Supporting Information

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A New Lignan from Leaves of *Ormosia xylocarpa*

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^{1}H-NMR and ^{13}C-NMR data of compound **2-6**

*Hedyotol C (**2**):* White power; $C_{31}H_{36}O_{11}$; HR-ESI-MS m/z 607 $[M + Na]^+$; ^{1}H-NMR (400MHz, DMSO-d_6) δ_H: 6.96 (1H, d, *J* = 1.6 Hz, H-2′), 6.89 (1H, d, *J* = 2.0 Hz, H-2′′), 6.78 (1H, m, H-5′), 6.75 (1H, d, *J* = 1.6 Hz, H-5′′), 6.72 (1H, d, *J* = 8.0 Hz, H-6′), 6.68 (1H, d, *J* = 8.0 Hz, H-6′′), 6.64 (2H, s, H-2, 6), 4.85 (1H, m, H-7′′), 4.65 (1H, d, *J* = 4.0 Hz, H-7′), 4.61 (1H, d, *J* = 4.0 Hz, H-7), 4.15 (2H, m, H-9′), 3.98 (1H, m, H-8′′), 3.78 (2H, overlapped, H-9), 3.76 (3H, s, 5′′-OCH_3), 3.74 (6H, s, 3, 5-OCH_3), 3.71 (3H, s, 3′′-OCH_3), 3.63 (1H, d, *J* = 11.2, 4.8 Hz, H-9′′a), 3.20 (1H, m, H-9′′b), 3.05 (2H, m, H-8, 8′). ^{13}C-NMR (100 MHz, DMSO-d_6) δ_C: 152.5 (C-3,5), 147.6 (C-3′′), 146.9 (C-3′), 146.0 (C-4′), 145.3 (C-4′′), 137.0 (C-1), 135.3(C-4), 133.0 (C-1′), 132.2 (C-1′′), 119.2 (C-6′), 118.7 (C-6′′), 115.2 (C-5′), 114.7 (C-5′′), 110.9 (C-2′), 110.4 (C-2′′), 103.3 (C-2, 6), 87.1 (C-8′′), 85.2 (C-7, 7′), 71.5 (C-7′′), 71.3 (C-9), 71.0 (C-9′), 60.2 (C-9′′), 56.0 (3, 5-OCH_3), 55.6 (3′-OCH_3), 55.5 (3′′-OCH_3), 53.9 (C-8′), 53.9 (C-8).

*Buddlenol C (**3**):* Light yellow solid; $C_{32}H_{38}O_{12}$; HR-ESI-MS m/z 615 $[M + H]^+$; ^{1}H-NMR (400MHz, DMSO-d_6) δ_H: 6.89 (1H, d, *J* = 2.0 Hz, H-2′), 6.75 (1H, d, *J* = 2.0 Hz, H-2′′), 6.72 (1H, d, *J* = 8.0 Hz, H-5′′), 6.64 (2H, s, H-2, 6), 6.59 (2H, s, H-2′, 6′), 4.81 (1H, m, H-7′′), 4.65 (1H, d, *J* = 4.0 Hz, H-7′), 4.61 (1H, d, *J* = 4.0 Hz, H-7), 4.15-4.02 (3H, overlapped, H-8′′, 9a, 9b), 3.79 (2H, overlapped, H-9), 3.76 (9H, s, 3′, 5′, 3′′-OCH_3), 3.72 (6H, s, 3, 5-OCH_3), 3.75 (1H, s, H-9′′a), 3.68 (1H, m, H-9′′b), 3.05 (2H, m, H-8, 8′). ^{13}C-NMR (100 MHz, MSO-d_6) δ_C: 152.6 (C-3,5), 147.5 (C-3′, 5′), 147.4 (C-3), 146.0 (C-4′′), 136.8 (C-1), 134.9(C-4), 134.3 (C-4′′), 132.5 (C-1′′), 132.2 (C-1′), 118.7 (C-6′′), 115.2 (C-5′′), 110.4 (C-2′′), 104.2 (C-2, 6), 103.3 (C-2′, 6′), 85.4 (C-8′′), 85.2 (C-7, 7′), 72.4 (C-7′′), 71.3 (C-9), 71.0 (C-9′), 59.9 (C-9′′), 56.0 (3, 5-OCH_3), 55.9 (3′, 5′-OCH_3), 55.6 (3′′-OCH_3), 53.8 (C-8′), 53.5 (C-8).

*(+)-Medioresinol (**4**):* Prismatic crystals; $C_{21}H_{24}O_7$; HR-ESI-MS m/z 389 $[M + H]^+$; ^{1}H-NMR (400MHz, DMSO-d_6) δ_H: 6.89 (1H, d, *J* = 1.6 Hz, H-2), 6.75 (1H, dd, *J* = 8.0, 1.6 Hz, H-5′), 6.72 (1H, d, *J* = 8.0 Hz, H-6), 6.59 (2H, s, H-2′, 6′), 4.60 (1H, m, H-7, 7′), 4.13 (2H, m, H-9a, 9′a), 3.76 (3H, s, 3′-OCH_3), 3.75(6H, s, 3, 5-OCH_3), 3.72 (1H, s, H-9b, 9′b), 3.05 (2H, m, H-8, 8′). ^{13}C-NMR (100 MHz, DMSO-d_6) δ_C: 147.9 (C-3, 5), 147.5 (C-3′), 145.9 (C-4′), 134.8(C-4), 132.2 (C-1′), 131.4 (C-1), 118.6 (C-6′), 115.1 (C-5′), 110.4 (C-2′), 103.6 (C-2, 6), 85.4 (C-7), 85.2(C-7′), 71.1 (C-9), 70.9 (C-9′), 56.0 (3, 5-OCH_3), 55.6 (3-OCH_3), 53.8 (C-8), 53.5 (C-8′).

*(+)-Isolariciresinol (**5**):* Light yellow power; $C_{20}H_{24}O_6$; HR-ESI-MS m/z 383.2 $[M + Na]^+$; ^{1}H-NMR (400MHz, DMSO-d_6) δ_H: 6.68 (1H, d, *J* = 8.0 Hz, H-5′), 6.64 (1H, d, *J* = 2.0 Hz, H-2′), 6.60 (1H, s, H-6), 6.35 (1H, dd, *J* = 8.0, 2.0 Hz, H-6′), 6.09 (1H, s, H-3), 3.74 (1H, d, *J* = 10.4 Hz, H-7), 3.70 (3H, s, 3′-OCH_3), 3.69 (3H, s, 5-OCH_3), 3.43 (2H, m, H-9′), 3.17 (2H, d, *J* = 4.8 Hz, H-7′), 2.68 (2H, m, H-9), 1.83 (1H, m, H-8), 1.61 (1H, m, H-8′). ^{13}C-NMR (100 MHz, DMSO-d_6) δ_C: 147.3 (C-3′), 145.5 (C-5), 144.6 (C-4′), 144.1 (C-4), 137.2 (C-1′), 132.7 (C-2), 127.2 (C-1), 121.5 (C-6′), 116.3 (C-3), 115.3 (C-5′), 113.2 (C-2′), 111.8 (C-6), 63.6 (C-9), 59.7 (C-9′), 55.7 (5-OCH_3), 55.5 (3′-OCH_3), 48.7 (C-7′), 45.9 (C-8′), 38.1 (C-8), 32.3 (C-7).

