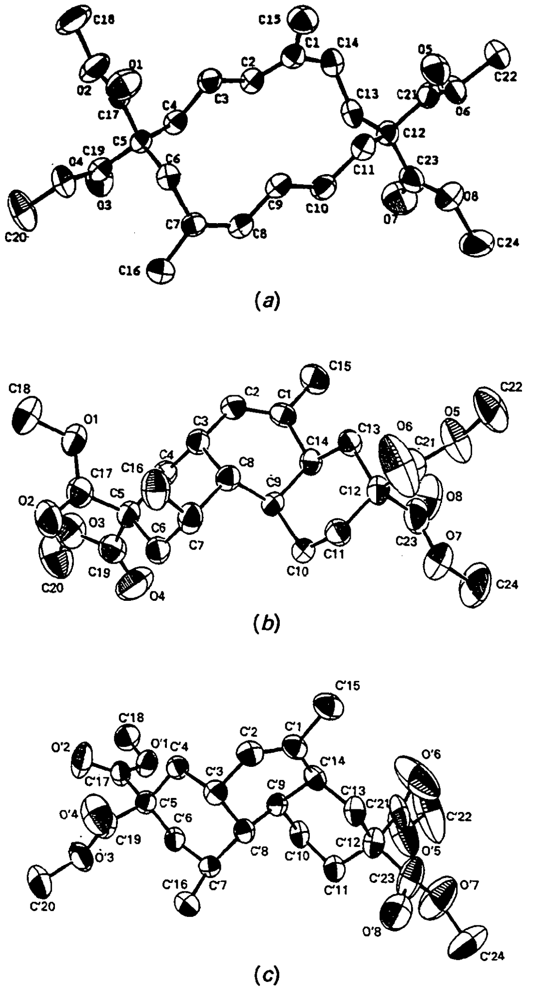

(a)

(b)

(c)

Fig. 2. *ORTEP* (Johnson, 1976) perspective views and atom numbering for both title compounds: (*a*) compound (I), (*b*) compound (II) molecule 1 and (*c*) compound (II) molecule 2.

If macrocycle (I) had an inherent preference to conserve the C(2)—C(1)—C(14)—C(13) synclinal form of butene seen here, then an alternate reaction to the Diels–Alder cycloaddition – plagued by considerable steric interactions in the transition state – might become favoured. In this way an ene/retro-ene/Diels–Alder sequence could proceed from (I) *via* a bicyclic intermediate (IV) and a macrocyclic *trans–cis–trans* (*TCT*) triene (V) (Fig. 1) to finally produce the tricyclic (*CAC*) (II) *cis–anti–cis* compound. Both crystal structures constitute a solid structural basis for further speculation on the cycloaddition pathway linking macrocycles to tricycles. No abnormally short intermolecular contacts were noted.

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Structure of 2-Anilino-4,6-dimethoxy-1,3,5-triazine

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Abstract. $C_{11}H_{12}N_4O_2$, $M_r = 232{\cdot}2$, monoclinic, $P2_1/c$, $a = 10{\cdot}980\,(1)$, $b = 6{\cdot}317\,(1)$, $c = 16{\cdot}207\,(2)$ Å, $\beta = 90{\cdot}64\,(1)°$, $V = 1124{\cdot}0$ Å^3, $D_x = 1{\cdot}372$ Mg m^{-3}, $Z = 4$, Cu $K\alpha$, $\lambda = 1{\cdot}54178$ Å, $\mu = 0{\cdot}78$ mm^{-1}, $F(000) = 488$, $T = 293$ K, final $R = 0{\cdot}058$ for 1434 observed $[F > 2\sigma(F)]$ reflections. The lengths of the N(amine)—C bonds linking the phenyl and *s*-triazine rings [1·415 (4) and 1·350 (4) Å, respectively] indicate extensive conjugation, as do the C(triazine)—OMe distances [1·342 (4) and 1·329 (3) Å]. The near pla-

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narity of the molecule is also consistent with such conjugation. Adjacent *s*-triazine rings are separated by 3·35 Å.

Introduction. In our program on the structure and activity of 1,3,5-triazines (Główka & Iwanicka, 1989*a*,*b*; Główka, Iwanicka & Kamiński, 1990) we have tried to relate electronic effects in *s*-triazine rings to geometric deformations of the aromatic systems. The present study is a continuation of this program.

