

Supporting Information

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Chemical Constituents from the Roots of *Calophyllum pisiferum* Planch. & Triana and Their Cytotoxic and Antioxidant Activities

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Table S1: Comparative ^{13}C NMR data of calopisifuran (**1**) and isodisparfuran A (Guilet *et al.*, 2001)

Position	δ_{C}^a calopisifuran (1) in CDCl_3	δ_{C}^a isodisparfuran A* in CDCl_3
1		
2	159.3	159.2
3	114.4	112.0
4	156.8	153.7
4a	104.9	100.0
5	163.0	154.2
6	103.9	115.0
7	156.1	162.7
8	109.8	106.1
8a	153.5	154.3
1'	139.0	137.1
2', 6'	127.7	127.9
3', 5'	127.2	128.1
4'	128.4	129.3
1''	204.3	207.3
2''	51.7	53.6
3''	25.0	25.6
4''	22.7	22.7
5''	22.7	22.7
2'''	143.9	146.6
3'''	104.7	104.9

^a Recorded in 125 MHz

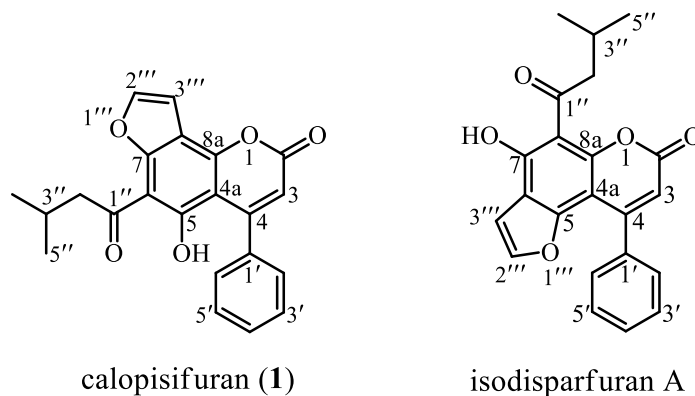


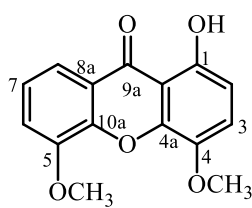
Figure S1: Structures of calopisifuran (**1**) and isodisparfuran A

Table S2: Comparative ^{13}C NMR data of 1-hydroxy-4,5-dimethoxyxanthone (**2**) and 1,8-dihydroxy-2-methoxyxanthone (*Witjeratne *et al.*, 2006)

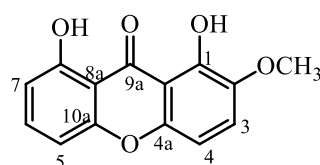
Position	δ_{C}^a 1-hydroxy-4,5-dimethoxyxanthone (2) in CDCl_3	δ_{C}^b 1,8-dihydroxy-2-methoxyxanthone * in CDCl_3
1	150.7	150.2
2	106.0	147.8
3	120.9	121.3
4	142.8	105.8
4a	149.8	149.7
5	148.5	107.1
6	116.1	137.6
7	123.4	110.4
8	116.9	161.4
8a	118.5	107.4
9	183.0	186.7
9a	109.2	108.1
10a	147.0	156.6

^a Recorded in 75 MHz

^b Recorded in 150 MHz



1-hydroxy-4,5-dimethoxyxanthone (**2**)



1,8-dihydroxy-2-methoxyxanthone

Figure S2: 1-hydroxy-4,5-dimethoxyxanthone (**2**) and 1,8-dihydroxy-2-methoxyxanthone

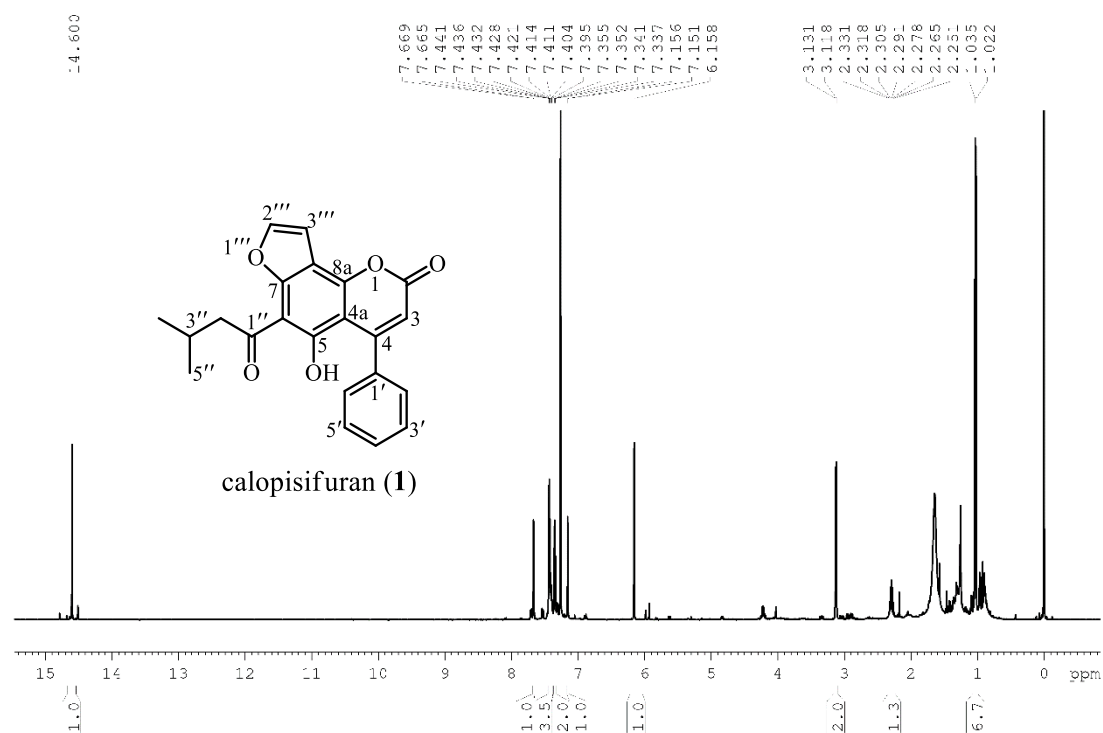


Figure S3: ^1H NMR (500 MHz, CDCl_3) spectrum of calopisifuran (1)

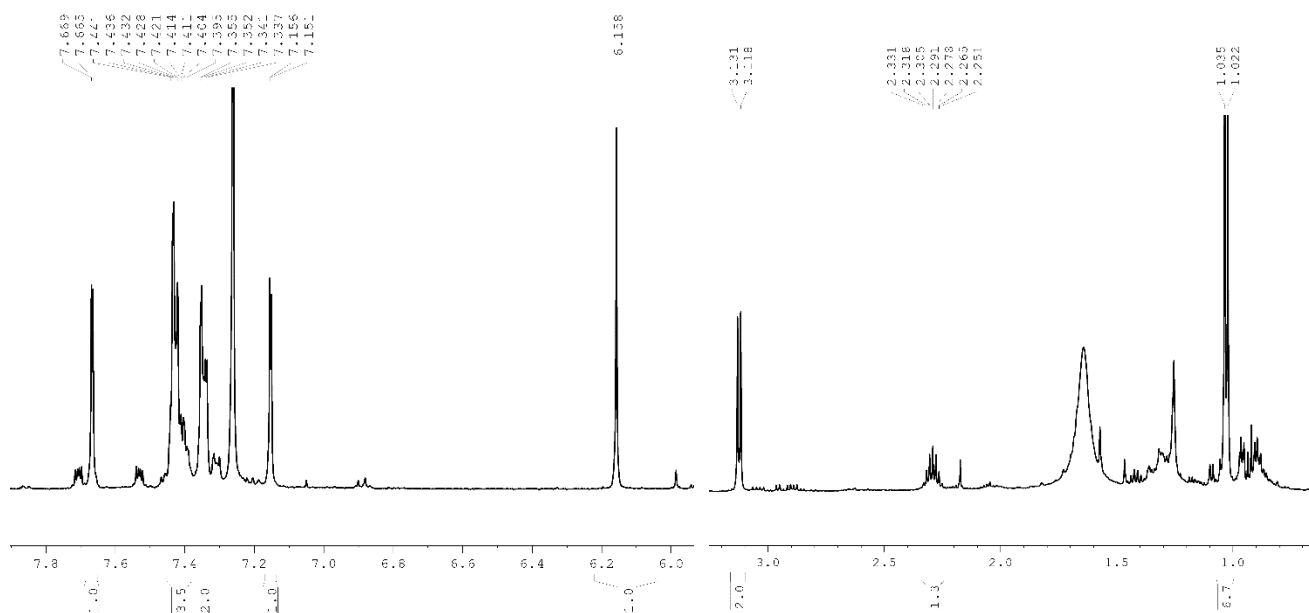


Figure S4: ^1H NMR (500 MHz, CDCl_3) spectrum of calopisifuran (1)
(From δ_{H} 1.0 ppm to δ_{H} 7.8 ppm)

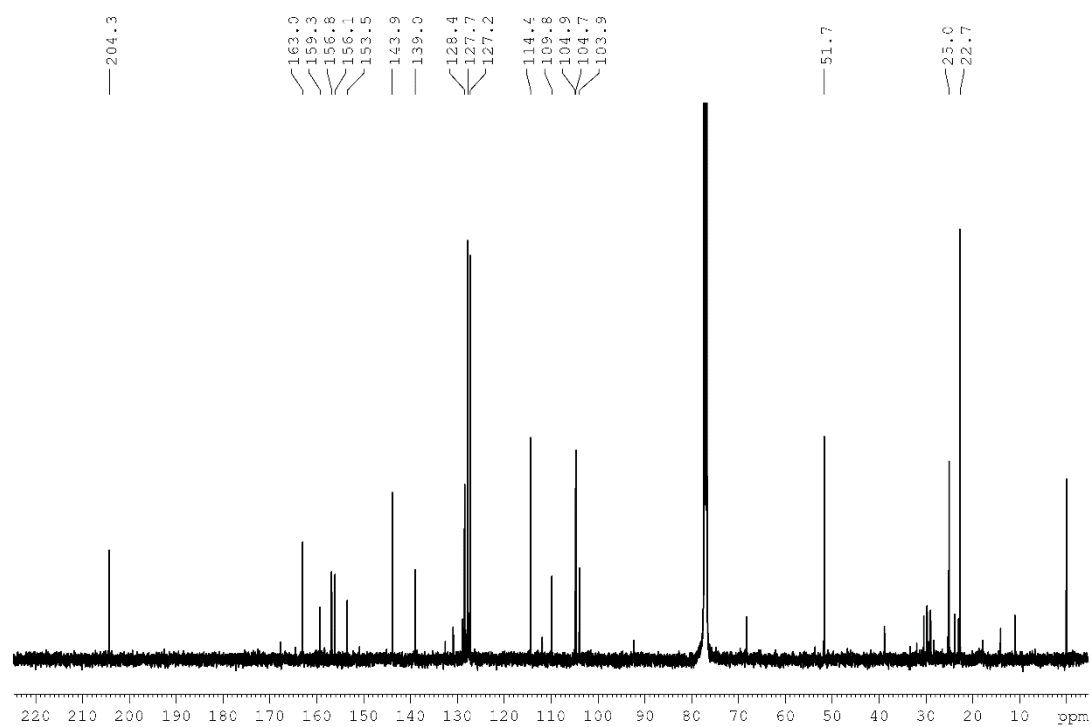


Figure S5: ^{13}C NMR (125 MHz, CDCl_3) spectrum of calopisifuran (**1**)