*5-Methoxy-(+)-isolariciresinol (**6**):* White power; $C_{21}H_{26}O_7$; HR-ESI-MS m/z 389 $[M - H]^-$; ^{1}H-NMR (400MHz, DMSO-d_6) δ_H: 6.60 (1H, s, H-2′), 6.35 (2H, s, H-2, 6), 6.11 (1H, s, H-5′), 3.74 (1H, d, *J* =

10.4 Hz, H-7), 3.70 (3H, s, 3′-OCH_3), 3.68 (6H, s, 3, 5-OCH_3), 3.45 (2H, m, H-9′), 3.18 (2H, m, H-7), 2.69 (2H, m, H-9), 1.85 (1H, m, H-8), 1.64 (1H, m, H-8′). ^{13}C-NMR (100 MHz, DMSO-d_6) δ_C: 147.8 (C-3,5), 145.6 (C-3′), 144.1 (C-4′), 136.2 (C-1), 133.7 (C-4), 132.6 (C-6′), 127.2 (C-1′), 116.2 (C-5′), 111.8 (C-2′), 106.6 (C-2, 6), 63.6 (C-9), 59.8 (C-9′), 56.1 (3, 5-OCH_3), 55.5 (3′-OCH_3), 46.5 (C-7′), 45.7 (C-8′), 38.1 (C-8), 32.3 (C-7).

(+)-Lyoniresinol (7): White square crystal; $C_{22}H_{28}O_8$; HR-ESI-MS m/z 419 $[M - H]^-$; ^{1}H-NMR (400MHz, DMSO-d_6) δ_H: 6.54 (1H, s, H-2′), 6.28 (2H, s, H-2, 6), 4.23 (1H, d, J = 5.2 Hz, H-7), 3.76 (3H, s, 3′-OCH_3), 3.62 (6H, s, 3, 5-OCH_3), 3.46 (2H, m, H-9′), 3.29 (3H, s, 5′-OCH_3), 3.23 (1H, m, H-9a), 3.16 (1H, m, H-9b), 2.61 (1H, dd, J = 14.8, 4.4 Hz, H-7), 2.42 (1H, dd, J = 14.8, 11.2 Hz, H-7′), 1.83 (1H, m, H-8), 1.42 (1H, m, H-8′). ^{13}C-NMR (100 MHz, DMSO-d_6) δ_C: 147.6 (C-3,5), 146.9 (C-5′), 146.4 (C-3′), 137.8 (C-1′), 137.2 (C-4), 133.4 (C-4′), 128.6 (C-1), 125.0 (C-2′), 106.7 (C-6′), 105.9 (C-2, 6), 64.6 (C-9), 62.2 (C-9′), 59.0 (5′-OCH_3), 56.1 (3, 5-OCH_3), 55.7 (3′-OCH_3), 46.7 (C-8′), 39.0 (C-8), 32.3 (C-7).

Bioassay for Antioxidant Activity

The samples (compounds **1**-**7**) were configured to a concentration gradient of 0.500, 0.250, 0.100. 0.050, 0.025, 0.010 mg/mL as sample solution. Vitamin C was used as a positive control group.The absorbance A were measured by a microplate reader. The effective concentration (IC_{50}) was calculated in IBM SPSS Statistics 26.0.

1. DPPH Free Radical Scavenging Test

DPPH was dissolved in methanol as working solution of 0.1mmol/L. 100 μL of DPPH working solution was added to 100μL of sample solution in a 96-well plate, shaking mixed, and protected from light at room temperature for 30 min. The absorbance value at 517nm was A_1. Methanol was used to replace the DPPH working solution to deduct the background absorption of the sample solution, and the absorbance value was A_2. Replace the sample solution with the same volume of methanol as a negative control, and the absorbance value is A_0. Vitamin C was used as a positive control group. The calculation formula was: Clearance rate = $[1- (A_1-A_2)/A_0] \times 100\%$.

2. $ABTS^+$ Free Radical Scavenging Test

Mix 5mL of 7mmol/L ABTS aqueous solution and 5mL of sample solution, and 2.45mmol/L $K_2S_2O_8$ aqueous solution, and placed it in the dark at 24 ℃ for 16 h to obtain $ABTS^+$ solution. Take 1mL of $ABTS^+$ solution and dilute it with distilled water until the absorbance value at 734nm was 0.700 ± 0.002. Take 40μL of the sample solution and mixed it with 160μL of $ABTS^+$ solution in a 96-well plate, the absorbance value at 734nm was A_j. Ultra-pure water was used to replace the $ABTS^+$ working solution to deduct the background absorption of the sample solution, and the absorbance value was A_i. Replace the sample solution with the same volume of methanol as a negative control, and the absorbance value is A_0. The calculation formula was: Clearance rate = $[A_0- (A_j -A_i)]/A_0 \times 100\%$.

3. ·OH Free Radical Scavenging Test

Mix 1.2mL of 20mmol/L $C_7H_5O_3Na$ and 4mL 1.5mmol/L $FeSO_4$ as working solution.Take 104μL of working solution and mixed it with 40μL sample solution in a 96-well plate, then added 56μL of 6mmol/L H_2O_2 and placed it at 37 ℃ water bath for 1 h, the absorbance value at 510nm was A_a. Ultra-pure water was used to replace the H_2O_2 to deduct the background absorption of the sample solution, and the absorbance value was A_b. Replace the sample solution with the same volume of methanol as a negative control, and the absorbance value is A_0. The calculation formula was: Clearance rate = $[A_0- (A_a -A_b)]/A_0 \times 100\%$.

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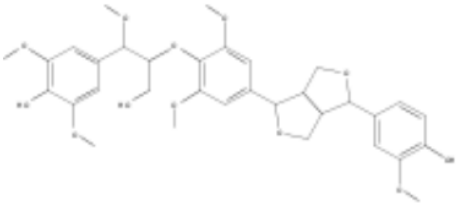

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☐ 95-98	45

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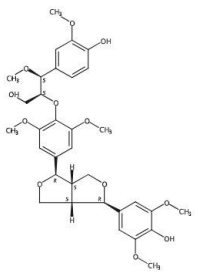

Absolute stereochemistry.

$C_{33}H_{40}O_{12}$
Benzenepropanol, β-[2,6-dimethoxy-4-[(1*R*,3a*S*,4*R*,6a*S*)-tetrahydro-4-(4-hydroxy-3,5-dimethoxyphenyl)-1*H*,3*H*-furo[3,4-*c*]furan-1-yl]phenoxy]-4-hydroxy-γ,3-dimethoxy-, (β*S*,γ*S*)-

▸ **Key Physical Properties**
Experimental Properties

Score: ≥ 99
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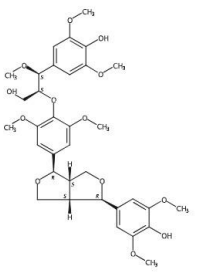
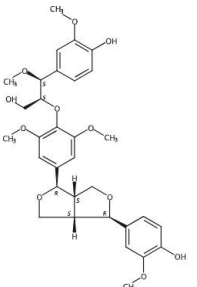


Absolute stereochemistry.