Experimental. A prismatic crystal of dimensions 0·28 × 0·13 × 0·03 mm was used for data collection (CAD-4 diffractometer, Cu $K\alpha$ radiation), lattice-parameter determination from θ values of 25 reflections in the range $10 < \theta < 31°$; 1756 reflections excluding controls (1610 unique) were measured in an $\omega/2\theta$ mode up to $\theta_{\max} = 60°$ only, because of the poor quality of the crystal; 1434 of these having $F_o > 2\sigma(F_o)$ were considered observed and used in the refinement; h, k, l ranges 0/12, 0/7 and $-18/18$. Three standards monitored every 2 h did not show significant changes in intensities. Absorption was corrected according to Walker & Stuart (1983); maximum and minimum absorption corrections were 1·29 and 1·05. The structure was solved with direct methods (Sheldrick, 1986) and refined by anisotropic full-matrix least squares (Sheldrick, 1976) on F [C-bonded H atoms 1·08 Å from C in rigid groups with isotropic temperature factors; for H on N(7) x, y, z and $U_{\rm iso}$ were refined]. All H atoms were identified in a difference Fourier synthesis at $R = 0·094$. The final cycle had 191 variables, $(\Delta/\sigma)_{\max} = 0·001$, $R = 0·058$, $wR = 0·068$, $w^{-1} = \sigma^2(F_o^2) + 0·0086F_o^2$ and isotropic extinction parameter $g = 0·006$ (Larson, 1967). In the final ΔF synthesis $\rho_{\max} = 0·11$ and $\rho_{\min} = -0·08$ e Å^{-3}. Scattering factors were those included in *SHELX*. The calculations were performed on an Amstrad PC 1512 microcomputer.

The final atomic parameters for non-H atoms are given in Table 1.*

Discussion. The atom-numbering scheme and a view of the molecule are shown in Fig. 1 and selected geometrical parameters are listed in Table 2. The molecule of 2-anilino-4,6-dimethoxy-1,3,5-triazine is roughly planar: the dihedral angle between the two rings is 8·4 (1)°. In consequence, the intramolecular H(13)···N(5) contact is only 2·27 Å. The spanning NH group shows conjugation of its lone-pair electrons with both aromatic systems so that the $\mathrm{N(1)}\text{—}\underset{\underset{\mathrm{N(7)}}{|}}{\mathrm{C(6)}}\text{—}\mathrm{N(5)}$ fragment has a guanidine-like structure. However, the conjugation is evidently stronger with the 1,3,5-triazine ring, judging by the relative lengths of the N(7)—C(6) and N(7)—C(8) bonds [1·350 (4) and 1·415 (4) Å, respectively]. The torsion angles N(5)—C(6)—N(7)—C(8) [−3·3 (6)] and C(6)—N(7)—C(8)—C(13) [−5·7 (6)°] are both near zero. In structures with a cyclohexyl group replacing the phenyl group of the title compound the bonds corresponding to C(6)—N(7) are indeed shorter than those observed in this study: 1·337 (2) Å in 2-cyclohexylamino-4,6-dimethoxy-1,3,5-triazine (Główka & Iwanicka, 1989*a*) and 1·322 (6) Å in 2-chloro-4-cyclohexylamino-6-methoxy-1,3,5-triazine

Table 1. *Positional and equivalent isotropic temperature parameters for non*-H *atoms*

$$B_{\rm eq} = (8\pi^2/3)\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$(Å^2)
N(1)	0·0356 (2)	0·0343 (4)	0·6619 (2)	4·00 (7)
C(2)	0·0097 (3)	−0·1327 (5)	0·6155 (2)	3·61 (8)
N(3)	0·0698 (2)	−0·2068 (4)	0·5520 (2)	3·71 (7)
C(4)	0·1676 (3)	−0·0905 (5)	0·5348 (2)	3·35 (8)
N(5)	0·2045 (2)	0·0828 (4)	0·5731 (1)	3·59 (7)
C(6)	0·1355 (3)	0·1381 (5)	0·6369 (2)	3·45 (8)
O(2)	−0·0906 (2)	−0·2349 (4)	0·6402 (1)	4·43 (6)
C(20)	−0·1226 (4)	−0·4308 (6)	0·5982 (2)	4·88 (11)
O(4)	0·2306 (2)	−0·1635 (4)	0·4713 (1)	4·52 (6)
C(40)	0·3404 (3)	−0·0532 (7)	0·4509 (2)	5·33 (11)
N(7)	0·1632 (3)	0·3121 (5)	0·6816 (2)	4·47 (8)
C(8)	0·2615 (3)	0·4563 (5)	0·6769 (2)	3·68 (8)
C(9)	0·2538 (3)	0·6310 (5)	0·7284 (2)	4·13 (8)
C(10)	0·3461 (4)	0·7799 (6)	0·7296 (2)	5·09 (11)
C(11)	0·4466 (4)	0·7555 (7)	0·6796 (2)	5·23 (11)
C(12)	0·4524 (3)	0·5868 (7)	0·6274 (2)	5·17 (11)
C(13)	0·3605 (3)	0·4344 (6)	0·6255 (2)	4·75 (11)

