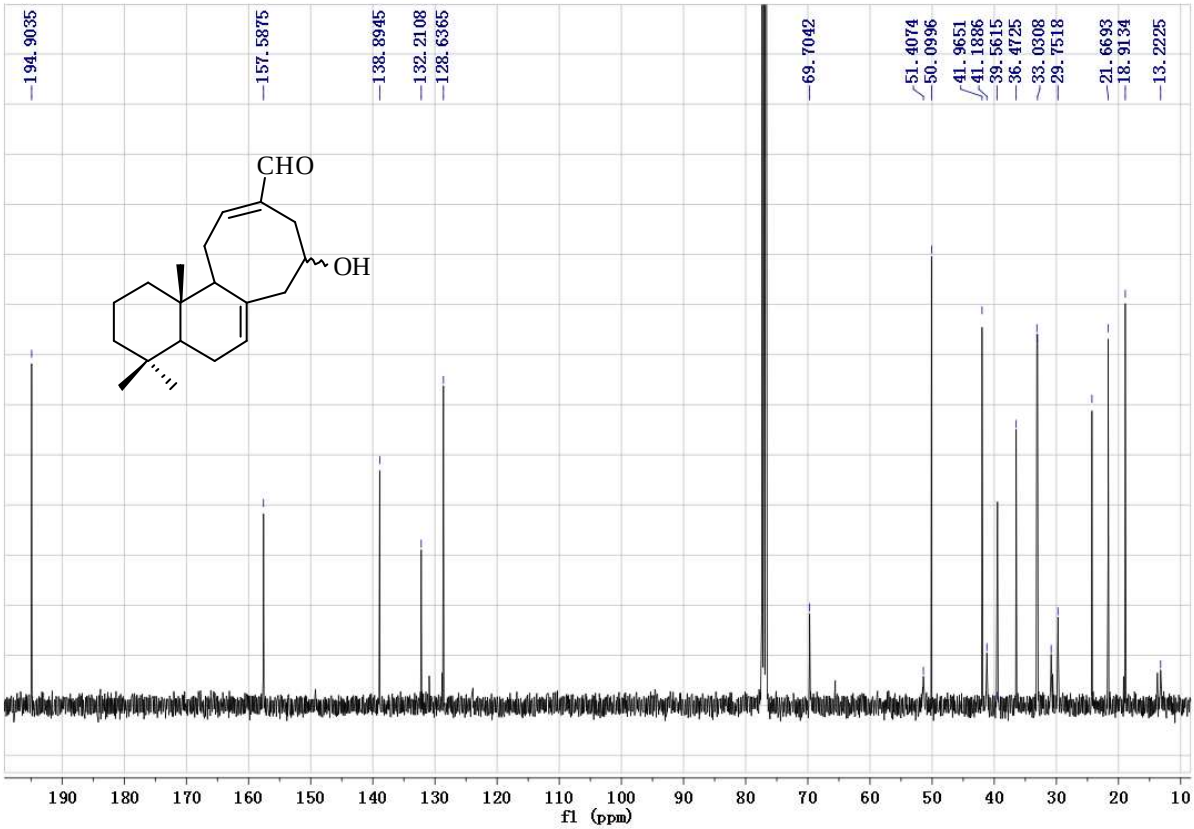


S38: ^{13}C-NMR (100 MHz, DMSO-d_6) Spectrum of Compound **7** Curcumenone



S39: ^{1}H-NMR (400 MHz, $CDCl_3$) Spectrum of Compound **8** Curcuminol D

Curcuminol D (8): ^{1}H-NMR ($CDCl_3$, 400 MHz): 0.79 (3H, s, H-20); 0.89 (3H, s, Me-19); 0.91 (3H, s, Me-18); 0.99 (1H, td, 3.9, 12.8, H-1a); 1.18 (1H, td, 3.3, 12.8, H-3a); 1.33 (1H, dd, 5.0, 12.3, H-5); 1.47 (1H, m, H-3b); 1.51 (1H, m, H-2a); 1.57 (1H, dt, H-2b); 1.87 (1H, m, H-1b); 1.96 (1H, m, H-6a); 2.12 (1H, dd, 3.4, 14.3, H-16a); 2.16 (1H, m, H-6b); 2.25 (1H, t, 12.3, H-14a); 2.32 (1H, m, H-11a); 2.40 (1H, d, 14.2, H-16b); 2.55 (1H, d, 11.7, H-9); 2.80 (1H, dd, 5.8, 20.0, H-11b); 3.11 (1H, dd, 5.5, 13.2, H-14b); 3.72 (1H, m, H-15); 5.66 (1H, s, Me-7); 6.80 (1H, s, H-12); 9.34 (1H, s, H-17). ^{13}C-NMR ($CDCl_3$, 400 MHz): 39.6 (C-1), 19.0 (C-2), 42.0 (C-3), 33.0 (C-4), 50.1 (C-5), 24.3 (C-6), 128.6 (C-7), 132.2 (C-8), 51.4 (C-9), 36.5 (C-10), 30.8 (C-11), 157.6 (C-12), 138.9 (C-13), 29.8 (C-14), 69.7 (C-15), 41.2 (C-16), 194.9 (C-17). [20]



S40: ^{13}C-NMR (100 MHz, $CDCl_3$) Spectrum of Compound **8** Curcuminol D