Supplementary Material

A mycophenolic acid derivative from the fungus *Penicillium* sp. SCSIO sof101

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Abstract

Mycophenolic acid (MPA) is a group of metabolite derived from several species of *Penicillium*, which shows potent bioactivity. In this study, a new derivative of MPA compound named penicacid D (I), was isolated from the marine derived fungus *Penicillium* sp. SCSIO sof101, along with seven known compounds (2-8). Their structures were elucidated based on the HR-ESI-MS and NMR data. Moreover, the $^1$H and $^{13}$C NMR data of compound 2 and the $^{13}$C NMR data of compound 3 are reported. Compounds 1, 4 and 6 exhibited weak activities against *Escherichia coli* (clinical isolation number 100385570) and *Acinetobacter baumannii* (clinical isolation number 100069).

Keywords: Mycophenolic acid derivative; *Penicillium* sp; antimicrobial
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**Figure S1** Key HMBC correlations of compounds 1 and 2.

![Diagram of compounds 1 and 2 with HMBC correlations]

**Figure S2.** HR-ESI-MS spectrum of compound 1

![HR-ESI-MS spectrum of compound 1]
Figure S3. $^1$H NMR (500 MHz) spectrum of compound 1 in CD$_3$OD

Figure S4. $^{13}$C NMR (125 MHz) spectrum of compound 1 in CD$_3$OD
Figure S5. HMQC spectrum of compound 1 in CD$_3$OD

Figure S6. HMBC spectrum of compound 1 in CD$_3$OD
Table S1 $^1$H-NMR (500 MHz) and $^{13}$C-NMR (125 MHz) spectroscopic data of compounds 1 and 3 in CD$_3$OD.

| position | 1 | 3 |
|----------|---|---|
| n        | $\delta_H$ (multi. $J$ in Hz) | $\delta_C$ | $\delta_H$ (multi. $J$ in Hz) | $\delta_C$ |
| 1        | 169.3 C | 6.49 (s) | 119.2 C | 119.6 C |
| 3        | 99.1 CH | 2.17 (s) | 10.9 CH | 10.9 CH |
| 3a       | 148.1 C | 5.20 (s) | 116.2 C | 116.2 C |
| 4        | 148.1 C | 3.99 (s) | 59.7 CH | 59.7 CH |
| 4-CH$_3$ | 2.17 (s) | 2.06 (s) | 10.1 CH | 10.1 CH |
| 5        | 162.3 C | 119.2 C | 119.2 C | 119.2 C |
| 5-OCH    | 158.7 C | 158.7 C | 158.7 C | 158.7 C |
| 6        | 118.9 C | 118.9 C | 118.9 C | 118.9 C |
| 7        | 158.7 C | 158.7 C | 158.7 C | 158.7 C |
| 7a       | 103.8 C | 103.8 C | 103.8 C | 103.8 C |
| 9        | 88.1 CH | 5.12 (q, 8.5) | 88.2 CH | 88.2 CH |
| 10       | 33.3 CH | 3.27 (dd, 8.5,15.6), 3.62 (dd, 8.5, 15.6) | 32.0 CH | 32.0 CH |
| 11       | 46.6 CH | 2.79 (m) | 2.89 (m) | 2.89 (m) |
| 11-CH    | 13.8 CH | 1.33 (d, 6.9) | 12.6 CH | 12.6 CH |
| 12       | 178.3 C | 178.3 C | 178.0 C | 178.0 C |
| position | $\delta_H$ (multi. $J$ in Hz) | $\delta_C$ |
|----------|------------------|----------|
| 1        |                  | 160.8 C  |
| 1a       |                  | 114.5 C  |
| 2        | 7.24 (s)         | 122.4 CH |
| 3        |                  | 153.4 C  |
| 4        | 7.67 (s)         | 118.3 CH |
| 4a       |                  | 132.2 C  |
| 5        | 7.15 (s)         | 110.6 CH |
| 5a       |                  | 132.3    |
| 6        |                  | 160.8 C  |
| 7        |                  | 107.5 C  |
| 8        |                  | 159.9 C  |
| 8a       |                  | 112.7 C  |
| 9        |                  | 187.8 C  |
| 10       |                  | 181.9 C  |
| 11       | 4.37 (d, 6.0)    | 76.5 CH  |
| 12       | 3.68 (p, 6.0)    | 70.2 CH  |
| 13       | 1.06 (d, 6.0)    | 19.2 CH$_3$ |

**Compound 2.** Red powder; $[\alpha]^{25}_D +170$ (c 0.1, MeOH); UV (MeOH) $\lambda_{\max}$ (log $e$) 221 (3.37), 272 (3.25), 432 (2.95) nm; $^1$H NMR and $^{13}$C NMR spectroscopic data, see Table S2; (-)HR-ESI-MS $m/z$ 363.0285 ([M − H]$, \text{calcd. for C}_{17}\text{H}_{13}\text{O}_7\text{Cl}, 363.0277)$