

Supporting Information

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A New Ingenane Diterpenoid from *Euphorbia jolkinii*

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Data File: E:\DATA\2022\1102\YEP4.lcd

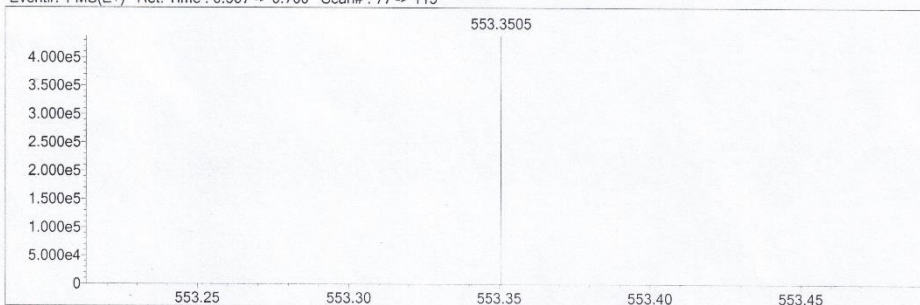
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H	1	5	100	F	1	0	0	Cl	1	0	0	Ag	1	0	0	H
2H	1	0	0	Na	1	0	0	Co	2	0	0	I	3	0	0	Na
B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	5	70	Si	4	0	0	Se	2	0	0					
N	3	0	10	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	5	Pd	2	0	0					

Error Margin (ppm): 5
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

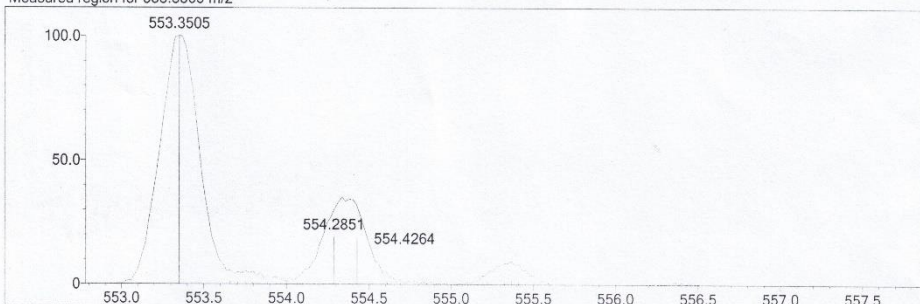
DBE Range: not fixed
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: OR

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 10000
 Max Results: 30

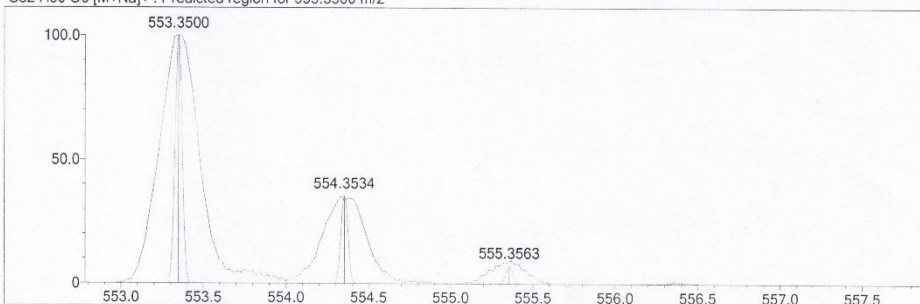
Event#: 1 MS(E+) Ret. Time : 0.507 -> 0.760 Scan#: 77 -> 115



Measured region for 553.3505 m/z



C32 H50 O6 [M+Na]+ : Predicted region for 553.3500 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C32 H50 O6	[M+Na]+	553.3505	553.3500	0.5	0.90	8.0

Figure S1: The HR-ESI-MS spectrum of 1

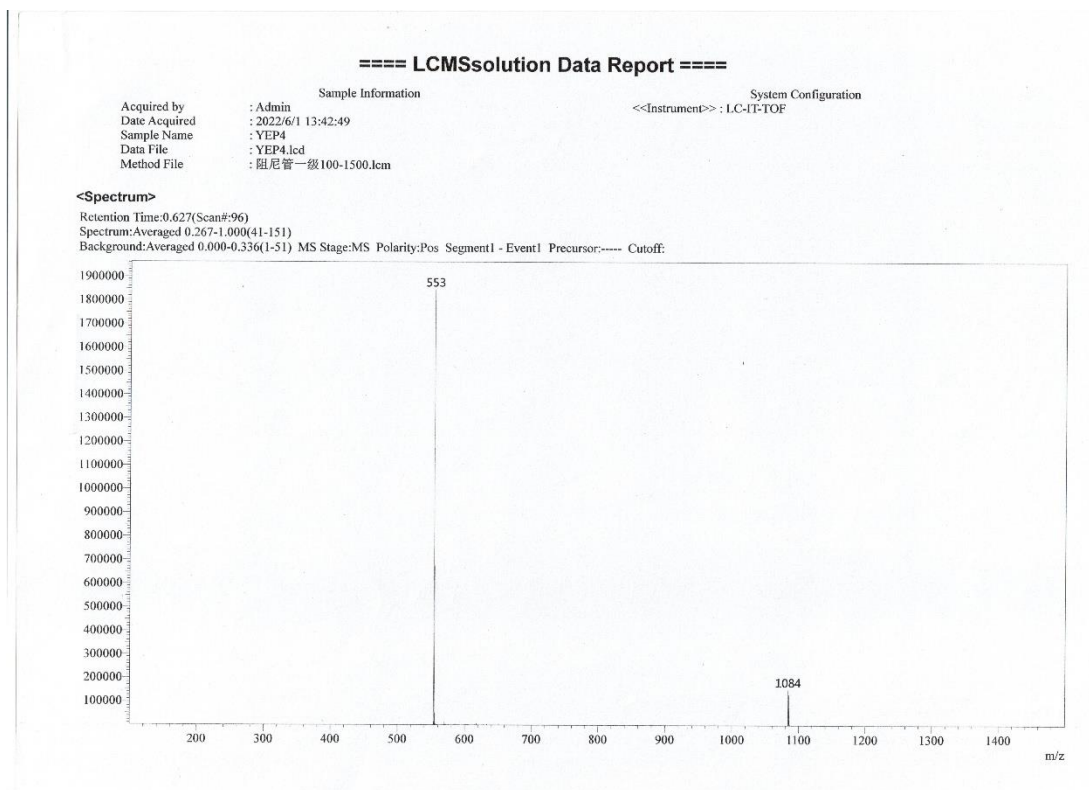


Figure S2: The ESI-MS spectrum of 1

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 24-FEB-2023

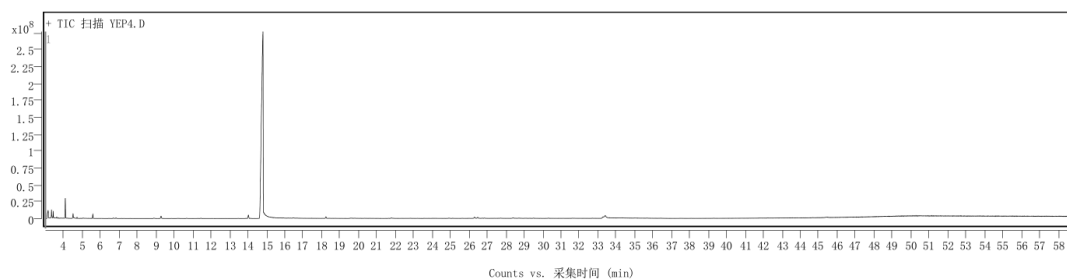
Set Temperature : 20.0

Time Delay : Disabled

Delay between Measurement : Disabled

<u>n</u>	<u>Average</u>	<u>Std.Dev.</u>	<u>% RSD</u>	<u>Maximum</u>	<u>Minimum</u>										
5	7.27	0.28	3.85	7.67	7.00	<u>S.No</u>	<u>Sample ID</u>	<u>Time</u>	<u>Result</u>	<u>Scale</u>	<u>OR °Arc</u>	<u>WLG.nm</u>	<u>Lg.mm</u>	<u>Conc.g/100ml</u>	<u>Temp.</u>
1	YEP4	12:17:29 PM	7.67	SR	0.023	589	100.00	0.300	20.2						
2	YEP4	12:17:35 PM	7.33	SR	0.022	589	100.00	0.300	20.1						
3	YEP4	12:17:42 PM	7.00	SR	0.021	589	100.00	0.300	20.1						
4	YEP4	12:17:53 PM	7.33	SR	0.022	589	100.00	0.300	20.0						
5	YEP4	12:17:59 PM	7.00	SR	0.021	589	100.00	0.300	20.0						

Figure S3: The optical rotation of 1



样品谱图

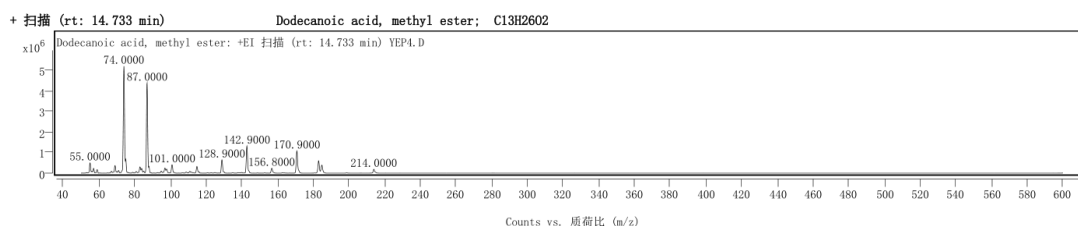


Figure S4: The GC-MS spectrum of the hydrolysis of dodecanoate unit of **1**

分析报告



谱图识别表														
最佳 ID 来源	名称	分子式	种类	m/z	差 (ppm)	CAS	分数	分数 (Lib)	分数 (DB)	分数 (MFG)	谱库/数据库			
Yes Lib 检索	Dodecanoic acid, methyl ester	C13H26O2				111-82-0	82.19	82.19			NIST20.L			
No Lib 检索	Undecanoic acid, 10-methyl-, methyl ester	C13H26O2				5129-56-6	83.92	83.92			NIST20.L			
No Lib 检索	Dodecanoic acid, methyl ester	C13H26O2				111-82-0	80.01	80.01			NIST20.L			
No Lib 检索	Dodecanoic acid, methyl ester	C13H26O2				111-82-0	79.27	79.27			NIST20.L			
No Lib 检索	Dodecanoic acid, methyl ester	C13H26O2				111-82-0	78.38	78.38			NIST20.L			
No Lib 检索	Dodecanoic acid, 2-methyl-	C13H26O2				2874-74-0	76.21	76.21			NIST20.L			
No Lib 检索	Dodecanoic acid, 2-methyl-	C13H26O2				2874-74-0	71.29	71.29			NIST20.L			
No Lib 检索	Methyl 11-methyl-dodecanoate	C14H28O2				1000336-45-1	69.93	69.93			NIST20.L			
No Lib 检索	Undecanoic acid, 10-methyl-, methyl ester	C13H26O2				5129-56-6	69.88	69.88			NIST20.L			
No Lib 检索	Methyl 13-methyltetradecanoate	C16H32O2				1000424-50-7	68.10	68.10			NIST20.L			
最佳名称														
Yes	Dodecanoic acid, methyl ester	C13H26O2		m/z (prec.)	111-82-0	CAS	24.683	RT (DB)	RT 差	分数	分数 (Lib)	分数 (Fwd)	分数 (Rev)	谱库/数据库
										82.19	82.19			NIST20.L

Figure S5: The library search data of hydrolysis of dodecanoate unit of **1**
GC-MS analysis detail

Column: DB-5MS capillary column (30 m × 0.25 mm, 0.25 μm); injector temperature: 250 °C; initial temperature: 40 °C, increased at 40 °C/min to 120 °C, held for 5 min; increased at 5 °C/min to 240 °C, held for 5 min; increased at 5 °C/min to 300 °C, held for 10 min; carrier gas: helium; flow rate: 1 mL/min; injection volume: 1 μL. Mass: El voltage, 70 eV; Mass scanned-mass range: m/z 50-600.

