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8-Methoxy-3-(4-methylbenzylidene)-6-(prop-1-enyl)chroman-4-one

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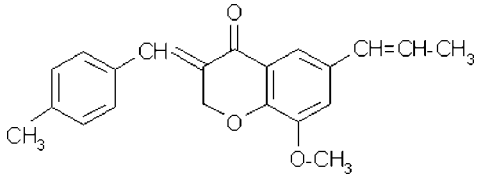
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.120; data-to-parameter ratio = 13.4.

In the title compound, $C_{21}H_{20}O_3$, the tolyl ring makes a dihedral angle of 31.11 (6)° with the benzene ring of the chromanone unit. The pyrone ring adopts a half-chair conformation. The molecular structure is stabilized by a weak intramolecular C—H···O interaction and the crystal packing is stabilized by weak intermolecular C—H···O interactions and a C—H···π interaction.

Related literature

For related lituerature, see: Puviarasan *et al.* (1998); Tillekeratne *et al.* (2001); Nissa *et al.* (2001); Kang *et al.* (2004); Wu, Xu, Wan *et al.* (2005); Wu, Xu, Zhou *et al.* (2005); Schollmeyer *et al.* (2005); Suresh *et al.* (2007).



Experimental

Crystal data

$C_{21}H_{20}O_3$
M_r = 320.37
Monoclinic, $P2_1/n$
a = 6.8550 (5) Å
b = 11.6264 (8) Å
c = 20.9669 (14) Å
β = 96.947 (1)°
V = 1658.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.18 × 0.11 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.984, T_{max} = 0.995
17310 measured reflections
2941 independent reflections
2054 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.120
S = 1.05
2941 reflections
220 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

Cg is the centroid of the C11/C14–C17/C12 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O2	0.93	2.39	2.784 (2)	106
C7—H7C···O2^{i}	0.96	2.57	3.512 (4)	166
C10—H10B···O2^{ii}	0.97	2.46	3.246 (4)	138
C21—H21B···Cg^{iii}	0.96	2.86	3.722 (2)	150

Symmetry codes: (i) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x-1, y, z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2242).

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supplementary materials

Acta Cryst. (2008). E**64**, o27 [**doi:10.1107/S1600536807060989**]

8-Methoxy-3-(4-methylbenzylidene)-6-(prop-1-enyl)chroman-4-one

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Comment

The chromanone moiety present in the title compound consisting of the pyrone ring and benzene ring plays an important role in many areas of medicines such as inhibition of HIV replication (Tillekeratne *et al.*, 2001). The naturally occurring classes of compounds to which they belong, the benzylidene chroman-4-ones, have identified as a potential source of new anti-fungal agents (Kang *et al.*, 2004).

The geometric parameters in the title compound agree with the reported values of similar structure (Puviarasan *et al.*, 1998; Wu, Xu, Wan *et al.*, 2005; Wu, Xu, Zhou *et al.*, 2005; Schollmeyer *et al.*, 2005; Nissa *et al.*, 2001; Suresh *et al.*, 2007). The methylphenyl ring makes a dihedral angle of 31.11 (6)° with the benzene ring of the chromanone unit.

The molecular structure is stabilized by a weak intramolecular C—H···O interaction and the crystal packing is stabilized by weak intermolecular C—H···O interactions and a C—H···π interaction involving the C11/C14—C17/C12 (Centroid *Cg*) ring.

Experimental

Baylis-Hillman reaction of *p*-tolualdehyde with methyl acrylate afforded methyl-3-hydroxy-3-(*p*-tolyl-)-2-methyene propanoate, which was converted to methyl-(2,2)–2-bromomethyl-3-(*p*-tolyl)-prop-2-enoate on treatment with hydrobromic acid in presence of concentrated sulfuric acid. The product was treated with isoeugenol in presence of potassium carbonate and acetone to give methyl-3-(*p*-tolyl)-2-(2-methoxy-4-prop-1-enyl)-phenoxy methyl-prop-2-enoate, which was hydrolysed by alkali solution to give the prop-2-enoic acid. This acid was cyclized with trifluoro acetic anhydride in dichloromethane to yield 3-(4-methyl)benzylidine-6-prop-1-enyl-8-methoxyhroman-4-one.

Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic CH, C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for CH_2, C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for CH_3.