$C_{34}H_{42}O_{13}$
Benzenepropanol, β-[2,6-dimethoxy-4-[(1*R*,3a*S*,4*R*,6a*S*)-tetrahydro-4-(4-hydroxy-3,5-dimethoxyphenyl)-1*H*,3*H*-furo[3,4-*c*]furan-1-yl]phenoxy]-4-hydroxy-γ,3,5-trimethoxy-, (β*S*,γ*S*)-

▸ **Key Physical Properties**
Experimental Properties

Score: ≥ 99
☐ 3. **2143535-27-5**
~3



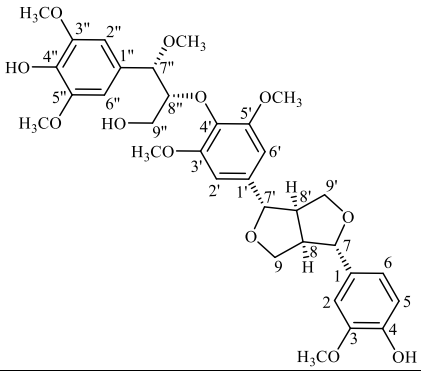
Absolute stereochemistry.,Rotation (-).

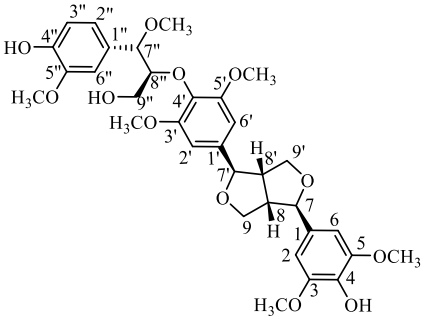
$C_{32}H_{38}O_{11}$
Benzenepropanol, β-[2,6-dimethoxy-4-[(1*R*,3a*S*,4*R*,6a*S*)-tetrahydro-4-(4-hydroxy-3-methoxyphenyl)-1*H*,3*H*-furo[3,4-*c*]furan-1-yl]phenoxy]-4-hydroxy-γ,3-dimethoxy-, (β*S*,γ*S*)-

▸ **Key Physical Properties**

Table S1: Comparison table for the NMR data with the most similar one

Position	compound **1** (DMSO-d_6)		most similar compound (chloroform-*d*)	
	δ_H	δ_C	δ_H	δ_C
1		132.2		134.1
2	6.88 (1H, d, *J* = 2.0 Hz)	115.2	6.70 (s)	104.5
3		147.7		152.8
4		146.0		148.3
5	6.72 (1H, d, *J* = 8.0 Hz)	110.4		152.8
6	6.75 (1H, dd, *J* = 8.0, 2.0 Hz)	118.7	6.70 (s)	104.5
7	4.61 (1H, d, *J* = 3.6 Hz)	85.2	4.67 (d, *J* =3.9 Hz)	86.8
8	3.05 (1H, m)	53.5	3.09(m)	55.2
9	4.14 (2H, m)	71.3	4.24 (dd, *J* =7.1, 15.0 Hz) 3.90 (obscured)	72.3
1′		136.8		134.3
2′, 6′	6.61 (2H, d, *J* = 2.0Hz)	103.2	6.68 (s)	104.2
3′, 5′		152.6		152.0
4′		134.7		136.7
7′	4.64 (1H, d, *J* = 3.6 Hz)	85.2	4.71 (d, *J* = 3.9 Hz)	86.6
8′	3.02 (1H, m)	53.8	3.09 (1H, m)	55.4
9′	3.77 (overlapped)	71.0	4.24 (dd, *J* = 7.1, 15.0 Hz) 3.90 (obscured)	72.3
1″		126.7		129.5
2″	6.54 (1H, m)	104.9	6.98 (d, *J* = 1.5 Hz)	111.9
3″		147.6		148.5
4″		134.7		146.9
5″		147.6	6.81 (d, *J* = 7.5 Hz)	115.1
6″	6.54 (1H, m)	104.9	6.84 (dd, *J* = 1.5, 7.5 Hz)	121.7
7″	4.39 (1H, d, *J* = 6.8 Hz)	82.6	4.56 (d, *J* = 6.8 Hz)	83.5
8″	4.19 (1H, m)	84.9	4.13 (m)	86.5
9″	3.65 (overlapped) 3.47 (overlapped)	59.8	3.80 (obscured), 3.52 (dd, *J* = 2.9, 11.7 Hz)	60.6
3-OCH_3	3.76 (3H, s)	55.6	3.82 s	57.4
5-OCH_3			3.82 s	57.4
3′, 5′-OCH_3	3.72 (6H, s)	56.0	3.84 s	56.8
3″-OCH_3	3.70 (3H, s)	55.9	3.86 s	57.0
5″-OCH_3	3.70 (3H, s)	55.9		
7″-OCH_3	3.71 (3H, s)	56.6	3.22 s	58.1





x-40. HRMS (ESI) m/z calcd for $C_{33}H_{40}O_{12}Na^+$ $(M+Na)^+$ 651.24120, found 651.24091.

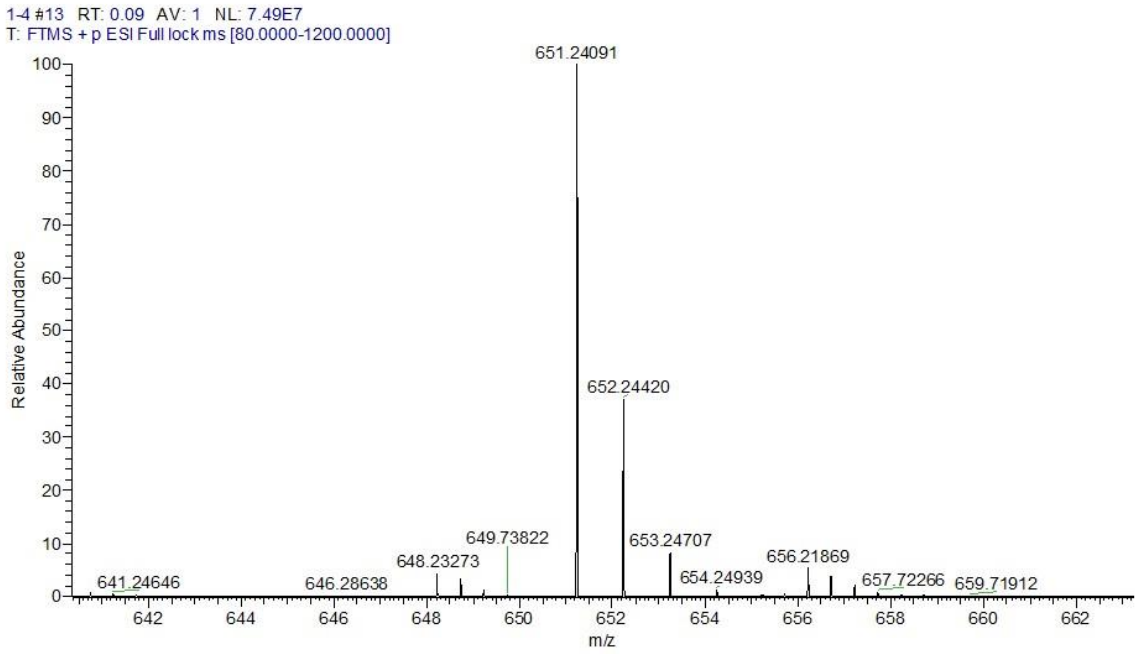


Figure S2: HR-ESI-MS spectrum of **1** (xylocarpalignan B)