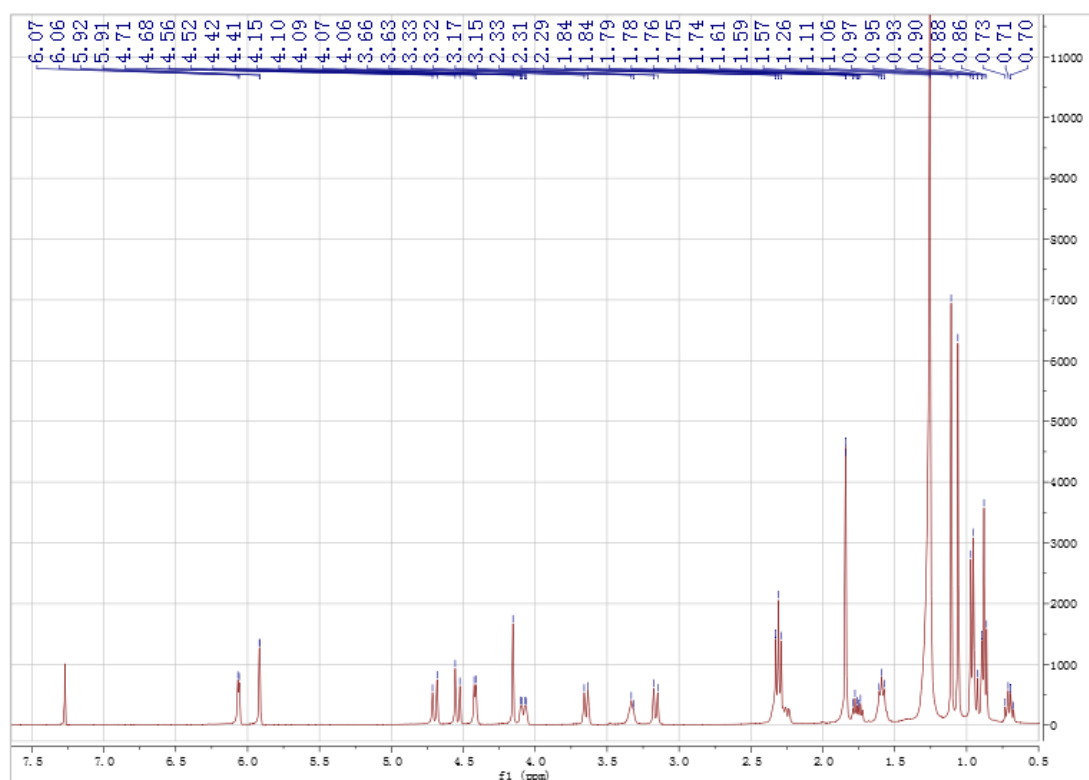


Figure S6: The ^1H -NMR (400 MHz, CDCl_3) spectrum of **1**

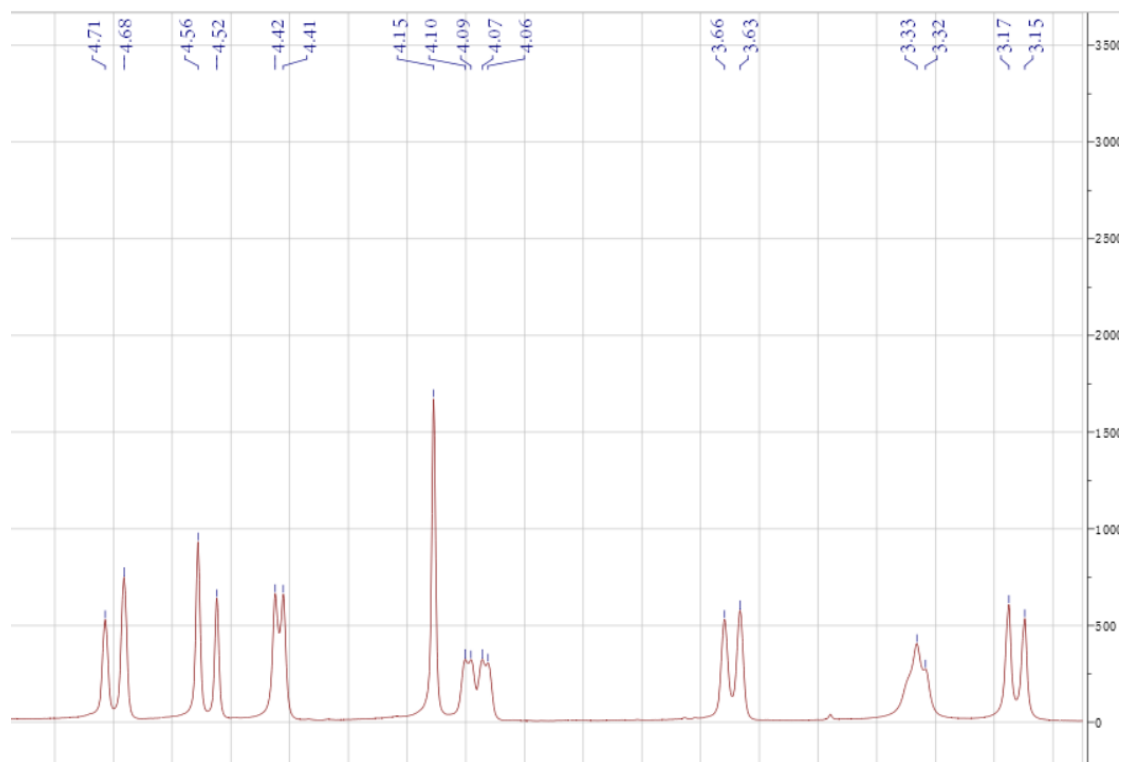


Figure S7: The ^1H -NMR (400 MHz, CDCl_3) spectrum of **1** (From δ_{H} 3.0 ppm to δ_{H} 4.8 ppm)

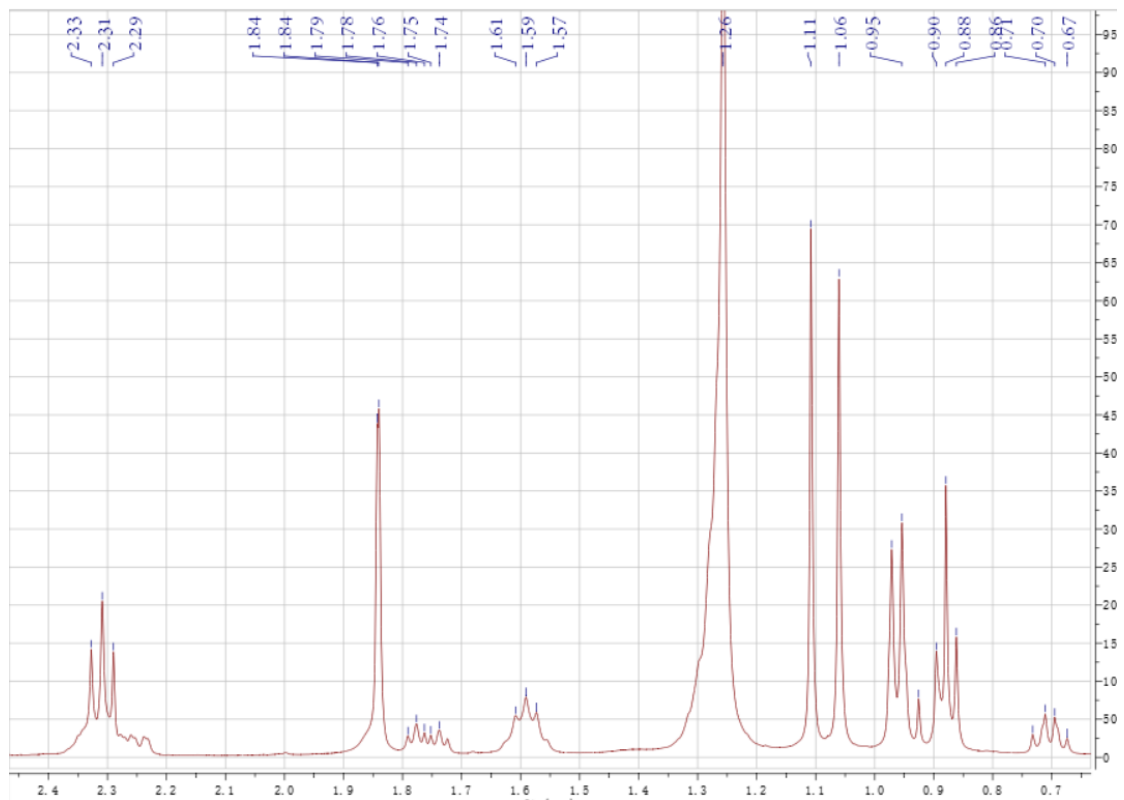


Figure S8: The ^1H -NMR (400 MHz, CDCl_3) spectrum of **1** (From δ_{H} 0 ppm to δ_{H} 2.4 ppm)

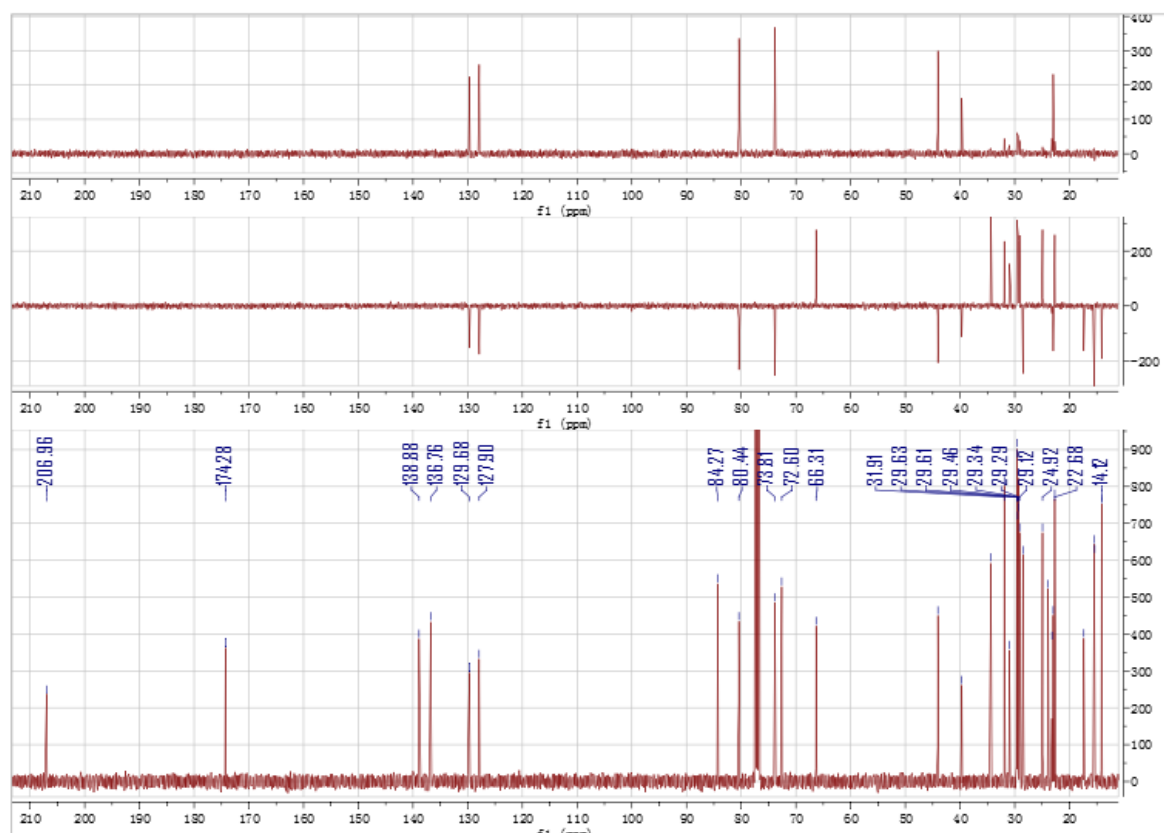


Figure S9: The ^{13}C NMR (100 MHz, CDCl_3) spectrum of **1**

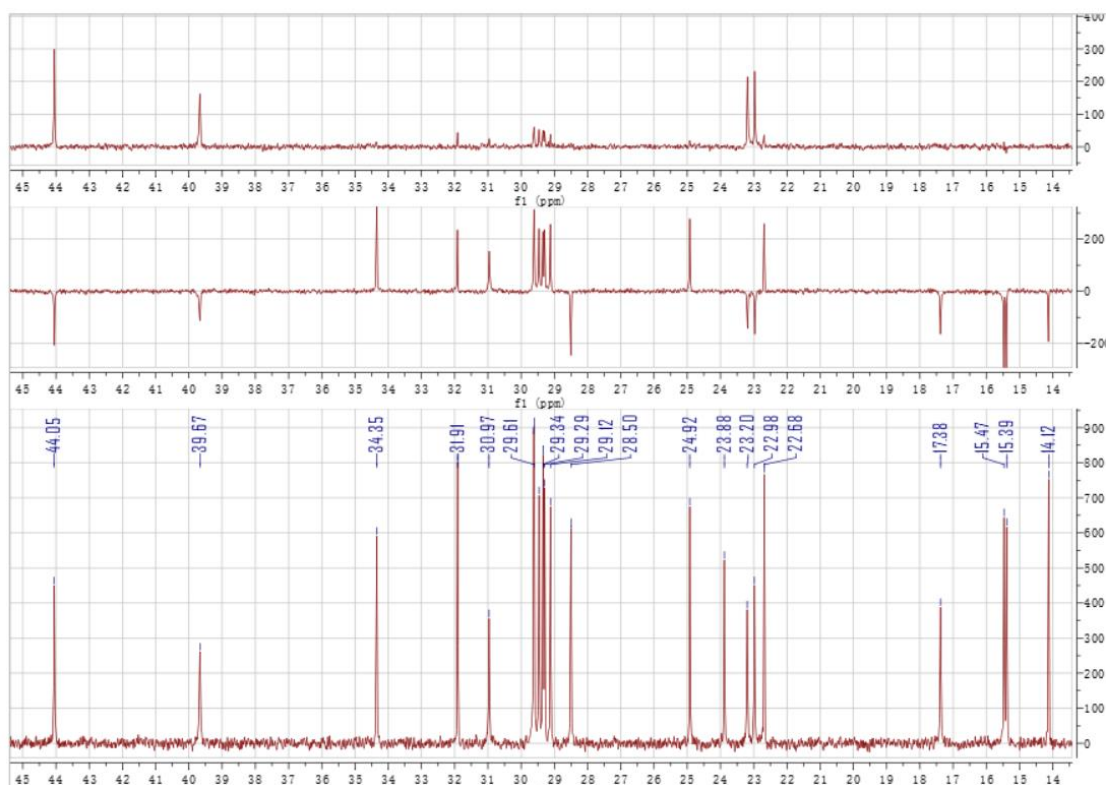


Figure S10: The ^{13}C NMR (100 MHz, CDCl_3) spectrum of **1** (From δ_c 14 ppm to δ_c 45 ppm)