Figures

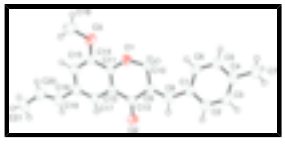

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

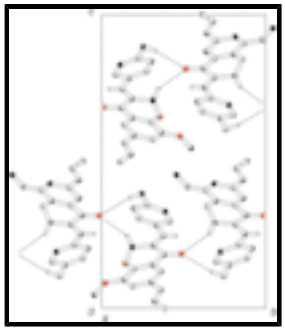

Fig. 2. A partial packing diagram of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

8-Methoxy-3-(4-methylbenzylidene)-6-(prop-1-enyl)chroman-4-one

Crystal data

$C_{21}H_{20}O_3$	$Z = 4$
$M_r = 320.37$	$F_{000} = 680$
Monoclinic, $P2_1/n$	$D_x = 1.283$ Mg m^{-3}
Hall symbol: -P 2yn	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.8550$ (5) Å	$\theta = 1.9$–27.2°
$b = 11.6264$ (8) Å	$\mu = 0.09$ mm^{-1}
$c = 20.9669$ (14) Å	$T = 293$ (2) K
$\beta = 96.947$ (1)°	Prism, yellow
$V = 1658.8$ (2) Å^3	0.18 × 0.11 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer	2941 independent reflections
Radiation source: fine-focus sealed tube	2054 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.039$
$T = 293$(2) K	$\theta_{max} = 25.1^\circ$
ω scan	$\theta_{min} = 2.0^\circ$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -8 \rightarrow 8$
$T_{min} = 0.984$, $T_{max} = 0.995$	$k = -13 \rightarrow 13$
17310 measured reflections	$l = -24 \rightarrow 24$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.120$	$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 0.331P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.006$

2941 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
220 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
O1	0.72176 (17)	0.14365 (10)	0.15211 (6)	0.0560 (4)
C11	0.5481 (2)	0.19760 (14)	0.13450 (8)	0.0431 (4)
O3	0.45043 (19)	0.02250 (10)	0.08579 (7)	0.0622 (4)
O2	0.66403 (19)	0.48556 (10)	0.18481 (7)	0.0616 (4)
C17	0.3351 (3)	0.36251 (16)	0.12538 (8)	0.0484 (5)
H17	0.3131	0.4391	0.1352	0.058*
C12	0.5149 (2)	0.31169 (14)	0.14850 (8)	0.0431 (4)
C14	0.4016 (3)	0.13375 (14)	0.09710 (9)	0.0467 (4)
C13	0.6739 (2)	0.38058 (14)	0.18298 (8)	0.0439 (4)
C9	0.8458 (2)	0.31532 (14)	0.21405 (8)	0.0429 (4)
C15	0.2262 (3)	0.18653 (16)	0.07531 (9)	0.0519 (5)
H15	0.1286	0.1442	0.0511	0.062*
C16	0.1906 (3)	0.30248 (16)	0.08862 (9)	0.0498 (5)
C8	0.9929 (2)	0.37410 (15)	0.24703 (8)	0.0461 (4)
H8	0.9749	0.4534	0.2468	0.055*
C19	0.0062 (3)	0.36065 (18)	0.06302 (10)	0.0593 (5)
H19	−0.0081	0.4355	0.0774	0.071*
C1	1.1769 (2)	0.33551 (15)	0.28342 (8)	0.0436 (4)
C20	−0.1372 (3)	0.32230 (19)	0.02369 (10)	0.0652 (6)
H20	−0.1260	0.2473	0.0092	0.078*
C10	0.8380 (3)	0.18735 (15)	0.20825 (10)	0.0562 (5)
H10A	0.9711	0.1588	0.2087	0.067*
H10B	0.7866	0.1565	0.2458	0.067*
C2	1.3272 (3)	0.41550 (16)	0.29596 (9)	0.0545 (5)
H2	1.3065	0.4906	0.2814	0.065*
C4	1.5439 (3)	0.27688 (17)	0.35240 (9)	0.0506 (5)
C3	1.5067 (3)	0.38657 (17)	0.32947 (9)	0.0568 (5)
H3	1.6042	0.4423	0.3366	0.068*

