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Ethyl 5-(ethoxycarbonyl)-3-(4-methoxyphenyl)-1*H*-pyrazole-1-acetate

Wen-Liang Dong,[a,b] Yan-Qing Ge[a] and Bao-Xiang Zhao[a]*

[a]School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100, People's Republic of China, and [b]Shandong University of Traditional Chinese Medicine, Jinan 250355, People's Republic of China
Correspondence e-mail: bxzhao@hotmail.com

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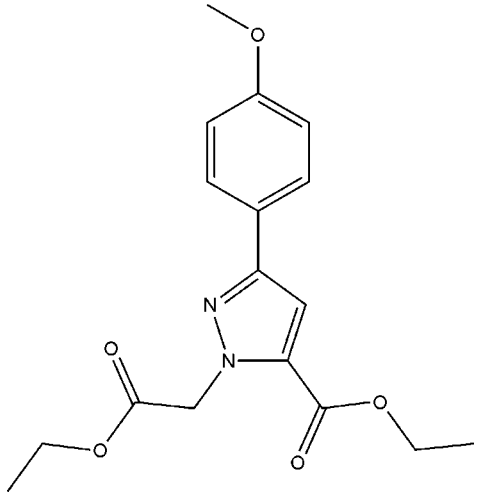
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.166; data-to-parameter ratio = 17.2.

In the title compound, $C_{17}H_{20}N_2O_5$, all bond lengths and angles show normal values. The dihedral angle between the pyrazole ring and the benzene ring is 6.98 (11)°. The molecules are linked by intermolecular C—H$\cdots\pi$ interactions.

Related literature

For related literature, see: Allen *et al.* (1987); Brough *et al.* (2005); Cheng *et al.* (2006); Dong *et al.* (2007); Sehon *et al.* (2006); Wei *et al.* (2006); Xia *et al.* (2007).



Experimental

Crystal data

$C_{17}H_{20}N_2O_5$
M_r = 332.35
Triclinic, $P\overline{1}$
a = 7.4267 (1) Å
b = 11.0511 (2) Å
c = 11.7139 (2) Å
α = 106.721 (1)°
β = 97.898 (1)°
γ = 106.796 (1)°
V = 855.59 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 (2) K
0.45 × 0.39 × 0.28 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.846, T_{max} = 0.974
13041 measured reflections
3806 independent reflections
2376 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.166
S = 1.06
3806 reflections
221 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
X—H$\cdots\pi$-ring interactions calculated by *PLATON* (Spek, 2003). Cg^i is a centroid of the pyrazole ring N1/N2/C8/C9/C10.

X—H$\cdots Cg$	X—H	H$\cdots Cg$	$X\cdots Cg$	X—H$\cdots Cg$
C1—H1$A\cdots Cg1^i$	0.96	2.89	3.731 (3)	147

Symmetry code: (i) $1+x, y, z$. $Cg1$ is the centroid of the the pyrazole ring.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2063).

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supplementary materials

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Ethyl 5-(ethoxycarbonyl)-3-(4-methoxyphenyl)-1*H*-pyrazole-1-acetate

W.-L. Dong, Y.-Q. Ge and B.-X. Zhao

Comment

The pyrazole unit is one of the core structures in a number of natural products. Many pyrazole derivatives are known to exhibit a wide range of biological properties such as antagonists (Sehon *et al.*, 2006), anti-inflammatory (Cheng *et al.*, 2006), inhibitors of the Hsp90 (Brough *et al.*, 2005), antitumor (Wei *et al.*, 2006; Xia *et al.*, 2007). In our previous paper, we reported the crystal structure of ethyl 3-(4-chlorophenyl)-5-(ethoxycarbonyl)-1*H*-pyrazole-1-acetate (Dong *et al.*, 2007). We report here the crystal structure of the title compound, (I).

In compound (I) (Fig. 1), all bond lengths and angles are normal (Allen *et al.*, 1987). The dihedral angles between the rings of the pyrazole and the benzene ring is 6.98 (11)^{o}. The two ethyl carboxylate groups are inclined to the attached pyrazole ring by 2.16 (9)^{o} and 75.95 (11)^{o}, respectively. The molecules are linked into a network parallel by C—H···π interactions (Table 1) involving the pyrazole ring (centroid *Cg*1). We report here the crystal structure of the title compound, (I).

