Supporting Information

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Secondary Metabolites from Marine-Derived Fungus

*Aspergillus carneus* GXIMD00519

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Table S1: Relative free energies\textsuperscript{a} and equilibrium populations\textsuperscript{b} of conformers for (1'S, 4'S, 5'S)-\textbf{1}\\

| conformer | $\Delta G$ | P (%) |
|-----------|-------------|-------|
| 1a        | 0.00        | 100.00|

\textsuperscript{a} B3LYP/6-31G(d), in kcal/mol. \textsuperscript{b} From $\Delta G$ values at 298.15 K. \textsuperscript{c} in MeOH, no imaginary frequency.

Figure S20: The optimized structures (left) and the calculated CD spectra of conformers (1'S 4'S, 5'S)-\textbf{1} in MeOH at M06-2X/def2TZVP level (right). $\sigma$ = 0.22 eV
Table S2: Relative free energies$^a$ and equilibrium populations$^b$ of conformers for (6S)-2$^c$

| conformer | $\Delta G$ (kcal/mol) | P (%) |
|-----------|------------------------|-------|
| 2a        | 0.00                   | 69.13 |
| 2b        | 1.03                   | 11.98 |
| 2c        | 1.15                   | 9.86  |
| 2d        | 1.20                   | 9.03  |

$^a$ B3LYP/6-31G(d), in kcal/mol. $^b$ From $G$ values at 298.15 K. $^c$ in MeOH, no imaginary frequency.
Figure S21: The optimized structures (left) and the calculated CD spectra of conformers (6S)-2 in MeOH at M06-2X/def2TZVP level (right). $\sigma = 0.3$ eV.
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Figure S23: The SciFinder searching results of compound 1
### Table S3: The structural comparison of similar compounds with 1

| No. | Similarity score | Similar chemical structure and CAS number | compound 1 |
|-----|------------------|----------------------------------------|------------|
| 1   | 95               | ![Chemical structure](image1)          | ![Chemical structure](image2) |
|     |                  | CAS NO. 28458-23-3 Absolute stereochemistry |            |
| 2   | 95               | ![Chemical structure](image3)          | ![Chemical structure](image4) |
|     |                  | CAS NO. 93922-50-0 Absolute stereochemistry |            |
| 3   | 95               | ![Chemical structure](image5)          | ![Chemical structure](image6) |
|     |                  | CAS NO. 99528-66-2 Relative stereochemistry |            |
| 4   | 95               | ![Chemical structure](image7)          | ![Chemical structure](image8) |
|     |                  | CAS NO. 99528-67-3 Relative stereochemistry |            |
Figure S24: The Scifinder searching results of compound 2
### Table S4: The structural comparison of similar compounds with 2

| No. | Similarity score | Chemical structure and CAS number | Chemical structure of compound 2 |
|-----|------------------|-----------------------------------|---------------------------------|
| 1   | 91               | ![Chemical structure](image)       | ![Chemical structure](image)    |
|     |                  | CAS NO. 824393-57-9               | Absolute stereochemistry        |
| 2   | 91               | ![Chemical structure](image)       | ![Chemical structure](image)    |
|     |                  | CAS NO. 2165716-67-4              | Absolute stereochemistry        |
| 3   | 91               | ![Chemical structure](image)       | ![Chemical structure](image)    |
|     |                  | CAS NO. 2307909-20-0              | Absolute stereochemistry        |
### Table S5: The NMR data comparison of similar compounds with 1

| Position | Compound 1<sup>a</sup> | nidurufin<sup>a,b</sup> (CAS NO. 28458-23-3) | 2'-epinidurufin<sup>c</sup> (CAS NO. 93922-50-0) |
|----------|------------------------|-----------------------------------------------|-----------------------------------------------|
| 1        | -                      | 158.1 (C)                                      | -                                              |
| 2        | -                      | 116.1 (C)                                      | 159.8 (C)                                      |
| 3        | -                      | 158.7 (C)                                      | 115.0 (C)                                      |
| 4        | 6.85, s                | 107.2 (CH)                                     | 158.4 (C)                                      |
| 4a       | -                      | 133.0 (C)                                      | -                                              |
| 5        | 6.94, d, J = 2.4       | 109.4 (CH)                                     | 134.6 (C)                                      |
| 6        | -                      | 166.2 (C)                                      | -                                              |
| 7        | 6.43, d, J = 2.4       | 107.9 (CH)                                     | 164.2 (C)                                      |
| 8        | -                      | 164.4 (C)                                      | -                                              |
| 8a       | -                      | 108.0 (C)                                      | -                                              |
| 9        | -                      | 188.3 (C)                                      | -                                              |
| 9a       | -                      | 108.4 (C)                                      | -                                              |
| 10       | -                      | 180.6 (C)                                      | -                                              |
| 10a      | -                      | 134.6 (C)                                      | -                                              |
| 1'       | 5.09, d, J = 3.0       | 65.7 (CH)                                      | 133.1 (C)                                      |
| 2'       | 2.32, ddt, J = 17.3, 8.3, 3.8 | 21.9 (CH<sub>2</sub>) | -                                              |
| 3'       | 1.64, d, J = 13.0      | 23.5 (CH<sub>2</sub>)                         | 136. (CH<sub>2</sub>)                          |
| 4'       | 3.55, t, J = 2.8       | 66.7 (CH)                                      | 1.82, m                                        |
| 5'       | -                      | 102.6 (C)                                      | 1.57, m                                        |
| 6'       | 1.49, s                | 24.0 (CH<sub>3</sub>)                         | 101.5 (C)                                      |

<sup>a</sup> in DMSO-<em>d<sub>6</sub></em>.

<sup>b</sup> reference: X. W. Luo, H. M. Lu, X. Q. Chen, X. F. Zhou, C. H. Gao and Y. H. Liu (2020). Secondary metabolites and their biological activities from the sponge derived fungus <em>Aspergillus versicolor</em>, <em>Chem. Nat. Comp.</em> <strong>56</strong>, 716-719.

<sup>c</sup> reference: R. A. Murphy Jr and M. P. Cava (1984). Stereochemistry of nidurufin: synthesis of 6,8-dideoxynidurufin and 6,8-dideoxyepinidurufin, <em>J. Am. Chem. Soc.</em> <strong>106</strong>, 7630-7632.