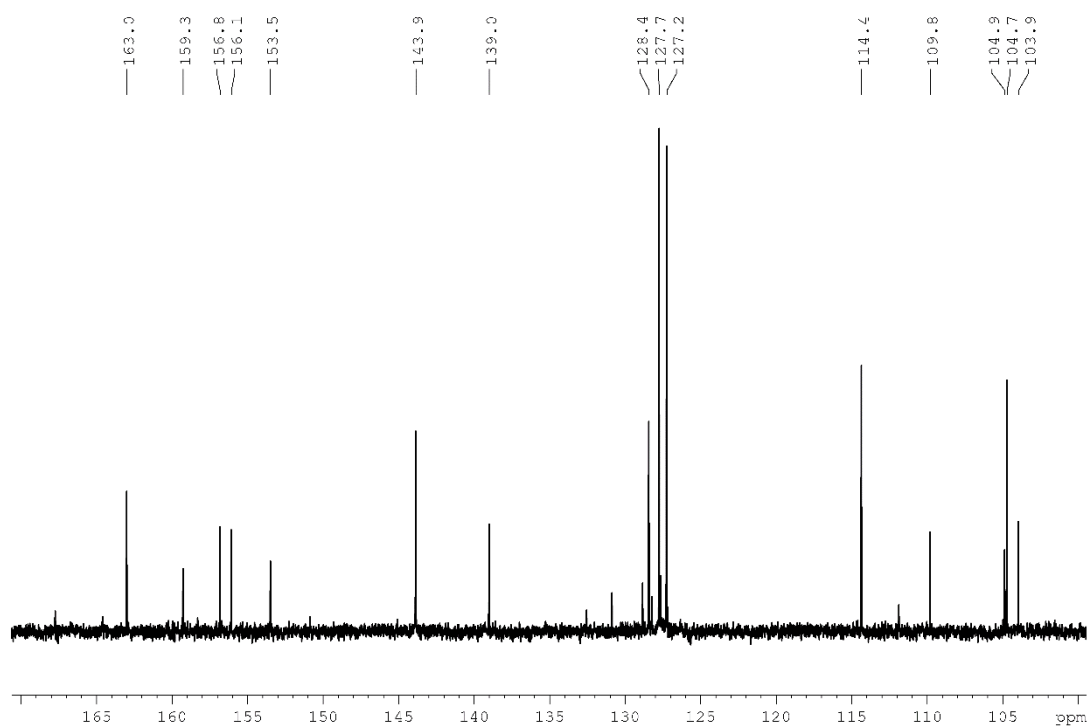


Figure S6: ^{13}C NMR (125 MHz, CDCl_3) spectrum of calopisifuran (**1**)
(From $\delta_{\text{C}} 105$ ppm to $\delta_{\text{C}} 165$ ppm)

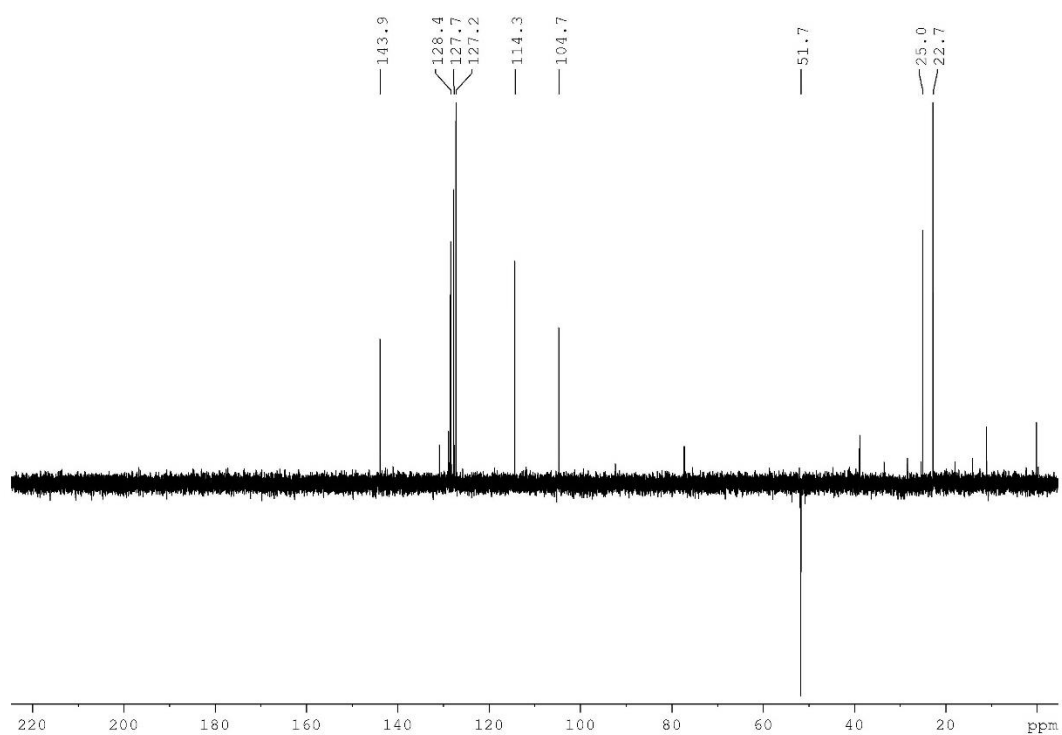


Figure S7: DEPT135 (125 MHz, CDCl₃) spectrum of calopisifuran (**1**)

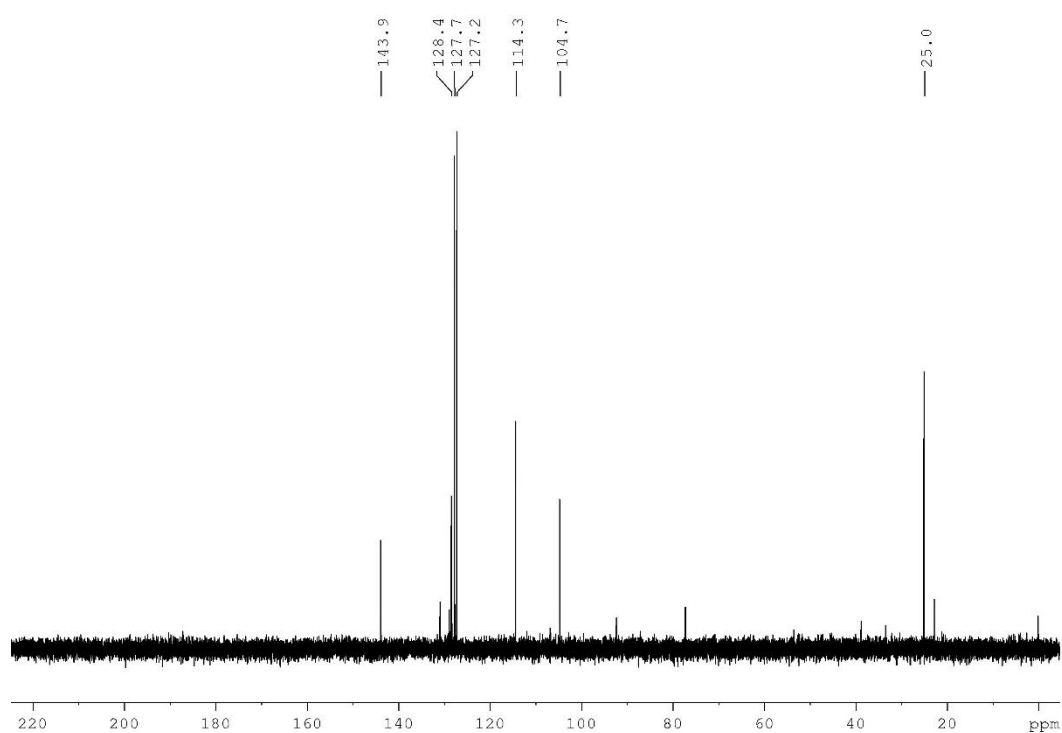


Figure S8: DEPT90 (125 MHz, CDCl₃) spectrum of calopisifuran (**1**)

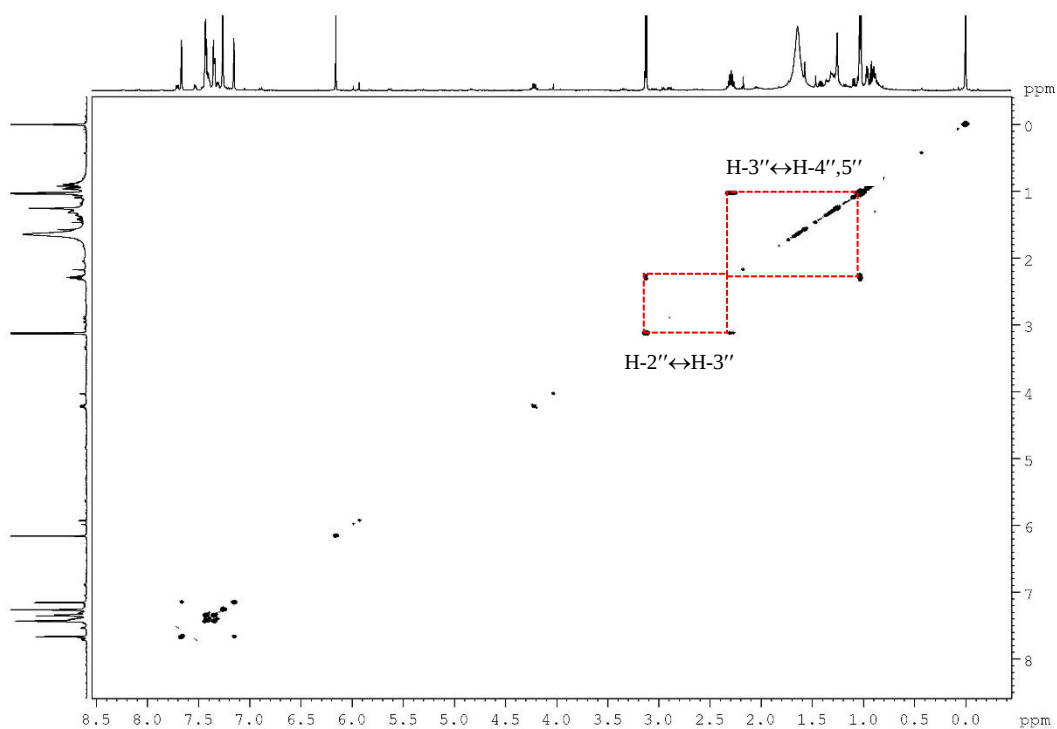


Figure S9: ^1H , ^1H -COSY spectrum of calopisifuran (**1**) in CDCl_3

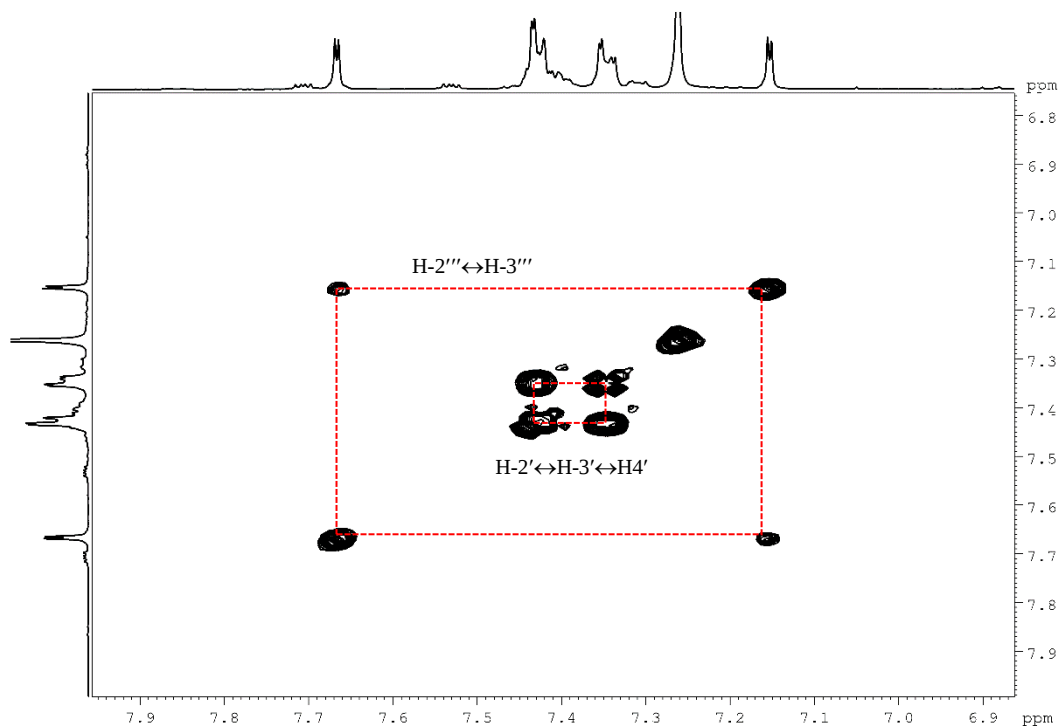


Figure S10: ^1H , ^1H -COSY spectrum of calopisifuran (**1**) in CDCl_3
(From δ_{H} 6.9 ppm to δ_{H} 7.9 ppm)

