C(26)—C(27) bond distances [1·509 (5) Å av.] are normal single bonds. The C—C bonds linking the thiophene groups to the C=N bonds, *e.g.* C(4)—C(5), are shorter [1·449 (4) Å av.], indicating that conjugation occurs between the C=N and thiophene moieties. Bond distances and angles within the thiophene group are unexceptional, *e.g.* C—S 1·709 (4) Å av., C—S—C 91·6 (2)° av. Complexation studies of S_3tren are underway.

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Anticancer Agent Development. 3. X-ray Structure of Dimethyl 1-Methoxy-6,7-methylenedioxy-4-(3,4,5-trimethoxyphenyl)-*trans*-3,4-dihydronaphthalene-2,3-dicarboxylate

BY JOHN R. PETERSON,*† HOANG D. DO AND ROBIN D. ROGERS*

The Michael Faraday Laboratories, Department of Chemistry, Northern Illinois University, DeKalb, IL 60115, *USA*

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Abstract. $C_{25}H_{26}O_{10}$, $M_r = 486{\cdot}48$, monoclinic, $P2_1/n$, $a = 13{\cdot}708$ (6), $b = 11{\cdot}755$ (4), $c = 15{\cdot}491$ (5) Å, $\beta = 108{\cdot}92$ (3)°, $V = 2361{\cdot}3$ Å^3, $Z = 4$, $D_x = 1{\cdot}37$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 0{\cdot}66$ cm^{-1}, $F(000) = 1024$, $T = 293$ K, final $R = 0{\cdot}051$ for 1884 observed [$F_o \geq 5\sigma(F_o)$] reflections. The 3-methoxycarbonyl group and the 4-aryl ring occupy quasiaxial positions in the observed structure. There is no crystallographically imposed symmetry. Several intermolecular van der Waals interactions of note occur in this compound.

Introduction. Synthetic congeners of the American mayapple constituent podophyllotoxin have sparked much interest in recent years as anticancer agents (Beers, Imakura, Dai, Li, Cheng & Lee, 1988; Jardine, 1980). The epipodophyllotoxin derivatives etoposide and teniposide are two such therapeutically useful preparations (Kaneko & Wong, 1987; Keller-Juslen, Kuhn, Wartburg & Stahelin, 1971). The natural products and the synthetic modifications elicit their antineoplastic effect by strikingly different mechanisms, however. The natural lignans induce metaphase arrest in dividing cells by reversible binding to tubulin, which in turn disrupts mitotic spindle formation and microtubule assembly (Jardine, 1980; Loike & Horwitz, 1976). In contrast, etoposide and teniposide neither bind nor inhibit tubulin or prevent microtubule assembly at relevant concentrations. These compounds instead exert their anticancer activity by arresting cell division at the S or G_2 phase of the cell cycle through an interaction with DNA topoisomerase II (Chow, MacDonald & Ross, 1988; Kohn, 1987). The latter interaction leads to an inhibition of DNA catenation activity and the production of DNA single- and double-strand breaks. In conjunction with our synthetic investigations on the podophyllotoxins (Peterson, Winter, Do & Rogers, 1989; Peterson, Do & Rogers, 1988), we are interested in ascertaining the molecular requirements associated with the specific manifestation of each of the above biological *modus operandi*. Such knowledge is anticipated to permit the scientifically sound design of new anticancer drugs that are based upon natural product models. Herein we describe the X-ray crystal structure and an analysis of the closest contacts between neighboring molecules in the crystal lattice for dimethyl 1-methoxy-6,7-methylene-

*Authors to whom correspondence should be addressed.
†Current address: Department of Pharmacognosy, School of Pharmacy, The University of Mississippi, University, MS 38677, USA.

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dioxy-4-(3,4,5-trimethoxyphenyl)-*trans*-3,4-dihydronaphthalene-2,3-dicarboxylate. The title compound and its congeneric series provide new molecular probes for structure–activity studies with regard to partial aromatization of the natural and *epi*-podophyllotoxin ring systems (Beers *et al.*, 1988).