C6	1.2140 (3)	0.22494 (16)	0.30760 (9)	0.0532 (5)
H6	1.1164	0.1691	0.3012	0.064*
C5	1.3935 (3)	0.19739 (17)	0.34087 (10)	0.0575 (5)
H5	1.4144	0.1227	0.3561	0.069*
C21	−0.3191 (3)	0.3854 (2)	−0.00093 (11)	0.0740 (7)
H21A	−0.3129	0.4622	0.0160	0.111*
H21B	−0.4310	0.3464	0.0122	0.111*
H21C	−0.3309	0.3884	−0.0470	0.111*
C7	1.7370 (3)	0.2454 (2)	0.39040 (10)	0.0685 (6)
H7A	1.7215	0.2423	0.4353	0.103*
H7B	1.8339	0.3022	0.3835	0.103*
H7C	1.7788	0.1716	0.3766	0.103*
C18	0.3117 (3)	−0.04441 (18)	0.04568 (11)	0.0714 (6)
H18A	0.1910	−0.0487	0.0645	0.107*
H18B	0.3629	−0.1205	0.0414	0.107*
H18C	0.2875	−0.0092	0.0041	0.107*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0484 (7)	0.0417 (7)	0.0717 (9)	0.0082 (6)	−0.0177 (6)	−0.0105 (6)
C11	0.0403 (9)	0.0413 (10)	0.0459 (10)	0.0016 (7)	−0.0016 (8)	0.0025 (7)
O3	0.0573 (8)	0.0466 (8)	0.0776 (10)	−0.0033 (6)	−0.0127 (7)	−0.0133 (7)
O2	0.0621 (8)	0.0375 (7)	0.0800 (10)	0.0054 (6)	−0.0125 (7)	−0.0039 (6)
C17	0.0456 (10)	0.0472 (10)	0.0509 (11)	0.0076 (8)	−0.0001 (9)	−0.0037 (8)
C12	0.0412 (9)	0.0423 (10)	0.0445 (10)	0.0036 (7)	−0.0003 (8)	0.0010 (7)
C14	0.0478 (10)	0.0407 (10)	0.0503 (10)	−0.0017 (8)	0.0006 (8)	−0.0019 (8)
C13	0.0445 (10)	0.0387 (10)	0.0474 (10)	0.0027 (7)	0.0010 (8)	−0.0017 (8)
C9	0.0424 (10)	0.0386 (9)	0.0462 (10)	0.0010 (7)	−0.0005 (8)	0.0009 (7)
C15	0.0420 (10)	0.0592 (12)	0.0517 (11)	−0.0058 (9)	−0.0056 (8)	−0.0034 (9)
C16	0.0427 (10)	0.0560 (11)	0.0494 (10)	0.0043 (8)	0.0005 (8)	−0.0014 (8)
C8	0.0466 (11)	0.0395 (9)	0.0512 (10)	−0.0006 (8)	0.0015 (8)	0.0011 (8)
C19	0.0462 (11)	0.0651 (13)	0.0639 (13)	0.0047 (9)	−0.0046 (10)	−0.0083 (10)
C1	0.0400 (9)	0.0448 (10)	0.0447 (10)	−0.0033 (8)	−0.0004 (8)	−0.0017 (8)
C20	0.0523 (12)	0.0696 (13)	0.0702 (14)	0.0056 (10)	−0.0074 (10)	−0.0053 (11)
C10	0.0514 (11)	0.0419 (10)	0.0685 (13)	0.0005 (8)	−0.0197 (10)	−0.0022 (9)
C2	0.0533 (11)	0.0458 (10)	0.0620 (12)	−0.0098 (9)	−0.0036 (9)	0.0048 (9)
C4	0.0388 (10)	0.0624 (12)	0.0496 (11)	−0.0015 (9)	0.0014 (8)	−0.0043 (9)
C3	0.0450 (11)	0.0589 (12)	0.0643 (12)	−0.0164 (9)	−0.0016 (9)	0.0006 (10)
C6	0.0446 (10)	0.0469 (10)	0.0643 (12)	−0.0085 (8)	−0.0086 (9)	0.0046 (9)
C5	0.0515 (11)	0.0480 (11)	0.0688 (13)	−0.0012 (9)	−0.0091 (10)	0.0063 (9)
C21	0.0482 (12)	0.0975 (17)	0.0734 (15)	0.0099 (11)	−0.0044 (11)	0.0110 (13)
C7	0.0460 (11)	0.0862 (16)	0.0692 (14)	0.0021 (10)	−0.0093 (10)	−0.0048 (12)
C18	0.0684 (14)	0.0598 (13)	0.0821 (16)	−0.0118 (11)	−0.0073 (12)	−0.0215 (11)

Geometric parameters (Å, °)

O1—C11	1.3567 (19)	C1—C6	1.394 (2)
O1—C10	1.432 (2)	C20—C21	1.484 (3)

