Supporting Information

***Rec. Nat. Prod*. 18:2 (2024) 290-295**

Phytosteroids from roots of *Psammosilene tunicoides* W.C.Wu et C.Y.Wu

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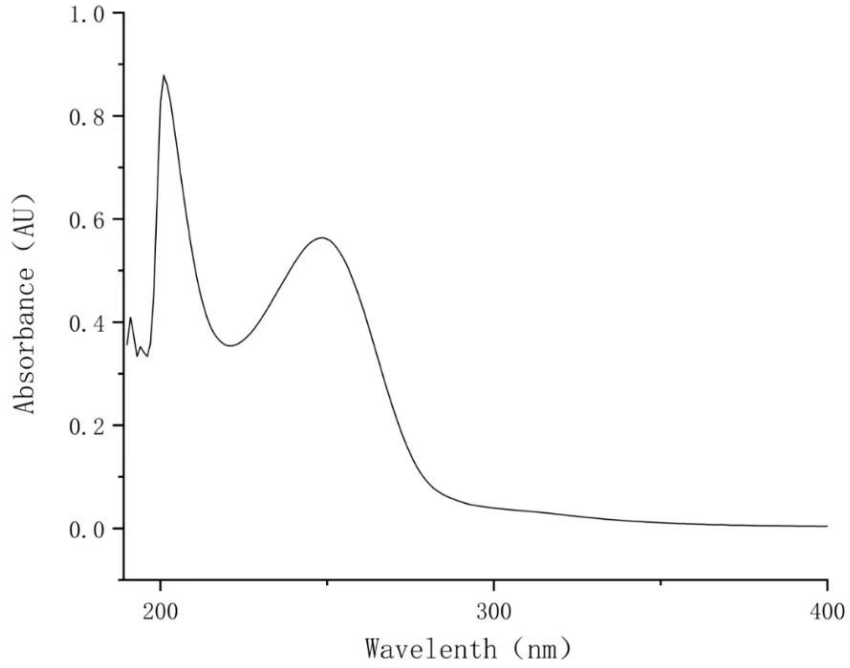


Figure S1: UV spectrum of **1** (furoecdysterone)

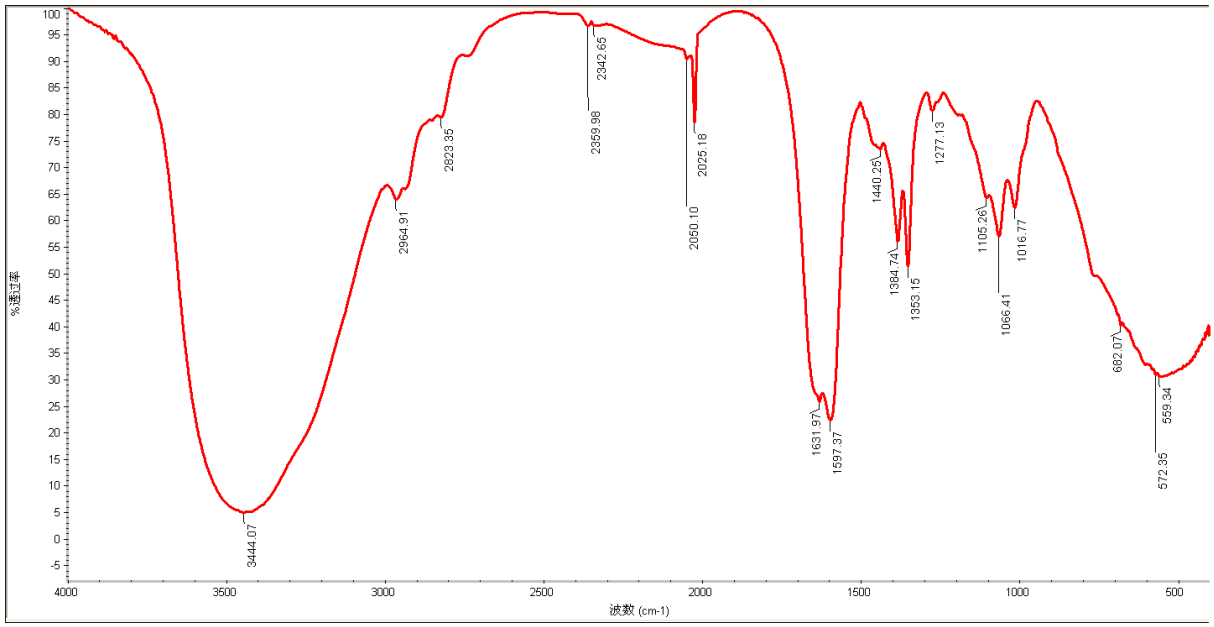


Figure S2: IR spectrum of **1** (furoecdysterone)

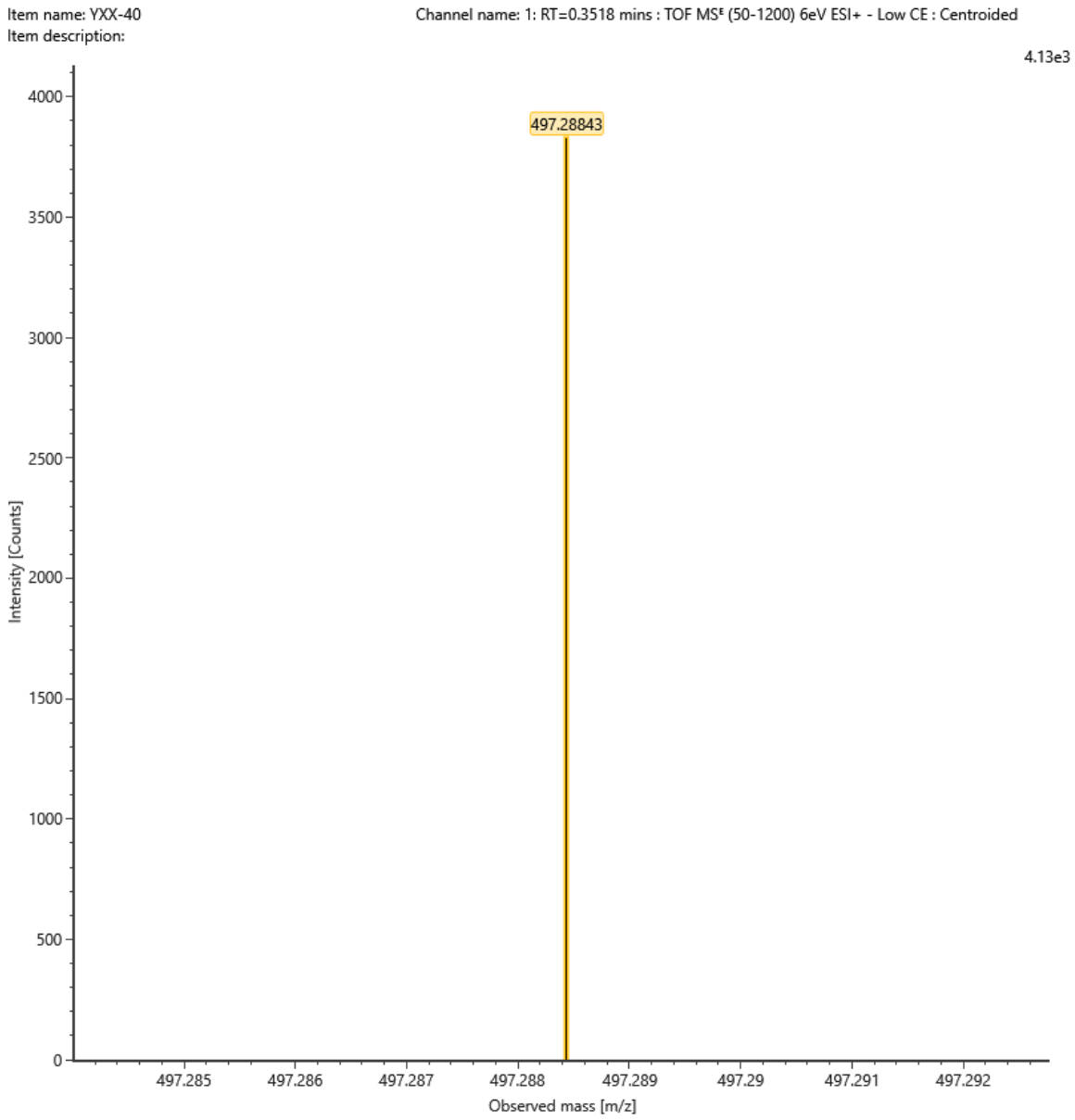
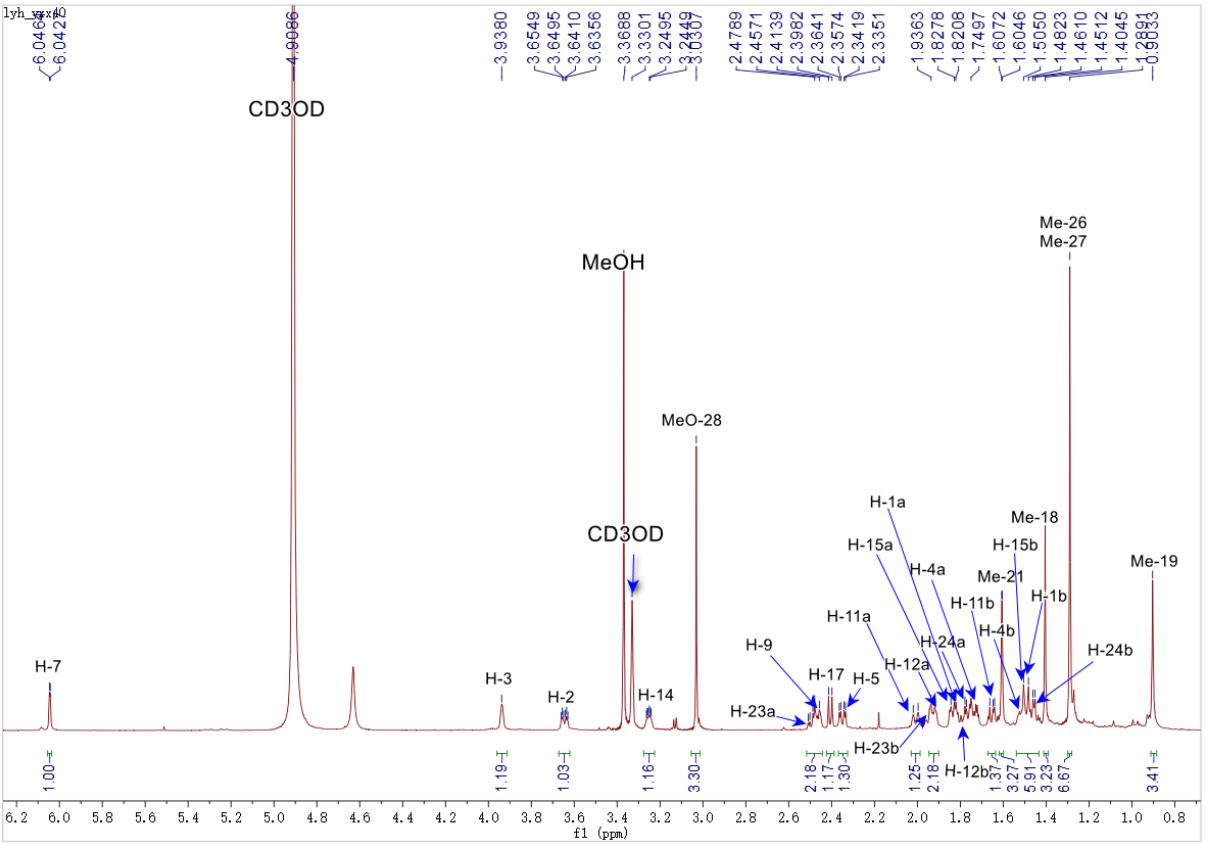
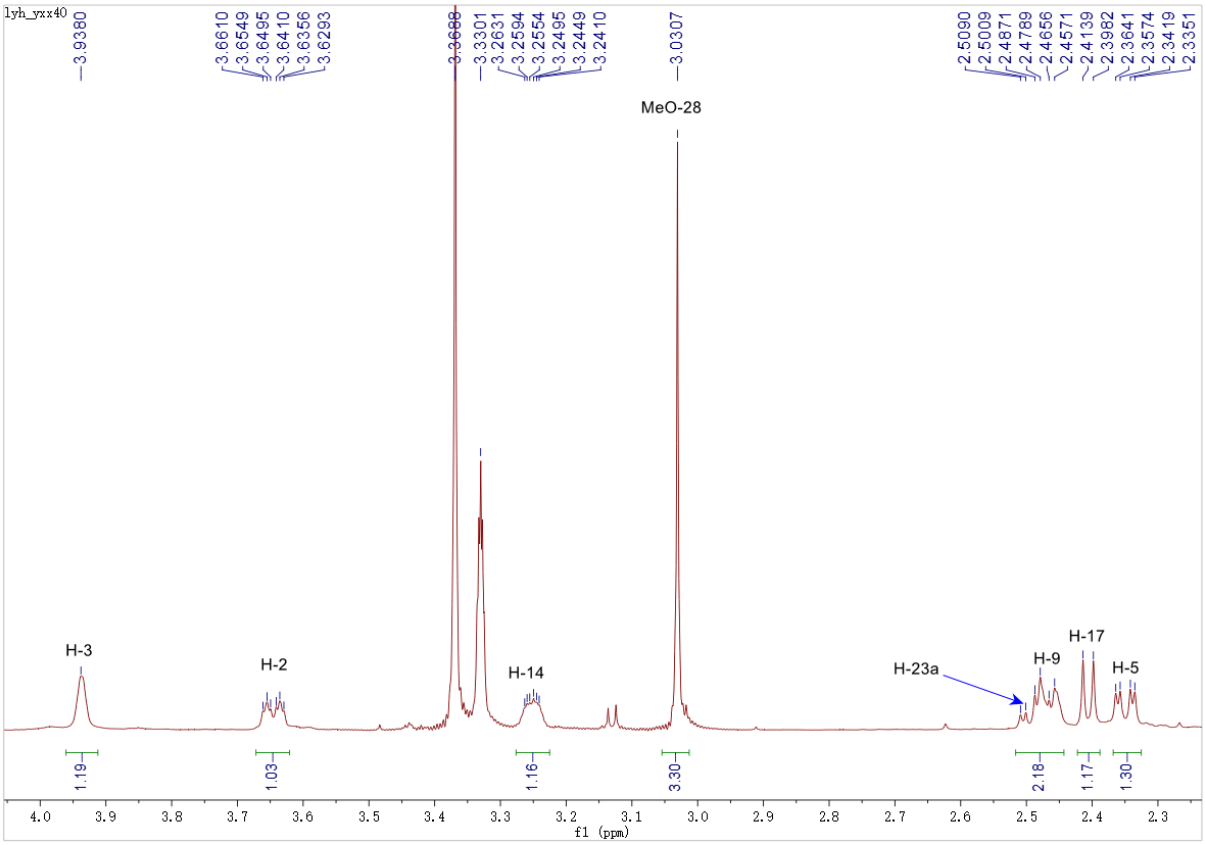


