

## Supporting Information

*Rec. Nat. Prod.* 17:6 (2023) 1085-1089

### A New Chromanone Derivative from *Calophyllum inophyllum* Resin and Its Antibacterial Activity

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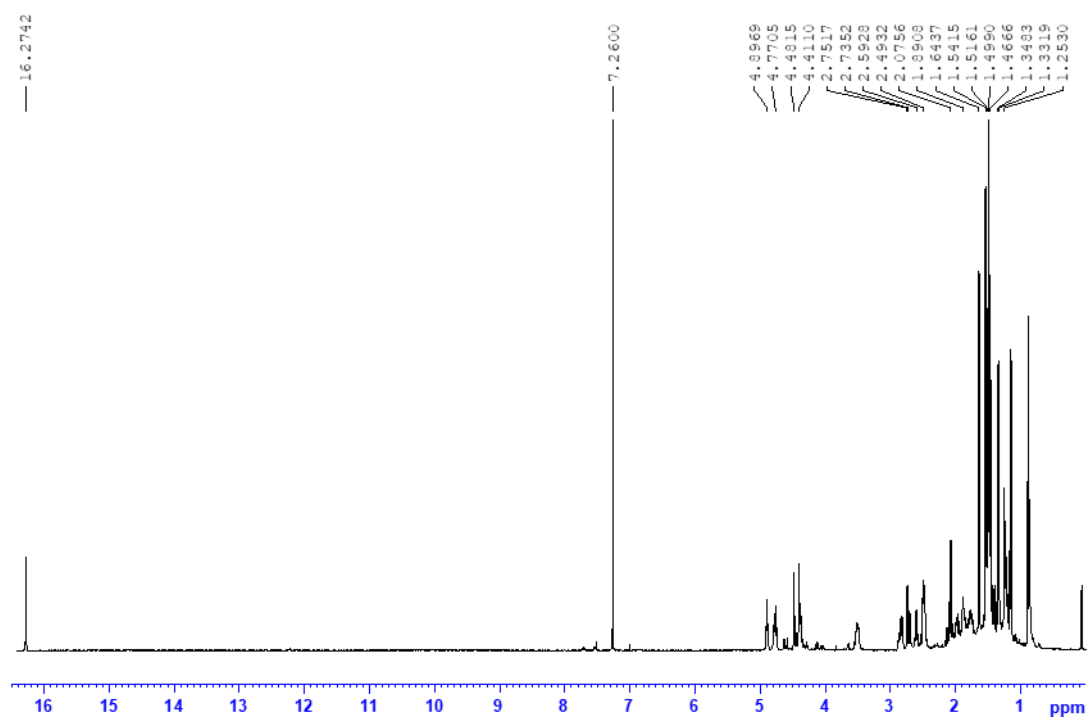
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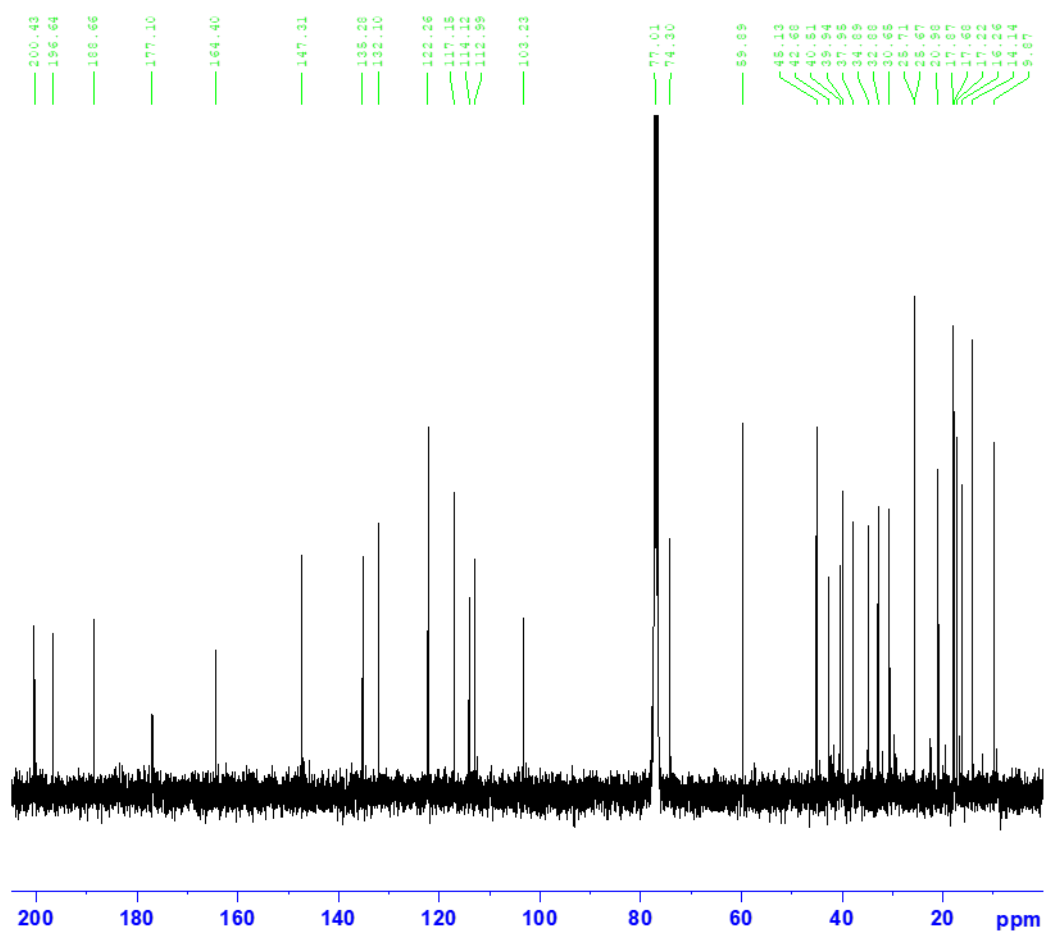
