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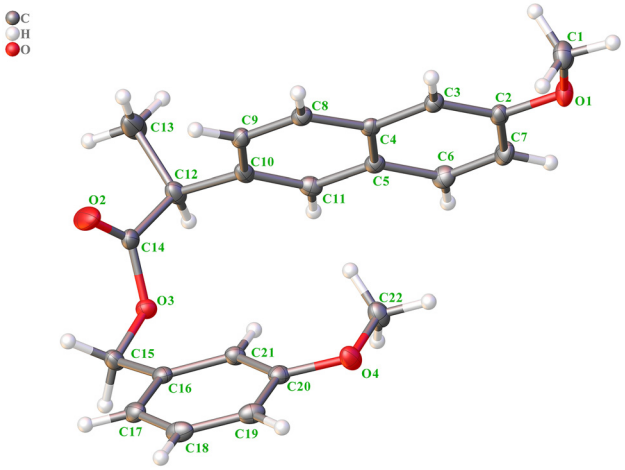
Crystal structure of 3-methoxybenzyl 2-(6-methoxynaphthalen-2-yl)propanoate, $C_{22}H_{22}O_4$



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Abstract

$C_{22}H_{22}O_4$, orthorhombic, $P2_12_12_1$ (no. 19), a = 5.861(2) Å, b = 8.140(2) Å, c = 37.654(8) Å, V = 1796.4(8) Å^3, Z = 4, $R_{gt}(F)$ = 0.0310, w$R_{ref}(F^2)$ = 0.0812, T = 100(2) K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of material

The compound was obtained commerciually (Bide Pharmatech Co., Ltd). Crystals suitable for the diffraction study were taken directly from the provided product.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.12 × 0.11 × 0.10 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.09 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II
θ_{max}, completeness:	27.5°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	61,610, 4,134, 0.032
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 4,042
$N(param)_{refined}$:	238
Programs:	Bruker[1], Olex2[2], SHELX[3]

2 Experimental details

Coordinates of hydrogen atoms were refined with constraints or restraints. The U_{iso} values were set to be 1.5U_{eq} of the carrier atom for methyl H atoms and 1.2U_{eq} for the remaining H atoms.

3 Comment

Naproxen is one of the most widely prescribed drugs for the treatment and management of inflammatory diseases. Long term use of naproxen can cause serious adverse reactions, such as erosion, narrowing, bleeding, and perforation in the gastrointestinal tract. The pharmacological effects of naproxen are related to the inhibition of COX-1 and COX-2 enzymes. However, due to poor selectivity, Naproxen is associated with severe gastrointestinal toxicity. Naproxen contains a free carboxyl group, which, when ionized, leads to an increase in acidity, a decrease in gastric pH, and complicates the problem.[4,5] Research has shown that using naproxen as a prodrug for esterification can reduce the gastrointestinal side effects of naproxen and improve its bioavailability.[6]

The title compound contains one naphthyl ring and two phenyl rings. The bond distances of C–O are 1.344(2) Å (C14–O3), 1.445(2) Å (C15–O3), 1.3744(19) Å (C20–O4), 1.428(2) Å (C22–O4), 1.3732(19) Å (C2–O1), 1.434(2) Å (C1–O1) and 1.205(2) Å (C14–O2). The bond distance of C14–O2 is shorter than others, indicating a double bond. The dihedral angels of ring 1 (C2–C3–C4–C5–C6–C7) and ring 2 (C4–C5–C8–C9–C10–C11), ring 1 (C2–C3–C4–C5–C6–C7) and ring 3 (C16–C17–C18–C19–C20–C21), ring 2 (C4–C5–C8–C9–C10–C11) and ring 3 (C16–C17–C18–C19–C20–C21) are 1.831(46)°, 57.895(47)°, and 56.358(49)°. The other bond distances and

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5864(3)	−0.0976(2)	0.49904(5)	0.0245(4)
H1A	0.582114	−0.145171	0.475142	0.037*
H1B	0.452688	−0.027139	0.502518	0.037*
H1C	0.585360	−0.185927	0.516717	0.037*
C2	0.8219(3)	0.0748(2)	0.53518(4)	0.0162(3)
C3	0.6778(3)	0.06430(19)	0.56386(4)	0.0148(3)
H3	0.541212	0.001838	0.562308	0.018*
C4	0.7343(3)	0.14778(19)	0.59602(4)	0.0138(3)
C5	0.9403(3)	0.24011(19)	0.59836(4)	0.0150(3)
C6	1.0815(3)	0.2508(2)	0.56770(4)	0.0190(3)
H6	1.217483	0.314217	0.568584	0.023*
C7	1.0243(3)	0.1709(2)	0.53694(4)	0.0196(3)
H7	1.120161	0.179757	0.516690	0.024*
C8	0.5889(3)	0.14127(19)	0.62625(4)	0.0156(3)
H8	0.448394	0.083386	0.624889	0.019*
C9	0.6494(3)	0.21786(19)	0.65743(4)	0.0168(3)
H9	0.550393	0.211503	0.677353	0.020*
C10	0.8579(3)	0.30641(19)	0.66034(4)	0.0163(3)
C11	0.9974(3)	0.3188(2)	0.63100(4)	0.0170(3)
H11	1.134230	0.381001	0.632551	0.020*
C12	0.9288(3)	0.3818(2)	0.69595(4)	0.0204(3)
H12	1.070205	0.448389	0.692311	0.024*
C13	0.9769(4)	0.2499(2)	0.72396(5)	0.0329(5)
H13A	1.012855	0.302675	0.746674	0.049*
H13B	1.106681	0.182618	0.716351	0.049*
H13C	0.842018	0.179959	0.726786	0.049*
C14	0.7384(3)	0.4949(2)	0.70842(4)	0.0177(3)
C15	0.5962(3)	0.7671(2)	0.70207(4)	0.0194(3)
H15A	0.664970	0.876854	0.705798	0.023*
H15B	0.510153	0.737656	0.723773	0.023*
C16	0.4346(3)	0.77421(19)	0.67091(4)	0.0157(3)
C17	0.2289(3)	0.8582(2)	0.67466(4)	0.0194(3)
H17	0.186647	0.902405	0.697066	0.023*
C18	0.0851(3)	0.8771(2)	0.64541(5)	0.0213(3)
H18	−0.054089	0.935725	0.647957	0.026*
C19	0.1429(3)	0.8113(2)	0.61267(5)	0.0192(3)
H19	0.044814	0.825600	0.592830	0.023*
C20	0.3469(3)	0.72360(19)	0.60906(4)	0.0166(3)
C21	0.4947(3)	0.70536(19)	0.63801(4)	0.0152(3)
H21	0.634077	0.647031	0.635428	0.018*
C22	0.5898(3)	0.5612(2)	0.57222(4)	0.0217(3)
H22A	0.593863	0.513450	0.548334	0.032*
H22B	0.586617	0.472960	0.589909	0.032*
H22C	0.725759	0.629186	0.575883	0.032*
O1	0.7901(2)	−0.00167(16)	0.50305(3)	0.0206(3)
O2	0.5752(3)	0.45553(16)	0.72590(4)	0.0342(3)
O3	0.7753(2)	0.64799(13)	0.69633(3)	0.0166(2)
O4	0.3901(2)	0.66046(15)	0.57589(3)	0.0209(3)

angles are in their normal ranges according to the previously reported compounds.[7–11]

Author contribution: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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