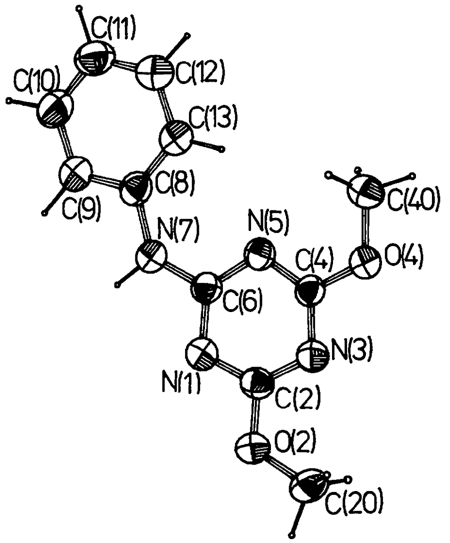

Fig. 1. Overall view and labelling scheme of atoms in 2-anilino-4,6-dimethoxy-1,3,5-triazine (Johnson, 1976).

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53507 (9 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Selected bond lengths* (Å), *bond angles* (°) *and torsion angles* (°)

N(1)—C(2)	1·324 (4)	C(2)—O(2)	1·342 (4)
N(1)—C(6)	1·345 (4)	O(2)—C(20)	1·453 (4)
N(3)—C(2)	1·315 (4)	C(4)—O(4)	1·329 (3)
N(3)—C(4)	1·333 (4)	O(4)—C(40)	1·434 (4)
N(5)—C(4)	1·320 (4)	C(6)—N(7)	1·350 (4)
N(5)—C(6)	1·334 (4)	N(7)—C(8)	1·415 (4)
C(2)—N(1)—C(6)	112·8 (3)	N(1)—C(2)—N(3)	128·5 (3)
C(2)—N(3)—C(4)	112·3 (3)	N(3)—C(4)—N(5)	127·1 (3)
C(4)—N(5)—C(6)	114·0 (3)	N(5)—C(6)—N(1)	125·3 (3)
C(2)—O(2)—C(20)	117·7 (3)	C(4)—O(4)—C(40)	117·1 (3)
C(6)—N(7)—C(8)	131·5 (3)		
N(3)—C(2)—O(2)—C(20)	3·9 (4)	N(5)—C(6)—N(7)—C(8)	−3·3 (6)
N(5)—C(4)—O(4)—C(40)	3·3 (4)	C(6)—N(7)—C(8)—C(13)	−5·7 (6)

(Główka & Iwanicka, 1991) while the bonds corresponding to N(7)—C(8) were found to be longer [1·457 (3) and 1·482 (6) Å, respectively] owing to the lack of conjugation with the cyclohexane ring. The methoxy groups of the title compound deviate slightly from the mean plane of the triazine system and the appropriate N—C—O—C torsional angles are 3·9 (4) and 3·3 (4)°. There is a partial stacking of parallel *s*-triazine rings with an interplanar distance of 3·35 Å.

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Structure of *N*-[4-Hydroxy-3,5-bis(1-pyrrolidinylmethyl)phenyl]-*N*′-(4-methoxyphenyl)urea

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Abstract. $C_{24}H_{32}N_4O_3$, $M_r = 424·55$, monoclinic, $P2_1/c$, $a = 15·740$ (1), $b = 17·279$ (3), $c = 8·757$ (2) Å, $\beta = 101·67$ (1)°, $V = 2332·4$ Å^3, $Z = 4$, $D_x = 1·209$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0·0873$ mm^{-1}, $F(000) = 912$, $T = 293$ K, $R = 0·057$ for 2095 observed reflections. The title molecule is chemically similar to several active type I antiarrhythmics but it is inactive. Structural results indicate that the lack of activity may be due to modifications of the lipophilic pharmacophore group rather than to conformational differences.

Introduction. In 1983, Stout and co-workers introduced a new family of antiarrhythmic agents originally from changrolin and based on 4-substituted 2,6-bis(1-pyrrolidinylmethyl)phenols (Stout, Mathier, Barcelon-Yang, Reynolds & Brown, 1983, 1984, 1985). Three active compounds [(1), (2) and (3)] have been studied by X-ray diffraction and molecular-mechanics calculations; the study indicated that these molecules adopt a similar shape, both in the crystal and *in vacuo* (Główka, Dargie & Codding, 1991). The limited flexibility of (1), (2) and (3), as compared to classical type I antiarrhythmics like lidocaine, mexiletine, procainamide and disopyramide, helped to establish the required spatial arrangement of binding groups in this class of drugs. In this paper, we present a study of an inactive but chemically similar

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