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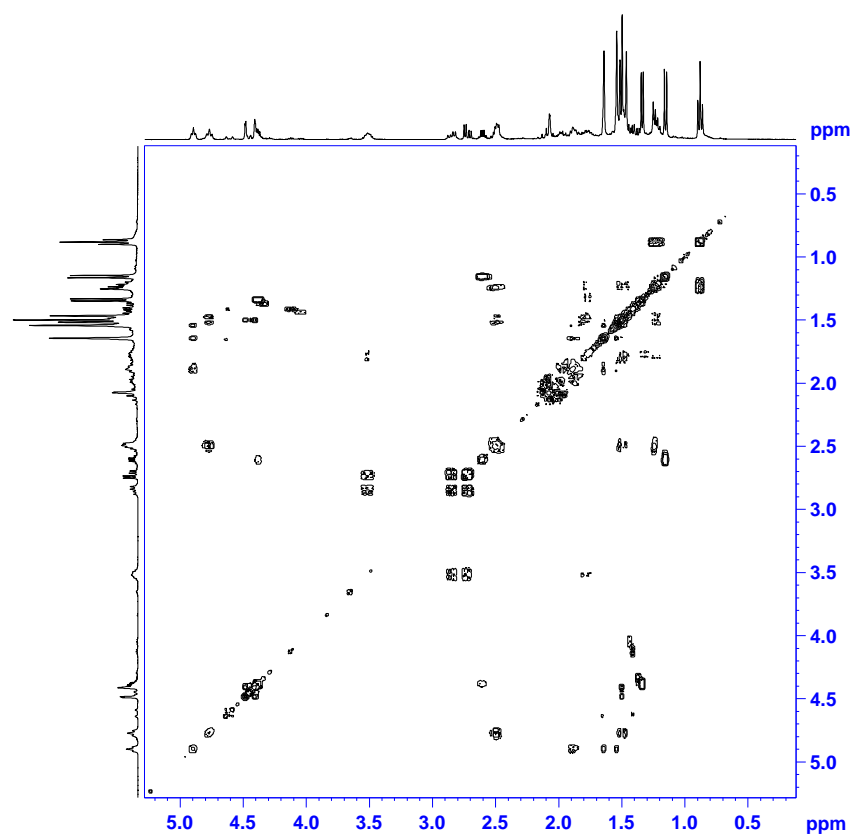
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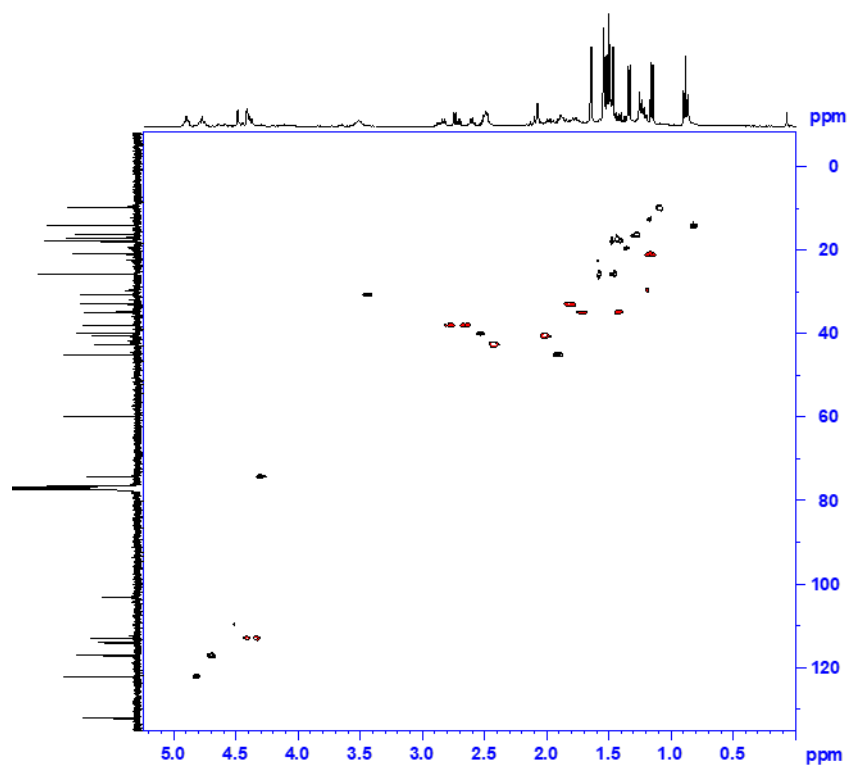
**Figure S1:**  $^1\text{H}$  NMR spectrum of calophylloidal acid B (**2**) in  $\text{CDCl}_3$



