Separation and Biological Activities of the Main Compounds from the Bark of *Myrica rubra* Siebold & Zucc

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Table S1. The partition coefficient (K values)of *Myrica rubra* main compounds in chloroform – methanol – water solvent systems

Chloroform–methanol–water (volume ratio)	Settling time (s)	Volume ratio (upper/lower)	K values			
			Myricetrin	Myricetin	Myricanol	Epigallocatechin gallate
4:1:2	8	5/6	13.1	12.6	0.1	7.0
4:3:2	15	1/1	6.7	5.9	0.2	2.8
10:8:3	18	2/5	4.0	3.2	0.7	2.0

Figure S1. Thin-Layer Chromatography detection of taraxerol (Rf=0.90) isolated from ethyl acetate extract of *Myrica rubra*. Developing solvent system:toluene – ethyl acetate- formic acid (3:5:1, v/v)

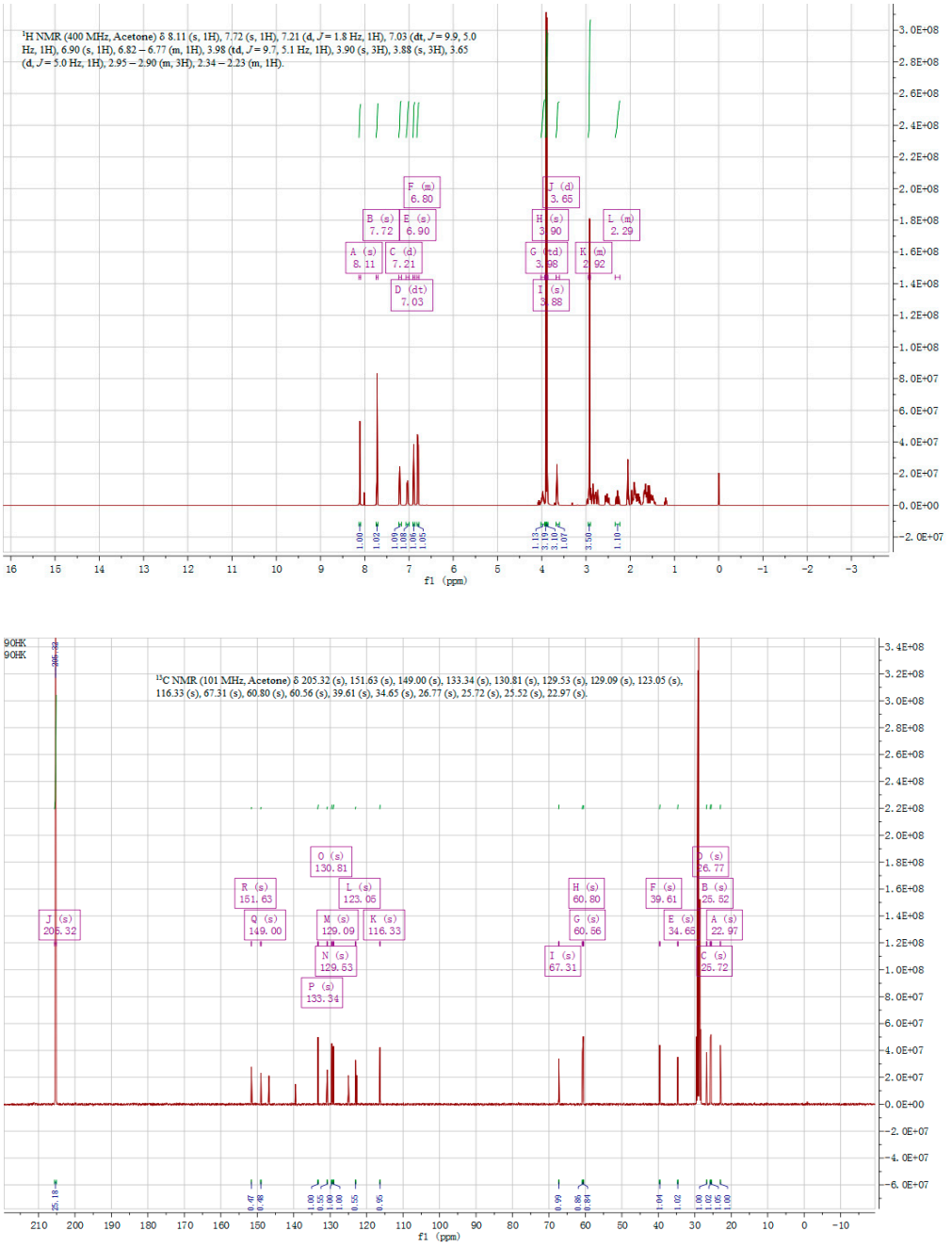

Figure S2. ^{1}H NMR，^{13}C NMR spectra of epigallocatechin gallate

^{1}HNMR (400 MHz, Acetone) δ 8.11 (s, 1H, OH), 7.72 (s, 1H, OH), 7.21 (d, *J* = 1.8 Hz, 1H, H-6”), 7.03 (dt, *J* = 9.9, 5.0 Hz, 1H, H-2”), 6.90 (s, 1H, H-6’), 6.82 – 6.77 (m, 1H, H-2’), 3.98 (td, *J* = 9.7, 5.1 Hz, 1H, H-8), 3.90 (s, 3H, H-6), 3.88 (s, 3H, H-3), 3.65 (d, *J* = 5.0 Hz, 1H, H-2), 2.95 – 2.90 (m, 3H, H-4a, 4b), 2.34 – 2.23 (m, 1H).

^{13}CNMR (101 MHz, Acetone) δ 205.32 (s, C=O), 151.63 (s, C-7), 149.00 (s, C-9), 133.34 (s, C-5), 130.81 (s, C-3’, 5’), 129.53 (s, C-3”, 5”), 129.09 (s, C-4”), 123.05 (s, C-4’), 116.33 (s, C-1’), 67.31 (s, C-1”), 60.80 (s, C-2”, 6”), 60.56 (s, C-2’, 6’), 39.61 (s, C-10), 34.65 (s, C-6), 26.77 (s, C-8), 25.72 (s, C-2), 25.52 (s, C-3), 22.97 (s, C-4).