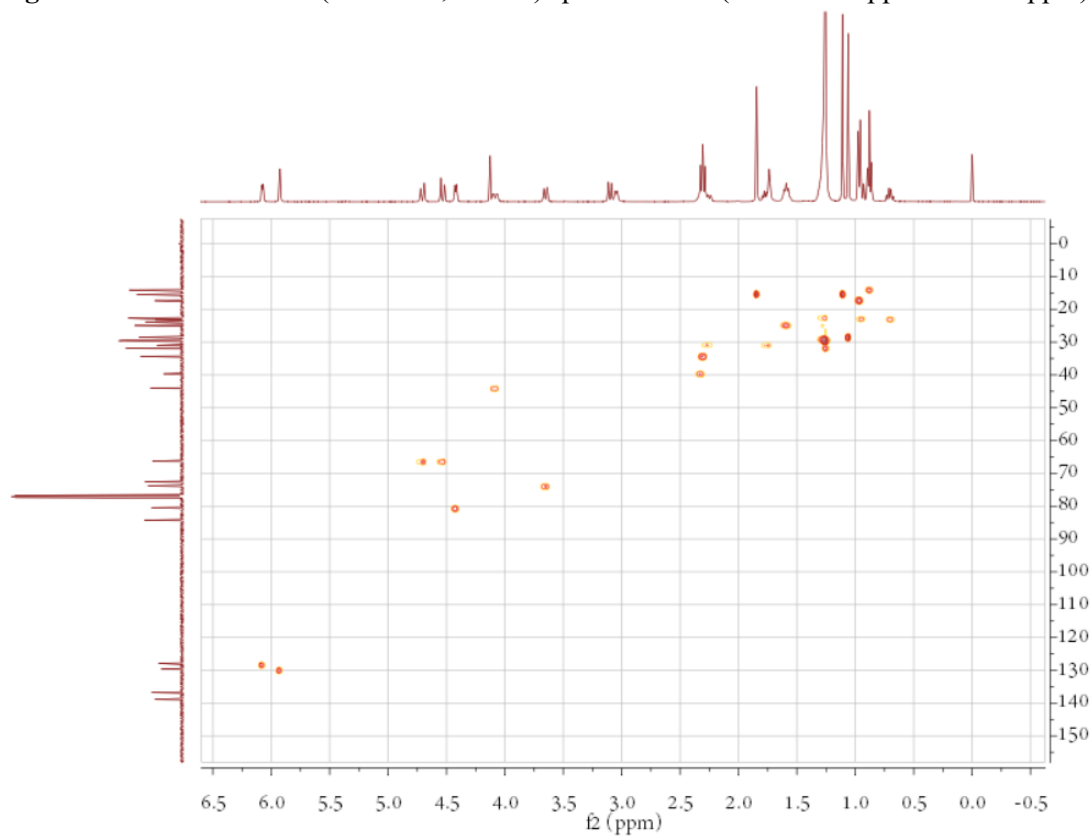


Figure S11: The HSQC spectrum of **1**

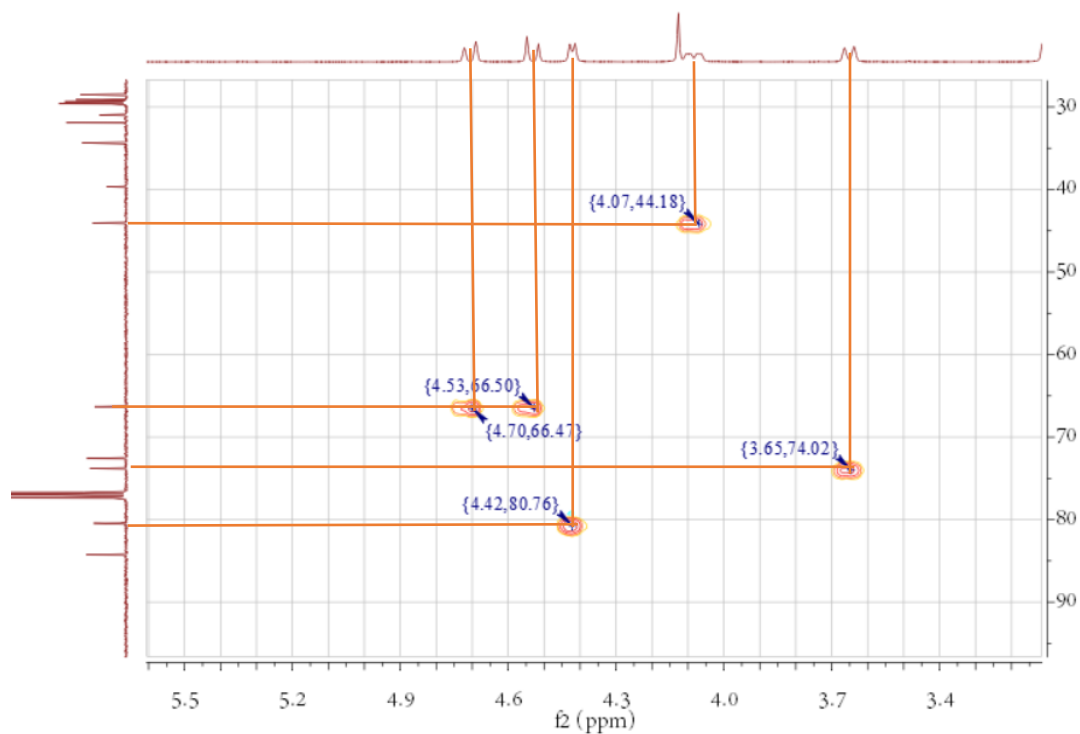


Figure S12: The HSQC spectrum of **1** (From δ_c 40 ppm to δ_c 90 ppm)

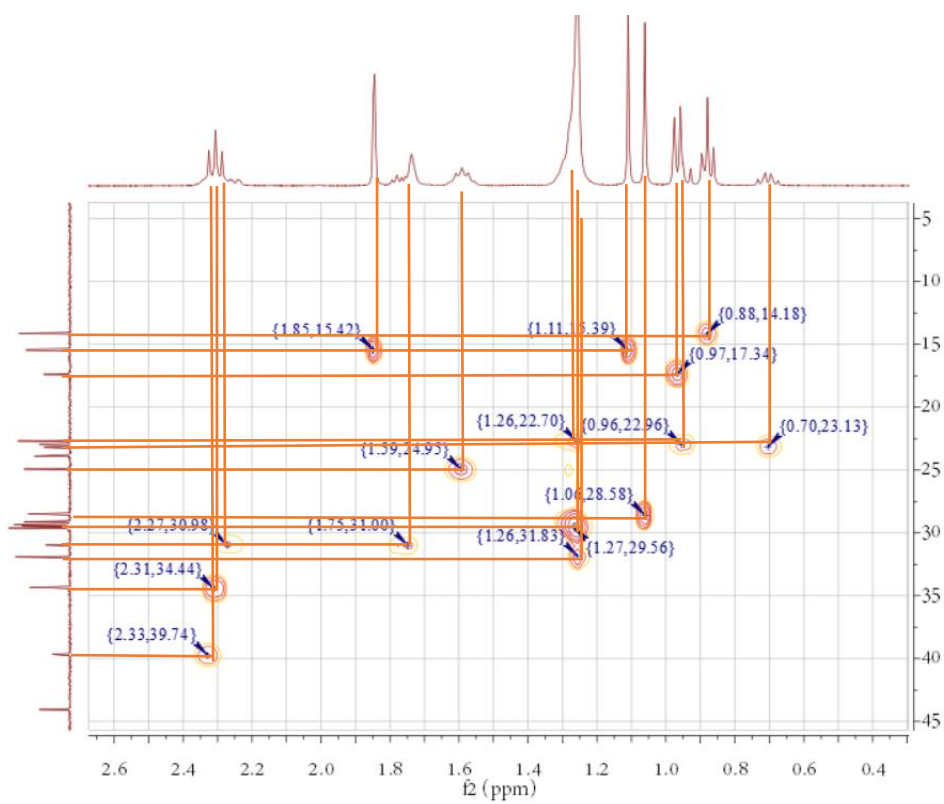


Figure S13: The HSQC spectrum of **1** (From δ_c 10 ppm to δ_c 40 ppm)