Experimental. The title dihydronaphthalene was obtained in 95% isolated yield by reaction of dimethyl 1-hydroxy-6,7-methylenedioxy-4-(3,4,5-trimethoxyphenyl)-*trans*-3,4-dihydronaphthalene-2,3-dicarboxylate with ethereal diazomethane at 273 K (Peterson *et al.*, 1989). The product was purified by flash chromatography on silica gel while eluting with 2% acetone in chloroform. Colorless, parallelepiped crystals (m.p. 433–435 K), suitable for X-ray analysis, were obtained by slow recrystallization from chloroform–pentane. The X-ray structure was in full agreement with the spectral and analytical data. Physical data: IR ($CHCl_3$) 2985, 2940, 2920, 2830, 1725, 1680, 1585, 1495, 1475, 1450, 1430, 1370, 1320, 1270, 1220, 1190, 1120, 1030, 1000, 925, 725 cm^{-1}; ^1H NMR ($CDCl_3$, 200 MHz) δ 7·19 (*s*, 1H), 6·64 (*s*, 1H), 6·28 (*s*, 2H), 6·00 (center *AB* quartet, J = 0·94 Hz, 2H), 4·50 (*d*, J = 2·42 Hz, 1H), 4·05 (*d*, J = 2·42 Hz, 1H), 3·87 (*s*, 3H), 3·80 (*s*, 3H), 3·76 (*s*, 3H), 3·75 (*s*, 6H), 3·63 (*s*, 3H); ^{13}C NMR ($CDCl_3$, 50 MHz) δ 173·00, 166·41, 162·20, 153·14, 149·59, 147·51, 137·25, 137·07, 133·73, 124·54, 109·50, 107·60, 104·93, 104·84, 101·60, 61·42, 60·75, 56·08, 52·43, 51·78, 48·71, 45·89. Analysis: calculated for $C_{25}H_{26}O_{10}$: C 61·73, H 5·39; found: C 61·63, H 5·32%. D_m not determined. Crystal 0·30 × 0·40 × 0·35 mm. Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$. Cell constants from setting angles of 25 reflections ($\theta > 18°$). Correction for Lorentz–polarization effect, no correction for absorption. $\theta_{max} = 46°$; h 0 to 15, k 0 to 12, l −16 to 16. Standard reflections observed every 3600 s of data collection time: 600, 060, 006. Variation = ±2%. 3578 reflections measured, 1884 independent observed reflections [$F_o \geq 5\sigma(F_o)$]. Structure solved utilizing *MULTAN* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) direct-methods program. Geometrically constrained H atoms were placed in calculated positions 0·95 Å from the bonded C atom and allowed to ride on that atom with B fixed at 5·5 $Å^2$. The methyl H atoms were located from a difference Fourier map and included with fixed contributions (B = 5·5 $Å^2$). Scattering factors from *International Tables for X-ray Crystallography* (1974); structure refined with *SHELX*76 (Sheldrick, 1976). $\sum w(|F_o| - |F_c|)^2$ minimized, $w = [\sigma(F_o)^2 + 0{\cdot}00006F_o^2]^{-1}$, 316 parameters varied. R = 0·051, wR = 0·051, S = 1·12. Δ/σ in final least-squares refinement cycle < 0·01, $\Delta\rho$ < 0·2 e $Å^{-3}$ in final difference map.

Table 1. *Final fractional coordinates and equivalent isotropic thermal parameters for* $C_{25}H_{26}O_{10}$

$B_{eq} = \frac{4}{3}[a^2\beta_{11} + b^2\beta_{22} + c^2\beta_{33} + ab(\cos\gamma)\beta_{12} + ac(\cos\beta)\beta_{13} + bc(\cos\alpha)\beta_{23}]$.

