Crystal structure of 2-[2-(4-chloro-phenyl)-acetylamino]-3-(3,4-dimethoxyphenyl)propionic acid methyl ester, $C_{20}H_{22}ClNO_5$

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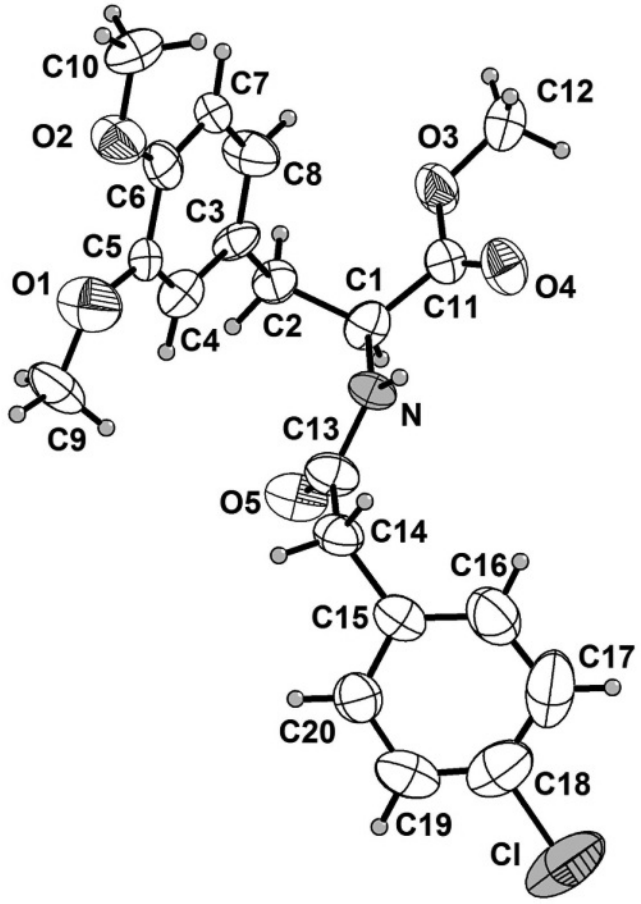

Abstract

$C_{20}H_{22}ClNO_5$, orthorhombic, $P2_12_12_1$ (no. 19), a = 5.001(1) Å, b = 13.085(3) Å, c = 29.765(6) Å, V = 1947.8 Å^3, Z = 4, $R_{gt}(F)$ = 0.0783, $wR_{ref}(F^2)$ = 0.1758, T = 293 K.

Table 1. Data collection and handling.

Crystal:	colourless needles, size 0.1×0.2×0.3 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	2.27 cm^{-1}
Diffractometer, scan mode:	Nonius cad4, $\omega/2\theta$
$2\theta_{max}$:	50.72°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4126, 3542
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1803
$N(param)_{refined}$:	244
Programs:	SHELX [4], DIAMOND [5]

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Source of material

The title compound was obtained from the reaction of *p*-chlorophenylacetic acid, thionyl chloride and (*R*)-methyl 2-amino-3-(3,4-dimethoxyphenyl)propanoate hydrochloride as described in literature [1] and recrystallized from $CHCl_3$-methanol to give crystals suitable for single-crystal X-ray diffraction.

Experimental details

In the crystal, H atoms were positioned geometrically with C–H = 0.93, 0.97 and 0.98 Å for aromatic, and methyl, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2 (or 1.5 for methyl groups) times U_{eq}(C).

Discussion

2-[2-(4-Chloro-phenyl)-acetylamino]-3-(3,4-dimethoxy-phenyl)-propionic acid methyl ester is the synthetic intermediate analogue of tetrahydroisoquinolines that are proven to be involved in some pathologies of the central nervous system. This family of compounds is also used in a number of cardiovascular diseases, for the treatment of cardiac ischemia or pulmonary embolism, and plays a role as a venous and arterial antithrombotic agent [1]. The geometrical parameters of this molecule are all in the expected ranges. In the crystal structure, intermolecular N–H···O hydrogen bonds link the molecules into chains along [100], in which may be effective in the stabilization of the structure.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(0A)	4*a*	0.3921	0.6879	0.8962	0.055
H(1A)	4*a*	0.8340	0.7589	0.9365	0.060
H(2A)	4*a*	0.9499	0.8427	0.8733	0.060
H(2B)	4*a*	0.8452	0.9268	0.9065	0.060
H(4A)	4*a*	0.7042	0.8044	0.8055	0.071
H(7A)	4*a*	0.1258	1.0756	0.8342	0.060
H(8A)	4*a*	0.4176	1.0136	0.8884	0.078
H(9A)	4*a*	0.5483	0.7523	0.6943	0.116
H(9B)	4*a*	0.5834	0.7194	0.7445	0.116
H(9C)	4*a*	0.7459	0.8122	0.7255	0.116
H(10A)	4*a*	–0.2207	1.0869	0.7344	0.095
H(10B)	4*a*	–0.0055	1.1322	0.7671	0.095
H(10C)	4*a*	–0.2246	1.0573	0.7854	0.095
H(12A)	4*a*	0.4669	1.0186	1.0135	0.143
H(12B)	4*a*	0.3868	0.9090	1.0300	0.143
H(12C)	4*a*	0.2131	0.9647	0.9936	0.143
H(14A)	4*a*	0.6439	0.5390	0.8211	0.067
H(14B)	4*a*	0.3968	0.5548	0.8531	0.067
H(16A)	4*a*	0.3841	0.4479	0.9257	0.105
H(17A)	4*a*	0.4594	0.2898	0.9597	0.134
H(19A)	4*a*	1.0841	0.2495	0.8699	0.106
H(20A)	4*a*	0.9717	0.4044	0.8367	0.089

