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#### Key indicators

Single-crystal X-ray study

$T = 293$  K

Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å

$R$  factor = 0.061

$wR$  factor = 0.170

Data-to-parameter ratio = 16.2

For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## 4'-(4-Chlorophenyl)-1'-methyl-4'',5'',6'',7''- tetrahydro-1*H*-indole-3-spiro-2'-pyrrolidine- 3'-spiro-2''-(thiazolo[3,2-*a*]pyrimidine)-2(3*H*),- 3''(2''*H*)-dione

The title compound,  $\text{C}_{23}\text{H}_{21}\text{ClN}_4\text{O}_2\text{S}$ , was synthesized by the intermolecular [3 + 2]-cycloaddition of azomethine ylide, derived from isatin and sarcosine by a decarboxylative route, and 2-(4-chlorobenzylidene)-6,7-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidin-3-one. In the molecule, the two spiro junctions link a planar 2-oxindole ring, a pyrrolidine ring in an envelope conformation and a 6,7-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidin-3-one ring. Two molecules are connected into a dimer by two  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds

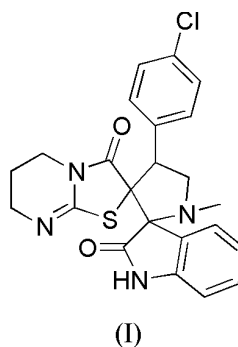
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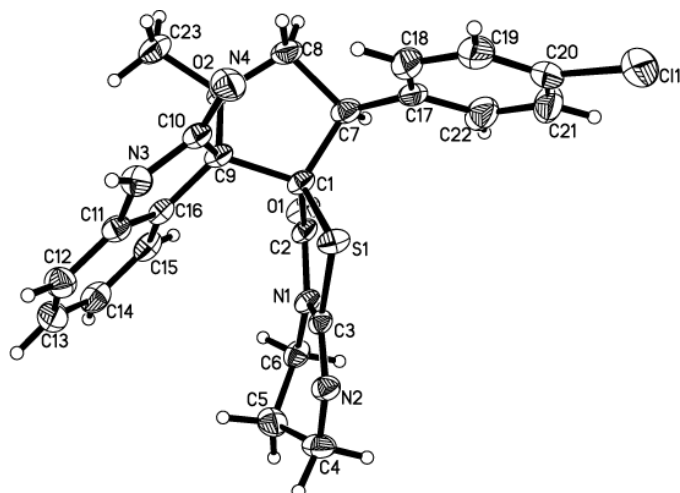
#### Comment

Spiro-compounds represent an important class of naturally occurring substances, which in many cases exhibit important biological properties (Kobayashi *et al.*, 1991; James *et al.*, 1991). 1,3-Dipolar cycloaddition reactions are widely used for the construction of spiro-compounds (Caramella & Grunanger, 1984). In this paper, the structure of the title compound, (I), is reported.

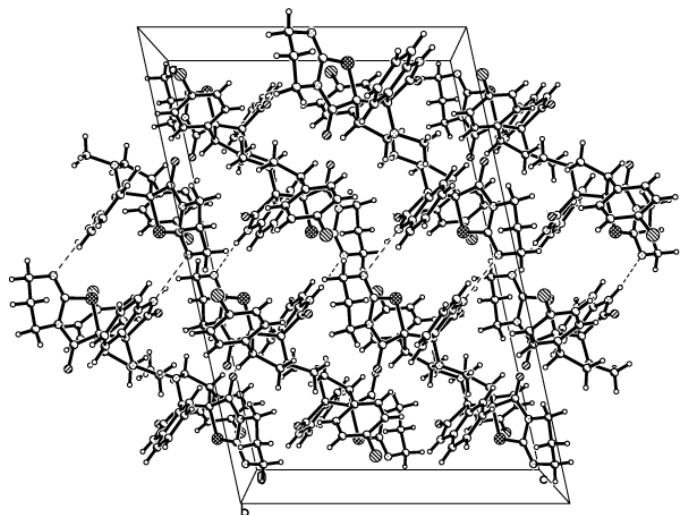


The compound was synthesized by the intermolecular [3 + 2]-cycloaddition of an azomethine ylide, derived from isatin and sarcosine by a decarboxylative route, and 2-(4-chlorobenzylidene)-6,7-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidin-3-one. The molecular structure of (I) is shown in Fig. 1.

