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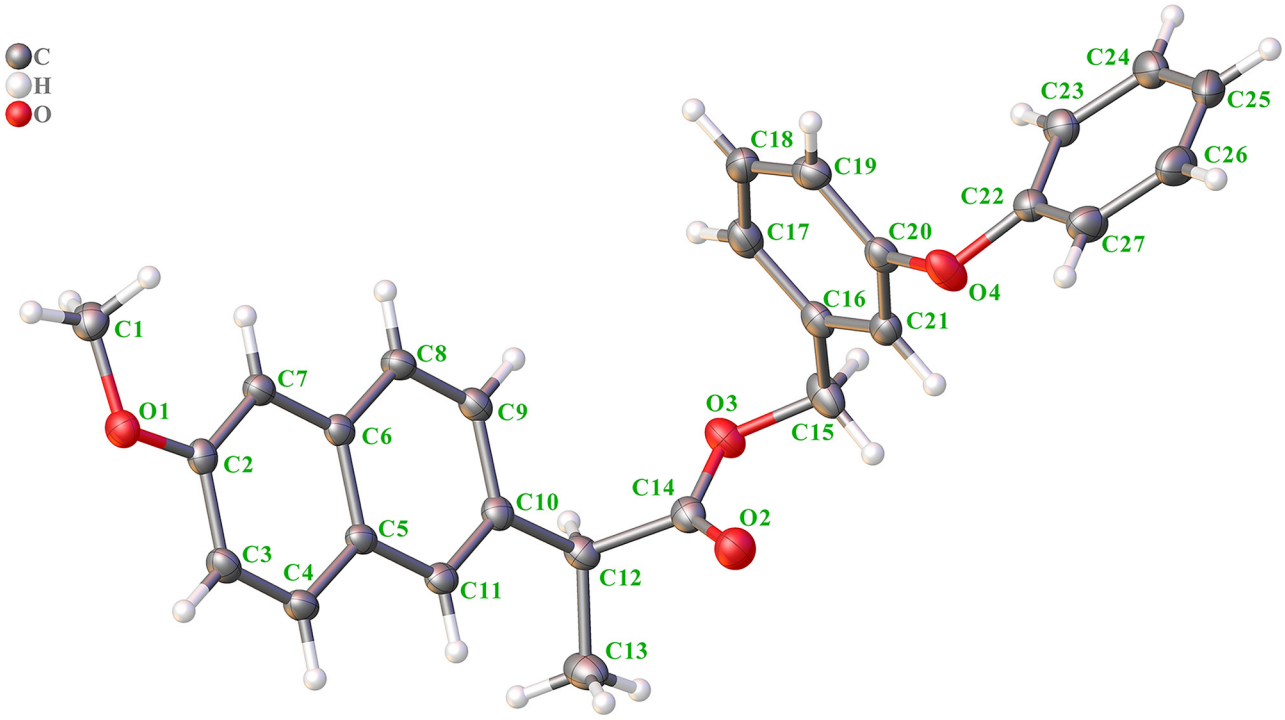
Crystal structure of 3-phenoxybenzyl 2-(6-methoxynaphthalen-2-yl)propanoate, $C_{27}H_{24}O_4$



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Abstract

$C_{27}H_{24}O_4$, orthorhombic, $P2_12_12_1$ (no. 19), a = 5.694(2) Å, b = 8.957(2) Å, c = 40.662(8) Å, V = 2073.7(10) Å^3, Z = 4, $R_{gt}(F)$ = 0.0339, $wR_{ref}(F^2)$ = 0.0837, 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.

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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:	27.6°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	77,707, 4,782, 0.044
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 4,511
$N(param)_{refined}$:	282
Programs:	Bruker,[1] Olex2,[2] SHELX[3]

1 Source of material

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

2 Experimental details

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.

