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

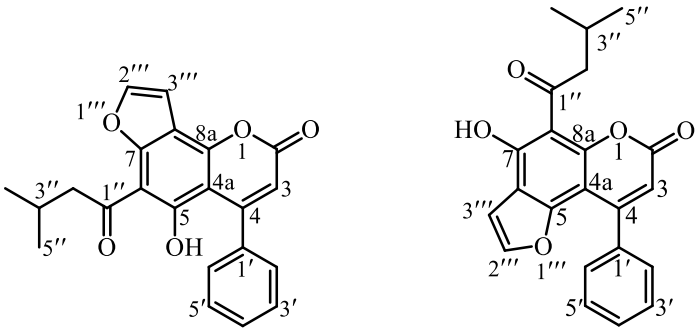
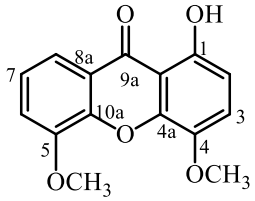


Figure S1: Structures of calopisifuran (**1**) and isodisparfuran A

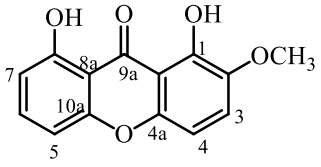
Table S2: Comparative ^{13}C NMR data of 1-hydroxy-4,5-dimethoxyxanthone (**2**) and 1,8-dihydroxy-2-methoxyxanthone (*Witjeratne *et al*., 2006)

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

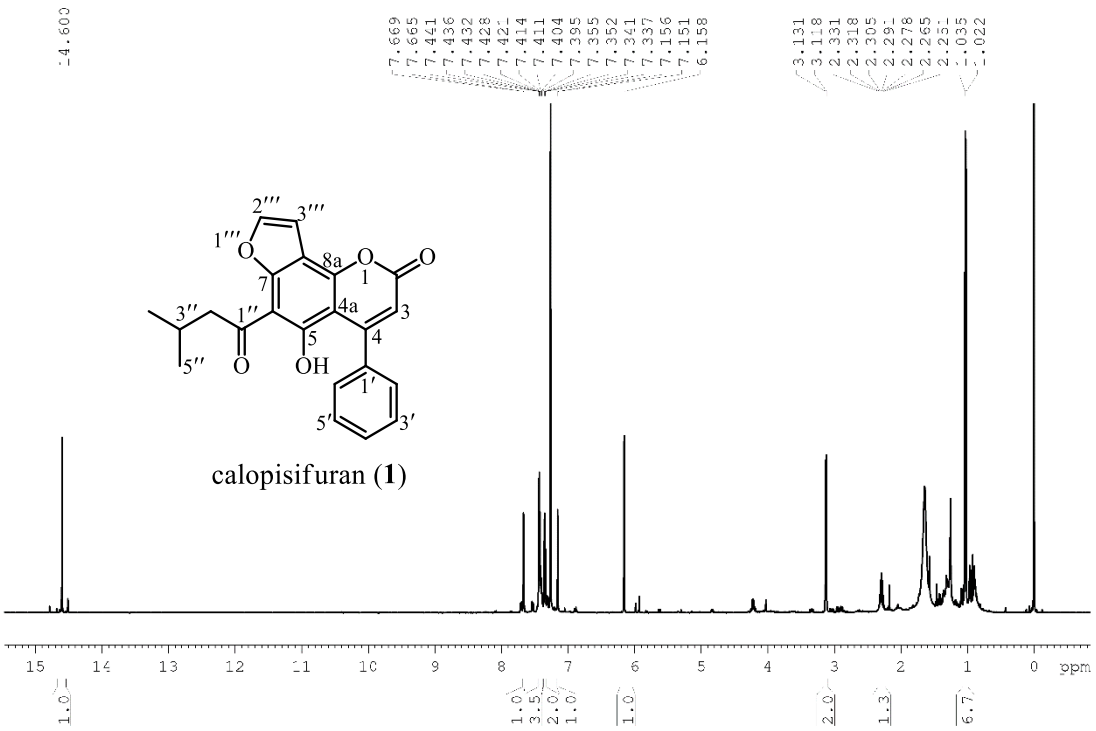


Figure S3: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of calopisifuran (**1**)

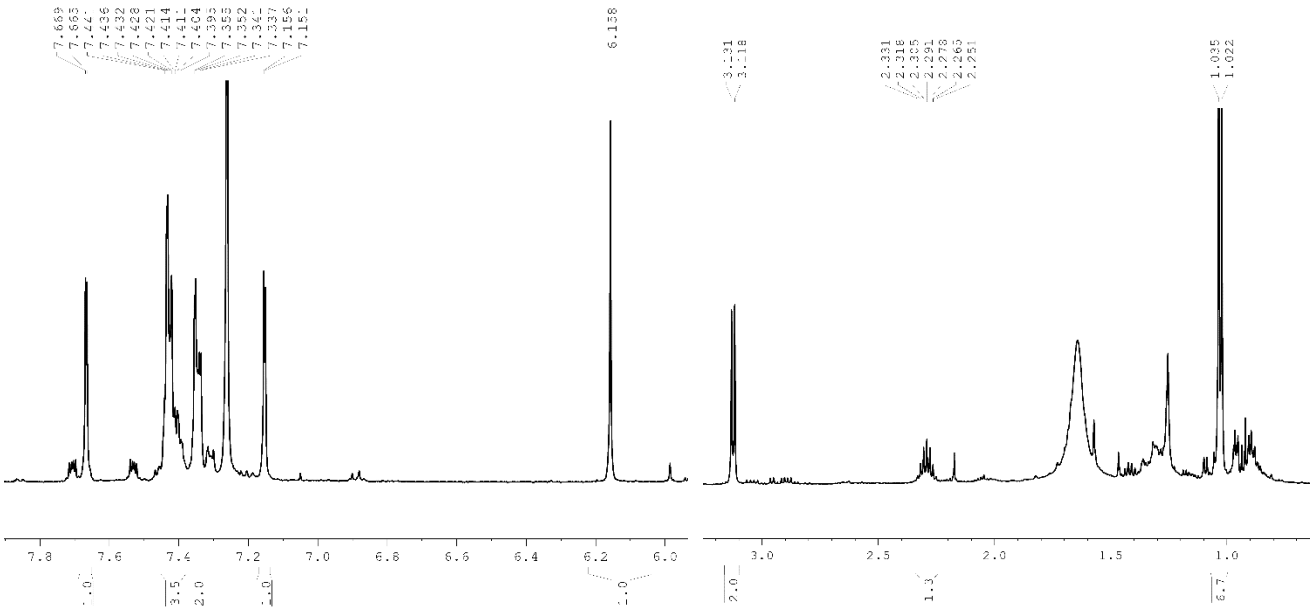


Figure S4: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of calopisifuran (**1**)
(From δ_H1.0 ppm to δ_H 7.8 ppm)

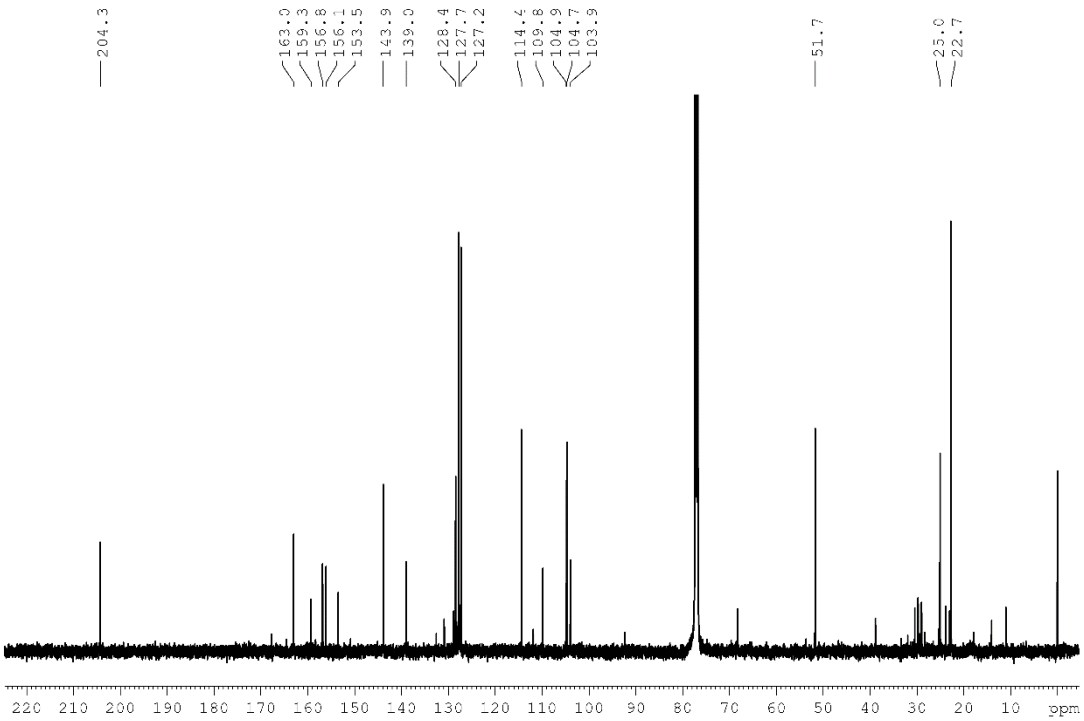


Figure S5: ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of calopisifuran (**1**)

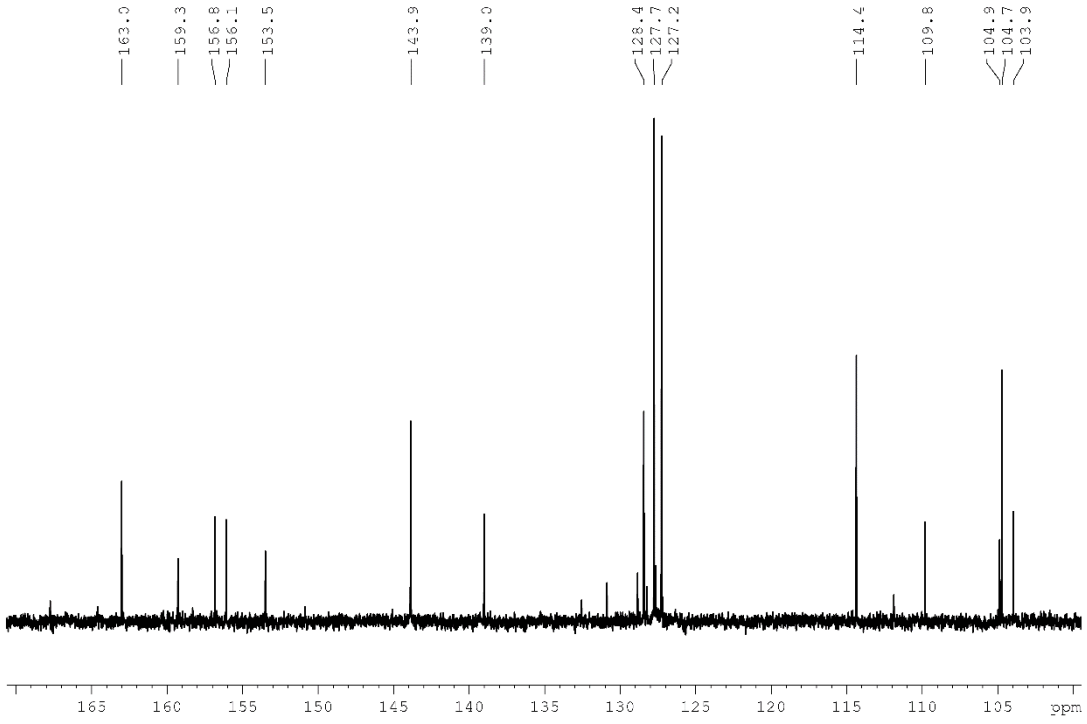


Figure S6: ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of calopisifuran (**1**)
(From δ_C105 ppm to δ_C 165 ppm)

