New Deoxyisoaustamide Derivatives from the Coral-Derived Fungus *Penicillium dimorphosporum* KMM 4689

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Abstract: Seven new deoxyisoaustamide derivatives (1–7) together with known compounds (8–10) were isolated from the coral-derived fungus *Penicillium dimorphosporum* KMM 4689. Their structures were established using spectroscopic methods, X-ray diffraction analysis and by comparison with related known compounds. The absolute configurations of some alkaloids were determined based on CD and NOESY data as well as biogenetic considerations. The cytotoxic and neuroprotective activities of some of the isolated compounds were examined and structure-activity relationships were discussed.

Keywords: *Penicillium dimorphosporum*, secondary metabolites, prenylated indole diketopiperazines, deoxyisoaustamide, neuroprotective activity; paraquat.
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![CD spectrum of 1]

Figure S2. CD spectrum of 2

![CD spectrum of 2]
CD spectrum of 3
Figure S4. CD spectrum of 4

Figure S5. CD spectrum of 5
Figure S6. CD spectrum of 6

Figure S7. CD spectrum of 7
CD spectrum of 8
Figure S9.

CD spectrum of 9
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Figure 71. Viability of human prostate PNT2 cells treated with the investigated compounds for 48 h. No significant cytotoxicity was observed for the concentrations of the drugs up to 100 µM.
Table S1 Selected crystal data and refinement parameters for structure 1.

| Parameter                        | Value                                      |
|----------------------------------|--------------------------------------------|
| Formula weight                   | 395.45                                     |
| Temperature (K)                  | 298(2)                                     |
| Radiation type                   | Mo Kα                                      |
| Space group                      | P2₁2₁2₁                                    |
| Unit cell dimensions (Å)         | a = 7.5507(3), b = 12.1354(6), c = 21.985(1) |
| V (Å³) / Z                       | 2014.5(2), 4                               |
| D calc (g/cm³)                   | 1.304                                      |
| μ, mm⁻¹                          | 0.091                                      |
| F(000)                           | 840                                        |
| Crystal size (mm)                | 0.45 × 0.41 × 0.28                         |
| θ range (°)                      | 1.853 - 32.041                             |
| Range of h, k and l              | -11<=h<=7, -16<=k<=18, -32<=l<=32           |
| Reflections                      | 35597/6978/6055                            |
| measured/ unique / with I>2σ(I)  | Rint = 0.0205                              |
| GooF                             | 1.030                                      |
| Final R indices [I>2sigma(I)]    | R1 = 0.0406, wR2 = 0.1116                  |
| R indices (all data)             | R1 = 0.0484, wR2 = 0.1179                  |
| Δρmin, Δρmax (e/Å³)              | -0.207, 0.208                              |
Table S2 Selected bond lengths (d, Å) in the structures 1.

| Bond                  | Distance (Å) |
|-----------------------|--------------|
| O(1)—C(4)            | 1.224(2)     |
| O(2)—C(9)            | 1.231(2)     |
| O(3)—C(6)            | 1.415(2)     |
| O(4)—C(5)            | 1.402(2)     |
| O(4)—C(22)           | 1.417(2)     |
| N(1)—C(4)            | 1.344(2)     |
| N(1)—C(3)            | 1.437(2)     |
| N(1)—C(10)           | 1.464(2)     |
| N(2)—C(9)            | 1.335(2)     |
| N(2)—C(5)            | 1.456(2)     |
| N(2)—C(8)            | 1.476(2)     |
| N(3)—C(18)           | 1.373(2)     |
| N(3)—C(19)           | 1.379(2)     |
| C(1)—C(2)            | 1.504(3)     |
| C(1)—C(19)           | 1.515(2)     |
| C(1)—C(20)           | 1.534(3)     |
| C(1)—C(21)           | 1.555(3)     |
| C(2)—C(3)            | 1.323(3)     |
| C(4)—C(5)            | 1.525(2)     |
| C(5)—C(6)            | 1.531(2)     |
| C(6)—C(7)            | 1.529(3)     |
| C(7)—C(8)            | 1.535(3)     |
| C(9)—C(10)           | 1.518(2)     |
| C(10)—C(11)          | 1.539(2)     |
| C(11)—C(12)          | 1.491(2)     |
| C(12)—C(19)          | 1.373(2)     |
| C(12)—C(13)          | 1.429(3)     |
| C(13)—C(14)          | 1.405(3)     |
| C(13)—C(18)          | 1.406(3)     |
| C(14)—C(15)          | 1.382(5)     |
| C(15)—C(16)          | 1.387(6)     |
| C(16)—C(17)          | 1.369(5)     |
| C(17)—C(18)          | 1.391(3)     |
Table S3 Hydrogen bonds for structure 1.

| D—H...A               | d(D—H) | d(H...A) | d(D...A) | <(DHA) |
|-----------------------|--------|----------|----------|--------|
| N(3)—H(3A)···O(1)\(^i\) | 0.94(3)| 2.01(3)  | 2.909(2) | 159(2) |
| O(3)—H(3)···O(2)\(^{ii}\) | 0.87(3)| 1.97(3)  | 2.825(2) | 170(3) |

Symmetry transformations used to generate equivalent atoms:
(ii)–x,y–1/2,–z+1/2;(iii) x–1/2,–y+3/2,–z