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## Structure Reports

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(±)-N-[4-Acetyl-5-methyl-5-(4-methylcyclohex-3-enyl)-4,5-dihydro-1,3,4-thiadiazol-2-yl]acetamide

Tebbaa Mohammed,<sup>a</sup> Nouredine Mazoir,<sup>a</sup> Jean-Claude Daran,<sup>b\*</sup> Moha Berraho<sup>a</sup> and Ahmed Benharref<sup>a</sup>

<sup>a</sup>Laboratoire de Chimie Biomoléculaire, Substances Naturelles et Réactivité, Faculté des Sciences, Semlalia, Université Cadi Ayyad, BP 2390 Marrakech, Morocco, and

<sup>b</sup>Laboratoire de Chimie de Coordination, 205 route de Narbonne, 31077 Toulouse Cedex 04, France

Correspondence e-mail: daran@cc-toulouse.fr

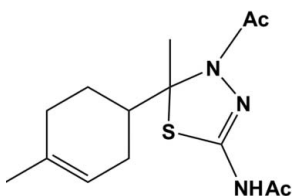
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Key indicators: single-crystal X-ray study;  $T = 180$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.037;  $wR$  factor = 0.113; data-to-parameter ratio = 25.1.

The new title thiadiazole compound,  $\text{C}_{14}\text{H}_{21}\text{N}_3\text{O}_2\text{S}$ , was semi-synthesized starting from 1-(4-methylcyclohex-3-enyl)-ethanone, a natural product isolated from *Cedrus atlantica* essential oil. The stereochemistry has been confirmed by single-crystal X-ray diffraction. The thiadiazoline ring is roughly planar, although it may be regarded as having a half-chair conformation. The cyclohexenyl ring has a half-chair conformation. The most interesting feature is the formation of a pseudo-ring formed by four molecules associated through  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds around a fourfold inversion axis, forming an  $R_4^2(28)$  motif.

## Related literature

For related literature, see: Aly *et al.* (2007); Beatriz *et al.* (2002); Bernstein *et al.* (1995); Cremer & Pople (1975); Demirbas *et al.* (2005); Etter *et al.* (1990); Farghaly *et al.* (2006); Invidiata *et al.* (1996); Kubota *et al.* (1982); Nizamuddin *et al.* (1999); Ourhriss *et al.* (2005); Paolo *et al.* (2005); Radul *et al.* (2005); Sun *et al.* (1999); Udipi *et al.* (2000).



## Experimental

## Crystal data

$\text{C}_{14}\text{H}_{21}\text{N}_3\text{O}_2\text{S}$   
 $M_r = 295.40$

Tetragonal,  $I4_1/a$   
 $a = 16.6855$  (3) Å

$c = 21.8961$  (8) Å  
 $V = 6096.0$  (3) Å<sup>3</sup>  
 $Z = 16$   
Mo  $K\alpha$  radiation

$\mu = 0.22$  mm<sup>-1</sup>  
 $T = 180$  (2) K  
 $0.29 \times 0.24 \times 0.08$  mm

## Data collection

Bruker APEXII CCD area-detector diffractometer  
Absorption correction: none  
87517 measured reflections

4637 independent reflections  
3849 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.032$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.113$   
 $S = 1.11$   
4637 reflections

185 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.39$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.26$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N3}-\text{H3}\cdots\text{O1}^i$	0.88	1.95	2.8223 (14)	171

Symmetry code: (i)  $y + \frac{1}{2}, -x + \frac{3}{2}, -z + \frac{3}{4}$ .

Data collection: APEX2 (Bruker, 2006); cell refinement: APEX2; data reduction: APEX2; program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEPIII (Burnett & Johnson, 1996), ORTEP-3 for Windows (Farrugia, 1997) and CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: WinGX (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2164).

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