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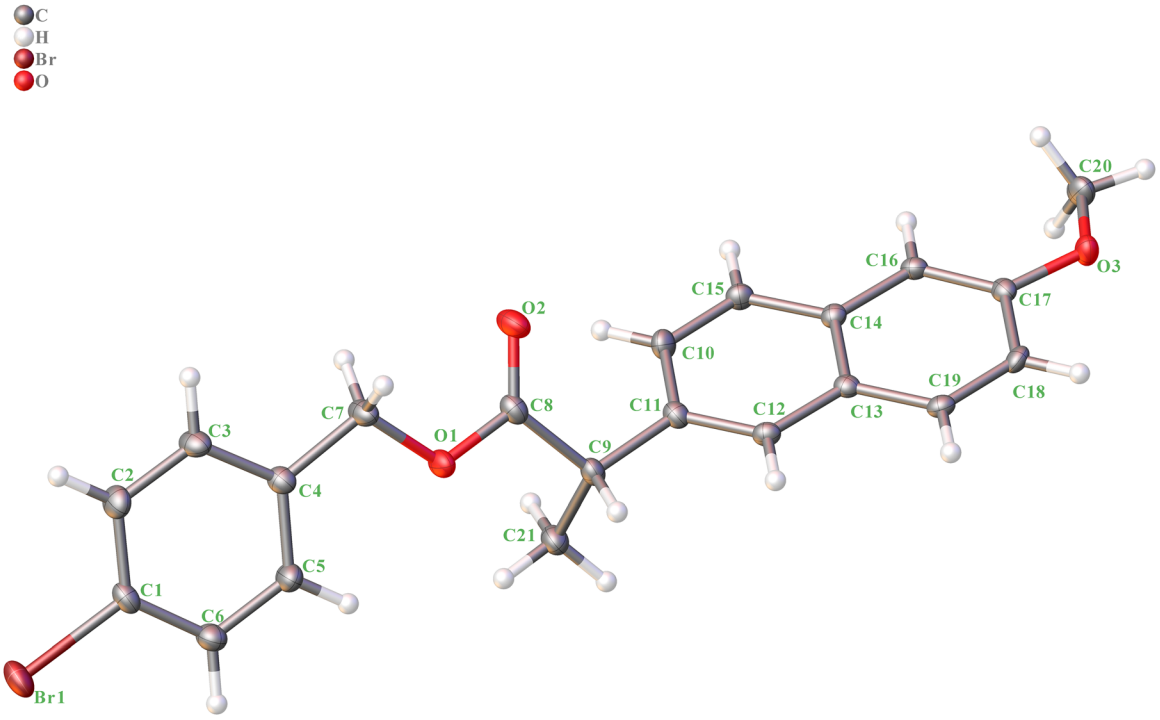
Crystal structure of 4-bromobenzyl 2-(6-methoxy-naphthalen-2-yl)propanoate, $C_{21}H_{19}BrO_3$



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Abstract

$C_{21}H_{19}BrO_3$, orthorhombic, $P2_12_12_1$ (no. 19), a = 6.011(2) Å, b = 11.630(2) Å, c = 25.165(5) Å, V = 1759.3(7) Å^3, Z = 4, $R_{gt}(F)$ = 0.0163, $wR_{ref}(F^2)$ = 0.0420, T = 100(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.12 × 0.11 × 0.10 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	2.35 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II
θ_{max}, completeness:	27.5°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	84,060, 4,020, 0.037
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3,879
$N(param)_{refined}$:	228
Programs:	Bruker,[1] Olex2,[2] SHELX[3]