Figure S3: HR-ESI-MS spectrum of **1** (furoecdysterone)





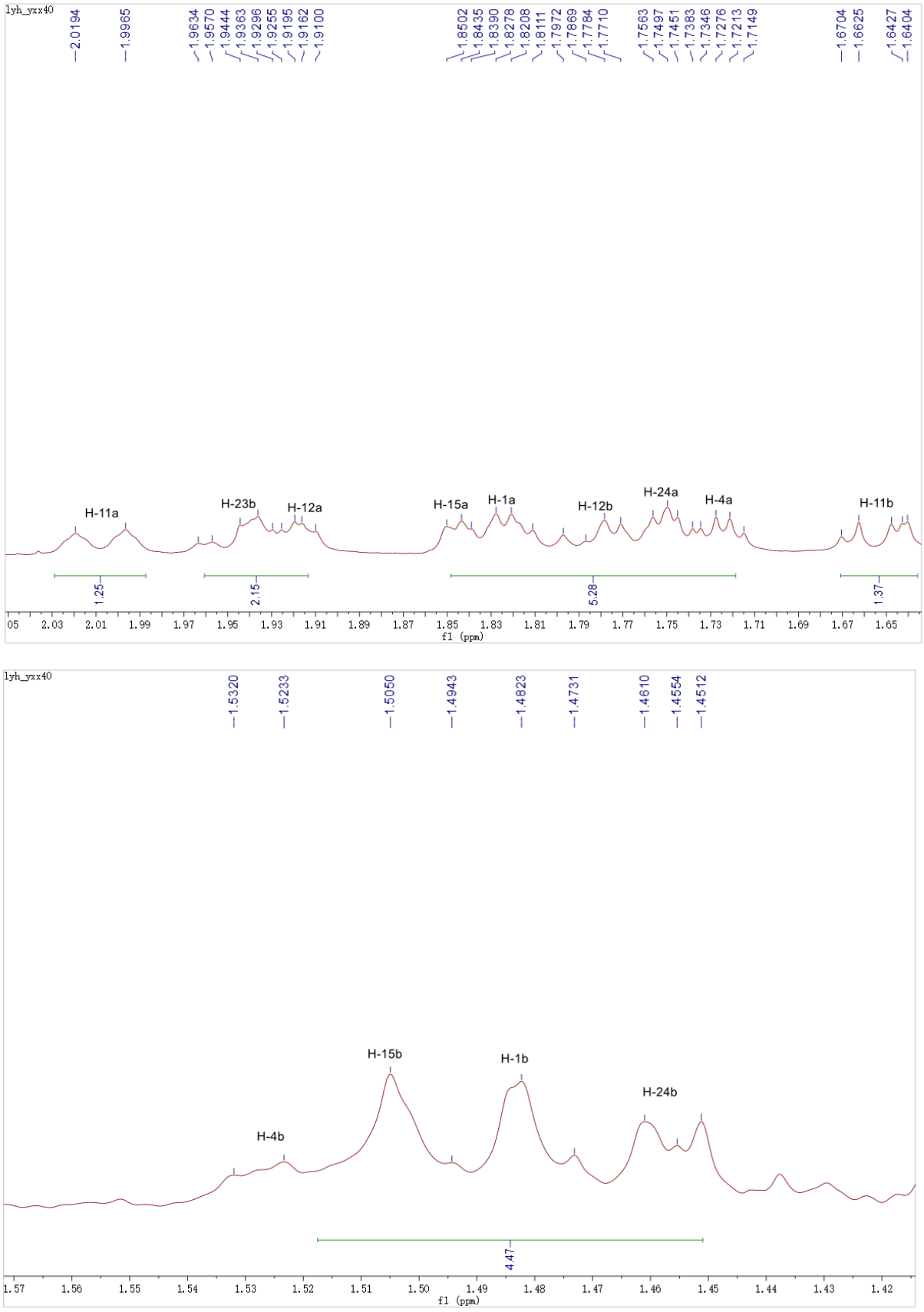


Figure S4: ^{1}H-NMR (400 MHz, CD_3OD) spectrum of **1** (furoecdysterone)

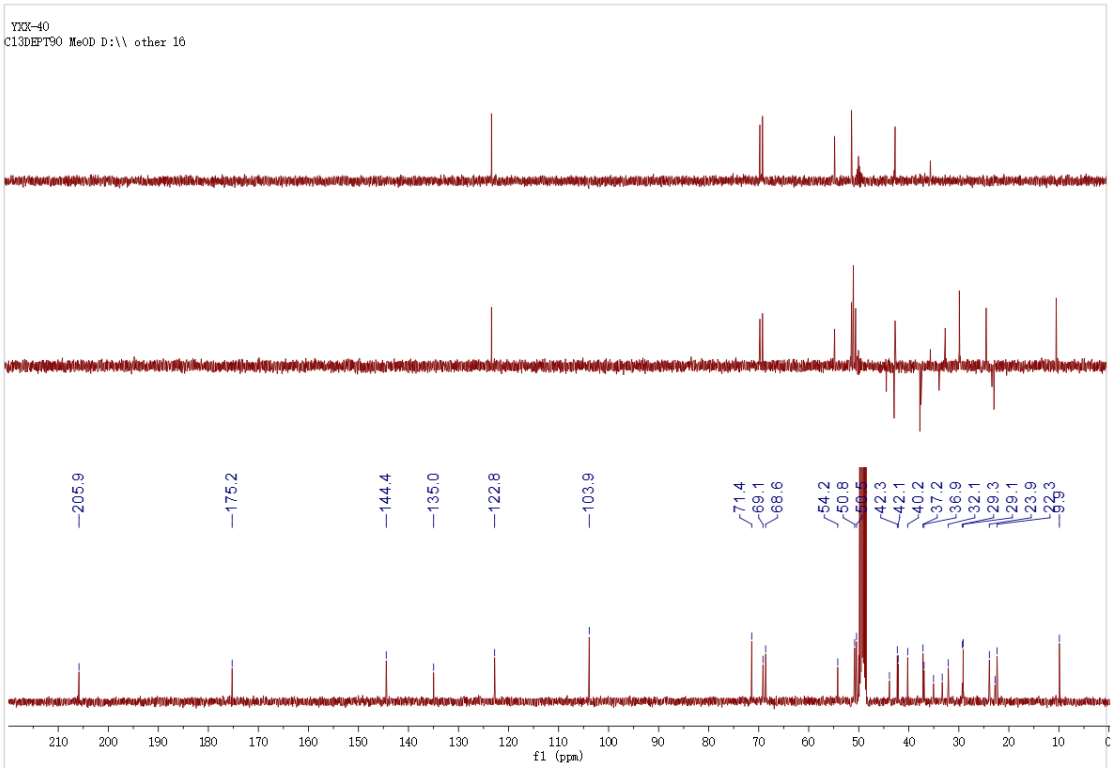


Figure S5: ^{13}C and DEPT NMR (100 MHz, CD_3OD) spectrum of **1** (furoecdysterone)