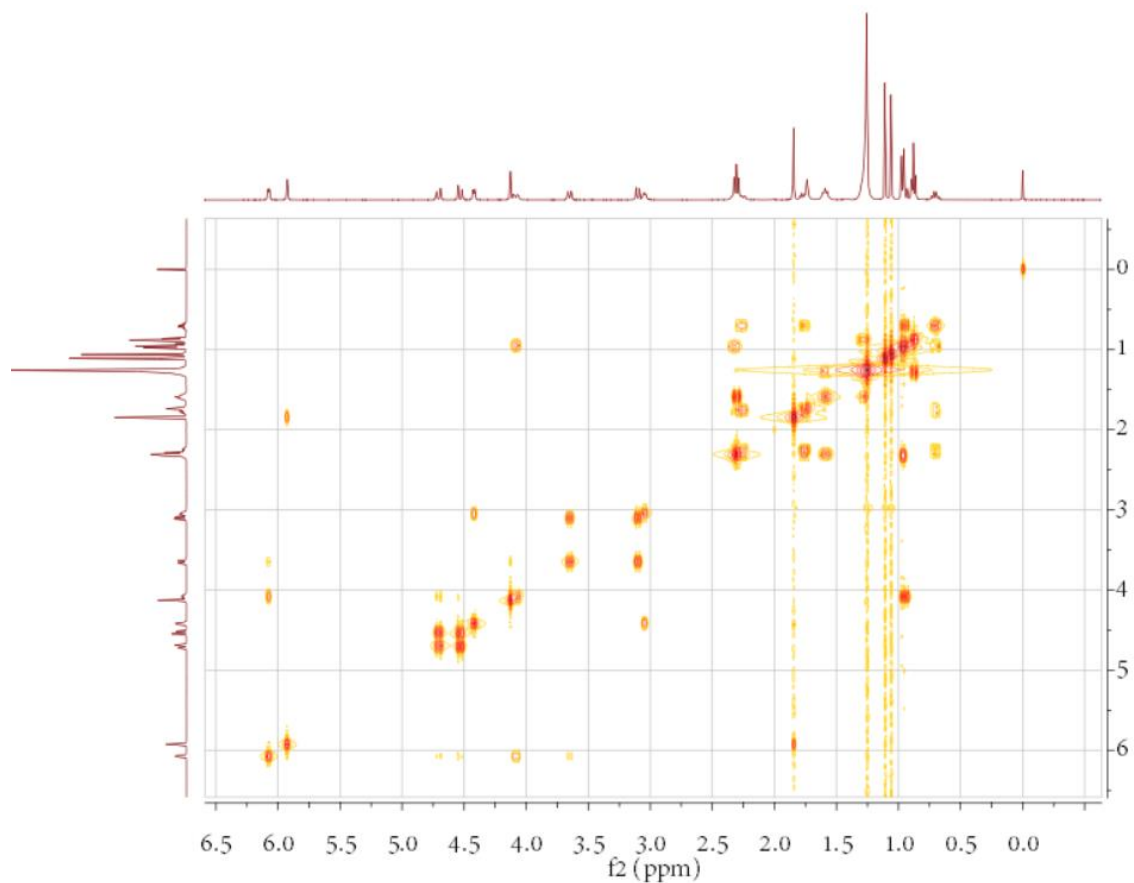


Figure S14: The ^1H - ^1H COSY spectrum of **1**

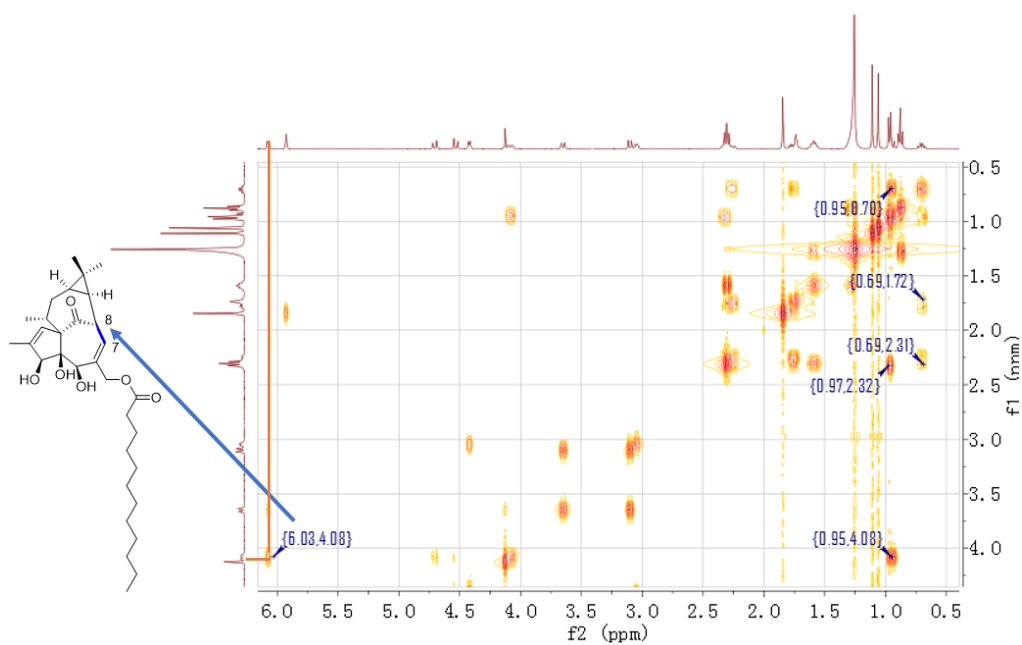


Figure S15: The ^1H - ^1H COSY of H-7/H-8 of **1**

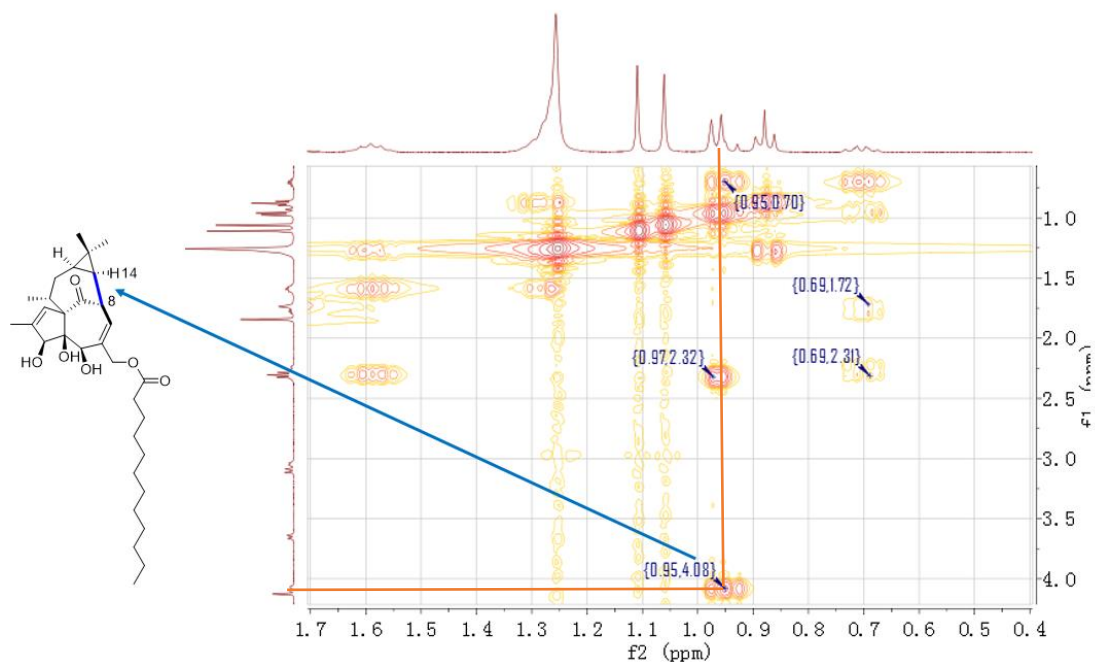


Figure S16: The ^1H - ^1H COSY of H-8/H-14 of **1**

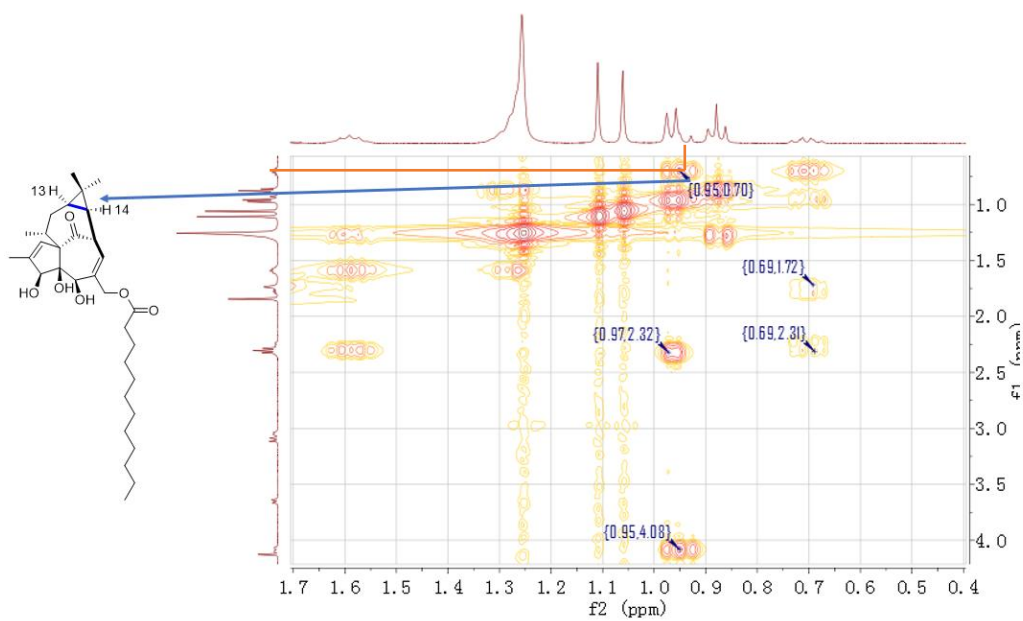


Figure S17: The ^1H - ^1H COSY of H-13/H-14 of **1**

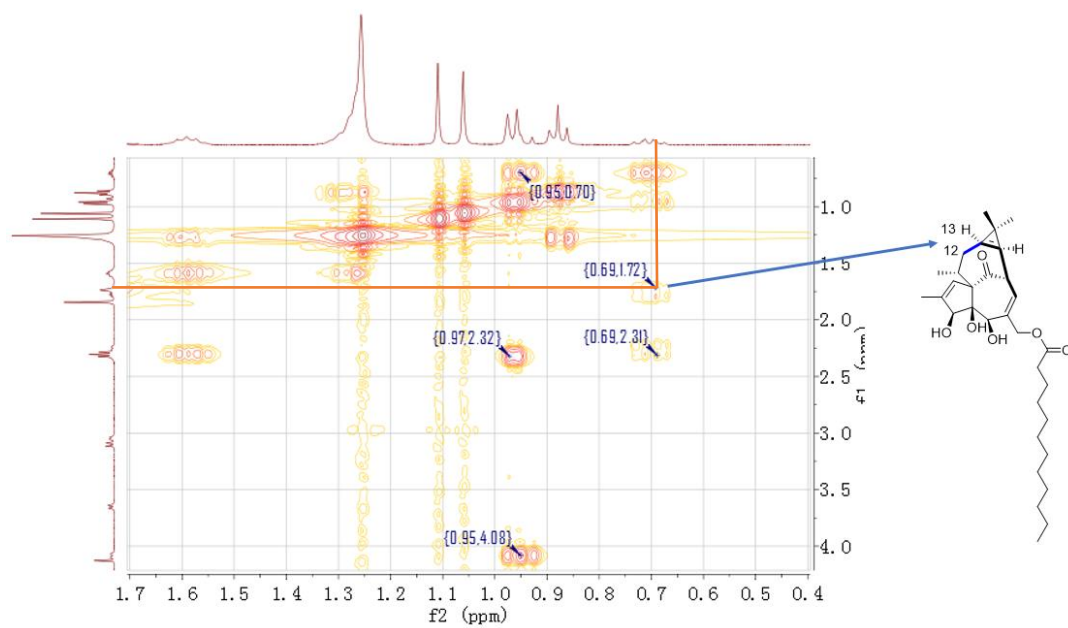


Figure S18: The ^1H - ^1H COSY of H-12/H-13 of **1**

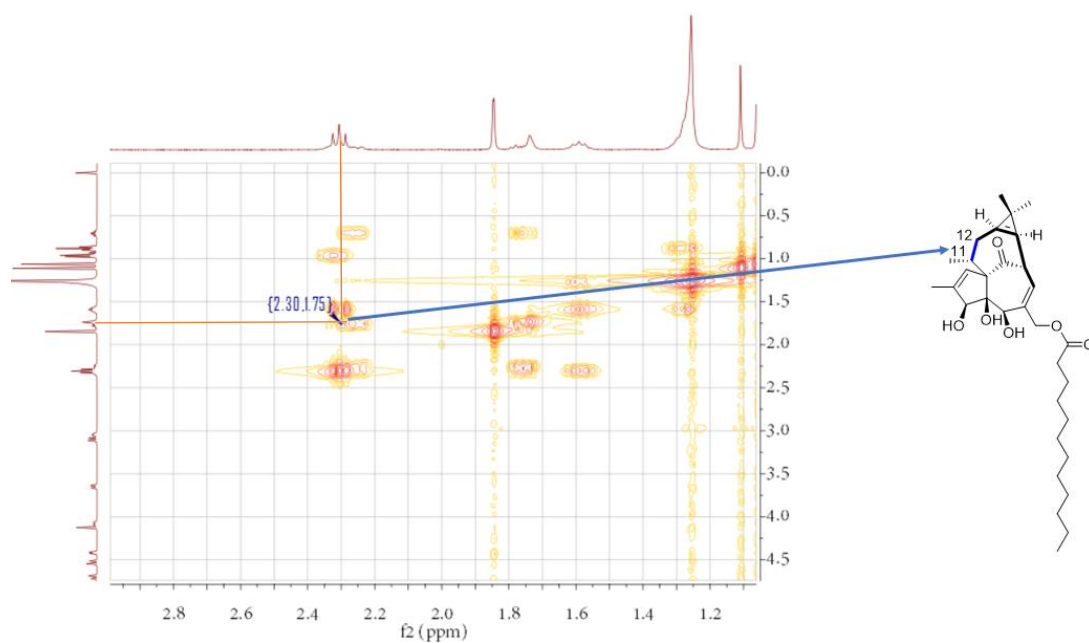


Figure S19: The ^1H - ^1H COSY of H-11/H-12 of **1**

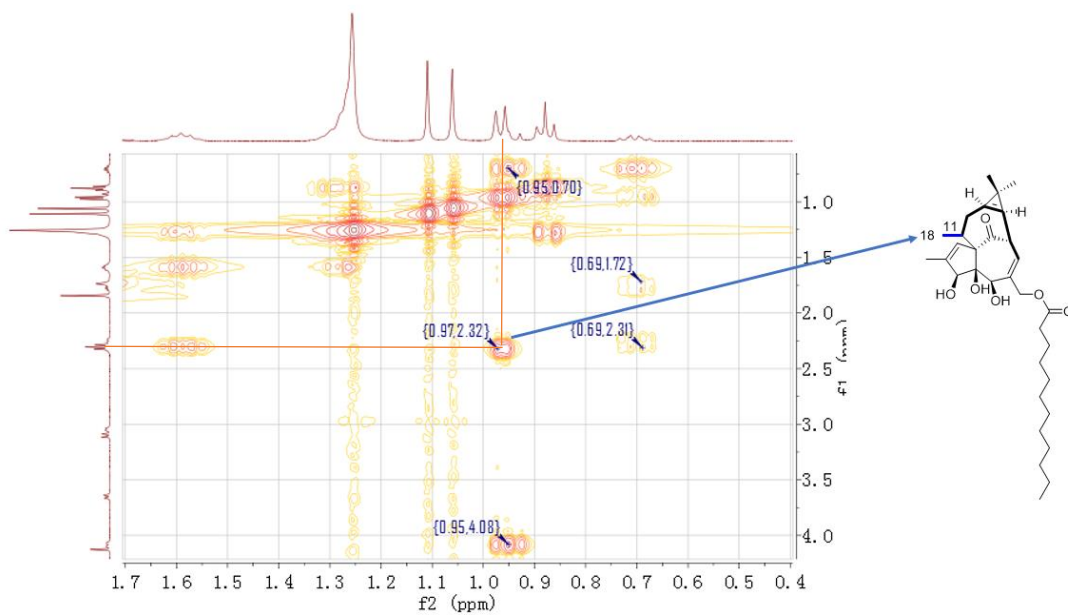


Figure S20: The ^1H - ^1H COSY of H-11/ CH_3 -18 of **1**

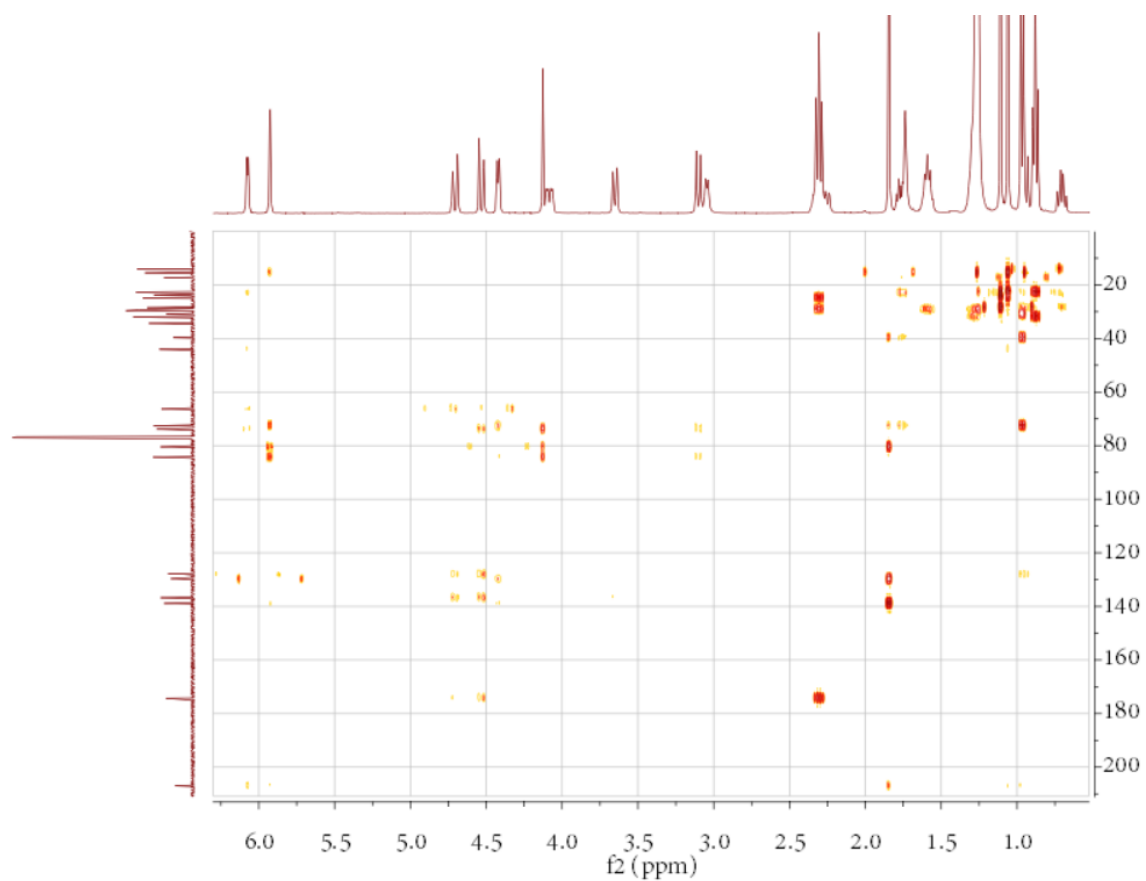


Figure S21: The HMBC spectrum of **1**

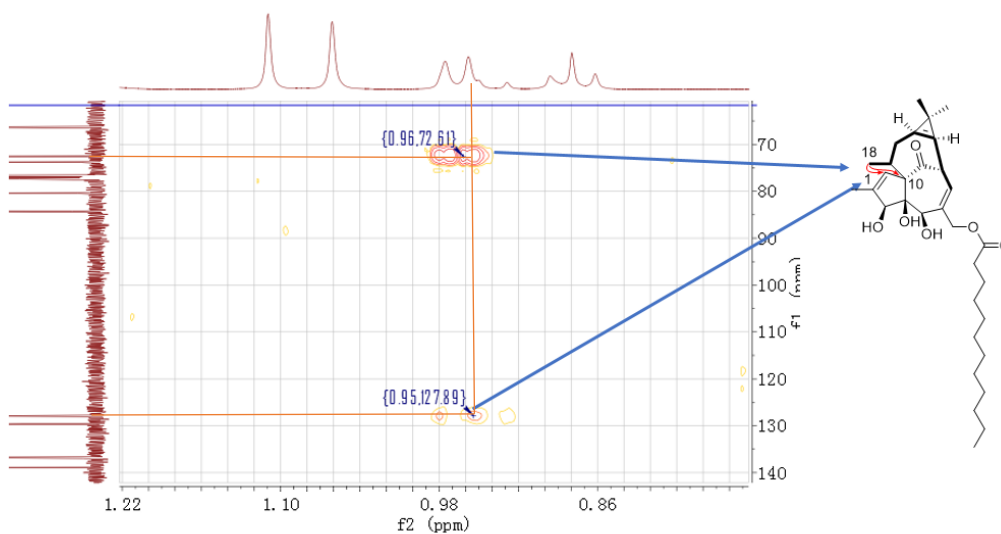


Figure S22: The HMBC correlations of CH_3 -18 to C-1 and C-10 of **1**

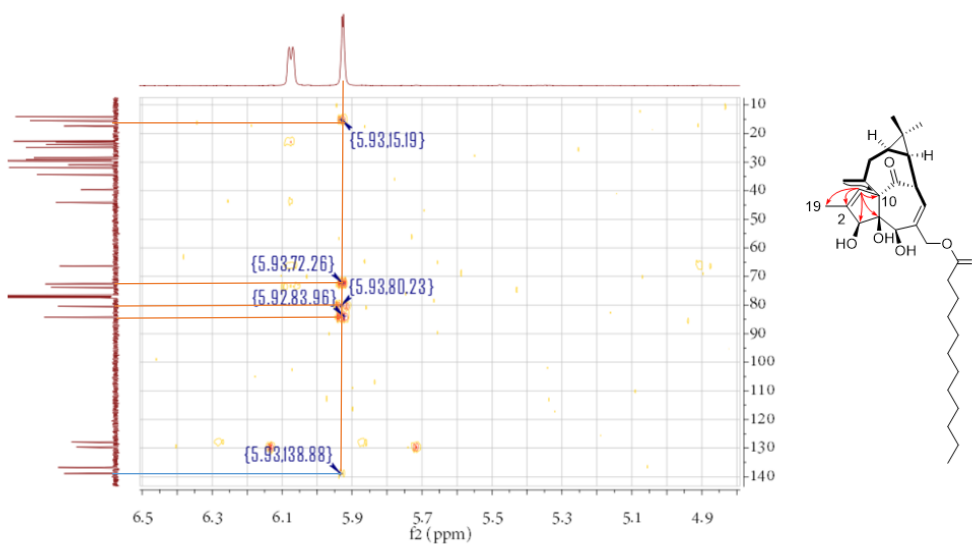


Figure S23: The HMBC correlations of H-1 to C-2, C-3, C-4, C-10 and C-19 of **1**