	x	y	z	B_{eq}
O(1)	1·0948 (3)	0·3377 (3)	0·3334 (2)	3·73
O(2)	1·0710 (3)	0·1436 (3)	0·3108 (3)	4·06
O(3)	0·7708 (2)	0·5024 (3)	0·3811 (2)	2·47
O(4)	0·4753 (3)	0·3791 (3)	0·3150 (2)	3·93
O(5)	0·5863 (3)	0·4882 (4)	0·4170 (3)	5·18
O(6)	0·5985 (3)	0·3426 (3)	0·1479 (2)	3·66
O(7)	0·5347 (3)	0·1678 (3)	0·1368 (2)	3·74
O(8)	0·6512 (3)	−0·1691 (3)	0·4977 (2)	3·95
O(9)	0·6864 (3)	−0·0381 (3)	0·6453 (2)	2·83
O(10)	0·7435 (3)	0·1786 (3)	0·6440 (2)	3·55
C(1)	0·8128 (4)	0·2086 (4)	0·3202 (3)	1·94
C(2)	0·8914 (4)	0·1404 (4)	0·3104 (3)	2·44
C(3)	0·9827 (4)	0·1922 (5)	0·3172 (3)	2·60
C(4)	0·9966 (4)	0·3084 (5)	0·3304 (3)	2·45
C(5)	0·9221 (4)	0·3777 (4)	0·3405 (3)	2·32
C(6)	0·8278 (4)	0·3254 (4)	0·3356 (3)	2·00
C(7)	0·7451 (4)	0·3934 (4)	0·3505 (3)	2·05
C(8)	0·6493 (4)	0·3549 (4)	0·3325 (3)	2·01
C(9)	0·6216 (3)	0·2397 (4)	0·2864 (3)	2·03
C(10)	0·7119 (3)	0·1544 (4)	0·3170 (3)	1·88
C(11)	0·7148 (4)	0·0998 (4)	0·4075 (3)	2·05
C(12)	0·6863 (4)	−0·0123 (4)	0·4089 (3)	2·50
C(13)	0·6780 (4)	−0·0587 (4)	0·4885 (3)	2·50
C(14)	0·6971 (4)	0·0069 (4)	0·5668 (3)	2·20
C(15)	0·7280 (4)	0·1188 (4)	0·5652 (3)	2·41
C(16)	0·7388 (4)	0·1652 (4)	0·4862 (3)	2·46
C(17)	0·6271 (6)	−0·2399 (5)	0·4189 (4)	5·63
C(18)	0·5842 (5)	−0·0366 (6)	0·6462 (4)	4·80
C(19)	0·7754 (5)	0·2945 (5)	0·6446 (3)	4·70
C(20)	0·5794 (4)	0·2446 (4)	0·1822 (3)	2·43
C(21)	0·5556 (5)	0·3522 (5)	0·0491 (3)	4·35
C(22)	0·5698 (4)	0·4169 (4)	0·3589 (3)	2·67
C(23)	0·3928 (4)	0·4282 (6)	0·3426 (4)	4·82
C(24)	1·1387 (5)	0·2361 (6)	0·3132 (4)	4·39
C(25)	0·8299 (4)	0·5121 (4)	0·4772 (3)	3·44

Discussion. Fractional coordinates and B_{eq} values are given in Table 1,* bond distances and angles in Table 2, and an *ORTEP* drawing (Johnson, 1976) in Fig. 1. A cell packing diagram is shown in Fig. 2.

The *trans*, quasidiaxial stereorelationship between the 3-methoxycarbonyl and 4-aryl groups is apparent upon examination of the *ORTEP* diagram. Indicative that both substituents indeed occupy quasiaxial positions is the C(11)—C(10)—C(9)—C(20) torsion angle of −148·7° and the small vicinal hydrogen-coupling constant of 2·42 Hz between C(10)—H and C(9)—H. It is important to note the absence of 1,3-quasidiaxial interactions when the molecule adopts this conformation (Ahmed, Lehrer & Stevenson, 1973; Ayres, 1969).

Several structural alterations were noted when the crystal structure of the title compound was compared with that for its desmethoxy synthetic precursor, dimethyl 1-hydroxy-6,7-methylenedioxy-4-(3,4,5-trimethoxyphenyl)-*trans*-3,4-dihydronaphthalene-2,3-

*Lists of structure factors, anisotropic thermal parameters, least-squares-planes results, torsion angles, and final fractional coordinates for H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51947 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond distances* (Å) *and angles* (°) *for* $C_{25}H_{26}O_{10}$

