α-Glucosidase Inhibitors from *Preussia minimoides*

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Abstract:

Extensive fractionation of an extract from the grain-based culture of the endophytic fungus *Preussia minimoides* led to the isolation of two new polyketides with novel skeletons, minimoidiones A (1) and B (2), along with the known compounds preussochromone C (3), corymbiferone (4), and 5-hydroxy-2,7-dimethoxy-8-methylnaphthoquinone (5). The structures of 1 and 2 were elucidated using 1D and 2D NMR data analysis, along with DFT calculations of 1H NMR chemical shifts. The absolute configuration of 1 was established by a single-crystal X-ray diffraction analysis and TDDFT-ECD calculations. Compounds 1–4 significantly inhibited yeast α-glucosidase.

*Preussia minimoides*

**Keywords:** *Preussia minimoides* | polyketides | antidiabetic drugs | diabetes treatment

**Article:**
The genus *Preussia* (Sporormiaceae) comprises species isolated from soil, wood, and plant debris. *Sporormiella* Ellis & Everh. is a similar genus, defined originally to include exclusively coprophilous species. Recent studies have demonstrated no difference between the two genera with respect to their habitat and other diagnostic morphological features. Thus, some authors consider it more appropriate to treat them as synonyms.\(^1\) *Preussia minimoides* (S.I. Ahmed & Cain) Valldos. & Guarro (Sporormiaceae) [Syn: *Sporormiella minimoides* S.I. Ahmed & Cain] is a prolific producer of many interesting polyketides and depsipeptides.\(^3\) Some of these metabolites possess interesting biological activities, including cytotoxicity (brocaenol A),\(^4\) antibacterial and antifungal activities (sporminarins A and B),\(^5\) and calmodulin inhibitory effects (corymbiferone C, corymbiferan lactone E, and 5-hydroxy-2,7-dimethoxy-8-methylnaphthoquinone).\(^6\)

The search for new α-glucosidase inhibitors and other antidiabetic drugs from natural sources has increased notably in recent years, considering that type II diabetes mellitus is one of the most challenging health problems of the 21st century. Therefore, as part of an effort to discover new α-glucosidases inhibitors useful for the development of antidiabetic drugs, we now report the isolation and structure elucidation of two new polyketides with novel skeletons, namely, minimoidiones A (1) and B (2), from an endophytic isolate of the fungus *P. minimoides* obtained from *Hintonia latiflora* (Sessé et Mociño ex DC.) Bullock (Rubiaceae).\(^6\)

### Results and Discussion

The defatted extract from moist rice cultures of *P. minimoides* inhibited the activity of yeast α-glucosidase (αGHY) with an IC\(_{50}\) of 38 μg/mL. Extensive fractionation of this extract yielded two novel polyketides, the benzo[de]anthracenedione 1 and the spiro[naphthalenephenalene]dione 2, which were given the trivial names minimoidiones A and
B, respectively. In addition, the known compounds preussochromone C (3),(7) corymbiferone (4),(8) and 5-hydroxy-2,7-dimethoxy-8-methylnaphthoquinone (5)(6) were isolated. Compound 3 was isolated for the first time from *P. minimoides*, and its NMR data were identical to those previously reported. Compounds 4 and 5 were previously obtained from the same isolate and were characterized by comparison with authentic samples.(6)

Minimoidione A (1) was isolated as yellow crystals. Its molecular formula, C_{21}H_{20}O_{7}, established from HRESIMS data, indicated a structure with 12 degrees of unsaturation. The IR (1651 cm\(^{-1}\)) and UV (maxima at 205, 221, 260, and 301 nm) spectra revealed absorptions indicative of conjugated ketone and aromatic moieties. Analysis of the \(^1\)H and \(^{13}\)C NMR data indicated the presence of 21 carbon atoms consisting of three methoxy groups, one additional methyl, six methines (four in the aromatic-vinylic region and two aliphatic), 11 nonprotonated carbons (two conjugated ketones, eight aromatic or olefinic, and one aliphatic), and two hydroxy groups (Table 1). On the basis of the 1D and 2D NMR data (Figures S4–S7), two partial substructures of 1 (a and b; Figure 1) were elucidated. Rings A and B of substructure a were assigned considering the HMBC correlations from H-2 to C-1/C-3/C-3a and from H-5 to C-3a/C-4/C-6/C-6a; the NOESY cross-peaks between H-2 and 1-OCH\(_3\) and from H-5 to 6-OCH\(_3\); and the presence of a phenolic hydroxy group at \(\delta\)H 13.21 (3-OH), which was chelated with the conjugated ketone group at \(\delta\)C 190.4 (C-4). On the other hand, diagnostic chemical shifts for the presence of a second \(\alpha,\beta\) unsaturated ketone system and the HMBC correlations from H-10 to C-8/C-9/C-11/C-11a, from H-8 to C-7/C-7a/C-9/7a-CH\(_3\), and from H-11a to C-10/C-11/C-11b assembled ring D of substructure b (Figure 1). Consideration of the molecular formula indicated that these partial structures have to be linked to form an additional ring (ring C). HMBC correlations from H-11a (\(\delta\)H 4.28) to C-1 (\(\delta\)C 163.4 in ring A)/C-10 (\(\delta\)C 100.4 at ring D)/C-11 (\(\delta\)C 175.1 at ring D)/C-11b (\(\delta\)C 108.9 at ring A) and from H-7 (\(\delta\)H 6.98, ring C) to C-6a/C-7a/C-8/C-11a (Figure 1) confirmed this tetracyclic system. Altogether, these correlations resulted in the planar structure of compound 1. The NOESY (Figure S6) interactions between 7a-CH\(_3\), H-8, and H-11a indicated that they had the same relative orientation. An X-ray diffraction analysis of 1 with Mo K\(\alpha\) radiation confirmed the proposed structure and the relative configuration at the chiral centers. An ORTEP drawing of the crystallographically determined structure of 1 is depicted in Figure 2.