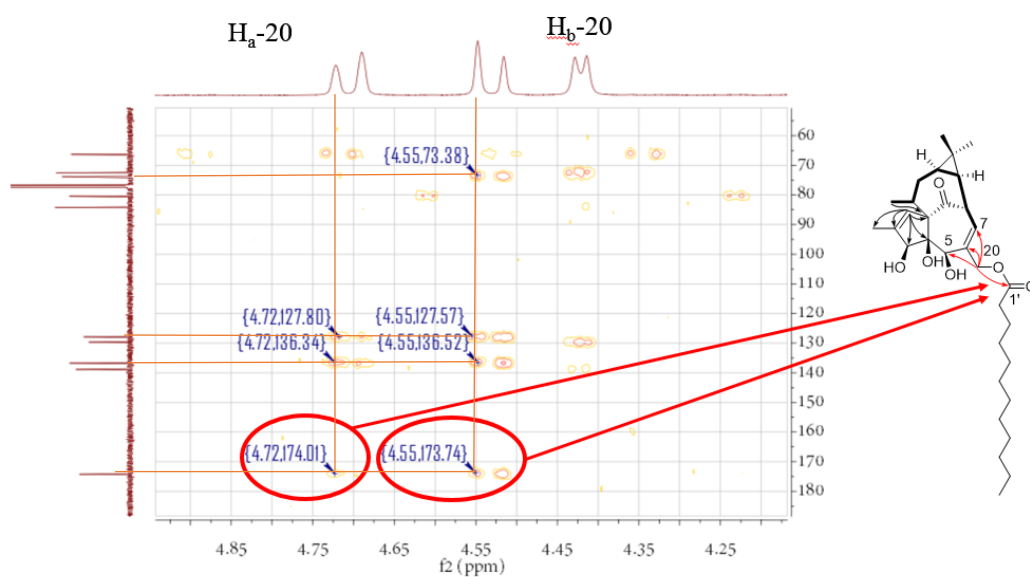


Figure S24: The HMBC correlations of H₂-20 to C-5, C-6, C-7, and C-1' of **1**



Figure S25: The HMBC correlations of H₂-2' to C-1' of **1**

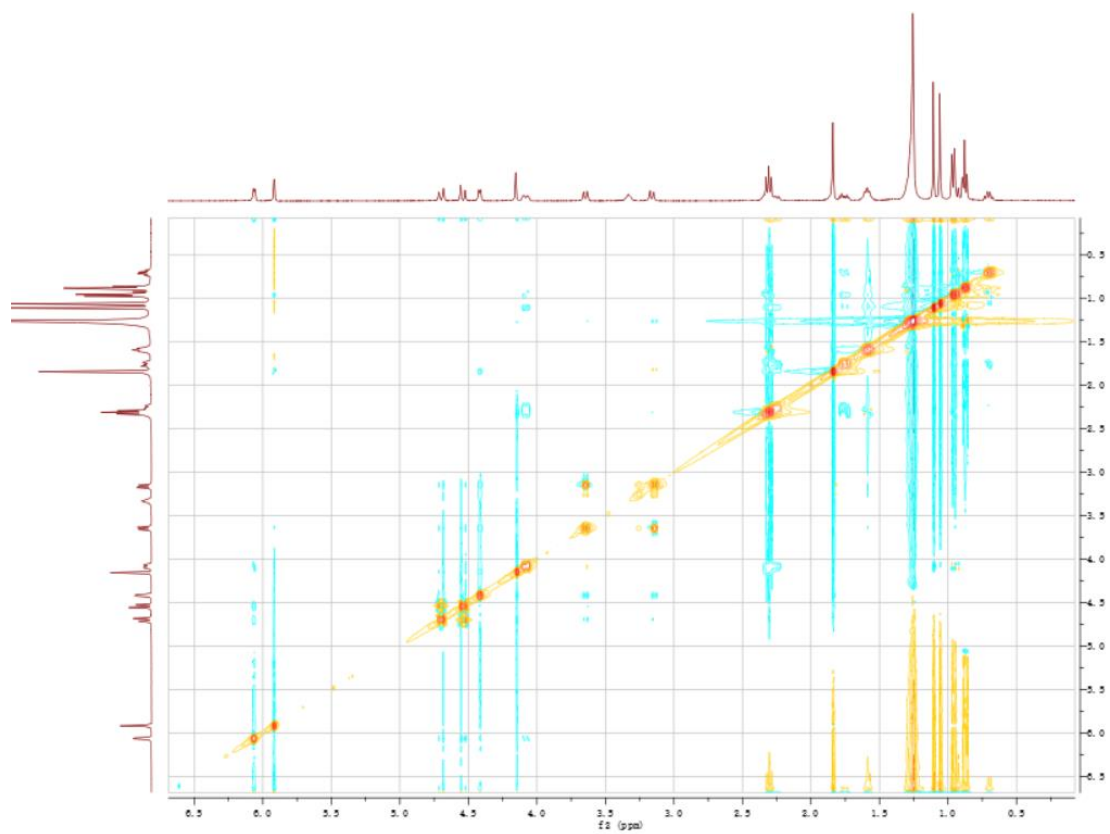


Figure S26: The ROESY spectrum of **1**

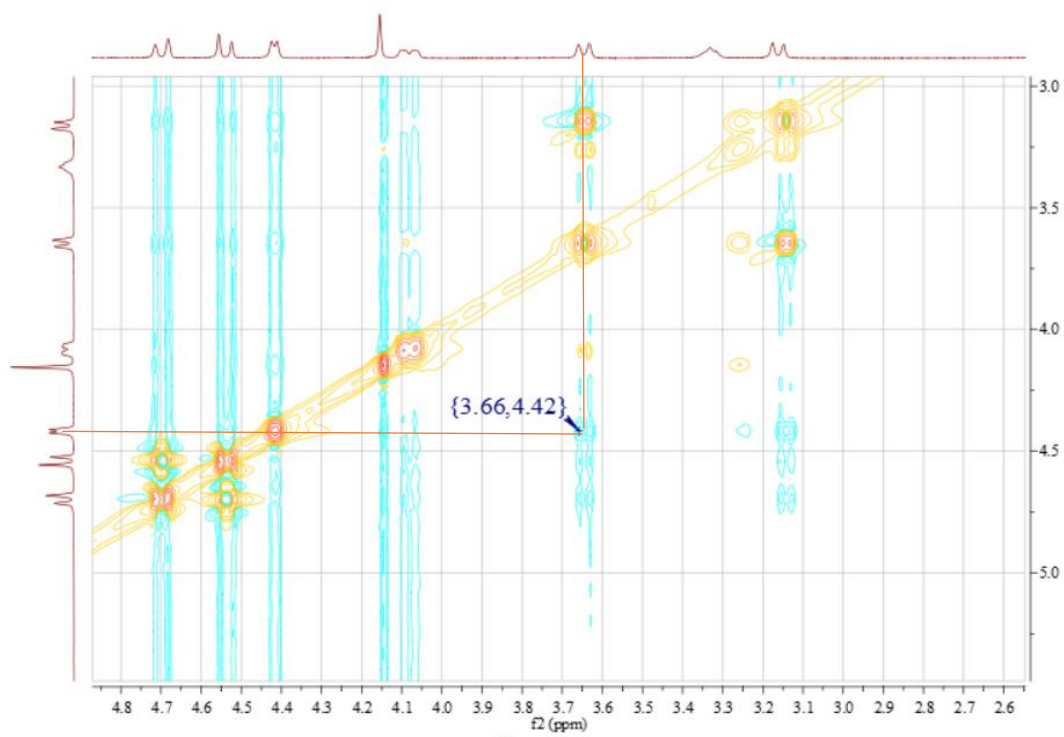


Figure S27: The ROESY correlation of H-5/H-3 of **1**

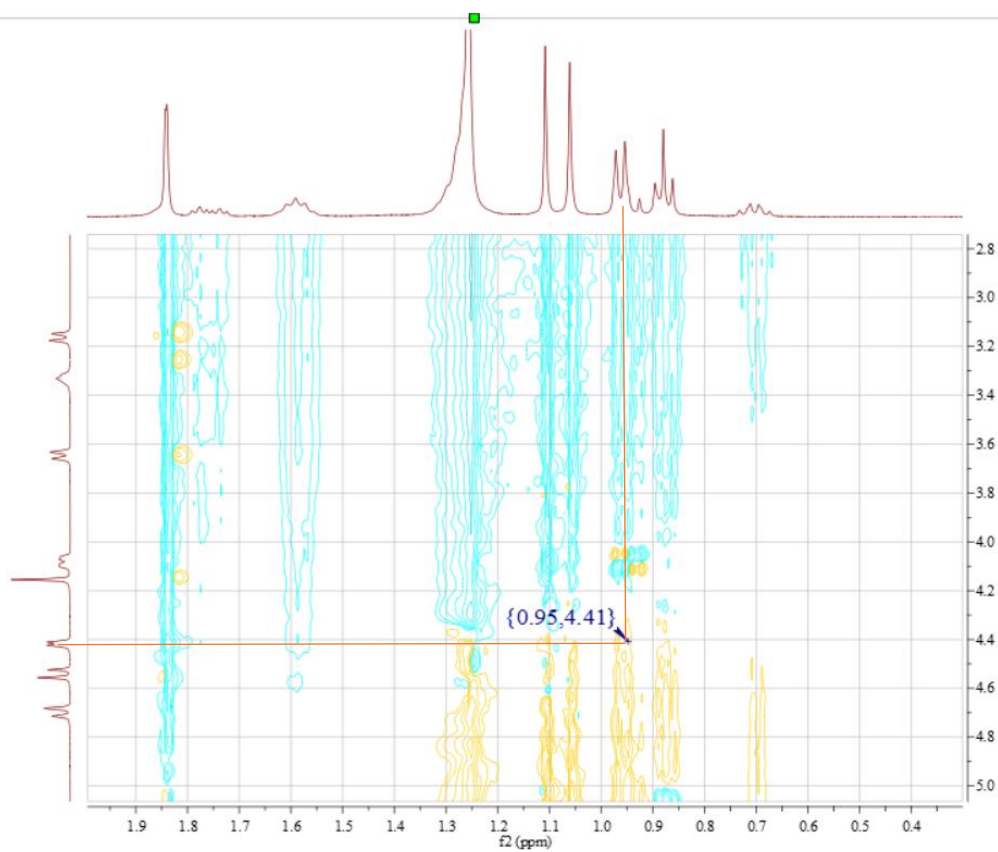


Figure S28: The ROESY correlation of H-3/CH₃-18 of **1**

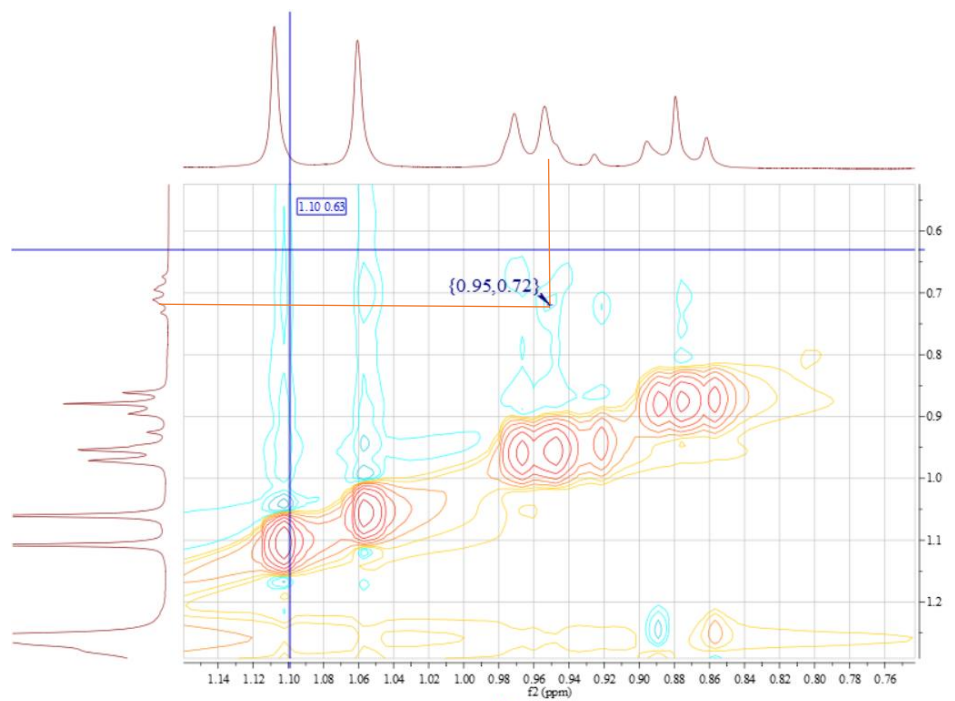


Figure S29: The ROESY correlation of CH₃-18/H-13 of **1**

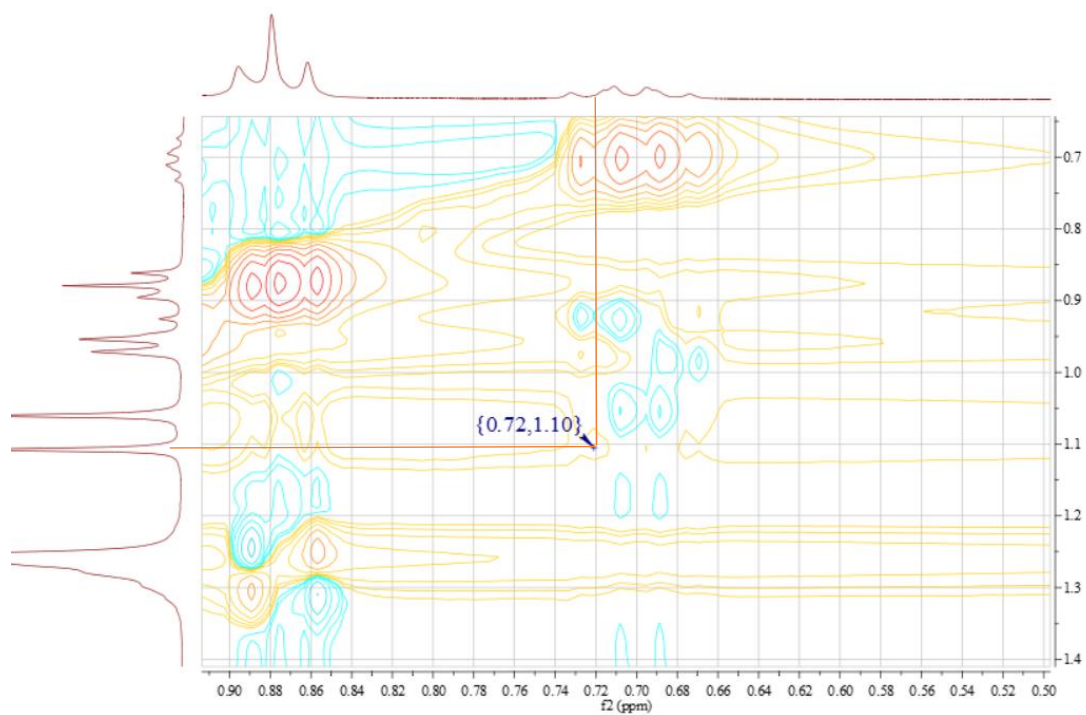


Figure S30: The ROESY correlation of $\text{CH}_3\text{-17/H-13}$ of **1**

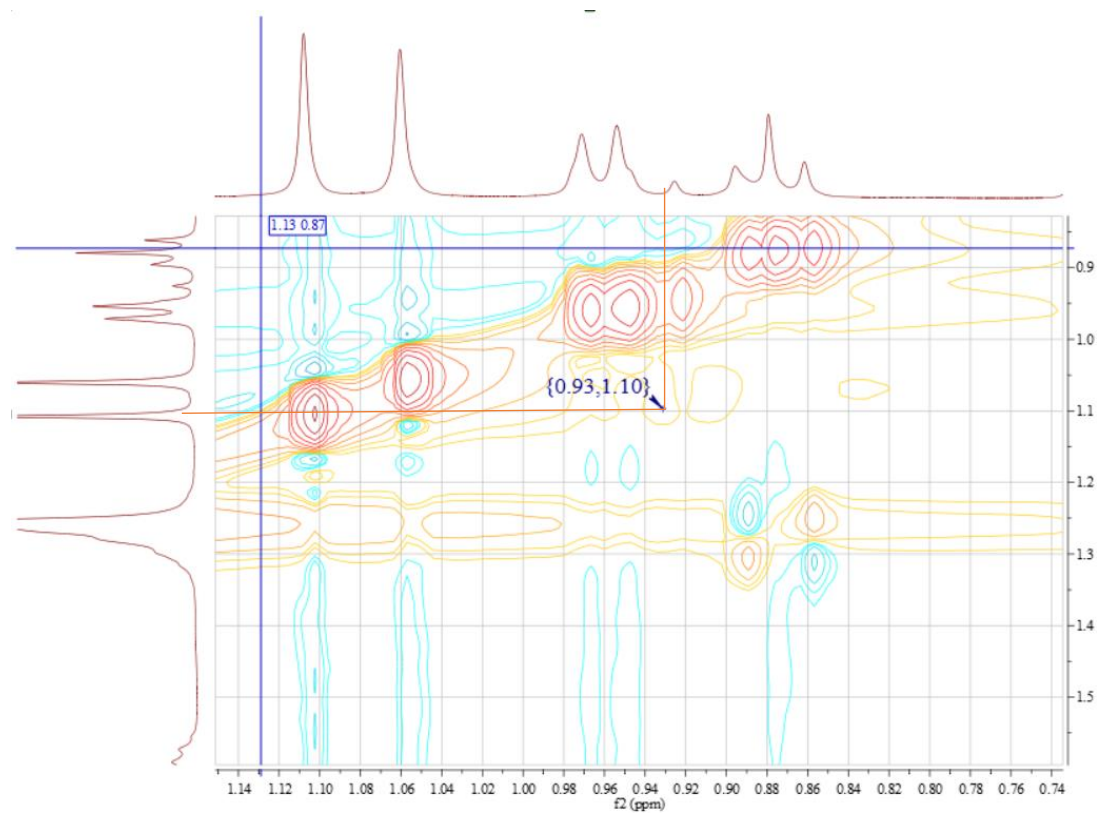


Figure S31: The ROESY correlation of $\text{CH}_3\text{-17/H-14}$ of **1**

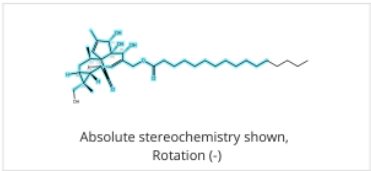
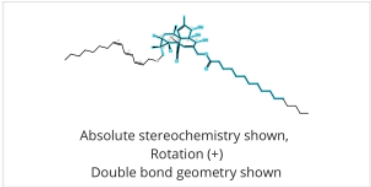
1																		
<p>184706-60-3</p>  <p>Absolute stereochemistry shown, Rotation (-)</p> <p>C₃₆H₅₈O₇ [(1<i>R</i>,1<i>aR</i>,2<i>S</i>,5<i>R</i>,5<i>aR</i>,6<i>S</i>,8<i>aS</i>,9<i>R</i>,10<i>R</i>)-1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-Octahydro-5,5<i>a</i>,6-trihydroxy-1-(hydroxymethyl)-1,7,9-trimethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodocen-4-yl]methyl hexadecanoate</p> <p> 1 Reference 0 Reactions 0 Suppliers </p>		<table border="1"> <thead> <tr> <th>Key Physical Properties</th> <th>Value</th> <th>Condition</th> </tr> </thead> <tbody> <tr> <td>Molecular Weight</td> <td>602.84</td> <td>-</td> </tr> <tr> <td>Boiling Point (Predicted)</td> <td>700.3±60.0 °C</td> <td>Press: 760 Torr</td> </tr> <tr> <td>Density (Predicted)</td> <td>1.15±0.1 g/cm³</td> <td>Temp: 20 °C; Press: 760 Torr</td> </tr> <tr> <td>pKa (Predicted)</td> <td>11.90±0.70</td> <td>Most Acidic Temp: 25 °C</td> </tr> </tbody> </table> <p>Experimental Properties Spectra</p>		Key Physical Properties	Value	Condition	Molecular Weight	602.84	-	Boiling Point (Predicted)	700.3±60.0 °C	Press: 760 Torr	Density (Predicted)	1.15±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr	pKa (Predicted)	11.90±0.70	Most Acidic Temp: 25 °C
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<p>1313435-00-5</p>  <p>Absolute stereochemistry shown, Rotation (+) Double bond geometry shown</p> <p>C₅₀H₈₀O₇ [(1<i>R</i>,1<i>aR</i>,2<i>S</i>,5<i>R</i>,5<i>aR</i>,6<i>S</i>,8<i>aS</i>,9<i>R</i>,10<i>aR</i>)-1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-Octahydro-5,5<i>a</i>,6-trihydroxy-1,7,9-trimethyl-11-oxo-1-[[2<i>Z</i>,4<i>E</i>,6<i>Z</i>]-2,4,6-tetradecatrien-1-yl]oxy)methyl]-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodocen-4-yl]methyl hexadecanoate</p> <p> 1 Reference 0 Reactions 0 Suppliers </p>		<table border="1"> <thead> <tr> <th>Key Physical Properties</th> <th>Value</th> <th>Condition</th> </tr> </thead> <tbody> <tr> <td>Molecular Weight</td> <td>793.17</td> <td>-</td> </tr> <tr> <td>Boiling Point (Predicted)</td> <td>818.9±65.0 °C</td> <td>Press: 760 Torr</td> </tr> <tr> <td>Density (Predicted)</td> <td>1.08±0.1 g/cm³</td> <td>Temp: 20 °C; Press: 760 Torr</td> </tr> <tr> <td>pKa (Predicted)</td> <td>11.90±0.70</td> <td>Most Acidic Temp: 25 °C</td> </tr> </tbody> </table>		Key Physical Properties	Value	Condition	Molecular Weight	793.17	-	Boiling Point (Predicted)	818.9±65.0 °C	Press: 760 Torr	Density (Predicted)	1.08±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr	pKa (Predicted)	11.90±0.70	Most Acidic Temp: 25 °C
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Boiling Point (Predicted)	818.9±65.0 °C	Press: 760 Torr																
Density (Predicted)	1.08±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr																
pKa (Predicted)	11.90±0.70	Most Acidic Temp: 25 °C																

Figure S32: The exact search report from scifinder of 1

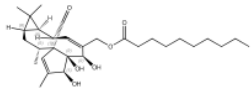
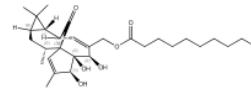
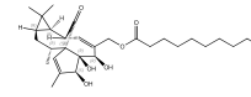
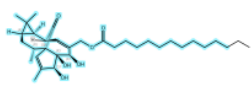
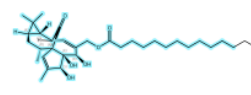
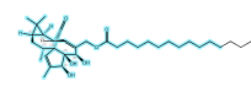