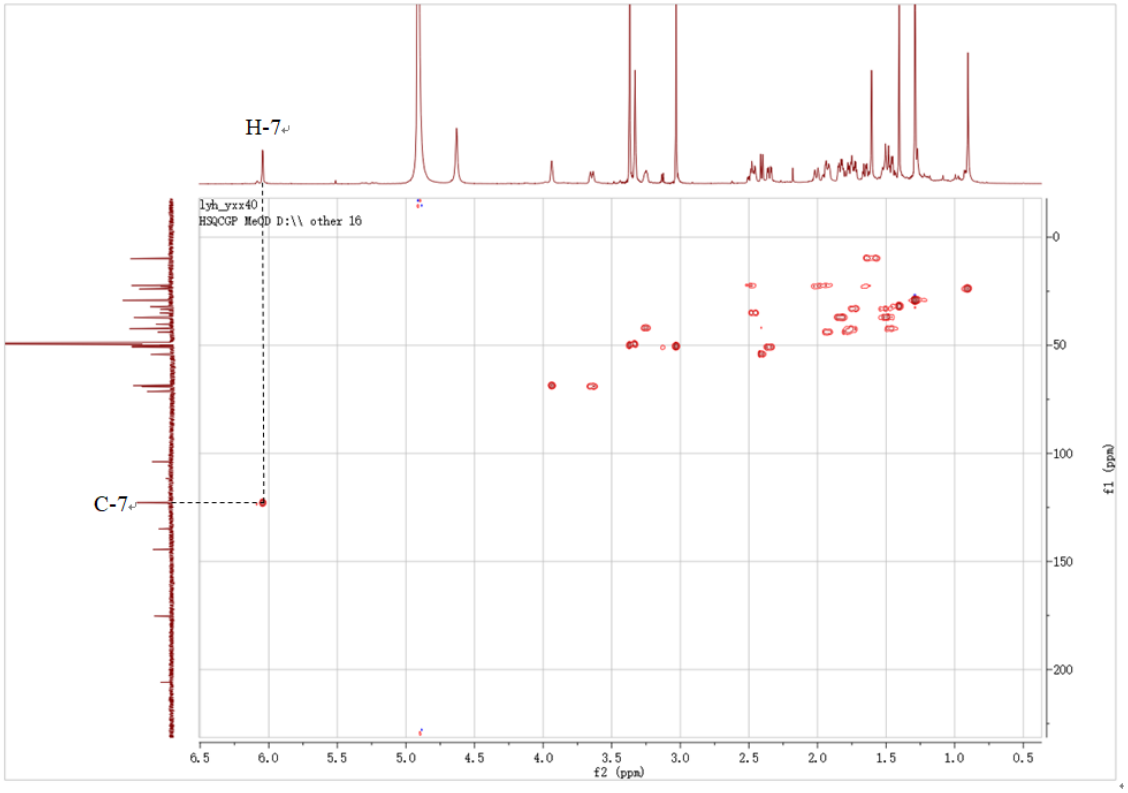


Figure S6: HSQC spectrum of **1** (furoecdysterone)

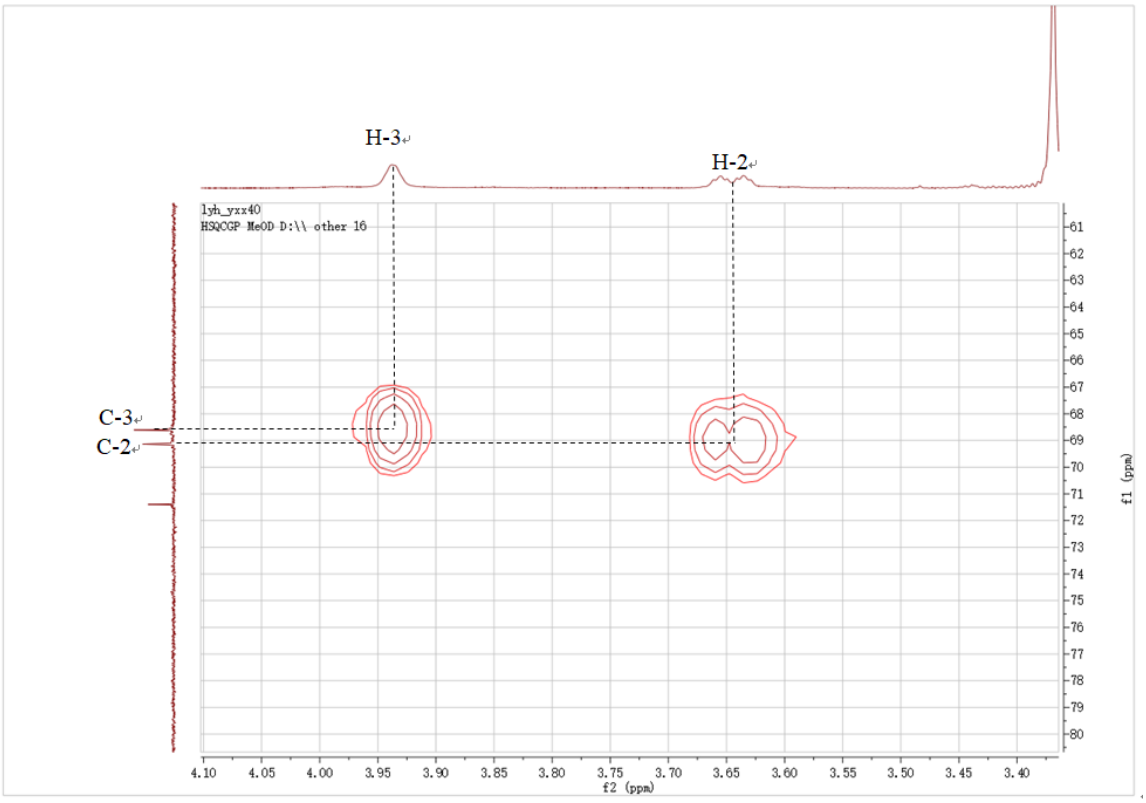


Figure S7: HSQC spectrum of **1** (furoecdysterone) (From δ_H 3.40 ppm to δ_H 4.00 ppm)

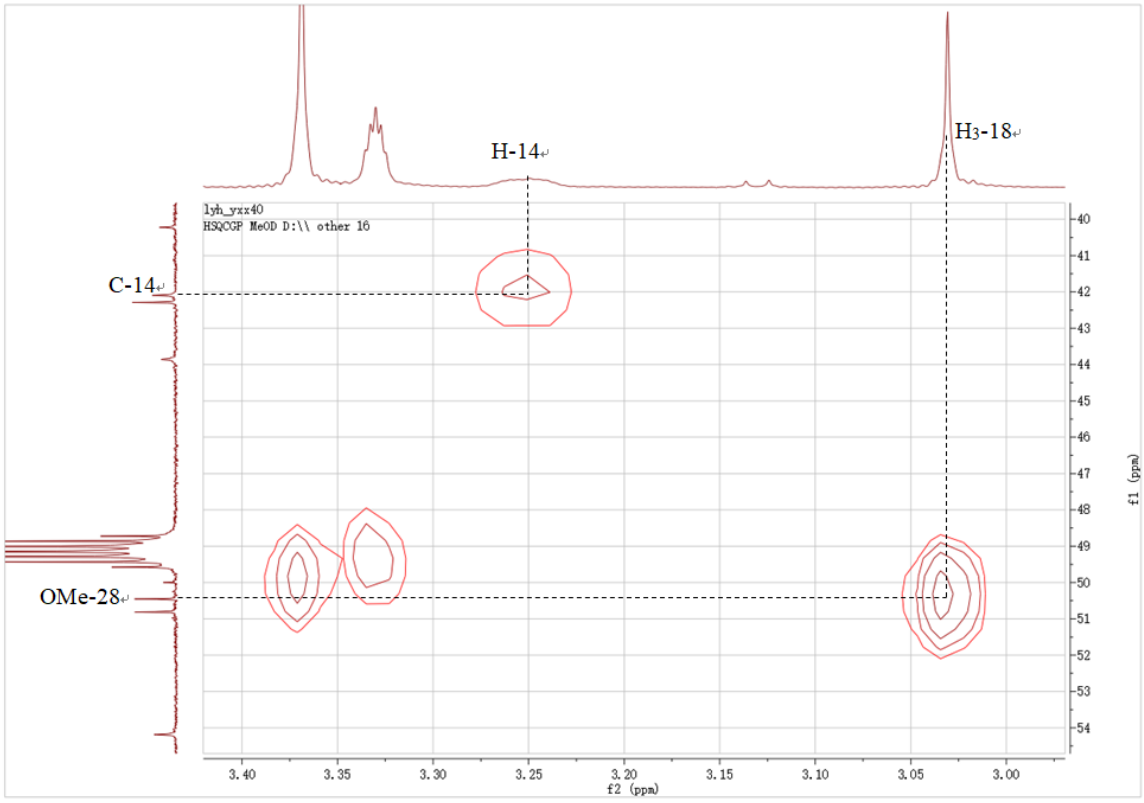


Figure S8: HSQC spectrum of **1** (furoecdysterone) (From δ_H 3.00 ppm to δ_H 3.40 ppm)

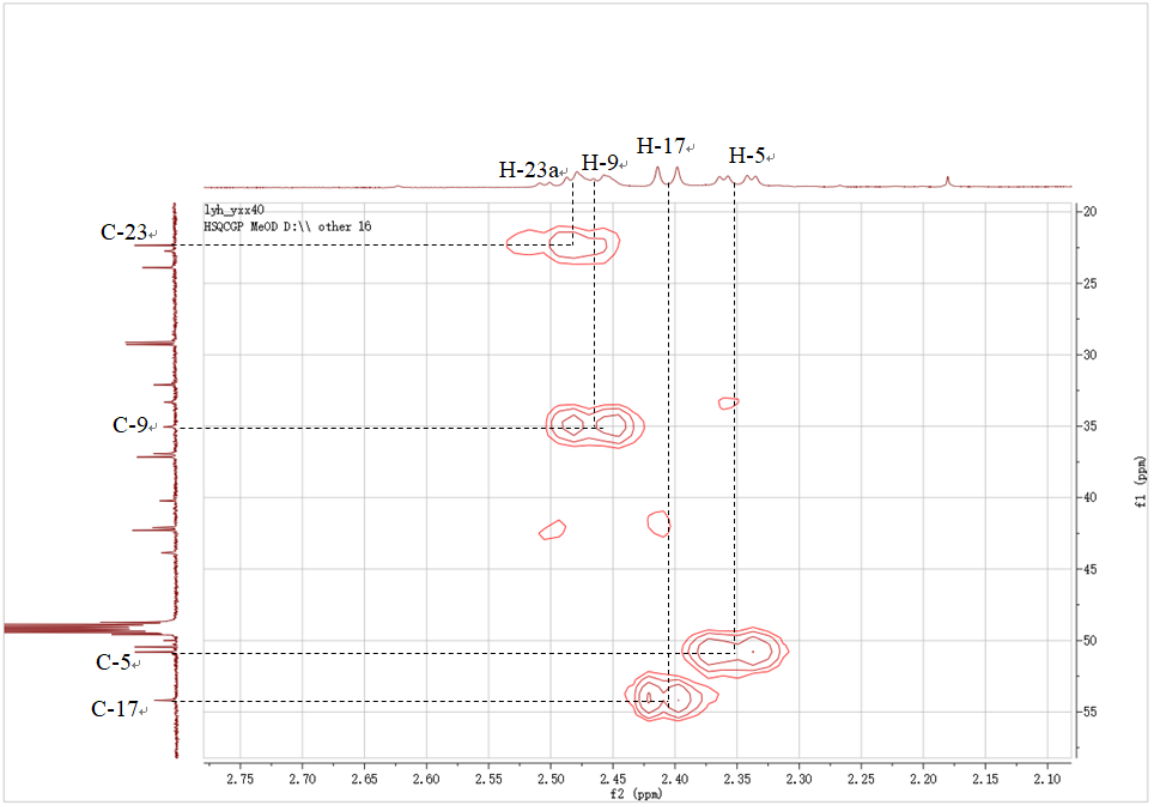


Figure S9: HSQC spectrum of **1** (furoecdysterone) (From δ_H 2.10 ppm to δ_H 2.75 ppm)

