Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Mycophenolate mofetil

Hemmige S. Yathirajan,[a] Basavegowda Nagaraj,[a] Santhosh L. Gaonkar,[a] Rajenahally S. Narasegowda,[a] Padmarajaiah Nagaraja[a] and Michael Bolte[b]*

[a]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, and [b]Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Marie-Curie-Straße 11, 60439 Frankfurt/Main, Germany

Correspondence e-mail: bolte@chemie.uni-frankfurt.de

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.118
Data-to-parameter ratio = 18.2

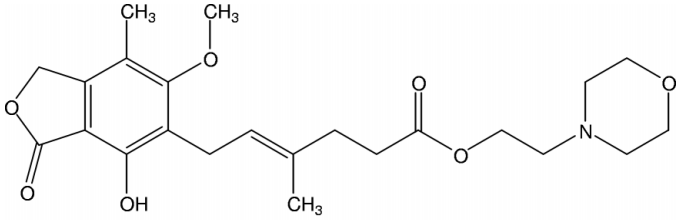
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 25 October 2004
Accepted 27 October 2004
Online 6 November 2004

The title compound, morpholinoethyl (*E*)-6-(1,3-dihydro-4-hydroxy-6-methoxy-7-methyl-3-oxo-2-benzofuran-5-yl)-4-methylhex-4-enoate, $C_{23}H_{31}NO_7$, belongs to the group of immunosuppresant drugs. Its crystal structure is stabilized by O—H···O and C—H···O hydrogen bonds.

Comment

The crystal structure of sodium mycophenolate has been reported by Rihs *et al.* (2000). We report here the crystal structure of morpholinoethyl (*E*)-6-(1,3-dihydro-4-hydroxy-6-methoxy-7-methyl-3-oxo-2-benzofuran-5-yl)-4-methylhex-4-enoate, (I), or mycophenolate mofetil, which is the mofetil ester of myophenolic acid, the active immunosuppresant (Moder, 2003). Mycophenolate mofetil is an active ingredient for immunosuppresant drugs used to prevent the body from rejecting a transplanted organ. Mycophenolate acts by blocking the action of a compound called inosine monophosphate dehydrogenase, which is required for the production of certain blood cells called T- and B-lymphocytes (Allison & Eugui, 1996).



(I)

A perspective view of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 1.6 plus three updates; Mogul Version 1.0; Allen, 2002). The morpholine ring adopts a chair conformation.

Experimental

The title compound was obtained as a gift from Thykn International (India). It was recrystallized from methanol to give colourless plates.

Crystal data

$C_{23}H_{31}NO_7$
M_r = 433.49
Monoclinic, $P2_1/c$
a = 20.784 (2) Å
b = 9.3210 (6) Å
c = 11.9373 (11) Å
β = 106.719 (7)°
V = 2214.8 (3) Å^3
Z = 4
D_x = 1.300 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 20 060 reflections
θ = 3.6–27.2°
μ = 0.10 mm^{-1}
T = 173 (2) K
Plate, colourless
0.42 × 0.36 × 0.22 mm

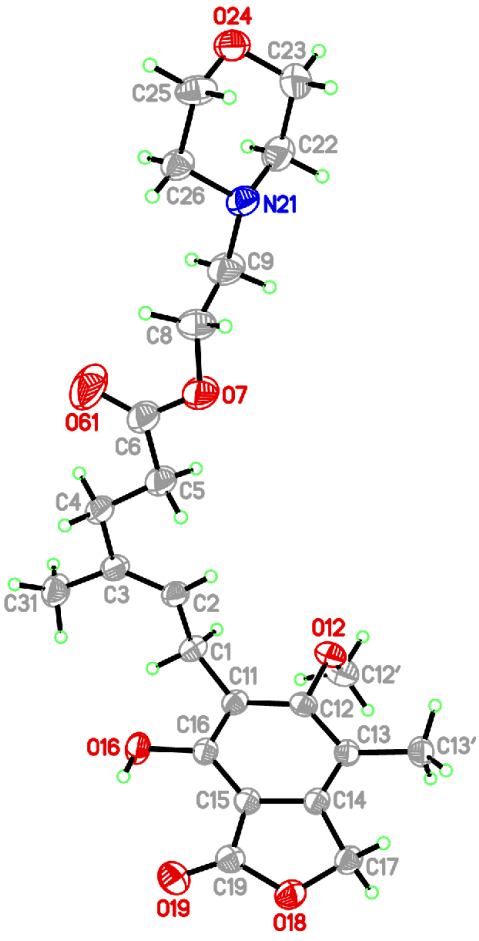


Figure 1
Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: none
30 508 measured reflections
5213 independent reflections
3770 reflections with $I > 2\sigma(I)$
$R_{int} = 0.063$
$\theta_{max} = 27.9°$
$h = -27 \rightarrow 27$
$k = -12 \rightarrow 12$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.118$
$S = 0.97$
5213 reflections
287 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.078P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.77$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O16—H16···O19	0.85 (2)	2.42 (2)	3.0717 (15)	134 (2)
O16—H16···O24^{i}	0.85 (2)	2.07 (2)	2.7664 (15)	139 (2)
C17—H17B···O19^{ii}	0.99	2.37	3.3205 (17)	162
C22—H22B···O61^{iii}	0.99	2.54	3.497 (3)	163

Symmetry codes: (i) $1-x, y-\frac{1}{2}, \frac{3}{2}-z$; (ii) $x, \frac{1}{2}-y, z-\frac{1}{2}$; (iii) $x, \frac{3}{2}-y, z-\frac{1}{2}$.

H atoms bonded to C atoms were refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C)] using a riding model, with C—H = 0.99, 0.98 and 0.95 Å for secondary CH, methyl and aromatic CH, respectively. The methyl groups were allowed to rotate but not to tip. The hydroxyl H atom was refined isotropically.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2003).

One of the authors (HSY) thanks Thykn International (India), Mumbai, for a gift sample of mycophenolate mofetil.

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Allison, A. C. & Eugui, E. M. (1996). *Clin. Transplant*, **10**, 77–84.
Moder, K. G. (2003). *Ann. Allergy Asthma Immunol.* **90**, 15–20.
Rihs, G., Papageorgiou, C. & Pfeffer, S. (2000). *Acta Cryst.* C**56**, 432–433.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1991). *SHELXTL-Plus.* Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.