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3419 (4)	0.2429 (2)	0.42314 (5)	0.0259 (4)
H1A	0.333227	0.200562	0.400950	0.039*
H1B	0.208511	0.310213	0.426653	0.039*
H1C	0.337000	0.162192	0.439386	0.039*
C2	0.5937 (3)	0.3956 (2)	0.45578 (4)	0.0197 (4)
C3	0.8002 (3)	0.4835 (2)	0.45642 (5)	0.0226 (4)
H3	0.898282	0.487481	0.437540	0.027*
C4	0.8601 (3)	0.5626 (2)	0.48389 (5)	0.0221 (4)
H4	0.999911	0.620449	0.483980	0.027*
C5	0.7154 (3)	0.5591 (2)	0.51228 (4)	0.0186 (4)
C6	0.5089 (3)	0.4715 (2)	0.51149 (4)	0.0186 (4)
C7	0.4495 (3)	0.3887 (2)	0.48284 (4)	0.0202 (4)
H7	0.311503	0.329094	0.482408	0.024*
C8	0.3634 (3)	0.4704 (2)	0.53975 (4)	0.0214 (4)
H8	0.223768	0.412332	0.539725	0.026*
C9	0.4210 (3)	0.5518 (2)	0.56712 (5)	0.0217 (4)
H9	0.320267	0.549578	0.585741	0.026*
C10	0.6279 (3)	0.6389 (2)	0.56811 (4)	0.0201 (4)
C11	0.7723 (3)	0.6413 (2)	0.54099 (5)	0.0202 (4)
H11	0.912300	0.698994	0.541506	0.024*
C12	0.6791 (4)	0.7285 (2)	0.59894 (5)	0.0221 (4)
H12	0.532818	0.783525	0.605143	0.026*
C13	0.8760 (4)	0.8418 (2)	0.59540 (5)	0.0310 (5)
H13A	1.023832	0.789722	0.590873	0.046*
H13B	0.891053	0.899026	0.615845	0.046*
H13C	0.840151	0.909900	0.577213	0.046*
C14	0.7399 (4)	0.6227 (2)	0.62686 (5)	0.0221 (4)
C15	0.6038 (5)	0.5132 (2)	0.67605 (5)	0.0310 (5)
H15A	0.495493	0.539489	0.694192	0.037*
H15B	0.766430	0.526899	0.684122	0.037*
C16	0.5682 (4)	0.3523 (2)	0.66699 (4)	0.0230 (4)
C17	0.3650 (4)	0.3065 (2)	0.65077 (5)	0.0270 (4)
H17	0.251304	0.378094	0.644194	0.032*
C18	0.3288 (4)	0.1562 (2)	0.64422 (5)	0.0270 (4)
H18	0.190007	0.125571	0.633145	0.032*
C19	0.4925 (4)	0.0504 (2)	0.65362 (5)	0.0254 (4)
H19	0.466270	−0.052555	0.649392	0.030*
C20	0.6951 (3)	0.0972 (2)	0.66929 (5)	0.0228 (4)
C21	0.7349 (3)	0.2462 (2)	0.67600 (5)	0.0221 (4)
H21	0.875500	0.276207	0.686711	0.027*
C22	0.8447 (3)	−0.1035 (2)	0.70209 (5)	0.0222 (4)
C23	0.6538 (4)	−0.1040 (2)	0.72307 (5)	0.0251 (4)
H23	0.527679	−0.036119	0.719795	0.030*
C24	0.6485 (4)	−0.2050 (3)	0.74902 (5)	0.0300 (5)
H24	0.517825	−0.205845	0.763543	0.036*
C25	0.8307 (4)	−0.3039 (3)	0.75395 (5)	0.0341 (5)
H25	0.826271	−0.372042	0.771846	0.041*
C26	1.0196 (4)	−0.3031 (3)	0.73266 (6)	0.0355 (5)
H26	1.145195	−0.371305	0.735958	0.043*
C27	1.0277 (4)	−0.2041 (2)	0.70656 (6)	0.0295 (5)
H27	1.157241	−0.204853	0.691838	0.035*
O1	0.5563 (3)	0.32440 (15)	0.42667 (3)	0.0234 (3)
O2	0.9227 (3)	0.55552 (17)	0.62968 (4)	0.0303 (3)
O3	0.5634 (3)	0.61321 (16)	0.64868 (3)	0.0277 (3)
O4	0.8732 (3)	−0.00454 (17)	0.67654 (4)	0.0297 (3)

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. In addition, 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] In this study, we prepared a new prodrug of naproxen that masked the free carboxylic acid groups of naproxen, thereby reducing related side effects.

The title compound contains one naphthyl ring and two phenyl rings. The bond distances of C–O are 1.429(2) Å (C1–O1), 1.361(2) Å (C2–O1), 1.207(3) Å (C14–O2), 1.343(2) Å (C14–O3),1.447(2) Å (C15–O3), 1.395(2) Å (C20–O4) and 1.375(2) Å (C22– O4). The bond distance of C14–O2 are shorter than others, indicating a double bond. The dihedral angels of ring 1 (C2–C3–C4–C5–C6–C7) and ring 2 (C5–C6–C8–C9–C10–C11), ring 1 (C2–C3–C4–C5–C6–C7) and ring 3 (C16–C17–C18–C19–C20–C21), ring 1 (C2–C3–C4–C5–C6–C7) and ring 4 (C22–C23–C24–C25–C26–C27), ring 2 (C5–C6–C8–C9–C10–C11) and ring 3 (C16–C17–C18–C19–C20–C21), ring 2 (C5–C6–C8–C9–C10–C11) and ring 4 (C22–C23–C24–C25–C26–C27), and ring 3 (C16–C17–C18–C19–C20–C21) and ring 4 (C22–C23–C24–C25–C26–C27) are 0.99(6)°, 81.35(6)°, 85.27(6)°, 80.37(6)°, 85.61(6)°, and 76.46(6)°. The other bond distances and angles are in their normal ranges.[7,8]

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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