O(1)—C(4)	1·377 (6)	O(1)—C(24)	1·417 (6)
O(2)—C(3)	1·372 (6)	O(2)—C(24)	1·422 (6)
O(3)—C(7)	1·372 (5)	O(3)—C(25)	1·451 (5)
O(4)—C(22)	1·328 (6)	O(4)—C(23)	1·451 (6)
O(5)—C(22)	1·197 (5)	O(6)—C(20)	1·330 (6)
O(6)—C(21)	1·455 (5)	O(7)—C(20)	1·185 (5)
O(8)—C(13)	1·369 (5)	O(8)—C(17)	1·424 (6)
O(9)—C(14)	1·378 (5)	O(9)—C(18)	1·406 (6)
O(10)—C(15)	1·364 (5)	O(10)—C(19)	1·429 (6)
C(1)—C(2)	1·391 (6)	C(1)—C(6)	1·397 (6)
C(1)—C(10)	1·509 (6)	C(2)—C(3)	1·365 (7)
C(3)—C(4)	1·385 (7)	C(4)—C(5)	1·355 (6)
C(5)—C(6)	1·412 (6)	C(6)—C(7)	1·465 (7)
C(7)—C(8)	1·331 (6)	C(8)—C(9)	1·520 (6)
C(8)—C(22)	1·474 (7)	C(9)—C(10)	1·544 (6)
C(9)—C(20)	1·529 (6)	C(10)—C(11)	1·531 (6)
C(11)—C(12)	1·377 (6)	C(11)—C(16)	1·387 (6)
C(12)—C(13)	1·386 (6)	C(13)—C(14)	1·388 (6)
C(14)—C(15)	1·385 (6)	C(15)—C(16)	1·392 (6)

C(4)—O(1)—C(24)	105·2 (4)	C(3)—O(2)—C(24)	105·3 (4)
C(7)—O(3)—C(25)	115·0 (3)	C(22)—O(4)—C(23)	116·1 (4)
C(20)—O(6)—C(21)	115·0 (4)	C(13)—O(8)—C(17)	117·4 (4)
C(14)—O(9)—C(18)	113·3 (4)	C(15)—O(10)—C(19)	117·1 (4)
C(2)—C(1)—C(6)	120·6 (5)	C(2)—C(1)—C(10)	119·2 (4)
C(6)—C(1)—C(10)	120·2 (5)	C(1)—C(2)—C(3)	117·2 (5)
O(2)—C(3)—C(2)	128·1 (5)	O(2)—C(3)—C(4)	109·8 (5)
C(2)—C(3)—C(4)	122·0 (5)	O(1)—C(4)—C(3)	109·7 (5)
O(1)—C(4)—C(5)	127·7 (5)	C(3)—C(4)—C(5)	122·5 (5)
C(4)—C(5)—C(6)	116·3 (5)	C(1)—C(6)—C(5)	121·2 (5)
C(1)—C(6)—C(7)	119·0 (5)	C(5)—C(6)—C(7)	119·7 (4)
O(3)—C(7)—C(6)	116·0 (4)	O(3)—C(7)—C(8)	121·0 (5)
C(6)—C(7)—C(8)	122·9 (4)	C(7)—C(8)—C(9)	118·7 (4)
C(7)—C(8)—C(22)	122·8 (4)	C(9)—C(8)—C(22)	118·4 (4)
C(8)—C(9)—C(10)	112·4 (4)	C(8)—C(9)—C(20)	114·5 (4)
C(10)—C(9)—C(20)	109·9 (4)	C(1)—C(10)—C(9)	111·8 (4)
C(1)—C(10)—C(11)	113·3 (4)	C(9)—C(10)—C(11)	109·5 (4)
C(10)—C(11)—C(12)	119·5 (4)	C(10)—C(11)—C(16)	120·0 (4)
C(12)—C(11)—C(16)	120·3 (4)	C(11)—C(12)—C(13)	119·7 (4)
O(8)—C(13)—C(12)	124·5 (4)	O(8)—C(13)—C(14)	114·6 (4)
C(12)—C(13)—C(14)	120·8 (4)	O(9)—C(14)—C(13)	121·0 (4)
O(9)—C(14)—C(15)	120·0 (4)	C(13)—C(14)—C(15)	119·0 (4)
O(10)—C(15)—C(14)	115·7 (4)	O(10)—C(15)—C(16)	123·7 (4)
C(14)—C(15)—C(16)	120·5 (4)	C(11)—C(16)—C(15)	119·6 (4)
O(6)—C(20)—O(7)	123·6 (5)	O(6)—C(20)—C(9)	113·5 (4)
O(7)—C(20)—C(9)	122·9 (5)	O(4)—C(22)—O(5)	122·3 (5)
O(4)—C(22)—C(8)	112·2 (4)	O(5)—C(22)—C(8)	125·3 (5)
O(1)—C(24)—O(2)	109·3 (4)		