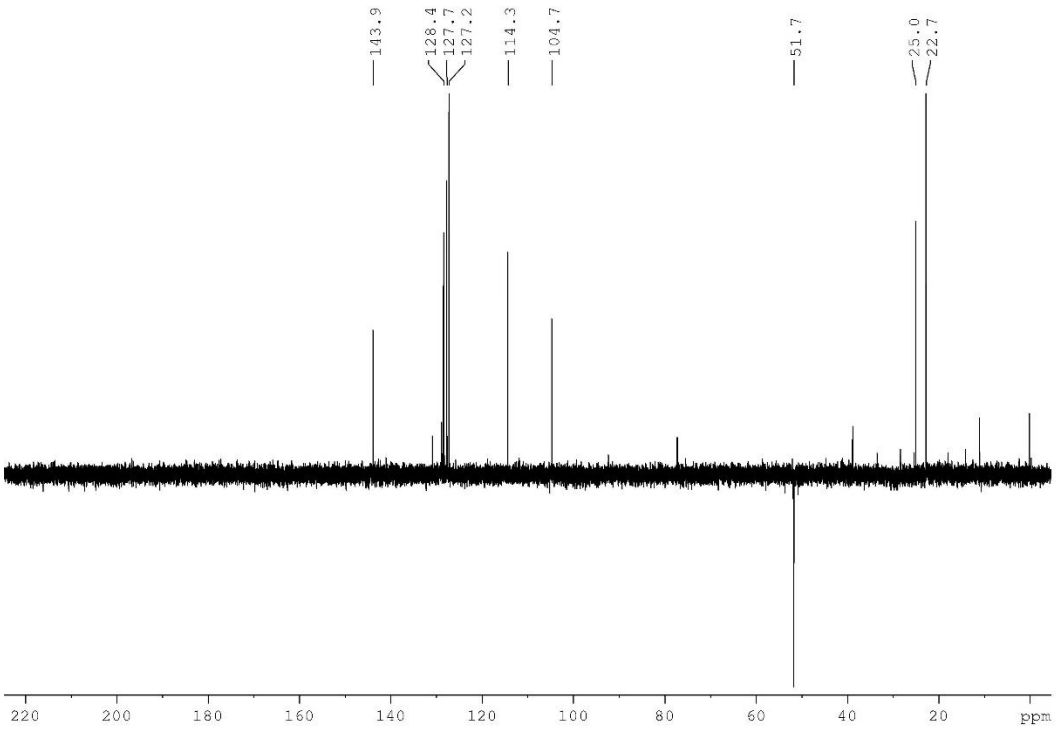


Figure S7: DEPT135 (125 MHz, $CDCl_3$) spectrum of calopisifuran (**1**)

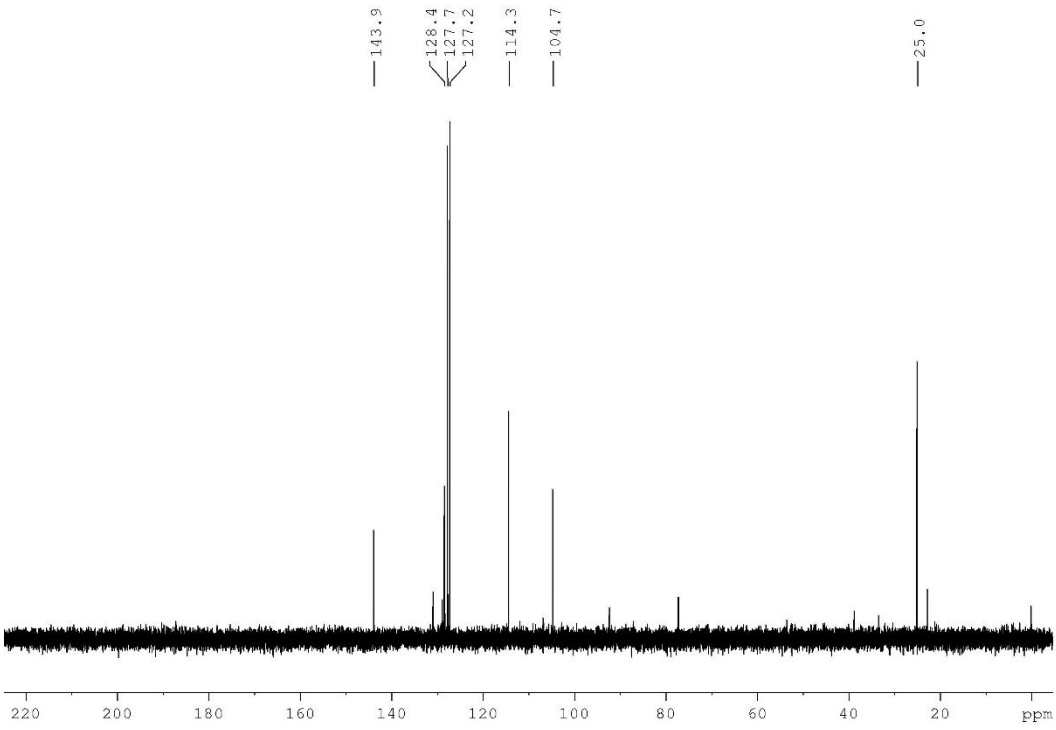


Figure S8: DEPT90 (125 MHz, $CDCl_3$) spectrum of calopisifuran (**1**)

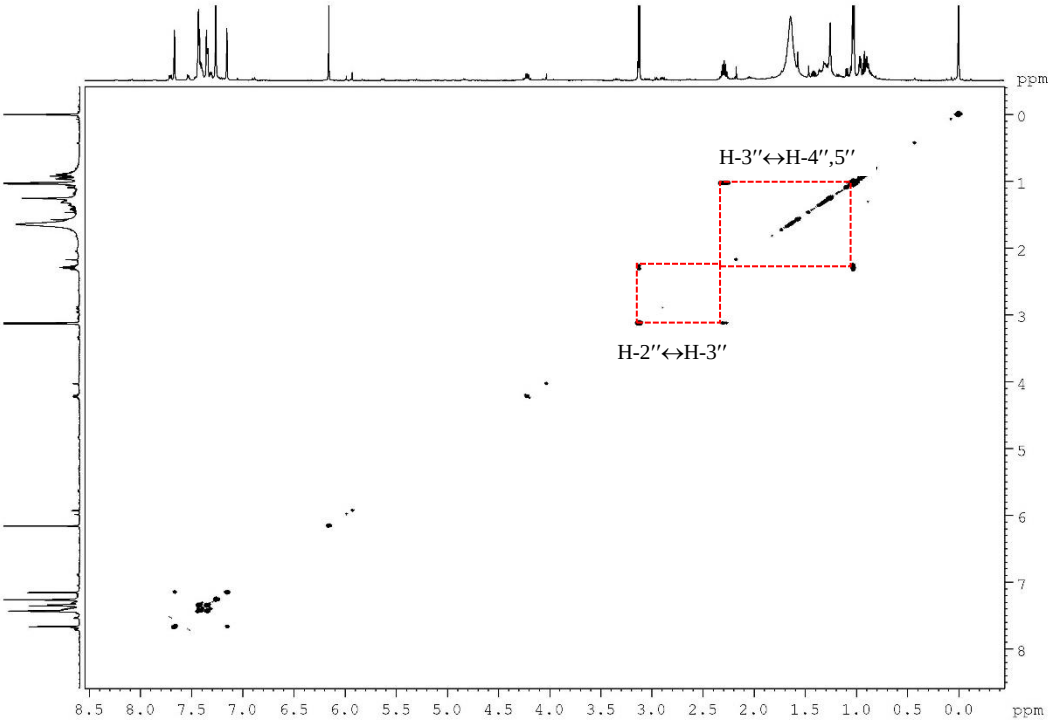


Figure S9: ^{1}H,^{1}H-COSY spectrum of calopisifuran (**1**) in $CDCl_3$

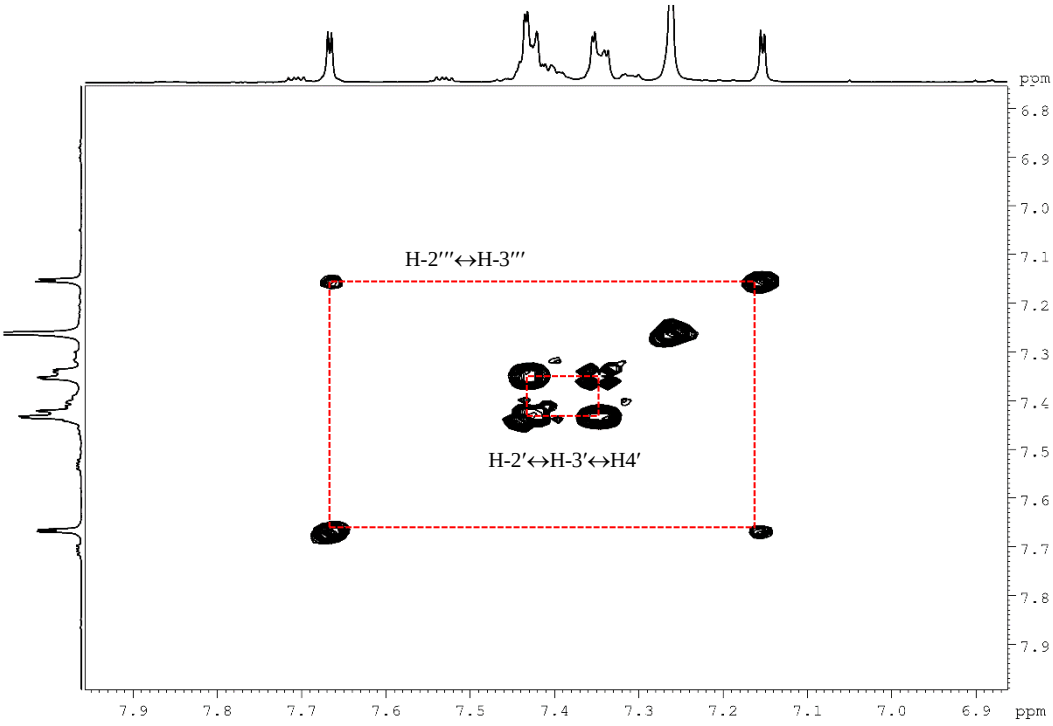


Figure S10: ^{1}H,^{1}H-COSY spectrum of calopisifuran (**1**) in $CDCl_3$
(From δ_H 6.9 ppm to δ_H 7.9 ppm)

