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β-Amyrin benzoate

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.039
wR factor = 0.101
Data-to-parameter ratio = 11.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The crystal structure of the pentacylic triterpenoid β-amyrin benzoate, $C_{37}H_{54}O_2$, is reported at 173 K. Short intramolecular C—H···O contacts are observed.

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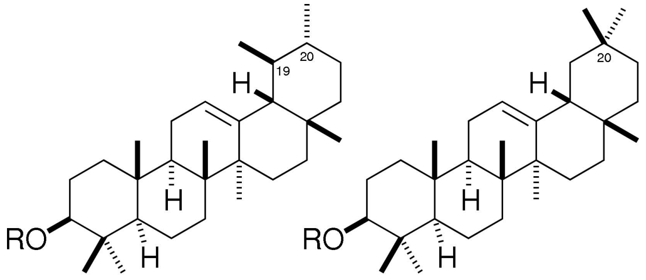
Comment

α-Amyrin, (1a), and β-amyrin, (2a), and their ester derivatives are pentacyclic triterpenoids, often found in equimolar amounts in plants that are ubiquitously distributed in the flora of the world. The two compounds have long been suspected of being responsible for a variety of beneficial effects and have been applied as herbal extracts in indigenous medicine. The investigation of traditional medicines has become increasingly important (Gurib-Fakim, 2006) and recent research has demonstrated that the amyrins (1a) and (2a) demonstrate, amongst others, antibacterial (Prinsloo & Meyer, 2006), antinociceptive (Otuki *et al.*, 2005) and liver-protective properties (Oliveira *et al.*, 2005).



1a R = H
1b R = COPh

2a R = H
2b R = COMe
2c R = COPh

The structures of (1a) and (2a) differ only in the arrangements of the methyl groups on C19 and C20. The X-ray crystal structures of the acetate, (1b), and benzoate, (1c), derivatives of α-amyrin have been reported [Grynpas & Lindley, 1979; refcodes ACAMYA and ACAMYB in the Cambridge Structural Database (CSD, Version 5.28, November 2006 release; Allen, 2002)]. In addition, the structure of β-amyrin acetate, (2b) (Yan *et al.*, 1989; refcode FUGWEJ01), is known. In this paper, we report the structure of β-amyrin benzoate, (2c).

The molecular structure of compound (2c) is shown in Fig. 1. The bond lengths and angles are comparable with values reported in the literature (Allen *et al.*, 1987).

The crystal structure does not contain any intermolecular hydrogen-bonding interactions between neighbouring molecules but does feature short intramolecular C—H···O contacts (Table 1 and Fig. 2) between the H atoms of the C23

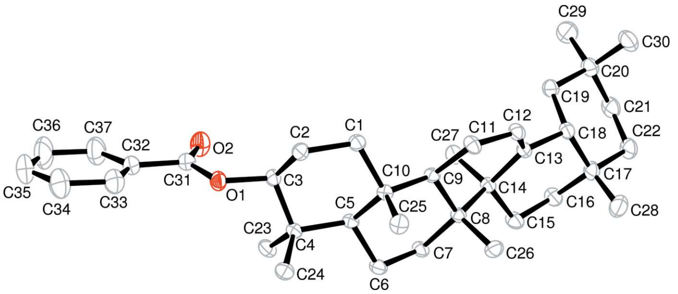


Figure 1
The molecular structure of (2c), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

methyl group and the C3 methine group and the O atoms of the benzoate group.

Although the absolute configuration of (2c) was not determined directly, it was inferred from the compound's occurrence as a natural product belonging to a well defined class of triterpenoids, and by comparison with the reported structure of β-amyrin acetate (Yan *et al.*, 1989).

Experimental

Crystals of (I) were dissolved in chloroform and grown by slow evaporation over a few days. The colourless crystals have a melting point of 507 K (literature value 505–508 K; Domínguez & Torres, 1972).

Crystal data

$C_{37}H_{54}O_2$
$M_r = 530.8$
Orthorhombic, $P2_12_12_1$
$a = 6.7897\ (1)$ Å
$b = 12.0370\ (2)$ Å
$c = 37.8246\ (6)$ Å
$V = 3091.31\ (8)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.07$ mm^{-1}
$T = 173\ (2)$ K
$0.64 \times 0.56 \times 0.16$ mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: integration (*XPREP*; Bruker, 1999)
$T_{\min} = 0.960$, $T_{\max} = 0.989$
45207 measured reflections
4236 independent reflections
3995 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.065$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.101$
$S = 1.06$
4236 reflections
360 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.30$ e Å^{-3}
$\Delta\rho_{\min} = -0.24$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C3—H3$\cdots$O2	1.00	2.26	2.7148 (19)	106
C23—H23$C\cdots$O1	0.98	2.54	2.933 (2)	104

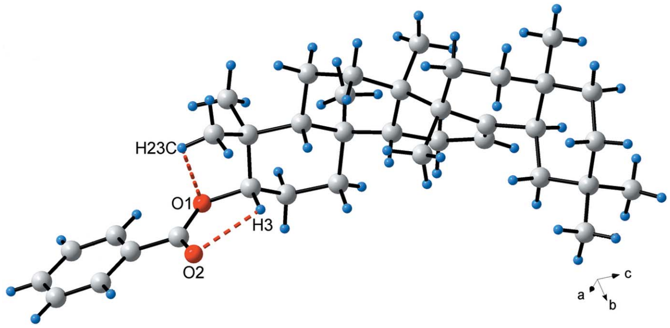


Figure 2
Intramolecular C—H$\cdots$O short contacts, shown as dashed red lines.

H atoms were positioned geometrically and allowed to ride on their respective parent atoms, with C—H bond lengths of 0.95 (acetylenic and aromatic CH), 1.00 (methine CH), 0.99 (methylene CH_2) and 0.98 Å (methyl CH_3), and with $U_{\rm iso}$(H) = 1.2 or 1.5 times $U_{\rm eq}$(C). In the absence of significant anomalous scattering effects, Friedel pairs have been merged.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2003).

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References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Brandenburg, K. (2001). *DIAMOND*. Release 2.1e. Crystal Impact GbR, Bonn, Germany.
Bruker (2004). *SAINT-Plus* (including *XPREP*). Version 7.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2005). *APEX2*. Version 1.0-27. Bruker AXS Inc., Madison, Wisconsin, USA.
Domínguez, X. A. & Torres, M. V. (1972). *Phytochemistry*, **11**, 848.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Grynpas, M. & Lindley, P. F. (1979). *J. Cryst. Mol. Struct.* **9**, 199–217.
Gurib-Fakim, A. (2006). *Mol. Aspects Med.* **27**, 1–93.
Oliveira, F. A., Chaves, M. H., Almeida, F. R. C., Lima, R. C. P. Jr, Silva, R. M., Maia, J. L., Brito, G. A. A. C., Santos, F. A. & Rao, V. S. (2005). *J. Ethnopharmacol.* **98**, 103–108.
Otuki, M. F., Ferreira, J., Lima, F. V., Meyre-Silva, C., Malheiros, A., Muller, L. A., Cani, G. S., Santos, A. R. S., Yunes, R. A. & Calixto, J. B. (2005). *J. Pharmacol. Exp. Ther.* **313**, 310–318.
Prinsloo, G. & Meyer, J. J. M. (2006). *S. Afr. J. Bot.* **72**, 482–483.
Sheldrick, D. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Yan, X.-Z., Kuo, Y.-H., Lee, T.-J., Shih, T.-S., Chen, C.-H., McPhail, D. R., McPhail, A. T. & Lee, K.-H. (1989). *Phytochemistry*, **28**, 1541–1543.

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