![Figure 1](image-url)
Figure 2. ORTEP drawing of compound 1.

Table 1. \(^1\)H (500 MHz) and \(^{13}\)C (125 MHz) NMR Data for Compound 1 in CDCl\(_3\)

<table>
<thead>
<tr>
<th>position</th>
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<th>(\delta_H) (in Hz)</th>
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<th>NOESY</th>
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<td>2</td>
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<tr>
<td>3</td>
<td>163.1 C</td>
<td></td>
<td></td>
<td></td>
</tr>
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<td>3a</td>
<td>106.8 C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3a(^1)</td>
<td>130.5 C</td>
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</tr>
<tr>
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<td>190.4 C</td>
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<tr>
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<td>6-OCH(_3)</td>
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<td>6a</td>
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</tr>
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<td>8, 11a</td>
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<td>8-OH</td>
<td>5.30, s</td>
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</table>

The absolute configuration at the stereogenic centers of 1 was deduced by comparison of the experimental and calculated electronic circular dichroism (ECD) spectra of the two possible enantiomers (7a\(^S\),8S,11a\(^S\) and 7a\(^R\),8R,11a\(^R\)), which were calculated using time-dependent
density functional theory (TDDFT). The calculated spectrum for the \(7aS,8S,11aS\) isomer showed good agreement with the experimental data (Figure 3).

![Figure 3](image)

**Figure 3.** Comparison of the experimental ECD spectrum of \(1\) (black) with those calculated at the B3LYP/6-31+G(d) level for enantiomers \(7aS,8S,11aS\) (red) and \(7aR,8R,11aR\) (blue).

Minimoidione B (2) was isolated as an optically inactive orange solid that analyzed for \(C_{26}H_{22}O_8\), which would require 16 double-bond equivalents. The IR spectrum showed characteristic absorptions for aromatic ring (1623 and 1461 cm\(^{-1}\)), hydroxy group (3437 cm\(^{-1}\)), and carbonyl groups (1653 cm\(^{-1}\)). The 1D and 2D NMR data (Table 2) included signals for four methoxy groups, one methylene, six aromatic or olefinic methines, and 16 nonprotonated carbons, including two conjugated ketone carbonyls, 14 aromatic, six of which were oxygenated, and one aliphatic. Finally, two phenolic chelated hydroxy groups were detected (\(\delta_H 13.30\) and 13.14). As in compound \(1\), detailed analysis of the 2D NMR spectra, in particular of the HMBC data, led to partial structures \(c\) and \(d\) indicated in Figure 4. Substructure \(e\) (rings A and B), identical to substructure \(a\) of compound \(1\), was elucidated on the basis of the HMBC cross-peaks from H-8' to C-6'a/C-7'/C-9, from H-5' to C-3'/C-4'/C-6', and from H-2' to C-1/C-3'/C-4'. Furthermore, the NOESY correlations from H-8' to 9'-OCH\(_3\) and H-5' to 4'-OCH\(_3\) and the chelated phenolic hydroxy group at \(\delta_H 13.14\) (7'-OH) completed the assembly. On the other hand, substructure \(d\) (including rings D and E and a methylene functionality) was established considering the following HMBC correlations: from H-6 to C-4a/C-5/C-7/C-8, from H-3 to C-1/C-2/C-4/C-4a, from H-8 to C-1/C-4a/C-7, and from H-1' to C-1/C-2/C-8a. The AB system for two meta-related protons observed in the \(^1\)H NMR between H-6 (\(\delta_H 6.35, d, J = 2.5\) Hz) and H-8 (\(\delta_H 6.24, d, J = 2.5\) Hz) and the NOESY correlations between H-3 and H-6 with the methoxy groups at C-2 and C-7, respectively, further supported substructure \(d\). These partial structures were linked to form an additional ring (ring C), based on the unsaturation count and the HMBC correlations from H-1a' and H-1b' (\(\delta_H 3.39\) and 3.19, dd, \(J = 18\) Hz) to C-2'/C-3a'/C-9'/C-10' (Figure 4). In addition, the correlations from H-1a' and H-1b' to C-1, from H-2' to C-1, from H-3 to C-1, and from H-8 to C-1 indicated that ring C was linked to ring D in a spiro fashion (Figure 4). The only asymmetric center of compound \(2\) was located at C-1, but the lack of optical activity and molecular symmetry indicated that the compound was a racemic mixture. On the basis of the above considerations, the structure of compound \(2\) was fully assembled.
Figure 4. Partial structures c and d and selected HMBC and key NOESY correlations of minimoidione B (2).