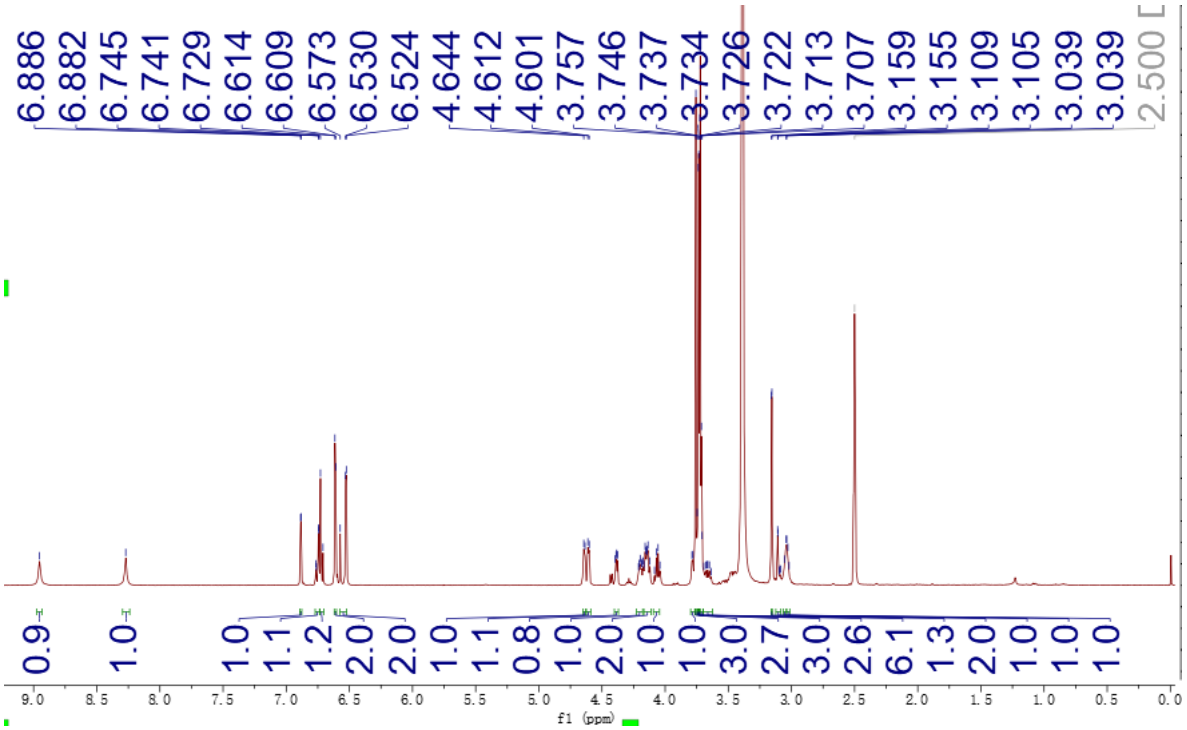


Figure S3: ^{1}H-NMR (400MHz，DMSO-d_6) spectrum of **1** xylocarpalignan B)

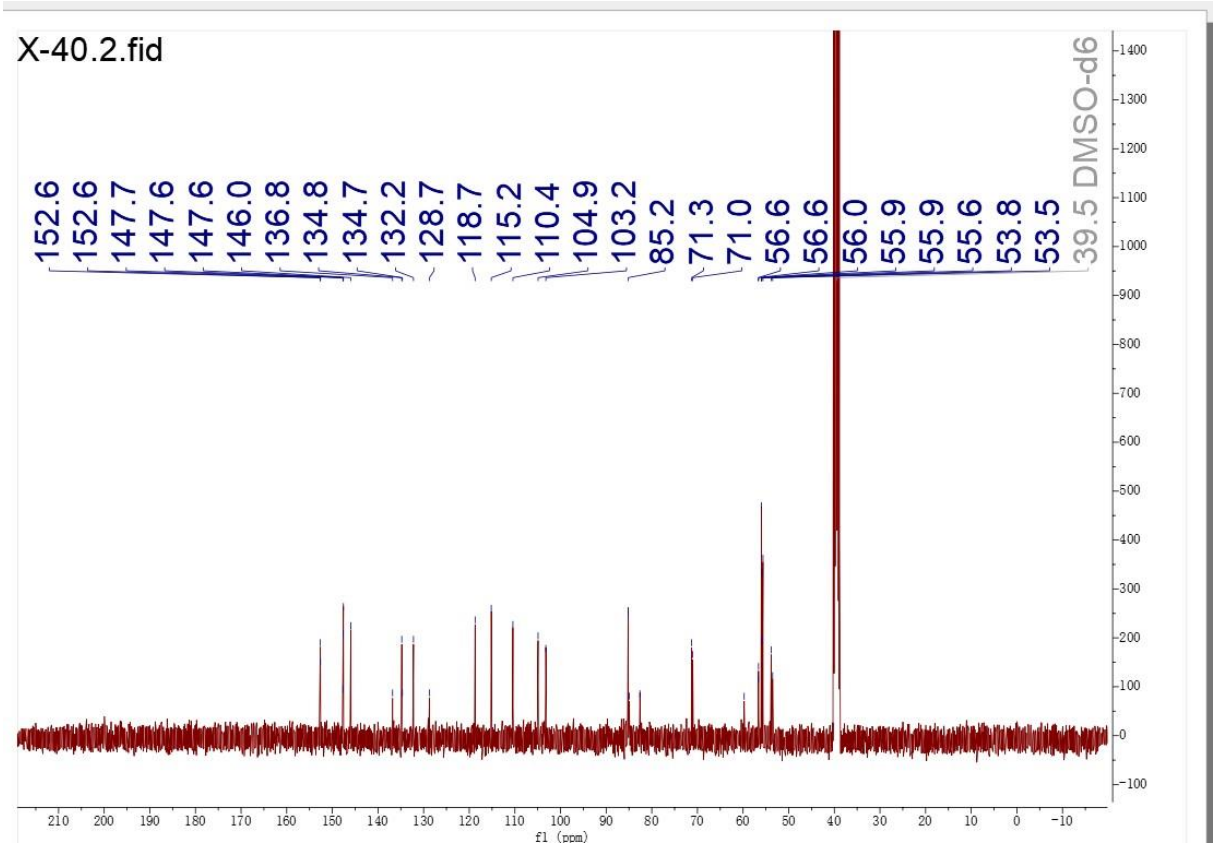


Figure S4: ^{13}C-NMR (100 MHz，DMSO-d_6) spectrum of **1** (xylocarpalignan B)