C11—C12	1.383 (2)	C20—H20	0.9300
C11—C14	1.408 (2)	C10—H10A	0.9700
O3—C14	1.364 (2)	C10—H10B	0.9700
O3—C18	1.422 (2)	C2—C3	1.383 (3)
O2—C13	1.2232 (19)	C2—H2	0.9300
C17—C16	1.370 (2)	C4—C3	1.376 (3)
C17—C12	1.400 (2)	C4—C5	1.384 (3)
C17—H17	0.9300	C4—C7	1.505 (2)
C12—C13	1.470 (2)	C3—H3	0.9300
C14—C15	1.378 (2)	C6—C5	1.377 (2)
C13—C9	1.484 (2)	C6—H6	0.9300
C9—C8	1.339 (2)	C5—H5	0.9300
C9—C10	1.493 (2)	C21—H21A	0.9600
C15—C16	1.404 (3)	C21—H21B	0.9600
C15—H15	0.9300	C21—H21C	0.9600
C16—C19	1.476 (2)	C7—H7A	0.9600
C8—C1	1.464 (2)	C7—H7B	0.9600
C8—H8	0.9300	C7—H7C	0.9600
C19—C20	1.284 (3)	C18—H18A	0.9600
C19—H19	0.9300	C18—H18B	0.9600
C1—C2	1.389 (2)	C18—H18C	0.9600
C11—O1—C10	116.25 (14)	O1—C10—H10A	108.4
O1—C11—C12	123.15 (15)	C9—C10—H10A	108.4
O1—C11—C14	116.80 (15)	O1—C10—H10B	108.4
C12—C11—C14	119.95 (15)	C9—C10—H10B	108.4
C14—O3—C18	117.44 (14)	H10A—C10—H10B	107.5
C16—C17—C12	121.75 (17)	C3—C2—C1	121.84 (17)
C16—C17—H17	119.1	C3—C2—H2	119.1
C12—C17—H17	119.1	C1—C2—H2	119.1
C11—C12—C17	119.46 (15)	C3—C4—C5	117.07 (17)
C11—C12—C13	119.72 (15)	C3—C4—C7	121.62 (17)
C17—C12—C13	120.65 (15)	C5—C4—C7	121.27 (18)
O3—C14—C15	125.96 (16)	C4—C3—C2	121.27 (17)
O3—C14—C11	115.04 (15)	C4—C3—H3	119.4
C15—C14—C11	119.00 (16)	C2—C3—H3	119.4
O2—C13—C12	121.22 (15)	C5—C6—C1	120.76 (17)
O2—C13—C9	122.71 (15)	C5—C6—H6	119.6
C12—C13—C9	116.06 (14)	C1—C6—H6	119.6
C8—C9—C13	118.29 (15)	C6—C5—C4	122.31 (18)
C8—C9—C10	124.61 (15)	C6—C5—H5	118.8
C13—C9—C10	117.05 (14)	C4—C5—H5	118.8
C14—C15—C16	121.81 (16)	C20—C21—H21A	109.5
C14—C15—H15	119.1	C20—C21—H21B	109.5
C16—C15—H15	119.1	H21A—C21—H21B	109.5
C17—C16—C15	118.03 (16)	C20—C21—H21C	109.5
C17—C16—C19	120.01 (17)	H21A—C21—H21C	109.5
C15—C16—C19	121.95 (16)	H21B—C21—H21C	109.5
C9—C8—C1	131.33 (16)	C4—C7—H7A	109.5
C9—C8—H8	114.3	C4—C7—H7B	109.5