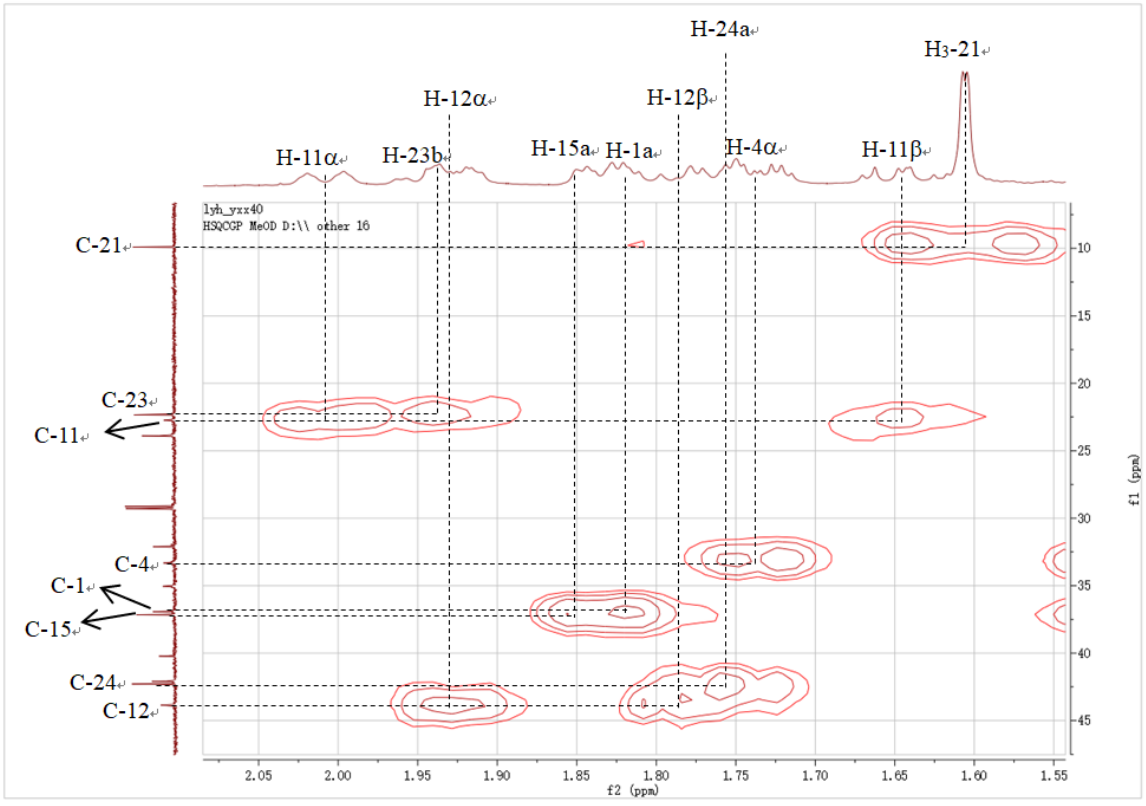


Figure S10: HSQC spectrum of **1** (furoecdysterone) (From δ_H 1.50 ppm to δ_H 2.05 ppm)

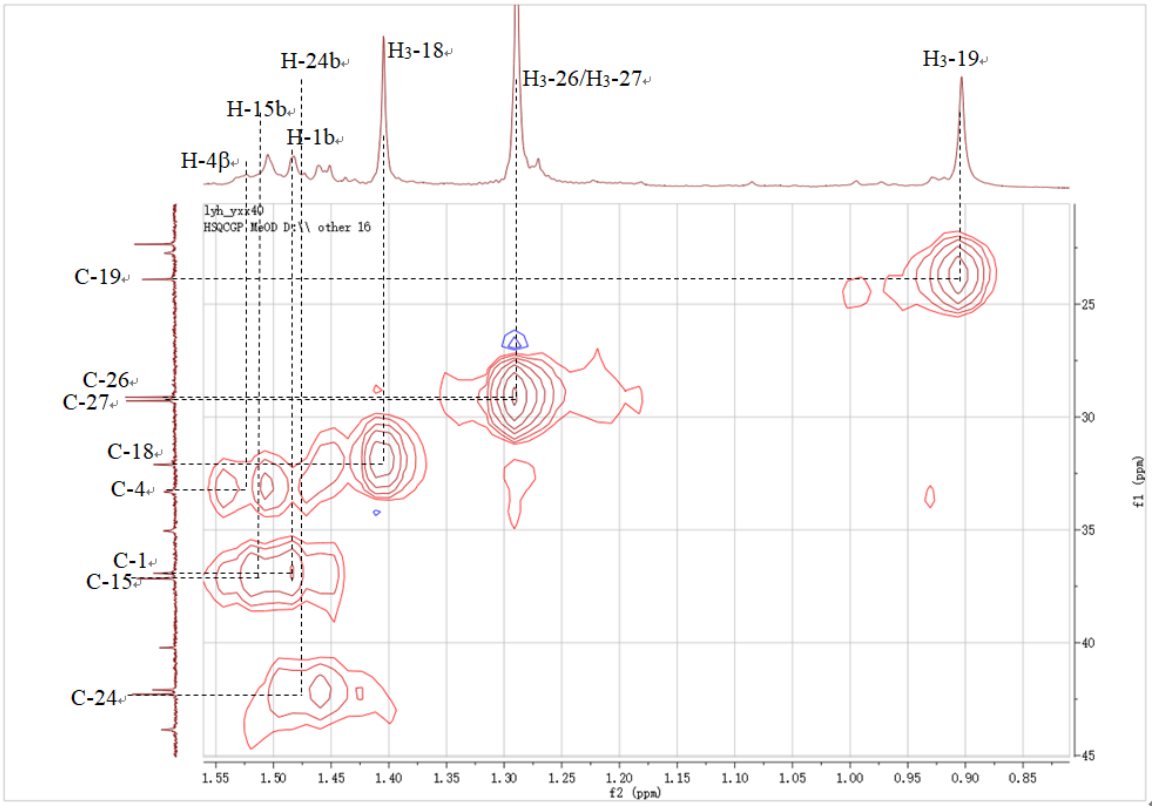


Figure S11: HSQC spectrum of **1** (furoecdysterone) (From δ_H 0.85 ppm to δ_H 1.55 ppm)