H(1)[C(17)]···O(5^{i})	2·28	C(17)···O(5^{i})	3·244 (7)
H(1)[C(24)]···H(1)[C(19^{ii})]	2·34	C(24)···H(1)[C(19^{ii})]	3·00
H(1)[C(24)]···O(10^{ii})	2·64	H(1)[C(24)]···C(19^{ii})	2·84
H(1)[C(19)]···H(2)[C(18^{iii})]	2·35	H(1)[C(19)]···O(9^{iii})	2·59
H(1)[C(19)]···C(18^{iii})	2·75		
H(3)[C(21)]···H(1)[C(25^{iv})]	2·35	O(7)···H(1)[C(5^{iv})]	2·51
H(1)[C(2)]···O(6^{iv})	2·68		
H(2)[C(17)]···H(3)[C(18^{v})]	2·62	H(1)[C(17)]···H(1)[C(23^{v})]	2·47
H(1)[C(18)]···H(1)[C(18^{v})]	2·65		
H(2)[C(23)]···O(10^{vi})	2·50		
O(8)···H(2)[C(24^{vii})]	2·54	O(9)···H(2)[C(24^{vii})]	2·66

Symmetry codes: (i) $x, y-1, z$; (ii) $\frac{1}{2}+x, \frac{1}{2}-y, z-\frac{1}{2}$; (iii) $\frac{3}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$; (iv) $\frac{3}{2}-x, y-\frac{1}{2}, \frac{1}{2}-z$; (v) $1-x, -y, 1-z$; (vi) $x-\frac{1}{2}, \frac{1}{2}-y, z-\frac{1}{2}$; (vii) $2-x, -y, 1-z$.

dicarboxylate (Peterson *et al.*, 1989). The same atom-numbering scheme is utilized for both compounds. Atoms C(1) through C(6), C(24), O(1) and O(2) of the title compound describe a plane to within 0·068 Å. Atoms C(7) and C(10) deviate from this plane by 0·065 and 0·004 Å, respectively. Surprisingly, atoms C(10), C(1), C(6), C(7) and C(8) of the title compound define a unique plane to within 0·090 Å, with the latter plane intersecting the former at an angle of 2·62°. This finding is in contrast to the 1-hydroxy precursor where atoms C(1) through C(8), C(10), C(24), O(1) and O(2) collectively lie in a plane. The dihydronaphthalene *B* ring of the title compound puckers about atom C(9) to relieve steric interactions between the C(20) and C(22) methoxycarbonyl groups. The C(1)—C(10)—C(9)—C(8) torsion angle of −43·9° and the 0·526 Å deviation of atom C(9) from the C(10)—C(1)—C(6)—C(7)—C(8) plane support this observation. Atom plane C(7), C(6), C(8) and O(3) intersects the C(10)—C(1)—C(6)—C(7)—C(8) plane at an angle of 10·77°, and carbonyl atom C(22) lies −0·195 Å out of the C(7), C(6), C(8) and O(3) plane of the title compound. This is again in contrast to the 1-hydroxy precursor where planarity is observed for atoms C(7), C(8), C(22), O(5) and O(3) to within 0·007 Å. Finally, the pendant aryl-ring atoms, C(11) through C(16), of the title compound describe a plane to within 0·019 Å.