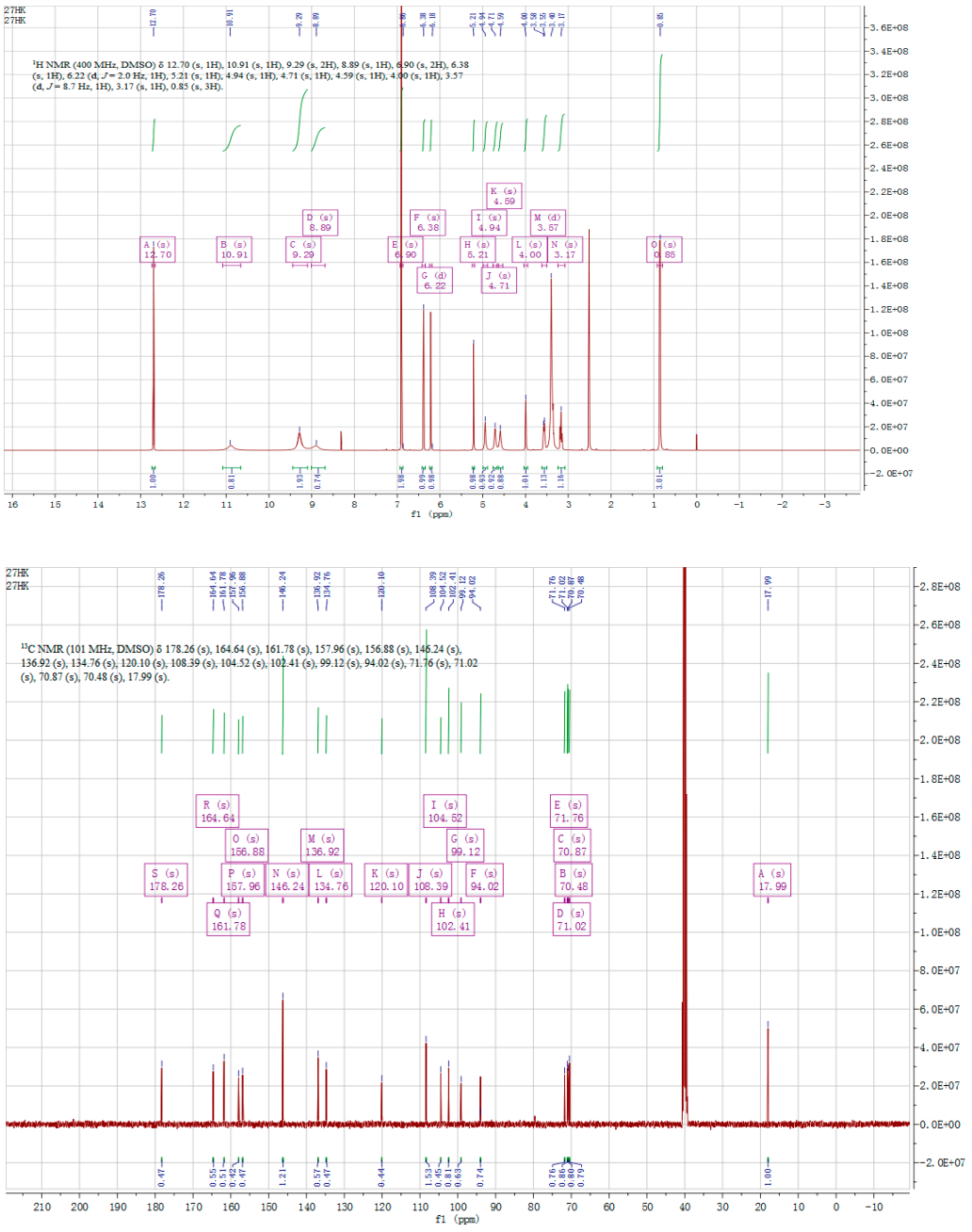

Figure S3. ^{1}H NMR，^{13}C NMR spectra of myricetrin

^{1}HNMR (400 MHz, DMSO) δ 12.70 (s, 1H, 5-OH), 10.91 (s, 1H, 7-OH), 9.29 (s, 2H, 3’, 5’-OH), 8.89 (s, 1H, 4’-OH), 6.90 (s, 2H, H-2’, 5’), 6.38 (s, 1H, H-6), 6.22 (d, *J* = 2.0 Hz, 1H, H-8), 5.21 (s, 1H, H-1”), 4.94 (s, 1H, OH), 4.71 (s, 1H, OH), 4.59 (s, 1H, OH), 4.00 (s, 1H, H-5”), 3.57 (d, *J* = 8.7 Hz, 1H, H-3”), 3.17 (s, 1H, H-4”), 0.85 (s, 3H, H-6”).

^{13}CNMR (101 MHz, DMSO) δ 178.26 (s, C-4), 164.64 (s, C-7), 161.78 (s), 157.96 (s, C-5), 156.88 (s, C-2, 9), 146.24 (s, C-3’, 5’), 136.92 (s, C-4’), 134.76 (s, C-3), 120.10 (s, C-1’), 108.39 (s, C-2’, 6’), 104.52 (s, C-10), 102.41 (s, C-1”), 99.12 (s, C-6), 94.02 (s, C-8), 71.76 (s, C-3”), 71.02 (s, C-2”), 70.87 (s, C-4”), 70.48 (s, C-5”), 17.99 (s, C-6”).

