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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(From $\delta_H$ 5.4 ppm to $\delta_H$ 8.0 ppm $\delta_C$ 72 ppm to $\delta_C$ 120 ppm)

**Figure S15**: HMBC spectrum of calopisifuran (1) in CDCl$_3$
(From $\delta_H$ 6.0 ppm to $\delta_H$ 8.0 ppm $\delta_C$ 125 ppm to $\delta_C$ 160 ppm)

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

**Figure S16**: NOESY spectrum of calopisifuran (1) in CDCl$_3$

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

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in CDCl$_3$

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(From $\delta_H$ 6.8 ppm to $\delta_H$ 8.1 ppm)

**Figure S25**: HMOC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (2) in CDCl$_3$

**Figure S26**: HMOC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (2) in CDCl$_3$
(From $\delta_H$ 6.0 ppm to $\delta_H$ 8.0 ppm $\delta_C$ 102 ppm to $\delta_C$ 126 ppm)

**Figure S27**: HMOC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (2) in CDCl$_3$
(From $\delta_H$ 3.8 ppm to $\delta_H$ 4.2 ppm $\delta_C$ 52 ppm to $\delta_C$ 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 $\delta_H$ 3.5 ppm to $\delta_H$ 8.0 ppm $\delta_C$ 135 ppm to $\delta_C$ 200 ppm)

**Figure S30**: HMBC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (2) in CDCl$_3$
(From $\delta_H$ 6.5 ppm to $\delta_H$ 8.2 ppm $\delta_C$ 100 ppm to $\delta_C$ 128 ppm)

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

**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 $\delta_H$ 3.0 ppm to $\delta_H$ 8.5 ppm)

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

Scifinder search report

S1: Calophyllum pisiferum research report
S2: Scifinder search report with 95-98 % similarity report of compound 1.
S3: Scifinder search report with 95-98 % similarity report of compound 2.

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Table S1: Comparative $^{13}$C NMR data of calopisifuran (1) and isodisparfuran A

(Guilet et al., 2001)

| Position | $\delta$* calopisifuran (1) in CDCl$_3$ | $\delta$* isodisparfuran A* in CDCl$_3$ |
|----------|----------------------------------------|----------------------------------------|
| 1        | 159.3                                  | 159.2                                  |
| 2        | 114.4                                  | 112.0                                  |
| 3        | 156.8                                  | 153.7                                  |
| 4        | 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                                  |

*Recorded in 125 MHz

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

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**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 | $\delta$ a 1-hydroxy-4,5-dimethoxyxanthone (2) in CDCl$_3$ | $\delta$ 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) ![Structure of 1-hydroxy-4,5-dimethoxyxanthone](image1.png)

1,8-dihydroxy-2-methoxyxanthone ![Structure of 1,8-dihydroxy-2-methoxyxanthone](image2.png)

**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 (I)

Figure S4: $^1$H NMR (500 MHz, CDCl$_3$) spectrum of calopisifuran (I)
(From $\delta_H$ 1.0 ppm to $\delta_H$ 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 $\delta_C$ 105 ppm to $\delta_C$ 165 ppm)

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**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 (I) in CDCl$_3$

**Figure S10:** $^1$H,$^1$H-COSY spectrum of calopisifuran (I) in CDCl$_3$
(From $\delta_{H}$ 6.9 ppm to $\delta_{H}$ 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 CDCl₃
(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 (CH₃)  | 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 (CH₃)  | 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

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 $\delta_H$ 7.0 ppm to $\delta_H$ 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**: $^1$H-$^1$H-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 $\delta_H$ 6.8 ppm to $\delta_H$ 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 CDCl₃
(From δH 6.0 ppm to δH 8.0 ppm δC 102 ppm to δC 126 ppm)

Figure S27: HMQC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (2) in CDCl₃
(From δH 3.8 ppm to δH 4.2 ppm δC 52 ppm to δC 61 ppm)
Figure S28: HMBC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (2) in CDCl₃

Figure S29: HMBC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (2) in CDCl₃
(From δH 3.5 ppm to δH 8.0 ppm δC 135 ppm to δC 200 ppm)
Figure S30: HMBC spectrum of 1-hydroxy-4,5-dimethoxyxanthone (2) in CDCl₃
(From δ_H 6.5 ppm to δ_H 8.2 ppm  δ_C 100 ppm to  δ_C 128 ppm)

Table S4. 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 (CH₃) | C-4 |
| 5-OMe    | 4.04, s       | 56.5 (CH₃) | 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 δH 3.0 ppm to δH 8.5 ppm)
**Figure S33**: HR-ESI-MS spectrum of 1-hydroxy-4,5-dimethoxyxanthone (2)

Scifinder search report

**S1: Calophyllum pisiferum** research report
S3: Scifinder search report with 95-98 % similarity report of compound 2.
C60 H50 O8
Shikimic-5-one, 1,4-dihydroxy-6-methoxy-

Key Physical Properties:
Molecular Weight 230.23
Boiling Point (Predicted)
Value: 108.6±0.3 °C (Condition: Press 760 Torr)
Density (Predicted)
Value: 1.426±0.05 g/mL (Condition: Temp 23 °C Press 760 Torr)
Molar Refractivity (Predicted)
Value: 7.79±0.25 (Condition: Molar Acidic Temp 25 °C)
Related Info:
- 2 References
- Reactions