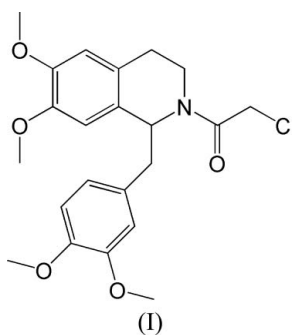


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yduangwenlong@126.com**Key indicators**Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.066  
 $wR$  factor = 0.173  
Data-to-parameter ratio = 15.6For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**2-Chloroacetyl-1-(3,4-dimethoxybenzyl)-6,7-  
dimethoxy-1,2,3,4-tetrahydroisoquinoline**

In the title compound,  $\text{C}_{22}\text{H}_{26}\text{ClNO}_5$ , there are two independent molecules in the asymmetric unit. The molecules are connected by  $\text{C}-\text{H}\cdots\text{O}$  interactions into one-dimensional chains running in the  $b$ -axis direction.

Received 1 September 2006  
Accepted 19 November 2006**Comment**

1-Benzyltetrahydroisoquinoline alkaloids occur widely in plants and have important biological activities. These naturally occurring products provide a basis for the development of therapeutic medicines with cardiovascular effects (Shama, 1972; Neumeyer *et al.*, 1977; Gibson & Tumbull, 1980). As part of a search for novel potent compounds with antiarrhythmic, calcium antagonistic, antihypertensive, neuromuscular blocking or platelet aggregation inhibitory activities, a series of substituted 1-benzyltetrahydroisoquinoline derivatives has been designed and synthesized (Huang *et al.*, 1990; Xu *et al.*, 1993; Zhang *et al.*, 2003; Wang *et al.*, 2005). *N*-Aminoacetylated tetrahydroisoquinolines are also useful as intermediates for the synthesis of isoquinoline derivatives. We report here the crystal structure of the title compound, (I).



There is a chiral C atom (C10) in (I), but the crystal structure is racemic. There are two independent molecules in the asymmetric unit, which has been chosen arbitrarily so that the molecules shown in Fig. 1 have opposite absolute configurations. Weak intermolecular  $\text{C}-\text{H}\cdots\text{O}$  interactions are observed (geometric details are given in Table 1). The molecules are linked into one-dimensional chains running in the  $b$ -axis direction by these  $\text{C}-\text{H}\cdots\text{O}$  interactions.

**Experimental**

The title compound was synthesized by acylation of tetrahydropapaverine and chloroacetyl chloride in dichloromethane, using anhydrous potassium carbonate as acid absorbing agent (He *et al.*, 1998). Single crystals were obtained by recrystallization from a mixture of ethyl acetate and ethanol (2:1).

## Crystal data

$C_{22}H_{26}ClNO_5$   
 $M_r = 419.89$   
 Monoclinic,  $P2_1/n$   
 $a = 16.380$  (3) Å  
 $b = 15.396$  (3) Å  
 $c = 16.536$  (3) Å  
 $\beta = 92.24$  (3)°  
 $V = 4167.0$  (14) Å<sup>3</sup>

$Z = 8$   
 $D_x = 1.339$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.22$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Block, colourless  
 $0.40 \times 0.40 \times 0.20$  mm

## Data collection

Enraf–Nonius CAD-4  
 diffractometer  
 $\omega/2\theta$  scans  
 Absorption correction:  $\psi$  scan  
 (North *et al.*, 1968)  
 $T_{\min} = 0.918$ ,  $T_{\max} = 0.958$   
 8446 measured reflections

8155 independent reflections  
 4379 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$   
 $\theta_{\text{max}} = 26.0^\circ$   
 3 standard reflections  
 every 200 reflections  
 intensity decay: none

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.066$   
 $wR(F^2) = 0.173$   
 $S = 1.02$   
 8155 reflections  
 524 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 1.23P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.26$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.36$  e Å<sup>-3</sup>  
 Extinction correction: *SHELXL97*  
 Extinction coefficient: 0.0039 (5)

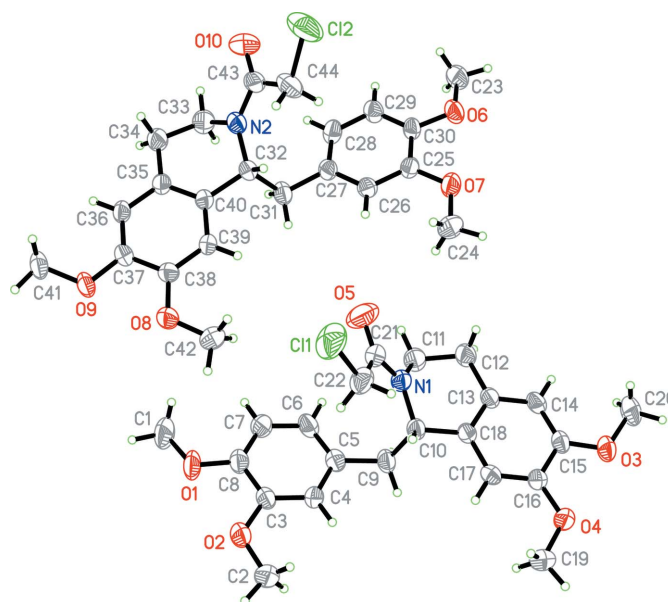


Figure 1

The asymmetric unit of the title compound, showing the atomic labelling. Displacement ellipsoids are drawn at the 50% probability level.

We are grateful for financial support by the National Natural Science Foundation of China (No. 30070861).

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C20-H20A\cdots O2^i$	0.96	2.51	3.383 (4)	152
$C22-H22A\cdots O8^{ii}$	0.97	2.57	3.400 (4)	144
$C22-H22A\cdots O9^{ii}$	0.97	2.35	3.241 (4)	153
$C44-H44B\cdots O3^{iii}$	0.97	2.40	3.272 (4)	149
$C44-H44B\cdots O4^{iii}$	0.97	2.42	3.270 (4)	147

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

All H atoms were located in a difference Fourier map and allowed to ride on their parent atoms at distances of 0.93 (aromatic), 0.96 (methyl) and 0.97 Å (methylene), with  $U_{\text{iso}}(\text{H})$  values of 1.2 or 1.5 times  $U_{\text{eq}}$  of the parent atom.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1997); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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