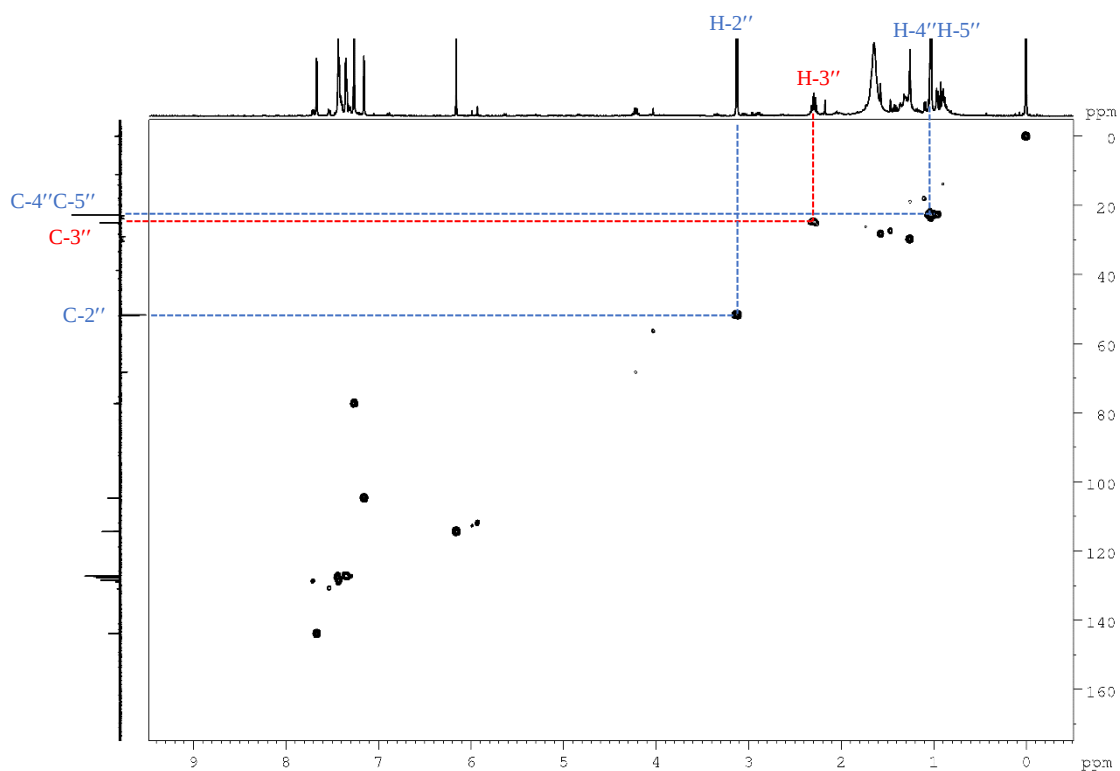


Figure S11: HMQC spectrum of calopisifuran (**1**) in CDCl₃

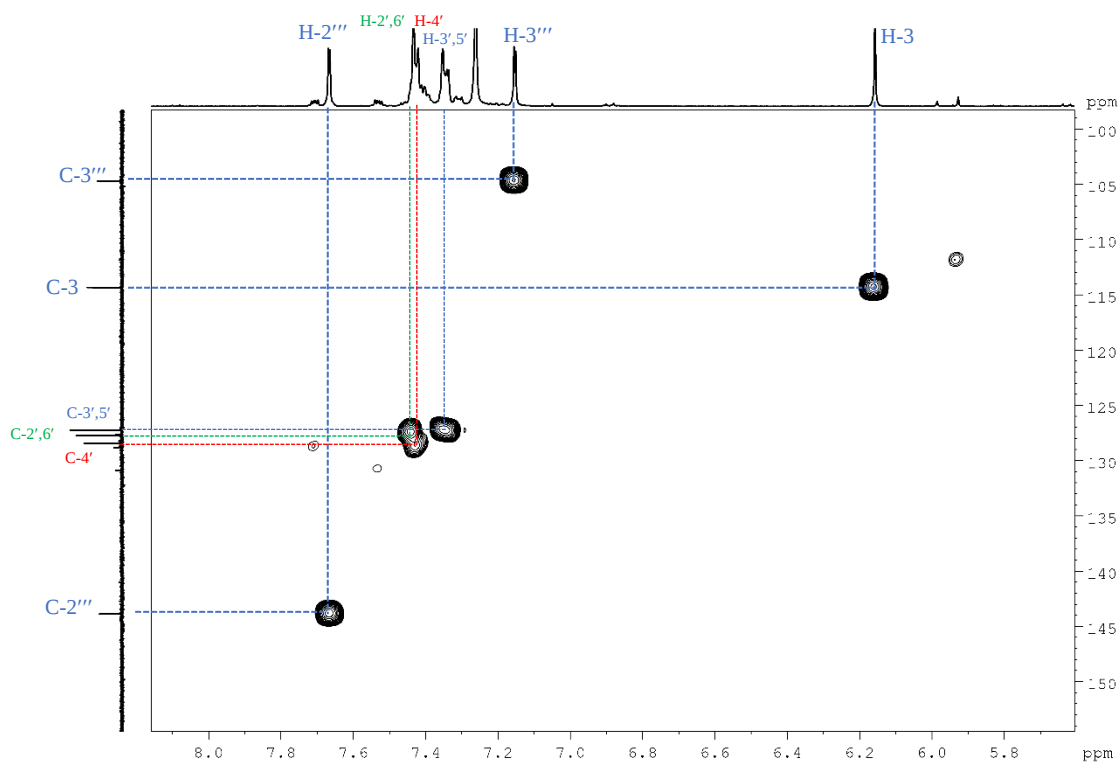


Figure S12: HMQC spectrum of calopisifuran (**1**) in CDCl₃
(From δ_H 5.8 ppm to δ_H 8.0 ppm and δ_C 100 ppm to δ_C 150 ppm)

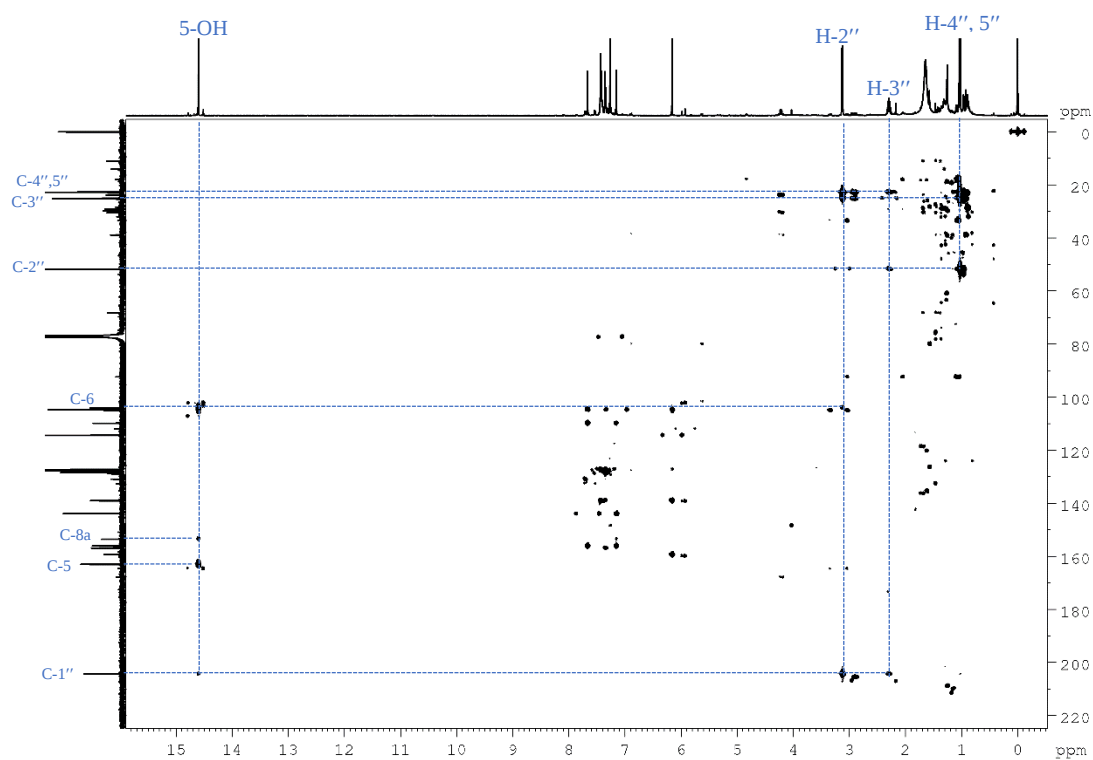


Figure S13: HMBC spectrum of calopisifuran (**1**) in CDCl₃

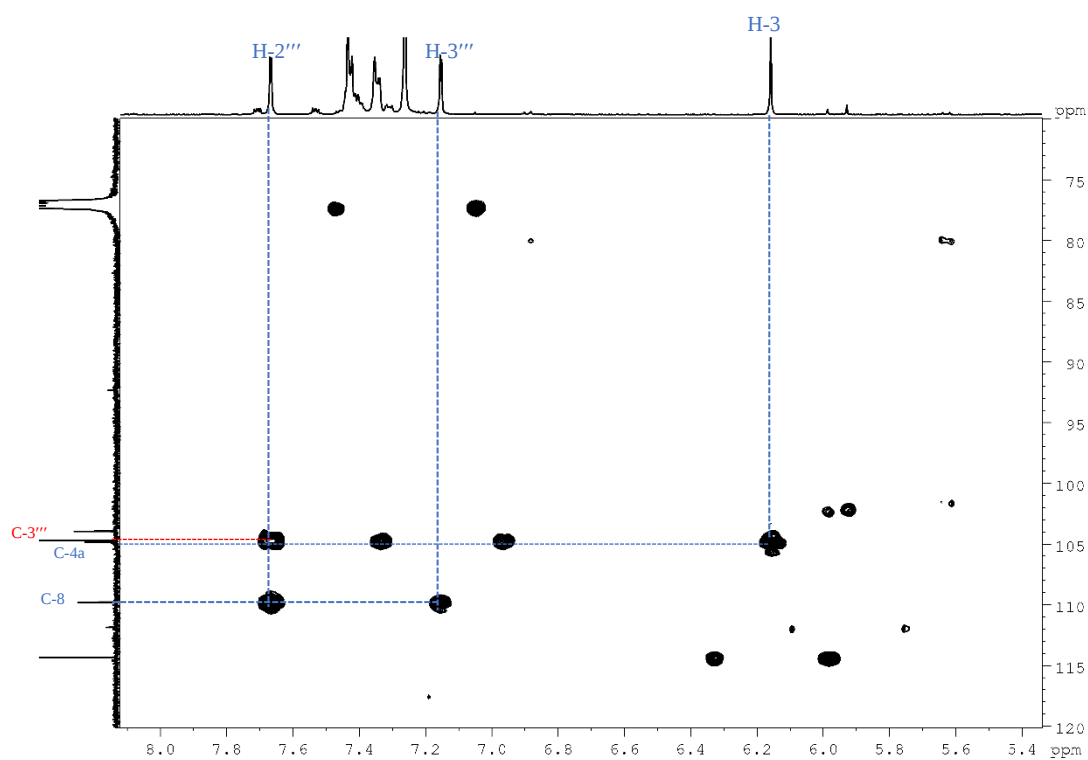


Figure S14: HMBC spectrum of calopisifuran (**1**) in CDCl₃
(From δ_H 5.4 ppm to δ_H 8.0 ppm δ_C 72 ppm to δ_C 120 ppm)

