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Crystal structure of benzo[d][1,3]dioxol-5-yl-2-(6-methoxynaphthalen-2-yl)propanoate, C_{21}H_{18}O_{5}

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Abstract

C_{21}H_{18}O_{5}, monoclinic, P_{21} (no. 4), a = 9.1511(4) Å, b = 5.6679(3) Å, c = 16.7731(9) Å, \( \beta = 93.435(2) \)°, V = 868.42(8) Å³, Z = 2, \( R_{gt} = 0.0410 \), \( wR_{ref} = 0.1204 \), T = 296(2) K.

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

Source of material

Naproxen acylchloride was synthesized according to the literature method [5]. Naproxen (0.01 mol, 2.30 g) was dissolved in dichloromethane (10 mL), and then oxalyl chloride (0.012 mol, 1.1 mL) and two drops of N,N-dimethylformamide were dropwise added at 0 °C. The solution was stirred for 2 h at room temperature. After the solvent and excess oxalyl chloride was removed by vacuum distillation, a yellow solid was obtained.

Experimental details

A suitable crystal was selected and tested on a Bruker D8 VENTURE diffractometer. Using OLEX2 [2], the structure was solved with the SHELXT [3] structure solution program using Intrinsic Phasing and refined with the SHELX [4] refinement package.

Comment

Naproxen is a well-known nonsteroidal anti-inflammatory drug. It is usually used for treating rheumatic, rheumatoid arthritis and osteoarthritis. However, it often brings...
gastrointestinal side effects such as ulcers, gastric perforation and bleeding in long-term administration because of its carboxylic acid group. In order to overcome the side effects, many researchers have transformed naproxen into a prodrug. Studies also found that many prodrugs can improve the liposolubility, especially suitable for transdermal delivery mode. Because sesamol has anti-inflammatory and antioxidant effects [6, 7], we synthesized a naproxen-sesamol ester as a prodrug based on the combination principles. We expect to reduce the side effects of naproxen and improve its bioavailability.

The title molecule consists of two moieties: the naphthalene moiety and the 1,2-methylenedioxybenzene group (see the figure). The naphthalene ring and 1,2-methylenedioxybenzene ring are not coplanar with a dihedral angle of 53.5°. One carbon–oxygen double bond exists in the compound, the C–O double bond distance (C13–O2) is 1.173(4) Å. The bond lengths of C1–O1 and C13–O3 are 1.427(4) and 1.327(4) Å, respectively. The other C–O bond lengths range from 1.372(4) to 1.429(4) Å. The C–C bond lengths from 1.352(5) to 1.518(4) Å. The torsion angles of C14–C12–C13–O2 and O3–C15–C16–C17 are −75.5(6)° and 178.3(2)°, respectively. All the bond lengths and angles are in the expected ranges [8].

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References