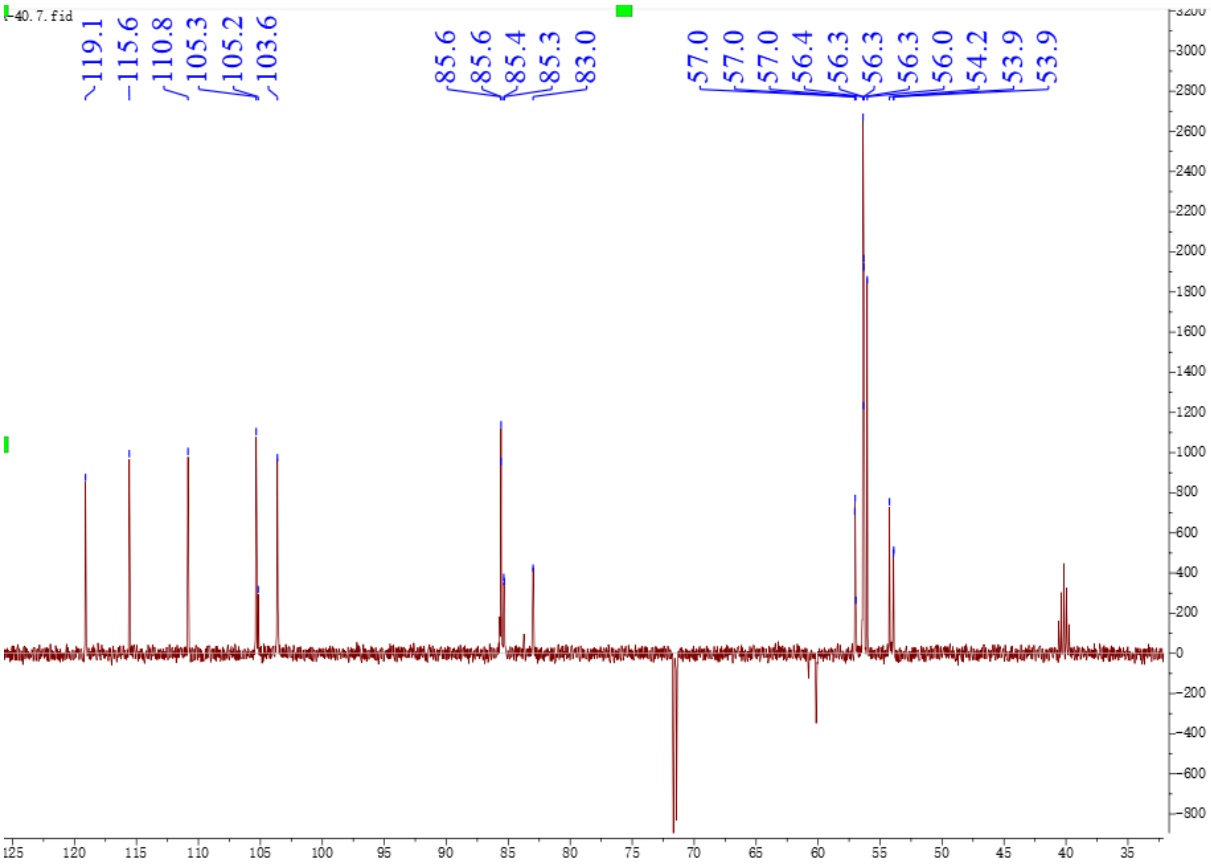


Figure S5:DEPT 135 (100 MHz，DMSO-d_6) spectrum of **1** (xylocarpalignan B)

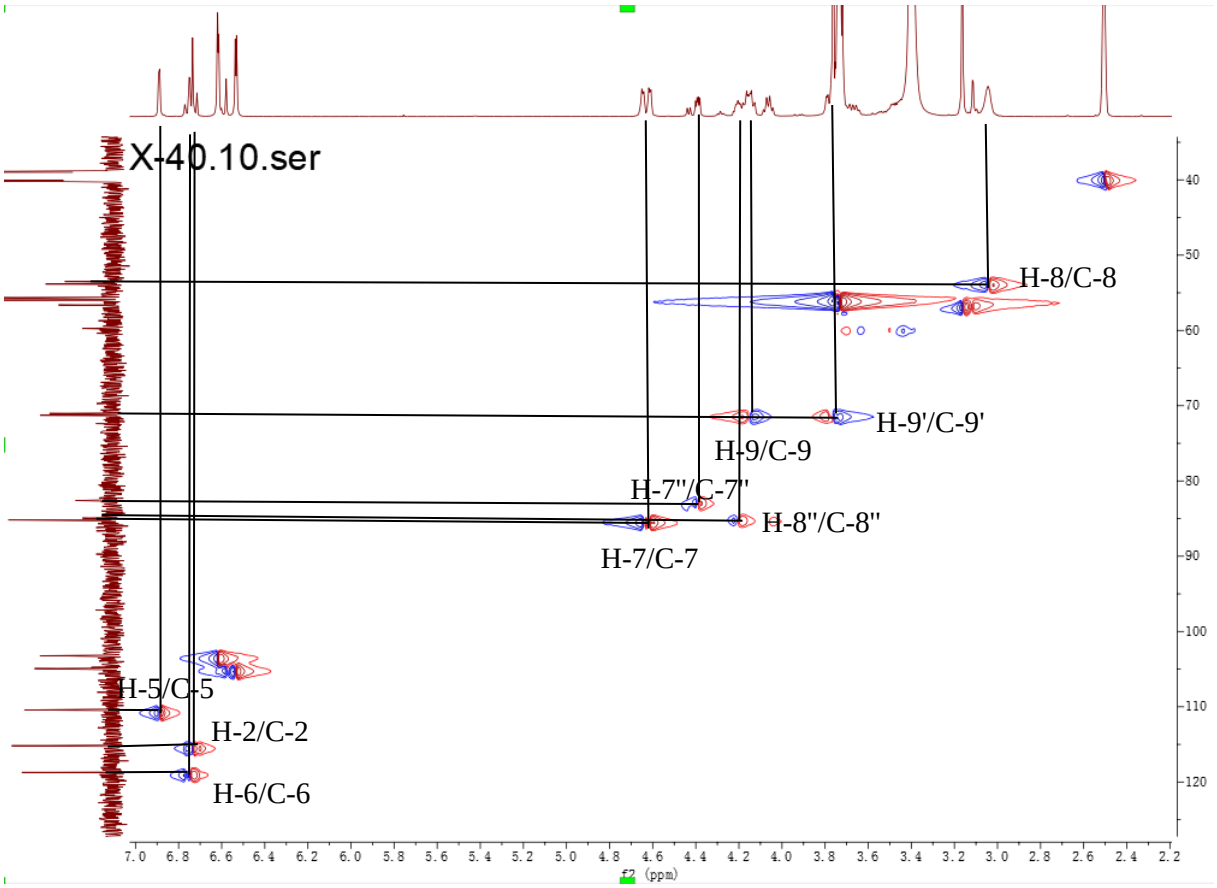


Figure S6: HSQC spectrum of **1** (xylocarpalignan B)