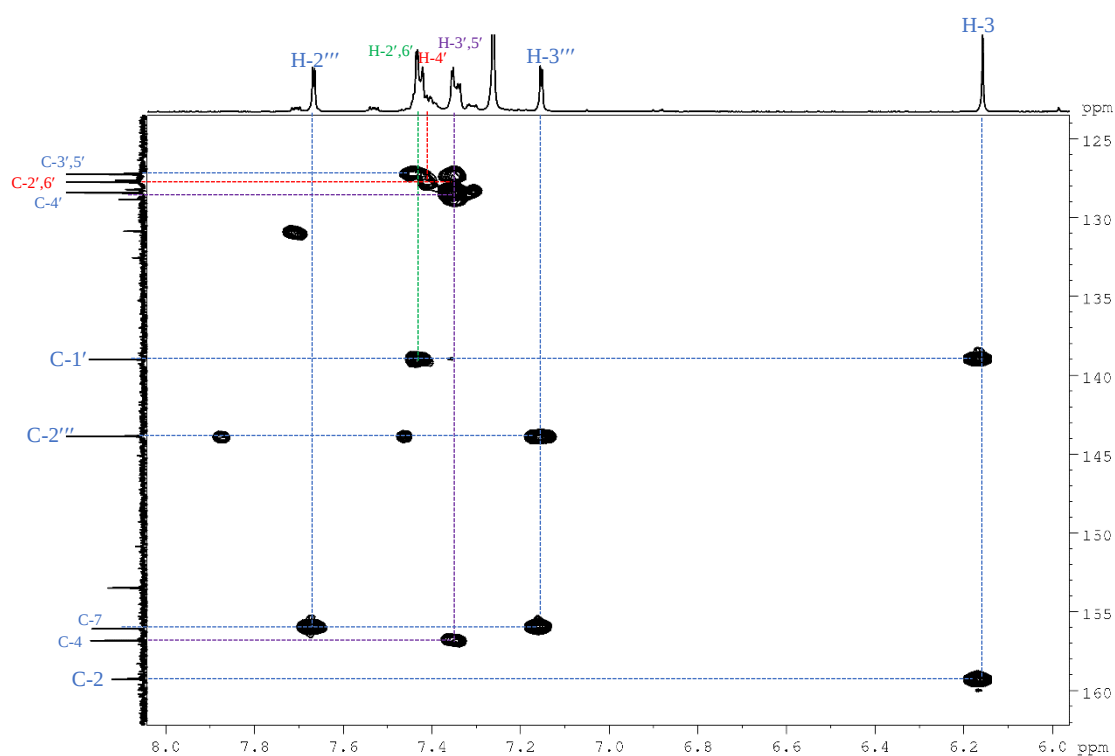


Figure S15: HMBC spectrum of calopisifuran (**1**) in CDCl_3
(From δ_{H} 6.0 ppm to δ_{H} 8.0 ppm δ_{C} 125 ppm to δ_{C} 160 ppm)

Table S3. All HMBC correlation of compound **1**

position	δ_{H} (J in Hz)	δ_{C} (type)	HMBC
3	6.16, s	114.4 (CH)	C-1', C-2, C-4a
2', 6'	7.44, br d	127.7 (CH)	C-1', C-3', 5'
3', 5'	7.35, m	127.2 (CH)	C-2', 6', C-4', C-4
4'	7.42, m	128.4 (CH)	C-2', 6'
2''	3.12, d (6.5)	51.7 (CH_2)	C-1'', C-3'', C-4'', 5'', C-6
3''	2.29, sep (6.5)	25.0 (CH)	C-1'', C-2'', C-4'', 5''
4'', 5''	1.02, d (6.5)	22.7 (CH_3)	C-2'', C-3''
2'''	7.66, d (2.0)	143.9 (CH)	C-3''', C-7, C-8
3'''	7.15, d (2.0)	104.7 (CH)	C-2''', C-7, C-8
5-OH	14.60, s		C-1'', C-5, C-6, C-8a

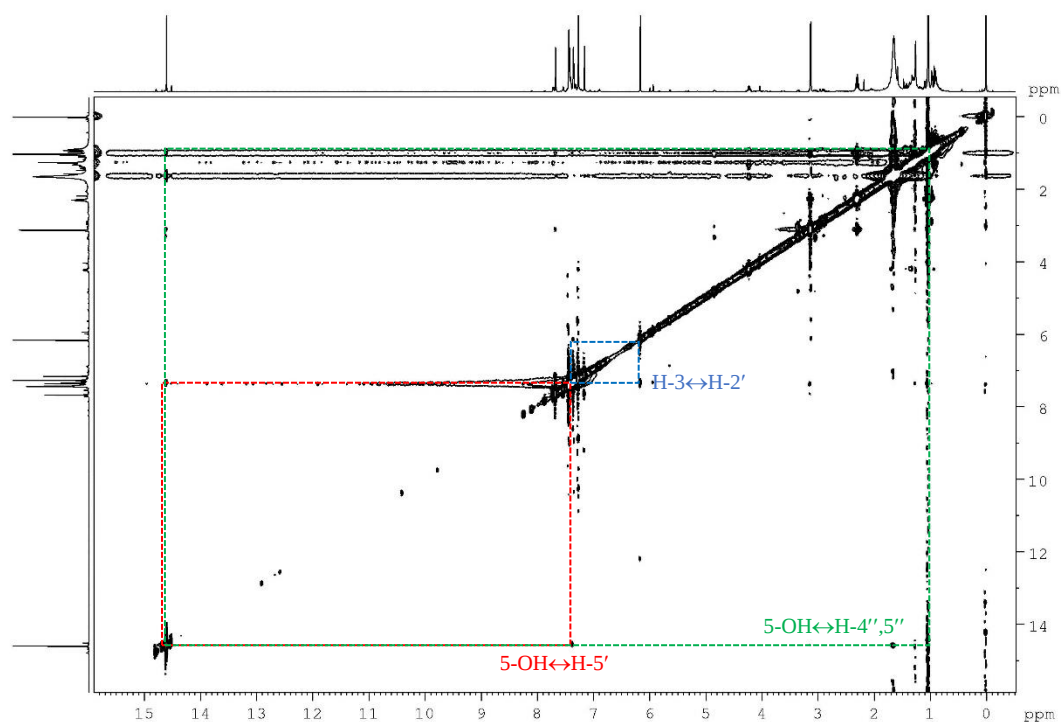


Figure S16: NOESY spectrum of calopisifuran (**1**) in CDCl₃

MS Spectrum Graph

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BG Mode:Averaged 5.800-5.899(872-886)

Mass Peaks:7 Base Peak:361.07(4608) MS Stage:MS Polarity:Neg Segment1 - Event2 Precursor:----- Cutoff: Ionization Mode:ESI

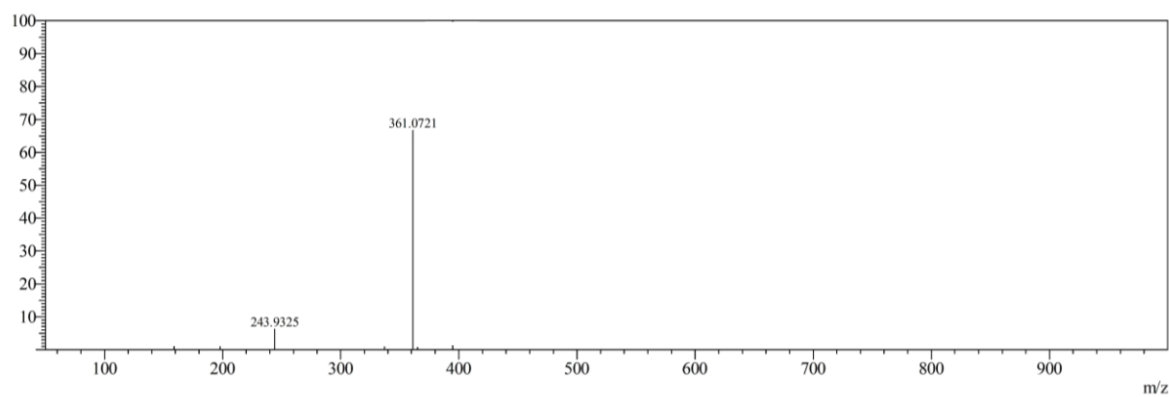


Figure S17: HR-ESI-MS spectrum of calopisifuran (**1**)

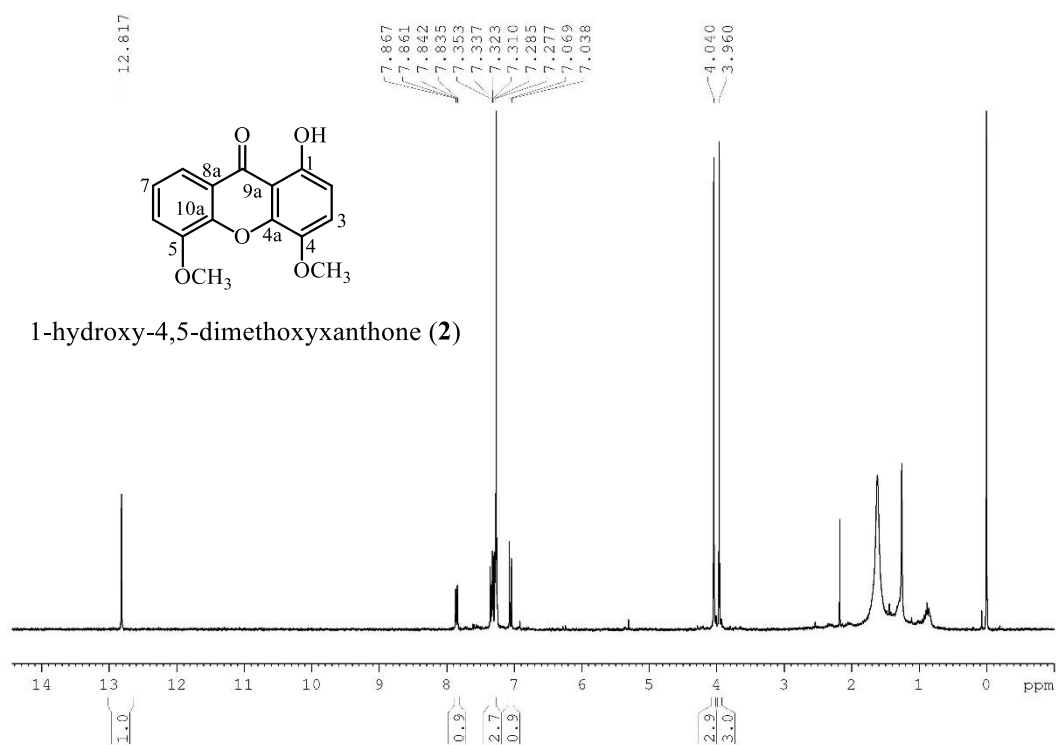


Figure S18: ¹H NMR (300 MHz, CDCl₃) spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**)

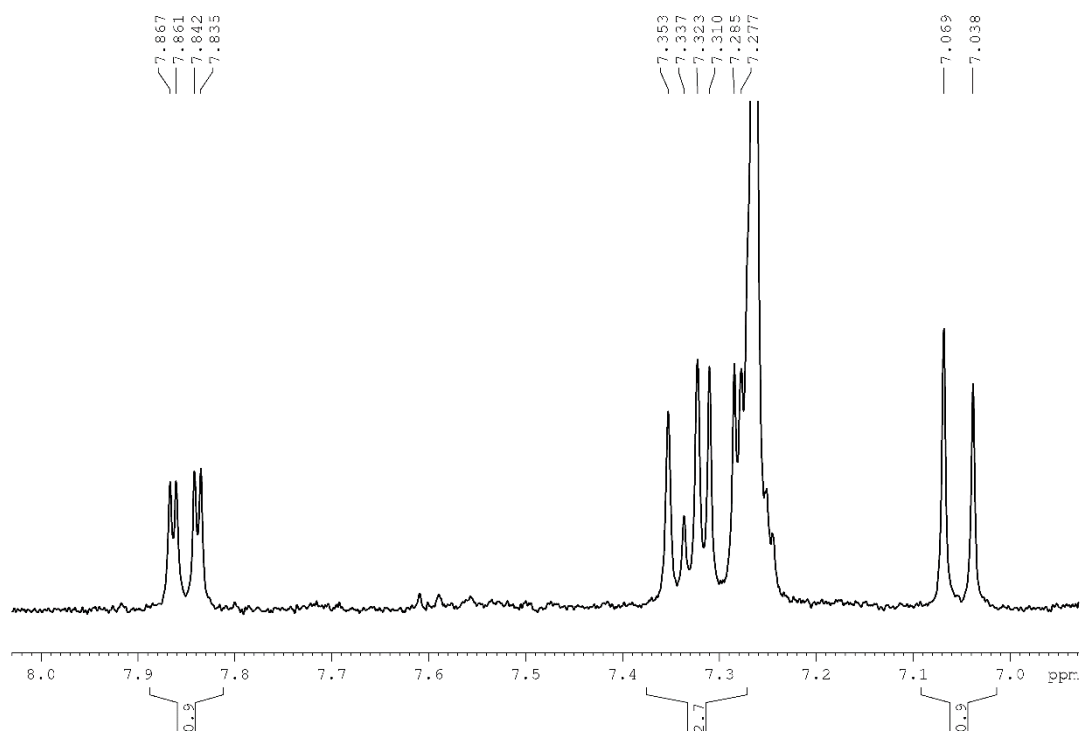


Figure S19: ¹H NMR (300 MHz, CDCl₃) spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**)
(From δ_H 7.0 ppm to δ_H 8.0 ppm)