Experimental

A mixture of ethyl 3-(4-methoxyphenyl)-1*H*-pyrazole-5-carboxylate (0.01 mol), ethyl chloroacetate (0.015 mol) and potassium carbonate (0.02 mol) in acetonitrile (50 ml) was heated to reflux for 15 h. The solvent was removed under reduced pressure, and the residue was dissolved in the mixture of water (50 ml) and ethyl acetate (50 ml). After separated, the water phase was extracted with ethyl acetate (25 ml), and then the organic phase was combined, dried over anhydrous magnesium sulfate and filtered. The solvent was removed under reduced pressure. The solid product was recrystallized from ethyl acetate (yield 55%). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a solution of the solid in ethyl acetate at room temperature for 6 d.

Refinement

All H atoms were placed in geometrically calculated positions and refined using a riding model with C—H = 0.97 Å (for CH_2 groups) and 0.96 Å (for CH_3 groups), their isotropic displacement parameters were set to 1.2 times (1.5times for CH_3 groups) the equivalent displacement parameter of their parent atoms.

Figures

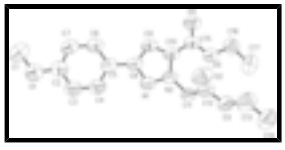

Fig. 1. The structure of the title molecule showing displacement ellipsoids drawn at the 50% probability level.

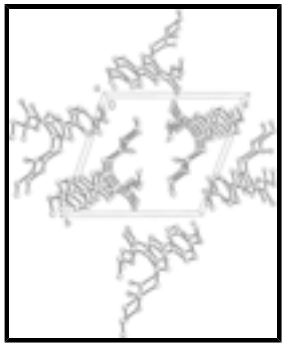

Fig. 2. Packing view of (I), shown down the *a* axis.

Ethyl 5-(ethoxycarbonyl)-3-(4-methoxyphenyl)-1*H*-pyrazole-1-acetate

Crystal data

$C_{17}H_{20}N_2O_5$	$Z = 2$
$M_r = 332.35$	$F_{000} = 352$
Triclinic, $P\overline{1}$	$D_x = 1.290$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.4267$ (1) Å	Cell parameters from 3567 reflections
$b = 11.0511$ (2) Å	$\theta = 3.0$–24.5°
$c = 11.7139$ (2) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 106.721$ (1)°	$T = 296$ (2) K
$\beta = 97.898$ (1)°	Prism, colourless
$\gamma = 106.796$ (1)°	0.45 × 0.39 × 0.28 mm
$V = 855.59$ (3) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	3806 independent reflections
Radiation source: fine-focus sealed tube	2376 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 296$(2) K	$\theta_{max} = 27.5^\circ$
φ and ω scans	$\theta_{min} = 2.3^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$h = -9 \rightarrow 9$
$T_{min} = 0.846$, $T_{max} = 0.974$	$k = -14 \rightarrow 14$
13041 measured reflections	$l = -15 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained
$wR(F^2) = 0.166$	$w = 1/[\sigma^2(F_o^2) + (0.0775P)^2 + 0.1127P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
3806 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
221 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
3 restraints	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.016 (4)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.7281 (3)	0.0919 (3)	0.9802 (3)	0.1071 (8)
H1A	−0.7815	0.0997	0.9043	0.161*
H1B	−0.8148	0.0990	1.0334	0.161*
H1C	−0.7110	0.0062	0.9639	0.161*
C2	−0.4043 (3)	0.2015 (2)	0.9716 (2)	0.0792 (5)
C3	−0.2328 (3)	0.3033 (2)	1.0311 (2)	0.0871 (6)
H3	−0.2183	0.3626	1.1091	0.104*
C4	−0.0829 (3)	0.3176 (2)	0.9754 (2)	0.0815 (6)
H4	0.0339	0.3872	1.0170	0.098*
C5	−0.0974 (3)	0.23132 (17)	0.85765 (17)	0.0676 (5)
C6	−0.2716 (3)	0.1283 (2)	0.7993 (2)	0.0783 (6)
H6	−0.2865	0.0685	0.7214	0.094*
C7	−0.4285 (3)	0.1127 (2)	0.8567 (2)	0.0823 (6)
H7	−0.5462	0.0432	0.8171	0.099*
C8	0.0682 (3)	0.25088 (16)	0.80054 (16)	0.0645 (5)
C9	0.0946 (3)	0.17110 (17)	0.69185 (17)	0.0674 (5)
H9	0.0062	0.0898	0.6365	0.081*
C10	0.2765 (3)	0.23673 (16)	0.68338 (16)	0.0640 (5)
C11	0.5351 (3)	0.46068 (18)	0.81994 (17)	0.0722 (5)
H11A	0.6397	0.4248	0.8165	0.087*
H11B	0.5551	0.5187	0.9038	0.087*
C12	0.5401 (3)	0.54247 (18)	0.73607 (18)	0.0744 (5)
C13	0.7510 (4)	0.7109 (3)	0.6817 (3)	0.1111 (9)
H13A	0.6755	0.7696	0.6977	0.133*