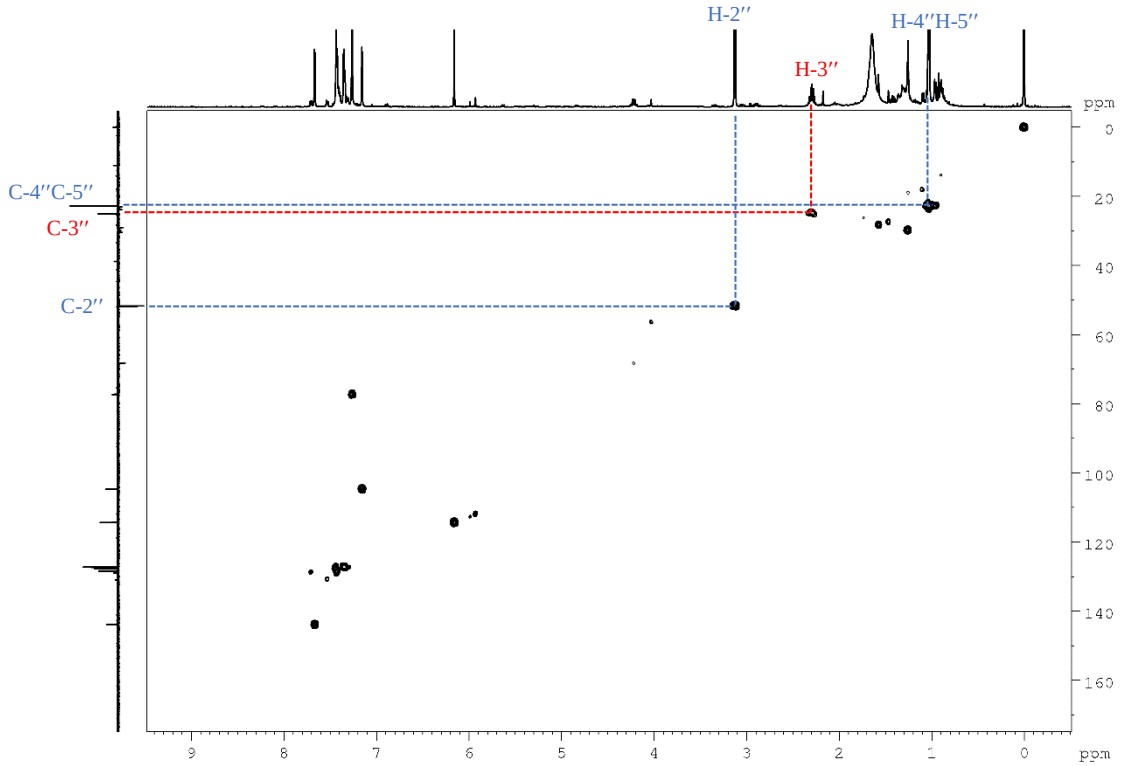


Figure S11: HMQC spectrum of calopisifuran (**1**) in $CDCl_3$

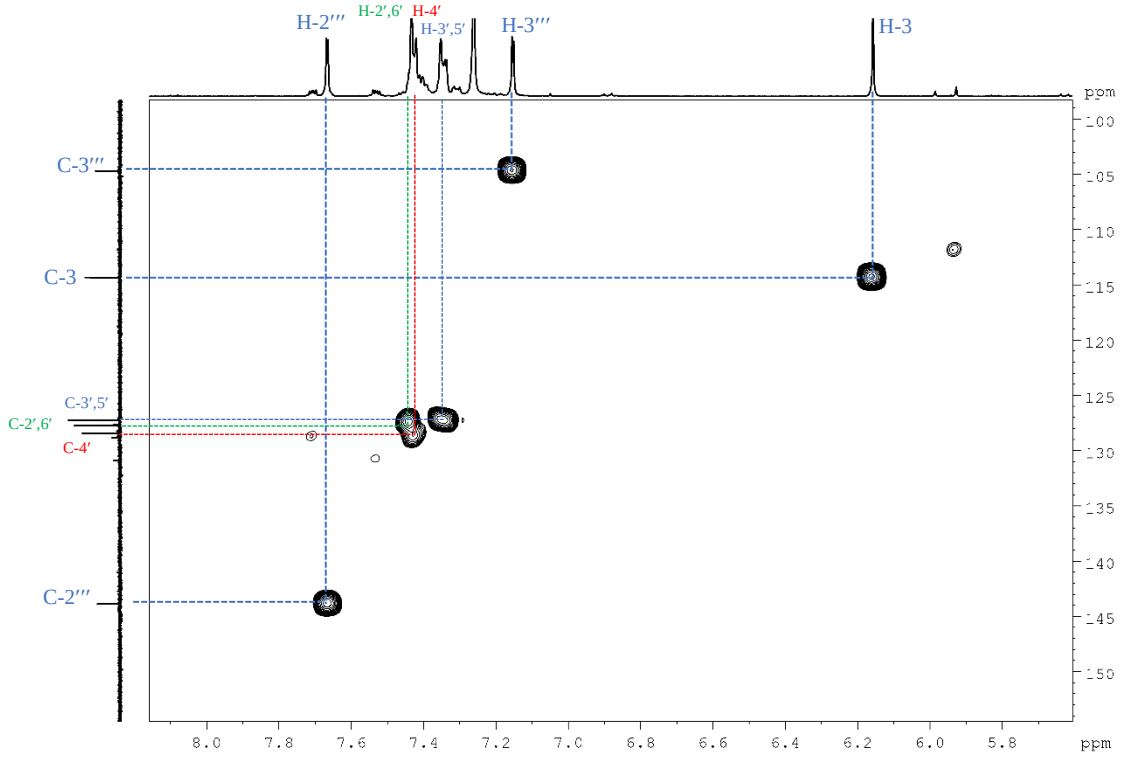


Figure S12: HMQC spectrum of calopisifuran (**1**) in $CDCl_3$
(From δ_H 5.8 ppm to δ_H 8.0 ppm and δ_C 100 ppm to δ_C 150 ppm)

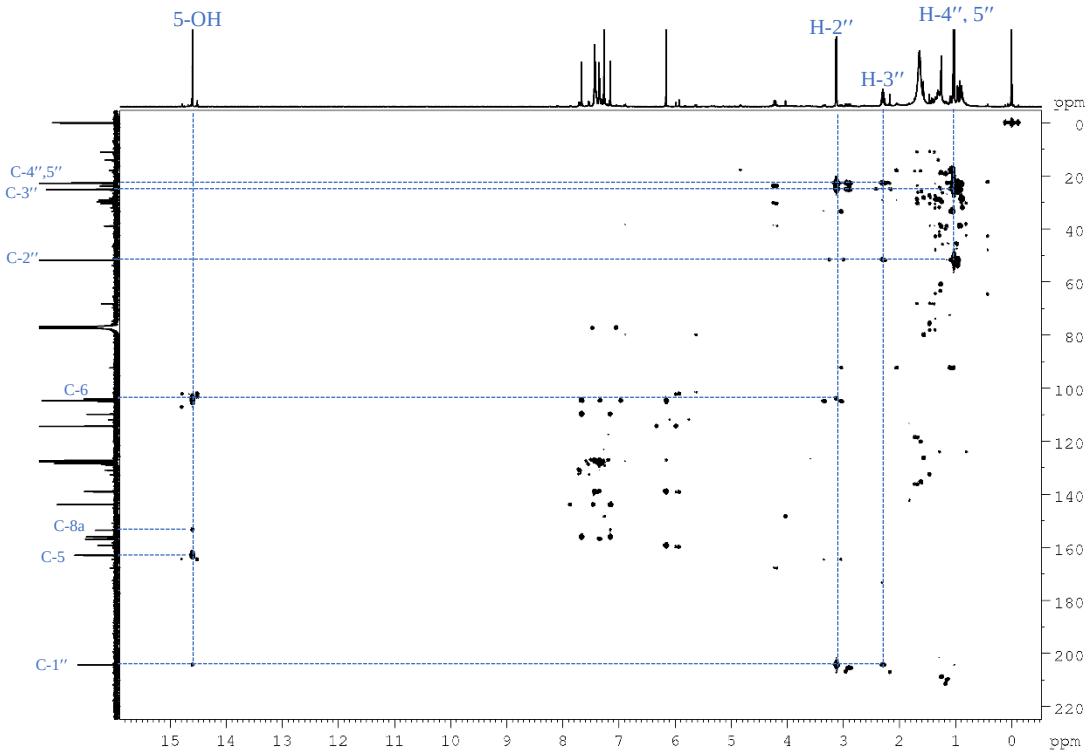


Figure S13: HMBC spectrum of calopisifuran (**1**) in $CDCl_3$

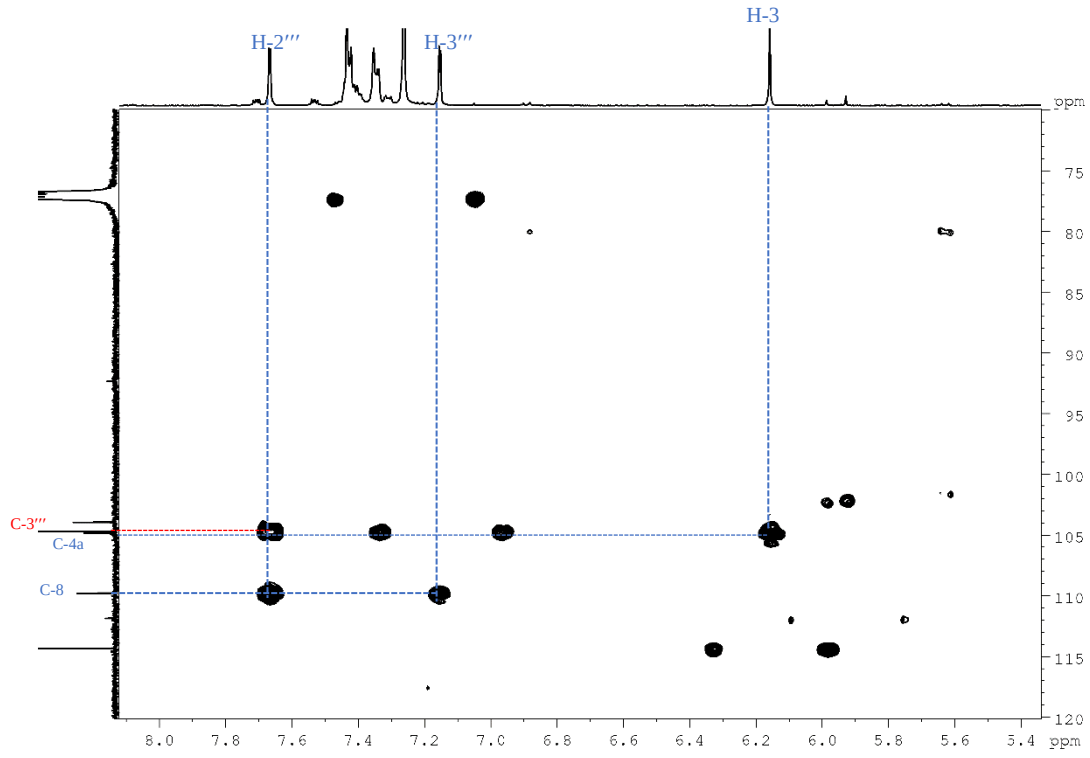


Figure S14: HMBC spectrum of calopisifuran (**1**) in $CDCl_3$
(From δ_H 5.4 ppm to δ_H 8.0 ppm δ_C 72 ppm to δ_C 120 ppm)