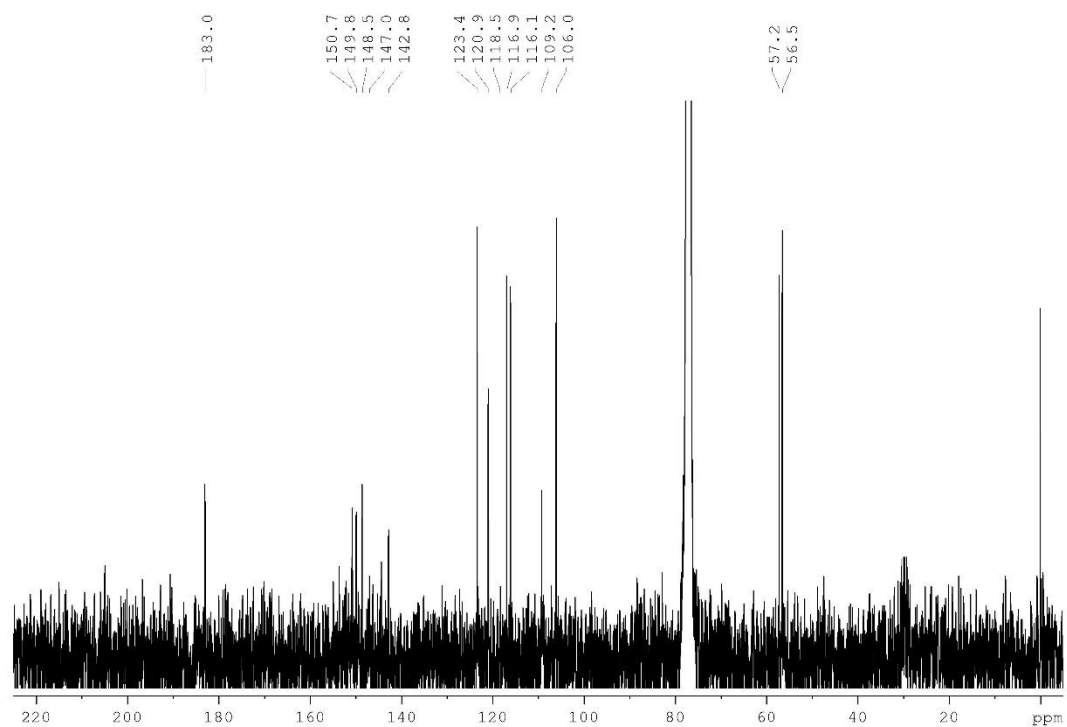


Figure S20: ^{13}C NMR (75 MHz, CDCl_3) spectrum of 1-hydroxy-4,5-dimethoxyxanthone (2)

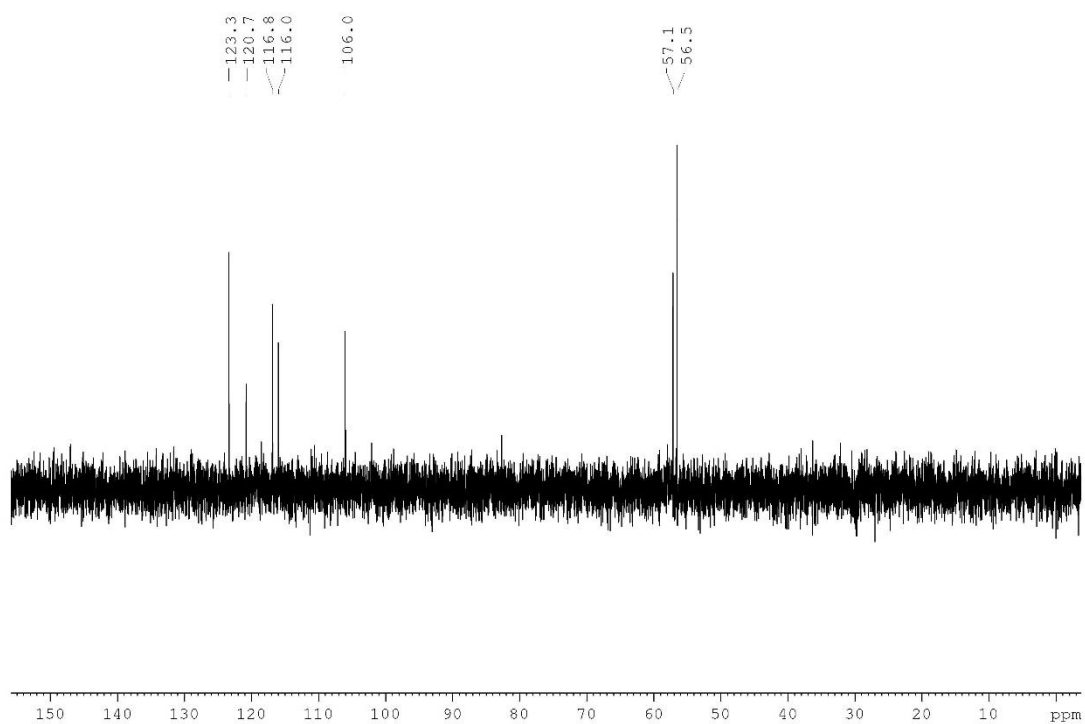


Figure S21: DEPT135 (75 MHz, CDCl_3) spectrum of 1-hydroxy-4,5-dimethoxyxanthone (2)

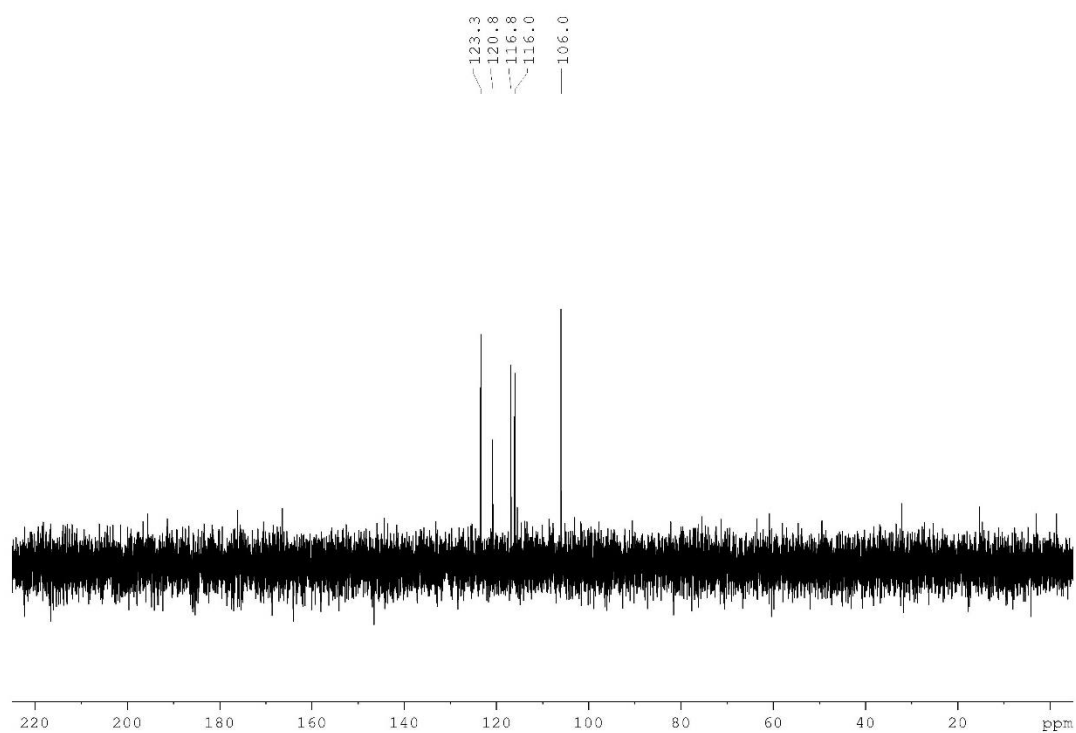


Figure S22: DEPT90 (75 MHz, CDCl_3) spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**)

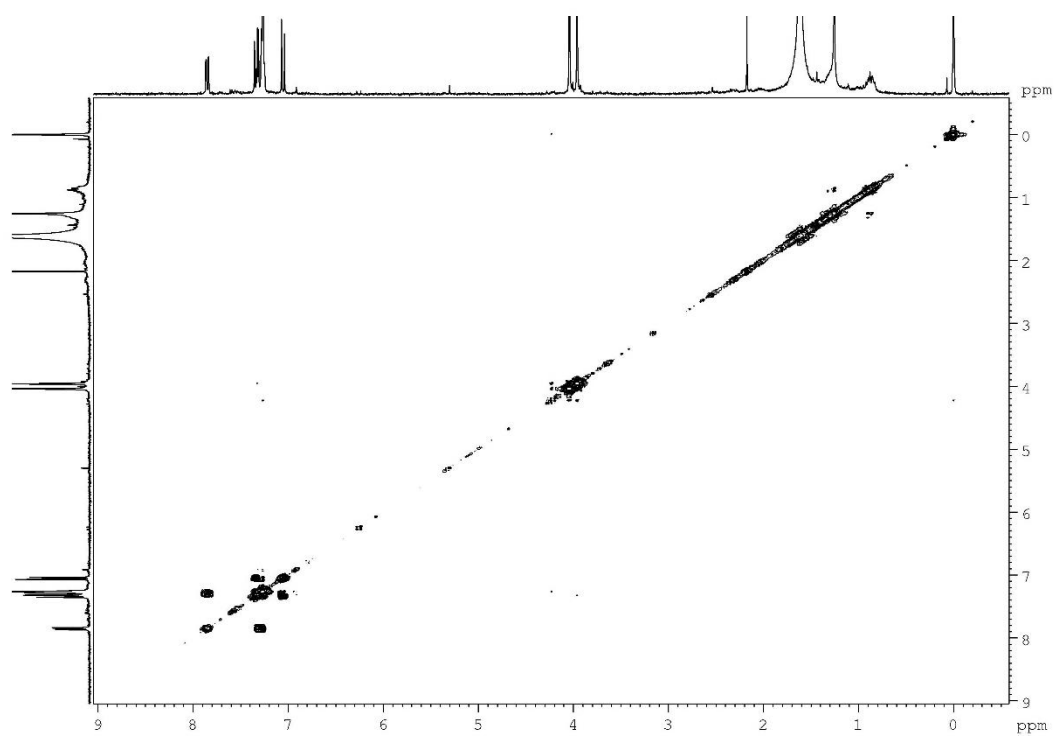


Figure S23: ^1H , ^1H -COSY spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in CDCl_3

