Supporting Information to:

New Furanoditerpenoids from *Croton jatrophoides*

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Crystal Structure Determination of Isoteucvin (2)

A crystal with dimensions ca. 0.15 × 0.40 × 0.40 mm was used for data collection. A total of 1713 unique reflections were measured within the range $0 \le h \le 10$, $0 \le k \le 14$, $0 \le l \le 21$. Of these, 1433 were above the significance level of 2.5 $\sigma(I_{obs})$ and were treated as observed. The range of (sin θ) / λ was 0.053–0.626 Å^{-1} ($4.7 \le \theta \le 74.8°$). Two reference reflections [(2 0 0),(1 2 2)] were measured hourly and showed no decrease during the 25-h collecting time. In addition, around 500 “Friedel” reflections were measured, which were used to determine the absolute configuration. Unit-cell parameters were refined by a least-squares fitting procedure using 23 reflections with $40.33 \le \theta \le 43.92°$. Corrections for Lorentz and polarization effects were applied. The structure was solved by the program package CRUNCH [1] and refined with XTAL [2] using scattering factors taken from Cromer and Mann and the International Tables for X-ray Crystallography [3], [4]. Structure validation, including the making of figures and tables, was carried out with PLATON [5]. The hydrogens were kept fixed at calculated positions, each with an isotropic atomic displacement parameter (U = 0.10 Å^2). Anisotropic full-matrix least-squares refinement on F converged to R_F = 0.078, R_{wF} = 0.089, (Δ/σ)max = 0.01, S = 1.04. A weighting scheme $w = [3. + 0.01*(\sigma(\text{Fobs}))^2 + 0.001/(\sigma(\text{Fobs}))]^{-1}$ was used. The secondary isotropic extinction coefficient refined to g = 2291(291) [6], [7]. The absolute-structure Flack parameter refined to Xabs = 0.2, indicating that the correct enantiomer had been refined [8]. However, the large s.u. (= 12) of Xabs implies that the absolute structure is not established unambiguously. A final difference Fourier map revealed a residual electron density between –0.34 and 0.37 eÅ^{-3}. The atom numbering of the refined crystal structure model is shown in **Fig. 1S**. The bond lengths and bond angles are close to values reported in the Cambridge Structural Database [9] for similar types of compounds.

Crystal Structure Determination of Jatrophoidin (3)

A crystal with dimensions ca. 0.20 × 0.30 × 0.75 mm was used for data collection. A total of 2022 unique reflections were measured within the range $0 \le h \le 8$, $0 \le k \le 19$, $-10 \le l \le 10$. Of these, 1884 were above the significance level of 2.5$\sigma(I_{obs})$ and were treated as observed. The range of (sin θ) / λ was 0.058–0.626 Å^{-1} ($5.1 \le \theta \le 74.8°$). Two reference reflections [($\bar{2}$ 0 2), (1 1 2)] were measured hourly and showed no decrease during the 70-h collecting time.

In addition, around 1500 “Friedel” reflections were measured, which were used to determine the absolute configuration. Unit-cell parameters were refined by a least-squares fitting procedure using 23 reflections with $40.00 \leq \theta \leq 50.61°$. Corrections for Lorentz and polarization effects were applied. The structure was solved by the program package CRUNCH [1] and refined with XTAL [2] using scattering factors taken from Cromer and Mann and the International Tables for X-ray Crystallography [3], [4]. Structure validation, including the making of figures and tables, was carried out with PLATON [5].The hydrogens were kept fixed at calculated positions, each with an isotropic atomic displacement parameter ($U = 0.10$ Å^2). Anisotropic full-matrix least-squares refinement on F converged to $R = 0.075$, $R_w = 0.070$, $(\Delta/\sigma)\text{max} = 0.10$, $S = 1.05$. A weighting scheme $w = [0.9 + 0.01*(\sigma(\text{Fobs}))^2 + 0.001/(\sigma(\text{Fobs}))]^{-1}$ was used. The secondary isotropic extinction coefficient refined to $g = 1236(92)$ [6], [7S]. The absolute structure Flack parameter refined to Xabs = –0.2(6), indicating that the correct enantiomer was refined [8]. A final difference Fourier map revealed a residual electron density between –0.23 and 0.28 eÅ^{-3}. The atom numbering of the refined crystal structure model is shown in **Fig. 2S**. The bond lengths and bond angles are close to values reported in the Cambridge Structural Database [9] for similar types of compounds.