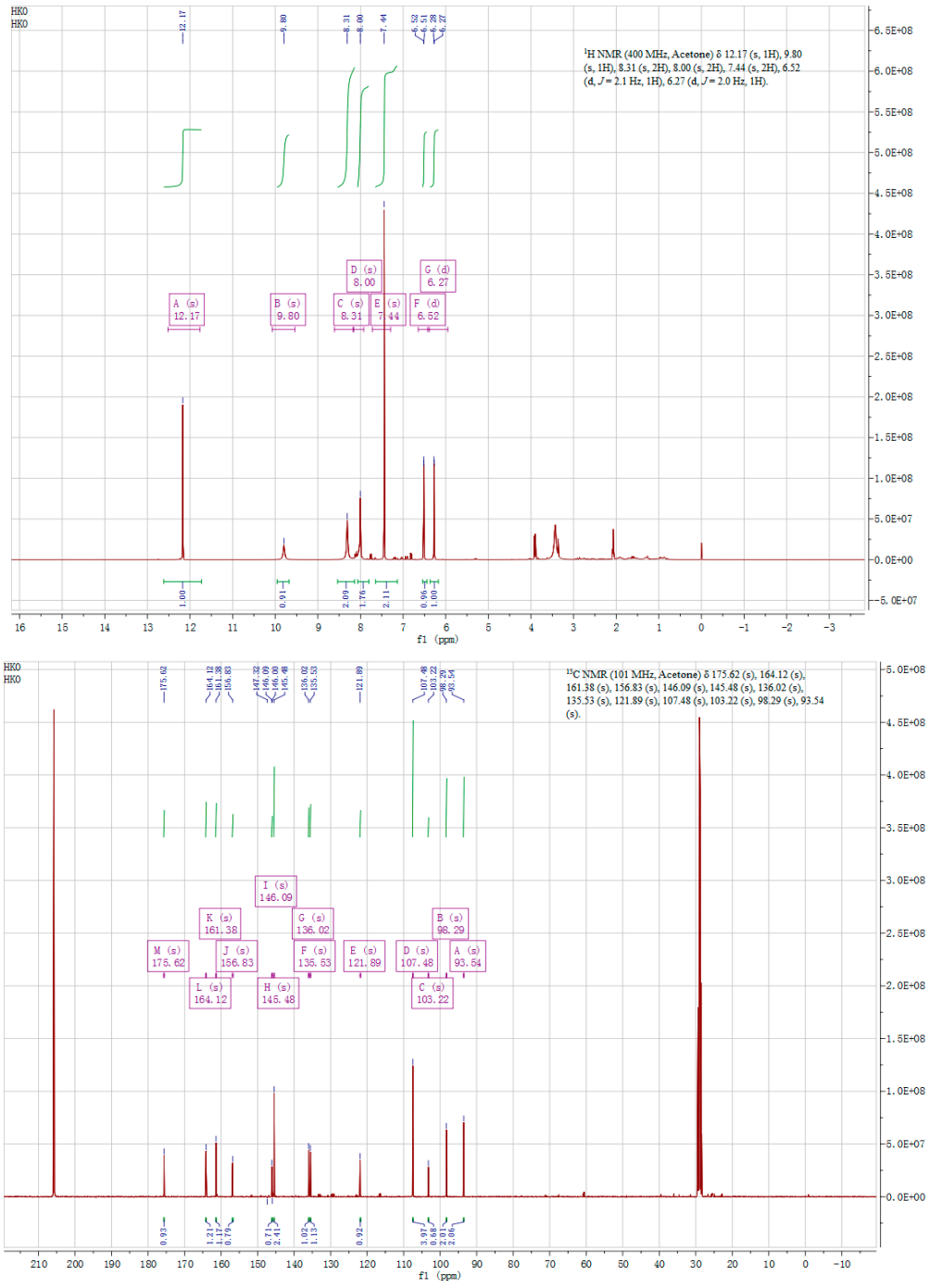

Figure S4. ^{1}H NMR，^{13}C NMR spectra of myricetin

^{1}H NMR (400 MHz, Acetone) δ 12.17 (s, 1H, 5-OH), 9.80 (s, 1H, 7-OH), 8.31 (s, 2H, OH), 8.00 (s, 2H, 3’, 5’-OH), 7.44 (s, 2H, H-2’, 6’), 6.52 (d, *J* = 2.1 Hz, 1H, H-8), 6.27 (d, *J* = 2.0 Hz, 1H, H-6).

^{13}C NMR (101 MHz, Acetone) δ 175.62 (s, C-4), 164.12 (s, C-7), 161.38 (s, C-5), 156.83 (s, C-9), 146.09 (s, C-3’, 5’), 145.48 (s, C-2), 136.02 (s, C-4’), 135.53 (s, C-3), 121.89 (s, C-1’), 107.48 (s, C-2’, 6’), 103.22 (s, C-10), 98.29 (s, C-6), 93.54 (s, C-8).