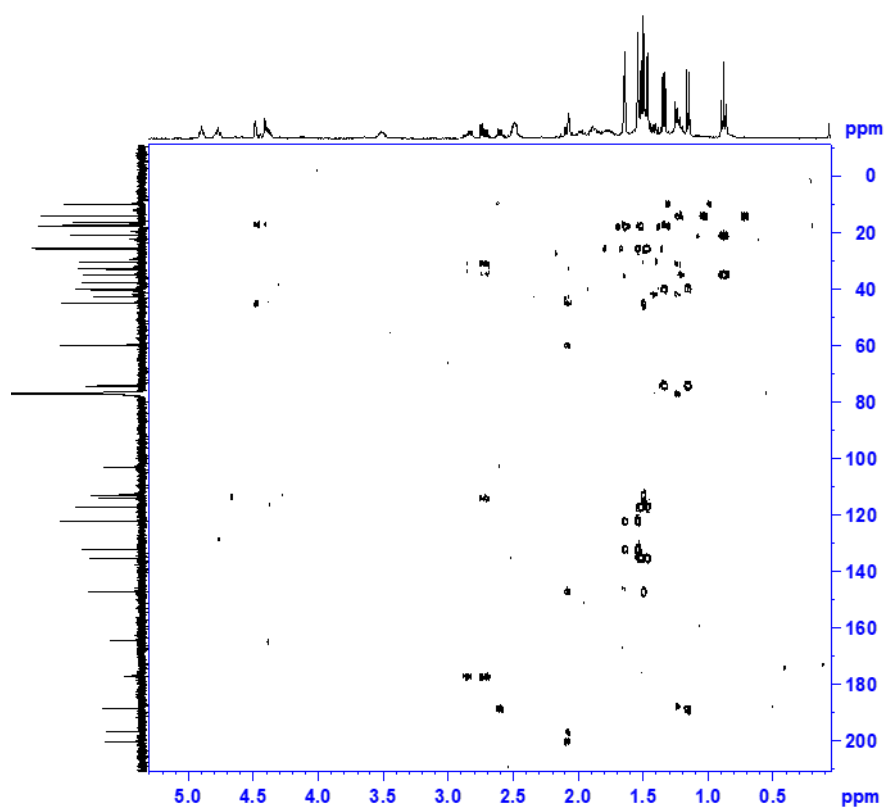
**Figure S2:**  $^{13}\text{C}$  NMR spectrum of calophylloic acid B (2) in  $\text{CDCl}_3$



