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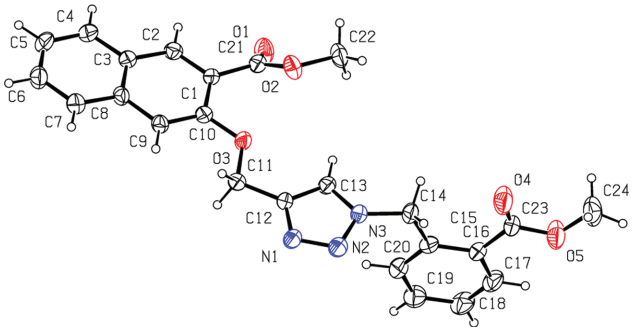
Crystal structure of methyl 3-((1-(2-(methoxycarbonyl)benzyl)-1H-1,2,3-triazol-4-yl)methoxy)-2-naphthoate, $C_{24}H_{21}N_3O_5$



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Abstract

$C_{24}H_{21}N_3O_5$, monoclinic, $P2_1/n$ (no. 14), $a = 5.8731(6)$ Å, $b = 12.4675(10)$ Å, $c = 28.912(3)$ Å, $\beta = 90.271(7)°$, $V = 2117.0(3)Å^3$, $Z = 4$, $R_{gt}(F) = 0.0797$, $wR_{ref}(F^2) = 0.1733$, $T = 293.23(10)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

Methyl 2-(azidomethyl)benzoate (200 mg, 1.05 mmol) and methyl 3-(prop-2-yn-1-yloxy)-2-naphthoate (250 mg, 1.05 mmol) were added to *tert*-butanol: water = 10 mL: 10 mL, then $CuSO_4·5H_2O$ (50 mg, 0.21 mmol) and VcNa (100 mg, 0.5 2 mmol) were added. The mixture was stirred at room temperature for 15 h. The solution was diluted with water and extracted with ethyl acetate. The organic layer was washed with water and dried over Na_2SO_4. After being filtered and concentrated, the residue was purified by silica gel column chromatography, eluted with ethyl acetate and petroleum ether (1:1, v/v) to give a white solid (yield 54%, 250 mg); **m.p.** 133.6–133.7 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$) d 8.32 (s, 1H, Ar-*H*), 8.04 (dd, $J = 8.0$, 1H, Ar-*H*), 7.87 (s, 1H, Ar-*H*), 7.78 (m, 2H, Ar-*H*), 7.45 (m, 4H, Ar-*H*), 7.36 (s, 1H, Ar-*H*), 7.11 (m, 1H, Ar-*H*), 5.99 (s, 2H, CH_2), 5.42 (s, 2H, CH_2), 3.91 (d, $J = 8.0$, 6H, CH_3). Single crystals of the title compound were obtained from dichloromethane.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.21 × 0.17 × 0.14 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	1.0 cm^{-1}
Diffractometer, scan mode:	SuperNova, ω-scans
$2\theta_{max}$, completeness:	52°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7894, 4175, 0.065
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1691
$N(param)_{refined}$:	291
Programs:	CrysAlis [7], SHELX [8], OLEX2 [9]

Experimental details

All H-atoms were placed in calculated positions and treated as riding: C—H = 0.93–0.97 Å, with $U_{iso} = 1.2$ or $1.5U_{eq}$(parent C-atom).

Discussion

1,2,3-Triazole is an important five-membered nitrogen-containing heterocyclic compound [1] and is a structure in a vast array of relevant compounds in distinct research areas such as crop protection, medicinal chemistry [2], and material sciences [3], because of its high metabolic stability, hydrogen-bonding capability, and amide bioequivalence [4, 5]. The alkyl substitution of function group at N(1) position of