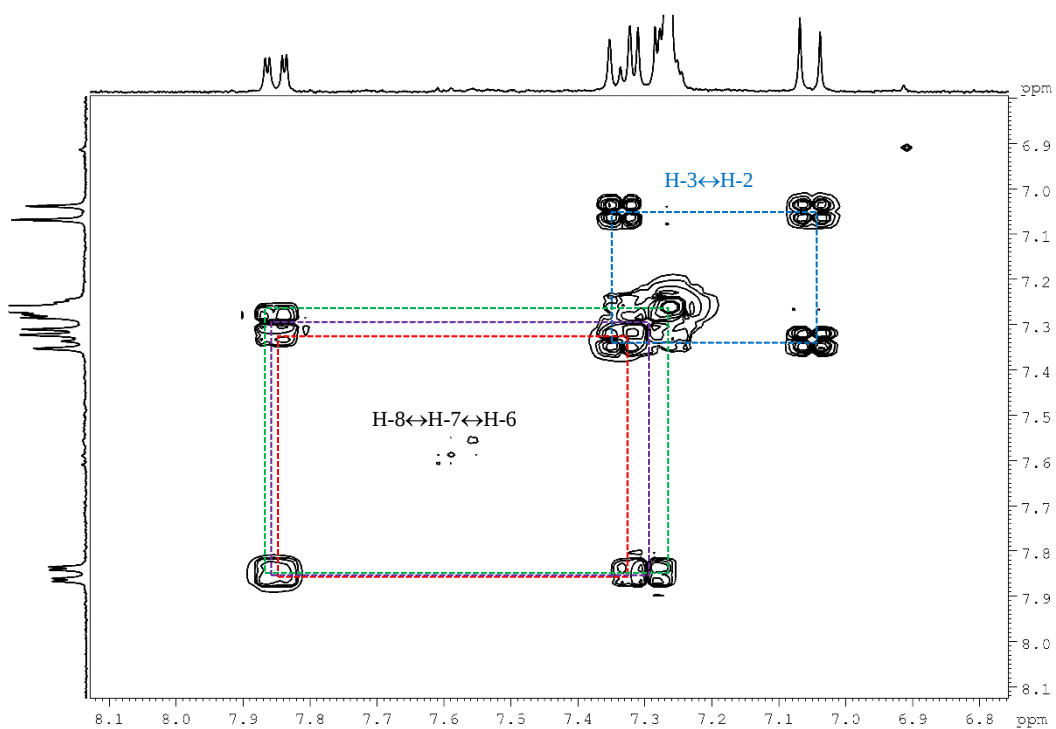


Figure S24: $^1\text{H}, ^1\text{H}$ -COSY spectrum of 1-hydroxy-4,5-dimethoxyxanthone (2) in CDCl_3 (From δ_{H} 6.8 ppm to δ_{H} 8.1 ppm)

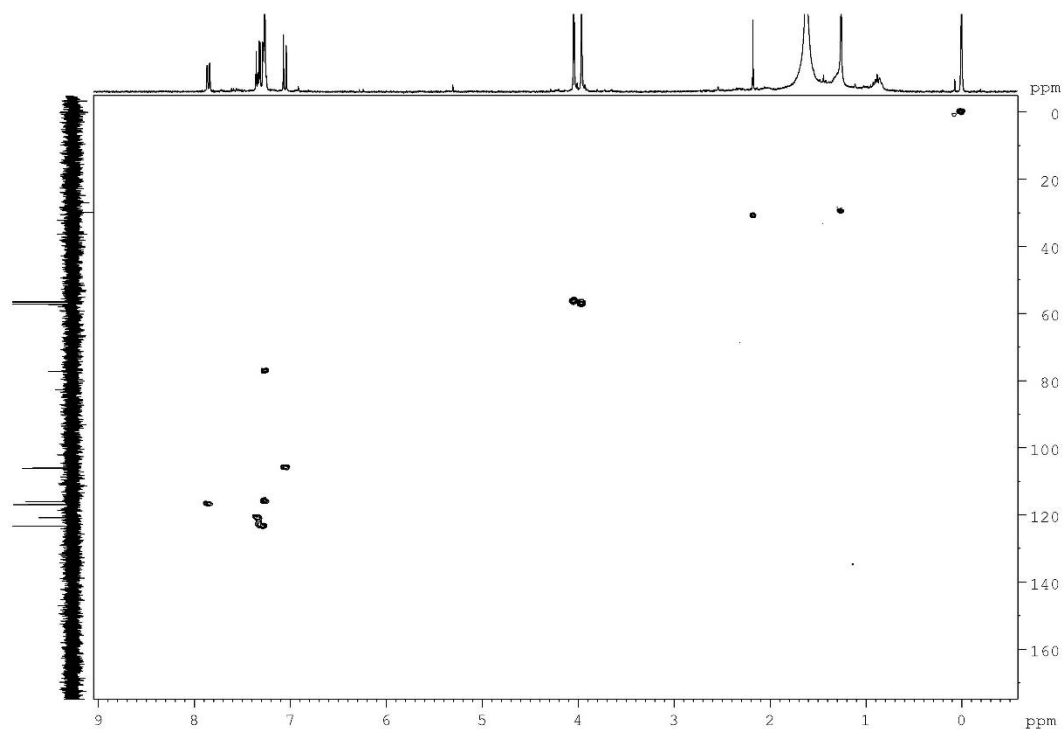


Figure S25: HMQC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (2) in CDCl_3

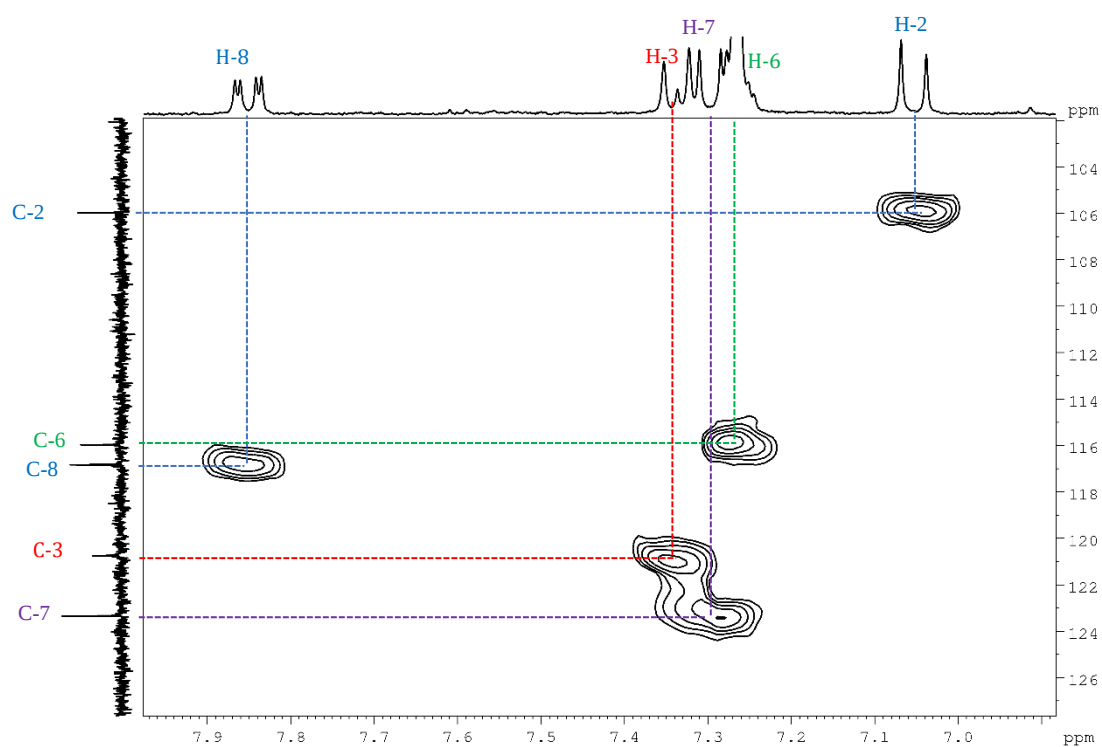


Figure S26: HMBC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in CDCl_3
(From δ_{H} 6.0 ppm to δ_{H} 8.0 ppm δ_{C} 102 ppm to δ_{C} 126 ppm)

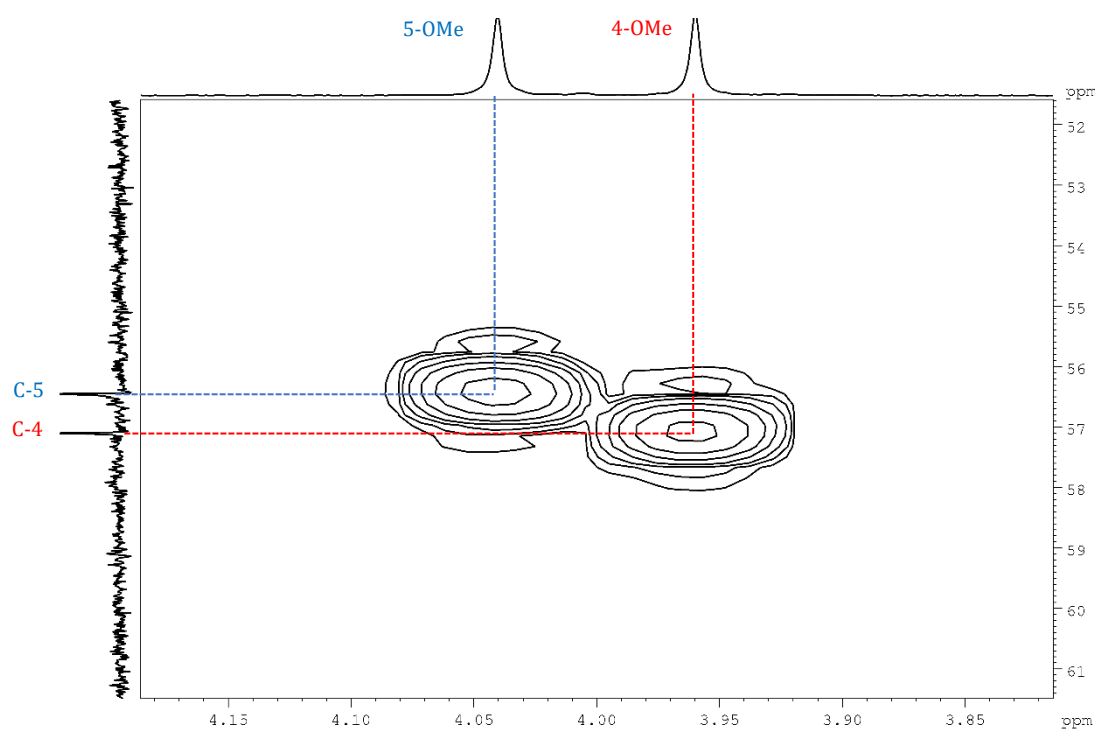


Figure S27: HMBC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in CDCl_3
(From δ_{H} 3.8 ppm to δ_{H} 4.2 ppm δ_{C} 52 ppm to δ_{C} 61 ppm)