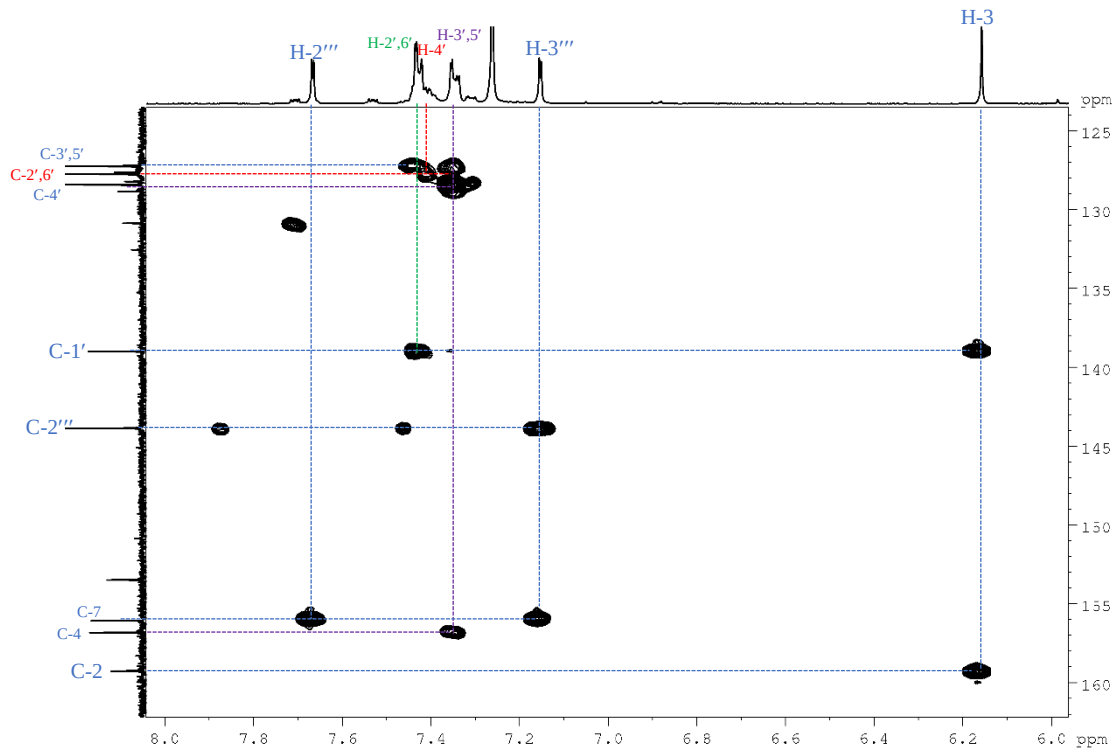


Figure S15: HMBC spectrum of calopisifuran (**1**) in $CDCl_3$
(From δ_H 6.0 ppm to δ_H 8.0 ppm δ_C 125 ppm to δ_C 160 ppm)

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

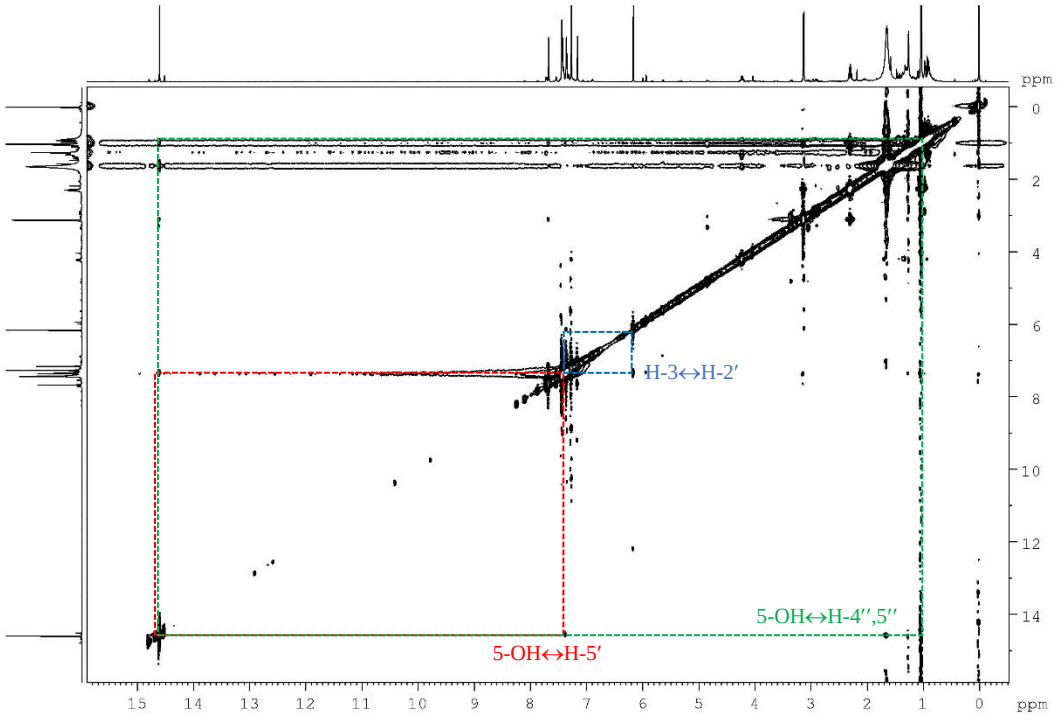


Figure S16: NOESY spectrum of calopisifuran (**1**) in CDCl

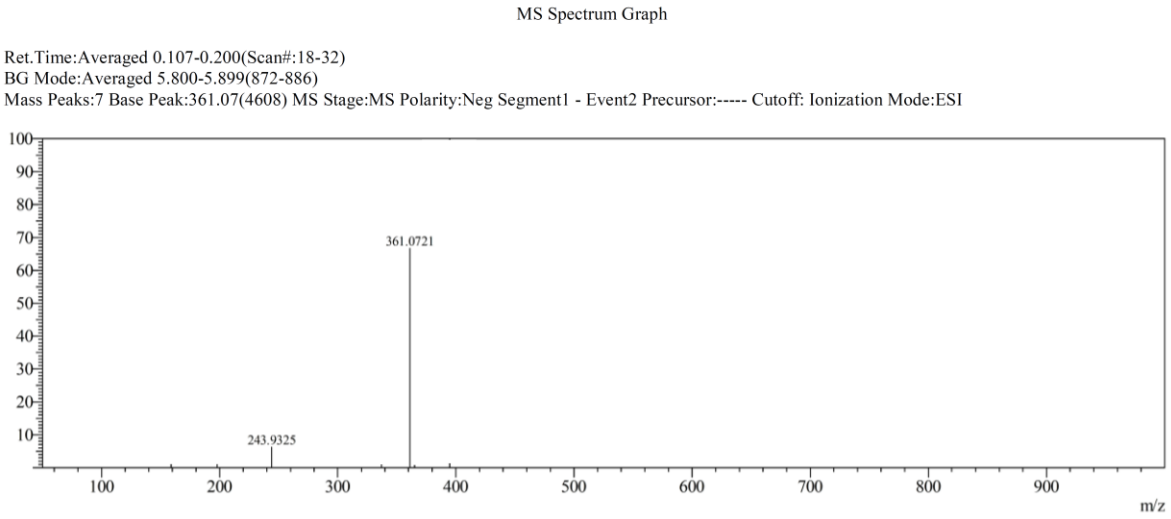


Figure S17: HR-ESI-MS spectrum of calopisifuran (**1**)

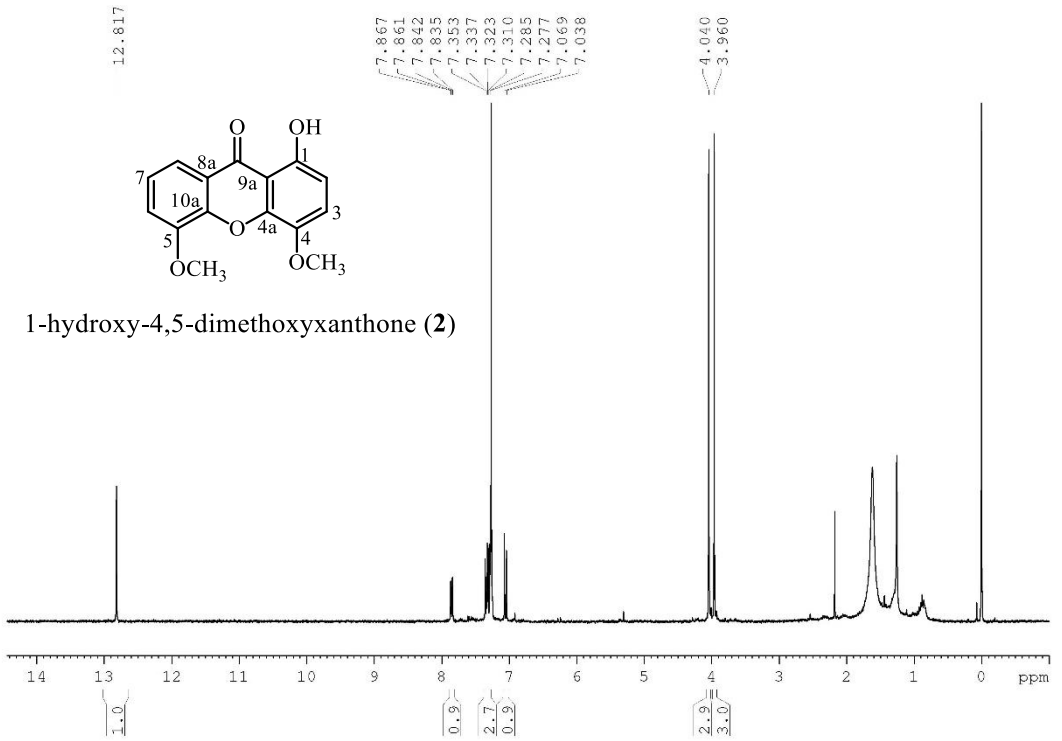


Figure S18: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**)

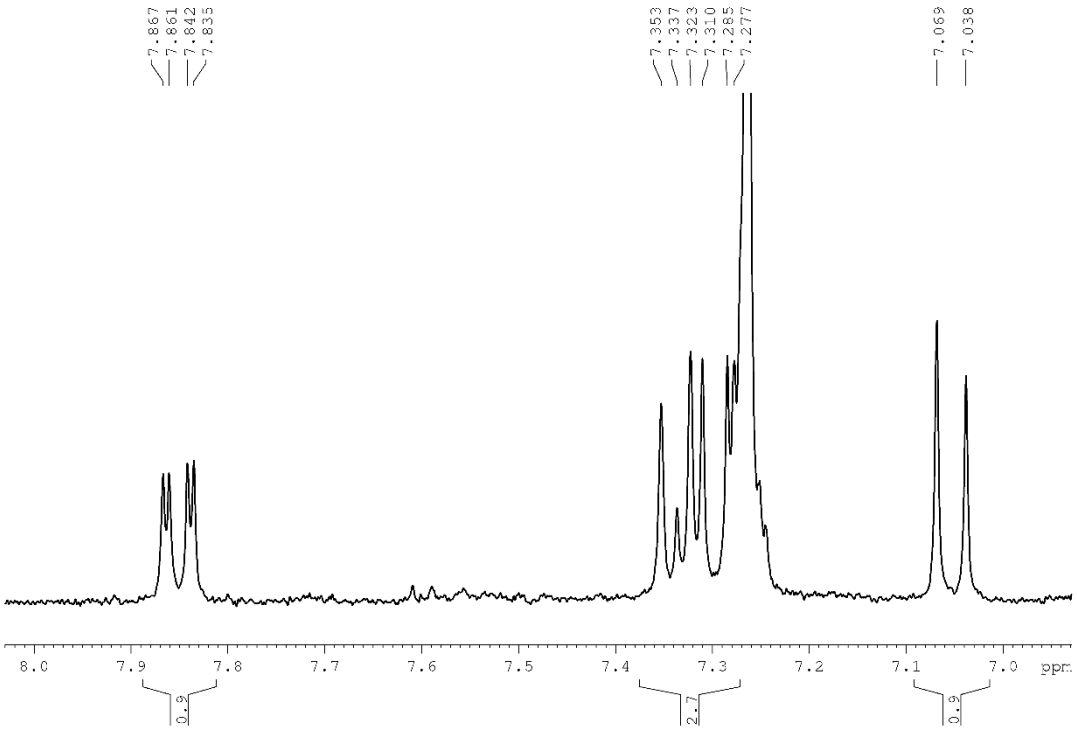


Figure S19: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) (From δ_H 7.0 ppm to δ_H 8.0 ppm)