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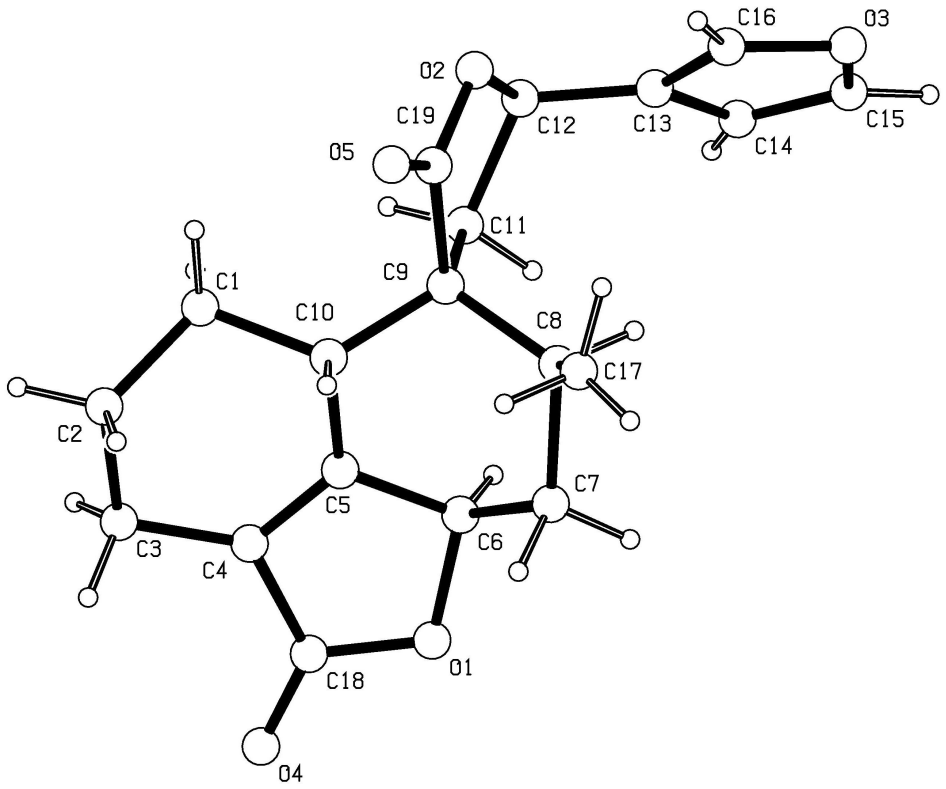

Fig. 1S Isoteucvin (**2**).

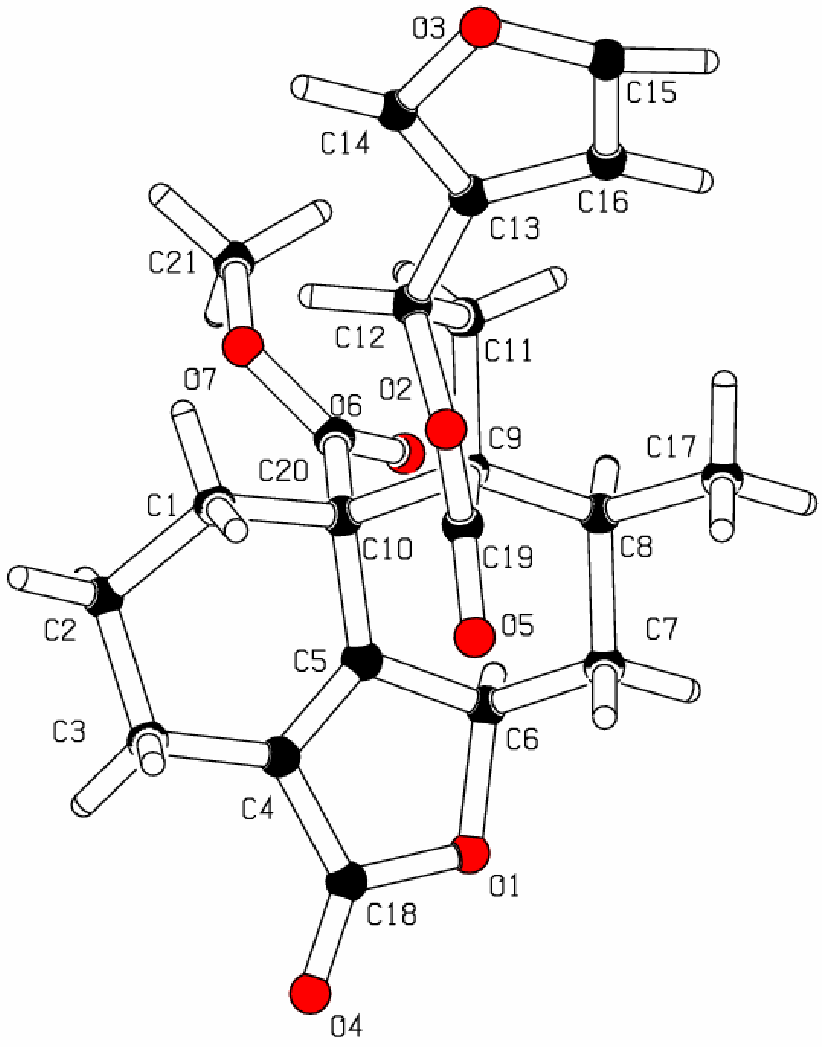

Fig. 2S Jatrophoidin (**3**).