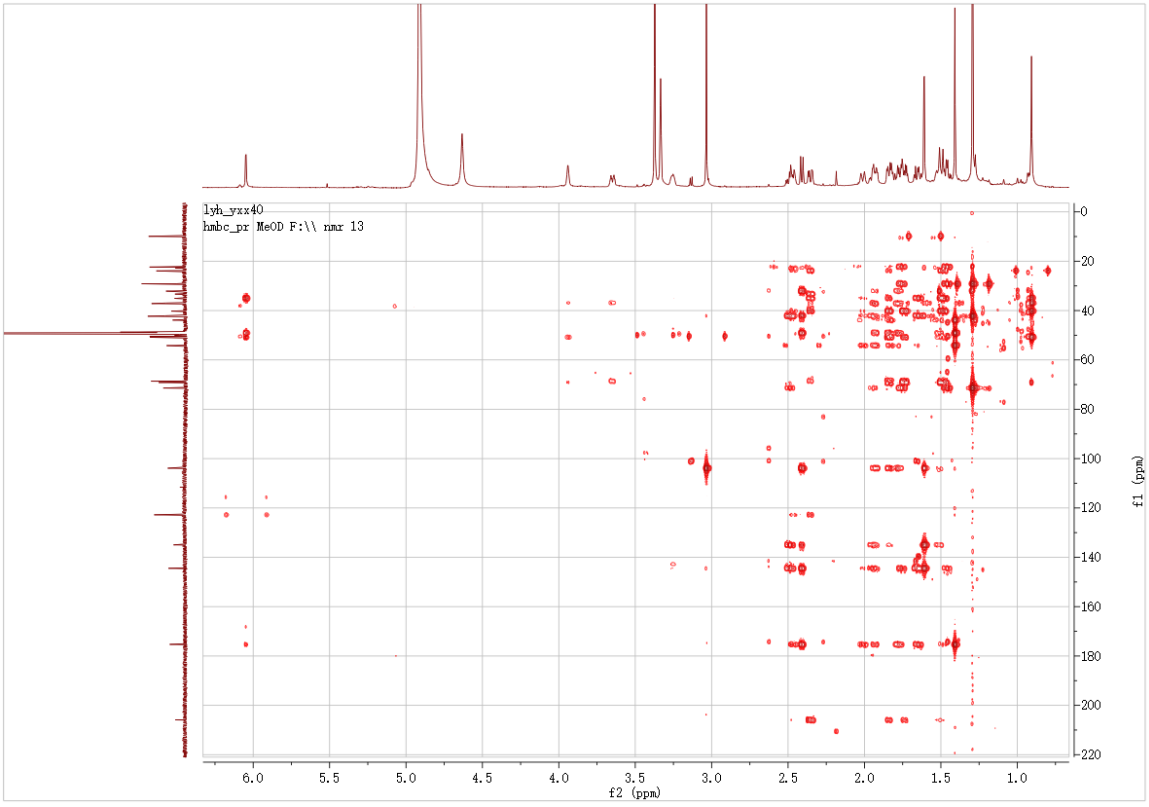
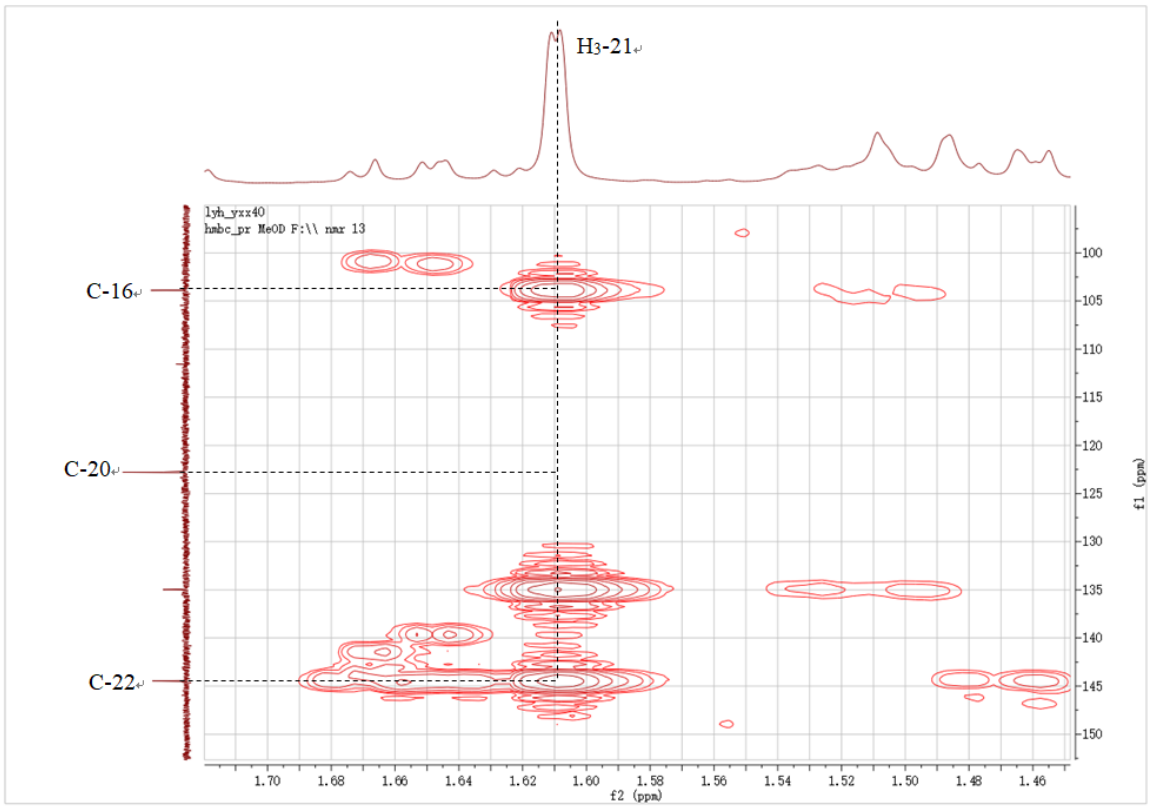
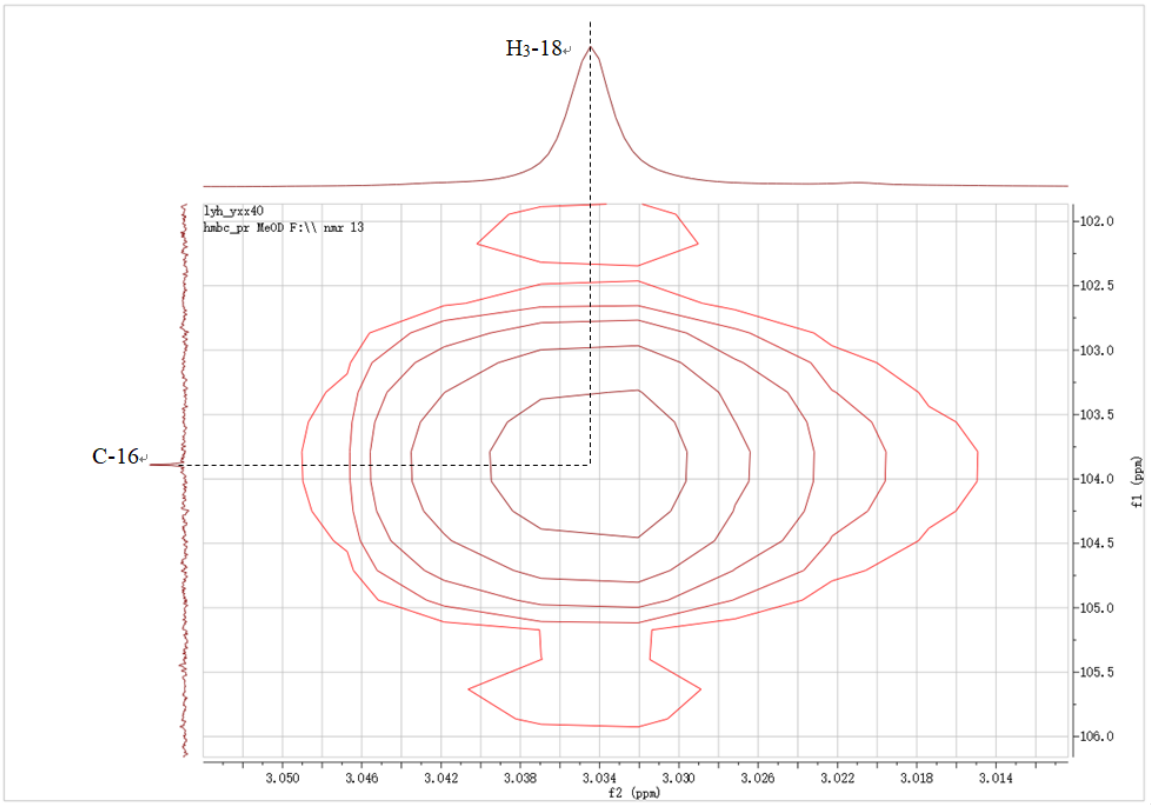
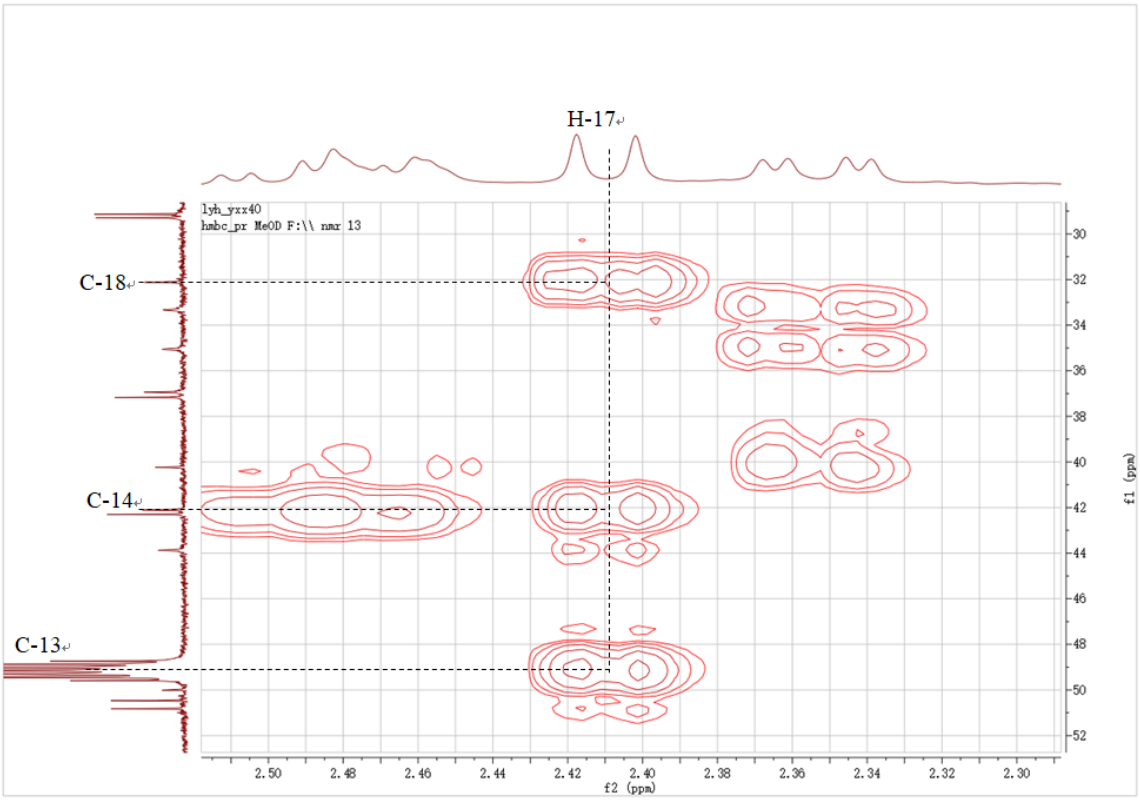
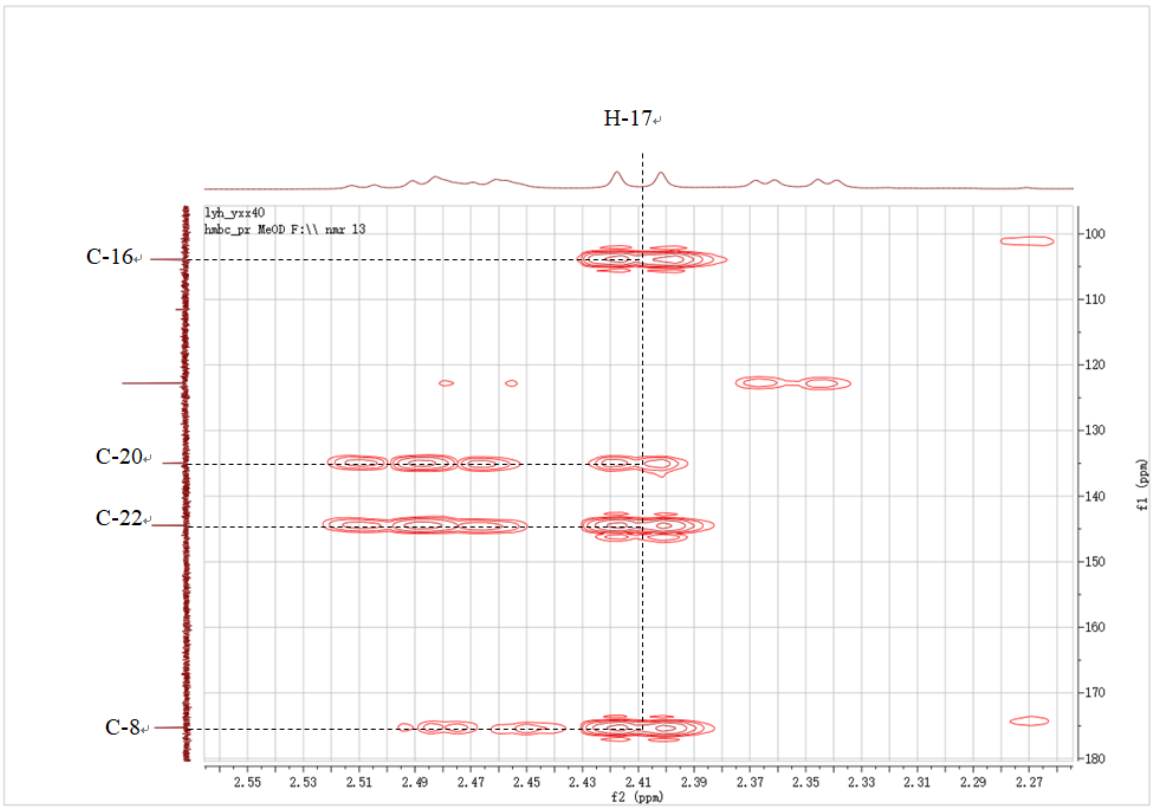


Figure S12: HMBC spectrum of **1** (furoecdysterone)