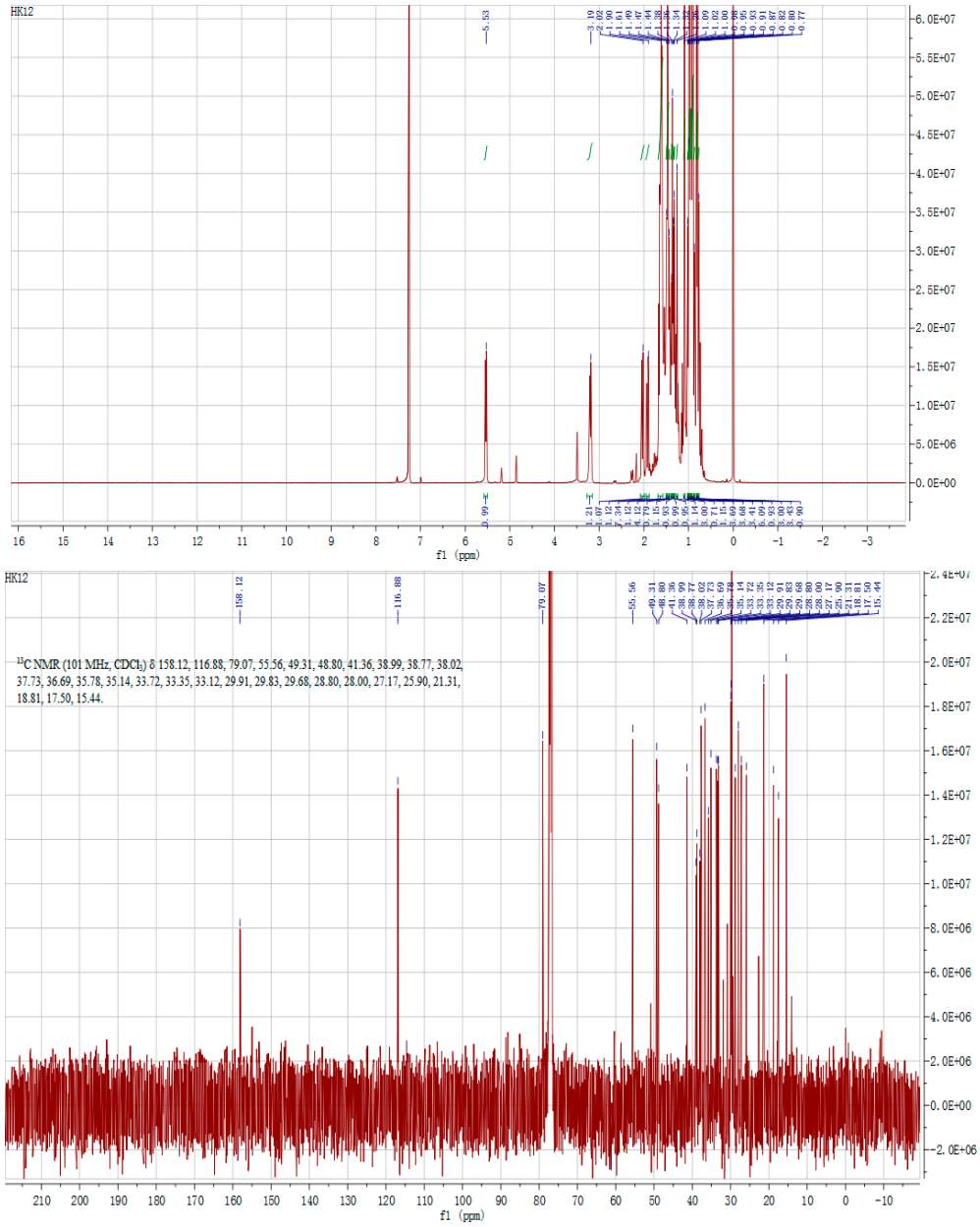

Figure S5. ^{1}H NMR，^{13}C NMR spectra of taraxerol

^{1}HNMR (400 MHz, $CDCl_3$) δ 5.53 (s, 1H, H-15), 3.19 (s, 1H, H-3), 2.02 (s, 1H, H-7), 1.90 (s, 1H, H-16), 1.64 (dd, *J* = 11.2, 5.3 Hz, 4H, C-1, 2, 11, 12), 1.61 (s, 3H, H-16, 2), 1.49 (s, 1H, H-6), 1.47 (s, 4H, H-6, 7, 11, 12), 1.44 (s, 1H, H-9), 1.38 (s, 1H, H-22), 1.36 (s, 1H, H-21), 1.34 (s, 1H), 1.32 (s, 1H, H-19), 1.26 (s, 1H, H-21), 1.09 (s, 3H, H-26), 1.02 (s, 1H, H-22), 1.00 (s, 1H, C-18), 0.98 (s, 3H, H-25), 0.95 (s, 3H, H-24), 0.93 (s, 3H, H-29), 0.91 (s, 6H, H-27, 30), 0.87 (s, 1H, H-5), 0.82 (s, 3H, H-23), 0.80 (s, 3H, H-28), 0.77 (s, 1H, H-1).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.15 (s, C-14), 116.91 (s, C-15), 79.10 (s, C-3), 55.60 (s, C-5), 49.35 (s, C-9), 48.85 (s, C-18), 41.40 (s, C-7), 38.92 (d, J = 22.6 Hz, C-8), 38.79 – 38.71 (m, C-4, 10), 38.05 (s, C-16), 37.69 (d, J = 14.1 Hz, C-1, 13), 36.73 (s, C-19), 35.81 (s, C-17), 35.18 (s, C-22), 33.75 (s, C-12), 33.38 (s, C-29), 33.15 (s, C-21), 29.91 (d, J = 7.9 Hz, C-28, 30), 28.83 (s, C-20), 28.03 (s, C-23), 27.21 (s, C-26), 25.92 (s, C-2), 21.34 (s, C-27), 18.84 (s, C-6), 17.53 (s, C-11), 15.46 (d, J = 2.8 Hz, C-25, 24).