<p>1 Similarity Score: 100</p> <p>83036-67-3</p>  <p>Absolute stereochemistry shown, Rotation (-)</p> <p>C₃₀H₄₆O₆ Decanoic acid, [(1<i>aR</i>,2<i>S</i>,5<i>R</i>,5<i>aR</i>,6<i>S</i>,8<i>aS</i>,9<i>R</i>,10<i>aR</i>)-1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-octahydro-5,5<i>a</i>,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-4-yl)methyl ester</p> <p>References: 10 Reaction: 1 Supplier: 1</p>	<p>2 Similarity Score: 100</p> <p>2389153-16-4</p>  <p>Absolute stereochemistry shown, Rotation (-)</p> <p>C₃₀H₄₆O₆ [(1<i>aS</i>,2<i>R</i>,5<i>R</i>,5<i>aR</i>,6<i>S</i>,8<i>a</i>,10<i>aR</i>)-1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-Octahydro-5,5<i>a</i>,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-4-yl)methyl decanoate</p> <p>Reference: 1 Reactions: 0 Suppliers: 0</p>	<p>3 Similarity Score: 100</p> <p>545404-39-5</p>  <p>Absolute stereochemistry shown</p> <p>C₃₀H₄₆O₆ [(1<i>aR</i>,2<i>R</i>,5<i>R</i>,5<i>aR</i>,6<i>S</i>,8<i>aS</i>,9<i>R</i>,10<i>aR</i>)-1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-Octahydro-5,5<i>a</i>,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-4-yl)methyl decanoate</p> <p>Reference: 1 Reactions: 0 Suppliers: 0</p>
<p>4 Similarity Score: 99</p> <p>113545-44-1</p>  <p>Absolute stereochemistry shown, Rotation (-)</p> <p>C₃₄H₅₄O₆ Tetradecanoic acid, [(1<i>aR</i>,2<i>S</i>,5<i>R</i>,5<i>aR</i>,6<i>S</i>,8<i>aS</i>,9<i>R</i>,10<i>aR</i>)-1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-octahydro-5,5<i>a</i>,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-4-yl)methyl ester</p> <p>References: 12 Reactions: 0 Supplier: 1</p>	<p>5 Similarity Score: 99</p> <p>2389153-12-0</p>  <p>Absolute stereochemistry shown, Rotation (-)</p> <p>C₃₄H₅₄O₆ [(1<i>aS</i>,2<i>R</i>,5<i>R</i>,5<i>aR</i>,6<i>S</i>,8<i>aR</i>,9<i>R</i>,10<i>aR</i>)-1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-Octahydro-5,5<i>a</i>,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-4-yl)methyl tetradecanoate</p> <p>Reference: 1 Reactions: 0 Suppliers: 0</p>	<p>6 Similarity Score: 99</p> <p>39071-33-5</p>  <p>Absolute stereochemistry shown</p> <p>C₃₆H₅₈O₆ Hexadecanoic acid, [(1<i>aR</i>,2<i>S</i>,5<i>R</i>,5<i>aR</i>,6<i>S</i>,8<i>aS</i>,9<i>R</i>,10<i>aR</i>)-1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-octahydro-5,5<i>a</i>,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-4-yl)methyl ester</p> <p>References: 23 Reactions: 0 Suppliers: 16</p>

Figure S33: The 99%-100% similarity search report from scifinder of **1**

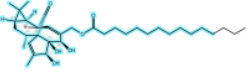
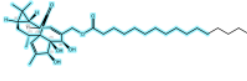
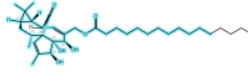
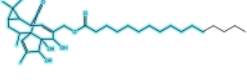
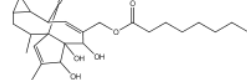

<p>7 Similarity Score: 99</p> <p>2869851-03-4</p>  <p>Absolute stereochemistry shown, Rotation (-)</p> <p>$C_{35}H_{56}O_6$</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>8 Similarity Score: 99</p> <p>2389153-14-2</p>  <p>Absolute stereochemistry shown, Rotation (-)</p> <p>$C_{36}H_{58}O_6$</p> <p>[[1a<i>S</i>,2<i>R</i>,5<i>R</i>,5a<i>R</i>,6<i>S</i>,8a,10a<i>R</i>]-1a,2,5,5a,6,9,10,10a-Octahydro-5,5a,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8a-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-4-yl]methyl hexadecanoate</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>9 Similarity Score: 99</p> <p>2702130-54-7</p>  <p>Relative stereochemistry shown</p> <p>$C_{36}H_{58}O_6$</p> <p>0 References 0 Reactions 1 Supplier</p>
<p>10 Similarity Score: 99</p> <p>74111-26-5</p>  <p>$C_{36}H_{58}O_6$</p> <p>Hexadecanoic acid, (1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8a-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-4-yl)methyl ester</p> <p>0 References 0 Reactions 2 Suppliers</p>	<p>11 Similarity Score: 99</p> <p>98649-87-7</p>  <p>$C_{28}H_{42}O_6$</p> <p>Octanoic acid, (1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8a-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-4-yl)methyl ester, [1a<i>R</i>-(1α,2β,5β,5aβ,6β,8α,9α,10α)]-</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>12 Similarity Score: 98</p> <p>240803-36-5</p>  <p>Absolute stereochemistry shown</p> <p>$C_{40}H_{66}O_6$</p> <p>[[1a<i>R</i>,2<i>S</i>,5<i>R</i>,5a<i>R</i>,6<i>S</i>,8a<i>S</i>,9<i>R</i>,10a<i>R</i>]-1a,2,5,5a,6,9,10,10a-Octahydro-5,5a,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8a-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-4-yl]methyl eicosanoate</p> <p>1 Reference 0 Reactions 0 Suppliers</p>