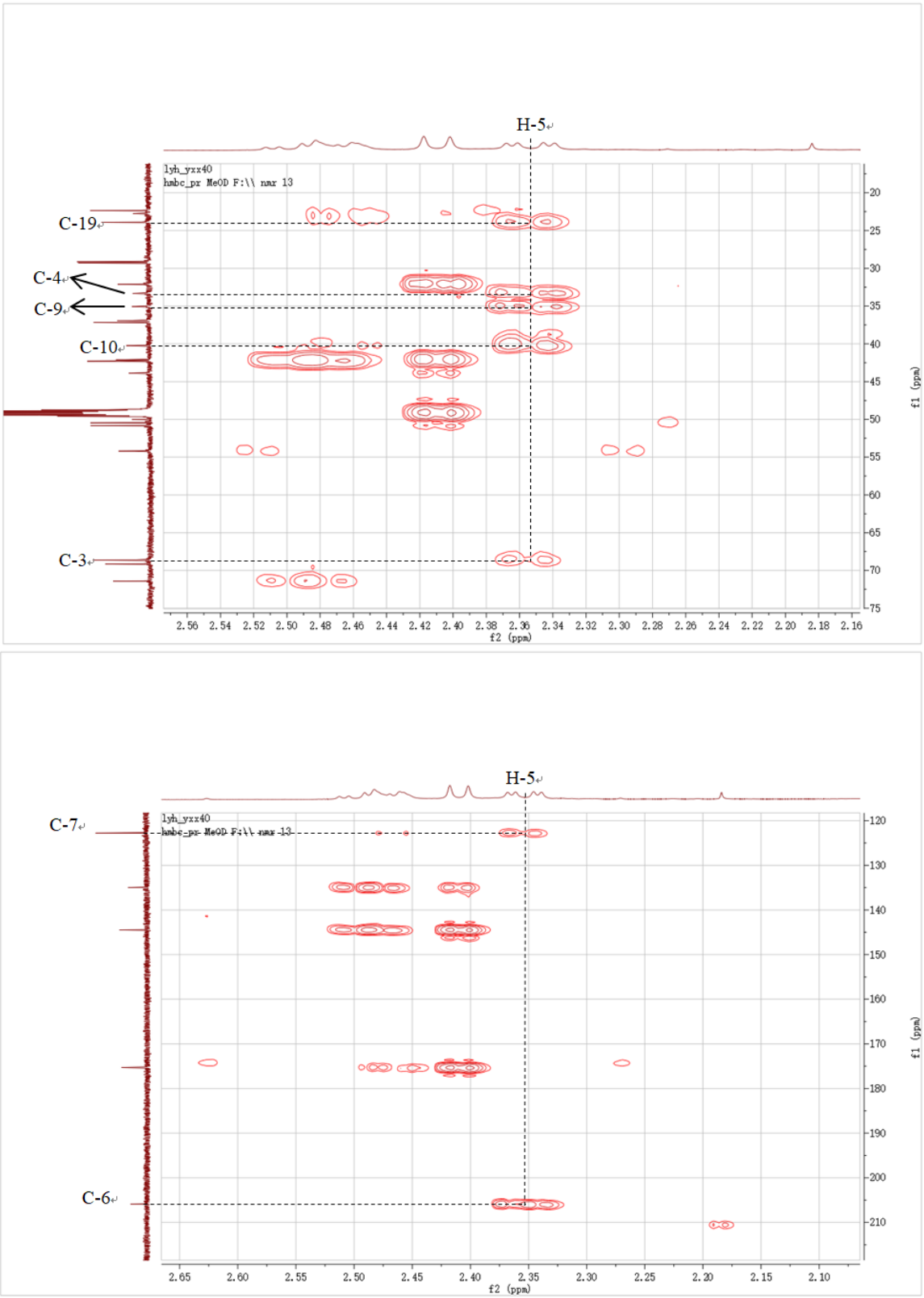


Figure S13: Key HMBC spectrum of **1** (furoecdysterone) (From δ_C 20 ppm to δ_C 210 ppm)

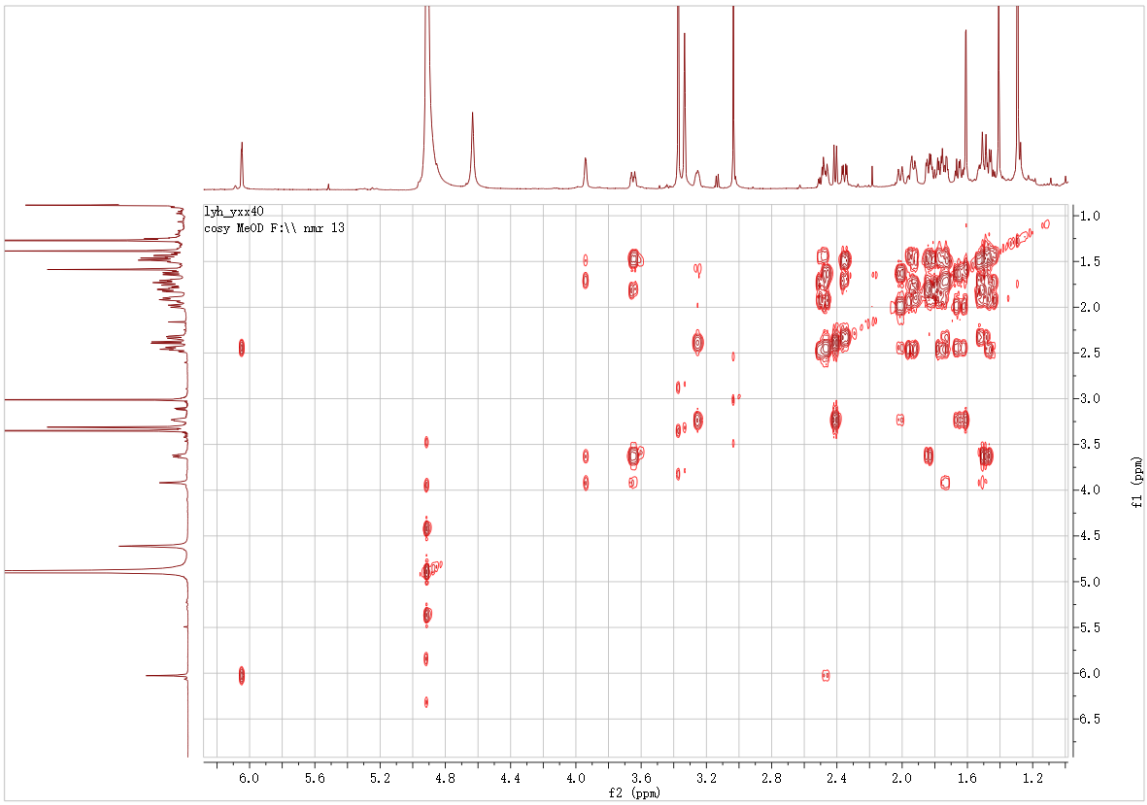


Figure S14: ^{1}H-^{1}H COSY spectrum of **1** (furoecdysterone)