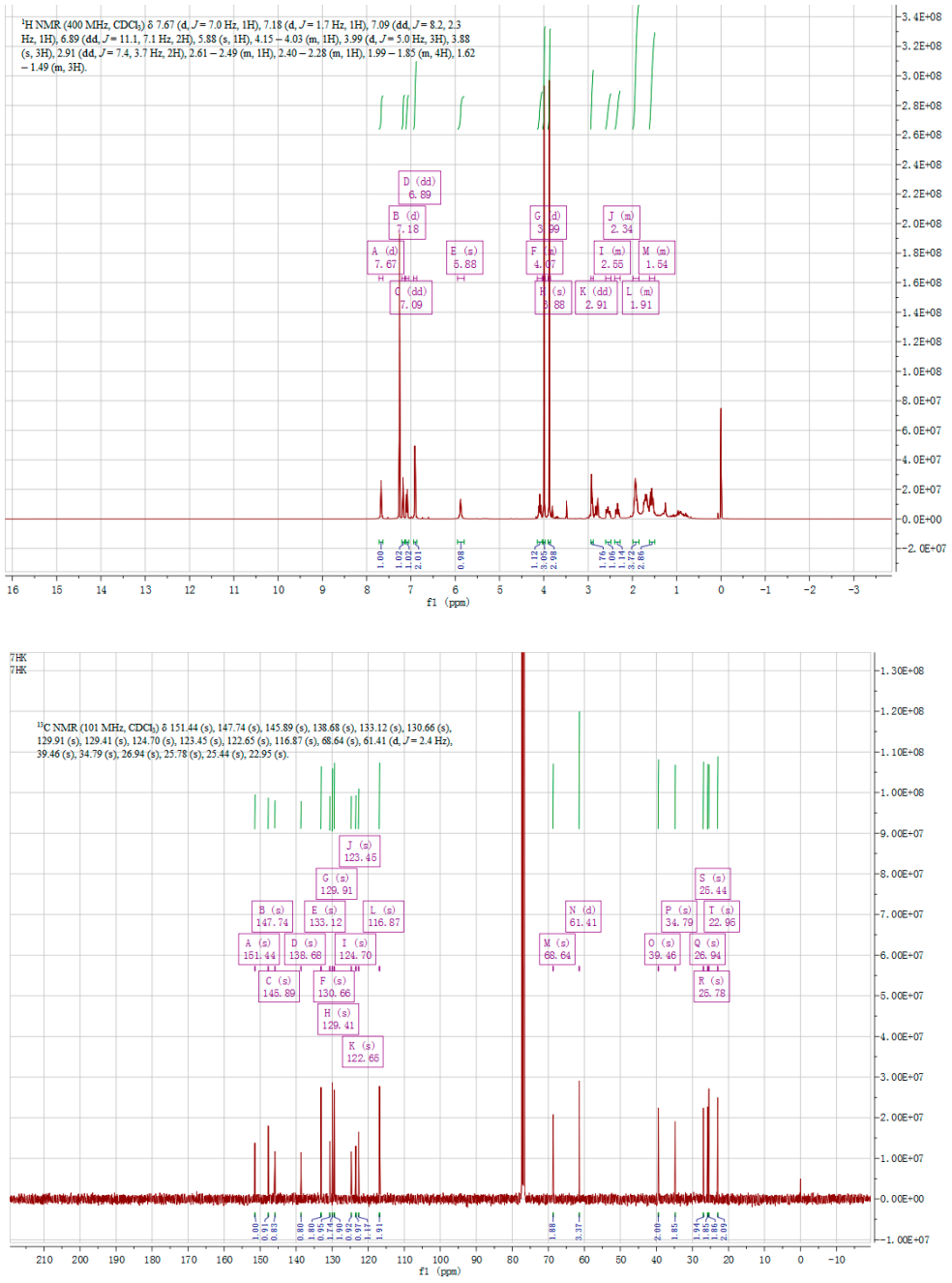

Figure S6. ^{1}H NMR，^{13}C NMR spectra of myricanol

^{1}HNMR (400 MHz, $CDCl_3$) δ 7.67 (d, J = 7.0 Hz, 1H, 17-OH), 7.18 (d, J = 1.7 Hz, 1H, H-18), 7.09 (dd, J = 8.2, 2.3 Hz, 1H, H-15), 6.89 (dd, J = 11.1, 7.1 Hz, 2H, H-16, 19), 5.88 (s, 1H, 5-OH), 4.15 – 4.03 (m, 1H, H-11), 3.99 (d, J = 5.0 Hz, 3H, H-20), 3.88 (s, 3H, H-21), 2.91 (dd, J = 7.4, 3.7 Hz, 2H, H-13), 2.61 – 2.49 (m, 1H, H-7), 2.40 – 2.28 (m, 1H, H-12), 1.99 – 1.85 (m, 4H, H-8, 10), 1.62 – 1.49 (m, 3H, H-9).

^{13}CNMR δ(ppm):(101 MHz, $CDCl_3$) δ 151.44 (s, C-17), 147.74 (s, C-5), 145.89 (s, C-3), 138.68 (s, C-4), 133.12 (s, C-18), 130.66 (s, C-14), 129.91 (s, C-15), 129.41 (s, C-19), 124.70 (s, C-1), 123.45 (s, C-2), 122.65 (s, C-6), 116.87 (s, C-16), 68.64 (s, C-11), 61.41 (d, *J* = 2.4 Hz, C-20, 21), 39.46 (s, C-10), 34.79 (s, C-12), 26.94 (s, C-13), 25.78 (s, C-7), 25.44 (s, C-8), 22.95 (s, C-9).