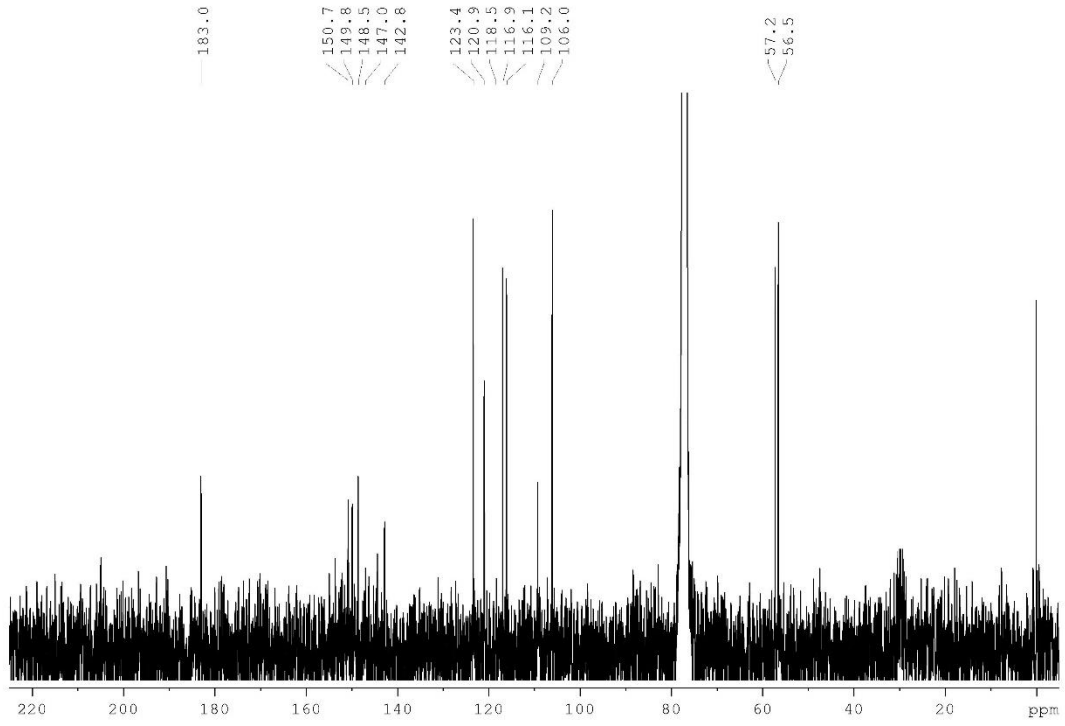


Figure S20: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**)

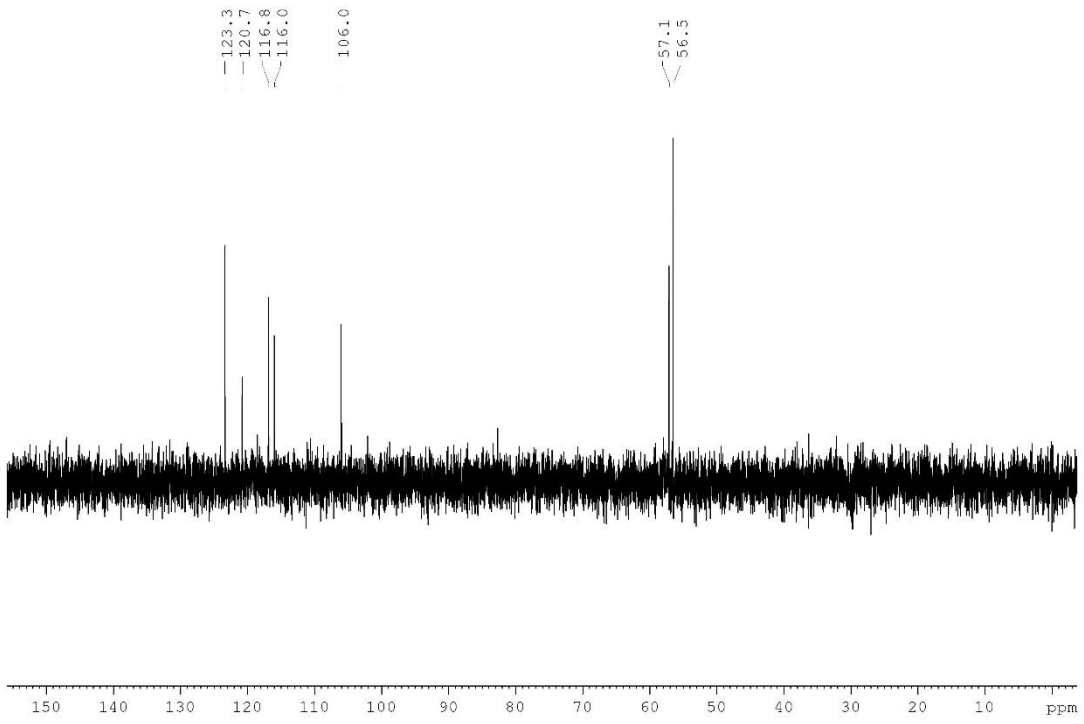


Figure S21: DEPT135 (75 MHz, $CDCl_3$) spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**)

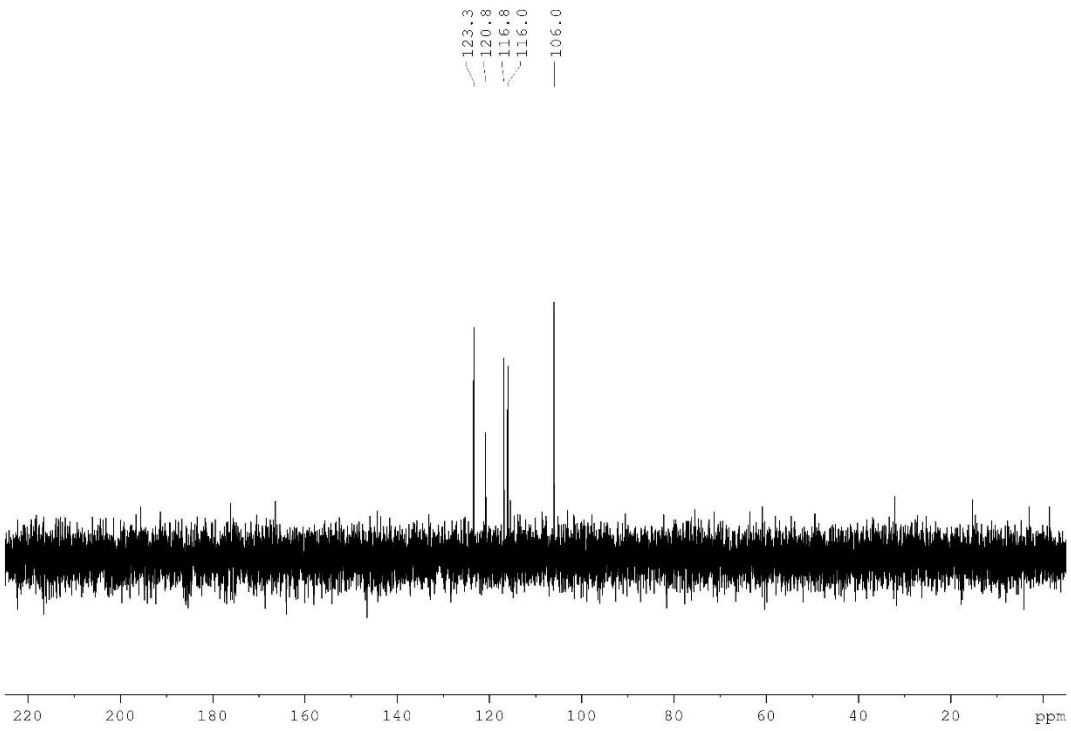


Figure S22: DEPT90 (75 MHz, $CDCl_3$) spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**)

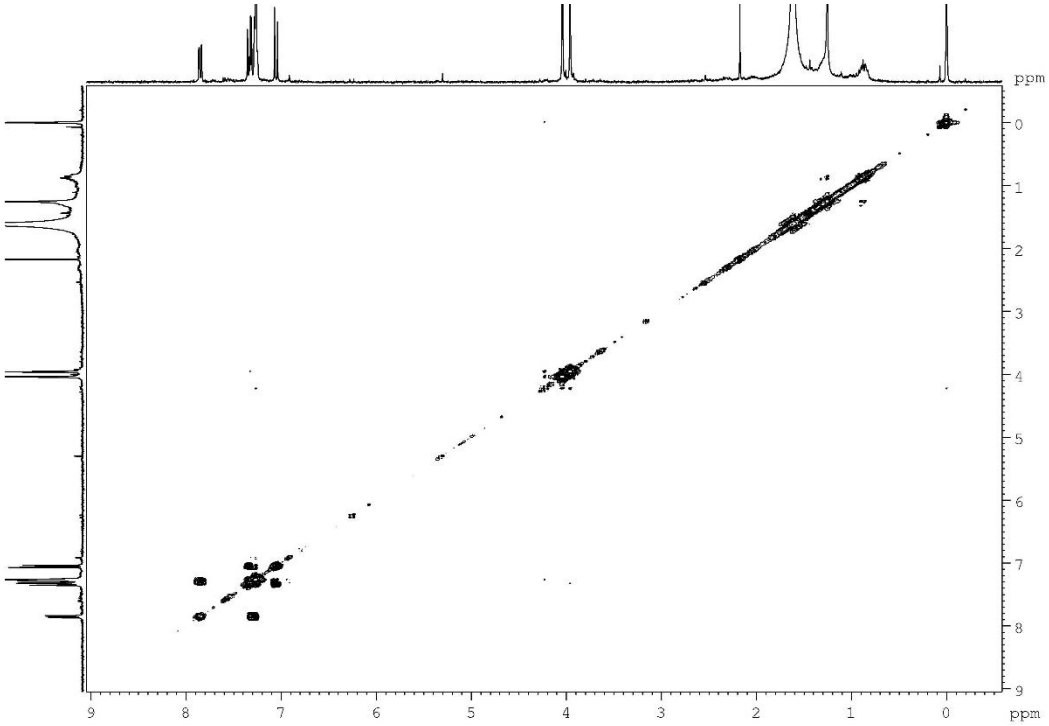


Figure S23: $^1H,^1H$-COSY spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in $CDCl_3$

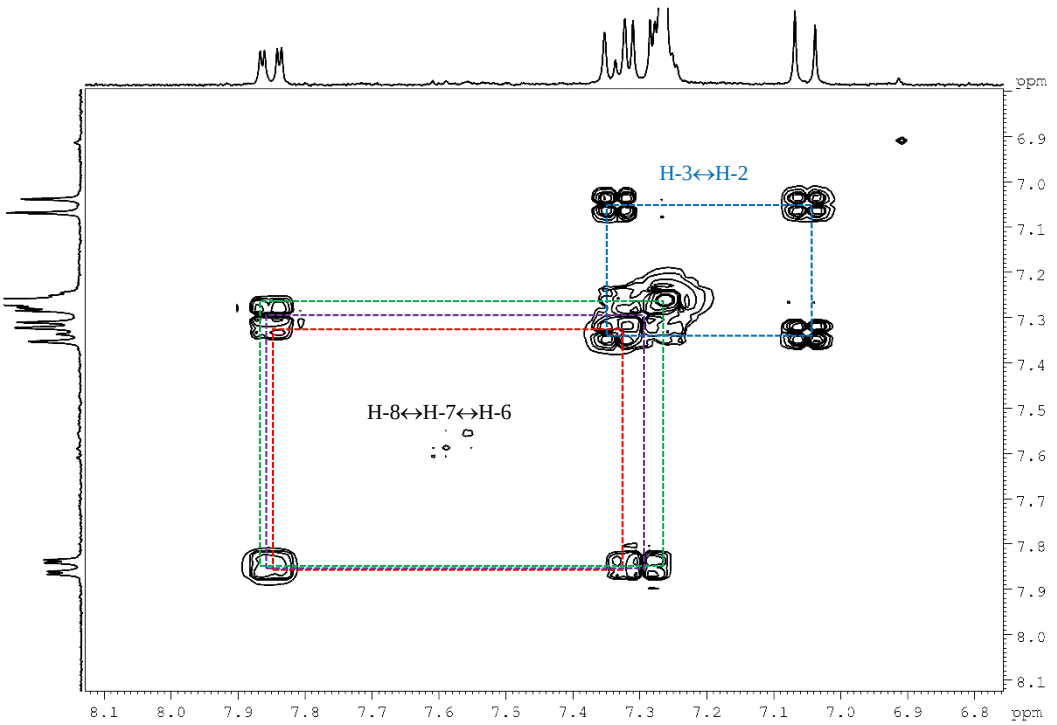


Figure S24: ^{1}H,^{1}H-COSY spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in $CDCl_3$ (From δ_H 6.8 ppm to δ_H 8.1 ppm)