H13B	0.7114	0.6574	0.5949	0.133*
C14	0.9606 (5)	0.7918 (3)	0.7167 (3)	0.1405 (13)
H14A	0.9996	0.8409	0.8034	0.211*
H14B	0.9843	0.8539	0.6730	0.211*
H14C	1.0335	0.7330	0.6963	0.211*
C15	0.3773 (3)	0.19420 (18)	0.58813 (18)	0.0714 (5)
C16	0.6729 (3)	0.2462 (3)	0.5236 (2)	0.0952 (7)
H16A	0.6079	0.2275	0.4395	0.114*
H16B	0.7006	0.1670	0.5287	0.114*
C17	0.8560 (4)	0.3647 (3)	0.5629 (3)	0.1128 (9)
H17A	0.8293	0.4383	0.5452	0.169*
H17B	0.9483	0.3412	0.5193	0.169*
H17C	0.9080	0.3909	0.6496	0.169*
N1	0.2268 (2)	0.36044 (14)	0.85650 (14)	0.0697 (4)
N2	0.3521 (2)	0.35071 (14)	0.78541 (14)	0.0664 (4)
O1	−0.5490 (2)	0.19486 (17)	1.03670 (16)	0.1040 (5)
O2	0.4038 (2)	0.53626 (15)	0.66541 (16)	0.1015 (5)
O3	0.7201 (2)	0.62366 (14)	0.75458 (13)	0.0866 (5)
O4	0.3061 (2)	0.08992 (16)	0.50282 (15)	0.1068 (6)
O5	0.55182 (19)	0.28057 (13)	0.60626 (13)	0.0793 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0884 (16)	0.0961 (16)	0.127 (2)	0.0173 (13)	0.0019 (14)	0.0497 (15)
C2	0.0858 (13)	0.0741 (12)	0.0800 (12)	0.0337 (11)	0.0114 (10)	0.0275 (9)
C3	0.0879 (15)	0.0757 (13)	0.0808 (14)	0.0253 (11)	0.0101 (12)	0.0105 (10)
C4	0.0789 (13)	0.0690 (12)	0.0812 (14)	0.0205 (10)	0.0088 (11)	0.0137 (10)
C5	0.0714 (11)	0.0561 (9)	0.0686 (11)	0.0195 (8)	0.0012 (9)	0.0217 (8)
C6	0.0816 (13)	0.0689 (11)	0.0720 (12)	0.0169 (10)	0.0042 (10)	0.0220 (9)
C7	0.0760 (12)	0.0665 (11)	0.0860 (13)	0.0112 (9)	−0.0028 (10)	0.0234 (9)
C8	0.0682 (11)	0.0522 (9)	0.0622 (10)	0.0151 (8)	−0.0010 (8)	0.0176 (8)
C9	0.0697 (11)	0.0500 (9)	0.0656 (11)	0.0123 (8)	−0.0031 (9)	0.0129 (8)
C10	0.0688 (11)	0.0497 (8)	0.0575 (10)	0.0127 (8)	−0.0034 (8)	0.0119 (7)
C11	0.0730 (11)	0.0625 (10)	0.0548 (10)	0.0035 (8)	−0.0051 (8)	0.0118 (8)
C12	0.0791 (12)	0.0573 (10)	0.0655 (11)	0.0093 (9)	−0.0017 (10)	0.0136 (8)
C13	0.129 (2)	0.0820 (15)	0.1059 (19)	0.0067 (14)	0.0078 (16)	0.0480 (14)
C14	0.146 (3)	0.106 (2)	0.127 (2)	−0.0186 (19)	0.021 (2)	0.0466 (18)
C15	0.0744 (12)	0.0624 (10)	0.0650 (11)	0.0193 (9)	0.0023 (9)	0.0152 (9)
C16	0.0941 (16)	0.1076 (17)	0.0903 (16)	0.0433 (14)	0.0266 (13)	0.0332 (13)
C17	0.0953 (17)	0.1129 (19)	0.150 (3)	0.0370 (15)	0.0466 (17)	0.0653 (19)
N1	0.0757 (10)	0.0590 (8)	0.0591 (9)	0.0129 (7)	0.0038 (8)	0.0144 (7)
N2	0.0691 (9)	0.0556 (8)	0.0563 (8)	0.0093 (7)	−0.0014 (7)	0.0127 (6)
O1	0.0940 (11)	0.0954 (11)	0.1023 (12)	0.0215 (9)	0.0206 (9)	0.0175 (9)
O2	0.0943 (10)	0.0906 (10)	0.1036 (12)	0.0156 (8)	−0.0142 (9)	0.0441 (9)
O3	0.0868 (9)	0.0727 (8)	0.0778 (9)	0.0016 (7)	0.0001 (7)	0.0287 (7)
O4	0.0975 (11)	0.0835 (10)	0.0917 (11)	0.0104 (8)	0.0154 (9)	−0.0146 (8)
O5	0.0756 (8)	0.0742 (8)	0.0753 (9)	0.0172 (7)	0.0137 (7)	0.0178 (7)