1 Source of materials

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

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.08234 (3)	−0.15505 (2)	0.74872 (2)	0.02566 (6)
C1	0.2394 (3)	−0.04140 (16)	0.70911 (7)	0.0182 (3)
C2	0.4405 (3)	−0.06943 (16)	0.68613 (8)	0.0210 (4)
H2	0.498387	−0.145251	0.688661	0.025*
C3	0.5568 (3)	0.01614 (16)	0.65912 (8)	0.0203 (4)
H3	0.695523	−0.001965	0.643087	0.024*
C4	0.4741 (3)	0.12762 (15)	0.65511 (7)	0.0167 (4)
C5	0.2693 (3)	0.15291 (16)	0.67810 (7)	0.0199 (3)
H5	0.209888	0.228343	0.675178	0.024*
C6	0.1503 (3)	0.06836 (17)	0.70544 (8)	0.0202 (4)
H6	0.010827	0.085738	0.721251	0.024*
C7	0.6089 (3)	0.21588 (16)	0.62514 (8)	0.0203 (4)
H7A	0.762476	0.218253	0.639308	0.024*
H7B	0.616282	0.194859	0.587061	0.024*
C8	0.6281 (3)	0.41768 (16)	0.61422 (7)	0.0174 (4)
C9	0.4976 (3)	0.52931 (15)	0.62140 (7)	0.0160 (3)
H9	0.362205	0.523626	0.598465	0.019*
C10	0.8387 (3)	0.66093 (16)	0.62498 (7)	0.0171 (3)
H10	0.904670	0.609787	0.649839	0.021*
C11	0.6264 (3)	0.63434 (15)	0.60312 (7)	0.0156 (3)
C12	0.5334 (3)	0.70879 (15)	0.56694 (7)	0.0142 (3)
H12	0.392398	0.691113	0.552002	0.017*
C13	0.6437 (3)	0.81172 (15)	0.55137 (7)	0.0132 (3)
C14	0.8556 (3)	0.83769 (15)	0.57347 (6)	0.0133 (3)
C15	0.9494 (3)	0.75952 (15)	0.61064 (7)	0.0155 (3)
H15	1.090752	0.775661	0.625788	0.019*
C16	0.9659 (3)	0.94206 (15)	0.55873 (7)	0.0138 (3)
H16	1.106488	0.960738	0.573638	0.017*
C17	0.8666 (3)	1.01518 (15)	0.52280 (7)	0.0143 (3)
C18	0.6562 (3)	0.98877 (15)	0.50027 (7)	0.0152 (3)
H18	0.590593	1.039986	0.475384	0.018*
C19	0.5473 (3)	0.88988 (15)	0.51424 (7)	0.0142 (3)
H19	0.406282	0.873161	0.499054	0.017*
C20	1.1470 (3)	1.15938 (17)	0.53247 (8)	0.0209 (4)
H20A	1.189780	1.234095	0.517645	0.031*
H20B	1.269563	1.104703	0.527902	0.031*
H20C	1.113889	1.168001	0.570394	0.031*
C21	0.4167 (3)	0.54378 (16)	0.67891 (7)	0.0207 (4)
H21A	0.326793	0.477016	0.689058	0.031*
H21B	0.326442	0.613693	0.681681	0.031*
H21C	0.545311	0.549880	0.702678	0.031*
O1	0.5056 (2)	0.32711 (11)	0.63099 (5)	0.0200 (3)
O2	0.8126 (2)	0.40755 (12)	0.59612 (6)	0.0247 (3)
O3	0.9537 (2)	1.11748 (11)	0.50539 (5)	0.0187 (3)

2 Experimental details

Coordinates of hydrogen atoms were refined without any 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, a potent non-steroidal anti-inflammatory drug (NSAID), blocks the activity of both COX-1 and COX-2 enzymes, which are key components of the cyclooxygenase pathway. Naproxen commonly causes gastrointestinal reactions, such as gastrointestinal bleeding.[1] These side effects may be linked to the carboxyl group present in naproxen. Esterifying the carboxyl group has been shown to reduce these side effects. Esterifying the carboxyl group has been shown to reduce these side effects.[2,3] Currently, naproxen is used clinically to treat or alleviate inflammation and pain caused by various conditions such as rheumatoid arthritis[4] and gout.[5] Additionally, naproxen has been found to exhibit anticancer activity against bladder [6] and prostate cancer.[7] Furthermore, studies have shown that naproxen acts against type A influenza viruses by binding to the viral nucleoprotein.[8] Therefore, the development of naproxen derivatives with fewer side effects is of significant importance.

The title compound contains one naphthyl ring and one phenyl ring. The bond distances of C–O are 1.372(2) Å (C17–O3), 1.433(2) Å (C20–O3), 1.353(2) Å (C8–O1), 1.442(2) Å (C7–O1) and 1.205(2) Å (C8–O2). The bond distance of C8–O2 are shorter than others, indicating a double bond. The bond of C–Br is 1.9057(19) Å (C1–Br1). The dihedral angels of ring 1 (C1–C2–C3–C4–C5–C6) and ring 2 (C10–C11–C12–C13–C14–C15), ring 1 (C1–C2–C3–C4–C5–C6) and ring 3 (C13–C14–C16–C17–C18–C19), and ring 2 (C10–C11–C12–C13–C14–C15) and ring 3 (C13–C14–C16–C17–C18–C19) are 56.58(5)°, 56.71(5)° and 0.78(5)°. The other bond distances and angles are in their normal ranges according to the previously reported compounds.[9–12]

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.
Competing interests: The authors declare no conflicts of interest regarding this article.

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