There are two spiro junctions in the molecule, which consists of a planar 2-oxindole ring, a pyrrolidine ring in an envelope conformation and a thiazolo[3,2-*a*]pyrimidine ring. Two molecules are connected into a centrosymmetric dimer by  $\text{N}3-\text{H}\cdots\text{N}2^i$  hydrogen bonds [symmetry code: (i)  $2 - x, y, \frac{1}{2} + z$ ], with an  $\text{N}\cdots\text{N}$  distance of 2.855 (2) Å and an  $\text{N}-\text{H}\cdots\text{N}$  angle of 166.9 (3)° (Fig. 2). The structure of 4'-(4-methoxyphenyl)-1'-methyl-4'',5'',6'',7''-tetrahydro-1*H*-indole-3-spiro-2'-pyrrolidine-3'-spiro-2''-(thiazolo[3,2-*a*]pyrimidine)-2(3*H*),-3''(2''*H*)-dione has been reported previously (Li *et al.*, 2003).



**Figure 1**  
The molecular structure of (I), drawn with 30% probability displacement ellipsoids.



**Figure 2**  
The crystal packing of (I), viewed along the *b* axis. Intermolecular N—H...N hydrogen bonds are shown as dashed lines.

## Experimental

A mixture of 2-(4-chlorobenzylidene)-6,7-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidin-3-one (1 mmol), isatin (1 mmol) and sarcosine (1 mmol) was refluxed in methanol (60 ml) until the disappearance of the starting material, as evidenced by thin-layer chromatography. When the reaction was complete, the solvent was removed *in vacuo* and the residue was separated by column chromatography (silica gel, petroleum ether/ethyl acetate = 5:1), giving the title compound, (I). IR (KBr): 3351.4 (—NH), 1724.4, 1689.7 (C=O)  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR ( $\delta$ ,

p.p.m.): 1.18 (*m*, 1H, —CH<sub>2</sub>), 1.66 (*m*, 1H, —CH<sub>2</sub>), 2.27 (*s*, 3H, N—CH<sub>3</sub>), 3.35 (*m*, 2H, CH<sub>2</sub>), 3.38 (*m*, 2H, CH<sub>2</sub>), 3.69 (*m*, 1H, —CH<sub>2</sub>), 4.09 (*m*, 1H, —CH<sub>2</sub>), 4.59 (*m*, 1H, —CH), 6.82–7.53 (*m*, 8H, ArH), 8.50 (*bs*, 1H, —NH); 20 mg of (I) was dissolved in 15 ml dioxane and the solution was kept at room temperature for 15 d; natural evaporation gave colorless single crystals of (I) suitable for X-ray analysis.

## Crystal data

$\text{C}_{23}\text{H}_{21}\text{ClN}_4\text{O}_2\text{S}$   
 $M_r = 452.95$   
Monoclinic,  $C2/c$   
 $a = 22.308$  (8) Å  
 $b = 13.224$  (5) Å  
 $c = 15.054$  (6) Å  
 $\beta = 102.250$  (8)°  
 $V = 4340$  (3) Å<sup>3</sup>  
 $Z = 8$

$D_x = 1.386$  Mg  $\text{m}^{-3}$   
Mo  $K\alpha$  radiation  
Cell parameters from 1009 reflections  
 $\theta = 3.0$ – $26.2^\circ$   
 $\mu = 0.30$   $\text{mm}^{-1}$   
 $T = 293$  (2) K  
Block, colorless  
 $0.40 \times 0.22 \times 0.20$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
Absorption correction: multi-scan (SADABS; Bruker, 1997)  
 $T_{\min} = 0.769$ ,  $T_{\max} = 0.942$   
17147 measured reflections

4454 independent reflections  
2952 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.054$   
 $\theta_{\max} = 26.4^\circ$   
 $h = -27 \rightarrow 27$   
 $k = -15 \rightarrow 16$   
 $l = -18 \rightarrow 18$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.061$   
 $wR(F^2) = 0.170$   
 $S = 1.04$   
4454 reflections  
275 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.084P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.57$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.57$  e Å<sup>-3</sup>

H atoms were positioned geometrically, with C—H = 0.93–0.98 Å, and refined with a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$ .

Data collection: SMART (Bruker, 1997); cell refinement: SMART; data reduction: SAINT (Bruker, 1997); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

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