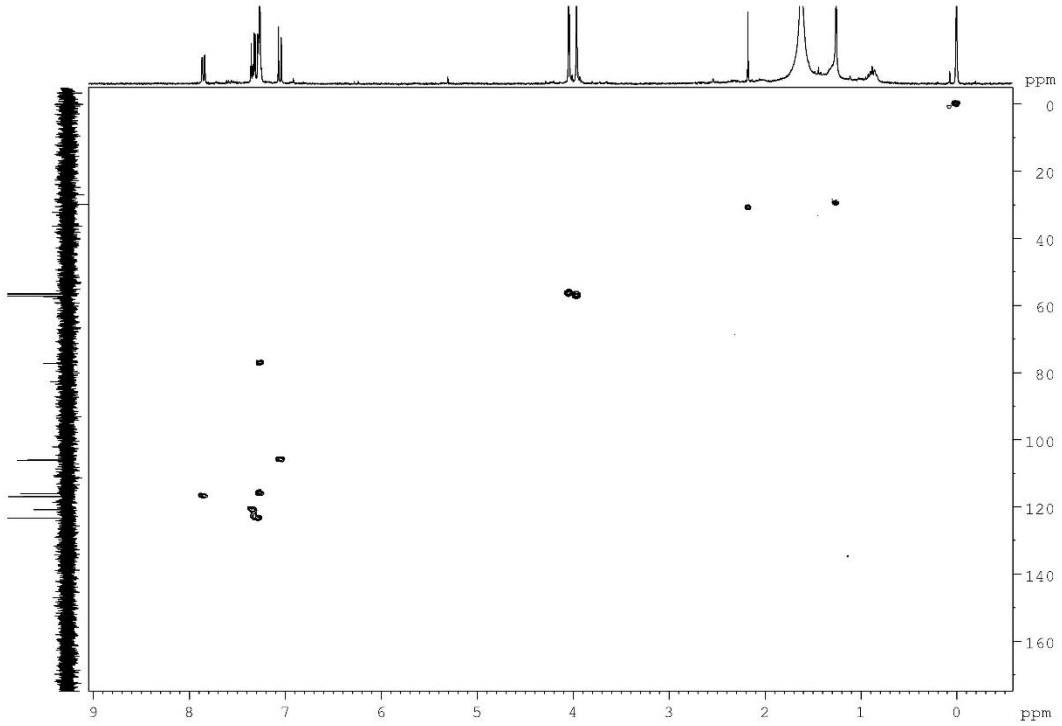


Figure S25: HMQC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in $CDCl_3$

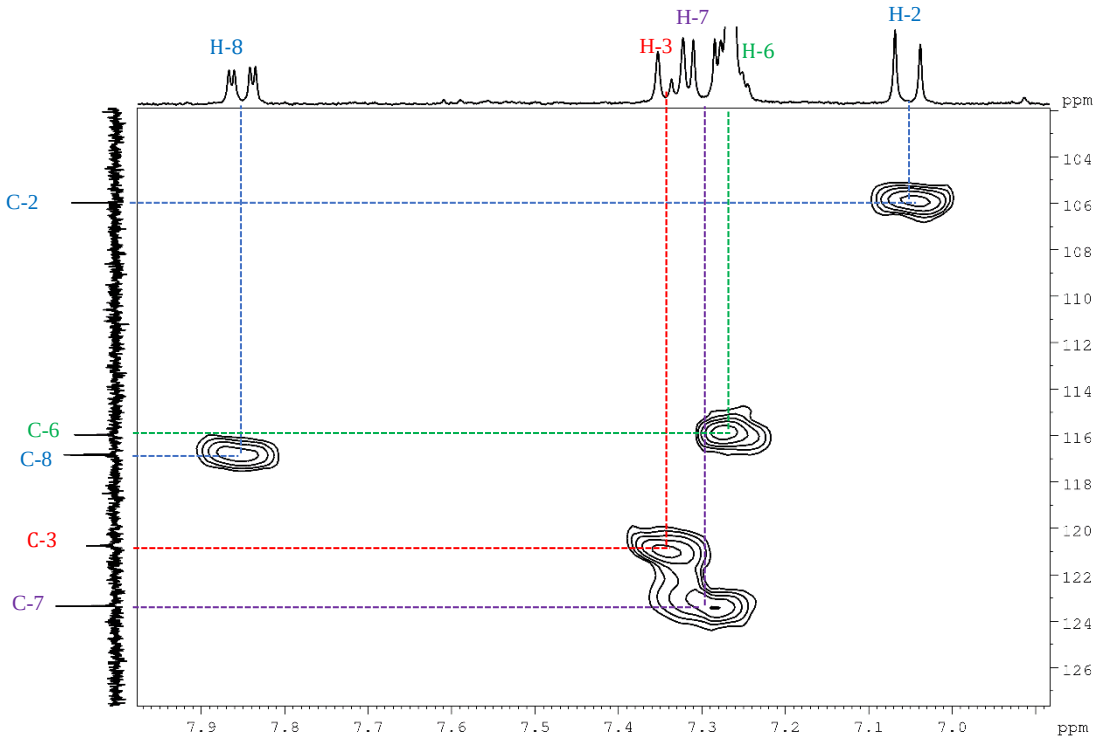


Figure S26: HMQC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in $CDCl_3$ (From δ_H 6.0 ppm to δ_H 8.0 ppm δ_C 102 ppm to δ_C 126 ppm)

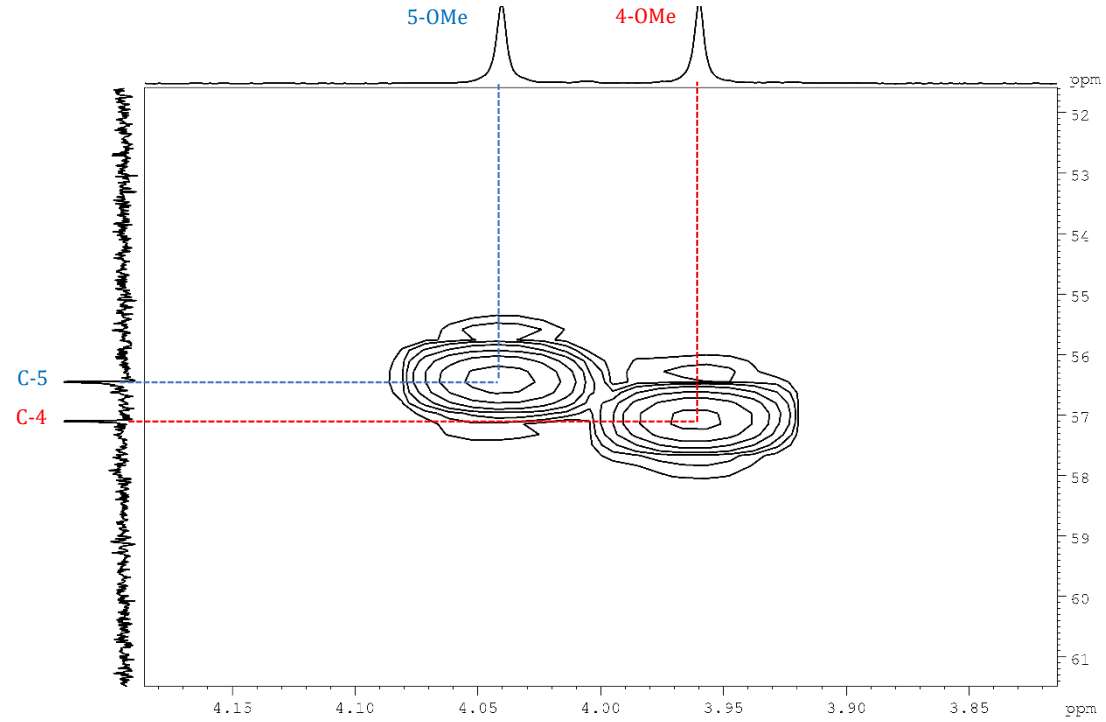


Figure S27: HMQC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in $CDCl_3$ (From δ_H 3.8 ppm to δ_H 4.2 ppm δ_C 52 ppm to δ_C 61 ppm)