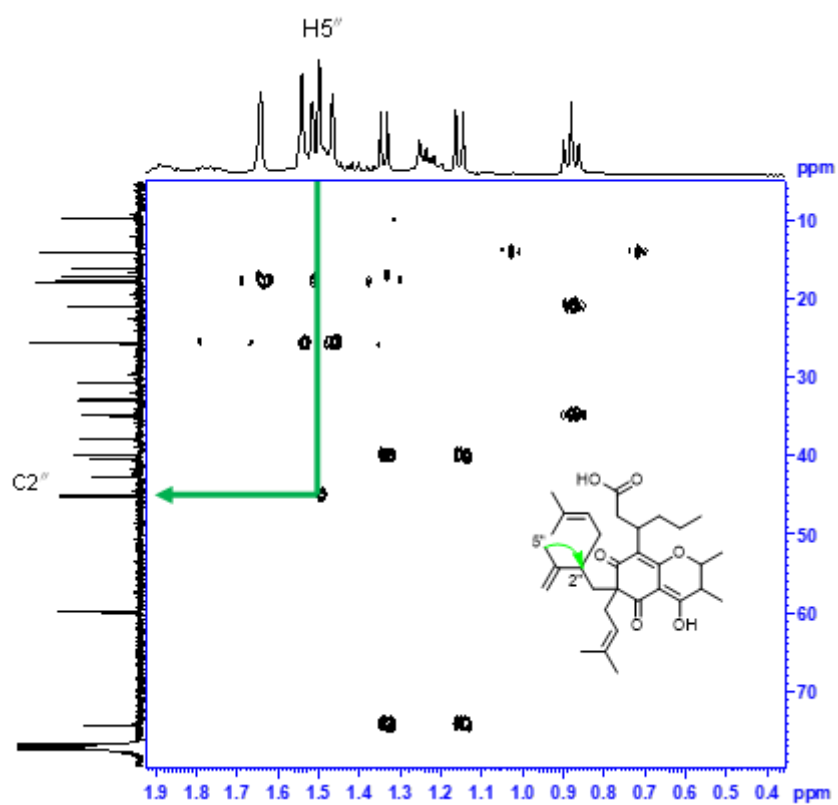
**Figure S3:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of calophylloidal acid B (**2**) in  $\text{CDCl}_3$