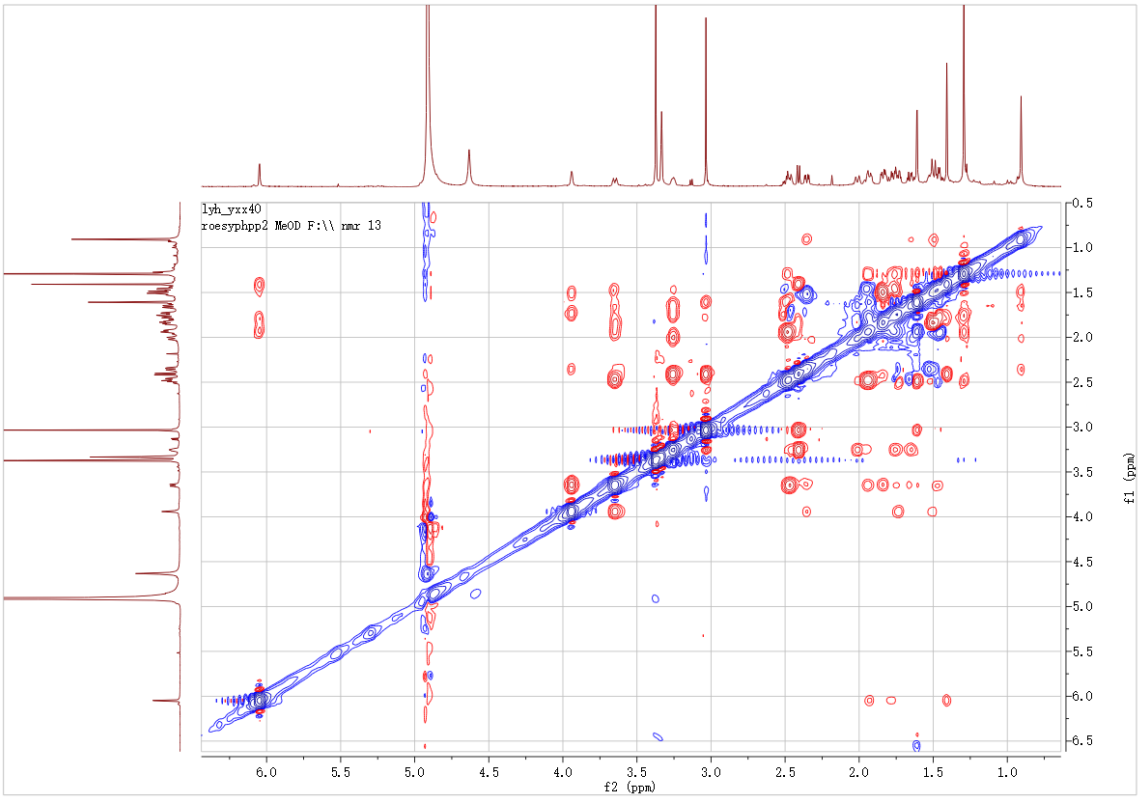
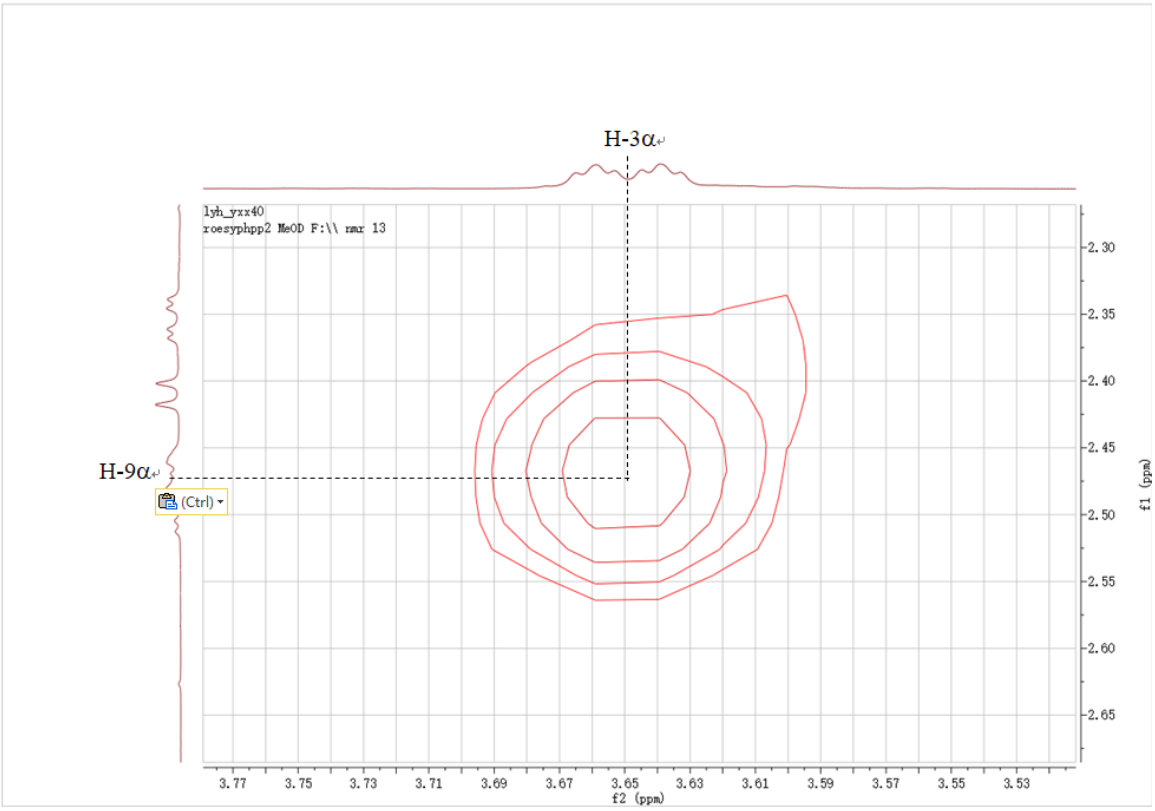
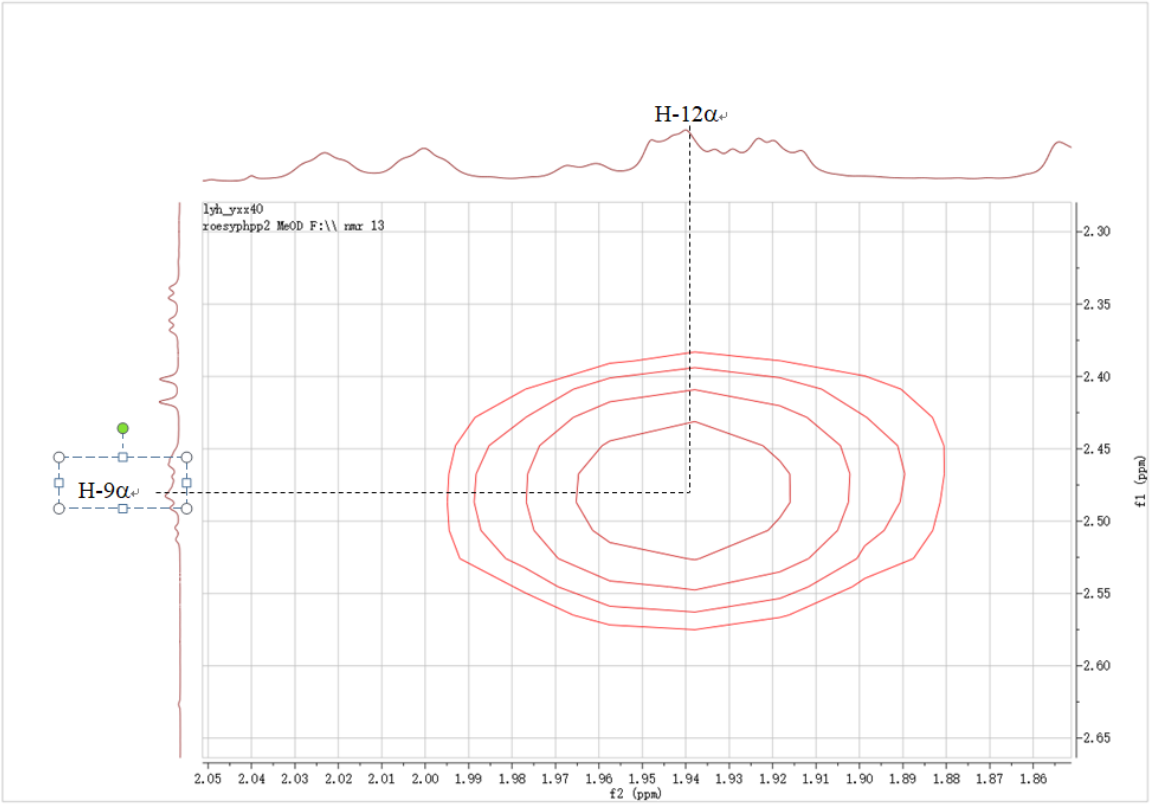
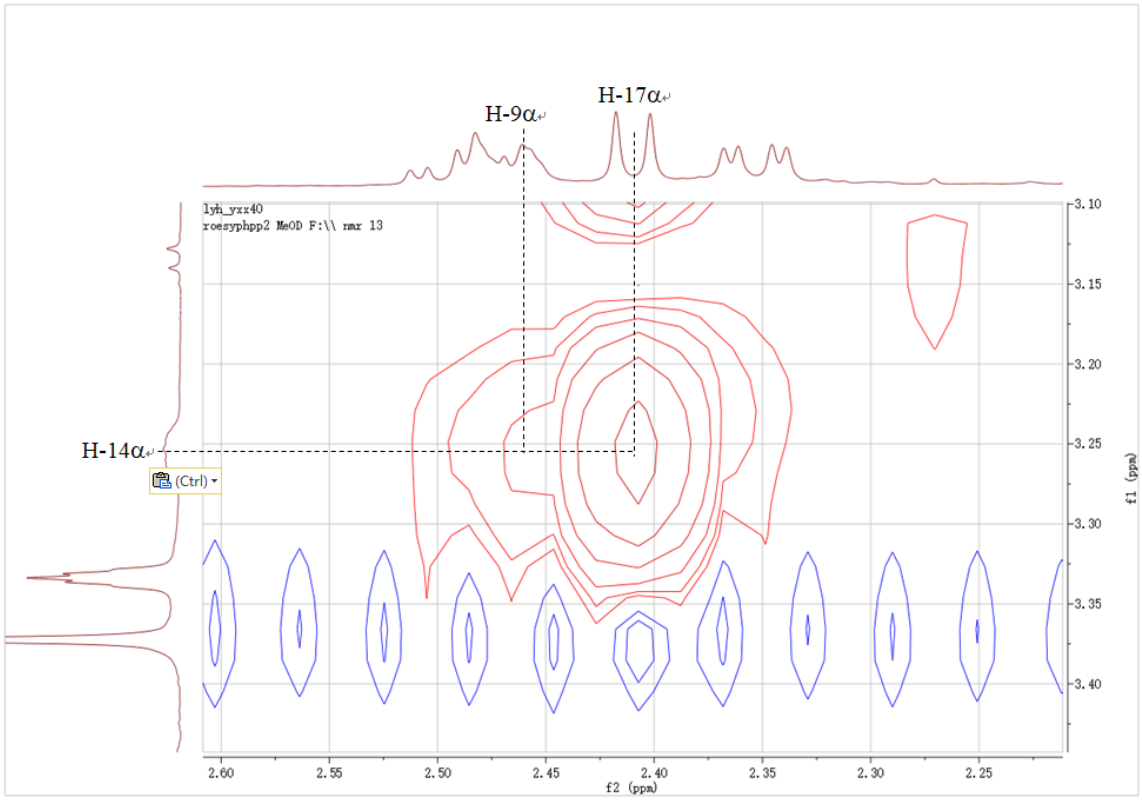
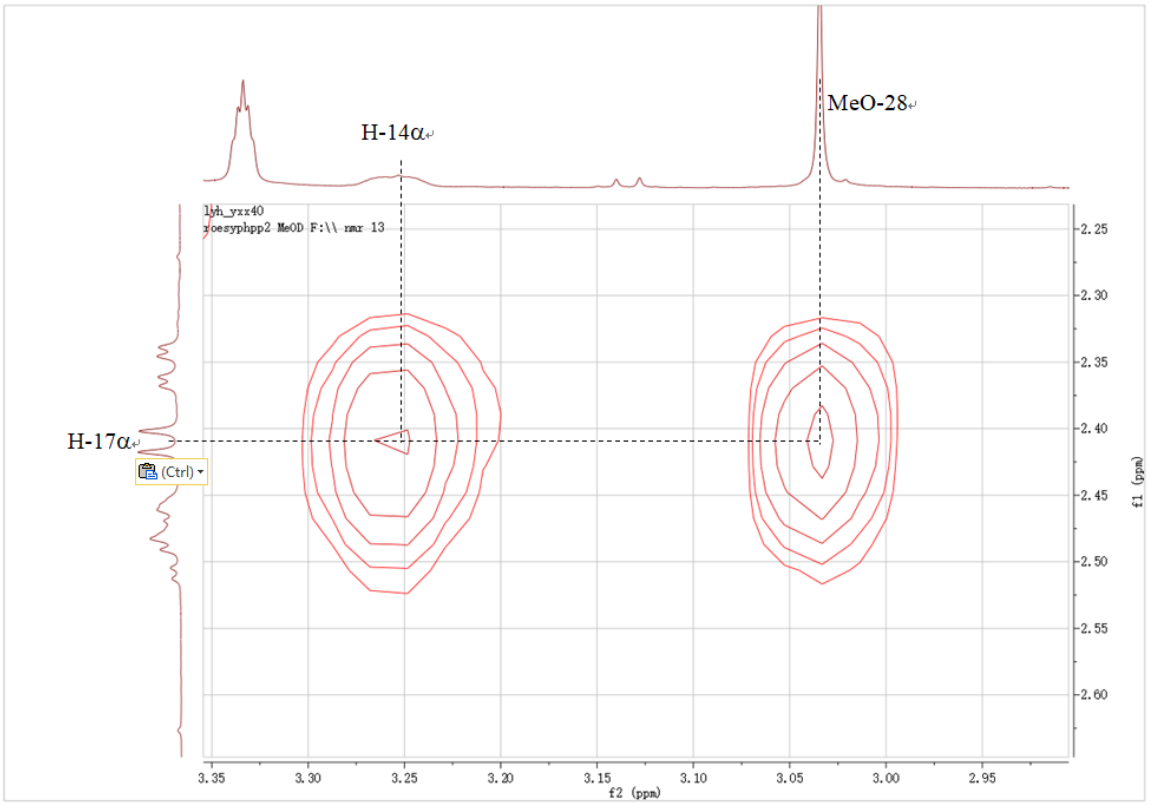


Figure S15: NOESY spectrum of **1** (furoecdysterone)









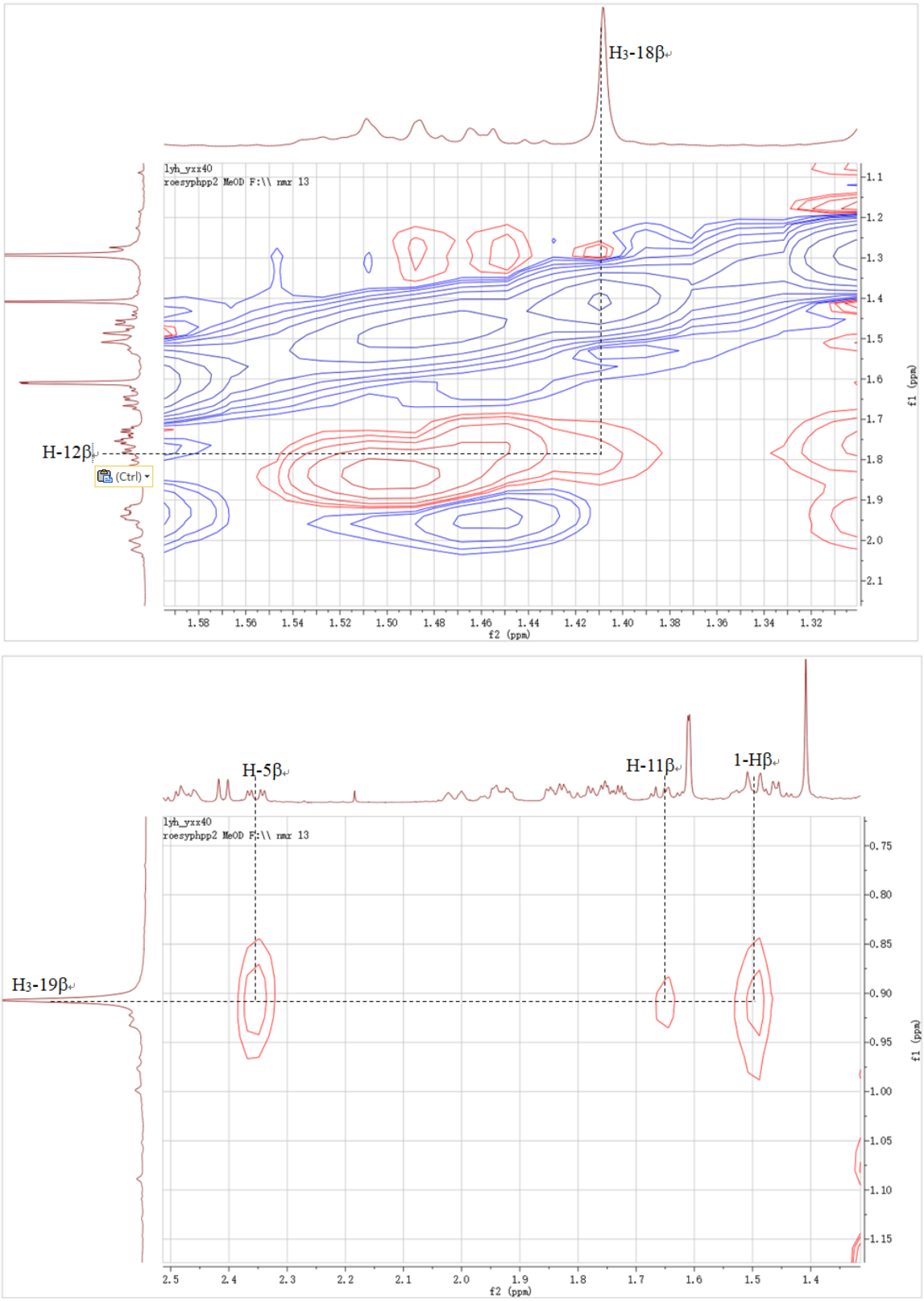


Figure S16: Key NOESY spectrum of **1** (furoecdysterone) (From δ_H 3.77 ppm to δ_H 1.40 ppm)

