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Tricoccin R2. Erratum

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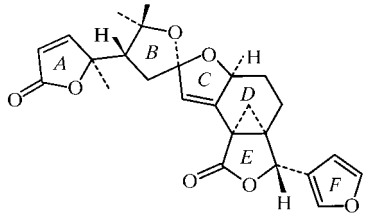
The crystal structure of the title compound, $C_{25}H_{26}O_7$, was published with erroneous positions for a C atom and the O atom in ring *F* [Sekar *et al.* (1996). *Acta Cryst.* (1996), C**52**, 92–94]. This has now been corrected and leads to a more sensible bond length and angle geometry.

Comment

During a comparative study of the molecular structure of Tricoccin R6 (Abdul Ajees *et al.*, 2001) with that of the related compound Tricoccin R2 (Sekar *et al.*, 1996) it was found that



Tricoccin R2

the geometry of the molecules in the two structures agreed well except in the region of ring *F* of Tricoccin R2. This could be traced to a wrong assignment of two of the atoms in ring *F* of Tricoccin R2. That is, the neighbours of atoms C21 and C22 in ring *F* of Tricoccin R2 are to be taken as O and C atoms, respectively, instead of C and O as in the original report. The structure of Tricoccin R2 thus modified was refined and converged to a lower *R* value and the final difference Fourier was better. There is now better agreement of the geometry of ring *F* of Tricoccin R2 with that of Tricoccin R6.

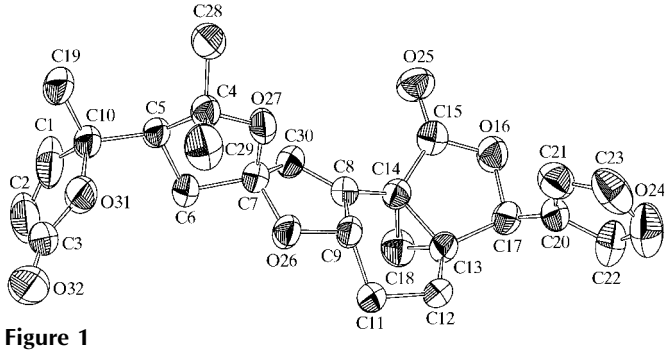


Figure 1
The molecular structure of the title compound with 30% probability displacement ellipsoids

Experimental

Crystal data

$C_{25}H_{26}O_7$
M_r = 438.46
Monoclinic, *C*2
a = 22.939 (1) Å
b = 6.574 (2) Å
c = 16.481 (2) Å
β = 114.67 (1)°
V = 2258.5 (7) Å^3
Z = 4
D_x = 1.289 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 20–30°
μ = 0.78 mm^{-1}
T = 293 (2) K
Needle, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical ψ scan (North *et al.*, 1968)
T_{min} = 0.961, T_{max} = 0.991
2312 measured reflections
2230 independent reflections
2054 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 70.3°
h = −25 → 27
k = 0 → 8
l = −19 → 0
2 standard reflections
frequency: 120 min
intensity decay: <1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.103
S = 1.07
2230 reflections
293 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 0.6138P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0018 (2)
Absolute structure: Flack (1983)
Flack parameter = 0.1 (3)

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *SDP* (Frenz, 1978); data reduction: *CAD*-4 *Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: VJ1131). Services for accessing these data are described at the back of the journal.

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