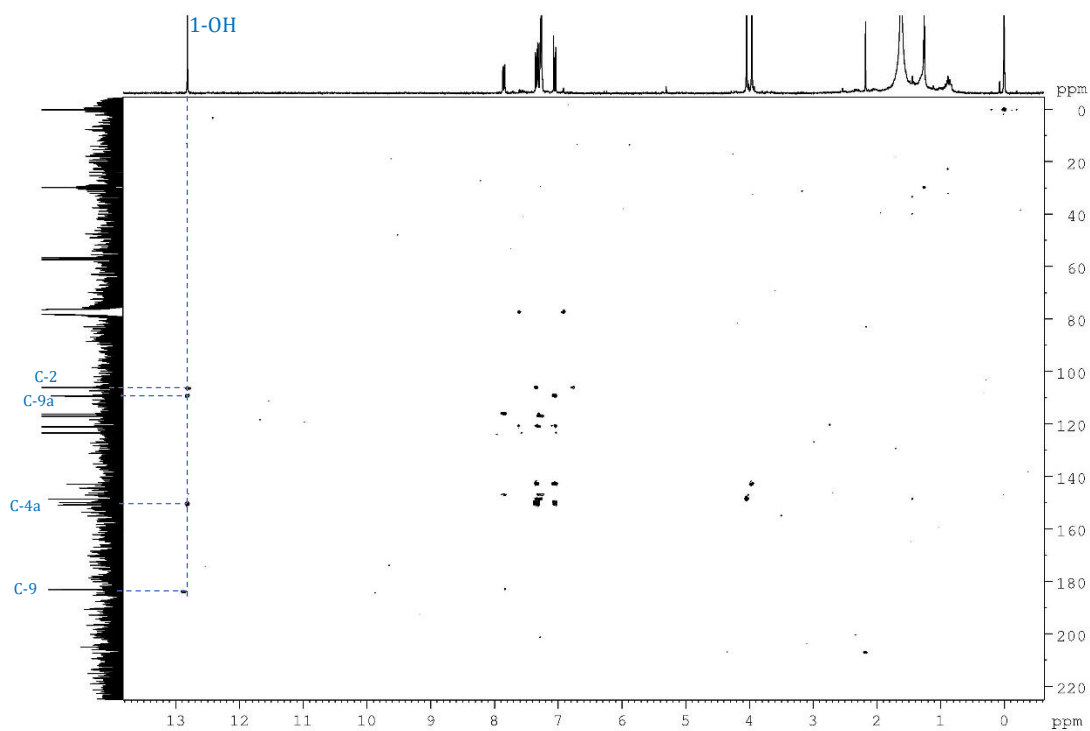


Figure S28: HMBC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in CDCl_3

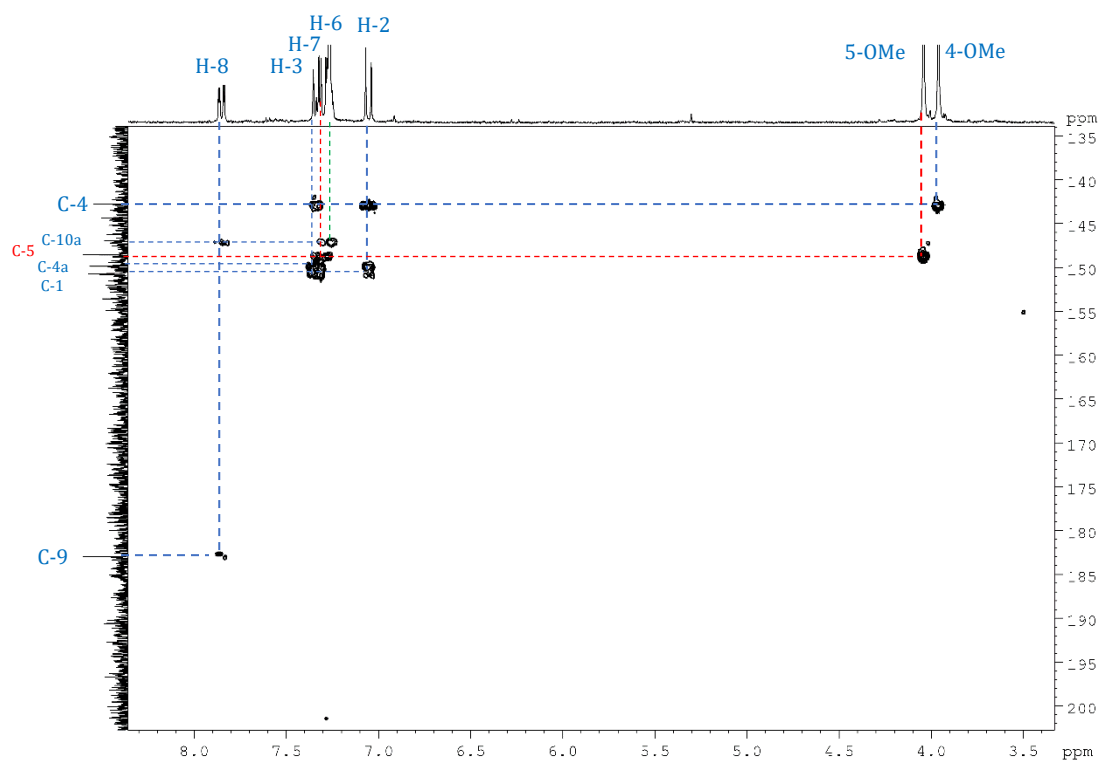


Figure S29: HMBC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in CDCl_3
(From δ_{H} 3.5 ppm to δ_{H} 8.0 ppm δ_{C} 135 ppm to δ_{C} 200 ppm)

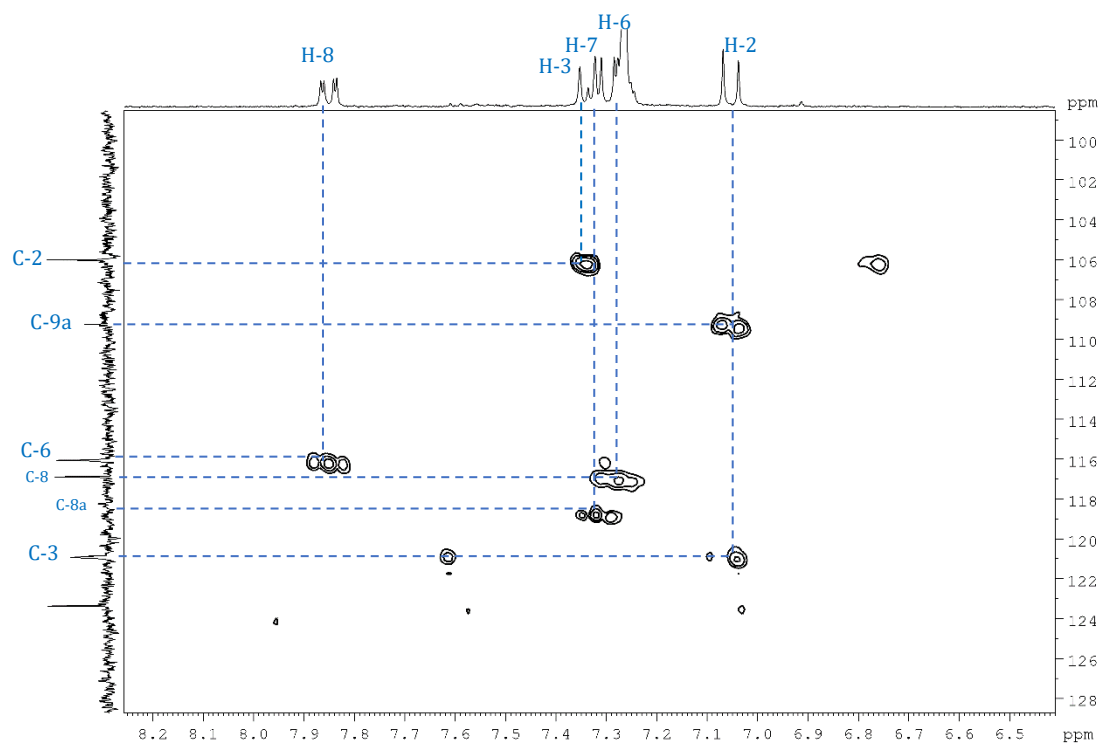


Figure S30:HMBC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in $CDCl_3$
(From δ_H 6.5 ppm to δ_H 8.2 ppm δ_C 100 ppm to δ_C 128 ppm)

TableS4. All HMBC correlation of compound **2**

position	δ_H (J in Hz)	δ_C (type)	HMBC
2	7.06, d (9.0)	106.0 (CH)	C-1, C-3, C-4, C-9a
3	7.33, d (9.0)	120.9 (CH)	C-1, C-2, C-4, C-4a
6	7.25, dd (8.5, 2.0)	116.1 (CH)	C-8, C-10a
7	7.32, t (8.5)	123.4 (CH)	C-5, C-8a
8	7.85, dd (8.5, 2.0)	116.9 (CH)	C-6, C-9, C-10a
1-OH	12.81, s		C-2, C-4a, C-9, C-9a
4-OMe	3.96, s	57.2 (CH_3)	C-4
5-OMe	4.04, s	56.5 (CH_3)	C-5

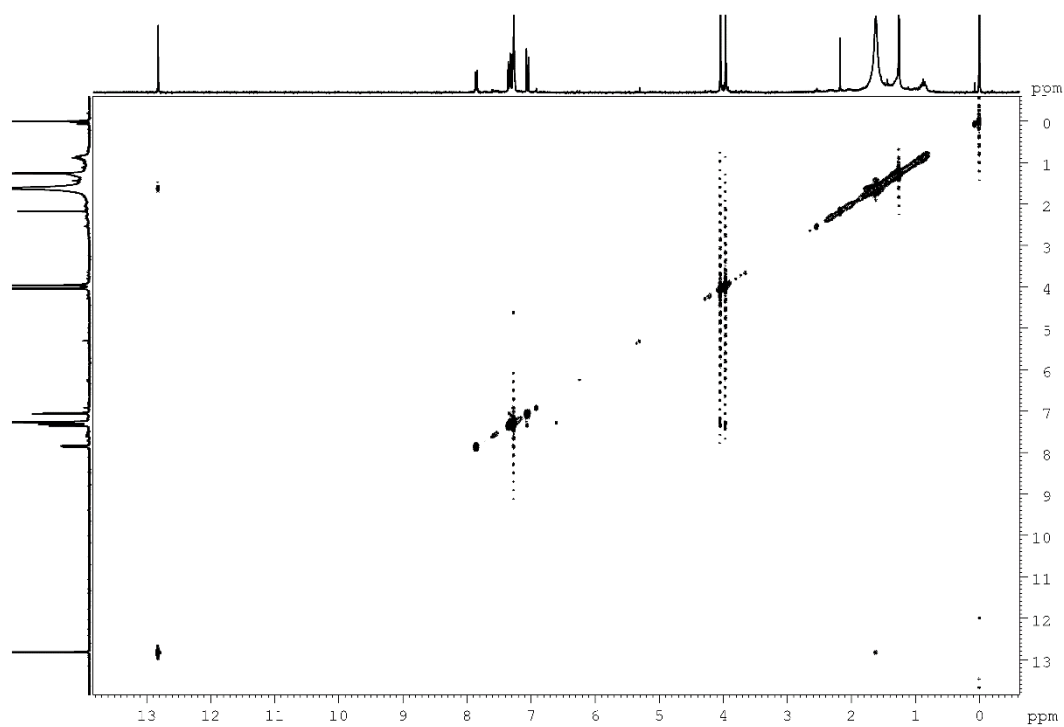


Figure S31: NOESY spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in CDCl₃

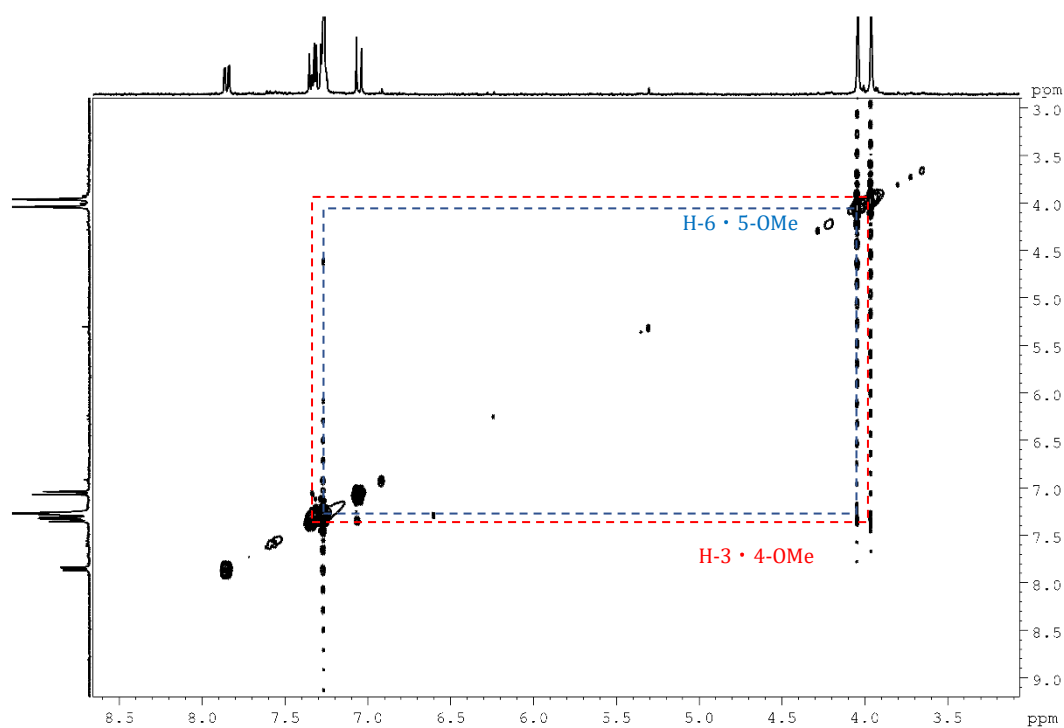


Figure S32: NOESY spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in CDCl₃
(From δ_{H} 3.0 ppm to δ_{H} 8.5 ppm)

MS Spectrum Graph

Ret.Time:Averaged 0.107-0.200(Scan#:18-32)

BG Mode:Averaged 5.800-5.899(872-886)

Mass Peaks:17 Base Peak:273.01(188922) MS Stage:MS Polarity:Pos Segment1 - Event2 Precursor:----- Cutoff: Ionization Mode:ESI