Table 2. $^1$H (500 MHz) and $^{13}$C (125 MHz) NMR Data for Compound 2 in CDCl₃

<table>
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<td>4a</td>
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<td>164.6 C</td>
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<tr>
<td>6</td>
<td>99.9 CH</td>
<td>6.35, d (2.5)</td>
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<td>8</td>
<td>106.4 CH</td>
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<td>8a</td>
<td>129.2 C</td>
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<td>7-OCH₃</td>
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<td>2'</td>
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<tr>
<td>4'</td>
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<td>13.14, s</td>
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All attempts to obtain suitable crystals of 2 for X-ray analysis failed. Therefore, in order to provide further evidence for our structural assignment of 2, $^1$H NMR chemical shifts were
calculated and compared with the experimental data according to the protocol of Willoughby and collaborators.\(^{(9)}\) Basically, this protocol involves a conformational search using molecular mechanics, geometry optimization using DFT, and chemical shift calculations using the GIAO method with the B3LYP/6-311+G(2d,p) level of theory. The computed \(^1\)H NMR chemical shifts of compound 2 (Tables S5 and S7) were all within 0.28 ppm of the corresponding experimental values. As can be seen in Tables S5 and S8, the matched mean absolute error was <0.17 ppm.\(^{(9)}\)

Figure 5. Model of binding for compounds 1 (yellow sticks) and the two stereoisomers of 2, \(R\) (cyan sticks) and \(S\) (green sticks), with \(\alpha\)GHY (blue cartoon, pdb 3A4A). The insets show details of the binding mode for 1 (A and E), 2\(R\) (B and F), and 2\(S\) (C and G).

Compounds 1–4 inhibited yeast \(\alpha\)-glucosidase (\(\alpha\)GHY), with IC\(_{50}\)’s ranging from 2.9 to 155 \(\mu\)M (Table S9). Among them, compound 2 showed the strongest effect (IC\(_{50}\) = 2.9 \(\mu\)M). In all cases, the activity was compared to that of an acarbose standard (IC\(_{50}\) = 877 \(\mu\)M). In order to envisage the putative binding mode of compounds 1 and 2 with \(\alpha\)GHY, docking analyses were carried out using the crystallized structure of \(\alpha\)GHY (pdb code 3A4A).\(^{(10, 11)}\) The docking protocol was validated reproducing the binding mode of acarbose at the catalytic domain (Figure S23).\(^{(12, 13)}\) Next, minimiodione A (1) and the \(R\) and \(S\) enantiomers of 2 were docked into the validated \(\alpha\)-glucosidase model. The results predicted that the \(R\) enantiomer of compound 2 binds in a site different from the catalytic domain [binding energy (\(\Delta G\)) = −7.7 kcal/mol]. This site was composed mainly by hydrophobic interactions including Pro488, Asn493, Phe494, Glu497, Phe563, Gly564, Tyr566, and Lys569 and hydrogen bonds between Lys373 and Lys568 (Figure 5C and F). On the other hand, docking of compound 1 and the \(S\) stereoisomer of 2 suggested that
they bind to the catalytic site of αGHY with higher affinities ($\Delta G = -8.5$ and $-10.4$ kcal/mol, respectively). The interactions in this site included hydrophobic contacts with Tyr158, Asp242, Phe314, Arg315, Tyr316, Glu411, and Asn415 and hydrophilic interactions with Ser240, His280, and Gln353 (Figure 5A, E, C, and G).

**Experimental Section**

**General Experimental Procedures**

Melting points were determined on a Fisher-Johns apparatus and are uncorrected. IR, UV, and ECD spectra were obtained on a PerkinElmer 400 FT-IR, a Shimadzu U160, and a JASCO model J720 spectrophotometer, respectively. Optical rotations were recorded at the sodium D-line wavelength using a PerkinElmer model 343 polarimeter at 20 °C. 1D and 2D NMR spectra were recorded on a 400 MHz Bruker Avance III (operating at 400 MHz for $^1$H and 100 MHz for $^{13}$C), a Varian Inova 300 MHz (operating at 300 MHz for $^1$H and 75 MHz for $^{13}$C), or a Varian Unity Inova 500 MHz (operating at 500 MHz for $^1$H and 125 MHz for $^{13}$C) spectrometer; spectra were recorded using CDCl$_3$ and tetramethylsilane as an internal standard. HRESIMS spectra were obtained using a Thermo LTQ Orbitrap XL mass spectrometer.

ESIMS analyses were performed on an SQD2 single-quadrupole mass spectrometer with an electrospray ion source. Data acquisition and processing was accomplished with the MassLynx software version 4.1 (Waters). HPLC was carried out on a Waters system equipped with a 2535 pump and a 2998 photodiode array detector; data acquisition and management of chromatographic output were performed with the Empower 3 software (Waters). Reagent-grade dichloromethane, $n$-hexane, and methanol and HPLC-grade acetonitrile and methanol (J.T. Baker) were regularly used in the extraction and isolation procedures. Silica gel 60 (70–230 mesh, Merck) and Sephadex LH-20 (General Electric) were used for column chromatography (CC). TLC analyses were performed on precoated silica gel 60 F$_{254}$ plates (Merck) using different mobile phases, and visualization of plates was carried out using a 10% Ce(SO$_4$)$_2$ solution in H$_2$SO$_4$ and heating.

**Isolation and Identification of P. minimoides**

The endophytic fungus *P. minimoides* was isolated from selected adult and healthy leaves of *H. latiflora*, collected by Sol Cristians in Huetamo (18°31.709′ N, 101°4.692′ W; 221 masl), State of Michoacan, Mexico, on July 2010. Identification of the plant was secured by the collector; a voucher specimen (131 336) was deposited at the Herbario de la Facultad de Ciencias (FCME), Mexico City, Mexico. The fungus was isolated as previously described.(6) The pure fungal strain was obtained after serial transfers on PDA plates and deposited into the Herbario Nacional de México (MEXU, voucher number 26355). The fungus was identified based on morphological characteristics, such as ascospore morphology.(6) Sequence data [internal transcribed spacer (ITS) and 28S rRNA] were deposited in GenBank as accessions KF557658 and KF557659, respectively. Data available at GenBank aligning with MEXU 26355 suggested this fungus is *P. minimoides*.