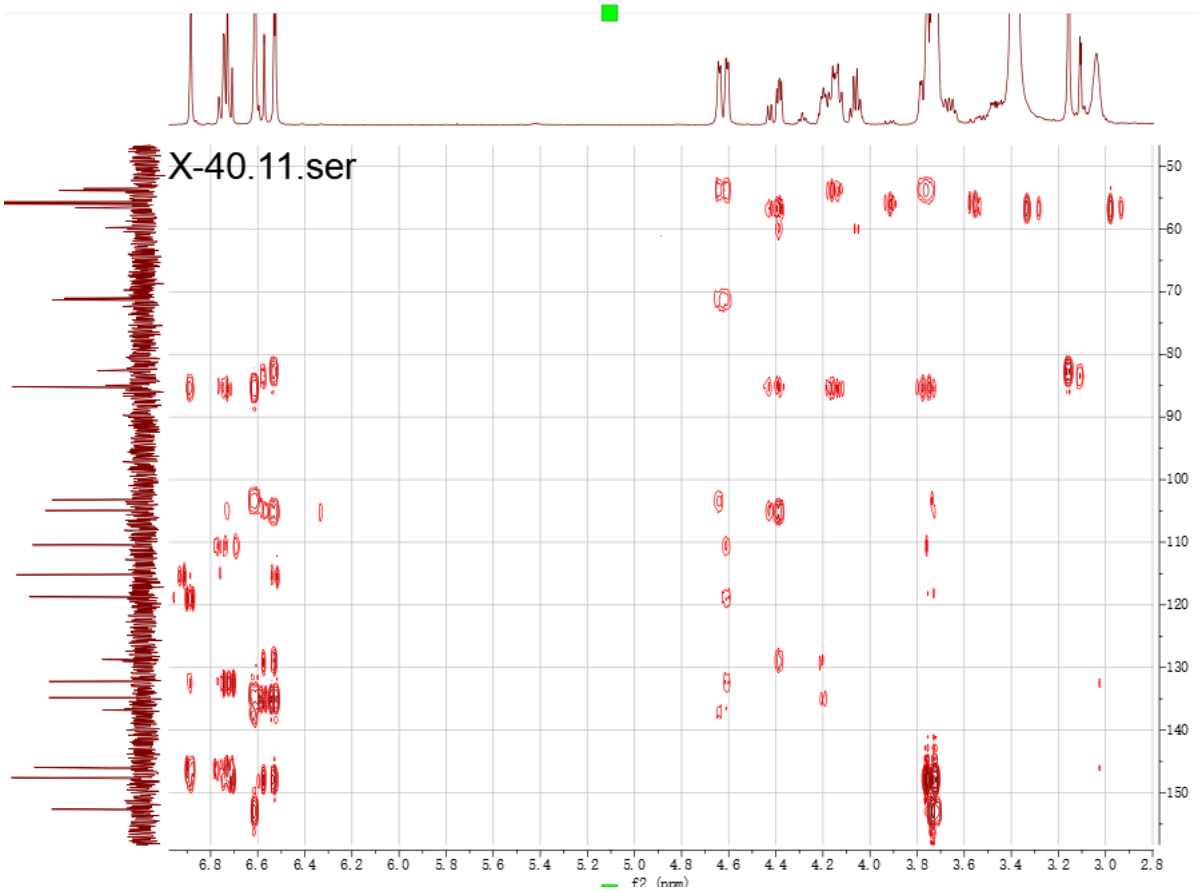


Figure S7: HMBC spectrum of **1** (xylocarpalignan B)

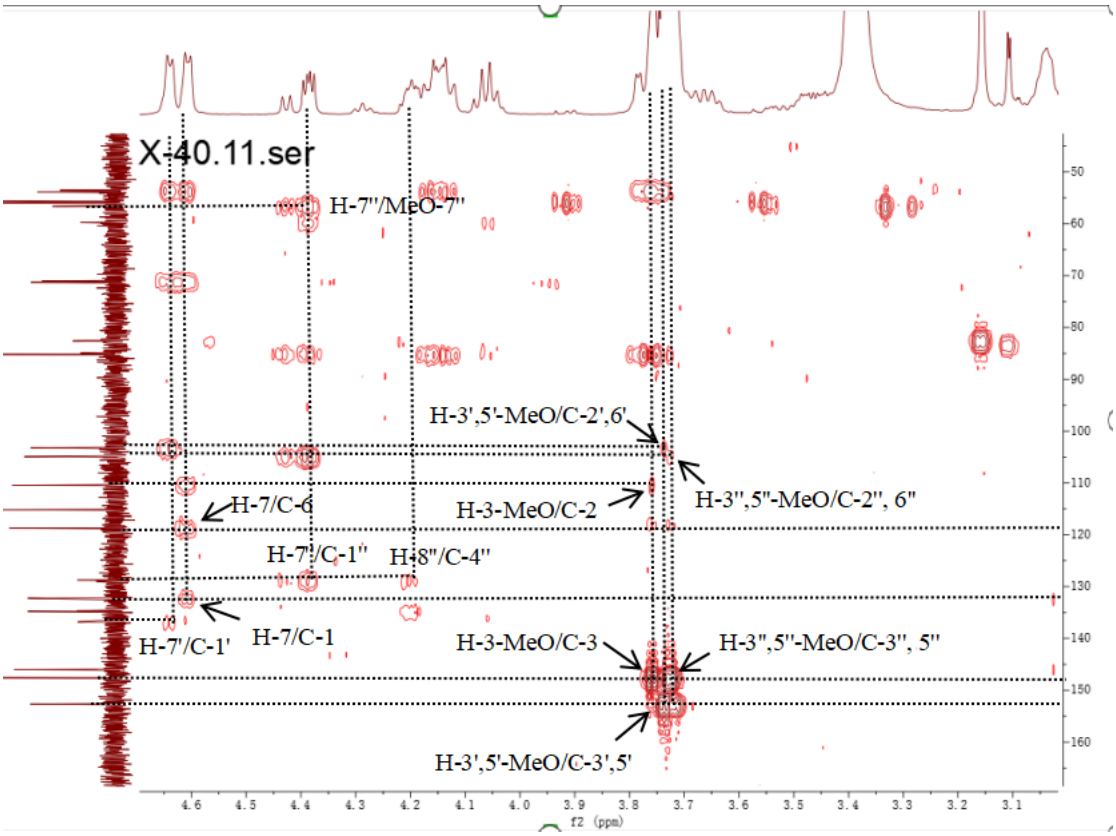


Figure S8: HMBC spectrum of **1** (xylocarpalignan B)(From δ_H 2.9 ppm to δ_H 4.9 ppm)