Geometric parameters (Å, °)

C1—O1	1.397 (3)	C11—C12	1.512 (3)
C1—H1A	0.9600	C11—H11A	0.9700
C1—H1B	0.9600	C11—H11B	0.9700
C1—H1C	0.9600	C12—O2	1.188 (2)
C2—C3	1.360 (3)	C12—O3	1.325 (2)
C2—C7	1.370 (3)	C13—O3	1.452 (3)
C2—O1	1.398 (3)	C13—C14	1.483 (4)
C3—C4	1.359 (3)	C13—H13A	0.9700
C3—H3	0.9300	C13—H13B	0.9700
C4—C5	1.402 (3)	C14—H14A	0.9600
C4—H4	0.9300	C14—H14B	0.9600
C5—C6	1.377 (2)	C14—H14C	0.9600
C5—C8	1.470 (3)	C15—O4	1.203 (2)
C6—C7	1.417 (3)	C15—O5	1.315 (2)
C6—H6	0.9300	C16—O5	1.455 (3)
C7—H7	0.9300	C16—C17	1.492 (3)
C8—N1	1.338 (2)	C16—H16A	0.9700
C8—C9	1.400 (3)	C16—H16B	0.9700
C9—C10	1.369 (3)	C17—H17A	0.9600
C9—H9	0.9300	C17—H17B	0.9600
C10—N2	1.368 (2)	C17—H17C	0.9600
C10—C15	1.469 (3)	N1—N2	1.338 (2)
C11—N2	1.449 (2)		
O1—C1—H1A	109.5	H11A—C11—H11B	108.0
O1—C1—H1B	109.5	O2—C12—O3	125.12 (19)
H1A—C1—H1B	109.5	O2—C12—C11	125.49 (19)
O1—C1—H1C	109.5	O3—C12—C11	109.39 (16)
H1A—C1—H1C	109.5	O3—C13—C14	107.6 (2)
H1B—C1—H1C	109.5	O3—C13—H13A	110.2
C3—C2—C7	121.2 (2)	C14—C13—H13A	110.2
C3—C2—O1	115.1 (2)	O3—C13—H13B	110.2
C7—C2—O1	123.7 (2)	C14—C13—H13B	110.2
C4—C3—C2	119.4 (2)	H13A—C13—H13B	108.5
C4—C3—H3	120.3	C13—C14—H14A	109.5
C2—C3—H3	120.3	C13—C14—H14B	109.5
C3—C4—C5	122.6 (2)	H14A—C14—H14B	109.5
C3—C4—H4	118.7	C13—C14—H14C	109.5
C5—C4—H4	118.7	H14A—C14—H14C	109.5
C6—C5—C4	117.2 (2)	H14B—C14—H14C	109.5
C6—C5—C8	122.06 (18)	O4—C15—O5	123.9 (2)
C4—C5—C8	120.78 (17)	O4—C15—C10	122.73 (19)
C5—C6—C7	120.6 (2)	O5—C15—C10	113.38 (15)
C5—C6—H6	119.7	O5—C16—C17	106.8 (2)
C7—C6—H6	119.7	O5—C16—H16A	110.4
C2—C7—C6	119.0 (2)	C17—C16—H16A	110.4
C2—C7—H7	120.5	O5—C16—H16B	110.4

