Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

6-[(2*E*)-3,7-Dimethylocta-2,6-dien-1-yl]-5,7-dihydroxy-8-(2-methylbutanoyl)-4-phenyl-2*H*-chromen-2-one–6-[(2*E*)-3,7-dimethylocta-2,6-dien-1-yl]-5,7-dihydroxy-8-(3-methylbutanoyl)-4-phenyl-2*H*-chromen-2-one (1/1) from *Mesua elegans*[1]

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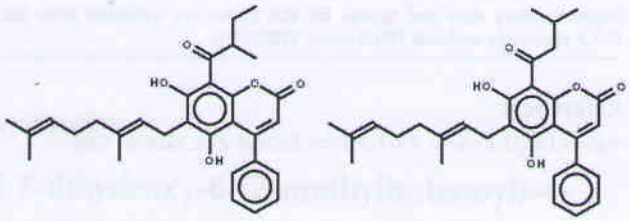
Received 23 February 2012; accepted 27 February 2012

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.066; wR factor = 0.208; data-to-parameter ratio = 14.7.

The title co-crystal, $C_{30}H_{34}O_5{\cdot}C_{30}H_{34}O_5$, comprises a 1:1 mixture of two mostly superimposed molecules with the same chemical formula that differ in the nature of the substituent (2-methylbutanoyl or 3-methylbutanoyl) bound at the exocyclic ketone. The lactone ring is close to planar (r.m.s. deviation = 0.058 Å) and the phenyl ring is twisted out of this plane [dihedral angle = 60.08 (9)°]. The geranyl substituent is almost normal to benzene ring to which it is connected [C—C—C_{ar}—C_{ar} (ar = aromatic) torsion angle = −87.8 (2)°]. Intramolecular O—H···O and O—H···π interactions are formed. In the crystal, supramolecular chains are formed along the a axis owing to C—H···O contacts, with the lactone carbonyl atom accepting two such bonds.

Related literature

For the spectroscopic characterization of the title material, see: Verotta *et al.* (2004) and for its acetylcholinesterase (AChE) inhibitory properties, see: Awang *et al.* (2010).



Experimental

Crystal data

$C_{30}H_{34}O_5{\cdot}C_{30}H_{34}O_5$
M_r = 949.14
Triclinic, $P\overline{1}$
a = 5.9426 (2) Å
b = 13.4688 (5) Å
c = 16.3275 (6) Å
α = 91.955 (3)°
β = 99.515 (3)°
γ = 95.834 (3)°
V = 1280.47 (8) Å^3
Z = 1
Cu $K\alpha$ radiation
μ = 0.66 mm^{-1}
T = 100 K
0.30 × 0.15 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.826, T_{max} = 0.968
25960 measured reflections
5330 independent reflections
4528 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.208
S = 1.01
5330 reflections
363 parameters
54 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

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

*Cg*1 is the centroid of the C10–C15 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4*o*···O5	0.85 (1)	1.54 (4)	2.35 (3)	158 (4)
O4—H4*o*···O5′	0.85 (1)	1.76 (4)	2.55 (3)	154 (3)
O3—H3*o*···*Cg*1	0.84 (2)	2.56 (4)	3.355 (2)	158 (4)
C2—H2···O2^{i}	0.95	2.47	3.408 (2)	169
C15—H15···O2^{ii}	0.95	2.59	3.351 (2)	137

Symmetry codes: (i) $-x+3, -y+1, -z+1$; (ii) $-x+2, -y+1, -z+1$.

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The authors thank the Ministry of Higher Education (Malaysia) for funding structural studies through the High-Impact Research scheme (UM.C/HIR/MOHE/SC/12), Ministry of Science and Technology grant (02–01-01-SF0329) and University of Malaya student's grant (PPP 369/2010B) for the isolation and elucidation of the co-crystal.

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