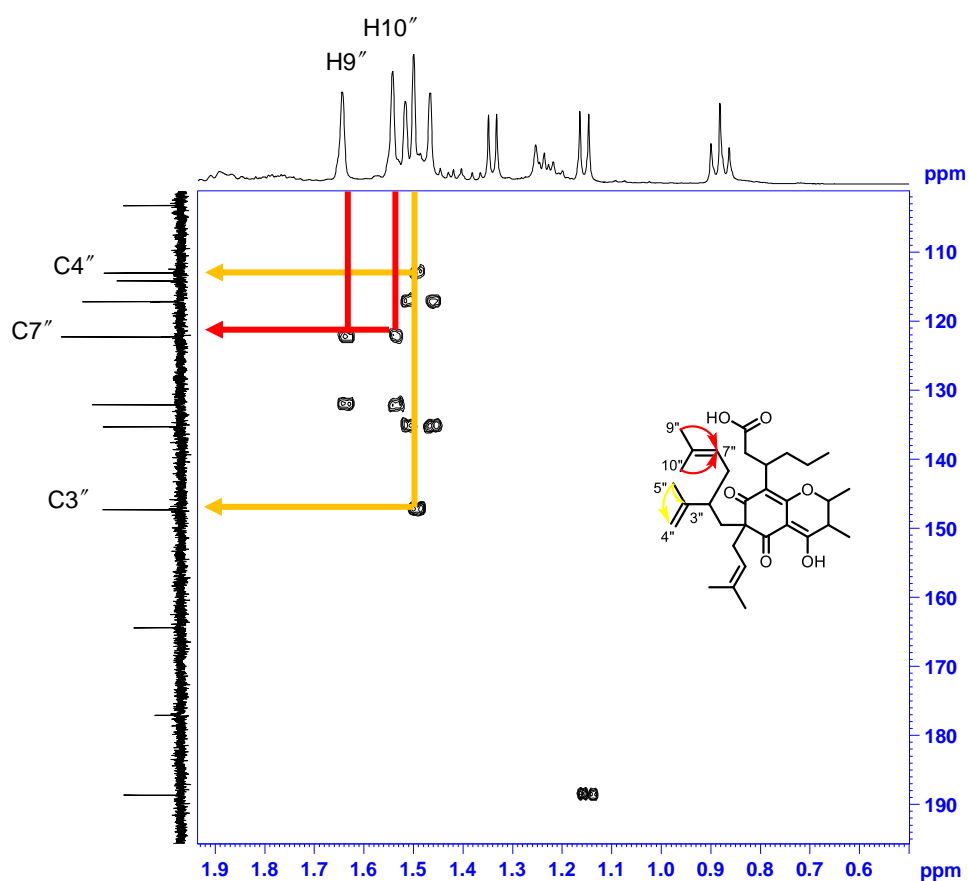
**Figure S4:** HSQC spectrum of calophylloic acid B (**2**) in  $\text{CDCl}_3$