**Fermentation, Extraction, and Isolation**
Erlenmeyer flasks with 50 mL of potato-dextrose broth (Difco) sterilized by autoclaving at 121 °C for 15 min were individually inoculated with 1 cm³ agar taken from a stock culture of *P. minimoides* on PDA plates. Cultures grown for 1 week were used to inoculate eight 2.8 L Fernbach flasks containing solid rice medium (200 g of white rice and 400 mL of H₂O). *P. minimoides* was cultured at room temperature for 45 days in static conditions with a 12/12 h daily light–dark period. After incubation, the solid medium was extracted exhaustively with a mixture of CH₂Cl₂–MeOH (8:2) via maceration. The extract was dried over Na₂SO₄ (anhydrous) and concentrated in vacuo to yield 7.3 g of a brownish oily residue. The extract was reconstituted with MeOH–MeCN (1:1) and partitioned with *n*-hexane to yield two primary fractions. The MeOH–MeCN fraction (5.4 g) inhibited the activity of the yeast α-glucosidase with an IC₅₀ of 38 μg/mL, and it was further fractionated via silica gel column chromatography, eluting with a gradient of *n*-hexane–CH₂Cl₂ (100:0 → 0:100) and CH₂Cl₂–MeOH (100:0 → 80:20) to afford nine secondary fractions (F₁–F₉). Fraction F₆ (184.8 mg) was subjected to Sephadex LH-20 CC eluting with CH₂Cl₂–MeOH (8:2) to afford six fractions (F₆₁–F₆₆). Fraction F₆IV (71.5 mg) was further purified by reversed-phase HPLC (Gemini C₁₈, 250 × 21.24 mm, 5 μm, Phenomenex) using as mobile phase 30:70 MeCN–H₂O (acidified with 0.1% formic acid) and increasing linearly to 50% MeCN over 30 min and finally to 100% MeCN for 5 min, at a flow rate of 21.24 mL/min. This process yielded 5.6 mg of 1 as yellow needles. Fraction F₄ (184.8 mg) was first washed with *n*-hexane (80 mL); the resulting residue (107.3 mg) was further purified by reversed-phase HPLC (Gemini C₁₈, 250 × 21.24 mm, 5 μm, Phenomenex) using as mobile phase 60:40 MeCN–H₂O (acidified with 0.1% formic acid) and increasing linearly to MeCN over 15 min, at a flow rate of 21.24 mL/min; this procedure afforded 11.6 mg of 2 as an orange solid and 20.3 mg of 4 as a yellow powder.

Fraction F₉ (425.9 mg) was purified by silica gel chromatography with a gradient of Hex–AcOEt (100:0 → 0:100) and AcOEt–MeOH (100:0 → 70:30) to afford seven fractions (F₉₁–F₉₇). Fraction F₉IV (48.8 g) was further purified by reversed-phase CC (Gemini C₁₈, 250 × 21.24 mm, 5 μm, Phenomenex) using as mobile phase 70:30 MeCN–H₂O (acidified with 0.1% formic acid) and increasing linearly to 50% MeCN over 30 min, at a flow rate of 21.24 mL/min, to obtain 3.2 mg of 3 as a yellow, amorphous solid. Fraction F₂ (68.2 mg) was washed with *n*-hexane (30 mL) and then subjected to Sephadex LH-20 chromatography eluting with CH₂Cl₂–MeOH (8:2) to afford five fractions (F₂₁–F₂₅). From fraction F₂IV spontaneously precipitated 16.3 mg of 5 as an orange powder.

**Minimoidione A (1):**

(C₂₁H₂₀O₇) yellow needles; mp 230–232 °C; [α]²⁰D +27.17 (1 mg/mL, CHCl₃); UV (MeOH, c 1.8) λₑₓ₅ max (log ε) 221 (−3.8), 243 (1.8), 258 (−0.1), 268 (0.3), 316 (−0.6) nm; IR (FTIR) νₑₓ₅ max 3640, 3119, 1670, 1616, 1246 cm⁻¹; ¹H and ¹³C NMR in Table 1; HRESIMS m/z 385.1270 [M + H]⁺, calcd 385.1282.

**Minimoidione B (2):**
(C_{26}H_{22}O_8) orange solid; mp 280–281 °C; [α]_{D}^{20} 0 (1 mg/mL, CHCl_3); IR (FTIR) ν_{max} 3065, 3916, 2956, 1587, 1572, 1229, 1214 cm^{-1}; ^1H and ^13C NMR in Table 2; HRESIMS m/z 463.1375 [M + H]^+, calcd 463.1387.

X-ray Crystal Structure Analysis of Compound 1

Single crystals suitable for X-ray analysis were obtained by recrystallization from CHCl_3–MeOH (8:2). A yellow crystal having approximate dimensions of 0.273 × 0.118 × 0.076 mm was mounted on a glass fiber. All measurements were made on a Bruker Smart Apex CCD diffractometer equipped with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) at 150 K. The structure was solved by the SHELXS-2013 method and refined using full-matrix least-squares on F^2. Suitable crystals of 1 were obtained by evaporation of CH_2Cl_2–MeOH (8:2). Crystallographic data for 1 have been deposited with the Cambridge Crystallographic Data Centre (CCDC) with the accession no. 1475816. These data are available, free of charge, from the CCDC via http://www.ccdc.cam.ac.uk/data_request/cif.