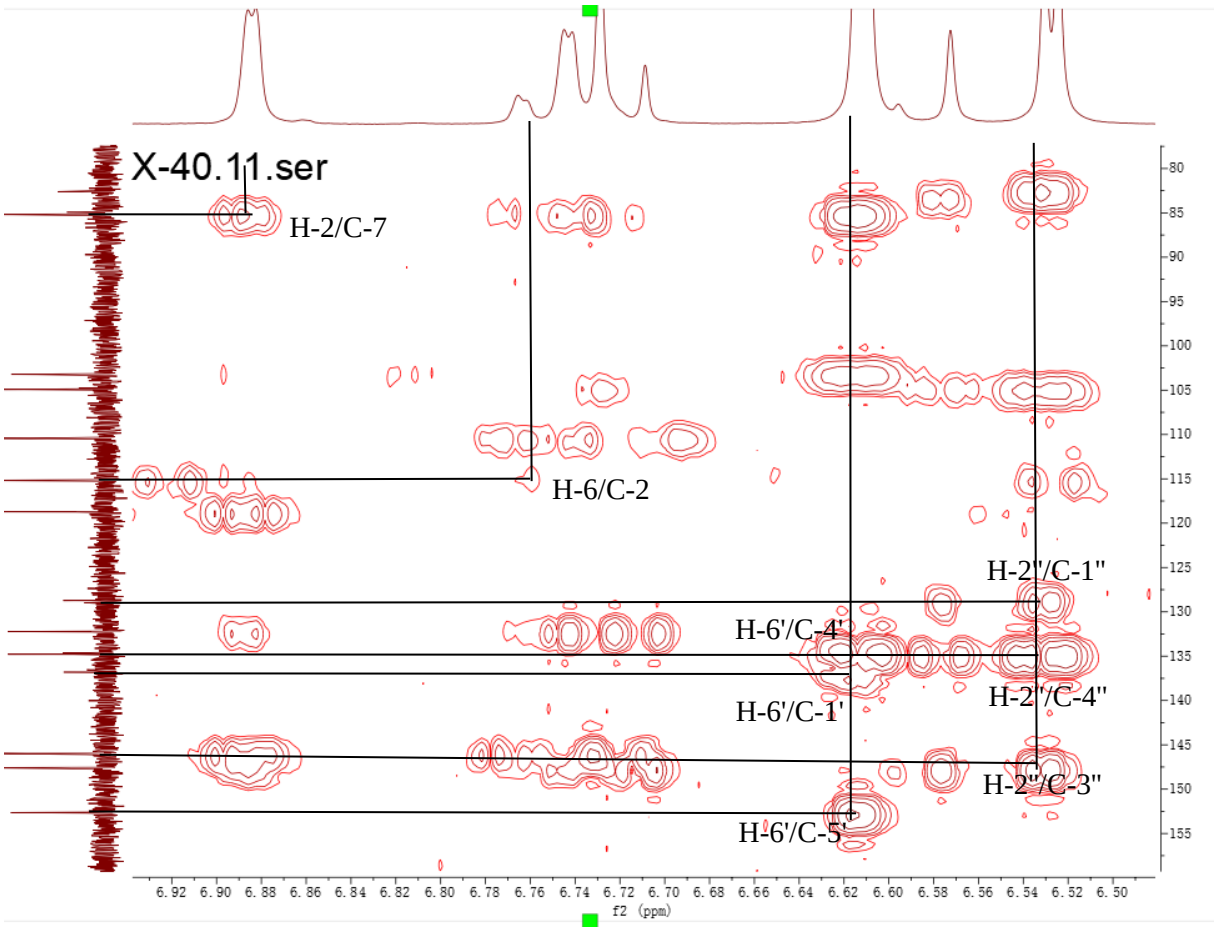


Figure S9: HMBC spectrum of **1** (xylocarpalignan B)(From δ_H 6.50 ppm to δ_H 6.92 ppm)

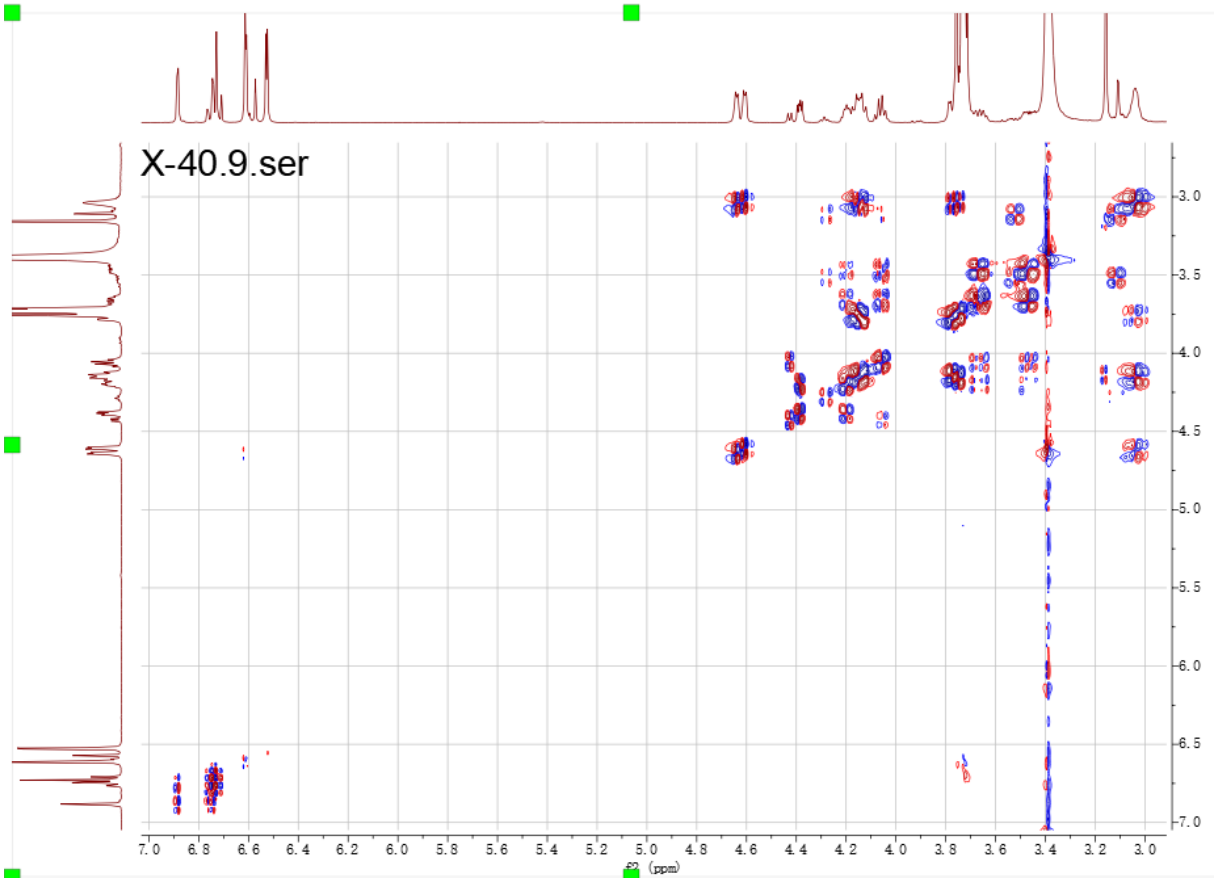


Figure S10: ^{1}H-^{1}H COSY spectrum of **1** (xylocarpalignan B)

