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Crystal structure of 2-(naphthalen-1-yl)ethyl 2-acetoxybenzoate, C_{21}H_{18}O_{4}

Abstract

C_{21}H_{18}O_{4}, monoclinic, P_{2}1/c (no. 14), a = 22.2457(10) Å, b = 5.0728(2) Å, c = 15.7045(7) Å, β = 110.012(2)^{\circ}, V = 1665.22(13) Å^{3}, Z = 4, R_{gt}(F) = 0.0434, wR_{ref}(F^2) = 0.1023, 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.

1 Source of materials

Aspirin acylchloride was synthesized according to the literature method [4]. 1-Naphthaleneethanol (0.01 mol, 1.72 g) and 4-(dimethylamino)-pyridin (DMAP, 0.0015 mol, 0.18 g) were dissolved in dry tetrahydrofuran (20 mL) and triethylamine (0.015 mol, 2 mL). The solution of aspirin acylchloride in dry tetrahydrofuran was dropwise added at 0 °C. The reaction mixture was stirred for 2 h at room temperature. The mixture was filtered to remove the solid and the filtrate was concentrated under vacuum to remove the solvent. The residue was dissolved in dichloromethane, successively washed with 5 % NaOH solution and water to pH = 7, and dried with anhydrous...
3 Comment

Aspirin is one of the most useful drugs in human history which has been used for over 100 years [5]. Furthermore, more and more new biological activities of aspirin had been uncovered. Aspirin has shown surprising well anti-tumor activities which made it become a hot spot to develop new anti-tumor drugs. Recently epidemiological studies have revealed a reduced incidence of cancer in individuals taking daily low-dose aspirin [6–8]. The anti-tumor mechanisms for aspirin is complex but there are some mainstreams. In order to achieve high efficiency, low toxicity and cost anti-tumor drugs, we chose aspirin as a core compound and modify its structures.

The title compound contains one naphthyl ring and one phenyl ring. The bond distances of C–O are 1.3432(17) Å (C13–O1), 1.4517(16) Å (C12–O1), 1.2102(17) Å (C13–O2), 1.4030(17) Å (C19–O3), 1.3605(18) Å (C20–O3) and 1.1964(19) Å (C20–O4), respectively. The bond distance of C13–O2 and C20–O4 are shorter than those of C13–O1, C12–O1, C19–O3 and C20–O3, indicating C13–O2 and C20–O4 are double bonds. The dihedral angle of ring 1 (C1–C2–C3–C4–C5–C6) and ring 2 (C3–C4–C10–C9–C8–C7) is 0.5°, indicating that these rings are almost coplanar. However, the dihedral angles of ring 3 (C14–C15–C16–C17–C18–C19) with ring 1 and ring 2 are 16.6° and 17.1°, respectively. The other bond distances and angles are in their normal ranges according to the previously reported compounds [9, 10].

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References