Crystal data for 1:

C_{21}H_{20}O_7, MW 384.37, monoclinic, space group P2_1/n, with unit cell parameters a = 9.1302(13) Å, b = 15.476(2) Å, c = 13.420(2) Å, α = 90°, β = 109.085(3)°, γ = 90°, Z = 4, T = 150(2) K, volume 1792.0(4) Å^3, F(000) 808, density(calcd) 1.425 Mg/m^3. Intensity data were collected in the range of 2.382–25.193° using a ω scan; 10 832 reflections collected, 3193 independent reflections [R(int) = 0.1193] were considered, observed, and used in the calculations. The final R_1 values were 0.0568 [I > 2σ(I)]. The final wR_2(F^2) values were 0.1138 [I > 2σ(I)], with a data–restraints–parameters ratio of 3193/2/263. The final R_1 values were 0.1021 (all data). The final wR_2(F^2) values were 0.1404 (all data).

Computational Section

Minimum energy structures for the different stereoisomers were built with Spartan’08 software (Wavefunction Inc.). Conformational analysis was performed with the Monte Carlo search protocol as implemented in the same software under the MMFF94 molecular mechanics force field. The resulting conformers were minimized using the DFT method at the B3LYP/6-311+G(2d,p) level of theory for NMR chemical shift prediction. NMR shielding tensors were computed with the gauge-independent atomic orbital (GIAO) method and the polarizable continuum model using the integral equation formalism variant (IEFPCM) as the SCRF method.(9) The TDDFT method at the B3LYP/6-31+G(d) level of theory was employed for ECD calculations using the same DFT-minimized conformers. The self-consistent reaction field with conductor-like continuum solvent model was used to perform the ECD calculations of the major conformers of both 1 enantiomers in MeOH. The calculated excitation energy (nm) and rotatory strength (R) in dipole velocity (R_{vel}) and dipole length (R_{len}) forms were simulated into an ECD curve. All calculations were performed employing the Gaussian’09 program package (Gaussian Inc.).

The minimized structures for docking simulations were prepared using Autodock Tools package v1.5.4 (ADT, http://mgltools.scripps.edu/).(14) For metabolites, addition of Gasteiger charges
and number of torsions were set, and nonpolar hydrogens were merged. The crystallographic structure of α-glucosidase from yeast was obtained from the Protein Data Bank (RCSB; pdb code 3A4A). For the receptor all hydrogens (polar and nonpolar) and Kollman charges were added, and solvation parameters were assigned by default.

Molecular docking studies were achieved with AutoDock Vina v1.1.2.(15) First, a blind docking was performed in order to establish the common site of interaction of the metabolites with the α-glucosidase. The search space for this preliminary docking was defined as a box size of 54 × 68 × 68 Å in the x, y, and z dimensions, with a grid spacing of 1.0 Å and the macromolecule set as the center of the box. The default parameters of exhaustiveness and number of modes were not altered. Next, a refined docking was performed with a smaller box of searching space (30 × 25 × 25 Å and 1.0 Å of grid spacing), setting as the center of the grid box the lower state pose obtained from the blind docking. The conformational states from the docking simulations were analyzed using the AutoDockTools program, which also identified the H-bonds and van der Waals interactions between the catalytic site of α-glucosidase and the ligand. The predicted docked complexes (protein–ligand) were those conformations showing the lowest binding energy. The estimated inhibition constant ($K_i$) was calculated from the docking energy displayed by AutoDock Vina following the equation $K_i = \exp(\Delta G \times 1000/RT)$, where $\Delta G$ is the docking energy, $R$ is the universal constant of an ideal gas (1.987 19 cal K$^{-1}$ mol$^{-1}$), and $T$ is the temperature (298.15 K). Preparation of the figures was accomplished with the PyMOL visualization tool (PyMOL Molecular Graphics System, version 1.7.4, Schrödinger, LLC)(16) and LigPlot⁺.(17)

**Assay for α-Glucosidase Inhibitors**

The fungal extract, fractions, compounds, and acarbose (positive control) were dissolved in MeOH. Aliquots of 0–40 μL of testing materials (triplicated) were incubated for 10 min with 20 μL of enzyme stock solution (0.4 units/mL in phosphate buffer solution 100 mM, pH 7). After incubation, 10 μL of substrate (pNPG 5 mM) was added and further incubated for 30 min at 37 °C,(18) and the absorbances were determined. For the extract and fractions, the inhibitory activity was determined as a percentage in comparison to the blank (MeOH) according to the following equation:

$$\% \alpha\text{GHY} = \left(1 - \frac{A_{415t}}{A_{415c}}\right) \times 100\%$$

where % αGHY is the percentage of inhibition, $A_{415t}$ is the corrected absorbance of the extract, fractions, or compound under testing ($A_{415\text{ end}} - A_{415\text{ initial}}$), and $A_{415c}$ is the absorbance of the blank ($A_{415\text{ blank end}} - A_{415\text{ blank initial}}$). The

$$\% \text{Inhibition} = \frac{A_{100}}{1 + \left(\frac{I}{IC_{50}}\right)}$$

IC$_{50}$ was calculated by regression analysis, using the following equation:

where $A_{100}$ is the maximum inhibition, $I$ is the inhibitor concentration, IC$_{50}$ is the concentration required to inhibit activity of the enzyme by 50%, and $s$ is the cooperative degree.(19)

**Supporting Information**

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jnatprod.6b00574.
1D and 2D NMR spectra of compounds 1–5, X-ray crystallographic data of 1, calculated DFT B3LYP/6-31+G(d) free energies, population and theoretical averaged rotatory strength values expressed in \( R_{\text{len}} \) for conformers of 7a\( R \),8\( R \),11a\( R \) and 7a\( S \),8\( S \),11a\( S \) enantiomers of 1, comparison of computed and experimental \(^1\)H NMR data for 1 and 2 (\( S \) and \( R \) enantiomers), and inhibitory effect of 14 evaluated with \( \alpha \)GHY (PDF)

The authors declare no competing financial interest.