**Figure S5:** HMBC spectrum of calophylloidic acid B (**2**) in  $\text{CDCl}_3$

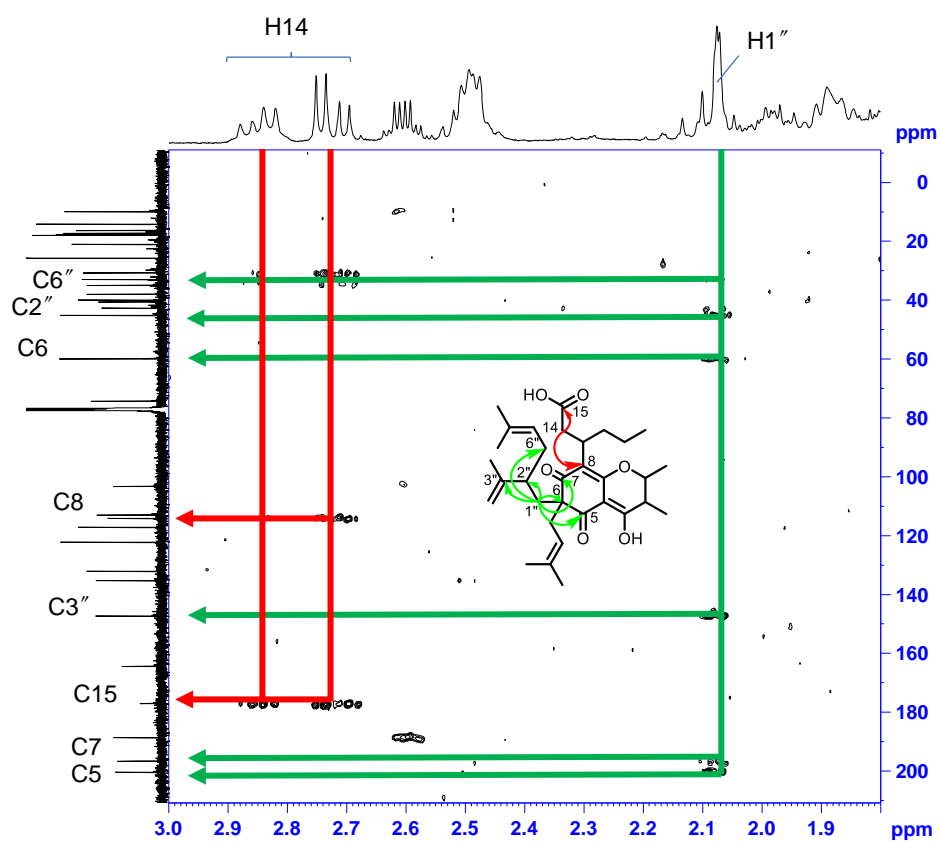


**Figure S6:** HMBC spectrum of calophylloidic acid B (**2**) (From  $\delta_c$  6.0 ppm to  $\delta_c$  80 ppm )

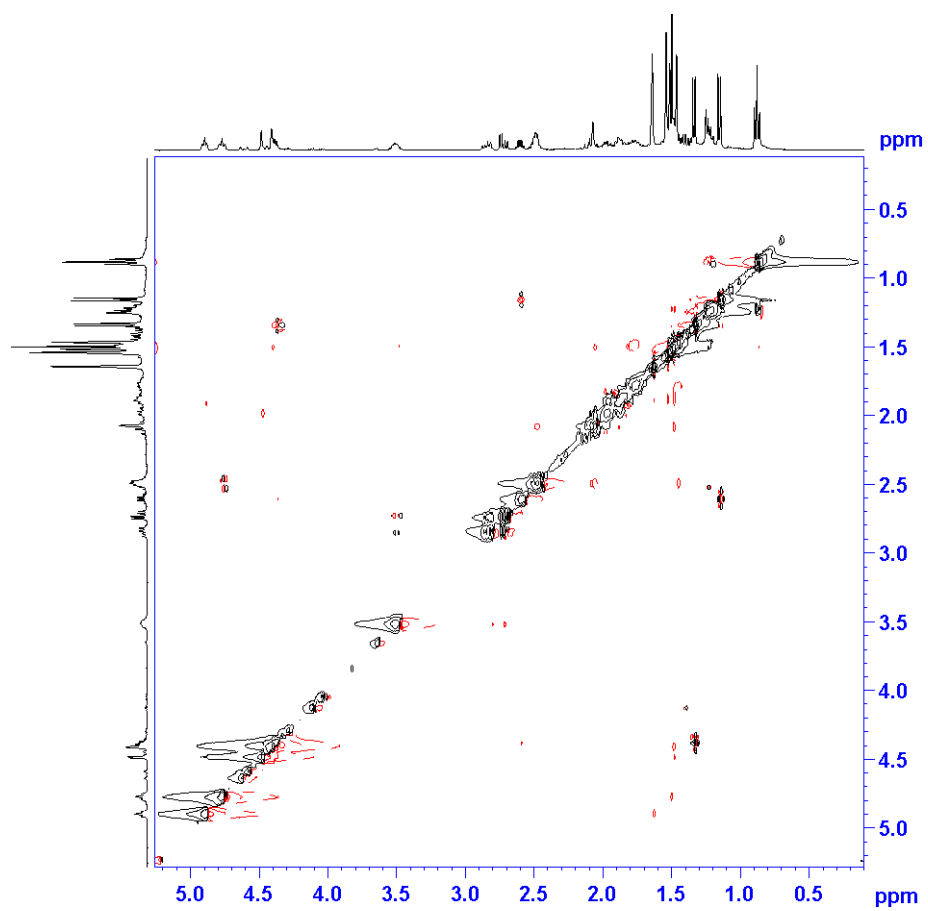


**Figure S7:** HMBC spectrum of calophylloic acid B (**2**) (From  $\delta_{\text{C}}$  100 ppm to  $\delta_{\text{C}}$  195 ppm)