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl	4*a*	0.8823(7)	0.1423(2)	0.94377(8)	0.267(3)	0.061(1)	0.105(2)	–0.016(2)	–0.057(2)	0.016(1)
N	4*a*	0.5625(7)	0.6968(3)	0.8966(1)	0.033(2)	0.049(3)	0.055(3)	0.013(2)	0.000(2)	–0.007(2)
O(1)	4*a*	0.3692(9)	0.8433(4)	0.7369(1)	0.106(4)	0.093(3)	0.058(3)	0.023(3)	–0.029(3)	–0.015(3)
C(1)	4*a*	0.681(1)	0.7852(4)	0.9194(2)	0.050(3)	0.046(3)	0.054(3)	–0.019(2)	–0.009(3)	–0.001(3)
O(2)	4*a*	0.0510(8)	0.9925(3)	0.7516(1)	0.074(3)	0.083(3)	0.058(3)	0.034(2)	–0.007(2)	0.002(2)
C(2)	4*a*	0.7921(9)	0.8684(4)	0.8885(2)	0.044(3)	0.056(3)	0.049(3)	0.015(2)	–0.006(2)	0.012(3)
C(3)	4*a*	0.584(1)	0.9028(4)	0.8532(2)	0.060(3)	0.032(3)	0.040(3)	0.002(3)	–0.021(3)	0.005(2)
O(3)	4*a*	0.5482(9)	0.9110(3)	0.9707(1)	0.108(3)	0.055(2)	0.067(3)	–0.025(2)	0.040(3)	–0.020(2)
O(4)	4*a*	0.2699(7)	0.7781(3)	0.9628(1)	0.050(2)	0.084(3)	0.063(3)	–0.010(2)	0.010(2)	–0.006(2)
C(4)	4*a*	0.580(1)	0.8554(4)	0.8117(2)	0.066(4)	0.053(4)	0.059(4)	0.000(3)	–0.001(3)	0.011(3)
O(5)	4*a*	0.9764(8)	0.6352(3)	0.8775(2)	0.060(2)	0.070(3)	0.083(3)	0.008(2)	–0.015(2)	–0.021(3)
C(5)	4*a*	0.391(1)	0.8833(4)	0.7788(2)	0.088(4)	0.046(3)	0.038(3)	0.007(3)	0.024(3)	0.008(3)
C(6)	4*a*	0.215(1)	0.9692(5)	0.7886(2)	0.046(3)	0.068(4)	0.064(4)	0.006(3)	0.024(3)	0.010(3)
C(7)	4*a*	0.232(1)	1.0187(4)	0.8283(2)	0.057(3)	0.044(3)	0.050(3)	0.005(3)	0.021(3)	0.002(3)
C(8)	4*a*	0.414(1)	0.9819(4)	0.8605(2)	0.073(4)	0.070(4)	0.052(4)	0.021(4)	–0.016(3)	–0.014(3)
C(9)	4*a*	0.579(1)	0.7764(5)	0.7243(2)	0.073(4)	0.080(5)	0.079(5)	–0.004(4)	0.023(4)	–0.040(4)
C(10)	4*a*	–0.112(1)	1.0731(4)	0.7602(2)	0.056(3)	0.045(3)	0.089(5)	0.001(3)	–0.018(3)	0.008(3)
C(11)	4*a*	0.477(1)	0.8189(5)	0.9535(2)	0.075(4)	0.054(4)	0.045(3)	0.006(3)	0.012(3)	0.002(3)
C(12)	4*a*	0.392(2)	0.9542(5)	1.0046(2)	0.138(6)	0.073(5)	0.074(5)	0.005(5)	0.042(5)	0.024(4)
C(13)	4*a*	0.733(1)	0.6280(4)	0.8758(2)	0.048(3)	0.052(3)	0.069(4)	–0.002(3)	–0.005(3)	–0.019(3)
C(14)	4*a*	0.588(1)	0.5426(4)	0.8523(2)	0.058(3)	0.057(4)	0.053(3)	0.018(3)	–0.003(3)	–0.004(3)
C(15)	4*a*	0.6561(9)	0.4400(4)	0.8769(2)	0.040(3)	0.057(4)	0.062(4)	–0.008(3)	–0.004(3)	–0.021(3)
C(16)	4*a*	0.518(1)	0.4058(6)	0.9143(3)	0.097(5)	0.084(5)	0.081(5)	–0.015(4)	0.024(4)	–0.023(5)
C(17)	4*a*	0.563(2)	0.3138(8)	0.9360(3)	0.141(8)	0.122(8)	0.072(5)	–0.045(7)	0.014(5)	0.014(5)
C(18)	4*a*	0.794(2)	0.2583(6)	0.9170(3)	0.126(7)	0.066(5)	0.088(6)	–0.003(5)	–0.031(5)	0.007(4)
C(19)	4*a*	0.943(2)	0.2887(6)	0.8808(3)	0.095(5)	0.074(5)	0.094(6)	0.013(4)	0.007(5)	–0.030(5)
C(20)	4*a*	0.873(1)	0.3808(5)	0.8611(2)	0.112(5)	0.069(4)	0.040(4)	0.013(4)	0.003(3)	–0.003(3)

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