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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}
O1	0.3280(6)	0.0699(3)	0.10043(12)	0.0723(11)
O2	0.6888(5)	0.0892(2)	0.07974(11)	0.0643(9)
O3	0.7194(5)	0.2874(2)	0.04533(10)	0.0526(8)
O4	1.7567(7)	0.2237(3)	0.20920(13)	0.0988(15)
O5	1.7817(6)	0.2529(3)	0.28410(12)	0.0878(12)
N1	1.1935(6)	0.4664(3)	0.06565(13)	0.0556(10)
N2	1.3469(6)	0.4501(3)	0.09827(14)	0.0590(11)
N3	1.2827(6)	0.3604(3)	0.12074(12)	0.0512(10)
C1	0.4100(7)	0.1698(3)	0.03266(15)	0.0447(11)
C2	0.2185(7)	0.1419(3)	0.00837(14)	0.0488(12)
H2	0.1300	0.0853	0.0191	0.059*
C3	0.1503(7)	0.1958(3)	−0.03227(16)	0.0490(12)
C4	−0.0488(8)	0.1677(3)	−0.05728(16)	0.0591(14)
H4	−0.1395	0.1116	−0.0470	0.071*
C5	−0.1088(9)	0.2222(4)	−0.09632(17)	0.0654(15)
H5	−0.2411	0.2040	−0.1123	0.079*
C6	0.0291(8)	0.3058(4)	−0.11228(17)	0.0646(14)
H6	−0.0112	0.3418	−0.1393	0.077*
C7	0.2224(8)	0.3355(3)	−0.08892(16)	0.0612(14)
H7	0.3125	0.3908	−0.1002	0.073*
C8	0.2851(7)	0.2825(3)	−0.04790(15)	0.0457(11)
C9	0.4791(7)	0.3148(3)	−0.02184(14)	0.0461(11)
H9	0.5651	0.3734	−0.0313	0.055*
C10	0.5391(7)	0.2595(3)	0.01732(15)	0.0459(11)
C11	0.8407(7)	0.3826(3)	0.03432(15)	0.0486(12)
H11A	0.7428	0.4449	0.0372	0.058*
H11B	0.8975	0.3794	0.0029	0.058*
C12	1.0328(7)	0.3885(3)	0.06798(15)	0.0452(11)
C13	1.0878(7)	0.3212(3)	0.10318(14)	0.0482(12)
H13	1.0079	0.2610	0.1130	0.058*
C14	1.4242(8)	0.3197(3)	0.15869(15)	0.0596(14)
H14A	1.5828	0.3342	0.1519	0.071*
H14B	1.4058	0.2425	0.1606	0.071*
C15	1.3662(7)	0.3689(3)	0.20507(16)	0.0504(12)
C16	1.4966(8)	0.3462(3)	0.24503(16)	0.0521(12)
C17	1.4378(9)	0.3940(4)	0.28658(16)	0.0662(14)
H17	1.5251	0.3795	0.3128	0.079*
C18	1.2559(9)	0.4617(4)	0.29033(18)	0.0752(16)
H18	1.2199	0.4925	0.3187	0.090*
C19	1.1262(9)	0.4838(4)	0.25163(18)	0.0714(15)
H19	1.0007	0.5290	0.2539	0.086*
C20	1.1823(8)	0.4389(4)	0.20964(17)	0.0619(14)
H20	1.0953	0.4558	0.1837	0.074*
C21	0.4668(8)	0.1048(3)	0.07396(17)	0.0510(12)
C22	0.7543(8)	0.0270(4)	0.12022(15)	0.0681(15)
H22A	0.6930	−0.0442	0.1177	0.102*
H22B	0.6957	0.0608	0.1475	0.102*
H22C	0.9173	0.0233	0.1222	0.102*
C23	1.6885(8)	0.2682(4)	0.24267(19)	0.0569(13)
C24	1.9697(9)	0.1777(4)	0.28644(19)	0.097(2)
H24A	2.0821	0.1968	0.2639	0.145*
H24B	1.9149	0.1066	0.2802	0.145*
H24C	2.0368	0.1799	0.3168	0.145*

1,2,3-triazole derivatives is attracting the attention of chemists [6]. In current study a number of alkyl-substituted 1,2,3-triazole derivatives in N(1) position were synthesized, which were used for the development of LPAR3 (Lysophosphatidic acid receptor 3) antagonist. Moreover, the crystal structure of these molecules were attempted to solve in order to gain the better understanding the binding pose of these molecules and LPAR3 in detail.

The crystal structure reveals that the triazole ring connects the benzyl and the naphthoate moiety. The dihedral angle between the triazole and the naphthyl moiety is 6.8°. The dihedral angle between triazole and benzyl moiety is 89.3°. In the crystal structure intermolecular π-π interactions and C—H$\cdots$π interactions play a role in the molecular packing. The bond lengths and angles derived from the title structure are within normal ranges.

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