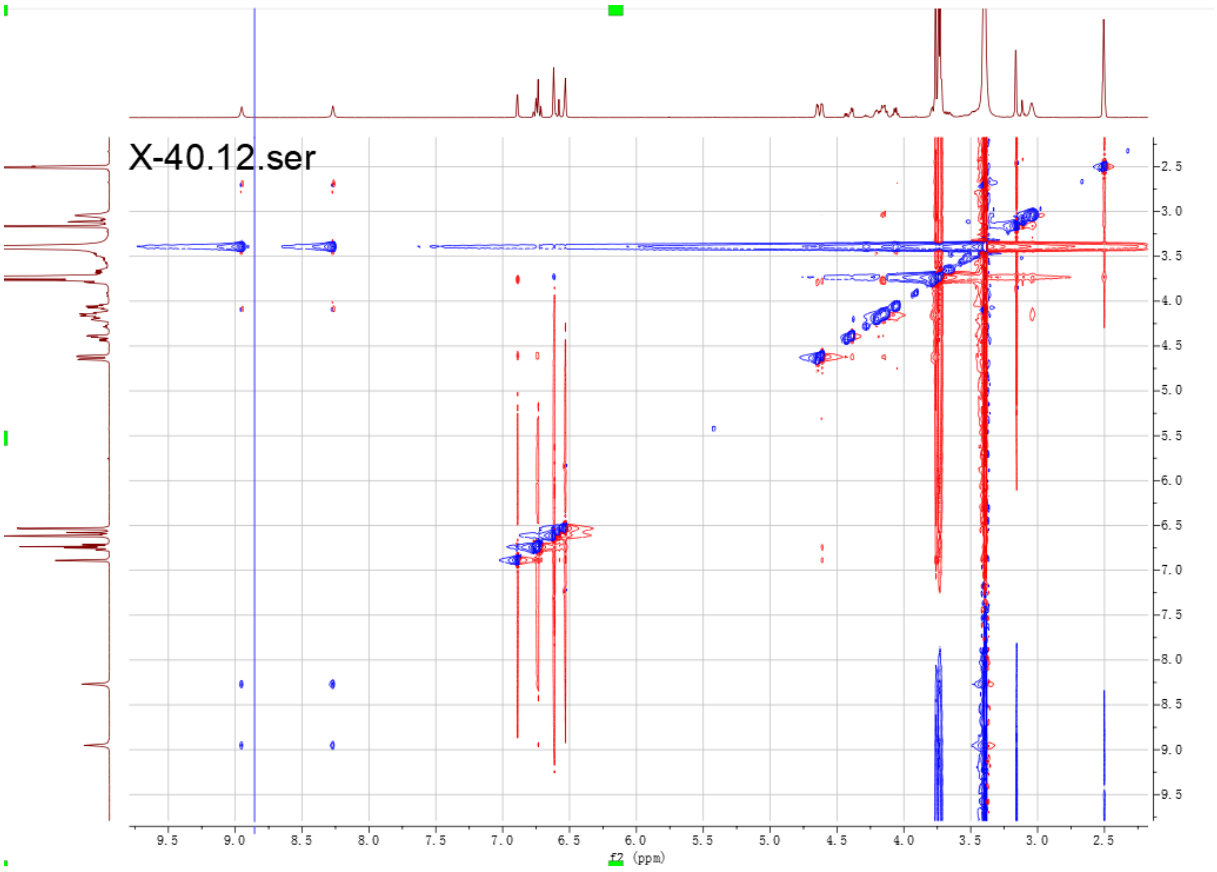


Figure S11: NOESY spectrum of **1** (xylocarpalignan B)

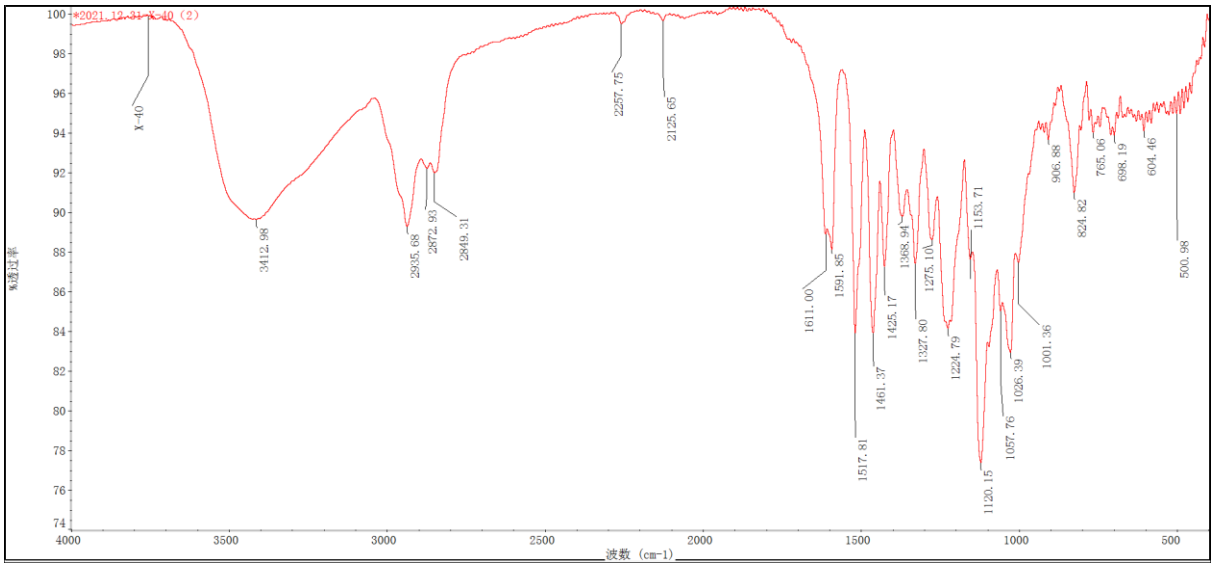


Figure S12: IR spectrum of **1** (xylocarpalignan B)

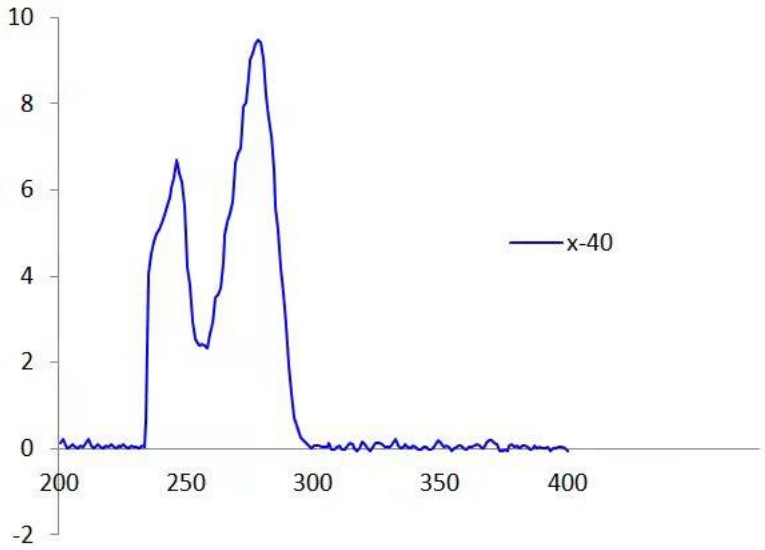


Figure S13: CD spectrum of **1** (xylocarpalignan B)