C1—C8—H8	114.3	H7A—C7—H7B	109.5
C20—C19—C16	129.0 (2)	C4—C7—H7C	109.5
C20—C19—H19	115.5	H7A—C7—H7C	109.5
C16—C19—H19	115.5	H7B—C7—H7C	109.5
C2—C1—C6	116.74 (16)	O3—C18—H18A	109.5
C2—C1—C8	117.80 (16)	O3—C18—H18B	109.5
C6—C1—C8	125.46 (15)	H18A—C18—H18B	109.5
C19—C20—C21	126.7 (2)	O3—C18—H18C	109.5
C19—C20—H20	116.7	H18A—C18—H18C	109.5
C21—C20—H20	116.7	H18B—C18—H18C	109.5
O1—C10—C9	115.55 (14)		
C10—O1—C11—C12	27.3 (2)	C12—C17—C16—C15	1.0 (3)
C10—O1—C11—C14	−156.35 (16)	C12—C17—C16—C19	−177.52 (17)
O1—C11—C12—C17	176.39 (16)	C14—C15—C16—C17	−1.2 (3)
C14—C11—C12—C17	0.2 (3)	C14—C15—C16—C19	177.31 (18)
O1—C11—C12—C13	1.2 (3)	C13—C9—C8—C1	178.65 (17)
C14—C11—C12—C13	−174.98 (16)	C10—C9—C8—C1	1.2 (3)
C16—C17—C12—C11	−0.6 (3)	C17—C16—C19—C20	173.4 (2)
C16—C17—C12—C13	174.58 (17)	C15—C16—C19—C20	−5.1 (3)
C18—O3—C14—C15	2.8 (3)	C9—C8—C1—C2	160.54 (19)
C18—O3—C14—C11	−177.03 (17)	C9—C8—C1—C6	−20.4 (3)
O1—C11—C14—O3	3.0 (2)	C16—C19—C20—C21	−179.4 (2)
C12—C11—C14—O3	179.47 (16)	C11—O1—C10—C9	−41.3 (2)
O1—C11—C14—C15	−176.79 (16)	C8—C9—C10—O1	−154.41 (17)
C12—C11—C14—C15	−0.4 (3)	C13—C9—C10—O1	28.1 (2)
C11—C12—C13—O2	165.08 (18)	C6—C1—C2—C3	1.5 (3)
C17—C12—C13—O2	−10.0 (3)	C8—C1—C2—C3	−179.40 (17)
C11—C12—C13—C9	−14.0 (2)	C5—C4—C3—C2	−0.5 (3)
C17—C12—C13—C9	170.86 (16)	C7—C4—C3—C2	−178.38 (18)
O2—C13—C9—C8	2.1 (3)	C1—C2—C3—C4	−0.5 (3)
C12—C13—C9—C8	−178.81 (16)	C2—C1—C6—C5	−1.5 (3)
O2—C13—C9—C10	179.76 (18)	C8—C1—C6—C5	179.48 (18)
C12—C13—C9—C10	−1.2 (2)	C1—C6—C5—C4	0.5 (3)
O3—C14—C15—C16	−178.93 (18)	C3—C4—C5—C6	0.5 (3)
C11—C14—C15—C16	0.9 (3)	C7—C4—C5—C6	178.39 (19)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O2	0.93	2.39	2.784 (2)	106
C7—H7C···O2^{i}	0.96	2.57	3.512 (4)	166
C10—H10B···O2^{ii}	0.97	2.46	3.246 (4)	138
C21—H21B···Cg^{iii}	0.96	2.86	3.722 (2)	150

Symmetry codes: (i) −*x*+5/2, *y*−1/2, −*z*+1/2; (ii) −*x*+3/2, *y*−1/2, −*z*+1/2; (iii) *x*−1, *y*, *z*.

Fig. 1

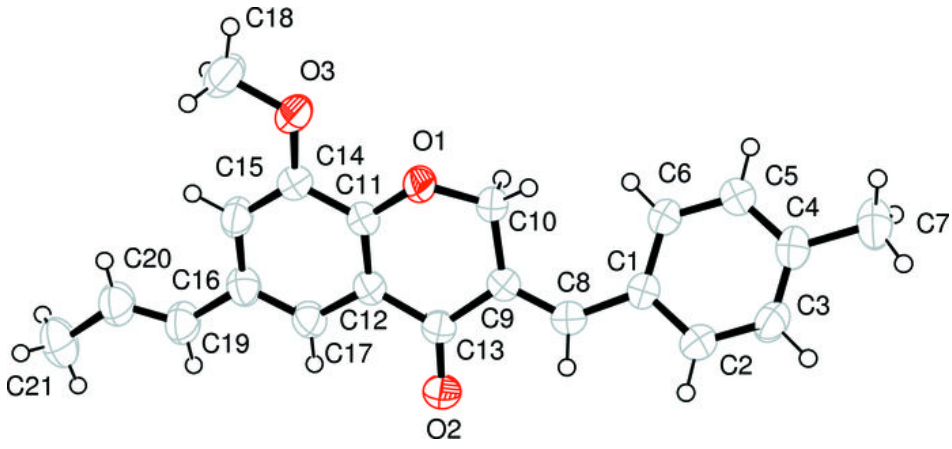
C18
O3
O1
C14
C15
C11
C10
C6
C5
C4
C7
C20
C16
C1
C8
C3
C12
C9
C19
C17
C13
C2
C21
O2

Fig. 2