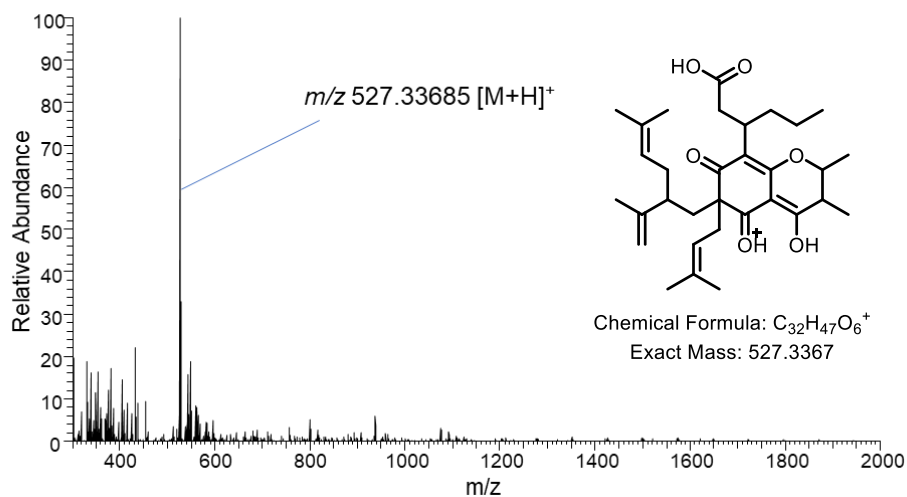


**Figure S8:** HMBC spectrum of calophylloidalic acid B (**2**) (From  $\delta_c$  0 ppm to  $\delta_c$  210 ppm)

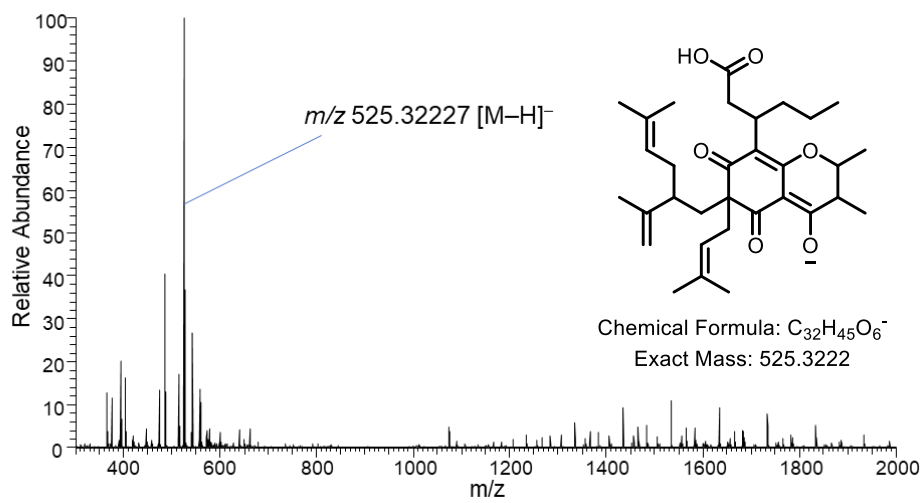


**Figure S9:** NOESY spectrum of calophylloidal acid B (2) in  $\text{CDCl}_3$

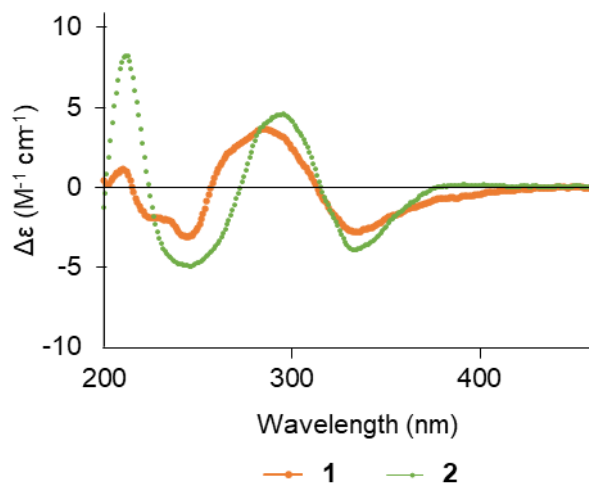
Positive mode



Negative mode



**Figure S10:** HRESIMS spectrum of calophylloic acid B (**2**).



**Figure S11:** ECD spectra of calophylloidic acid A (**1**) and B (**2**) in acetonitrile

## Initiating Search

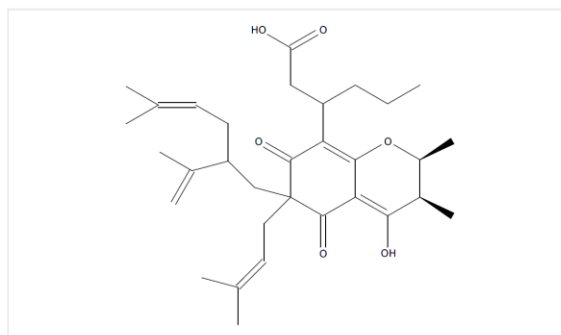
September 15, 2023, 9:23AM

## Substances:


Filtered By:

Similarity: 95-98

Number of Components: 1

Structure Match: **Similarity**

## Search Tasks

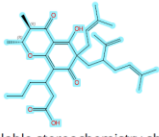
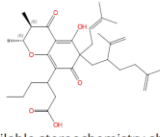
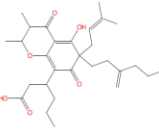
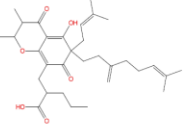
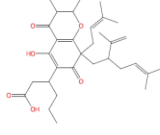
Task	Search Type	View
Exported: Returned Substance Results + Filters (5)	 Substances	<a href="#">View Results</a>

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Similarity	Count
95-98	5
90-94	8
85-89	13
80-84	24
75-79	39
70-74	175
65-69	2,263
60-64	15,388

**Substances** (5)[View in SciFinder®](#)

<p>1 Similarity Score: 96</p> <p>29077-61-0</p>  <p>Available stereochemistry shown</p> <p><b>C<sub>32</sub>H<sub>46</sub>O<sub>6</sub></b>  <i>rel</i>-(2<i>R</i>,3<i>R</i>)-3,4,6,7-Tetrahydro-5-hydroxy-2,3-dimethyl-6-(3-methyl-2-buten-1-yl)-6-[5-methyl-2-(1-methylethenyl)-4-hexen-1-yl]-4,7-dioxo-β-propyl-2<i>H</i>-1-benzopyran-8-propanoic acid</p> <p>References: 4 Reactions: 2 Suppliers: 0</p>	<p>2 Similarity Score: 96</p> <p>29077-60-9</p>  <p>Available stereochemistry shown</p> <p><b>C<sub>32</sub>H<sub>46</sub>O<sub>6</sub></b>  <i>rel</i>-(2<i>R</i>,3<i>R</i>)-3,4,6,7-Tetrahydro-5-hydroxy-2,3-dimethyl-6-(3-methyl-2-buten-1-yl)-6-[5-methyl-2-(1-methylethenyl)-5-hexen-1-yl]-4,7-dioxo-β-propyl-2<i>H</i>-1-benzopyran-8-propanoic acid</p> <p>References: 11 Reactions: 3 Suppliers: 0</p>	<p>3 Similarity Score: 96</p> <p>22879-64-7</p>  <p><b>C<sub>32</sub>H<sub>46</sub>O<sub>6</sub></b>  2<i>H</i>-1-Benzopyran-8-propanoic acid, 3,4,6,7-tetrahydro-5-hydroxy-2,3-dimethyl-6-(3-methyl-2-butenyl)-6-(7-methyl-3-methylene-6-octenyl)-4,7-dioxo-β-propyl-</p> <p>Reference: 1 Reactions: 0 Suppliers: 0</p>
<p>4 Similarity Score: 96</p> <p>25329-60-6</p>  <p><b>C<sub>32</sub>H<sub>46</sub>O<sub>6</sub></b>  8-Chromanpropionic acid, 6,7-dihydro-5-hydroxy-2α,3β-dimethyl-6-(3-methyl-2-butenyl)-6-(7-methyl-3-methylene-6-octenyl)-4,7-dioxo-α-propyl-</p> <p>References: 0 Reactions: 0 Suppliers: 0</p>	<p>5 Similarity Score: 95</p> <p>142382-37-4</p>  <p><b>C<sub>32</sub>H<sub>46</sub>O<sub>6</sub></b>  2<i>H</i>-1-Benzopyran-6-propanoic acid, 3,4,7,8-tetrahydro-5-hydroxy-2,3-dimethyl-8-(3-methyl-2-butenyl)-8-[5-methyl-2-(1-methylethenyl)-4-hexenyl]-4,7-dioxo-β-propyl-</p> <p>References: 5 Reactions: 2 Suppliers: 0</p>	

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