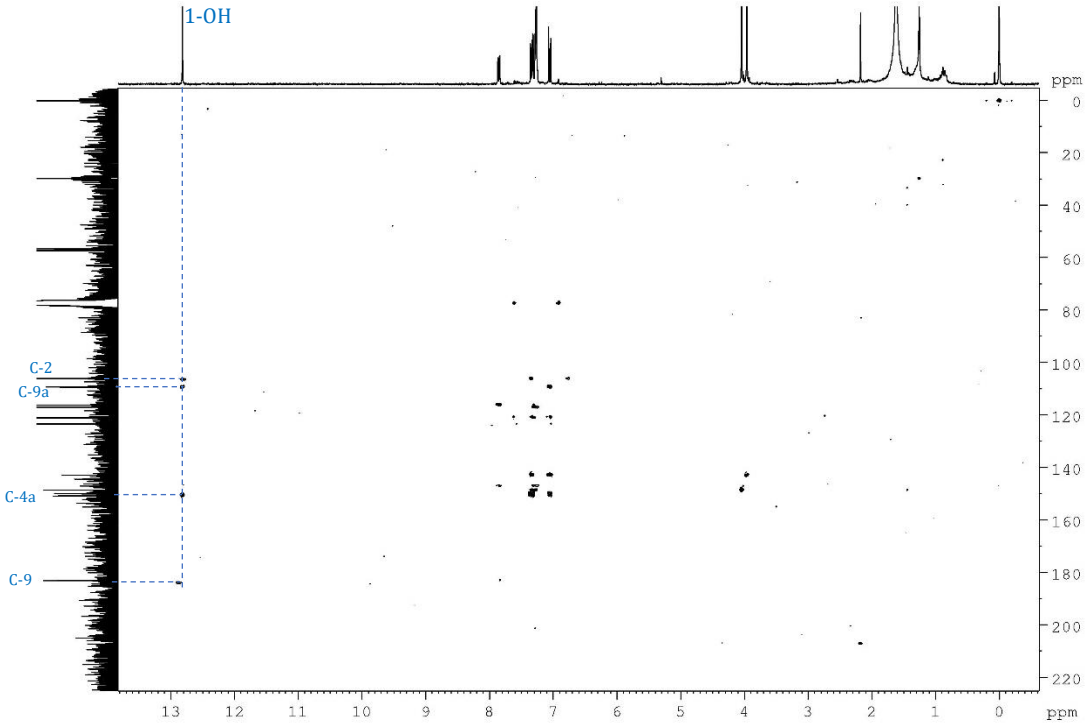


Figure S28: HMBC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in $CDCl_3$

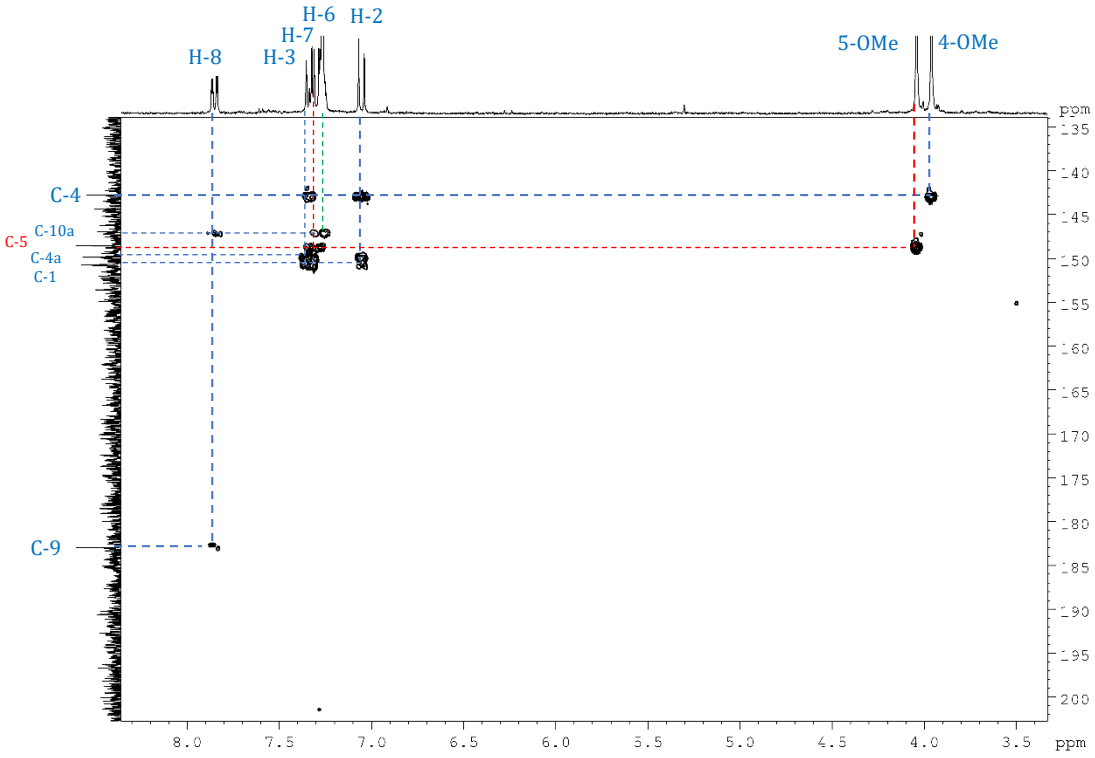


Figure S29: HMBC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in $CDCl_3$
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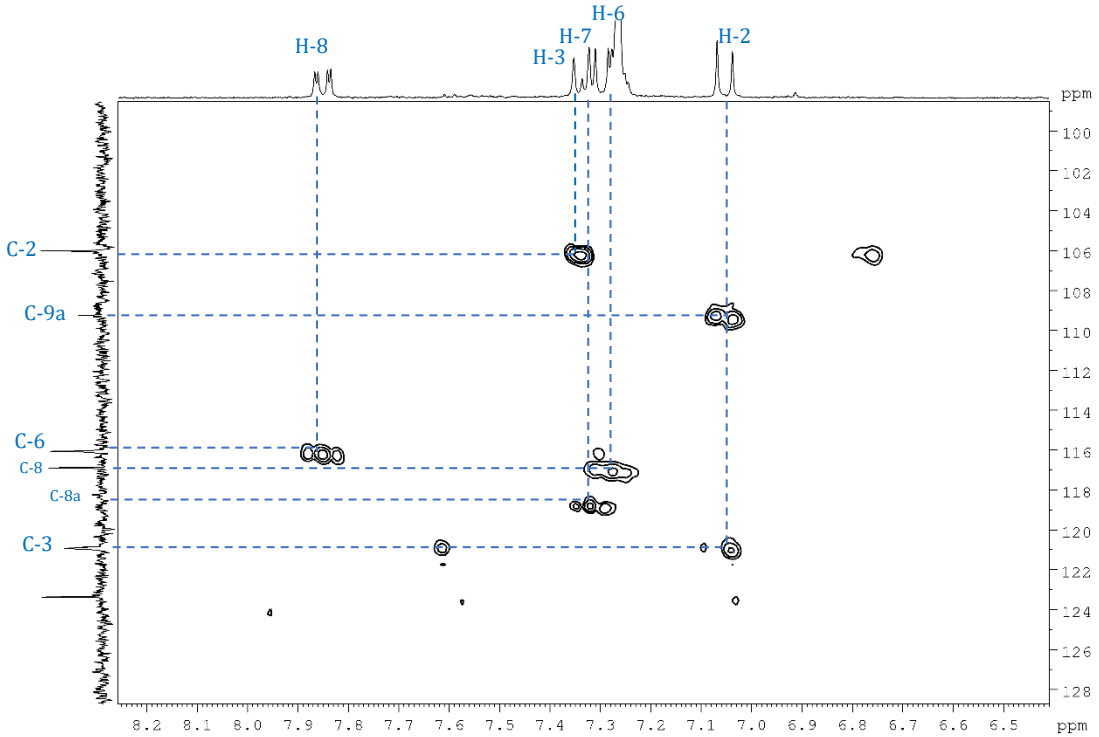

Figure S30:HMBC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in $CDCl_3$ (From δ_H 6.5 ppm to δ_H 8.2 ppm δ_C 100 ppm to δ_C 128 ppm)

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

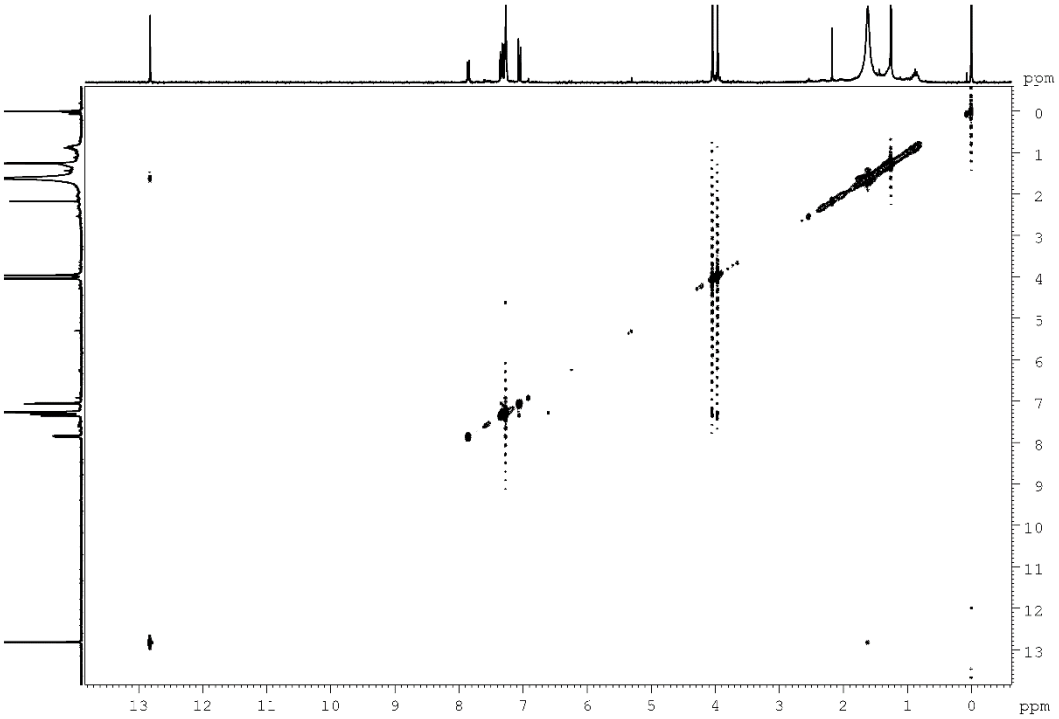

Figure S31: NOESY spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in $CDCl_3$

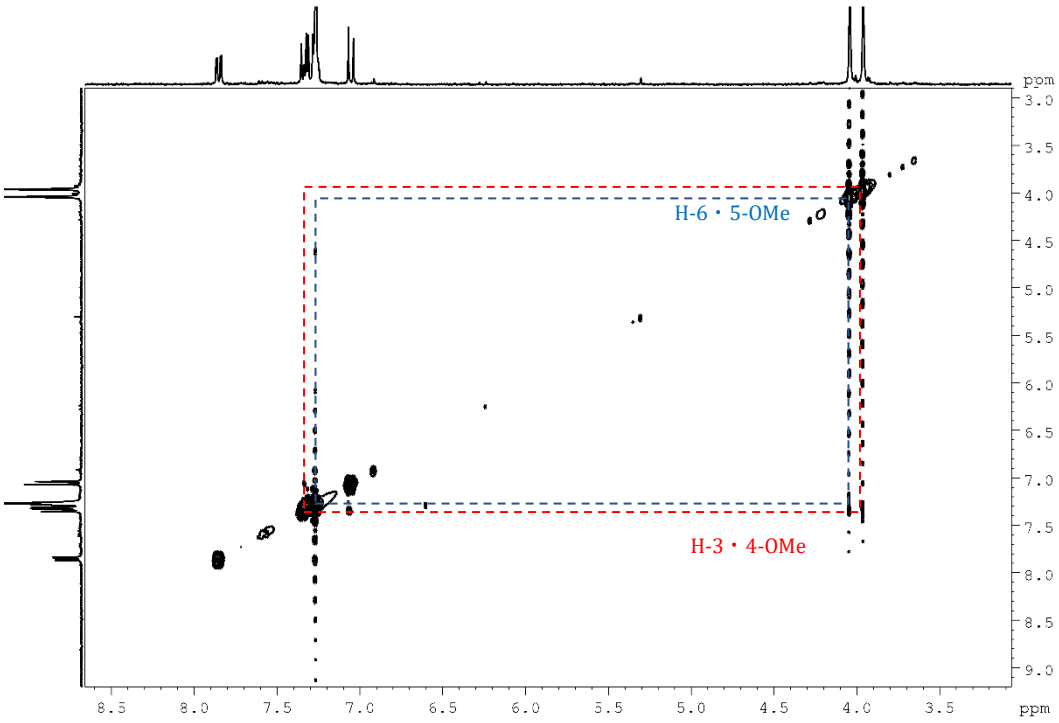

Figure S32: NOESY spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**) in $CDCl_3$ (From δ_H 3.0 ppm to δ_H 8.5 ppm)

MS Spectrum Graph

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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