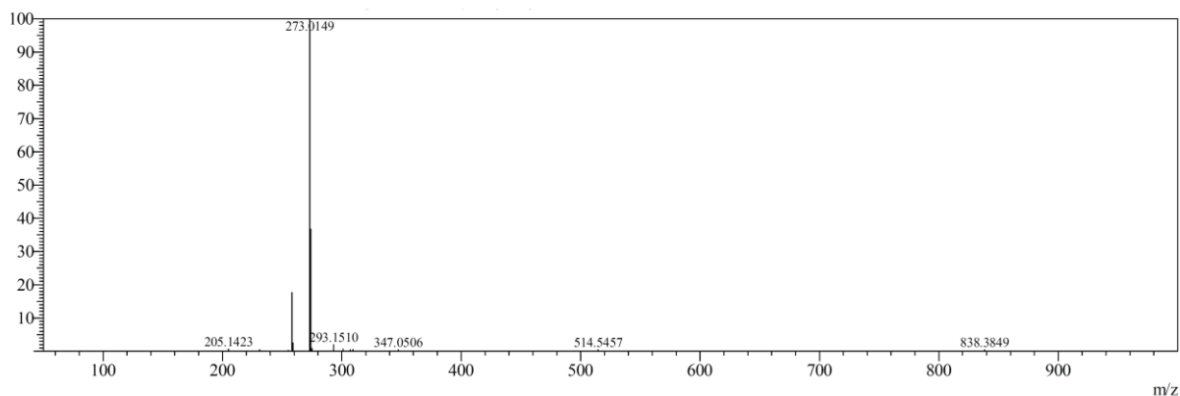


Figure S33: HR-ESI-MS spectrum of 1-hydroxy-4,5-dimethoxyxanthone (2)

Scifinder search report

S1: *Calophyllum pisiferum* research report

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Research Topic "Calophyllum pisiferum"

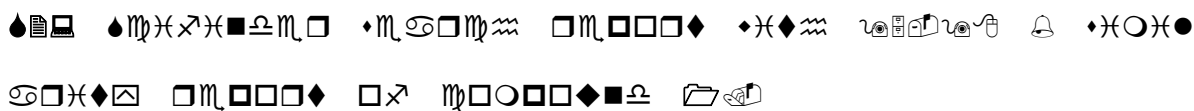
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	References
☐ No References were found containing both of the concepts "Calophyllum" and "pisiferum".	0
☐ 1936 references were found containing either the concept "Calophyllum" or the concept "pisiferum".	1936

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☒ 95-98	2
☐ 90-94	3
☐ 85-89	32
☐ 80-84	63
☐ 75-79	175
☐ 70-74	600
☐ 65-69	2439
☐ 0-64 (least similar)	10842

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Score: 98 1. 247593-01-7 C₂₁ H₁₆ O₅ 2H-Furo[2,3-h]-1-benzopyran-2-one, 5-hydroxy-6-(1-oxobutyl)-4-phenyl- Key Physical Properties: Molecular Weight 348.35 Boiling Point (Predicted) Value: 562.0±50.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.344±0.06 g/cm3 Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 6.06±0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 1 References Spectra	Score: 97 2. 342389-84-8 C₂₂ H₁₈ O₅ 7H-Furo[2,3-f][1]benzopyran-7-one, 4-hydroxy-5-(3-methyl-1-oxobutyl)-9-phenyl- Key Physical Properties: Molecular Weight 362.38 Boiling Point (Predicted) Value: 485.7±34.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.312±0.06 g/cm3 Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 5.12±0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 2 References Spectra	

S3: Scifinder search report with 95-98 % similarity report of compound 2.

SciFinder - Similarity Candidates x +

← → ↻ scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf ☆ ⚙️ A อนุชิต ใจหาญ

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Explore Saved Searches SciPlanner

Chemical Structure similarity

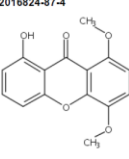
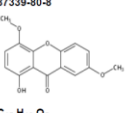
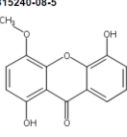
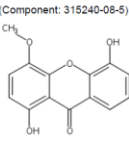
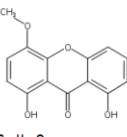
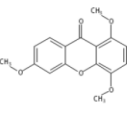
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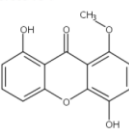
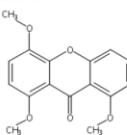
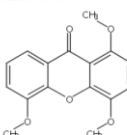
Select All Deselect All

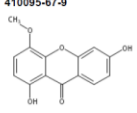
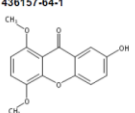
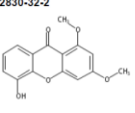
1 of 8 Similarity Candidates Selected

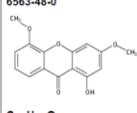
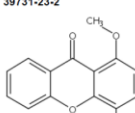
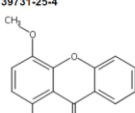
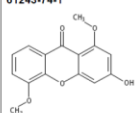
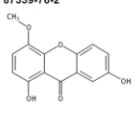
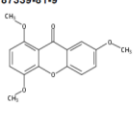
	Substances
☐ ≥ 99 (most similar)	0
☒ 95-98	20
☐ 90-94	81
☐ 85-89	334
☐ 80-84	640
☐ 75-79	783
☐ 70-74	3225
☐ 65-69	8350
☐ 0-64 (least similar)	24275

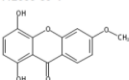
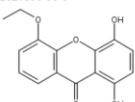
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Score: 98 1. 2016824-87-4  C₁₈H₁₂O₅ 9H-Xanthen-9-one, 8-hydroxy-1,4-dimethoxy- Key Physical Properties: Molecular Weight 272.25 Boiling Point (Predicted) Value: 483.7±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.360±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 6.95±0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 1 References	Score: 97 2. 87339-80-8  C₁₈H₁₂O₅ 9H-Xanthen-9-one, 1-hydroxy-4,7-dimethoxy- Key Physical Properties: Molecular Weight 272.25 Boiling Point (Predicted) Value: 483.7±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.360±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 7±-0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 1 References	Score: 97 3. 315240-08-5  C₁₈H₁₂O₅ 9H-Xanthen-9-one, 1,5-dihydroxy-4-methoxy- Key Physical Properties: Molecular Weight 258.23 Boiling Point (Predicted) Value: 510.8±50.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.480±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 7.54±0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 5 References
Score: 97 4. 1404478-66-5 (Component: 315240-08-5)  C₁₈H₁₀O₅ · H₂O 9H-Xanthen-9-one, 1,5-dihydroxy-4-methoxy-, hydrate (1:1) Related Info: ~ 1 References	Score: 97 5. 1605285-02-6  C₁₈H₁₀O₅ 9H-Xanthen-9-one, 1,8-dihydroxy-4-methoxy- Key Physical Properties: Molecular Weight 258.23 Boiling Point (Predicted) Value: 519.9±50.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.480±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 6.76±0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 1 References Reactions	Score: 96 6. 61234-59-1  C₁₈H₁₄O₅ 9H-Xanthen-9-one, 1,4,6-trimethoxy- Key Physical Properties: Molecular Weight 286.28 Melting Point (Experimental) Value: 158-160 °C Condition: Solv: ethanol (64-17-5) Boiling Point (Predicted) Value: 456.6±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.268±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr Related Info: ~ 2 References ~ 5 Commercial Sources Experimental Properties

Score: 96 7. 87339-75-1  C₁₈H₁₀O₅ 9H-Xanthen-9-one, 4,8-dihydroxy-1-methoxy- Key Physical Properties: Molecular Weight 258.23 Boiling Point (Predicted) Value: 510.8±50.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.480±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 6.99±0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 5 References ~ 2 Commercial Sources Spectra	Score: 96 8. 87339-86-4  C₁₈H₁₄O₅ 9H-Xanthen-9-one, 1,4,8-trimethoxy- Key Physical Properties: Molecular Weight 286.28 Boiling Point (Predicted) Value: 456.6±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.268±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr Related Info: ~ 1 References	Score: 96 9. 182675-54-3  C₁₈H₁₄O₅ 9H-Xanthen-9-one, 1,4,6-trimethoxy- Key Physical Properties: Molecular Weight 286.28 Boiling Point (Predicted) Value: 456.6±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.268±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr Related Info: ~ 1 References
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Score: 96 10. 410095-67-9  C₁₄H₁₀O₅ 9H-Xanthen-9-one, 1,6-dihydroxy-4-methoxy- Key Physical Properties: Molecular Weight 258.23 Melting Point (Experimental) Value: 165-167 °C Boiling Point (Predicted) Value: 519.9±50.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.480±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 6.96±0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 4 References ~ 3 Commercial Sources Spectra Experimental Properties	Score: 96 11. 436157-64-1  C₁₅H₁₂O₅ 9H-Xanthen-9-one, 7-hydroxy-1,4-dimethoxy- Key Physical Properties: Molecular Weight 272.25 Boiling Point (Predicted) Value: 483.7±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.360±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 9.05±0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 10 References ~ 2 Commercial Sources	Score: 95 12. 2830-32-2  C₁₅H₁₂O₅ 9H-Xanthen-9-one, 5-hydroxy-1,3-dimethoxy- Key Physical Properties: Molecular Weight 272.25 Melting Point (Experimental) Value: 271-272 °C Boiling Point (Predicted) Value: 483.7±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.360±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 7.96±0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 18 References ~ 3 Commercial Sources Experimental Properties
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Score: 95 13. 6563-48-0  C₁₅H₁₂O₅ 9H-Xanthen-9-one, 1-hydroxy-3,5-dimethoxy- Key Physical Properties: Molecular Weight 272.25 Melting Point (Experimental) Value: 168-169 °C Boiling Point (Predicted) Value: 483.7±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.360±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 6.71±0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 60 References ~ 5 Commercial Sources Spectra Experimental Properties	Score: 95 14. 39731-23-2  C₁₅H₁₂O₄ 9H-Xanthen-9-one, 1,4-dimethoxy- Key Physical Properties: Molecular Weight 256.25 Boiling Point (Predicted) Value: 423.3±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.270±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr Related Info: ~ 1 References	Score: 95 15. 39731-25-4  C₁₄H₁₀O₄ 9H-Xanthen-9-one, 1-hydroxy-4-methoxy- Key Physical Properties: Molecular Weight 242.23 Boiling Point (Predicted) Value: 452.6±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.375±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 7.73±0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 2 References ~ 2 Commercial Sources
Score: 95 16. 61243-74-1  C₁₅H₁₂O₅ 9H-Xanthen-9-one, 3-hydroxy-1,5-dimethoxy- Key Physical Properties: Molecular Weight 272.25 Boiling Point (Predicted) Value: 483.7±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.360±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 6.96±0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 6 References Reactions ~ 6 Commercial Sources	Score: 95 17. 87339-76-2  C₁₄H₁₀O₅ 9H-Xanthen-9-one, 1,7-dihydroxy-4-methoxy- Key Physical Properties: Molecular Weight 258.23 Boiling Point (Predicted) Value: 519.9±50.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.480±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 7.69±0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 37 References ~ 13 Commercial Sources Spectra	Score: 95 18. 87339-81-9  C₁₅H₁₄O₅ 9H-Xanthen-9-one, 1,4,7-trimethoxy- Key Physical Properties: Molecular Weight 286.28 Melting Point (Experimental) Value: 156-158 °C Condition: Solv: methanol (57-55-1) Boiling Point (Predicted) Value: 456.6±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.268±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr Related Info: ~ 6 References Reactions ~ 2 Commercial Sources Spectra Experimental Properties

Score: 95 19. 412339-59-4  C₁₄H₁₀O₅ 9H-Xanthen-9-one, 1,4-dihydroxy-6-methoxy- Key Physical Properties: Molecular Weight 258.23 Boiling Point (Predicted) Value: 508.5±50.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.480±0.06 g/cm3 Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 7.78±0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 2 References Reactions	Score: 95 20. 2621396-05-0  C₁₅H₁₂O₅ 9H-Xanthen-9-one, 5-ethoxy-1,4-dihydroxy- Key Physical Properties: Molecular Weight 272.25 Boiling Point (Predicted) Value: 512.8±50.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.425±0.06 g/cm3 Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 7.82±0.20 Condition: Most Acidic Temp: 25 °C Related Info: ~ 1 References	
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