CAS SciFinder^{n}

Task History

Initiating Search

January 21, 2024, 12:56PM

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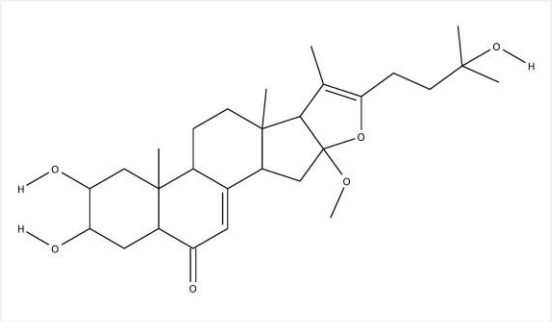

Search Tasks

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Returned All Results	All	View Results
Exported: Returned Substance Results + Filters (13) Filtered By: Structure Match: Similarity Similarity: 85-89 Number of Components: 1	Substances	View Results

CAS SciFinder^{n}

Substances (13)

View in SciFinder^{n}

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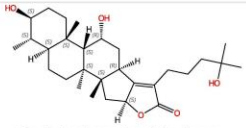


Absolute stereochemistry shown, Rotation (+)

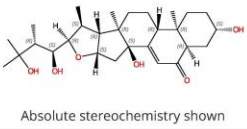
$C_{29}H_{46}O_5$

1 Reference | 2 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	474.67	-
Boiling Point (Predicted)	629.2±55.0 °C	Press: 760 Torr
Density (Predicted)	1.17±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	14.69±0.70	Most Acidic Temp: 25 °C

2

1021913-46-1



Absolute stereochemistry shown

$C_{28}H_{44}O_6$

(3β,5β,16β,22*R*,23*S*)-16,22-Epoxy-3,14,23,25-tetrahydroxyergost-7-en-6-one

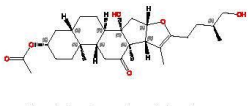
2 References | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	476.65	-
Boiling Point (Predicted)	658.0±55.0 °C	Press: 760 Torr
Density (Predicted)	1.23±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	13.60±0.70	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

3

201465-96-5



Absolute stereochemistry shown

$C_{29}H_{44}O_6$

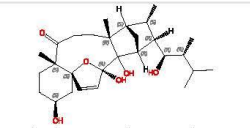
Furost-20(22)-en-12-one, 3-(acetyloxy)-14,26-dihydroxy-, (3β,5α,14β,25*R*)-

1 Reference | 3 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	488.66	-
Boiling Point (Predicted)	607.5±55.0 °C	Press: 760 Torr
Density (Predicted)	1.19±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	13.68±0.70	Most Acidic Temp: 25 °C

4

2258672-73-8



Absolute stereochemistry shown

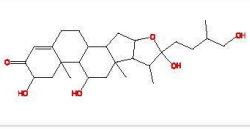
$C_{28}H_{44}O_6$

1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	476.65	-
Boiling Point (Predicted)	618.8±55.0 °C	Press: 760 Torr
Density (Predicted)	1.23±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.32±0.70	Most Acidic Temp: 25 °C

5

78527-42-1



$C_{27}H_{42}O_6$

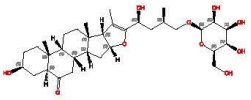
Furost-4-en-3-one, 2,11,22,26-tetrahydroxy-, (2β,11α,25*R*)-

0 References | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	462.62	-
Boiling Point (Predicted)	643.6±55.0 °C	Press: 760 Torr
Density (Predicted)	1.25±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.61±0.70	Most Acidic Temp: 25 °C

6

1824690-85-8



Absolute stereochemistry shown, Rotation (-)

$C_{33}H_{52}O_{10}$

(3β,5α,23*R*,25*R*)-26-(β-D-Glucopyranosyloxy)-3,23-dihydroxyfurost-20(22)-en-6-one

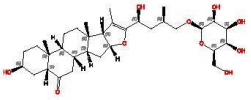
1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	608.76	-
Boiling Point (Predicted)	793.6±60.0 °C	Press: 760 Torr
Density (Predicted)	1.33±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.93±0.70	Most Acidic Temp: 25 °C

Spectra

7

1612247-10-5



Absolute stereochemistry shown

$C_{33}H_{52}O_{10}$

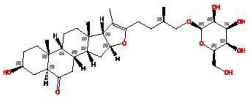
(3β,5α,23*S*,25*R*)-26-(β-D-Glucopyranosyloxy)-3,23-dihydroxyfurost-20(22)-en-6-one

1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	608.76	-
Boiling Point (Predicted)	793.6±60.0 °C	Press: 760 Torr
Density (Predicted)	1.33±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.93±0.70	Most Acidic Temp: 25 °C

8

1824690-84-7



Absolute stereochemistry shown, Rotation (-)

$C_{33}H_{52}O_{9}$

(3β,5α,25*R*)-26-(β-D-Glucopyranosyloxy)-3-hydroxyfurost-20(22)-en-6-one

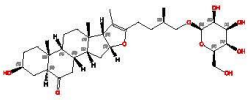
3 References | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	592.76	-
Boiling Point (Predicted)	751.9±60.0 °C	Press: 760 Torr
Density (Predicted)	1.29±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.94±0.70	Most Acidic Temp: 25 °C

Spectra

9

1612247-09-2



Absolute stereochemistry shown

$C_{33}H_{52}O_9$

(3β,5α,17β,25*R*)-26-(β-D-Glucopyranosyloxy)-3-hydroxyfurost-20(22)-en-6-one

1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	592.76	-
Boiling Point (Predicted)	751.9±60.0 °C	Press: 760 Torr
Density (Predicted)	1.29±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.94±0.70	Most Acidic Temp: 25 °C

10

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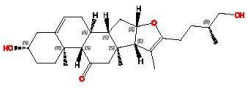


Absolute stereochemistry shown

$C_{27}H_{40}O_4$

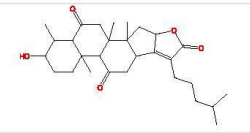
Furosta-5,20(22)-dien-11-one, 3,26-dihydroxy-, (3β,25*R*)-

2 References | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	428.61	-
Boiling Point (Predicted)	584.2±50.0 °C	Press: 760 Torr
Density (Predicted)	1.17±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	14.95±0.70	Most Acidic Temp: 25 °C

11

90248-41-2



$C_{29}H_{42}O_5$

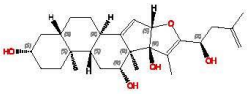
29-Nor-9β,13α,14β-dammar-17-en-21-oic acid, 3α,16β-dihydroxy-6,11-dioxo-, γ-lactone

2 References | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	470.64	-
Boiling Point (Predicted)	625.4±55.0 °C	Press: 760 Torr
Density (Predicted)	1.17±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	14.85±0.70	Most Acidic Temp: 25 °C

12

223260-38-6



Absolute stereochemistry shown

$C_{27}H_{40}O_5$

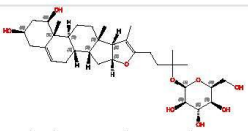
Furosta-14,20(22),25-triene-3,12,17,23-tetrol, (3β,5α,12β,23*R*)-

1 Reference | 7 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	444.60	-
Boiling Point (Predicted)	624.1±55.0 °C	Press: 760 Torr
Density (Predicted)	1.23±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.10±0.70	Most Acidic Temp: 25 °C

13

918344-57-7



Absolute stereochemistry shown

$C_{33}H_{52}O_9$

(1β,3β)-1,3-Dihydroxyfurosta-5,20(22)-dien-25-yl β-D-glucopyranoside

0 References | 0 Reactions | 0 Suppliers

Figure S17: Scifinder similarity report for **1** (furoecdysterone)

Table S1: A comparison of the ^{13}C NMR spectra data (δ_C, mult.) of **1** (furoecdysterone) and the most similar compounds

No.	furoecdysterone (**1**)	(20*S*,22*R*,24*R*)-16,22-epoxy-3β,14α,23β,25-tetrahydroxyergost-7-en-6-one[a]	22-deoxyecdysterone (**3**)
1	36.9, CH_2	36.5, CH_2	37.3, CH_2
2	68.6, CH	29.6, CH_2	68.7, CH
3	69.1, CH	63.8, CH	68.5, CH
4	33.3, CH_2	34.2, CH_2	32.8, CH_2
5	50.8, CH	51.6, CH	53.3, CH
6	205.9, C	202.9, C	206.5, C
7	122.8, CH	120.9, CH	122.1, CH
8	175.3, C	165.1, C	168.1, C
9	35.0, CH	35.2, CH	35.0, CH
10	40.2, C	37.0, C	39.3, C
11	22.7, CH_2	22.0, CH_2	22.0, CH_2
12	43.9, CH_2	32.9, CH_2	31.6, CH_2
13	49.3, C	49.1, C	48.1, C
14	42.1, CH	84.1, C	85.5, C
15	37.2, CH_2	41.0, CH_2	32.4, CH_2
16	103.9, C	82.8, CH	21.5, CH_2
17	54.2, CH	61.4, CH	51.8, CH
18	32.1, CH_3	17.8, CH_3	18.1, CH_3
19	23.9, CH_3	24.0, CH_3	26.5, CH_3
20	135.0, C	37.0, CH	75.9, C
21	9.9, CH_3	17.0, CH_3	24.4, CH_3
22	144.4, C	84.1, CH	45.5, CH_2
23	22.3, CH_2	69.8, CH	20.1, CH_2
24	42.3, CH_2	43.1, CH	45.9, CH_2

25	71.4, C	73.3, C	71.5, C
26	29.1, CH_3	29.5, CH_3	29.1, CH_3
27	29.3, CH_3	28.9, CH_3	29.3, CH_3
28	50.5, CH_3	7.8, CH_3	_

[a] Data taken from Zhou et al. (2007)