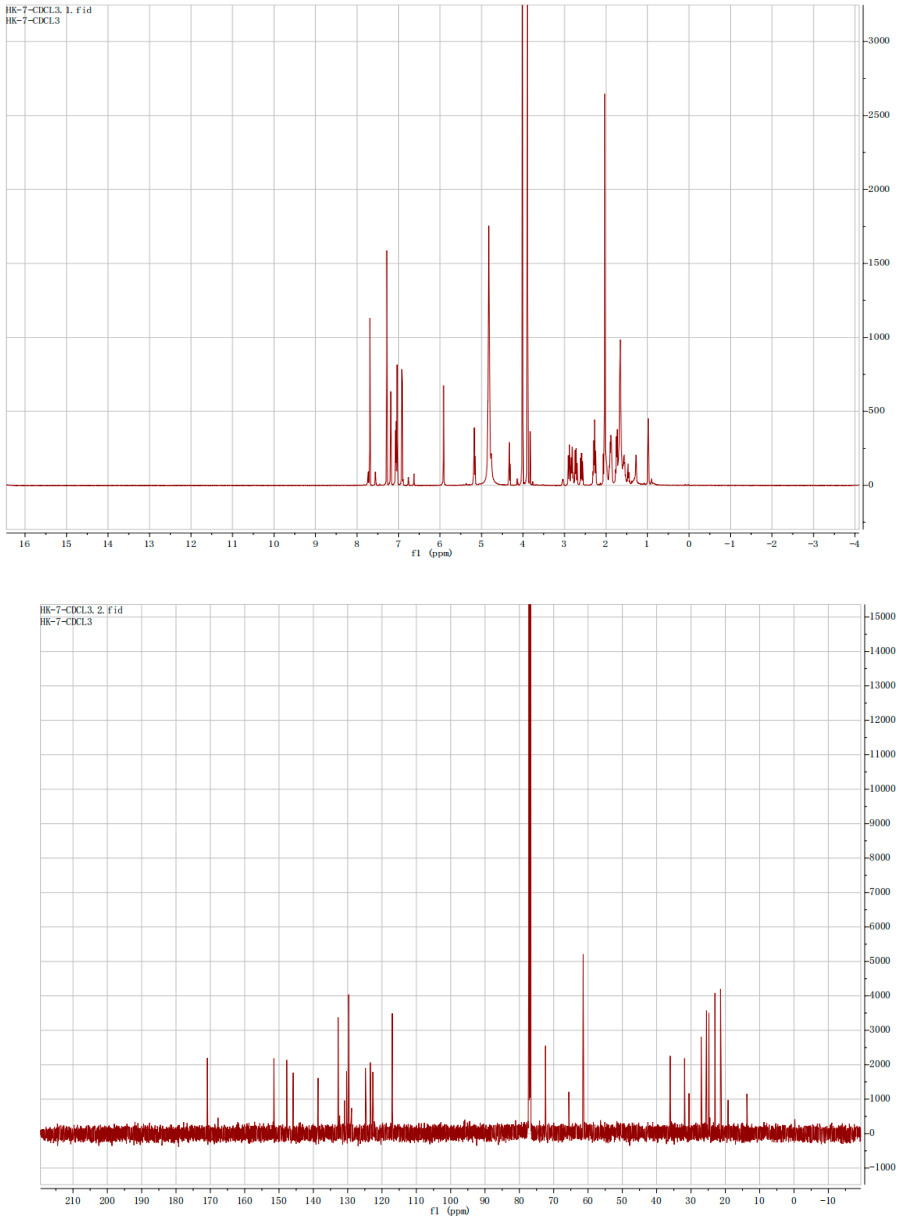

Figure S7. ^{1}H NMR，^{13}C NMR spectra of 11-*O*-acetylmyricanol

^{1}HNMR (600 MHz, $CDCl_3$) δ 7.69 (s, 1H, 17-OH), 7.19 (d, *J* = 2.3 Hz, 1H, H-18), 7.06 (dd, *J* = 8.3, 2.3 Hz, 1H, H-15), 7.03 (s, 1H, H-19), 6.91 (d, *J* = 8.3 Hz, 1H, H-16), 5.91 (s, 1H, 5-OH), 5.17 (t, *J* = 9.7 Hz, 1H, H-11), 4.01 (s, 3H, H-20), 3.89 (s, 3H, H-21), 2.89-2.72 (m, 2H, H-13), 2.82-2.58 (m, 2H, H-7), 2.27-2.00 (m, 2H, H-12), 2.27-1.89 (m, 2H, H-8), 2.03 (s, 3H, H-23), 1.86-1.65 (m, 2H, H-10), 1.73-1.56 (m, 2H, H-9).

^{13}CNMR δ(ppm):(150 MHz, $CDCl_3$) δ 21.4 (s, C-23), 23.0 (s, C-9), 24.8 (s, C-8), 25.5 (s, C-7), 27.0 (s, C-13), 31.9 (s, C-12), 36.1 (s, C-10), 61.4(s, C-20, 21), 72.4 (s, C-11), 117.0 (s, C-16), 122.7 (s, C-6), 123.4 (s, C-2), 124.8 (s, C-1), 129.6 (s, C-19), 129.7 (s, C-15), 130.3 (s, C-14), 132.8 (s, C-18), 138.6 (s, C-4), 145.9 (s, C-3), 147.7 (s, C-5), 151.5(s, C-17), 170.9 (s, C-22).