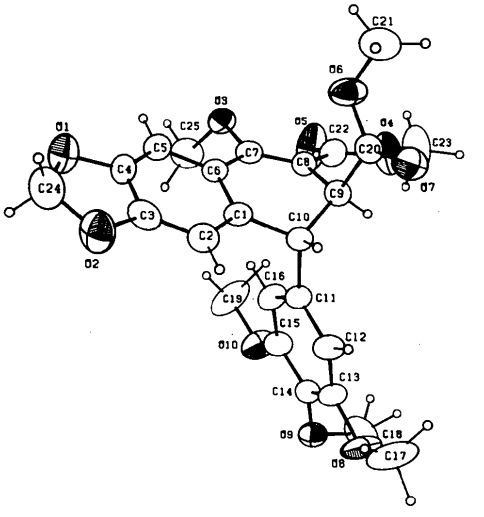

Fig. 1. Thermal-ellipsoid plot of the title compound showing the atom-numbering scheme. The H-atom radii are arbitrarily reduced.

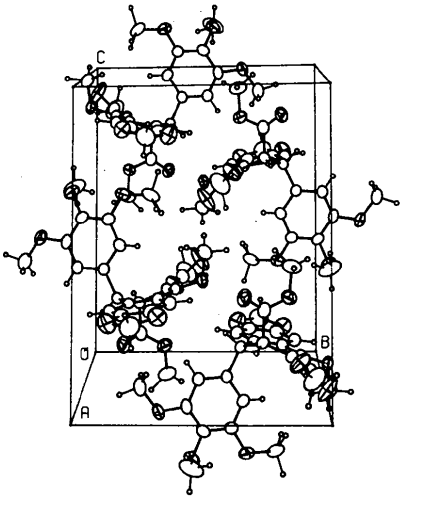

Fig. 2. Cell-packing diagram of the title compound.

This plane intersects the *B* ring plane, comprised of atoms C(10), C(1), C(6), C(7) and C(8), at an angle of 72·70°. The latter angle is substantially smaller than that observed in the 1-hydroxy precursor, where the pendant aryl ring was nearly perpendicular (88·0°) to the dihydronaphthalene ring plane. These pronounced structural changes of the title compound in comparison to its 1-hydroxy precursor are most easily explained by the disruption of the strong hydrogen bond between O atoms O(3) and O(5) in the latter.

An analysis of the closest intermolecular contact distances reveals that van der Waals forces are likely to be the dominant stabilizing force in the crystal lattice of the title compound. Several such interactions were noted to occur between neighboring molecules and the shortest of these have been tabulated with their symmetry relationships in Table 2.

In conclusion, several topographical alterations are found between the title compound and its 1-hydroxy precursor as a result of simple methyl substitution for an H atom. The capacity of a podophyllotoxin analogue to bind to tubulin or to trap a DNA–topoisomerase II complex is dramatically affected by what often appear to be minor chemical modifications (Chow *et al.*, 1988; Kohn, 1987; Jardine, 1980; Loike & Horwitz, 1976). Extensive chemical, structural and biological investigations of these and other podophyllotoxin derivatives are now in progress in our laboratories to ascertain the molecular requirements associated with these biological modes of action.

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Structure of Methyl 5-Phenyl-2-propionyl-3-pyrrolecarboxylate

BY M. NETHAJI, VASANTHA PATTABHI* AND V. G. THAILAMBAL

Department of Crystallography and Biophysics,† University of Madras, Guindy Campus, Madras-600 025, *India*

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Abstract. $C_{15}H_{15}NO_3$, $M_r = 257{\cdot}4$, monoclinic, $P2_1/n$, $a = 10{\cdot}070\ (2)$, $b = 5{\cdot}335\ (3)$, $c = 24{\cdot}23\ (1)$ Å, $\beta = 91{\cdot}60\ (3)°$, $V = 1301\ (2)$ Å^3, $Z = 4$, D_m (flotation) = $1{\cdot}312\ (3)$, $D_x = 1{\cdot}314$ g cm^{-3}, Cu $K\alpha(\lambda = 1{\cdot}5418$ Å), $\mu = 6{\cdot}64$ cm^{-1}, $F(000) = 544$, $T = 295$ K, final $R(F) = 0{\cdot}037$, $wR = 0{\cdot}035$ for 850 significant reflections, $I \geq 2{\cdot}5\sigma(I)$. The phenyl ring and the pyrrole ring are

* To whom correspondence should be addressed.
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