‡Taken in part from the Ph.D. thesis of Manuel Rangel-Grimaldo.

Dedicated to Professor Phil Crews, of the University of California, Santa Cruz, for his pioneering work on bioactive natural products.

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References


α-Glucosidase Inhibitors from *Preussia minimoides*‡

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Figure S20. $^{13}$C-NMR spectrum of 5-hydroxy-2,7-dimethoxy-8-methylnaphthoquinone (5) in CDCl$_3$. 
**Preussochromone C (3):** yellow powder; mp: 243-245 °C; $[\alpha]^{25}_D +151$ (1 mg/mL, MeOH); DC (c 0.01 mg/mL, CHCl$_3$) $\lambda_{\text{max}} (\Delta\varepsilon)$ 336 (+2.1), 296 (-0.1), 255 (+6.9); $^1$H-RMN (500 MHz, CDCl$_3$) $\delta_H$ (ppm): 13.15 (1H, s, OH-1), 6.53 (1H, s, H-2), 5.63 (1H, s, H-7), 4.81 (1H, d, $J = 12$ Hz, CH$_2$-10a), 4.21 (1H, d, $J = 12$ Hz, CH$_2$-10b), 3.97 (3H, s, CH$_3$O-12), 3.88 (3H, s, CH$_3$O-11); $^{13}$C-RMN (175 MHz, CDCl$_3$) $\delta_C$ (ppm): 189.1 (C-8), 173.1 (C-6), 166.4 (C-1), 165.4 (C-3), 159.5 (C-9), 145.4 (C-4a), 105.2 (C-8a), 104.7 (C-4), 100.5 (C-7), 100.1 (C-2), 69.5 (C-10), 63.5 (C-5), 56.6 (CH$_3$O-12), 56.3 (CH$_3$O-11); ESIMS m/z 293 [M+H]$^+$.  

**Corymbiferone (4):** yellow powder; mp: 255-257 °C; UV (MeOH) $\lambda_{\text{max}}$: 212, 245, 276, 364 nm; IR (FTIR-ATR) $\nu_{\text{max}}$: 3474, 3074, 2949, 1741, 1647, 1588, 1561, 1381 cm$^{-1}$; $^1$H-RMN (700 MHz, CDCl$_3$) $\delta_H$ (ppm): 14.56 (1H, s, OH-8), 8.25 (1H, s, H-10), 6.57 (1H, s, H-7), 5.92 (1H, s, H-2), 4.06 (3H, s, CH$_3$O-6), 3.96 (3H, s, CH$_3$O-3); $^{13}$C-RMN (175 MHz, CDCl$_3$) $\delta_C$ (ppm): 188.5 (C-1), 170.4 (C-8), 167.5 (C-6), 165.0 (C-3), 156.0 (C-9), 152.1 (C-10), 136.9 (C-4a), 107.9 (C-4), 105.0 (C-8a), 101.3 (C-2), 99.9 (C-7), 99.6 (C-5), 56.9 (CH$_3$O-6), 56.3 (CH$_3$O-3); ESIMS m/z 275 [M+H]$^+$.  

**5-Hydroxy-2,7-dimethoxy-8-methylnaphthoquinone (5):** orange powder; mp: 165–167 °C; UV (MeOH) $\lambda_{\text{max}}$ (log $\varepsilon$): 220 (4.5), 265 (4.1), 297 (4.0) nm; IR (FTIR-ATR) $\nu_{\text{max}}$: 3067, 1678, 1632, 1600, 1434, 1373, 1237 cm$^{-1}$; $^1$H-RMN (500 MHz, CDCl$_3$) $\delta_H$ (ppm): 13.28 (1H, s, OH-5), 6.63 (1H, s, H-6), 6.02 (1H, s, H-3), 3.90 (3H, s, CH$_3$O-7), 3.88 (3H, s, CH$_3$O-2), 2.52 (3H, s, CH$_3$-8); $^{13}$C-RMN (125 MHz, CDCl$_3$) $\delta_C$ (ppm): 189.4 (C-4), 181.2 (C, C-1), 164.2 (C, C-7), 162.8 (C, C-5), 161.0 (C, C-2), 128.8 (C, C-8a), 126.8 (C, C-8), 108.4 (C, C-5a), 108.3 (CH, C-3), 104.2 (CH, C-6), 56.5 (CH$_3$, OCH$_3$-2), 56.2 (CH$_3$, OCH$_3$-7), 12.6 (CH$_3$, C-8); HRESIMS m/z 249.0680 [M+H]$^+$ (calcd for C$_{13}$H$_{12}$O$_5$, 248.0684).
Table S1. Geometry Optimization and $^1$H NMR Single-Point Calculations at DFT B3LYP/6-311+G(2d,p) Level of Theory for Minimoidione A (1).

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| Conformer | Calculated chemical shift ($\delta$) | $\delta_{calcd}$ | $\delta_{exp}$ | $|\delta_{exp}-\delta_{calcd}|$ |
|-----------|-------------------------------------|------------------|----------------|-----------------------------|
| 02        | 26.234 26.234 25.6745 25.6746     | 5.42214727 5.42214727 5.94631816 5.94622447 | 5.42 5.65 0.2277 |
| 04        | 27.491 27.491 27.4635 27.4634    | 4.24451939 4.24451939 4.27028293 4.27037662 | 4.24 4.28 0.0355 |

$^*$Computed with B3LYP/6-311+G(2d,p)//B3LYP/6-311+G(2d,p).
Table S2. Comparison of Computed and Experimental $^1$H NMR Data for 1.

