SUPPLEMENTARY MATERIAL

A new $\alpha$-pyrone from the mangrove endophytic fungus

*Phomopsis* sp. HNY29-2B

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Abstract

A new $\alpha$-pyrone derivative, phomopyrone A (1), together with two known compounds (2–3), was isolated from the culture of the mangrove endophytic fungus Phomopsis sp. HNY29-2B. Their structures were determined by detailed analysis of spectroscopic data. The configuration of 1 was further confirmed by X-ray diffraction. All isolated compounds were evaluated for antibacterial and antioxidative activities. Compound 2 exhibited antibacterial activities with MIC values of 25 and 50 $\mu$M against Bacillus subtilis and Pseudomonas aeruginosa, and compound 3 showed activities against Staphylococcus aureus and Bacillus subtilis with MIC values of 25 and 50 $\mu$M, respectively.

Keywords

$\alpha$-pyrone; endophytic fungus; Phomopsis sp.; antibacterial activity
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Table S1. $^1$H and $^{13}$C NMR data of 1 (500 and 125 MHz, CDCl$_3$, δ in ppm).

| position | δ$_C$, type | δ$_H$, mult (J in Hz) | HMBC (H→C) |
|----------|-------------|------------------------|-------------|
| 2        | 164.8, C    |                        |             |
| 3        | 104.6, C    |                        |             |
| 4        | 167.1, C    |                        |             |
| 5        | 91.6, CH    | 6.12, s                | 3, 4, 6, 8  |
| 6        | 162.5, C    |                        |             |
| 7        | 54.9, CH$_2$| 4.55, s                | 2, 3, 4     |
| 8        | 127.0, C    |                        |             |
| 9        | 131.6, CH   | 6.73, q (7.2)          | 6, 10, 11   |
| 10       | 14.5, CH$_3$| 1.86, d (7.2)          | 8, 9        |
| 11       | 12.3, CH$_3$| 1.90, s                | 6, 8, 9     |
| 4-OCH$_3$| 56.5, CH$_3$| 3.93, s                | 4           |

Table S2. Antibacterial biological activities of compounds 1–3.

| compounds | antibacterial activity MIC (μM) |
|-----------|---------------------------------|
|           | B. subtilis$^a$ | P. aeruginosa$^b$ | S. aureus$^c$ |
| 1         | >100               | >100               | >100           |
| 2         | 25                 | 50                 | >100           |
| 3         | 50                 | >100               | 25             |
| ciprofloxacin$^d$ | 0.5                 | 0.5               | 0.5            |

$^a$Bacillus subtilis. $^b$Pseudomonas aeruginosa. $^c$Staphylococcus aureus.

$^d$Ciprofloxacin was tested as positive control.
**Figure S1.** Selected HMBC (arrow) correlations of phomopyrone A (1).

![Figure S1](image)

**Figure S2.** $^1$H NMR spectrum of 1 in CDCl$_3$
Figure S3. $^{13}$C NMR spectrum of 1 in CDCl$_3$
**Figure S5.** DEPT-135 spectrum of 1 in CDCl₃

**Figure S6.** HSQC spectrum of 1 in CDCl₃
Figure S7. $^1$H–$^1$H COSY spectrum of 1 in CDCl$_3$

Figure S8. HMBC spectrum of 1 in CDCl$_3$
Figure S9. HREIMS spectrum of 1