C6—C7—H7	120.5	C17—C16—H16B	110.4
N1—C8—C9	110.03 (17)	H16A—C16—H16B	108.6
N1—C8—C5	119.14 (17)	C16—C17—H17A	109.5
C9—C8—C5	130.83 (16)	C16—C17—H17B	109.5
C10—C9—C8	106.19 (15)	H17A—C17—H17B	109.5
C10—C9—H9	126.9	C16—C17—H17C	109.5
C8—C9—H9	126.9	H17A—C17—H17C	109.5
N2—C10—C9	106.01 (17)	H17B—C17—H17C	109.5
N2—C10—C15	125.70 (17)	C8—N1—N2	105.97 (15)
C9—C10—C15	128.25 (16)	N1—N2—C10	111.79 (15)
N2—C11—C12	111.51 (14)	N1—N2—C11	118.33 (14)
N2—C11—H11A	109.3	C10—N2—C11	129.73 (18)
C12—C11—H11A	109.3	C1—O1—C2	117.6 (2)
N2—C11—H11B	109.3	C12—O3—C13	116.71 (17)
C12—C11—H11B	109.3	C15—O5—C16	118.99 (16)
C7—C2—C3—C4	0.2 (3)	C9—C10—C15—O4	−0.7 (3)
O1—C2—C3—C4	179.65 (19)	N2—C10—C15—O5	−2.6 (3)
C2—C3—C4—C5	0.3 (3)	C9—C10—C15—O5	179.77 (16)
C3—C4—C5—C6	−0.7 (3)	C9—C8—N1—N2	−0.21 (18)
C3—C4—C5—C8	179.64 (18)	C5—C8—N1—N2	179.32 (14)
C4—C5—C6—C7	0.6 (3)	C8—N1—N2—C10	0.48 (19)
C8—C5—C6—C7	−179.75 (16)	C8—N1—N2—C11	176.47 (14)
C3—C2—C7—C6	−0.3 (3)	C9—C10—N2—N1	−0.56 (19)
O1—C2—C7—C6	−179.68 (18)	C15—C10—N2—N1	−178.58 (15)
C5—C6—C7—C2	−0.1 (3)	C9—C10—N2—C11	−175.96 (16)
C6—C5—C8—N1	173.34 (16)	C15—C10—N2—C11	6.0 (3)
C4—C5—C8—N1	−7.0 (2)	C12—C11—N2—N1	−106.75 (19)
C6—C5—C8—C9	−7.2 (3)	C12—C11—N2—C10	68.4 (2)
C4—C5—C8—C9	172.38 (18)	C3—C2—O1—C1	−179.77 (19)
N1—C8—C9—C10	−0.12 (19)	C7—C2—O1—C1	−0.4 (3)
C5—C8—C9—C10	−179.58 (16)	O2—C12—O3—C13	−0.3 (3)
C8—C9—C10—N2	0.40 (18)	C11—C12—O3—C13	−179.51 (19)
C8—C9—C10—C15	178.35 (16)	C14—C13—O3—C12	−179.8 (2)
N2—C11—C12—O2	13.2 (3)	O4—C15—O5—C16	−4.0 (3)
N2—C11—C12—O3	−167.54 (16)	C10—C15—O5—C16	175.57 (16)
N2—C10—C15—O4	176.88 (19)	C17—C16—O5—C15	177.34 (17)

X—H···π-ring interactions calculated by PLATON (Spek, 2003). Cg^{i} is a centroid of the pyrazole ring N1/N2/C8/C9/C10.

X—H···*Cg*	*X*—H	H···*Cg*	*X*···*Cg*	*X*—H···*Cg*
C1—H1A···*Cg*1^{i}	0.96	2.89	3.731 (3)	147

Symmetry code: (i) 1 + *x*,*y*,*z*.

Fig. 1

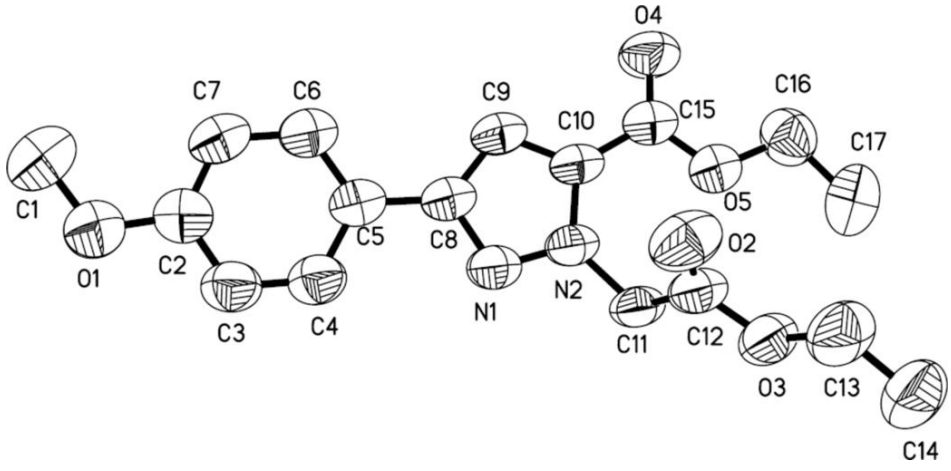
O4
C7
C6
C9
C10
C15
C16
C17
C1
O5
C5
C8
O2
O1
C2
N2
C3
C4
N1
C11
C12
O3
C13
C14

Fig. 2