Figure S34: The 98%-99% similarity search report from scifinder of 1

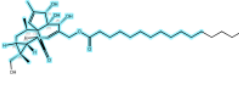
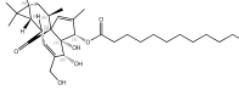
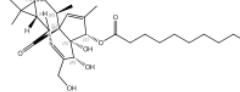
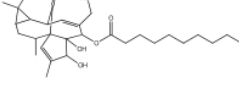
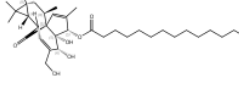
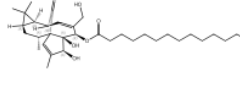
<p>13 Similarity Score: 98</p> <p>184706-60-3</p>  <p>Absolute stereochemistry shown, Rotation (-)</p> <p>C₃₆H₅₈O₇ [[1<i>R</i>,1<i>aR</i>,2<i>S</i>,5<i>R</i>,5<i>aR</i>,6<i>S</i>,8<i>aS</i>,9<i>R</i>,10<i>R</i>]-1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-Octahydro-5,5<i>a</i>,6-trihydroxy-1-(hydroxymethyl)-1,7,9-trimethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-4-yl]methyl hexadecanoate</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>14 Similarity Score: 98</p> <p>67021-88-9</p>  <p>Absolute stereochemistry shown</p> <p>C₃₂H₅₀O₆ Dodecanoic acid, (1<i>aR</i>,2<i>S</i>,5<i>R</i>,5<i>aS</i>,6<i>S</i>,8<i>aS</i>,9<i>R</i>,10<i>aR</i>)-1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-octahydro-5,5<i>a</i>-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-6-yl ester</p> <p>16 References 70 Reactions 0 Suppliers</p>	<p>15 Similarity Score: 98</p> <p>82425-34-1</p>  <p>Absolute stereochemistry shown</p> <p>C₃₀H₄₆O₆ Decanoic acid, 1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-octahydro-5,5<i>a</i>-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-6-yl ester, [1<i>aR</i>-(1<i>a</i>,2<i>β</i>,5<i>β</i>,5<i>aβ</i>,6<i>β</i>,8<i>aα</i>,9<i>α</i>,10<i>aα</i>)]-</p> <p>5 References 3 Reactions 4 Suppliers</p>
<p>16 Similarity Score: 98</p> <p>83036-66-2</p>  <p>Absolute stereochemistry shown, Rotation (+)</p> <p>C₃₀H₄₆O₆ Decanoic acid, 1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-octahydro-5,6-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-5-yl ester, [1<i>aR</i>-(1<i>a</i>,2<i>β</i>,5<i>β</i>,5<i>aβ</i>,6<i>β</i>,8<i>aα</i>,9<i>α</i>,10<i>aα</i>)]-</p> <p>1 Reference 1 Reaction 0 Suppliers</p>	<p>17 Similarity Score: 98</p> <p>83036-62-8</p>  <p>Absolute stereochemistry shown, Rotation (+)</p> <p>C₃₄H₅₄O₆ 3-<i>O</i>-Tetradecanoylingenol</p> <p>21 References 8 Reactions 5 Suppliers</p>	<p>18 Similarity Score: 98</p> <p>113545-45-2</p>  <p>Absolute stereochemistry shown</p> <p>C₃₄H₅₄O₆ Tetradecanoic acid, (1<i>aR</i>,2<i>S</i>,5<i>R</i>,5<i>aR</i>,6<i>S</i>,8<i>aS</i>,9<i>R</i>,10<i>aR</i>)-1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-octahydro-5<i>a</i>,6-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-5-yl ester</p> <p>2 References 0 Reactions 1 Supplier</p>

Figure S35: the 98% similarity search report from scifinder of **1**

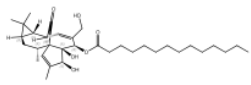
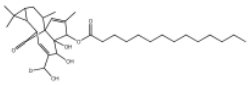
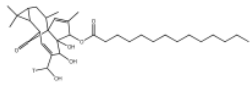
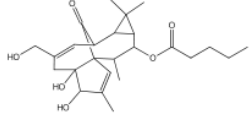
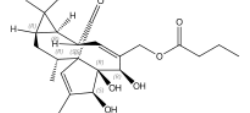
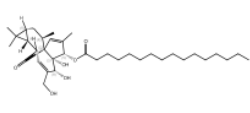
<p>19 Similarity Score: 98</p> <p>2389153-18-6</p>  <p>Absolute stereochemistry shown, Rotation (+)</p> <p>C₃₄H₅₄O₆ (1<i>a</i><i>S</i>,2<i>R</i>,5<i>R</i>,5<i>a</i><i>R</i>,6<i>S</i>,8<i>a</i><i>R</i>,9<i>R</i>,10<i>a</i><i>R</i>)-1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-Octahydro-5<i>a</i>,6-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-5-yl tetradecanoate</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>20 Similarity Score: 98</p> <p>143725-48-8</p>  <p>C₃₄H₅₃DO₆ Tetradecanoic acid, 1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-octahydro-5,5<i>a</i>-dihydroxy-4-(hydroxymethyl)-<i>d</i>-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-6-yl ester, [1<i>a</i><i>R</i>-(1<i>a</i><i>a</i>,2<i>β</i>,5<i>β</i>,5<i>a</i><i>β</i>,6<i>β</i>,8<i>a</i><i>a</i>,9<i>a</i>,10<i>a</i><i>a</i>)]-</p> <p>1 Reference 1 Reaction 0 Suppliers</p>	<p>21 Similarity Score: 98</p> <p>143725-47-7</p>  <p>C₃₄H₅₃O₆T Tetradecanoic acid, 1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-octahydro-5,5<i>a</i>-dihydroxy-4-(hydroxymethyl)-<i>d</i>-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-6-yl ester, [1<i>a</i><i>R</i>-(1<i>a</i><i>a</i>,2<i>β</i>,5<i>β</i>,5<i>a</i><i>β</i>,6<i>β</i>,8<i>a</i><i>a</i>,9<i>a</i>,10<i>a</i><i>a</i>)]-</p> <p>1 Reference 1 Reaction 0 Suppliers</p>
<p>22 Similarity Score: 98</p> <p>129344-79-2</p>  <p>C₂₅H₃₆O₆ Pentanoic acid, 1,1<i>a</i>,2,5,5<i>a</i>,6,9,10-octahydro-5<i>a</i>,6-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-10<i>a</i><i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-10<i>a</i>-yl ester, [1<i>a</i><i>R</i>-(1<i>a</i><i>a</i>,2<i>β</i>,5<i>a</i><i>β</i>,6<i>β</i>,8<i>a</i><i>a</i>,9<i>a</i>,10<i>a</i><i>a</i>)]-</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>23 Similarity Score: 98</p> <p>1448352-33-7</p>  <p>Absolute stereochemistry shown</p> <p>C₂₄H₃₄O₆ [[1<i>a</i><i>R</i>,2,5,5<i>R</i>,5<i>a</i><i>R</i>,6,5,8<i>a</i>,9<i>R</i>,10<i>a</i><i>R</i>]-1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-Octahydro-5,5<i>a</i>,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-4-yl]methyl butanoate</p> <p>2 References 1 Reaction 0 Suppliers</p>	<p>24 Similarity Score: 97</p> <p>52557-26-3</p>  <p>Absolute stereochemistry shown</p> <p>C₃₆H₅₈O₆ Euphorbia factor I₁</p> <p>25 References 3 Reactions 15 Suppliers</p>

Figure S36: the 97%-98% similarity search report from scifinder of **1**

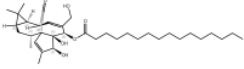
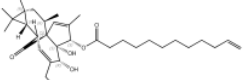
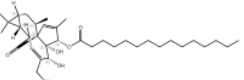
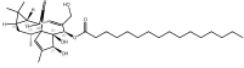
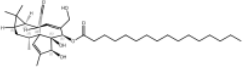
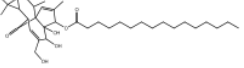
<p>25 Similarity Score: 97</p> <p>37394-33-5</p>  <p>Absolute stereochemistry shown</p> <p>C₃₆H₅₈O₆ Hexadecanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-4-(hydroxy methyl)-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8a-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclododecen-5-yl ester, [1<i>aR</i>-(1<i>aα</i>,2<i>β</i>,5<i>β</i>,5<i>aβ</i>,6<i>β</i>,8<i>aα</i>,9<i>α</i>,10<i>aα</i>)]-</p> <p>References: 6 Reactions: 0 Suppliers: 1</p>	<p>26 Similarity Score: 97</p> <p>1453471-31-2</p>  <p>Absolute stereochemistry shown</p> <p>C₃₂H₄₈O₆ (1<i>aR</i>,2<i>S</i>,5<i>R</i>,5<i>aS</i>,6<i>S</i>,8<i>aS</i>,9<i>R</i>,10<i>aR</i>)-1a,2,5,5a,6,9,10,10a-Octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8a-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclododecen-6-yl 11-dodecanoate</p> <p>References: 3 Reactions: 0 Suppliers: 0</p>	<p>27 Similarity Score: 97</p> <p>363136-24-7</p>  <p>Absolute stereochemistry shown</p> <p>C₃₅H₅₆O₆ (1<i>aR</i>,2<i>S</i>,5<i>R</i>,5<i>aS</i>,6<i>S</i>,8<i>aS</i>,9<i>R</i>,10<i>aR</i>)-1a,2,5,5a,6,9,10,10a-Octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8a-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclododecen-6-yl pentadecanoate</p> <p>References: 2 Reactions: 0 Suppliers: 0</p>
<p>28 Similarity Score: 97</p> <p>2389161-15-1</p>  <p>Absolute stereochemistry shown, Rotation (+)</p> <p>C₃₆H₅₈O₆</p> <p>Reference: 1 Reactions: 0 Suppliers: 0</p>	<p>29 Similarity Score: 97</p> <p>82468-50-6</p> <p>37394-33-5</p>  <p>Absolute stereochemistry shown</p> <p>C₃₆H₅₄O₆ Hexadecadienoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-4-(hydroxy methyl)-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8a-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclododecen-5-yl ester, [1<i>aR</i>-(1<i>aα</i>,2<i>β</i>,5<i>β</i>,5<i>aβ</i>,6<i>β</i>,8<i>aα</i>,9<i>α</i>,10<i>aα</i>)]-</p> <p>Reference: 1 Reactions: 0 Suppliers: 0</p>	<p>30 Similarity Score: 97</p> <p>2738924-02-0</p>  <p>C₃₆H₅₈O₆</p> <p>References: 0 Reactions: 0 Supplier: 1</p>

Figure S37: the 97% similarity search report from scifinder of 1

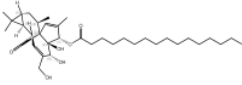
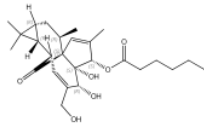
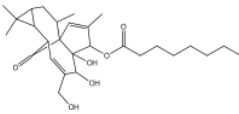
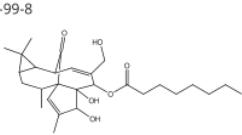
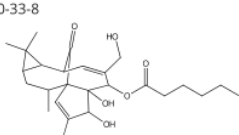
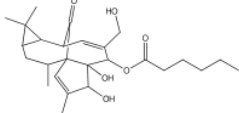
<p>31 Similarity Score: 97</p> <p>2704973-14-6</p>  <p>Relative stereochemistry shown</p> <p>C₃₆H₅₈O₆</p> <p>0 References 0 Reactions 1 Supplier</p>	<p>32 Similarity Score: 97</p> <p>83036-61-7</p>  <p>Absolute stereochemistry shown</p> <p>C₂₆H₃₈O₆</p> <p>Hexanoic acid, (1a<i>R</i>,2<i>S</i>,5<i>R</i>,5a<i>S</i>,6<i>S</i>,8a<i>S</i>,9<i>R</i>,10a<i>R</i>)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8a-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-6-yl ester</p> <p>16 References 44 Reactions 4 Suppliers</p>	<p>33 Similarity Score: 97</p> <p>77508-66-8</p>  <p>C₂₈H₄₂O₆</p> <p>Octanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8a-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-6-yl ester, [1a<i>R</i>-(1aα,2β,5β,5aβ,6β,8aα,9α,10aα)]-</p> <p>4 References 1 Reaction 0 Suppliers</p>
<p>34 Similarity Score: 97</p> <p>82438-00-4</p>  <p>C₂₈H₄₀O₆</p> <p>Octenoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8a-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-5-yl ester, [1a<i>R</i>-(1aα,2β,5β,5aβ,6β,8aα,9α,10aα)]-</p> <p>2 References 0 Reactions 0 Suppliers</p>	<p>35 Similarity Score: 97</p> <p>119000-34-9</p>  <p>C₂₆H₃₄O₆</p> <p>Hexadienoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8a-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-5-yl ester, [1a<i>R</i>-(1aα,2β,5β,5aβ,6β,8aα,9α,10aα)]-</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>36 Similarity Score: 97</p> <p>119000-33-8</p>  <p>C₂₆H₃₈O₆</p> <p>Hexanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8a-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-5-yl ester, [1a<i>R</i>-(1aα,2β,5β,5aβ,6β,8aα,9α,10aα)]-</p> <p>0 References 0 Reactions 0 Suppliers</p>

Figure S38: the 97% similarity search report from scifinder of 1

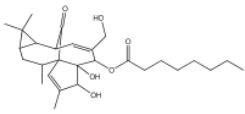
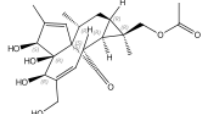
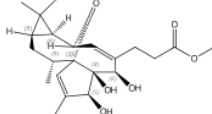
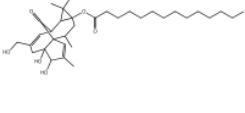
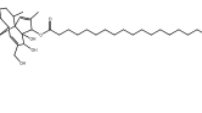
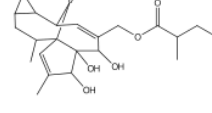
<p>37 Similarity Score: 97</p> <p>82437-99-8</p>  <p>C₂₈H₄₂O₆ Octanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-4-(hydroxy methyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, [1aR-(1aα,2β,5β,5aβ,6β,8aα,9α,10aα)]-</p> <p>References: 0 Reactions: 0 Suppliers: 0</p>	<p>38 Similarity Score: 97</p> <p>88262-83-3</p>  <p>Absolute stereochemistry shown</p> <p>C₂₂H₃₀O₇ (1R,1aR,2S,5R,5aR,6S,8aS,9R,10aR)-1-[(Acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-4-(hydroxy methyl)-1,7,9-trimethyl-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-11-one</p> <p>Reference: 1 Reactions: 0 Suppliers: 0</p>	<p>39 Similarity Score: 97</p> <p>2222491-26-9</p>  <p>Absolute stereochemistry shown, Rotation (+)</p> <p>C₂₃H₃₂O₆ Methyl (1aR,2S,5R,5aR,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecene-4-propanoate</p> <p>Reference: 1 Reactions: 2 Suppliers: 0</p>
<p>40 Similarity Score: 96</p> <p>129317-91-5</p>  <p>C₃₄H₅₄O₆ Tetradecanoic acid, 1,1a,2,5,5a,6,9,10-octahydro-5a,6-dihydroxy-4-(hydroxy methyl)-1,1,7,9-tetramethyl-11-oxo-10aH-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-10a-yl ester, [1aR-(1aα,2β,5aβ,6β,8aα,9α,10aα)]-</p> <p>Reference: 1 Reactions: 0 Suppliers: 0</p>	<p>41 Similarity Score: 96</p> <p>83036-63-9</p>  <p>C₄₀H₆₆O₆ Eicosanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxy methyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, [1aR-(1aα,2β,5β,5aβ,6β,8aα,9α,10aα)]-</p> <p>Reference: 1 Reaction: 1 Suppliers: 0</p>	<p>42 Similarity Score: 96</p> <p>74690-94-1</p>  <p>C₂₅H₃₆O₆ Butanoic acid, 2-methyl-, (1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl) methyl ester, [1aR-[1aα,2β,4(S*),5β,5aβ,6β,8aα,9α,10aα]]-</p> <p>Reference: 1 Reactions: 0 Suppliers: 0</p>