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MAE = $\frac{1}{N} \sum_{i=1}^{N} |\delta_{\text{calc.}} - \delta_{\text{exp.}}|$

Mean absolute error (MAE): 0.158

*Chemical shifts were derived from application of scaling factors (slope = −1.0674, intercept = 32.0216) to the $^1$H NMR shielding tensors computed at the B3LYP/6-311+G(2d,p) level of theory.
Table S3. Calculated DFT B3LYP/6-31+G(d) Free Energies, Population and Theoretical Averaged Rotatory Strength Values Expressed in $R(len)$ for Conformers of 7aS,8S,11aS Enantiomer of 1.

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| 30         | -6.661 | -6.662 | 2.304  | 0.439  | -6.658              | 206.99           

$^a$DFT B3LYP/6-31+G(d) Gibbs free energies in kcal mol$^{-1}$ relative to the absolute G value for the global minimum $-840032.1537$ kcal mol$^{-1}$. $^b$In percent from $\Delta G$ values at 298 K and 1 atm. $^c$DFT B3LYP/6-31+G(d) Rotatory strength values expressed in $R(len)$. $^d$Calculated with the equation $\Sigma iR(len)i \times Pi$, where $R(len)i$ is the theoretical $R(len)$ value calculated for the $n = 1-30$ excitation state and $Pi$ is the population for the $i^{th}$ conformer. $^e$Averaged excitation state.
### Table S4. Calculated DFT B3LYP/6-31+G(d) Free Energies, Population and Theoretical Averaged Rotatory Strength Values Expressed in $R_{\text{len}}$ for Conformers of 7aR,8R,11aR Enantiomer of 1.

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<td>1.450</td>
<td>23.755</td>
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$^a$DFT B3LYP/6-31+G(d) Gibbs free energies in kcal mol$^{-1}$ relative to the absolute G value for the global minimum −840032.1537 kcal mol$^{-1}$. $^b$In percent from $\Delta G$ values at 298 K and 1 atm. $^c$DFT B3LYP/6-31+G(d) Rotatory strength values expressed in $R_{\text{len}}$. $^d$Calculated with the equation $\Sigma_i R(len)_i \times P_i$, where $R(len)_i$ is the theoretical $R_{\text{len}}$ value calculated for the $n = 1$-30 excitation state and $P_i$ is the population for the $i$th conformer. $^e$Averaged excitation state.
**Figure S21.** Calculated ECD at DFT B3LYP/6-31+G(d) theory Level for 7aS,8S,11aS enantiomer of 1.

**Figure S22.** Calculated ECD at DFT B3LYP/6-31+G(d) theory Level for 7aR,8R,11aR enantiomer of 1.
Table S5. Geometry Optimization and $^1$H NMR Single-Point Calculations at DFT B3LYP/6-311+G(2d,p) Level of Theory for R Enantiomer of Minimoidione B (2).

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<th>Energy (kcal/mol)</th>
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Conformers Calculated chemical shift ($\delta$)

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*Computed with B3LYP/6-311+G(2d,p)//B3LYP/6-311+G(2d,p).
Table S6. Comparison of computed and experimental $^1$H NMR data for $R$ enantiomer of 2.

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*Chemical shifts were derived from application of scaling factors (slope = $-1.0674$, intercept = 32.0216) to the $^1$H NMR shielding tensors computed at the B3LYP/6-311+G(2d,p) Level of theory.

Mean absolute error (MAE): 0.166
Table S7. Geometry Optimization and $^1$H NMR Single-Point Calculations at DFT B3LYP/6-311+G(2d,p) Level of Theory for $S$ Enantiomer of Minimoidione B (2).

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<th>Energy (kcal/mol)</th>
<th>∆G (kcal/mol)</th>
<th>Molar Fraction</th>
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</table>

| Conformer | Calculated chemical shift (δ) | $\Delta$calcd* | $\Delta$exp | $|\Delta$exp$-\Delta$calcd$|$ |
|-----------|-------------------------------|-----------------|-------------|--------------------------|
| 01 02 03  |                               |                 |             |                          |
| 25.3816   | 25.3549 25.3816               | 6.22072325      | 6.22072325  | 6.22 6.45 0.2282         |
| 26.1652   | 26.1343 26.1653               | 5.48660296      | 5.48650927  | 5.49 5.75 0.2673         |
| 28.7284   | 28.7055 28.7284               | 3.08525389      | 3.08525389  | 3.09 3.19 0.0103         |
| 25.3947   | 25.293 25.3947                | 6.20845044      | 6.20845044  | 6.21 6.36 0.1484         |
| 26.3886   | 26.389 26.3886                | 5.27730935      | 5.27730935  | 5.28 5.70 0.4255         |
| 17.9758   | 18.302 17.9758                | 13.1588908      | 13.1588908  | 13.16 13.30 0.1397       |
| 28.0592   | 28.0511 28.0592               | 3.71219786      | 3.71219786  | 3.71 3.79 0.0827         |
| 28.0671   | 28.0594 28.0671               | 3.7047967       | 3.7047967   | 3.70 3.79 0.0901         |
| 27.7667   | 27.7495 27.7667               | 3.98622822      | 3.98622822  | 3.99 3.79 0.1913         |
| 28.2354   | 28.2188 28.2354               | 3.54712385      | 3.54712385  | 3.55 3.84 0.2928         |
| 27.8571   | 27.8511 27.8571               | 3.90153644      | 3.90153644  | 3.90 3.84 0.0616         |
| 28.2343   | 28.2188 28.2343               | 3.54815439      | 3.54815439  | 3.55 3.84 0.2917         |
| 28.3916   | 28.3765 28.3916               | 3.40078696      | 3.40078696  | 3.40 3.80 0.4027         |
| 28.4171   | 28.3821 28.4171               | 3.37689713      | 3.37689713  | 3.38 3.80 0.4266         |
| 28.2079   | 28.1835 28.2079               | 3.57288739      | 3.57288739  | 3.57 3.80 0.2306         |
| 27.8766   | 27.9316 27.8766               | 3.88326775      | 3.88326775  | 3.88 3.67 0.2107         |
| 28.1085   | 28.2608 28.1085               | 3.66601087      | 3.66601087  | 3.67 3.67 0.0066         |
| 28.1235   | 28.2259 28.1235               | 3.65195803      | 3.65195803  | 3.65 3.67 0.0206         |

