Supporting Information

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

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Figure S1: ¹H NMR spectrum of calophylloidic acid B (2) in CDCl₃



Figure S2: ¹³C NMR spectrum of calophylloidic acid B (2) in CDCl₃



Figure S3: ¹H-¹H COSY spectrum of calophylloidic acid B (2) in CDCl₃



Figure S4: HSQC spectrum of calophylloidic acid B (2) in CDCl₃



Figure S5: HMBC spectrum of calophylloidic acid B (2) in CDCl₃



Figure S6: HMBC spectrum of calophylloidic acid B (2) (From δ_C 6.0 ppm to δ_C 80 ppm)



Figure S7: HMBC spectrum of calophylloidic acid B (2) (From δ_C 100 ppm to δ_C 195 ppm)



Figure S8: HMBC spectrum of calophylloidic acid B (2) (From $\delta_C 0$ ppm to $\delta_C 210$ ppm)



Figure S9: NOESY spectrum of calophylloidic acid B (2) in CDCl₃



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



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

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Task History

September 15, 2023, 9:23AM

Initiating Search

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	View Results

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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

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Substances (5)

1 Similarity Score: 96 2 Similarity Score: 96 3 Similarity Score: 96 29077-61-0 29077-60-9 22879-64-7 Available stereochemistry shown Available stereochemistry shown C₃₂H₄₆O₆ C₃₂H₄₆O₆ C₃₂H₄₆O₆ 2H-1-Benzopyran-8-propanoic acid, 3,4,6, rel-(2R,3R)-3,4,6,7-Tetrahydro-5-hydroxyrel-(2R,3R)-3,4,6,7-Tetrahydro-5-hydroxy-7-tetrahydro-5-hydroxy-2,3-dimethyl-6-(3-2,3-dimethyl-6-(3-methyl-2-buten-1-yl)-6-2,3-dimethyl-6-(3-methyl-2-buten-1-yl)-6methyl-2-butenyl)-6-(7-methyl-3-[5-methyl-2-(1-methylethenyl)-4-hexen-1-[5-methyl-2-(1-methylethenyl)-5-hexen-1methylene-6-octenyl)-4,7-dioxo-β-propylyl]-4,7-dioxo-β-propyl-2*H*-1-benzopyranyl]-4,7-dioxo-β-propyl-2*H*-1-benzopyran-8-propanoic acid 8-propanoic acid Д З 0 **1 4** ₽ 2 11 1 0 🛛 0 0 References Reactions Suppliers References Reactions Suppliers Reference Reactions Suppliers 4 Similarity Score: 96 5 Similarity Score: 95 25329-60-6 142382-37-4 C₃₂H₄₆O₆ C₃₂H₄₆O₆ 8-Chromanpropionic acid, 6,7-dihydro-5-2H-1-Benzopyran-6-propanoic acid, 3,4,7, hydroxy-2α,3β-dimethyl-6-(3-methyl-2-8-tetrahydro-5-hydroxy-2,3-dimethyl-8-(3butenyl)-6-(7-methyl-3-methylene-6methyl-2-butenyl)-8-[5-methyl-2-(1octenyl)-4,7-dioxo-a-propylmethylethenyl)-4-hexenyl]-4,7-dioxo-βpropyl-0 0 🛛 0 5 ₽ 2 0 References Reactions References Reactions Suppliers Suppliers

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