Dong-li Jiang, Yang Liu, Ying Cui and Rui Li*

Crystal structure of 3,4-dimethoxybenzyl 2-(6-methoxynaphthalen-2-yl)propanoate, C$_{23}$H$_{24}$O$_5$

Abstract
C$_{23}$H$_{24}$O$_5$, monoclinic, C2 (no. 4), a = 23.958(2) Å, b = 5.8145(5) Å, c = 17.839(3) Å, β = 129.974(3)°, V = 1904.3(4) Å$^3$, Z = 4, R$_{gt}$(F) = 0.0435, wR$_{ref}$(F$^2$) = 0.1140, T = 153(2) K.

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
Naproxen acylchloride was synthesized according to the literature method.$^4$ 3,4-Dimethoxybenzyl alcohol (0.01 mol, 1.69 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 naproxen acylchloride in dry tetrahydrofuran was dropwise added at 0°C. The reaction mixture was stirred for 2 h at room temperature. The mixture was filtrated to remove the solid and the filtrate was concentrated under vacuum to remove the solvent. The residue was

Table 1: Data collection and handling.

| Crystal: | Colorless block |
| Size: | 0.12 × 0.11 × 0.10 mm |
| Wavelength: | Mo Kα radiation (0.71073 Å) |
| μ: | 0.09 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker Apex-II, ϕ and ω |
| θ$_{max}$, completeness: | 27.7°, >99% |
| N(hkl)$_{measured}$, N(hkl)$_{unique}$, R$_{int}$. | 31,278, 4413, 0.050 |
| Criterion for I$_{obs}$, N(hkl)$_{gt}$: | I$_{obs}$ > 2σ(I$_{obs}$), 3832 |
| N(param)$_{refined}$: | 257 |
| Programs: | Bruker,$^1$ OLEX2,$^2$ SHELX$^3$ |

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dissolved in dichloromethane, successively washed with 5% NaOH solution and water to pH = 7, and dried with anhydrous Na2SO4. The solution was filtrated, and concentrated under vacuum to obtain crude product. The crude product was purified by recrystallization in ethanol. The crystals were obtained from tetrahydrofuran solution.

2 Experimental details

Coordinates of hydrogen atoms were refined with constraints. The Uiso values were set to 1.5Ueq of the carrier atom for methyl H atoms and 1.2Ueq for the remaining H atoms.

3 Comment

Naproxen is one of the strongest non-steroidal anti-inflammatory drugs (NSAIDs), inhibits the cyclooxygenase (COX) enzymes both COX-1 and COX-2. Inhibits both COX-1 and COX-2 which are the enzymes of cyclooxygenase (COX). Naproxen displays analgesic, anti-inflammatory, and antipyretic activity. In addition, the researchers reported anticancer 1 activities of naproxen derivatives.3 In cure of advancing prostate cancer, naproxen was discovered to be reliable and effective with early repetitive disease in a phase II clinical trial.4 By inducing apoptosis and cell cycle arrest toward bladder cancer cells, naproxen displayed anticancer influences. Naproxen inhibited protein kinase B (AKT) phosphorylation and induced apoptosis in rat urinary bladder cancers. 5 In order to achieve high efficiency, low toxicity and cost anti-tumor drugs, we chose naproxen as a core compound and modify its structures.

There is one title molecule in the asymmetric unit. The title compound contained one pyridine ring and one naphthyl moiety. The bond distances of C–O are 1.467(3) Å (C9–O3), 1.347(3) Å (C10–O3), 1.377(3) Å (C4–O1), 1.428(4) Å (C1–O1), 1.379(3) Å (C21–O5), 1.419(4) Å (C23–O3), 1.370(3) Å (C3–O2), 1.431(4) Å (C2–O2), and 1.210(4) Å (C10–O4), respectively. The bond distance of C10–O4 is shorter than those of C9–O3, C10–O3, C4–O1, C4–O1, C1–O1, C21–O5, C23–O3, C3–O2 and C2–O2, indicating C10–O4 is double bond. The dihedral angles of ring 1 (C3–C4–C5–C6–C7–C8) and ring 2 (C13–C14–C15–C16–C17–C18), ring 1 (C3–C4–C5–C6–C7–C8) and ring 3 (C16–C17–C19–C20–C21–C22), ring 2 (C13–C14–C15–C16–C17–C18) and ring 3 (C16–C17–C19–C20–C21–C22) are 7.06°, 7.511°, 3.201°, respectively. The other bond distances and angles are in their normal ranges according to the previously reported compounds.8–10
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References