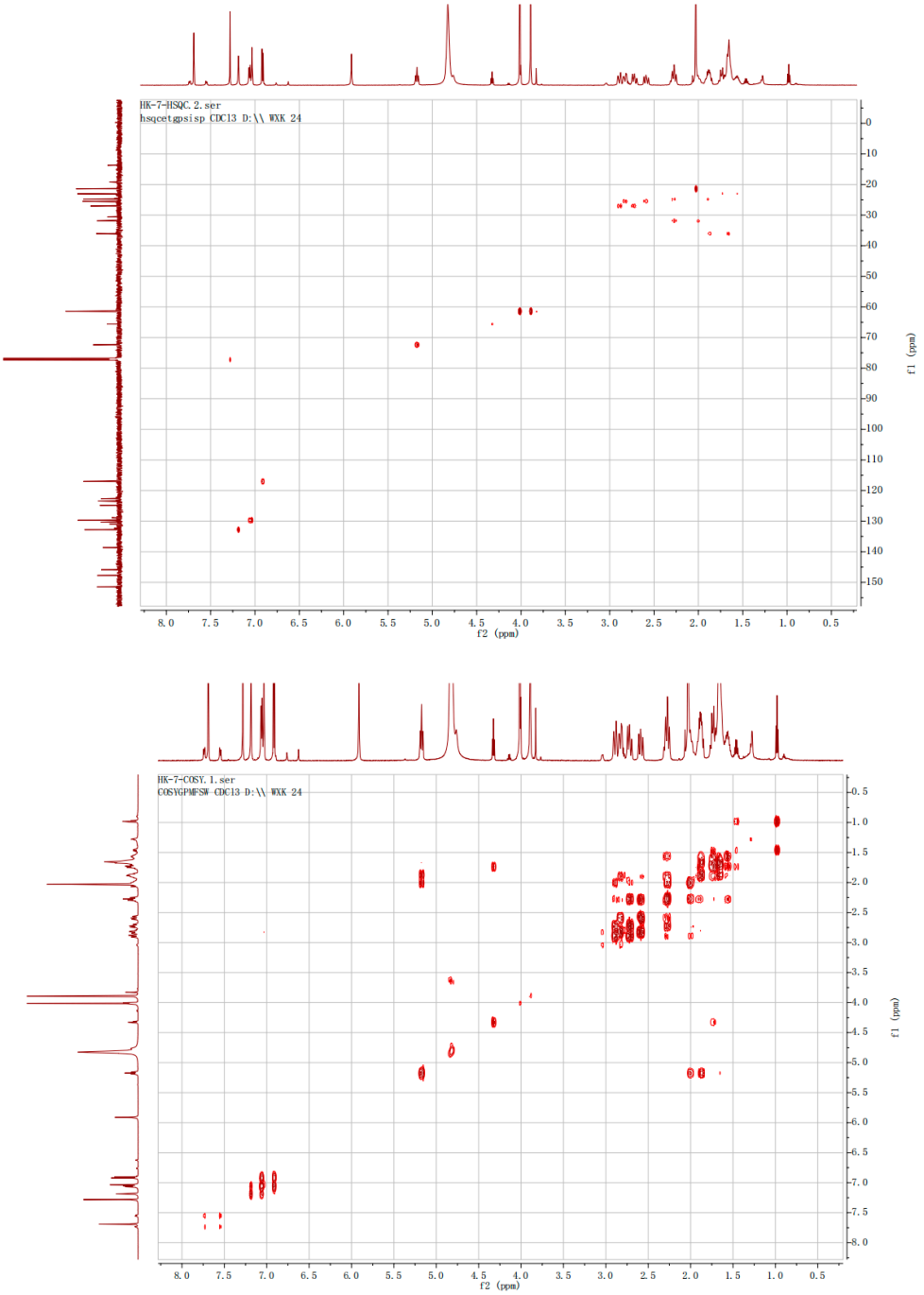

Figure S8. HSQC, HH-COSY spectra of 11-*O*-acetylmyricanol

HH-COSY:δ2.27-1.89(m, 1H, H-8) and δ2.82-2.58(m, 1H, H-7), δ1.73-1.56 (m, 1H, H-9); δ5.17 (t, J=9.7 Hz, 1H, H-11) and δ1.86-1.65 (m, 1H, H-10), δ2.27-2.00 (m, 1H, H-8); δ2.89-2.72 (m, 1H, H-13) and δ2.27-2.00 (m, 1H, H-8); δ7.06 (dd, J = 8.3, 2.3 Hz, 1H, H-15) and δ6.91 (d, J = 8.3 Hz, 1H, H-16) are signals from adjacent ortho-hydrogens.