Figure S39: the 96%-97% similarity search report from scifinder of 1

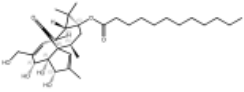
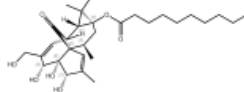
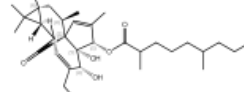
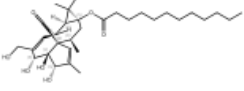
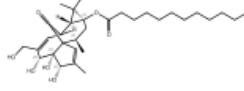
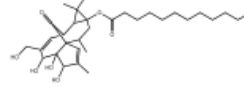
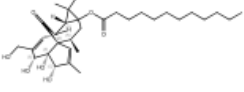
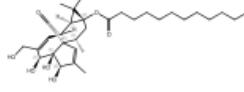
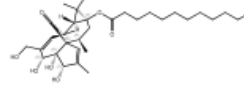
<p>43 Similarity Score: 96</p> <p>54706-70-6</p>  <p>Absolute stereochemistry shown, Rotation (-)</p> <p>C₃₂H₅₀O₇ Dodecanoic acid, (1<i>a</i>,<i>R</i>,2<i>S</i>,5<i>R</i>,5<i>a</i>,<i>R</i>,6<i>S</i>,8<i>a</i>,<i>S</i>,9<i>R</i>,10<i>a</i>,<i>S</i>)-1,1<i>a</i>,2,5,5<i>a</i>,6,9,10-octahydro-5,5<i>a</i>,6-trihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-10<i>a</i>-<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-10<i>a</i>-yl ester</p> <p>13 References 541 Reactions 37 Suppliers</p>	<p>44 Similarity Score: 96</p> <p>2254316-15-7</p>  <p>Absolute stereochemistry shown</p> <p>C₃₀H₄₆O₇ (1<i>a</i>,<i>R</i>,2<i>S</i>,5<i>R</i>,5<i>a</i>,<i>R</i>,6<i>S</i>,8<i>a</i>,<i>S</i>,9<i>R</i>,10<i>a</i>,<i>S</i>)-1,1<i>a</i>,2,5,5<i>a</i>,6,9,10-Octahydro-5,5<i>a</i>,6-trihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-10<i>a</i>-<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-10<i>a</i>-yl decanoate</p> <p>1 Reference 3 Reactions 0 Suppliers</p>	<p>45 Similarity Score: 96</p> <p>403805-88-9</p>  <p>Available stereochemistry shown, Rotation (-)</p> <p>C₃₁H₄₈O₆ (1<i>a</i>,<i>R</i>,2<i>S</i>,5<i>R</i>,5<i>a</i>,<i>S</i>,6<i>S</i>,8<i>a</i>,<i>S</i>,9<i>R</i>,10<i>a</i>,<i>R</i>)-1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-Octahydro-5,5<i>a</i>-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1<i>a</i>-<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-6-yl 2,6-dimethylnonanoate</p> <p>1 Reference 0 Reactions 0 Suppliers</p>
<p>46 Similarity Score: 96</p> <p>2748602-26-6</p>  <p>Relative stereochemistry shown</p> <p>C₃₂H₅₀O₇</p> <p>0 References 0 Reactions 1 Supplier</p>	<p>47 Similarity Score: 96</p> <p>2714897-58-0</p>  <p>Relative stereochemistry shown</p> <p>C₃₂H₅₀O₇</p> <p>0 References 0 Reactions 1 Supplier</p>	<p>48 Similarity Score: 96</p> <p>2700206-52-4</p>  <p>C₃₂H₅₀O₇</p> <p>0 References 0 Reactions 4 Suppliers</p>
<p>49 Similarity Score: 96</p> <p>2561421-90-5</p>  <p>Relative stereochemistry shown</p> <p>C₃₂H₅₀O₇</p> <p>0 References 0 Reactions 1 Supplier</p>	<p>50 Similarity Score: 96</p> <p>2512196-32-4</p>  <p>Relative stereochemistry shown</p> <p>C₃₂H₅₀O₇</p> <p>0 References 0 Reactions 5 Suppliers</p>	<p>51 Similarity Score: 96</p> <p>2512189-22-7</p>  <p>Relative stereochemistry shown</p> <p>C₃₂H₅₀O₇</p> <p>0 References 0 Reactions 1 Supplier</p>

Figure S40: the 96% similarity search report from scifinder of **1**

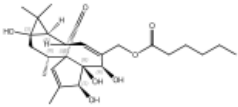
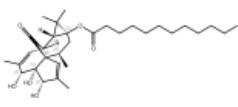
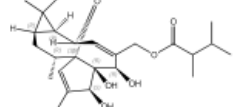
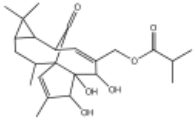
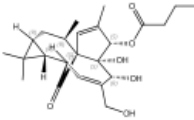
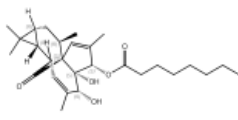
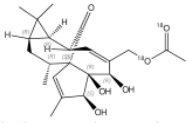
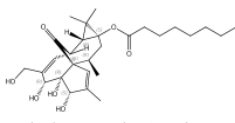
<p>52 Similarity Score: 96</p> <p>2254317-05-8</p>  <p>Absolute stereochemistry shown</p> <p>C₂₆H₃₈O₇</p> <p>1 Reference 1 Reaction 0 Suppliers</p>	<p>53 Similarity Score: 96</p> <p>2254316-17-9</p>  <p>Absolute stereochemistry shown</p> <p>C₃₂H₅₀O₆</p> <p>(1<i>aR</i>,2<i>S</i>,5<i>R</i>,5<i>aS</i>,6<i>S</i>,8<i>aS</i>,9<i>R</i>,10<i>aS</i>)-1,1<i>a</i>,2,5,5<i>a</i>,6,9,10-Octahydro-5,5<i>a</i>,6-trihydroxy-1,1,4,7,9-pentamethyl-11-oxo-10<i>aH</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-10<i>a</i>-yl dodecanoate</p> <p>1 Reference 1 Reaction 0 Suppliers</p>	<p>54 Similarity Score: 96</p> <p>2615930-06-6</p>  <p>Absolute stereochemistry shown</p> <p>C₂₆H₃₈O₆</p> <p>1 Reference 0 Reactions 0 Suppliers</p>
<p>55 Similarity Score: 96</p> <p>74690-91-8</p>  <p>C₂₄H₃₄O₆</p> <p>Propanoic acid, 2-methyl-, (1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-octahydro-5,5<i>a</i>,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-4-yl) methyl ester, [1<i>aR</i>-(1<i>a</i>α,2β,5β,5<i>a</i>β,6β,8<i>a</i>α,9<i>\alpha,10<i>a</i>α)]-</i></p> <p>2 References 0 Reactions 0 Suppliers</p>	<p>56 Similarity Score: 96</p> <p>77508-67-9</p>  <p>Absolute stereochemistry shown</p> <p>C₂₄H₃₄O₆</p> <p>Butanoic acid, 1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-octahydro-5,5<i>a</i>-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-6-yl ester, [1<i>aR</i>-(1<i>a</i>α,2β,5β,5<i>a</i>β,6β,8<i>a</i>α,9<i>\alpha,10<i>a</i>α)]-</i></p> <p>5 References 3 Reactions 1 Supplier</p>	<p>57 Similarity Score: 96</p> <p>2244983-56-8</p>  <p>Absolute stereochemistry shown</p> <p>C₂₈H₄₂O₅</p> <p>(1<i>aR</i>,2<i>S</i>,5<i>R</i>,5<i>aS</i>,6<i>S</i>,8<i>aS</i>,9<i>R</i>,10<i>aR</i>)-1<i>a</i>,2,5,5<i>a</i>,6,9,10,10<i>a</i>-Octahydro-5,5<i>a</i>-dihydroxy-1,1,4,7,9-pentamethyl-11-oxo-1<i>H</i>-2,8<i>a</i>-methanocyclopenta[<i>a</i>]cyclopropa[<i>e</i>]cyclodecen-6-yl octanoate</p> <p>1 Reference 2 Reactions 1 Supplier</p>

Figure S41: the 96% similarity search report from scifinder of 1

Substances (2)

[View in SciFinder®](#)

1	Similarity Score: 96	2	Similarity Score: 95
2088758-65-8		2254316-22-6	
$C_{22}H_{30}O_6$	Absolute stereochemistry shown, Rotation (+)	$C_{28}H_{42}O_7$	Absolute stereochemistry shown
1 Reference	3 Reactions	0 Suppliers	1 Reference
		5 Reactions	0 Suppliers

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Figure S42: the 95% similarity search report from scifinder of 1



Figure S43: The image of the *Euphorbia jolkinii*

The herbarium number of *Euphorbia jolkinii* registered at <https://sweetgum.nybg.org/science/ih/> was 4048695.

Table S1: The NMR data of the compound **1-3** (¹H NMR 400 MHz, ¹³C NMR 100 MHz, in CDCl₃)*

	1	2	3	1	2	3
	δ_C	δ_C	δ_C	δ_H	δ_H	δ_H
1	129.7	129.1	129.3	5.92, d (1.5)	5.90, br.s	5.90, br.s
2	138.9	139.0	139.0			
3	80.4	80.1	80.2	4.42, d (5.5)	4.42, d (5.5)	4.42, d (5.5)
4	84.3	84.2	84.2			
5	73.8	73.8	73.8	3.65, d (10.6)	3.64, d (11.0)	3.64, d (10.9)
6	136.8	136.8	136.7			
7	127.9	127.4	127.6	6.07, d (3.7)	6.05, d (3.9)	6.05, d (3.7)
8	44.0	44.0	44.0	4.07, dd (3.8, 11.7)	4.08, dd (3.8, 11.5)	4.08, dd (3.8, 11.7)
9	207.0	207.5	207.3			
10	72.6	72.6	72.6			
11	39.7	39.5	39.6	2.32, m	2.32, m	2.32, m
12	31.0	30.9	30.9	2.25, m	2.25, m	2.25, m
				1.74, brs	1.74, brs	1.74, brs
13	23.2	23.2	23.1	0.70, dd (8.5, 14.9)	0.70, dd (8.2, 15.0)	0.70, dd (8.5, 14.9)
14	23.0	22.9	22.9	0.94, m	0.94, m	0.94, m
15	23.9	23.8	23.9			
16	28.5	28.5	28.5	1.06, s	1.06, s	1.06, s
17	15.5	15.5	15.5	1.11, s	1.11, s	1.11, s
18	17.4	17.4	17.4	0.97, d (6.9)	0.95, d (6.9)	0.97, d (6.9)
19	15.4	15.4	15.4	1.84, d (1.1)	1.83, br.s	1.83, br.s
20	66.3	66.3	66.3	4.70, d (12.9)	4.69, d (12.9)	4.69, d (12.9)
				4.53, d (12.9)	4.54, d (12.9)	4.54, d (12.9)
1'	174.3	174.5	174.4			
2'	34.4	34.3	34.3	2.30, t (6.5)	2.30, t (6.5)	2.30, t (6.5)
3'	24.9	24.9	24.9	1.59, m	1.59, m	1.59, m
4'	29.1	29.3	29.3	1.26, m	1.25, m	1.26, m
5'	29.3	29.5	29.5	1.26, m	1.25, m	1.26, m
6'	29.6	29.7	29.7	1.26, m	1.25, m	1.26, m
7'	29.6	29.7	29.7	1.26, m	1.25, m	1.26, m

8'	29.5	29.7	29.7	1.26, m	1.25, m	1.26, m
9'	29.3	29.7	29.6	1.26, m	1.25, m	1.26, m
10'	31.9	29.7	29.6	1.26, m	1.25, m	1.26, m
11'	22.7	29.7	29.6	1.26, m	1.25, m	1.26, m
12'	14.1	29.7	29.5	0.88, t (6.8)	1.25, m	1.26, m
13'		29.7	22.7		1.25, m	1.26, m
14'		29.5	14.1		1.25, m	0.88, t (6.8)
15'		22.7			1.25, m	
16'		14.1			0.88, t (6.7)	

As the ^1H NMR and ^{13}C NMR data shown in the Table S1, these data were very similar, while the differences were the molecular formula of compound **2** was $\text{C}_{36}\text{H}_{58}\text{O}_6$ by ESI-MS m/z 585 ($[\text{M}-\text{H}]^-$), and compound **3** was $\text{C}_{34}\text{H}_{54}\text{O}_6$ by ESI-MS m/z 1139 ($[\text{2M}+\text{Na}]^+$).

S1:Cytotoxic Activity Assay

Firstly, prepared the single cell suspension with the 10% fetal bovine serum (DMEM or RPMI1640), inoculated 5000 cells each well onto the 96-well plate, and the volume of each well was 100 μL . Cells were inoculated and cultured 24 hours in advance. Secondly, the testing compound was dissolved with DMSO in 40 μM , 8 μM , 1.6 μM , 0.32 μM and 0.064 μM , the final volume of each hole was 200 μL . After 48 hours of culturing at 37 $^\circ\text{C}$, removed the culture solution in the hole, and added 20 μL MTS solution to each hole and culture solution 100 μL , set 3 blank holes. Then hatched for 4 hours to measure the light absorption value after the reaction was fully carried out. Finally, set the wavelength of the multifunctional enzyme marker at 492 nm to read the light absorption value, and then calculated IC_{50} value of the tested compound by the Reed and Muench method, the Positive control were cisplatin (DDP) and paclitaxel (Taxol).