*Computed with B3LYP/6-311+G(2d,p)//B3LYP/6-311+G(2d,p).
Table S8. Comparison of computed and experimental $^1$H NMR data for $S$ enantiomer of 2.

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<td>4'-OCH$_3$</td>
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<tr>
<td>OH-5</td>
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<td>13.16</td>
</tr>
<tr>
<td>OH-7'</td>
<td>13.14</td>
<td>12.92</td>
</tr>
<tr>
<td>MAE</td>
<td></td>
<td>0.169</td>
</tr>
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*Chemical shifts were derived from application of scaling factors (slope = −1.0674, intercept = 32.0216) to the $^1$H NMR shielding tensors computed at the B3LYP/6-311+G(2d,p) Level of theory.

Mean absolute error (MAE): 0.169

$$MAE = |\Delta \delta_{\text{ave}}| = \frac{1}{N} \sum_{i=1}^{N} |\delta_{i}^{\text{comp}} - \delta_{i}^{\text{exp}}|$$
Table S9. Inhibitory Effect and docking binding energies (ΔG) of Compounds 1–4 Tested Against Yeast α-Glucosidase (αGHY)

<table>
<thead>
<tr>
<th>compound</th>
<th>IC$_{50}$ (µM)</th>
<th>ΔG (kcal mol$^{-1}$)</th>
</tr>
</thead>
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<tr>
<td>minimoidione A (1)</td>
<td>95.2 ± 0.8</td>
<td>–8.5</td>
</tr>
<tr>
<td>minimoidione B (2)</td>
<td>2.9 ± 0.47</td>
<td>–7.7 (R)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>–10.3 (S)</td>
</tr>
<tr>
<td>preussochromone C (3)</td>
<td>66.5 ± 0.97</td>
<td>–7.9</td>
</tr>
<tr>
<td>corymbiferone (4)</td>
<td>155.5 ± 4.25</td>
<td>–7.6</td>
</tr>
<tr>
<td>acarbose*</td>
<td>876.9 ± 38.8</td>
<td>–9.9</td>
</tr>
</tbody>
</table>

*Acarbose was used as positive control for αGHY.

Figure S23. 2D Representation of the interactions among αGHY and acarbose in the predicted binding site.
**Table S10.** Crystal Data and Structure Refinement for Minimoidione A (1).

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<td>Empirical formula</td>
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<tr>
<td>Formula weight</td>
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</tr>
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<td>Temperature</td>
<td>150(2) K</td>
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<tr>
<td>Wavelength</td>
<td>0.71073 Å</td>
</tr>
<tr>
<td>Crystal system</td>
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</tr>
<tr>
<td>Space group</td>
<td>P 2/n</td>
</tr>
<tr>
<td>Unit cell dimensions</td>
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</tr>
<tr>
<td></td>
<td>b = 15.476(2) Å, β = 109.085(3)°</td>
</tr>
<tr>
<td></td>
<td>c = 13.420(2) Å, γ = 90°</td>
</tr>
<tr>
<td>Volume</td>
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<tr>
<td>Z</td>
<td>4</td>
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<tr>
<td>Density (calculated)</td>
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<td>Absorption coefficient</td>
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<tr>
<td>F(000)</td>
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</tr>
<tr>
<td>Crystal size</td>
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<tr>
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<tr>
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<td>Reflections collected</td>
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<tr>
<td>Independent reflections</td>
<td>3193 [R(int) = 0.1193]</td>
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<td>Completeness to theta = 25.193°</td>
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<td>Refinement method</td>
<td>Full-matrix least-squares on F²</td>
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<td>Data / restraints / parameters</td>
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<tr>
<td>Goodness-of-fit on F²</td>
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<tr>
<td>R indices (all data)</td>
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<tr>
<td>Largest diff. peak and hole</td>
<td>0.354 and -0.426 e.Å⁻³</td>
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</table>
Atomic coordinates \((\times 10^4)\) and equivalent isotropic displacement parameters \((\text{Å}^2 \times 10^3)\) for preussaminimoidione I (1). U(eq) is defined as one third of the trace of the orthogonalized \(U^i\) tensor.

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Bond lengths [Å] and angles [°] for minimoidione A (1).

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Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for minimoidione A (1). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^* U_{11} + \ldots + 2hk a^* b^* U_{12}]$

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Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\AA^2 \times 10^{-3}$) for minimoidione A (1).

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Hydrogen bonds for minimoidione A (1) [Å and °].

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<th>d(H...A)</th>
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Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+2