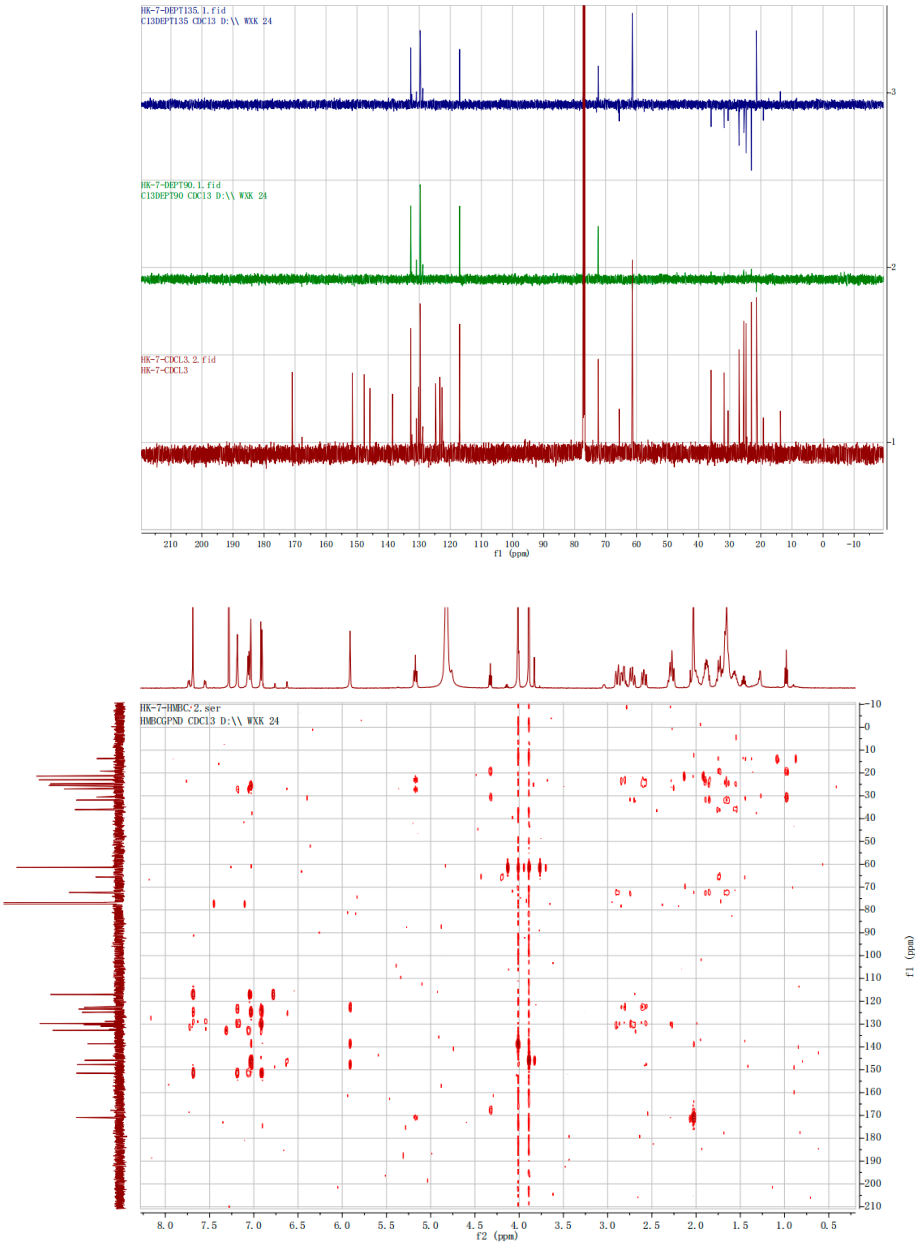

Figure S9. DEPT, HMBC spectra of 11-*O*-acetylmyricanol

DEPT:1 high field methyl group, 2 methoxy, 6 methylene CH2, 1 sp3-hybridized CH, 4 sp2-hybridized CH, 9 quaternary carbons containing 1 ester group and 2 benzene rings.

HMBC:$^{3}J_{H\text{-}C}$ coupling between 2.82-2.58(m, 1H, H-7) and δ147.7(C5), δ129.6 (C19), δ23.0 (C9); δ2.27-1.89(m, 1H, H-8) and δ122.7(C6); δ5.17 (t, J=9.7 Hz, 1H, H-11) and δ23.0(C9), δ27.0(C13), δ170.9(C22); δ2.27-2.00(m, 1H, H-12) and δ130.3(C14); δ6.91(d, J=8.3Hz, 1H, H-16) and δ124.8(C1); δ7.19 (d, J=2.3Hz, 1H, H-18) and δ129.7(C15), δ123.4(C2), δ27.0(C13); δ4.01 (s, 3H, H-20) and δ138.6(C4); δ3.89(s, 3H, H-21) and δ145.9(C3); δ5.91 (s, 1H, 5-OH) and δ138.6(C4), δ122.7(C6); δ7.69 (s, 1H, 17-OH) and δ124.8(C1), δ117.0(C16). $^{2}J_{H\text{-}C}$ coupling between δ5.17 (t, J=9.7 Hz, 1H, H-11) and δ36.1(C10); δ5.91 (s, 1H, 5-OH) and δ147.7(C5); δ7.69 (s, 1H, 17-OH) and δ151.5(C17); δ2.03(s, 3H, H-23) and δ170.9(C22).

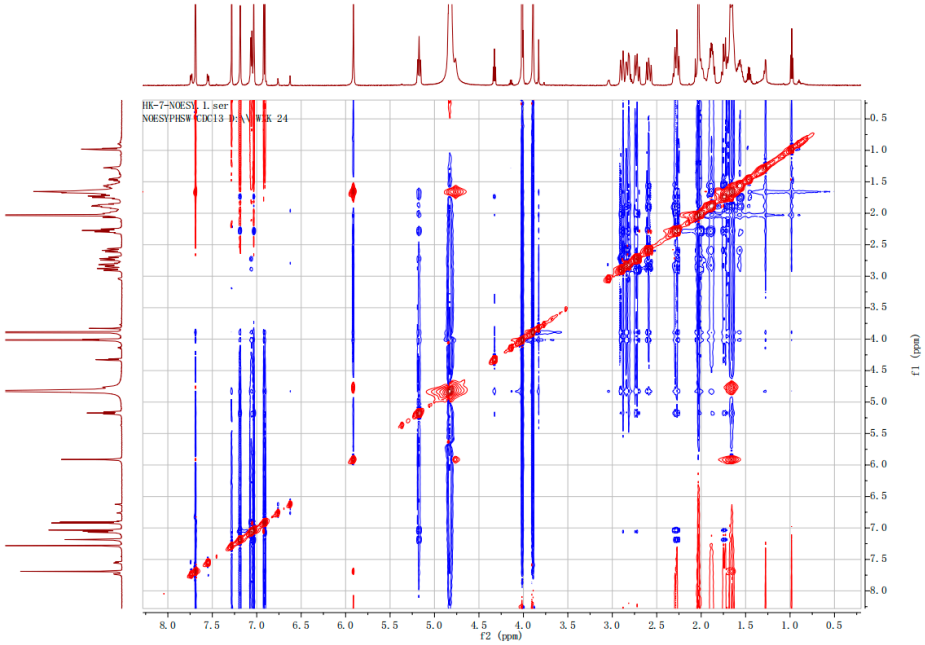

Figure S10. NOESY spectra of 11-*O*-acetylmyricanol

NOESY: The spatial positions of the three adjacent hydrogens are δ 5.17 (t, J = 9.7 Hz, 1H, H-11), δ 7.19 (d, J = 2.3 Hz, 1H, H-18) and δ 7.03 (s, 1H, H-19).

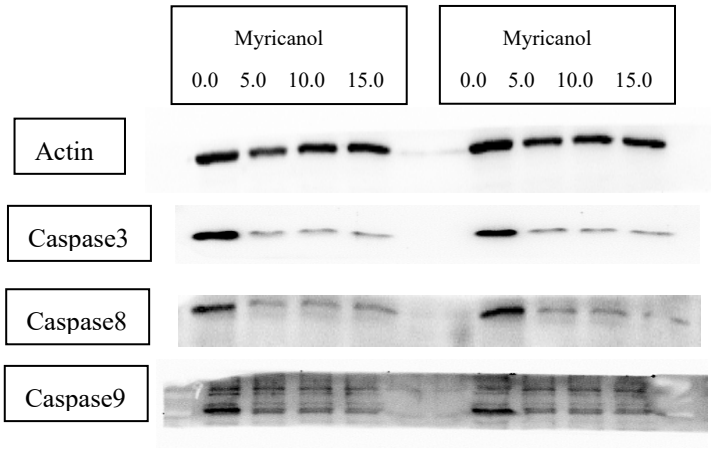

Figure S11. The uncropped western blot gels of actin, caspase 3, caspase 8, and caspase 9.