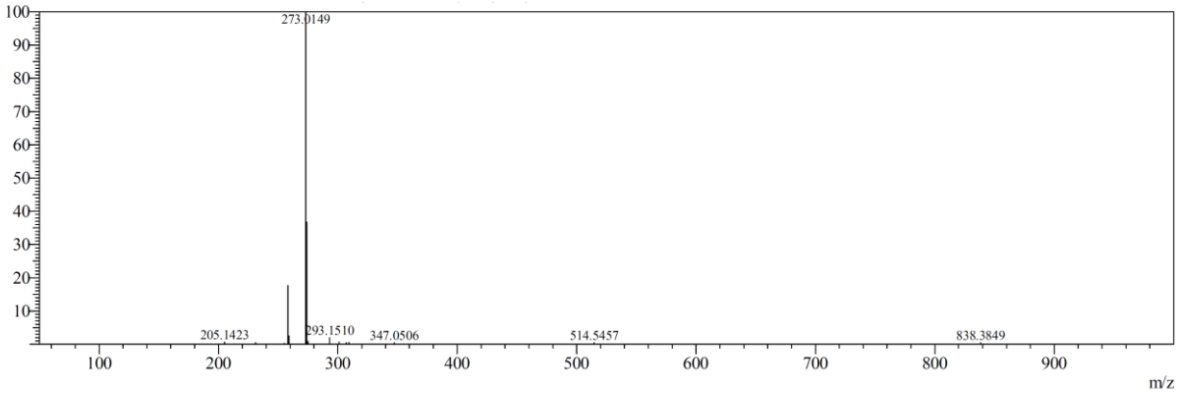
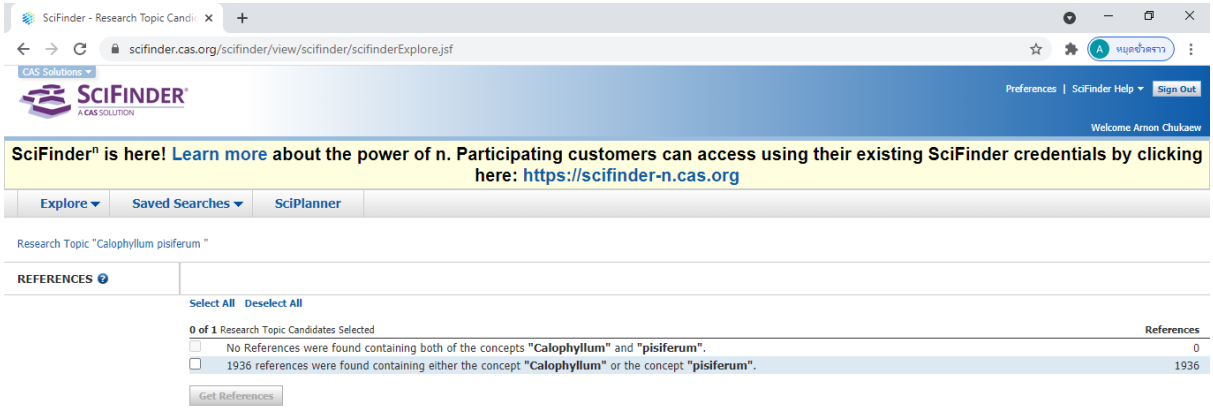
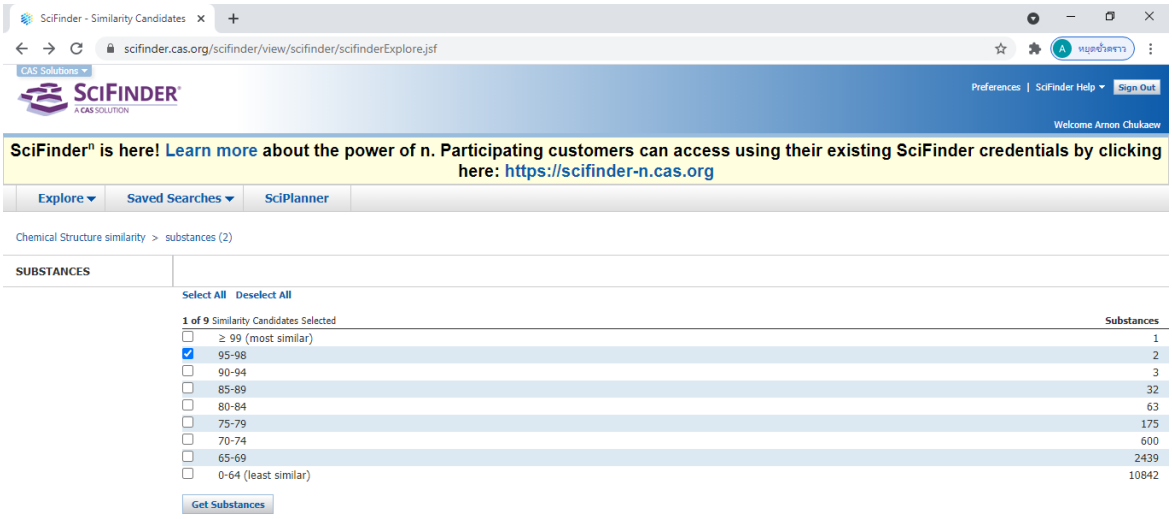


Figure S33: HR-ESI-MS spectrum of 1-hydroxy-4,5-dimethoxyxanthone (**2**)

Scifinder search report

S1: *Calophyllum pisiferum* research report

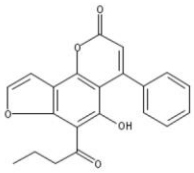




Score: 98

1.

247593-01-7



$C_{21}H_{16}O_5$

2*H*-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

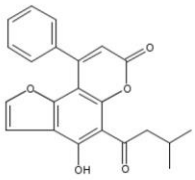
Related Info:

~ 1 References
Spectra

Score: 97

2.

342389-84-8



$C_{22}H_{18}O_5$

7*H*-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

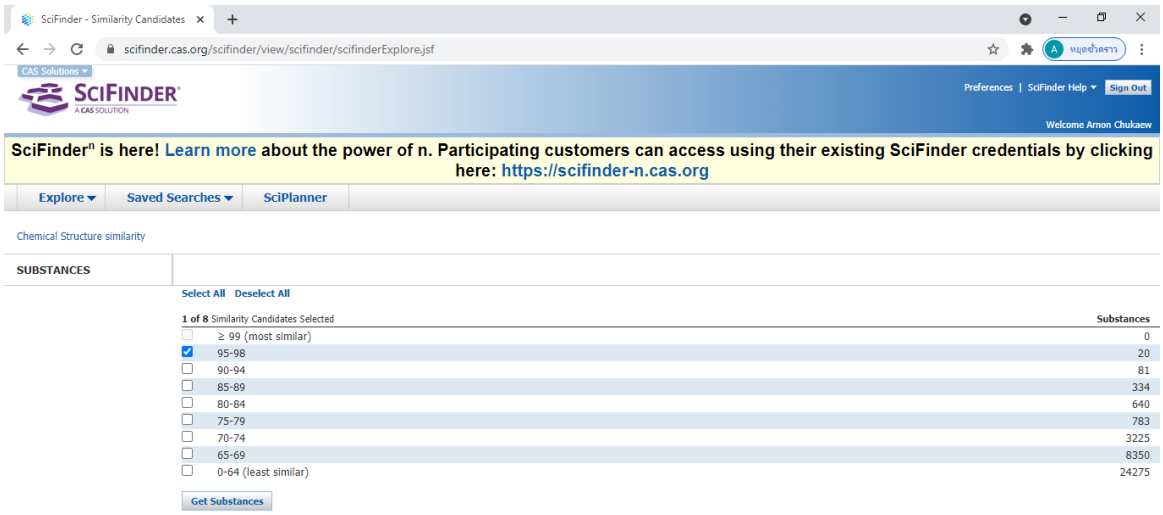
Density (Predicted)
Value: 1.312±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)
Value: 5.12±0.20 | Condition: Most Acidic Temp: 25 °C

Related Info:

~ 2 References
Spectra

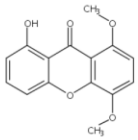
S3: Scifinder search report with 95-98 % similarity report of compound **2**.



Score: 98

1.

2016824-87-4



$C_{15}H_{12}O_5$
9*H*-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

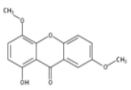
Related Info:

~ 1 References

Score: 97

2.

87339-80-8



$C_{15}H_{12}O_5$
9*H*-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

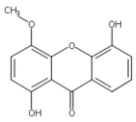
Related Info:

~ 1 References

Score: 97

3.

315240-08-5



$C_{14}H_{10}O_5$
9*H*-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:

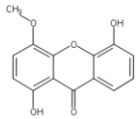
~ 5 References

Score: 97

4.

1404478-66-5

(Component: 315240-08-5)



• H_2O

$C_{14}H_{10}O_5$, H_2O
9*H*-Xanthen-9-one, 1,5-dihydroxy-4-methoxy-, hydrate (1:1)

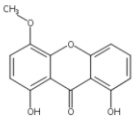
Related Info:

~ 1 References

Score: 97

5.

1605285-02-6



$C_{14}H_{10}O_5$
9*H*-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

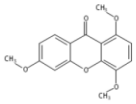
Related Info:

~ 1 References
Reactions

Score: 96

6.

61234-59-1



$C_{16}H_{14}O_5$
9*H*-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

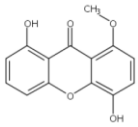
Related Info:

~ 2 References
~ 5 Commercial Sources
Experimental Properties

Score: 96

7.

87339-75-1



$C_{14}H_{10}O_5$
9*H*-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

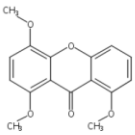
Related Info:

~ 5 References
~ 2 Commercial Sources
Spectra

Score: 96

8.

87339-86-4



$C_{16}H_{14}O_5$
9*H*-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

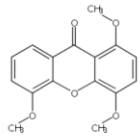
Related Info:

~ 1 References

Score: 96

9.

182675-54-3



$C_{16}H_{14}O_5$
9*H*-Xanthen-9-one, 1,4,5-trimethoxy-

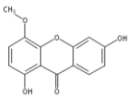
Key Physical Properties:

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
10.
410095-67-9



$C_{14}H_{10}O_5$
9*H*-Xanthen-9-one, 1,6-dihydroxy-4-methoxy-

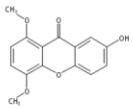
Key Physical Properties:

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



$C_{15}H_{12}O_5$
9*H*-Xanthen-9-one, 7-hydroxy-1,4-dimethoxy-

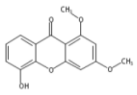
Key Physical Properties:

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



$C_{15}H_{12}O_5$
9*H*-Xanthen-9-one, 5-hydroxy-1,3-dimethoxy-

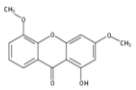
Key Physical Properties:

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

Score: 95
13.
6563-48-0



$C_{15}H_{12}O_5$
9*H*-Xanthen-9-one, 1-hydroxy-3,5-dimethoxy-

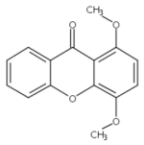
Key Physical Properties:

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



$C_{15}H_{12}O_4$
9*H*-Xanthen-9-one, 1,4-dimethoxy-

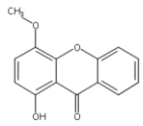
Key Physical Properties:

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



$C_{14}H_{10}O_4$
9*H*-Xanthen-9-one, 1-hydroxy-4-methoxy-

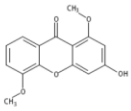
Key Physical Properties:

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



$C_{15}H_{12}O_5$
9*H*-Xanthen-9-one, 3-hydroxy-1,5-dimethoxy-

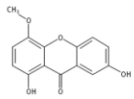
Key Physical Properties:

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: 6.98±0.20 | Condition: Most Acidic Temp: 25 °C

Related Info:

~ 6 References
Reactions
~ 6 Commercial Sources

Score: 95
17.
87339-76-2



$C_{14}H_{10}O_5$
9*H*-Xanthen-9-one, 1,7-dihydroxy-4-methoxy-

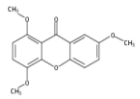
Key Physical Properties:

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



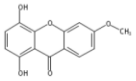
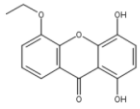
$C_{16}H_{14}O_5$
9*H*-Xanthen-9-one, 1,4,7-trimethoxy-

Key Physical Properties:

Molecular Weight
286.28
Melting Point (Experimental)
Value: 156-158 °C | Condition: Solv: methanol (67-56-1)
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**  **$C_{14}H_{10}O_5$** 9*H*-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**  **$C_{15}H_{12}O_5$** 9*H*-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	