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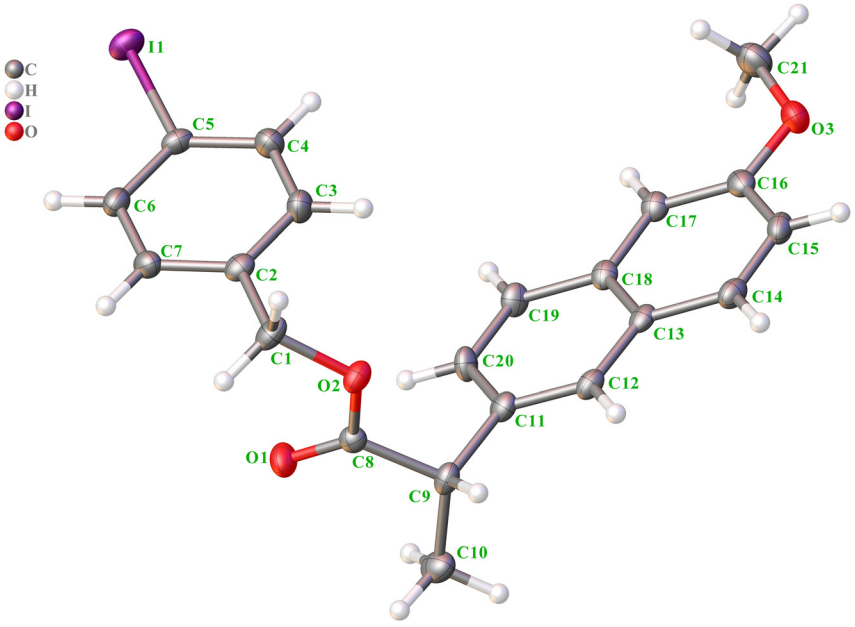
Crystal structure of 4-iodobenzyl 2-(6-methoxynaphthalen-2-yl) propanoate, $C_{21}H_{19}IO_3$



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Abstract

$C_{21}H_{19}IO_3$, monoclinic, $P2_1$ (no. 4), a = 11.8252 (4) Å, b = 5.4966 (2) Å, c = 14.9468 (5) Å, β = 106.888 (1)°, V = 929.62 (6) Å^3, Z = 2, $R_{gt}(F)$ = 0.0134, $wR_{ref}(F^2)$ = 0.0319, 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 the material

The compound was obtained commercially (Bide Pharmatech Co., Ltd). Its single crystals were obtained from tetrahydrofuran.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.15 × 0.13 × 0.12 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	1.74 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	27.6°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	32,753, 4,293, 0.026
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4,179
$N(param)_{refined}$:	228
Programs:	Olex2,[1] SHELX[2,3]

2 Experimental details

The C-bound H atoms were geometrically placed and refined as riding with U_{ISO}(H) = 1.2–1.5 U_{eq}(C) using the appropriate *SHELXL* commands. The N-bound H atoms were freely refined.

3 Comment

Naproxen is a commonly used nonselective nonsteroidal anti-inflammatory drug. The title compound is a Naproxen ester. A view on the structure of the ester is shown in the figure. One carbon-oxygen double bond exists in the compound, the C–O double bond distance (C8–O1) is 1.201 (3) Å. And there is a

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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}
C1	0.8392 (2)	0.7598 (4)	0.45239 (15)	0.0228 (5)
H1A	0.809003	0.918724	0.466617	0.027*
H1B	0.926641	0.765851	0.474167	0.027*
C2	0.7966 (2)	0.5625 (4)	0.50440 (15)	0.0189 (4)
C3	0.68138 (18)	0.4732 (7)	0.47328 (14)	0.0238 (5)
H3	0.629204	0.533698	0.416740	0.029*
C4	0.6417 (2)	0.2967 (5)	0.52382 (16)	0.0239 (5)
H4	0.562908	0.237760	0.502378	0.029*
C5	0.7190 (2)	0.2079 (4)	0.60615 (15)	0.0195 (4)
C6	0.8342 (2)	0.2927 (4)	0.63746 (16)	0.0211 (5)
H6	0.886642	0.230146	0.693487	0.025*
C7	0.87238 (17)	0.4687 (8)	0.58680 (13)	0.0208 (4)
H7	0.951366	0.526514	0.608432	0.025*
C8	0.85481 (19)	0.5384 (4)	0.32020 (15)	0.0171 (4)
C9	0.8060 (2)	0.5099 (4)	0.21472 (15)	0.0197 (5)
H9	0.798832	0.675207	0.185646	0.024*
C10	0.8898 (2)	0.3587 (5)	0.17675 (17)	0.0285 (5)
H10A	0.895002	0.193590	0.202398	0.043*
H10B	0.968364	0.433644	0.195050	0.043*
H10C	0.859891	0.351544	0.108404	0.043*
C11	0.68293 (19)	0.3973 (4)	0.19153 (14)	0.0186 (5)
C12	0.58818 (19)	0.4972 (4)	0.12560 (14)	0.0181 (5)
H12	0.598832	0.641666	0.094111	0.022*
C13	0.4747 (2)	0.3882 (3)	0.10375 (14)	0.0173 (5)
C14	0.37470 (19)	0.4890 (5)	0.03606 (15)	0.0210 (6)
H14	0.383911	0.631397	0.002838	0.025*
C15	0.2662 (2)	0.3837 (4)	0.01843 (15)	0.0231 (5)
H15	0.200730	0.453326	−0.027060	0.028*
C16	0.24989 (19)	0.1725 (4)	0.06691 (15)	0.0206 (4)
C17	0.34416 (19)	0.0650 (4)	0.13131 (15)	0.0189 (4)
H17	0.333120	−0.079369	0.162671	0.023*
C18	0.45835 (19)	0.1721 (4)	0.15051 (15)	0.0175 (4)
C19	0.5578 (2)	0.0706 (4)	0.21780 (16)	0.0202 (4)
H19	0.548889	−0.074398	0.249664	0.024*
C20	0.6667 (2)	0.1801 (4)	0.23725 (15)	0.0197 (4)
H20	0.732252	0.108832	0.282147	0.024*
C21	0.1106 (2)	−0.0984 (5)	0.10118 (19)	0.0310 (7)
H21A	0.025938	−0.135967	0.080323	0.046*
H21B	0.132847	−0.045606	0.166614	0.046*
H21C	0.155839	−0.243945	0.095473	0.046*
I1	0.66241 (2)	−0.04940 (4)	0.68756 (2)	0.02517 (4)
O1	0.93104 (14)	0.4144 (4)	0.37006 (11)	0.0261 (5)
O2	0.80061 (14)	0.7204 (3)	0.35175 (11)	0.0197 (3)
O3	0.13548 (14)	0.0913 (3)	0.04464 (12)	0.0269 (4)

carbon-iodine bond in the compound, the C–I bond distance (C5–I1) is 2.098 (2) Å.The dihedral angle of naphthalene ring and iodine-substituted benzene ring is 14.798(49)°. All the bond lengths and angles are in the expected ranges.[4–7]

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

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

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