Related literature. The title molecule, formed by an unusual reaction pathway from *cis*-1,2-dihydrocatechol (Banwell, Mackay, Reum, Richards & Stasi, 1992), is a member of the synthetically and biologically important aminoconduritol class of compounds (Balci, Suteyaz & Secen, 1990).

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Structure of *N*-(2-Furylmethyl)-α-cyano-2-furanacrylamide

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Abstract. $C_{13}H_{10}N_2O_3$, $M_r = 242.2$, triclinic, $P\bar{1}$, $a = 5.305$ (1), $b = 9.486$ (2), $c = 11.437$ (3) Å, $\alpha = 94.1$ (2), $\beta = 93.8$ (2), $\gamma = 93.6$ (2)°, $V = 571$ (1) Å^3, $Z = 2$, $D_x = 1.41$ g cm^{-3}, graphite-monochromated Mo $K\alpha$ radiation, $\lambda = 0.7107$ Å, $\mu = 0.96$ cm^{-1}, $F(000) = 252$, room temperature, $R = 0.048$ for 2586 observed reflections with $I \geq 3\sigma(I)$. There is an intramolecular hydrogen bond N(1)—H(6)···N(2) with N(1)···N(2) = 3.108 (5) Å. The structure is built up by discrete molecules linked by van der Waals forces.

Experimental. Intensity data were obtained from a prismatic crystal, 0.2 × 0.2 × 0.3 mm, on an Enraf–Nonius CAD-4 diffractometer using the ω–2θ scan mode. Unit-cell parameters were determined from least-squares refinement of 25 automatically centred reflections in the range $11 \leq \theta \leq 15°$. Three standard reflections showed intensity variation <5%. 2897 reflections were measured ($1 \leq \theta \leq 26°$; $0 \leq h \leq 6$, $-12 \leq k \leq 12$, $-14 \leq l \leq 14$) of which 2586 with $I \geq 3\sigma(I)$ were used for refinement. Lorentz and polarization corrections were applied, but absorption was ignored. The structure was solved by direct methods (Sheldrick, 1976) and refined using a full-matrix least-squares routine based on F. Non-H atoms were refined with anisotropic displacement parameters; H atoms were located from a difference Fourier map and refined isotropically. $R = 0.048$, $wR = 0.065$ $\{w = [\sigma^2(F) + 0.014F^2]^{-1}\}$; $\Delta\rho_{max} = 0.21$, $\Delta\rho_{min} = -0.42$ e Å^{-3}; $(\Delta/\sigma)_{max} = 0.32$. 203 parameters were refined. All refinement calculations were carried out using *SHELX*76 (Sheldrick, 1976). Atomic scattering factors were those stored in *SHELX*76. Positional parameters and equivalent isotropic displacement parameters are given in Table 1.† Bond lengths, bond angles and selected torsion angles are listed in Table 2. The numbering system for the molecule can be found in Fig. 1.

Related literature. The title compound was synthesized and spectroscopically investigated by Bartroli, Lamí & Díaz (1984). Research on bioactivity by Bermello (1990) using Golender & Rezenblit (1983) algorithms showed fungicide and bactericide proper-

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† Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, and bond distances, bond angles and torsion angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55537 (19 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AB0276]

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Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and equivalent isotropic displacement parameters* ($Å^2 \times 10^4$) *for non-H atoms*

$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j$.

	x	y	z	U_{eq}
C(1)	−2706 (3)	−461 (2)	1243 (1)	532 (5)
C(2)	−537 (3)	−775 (1)	1779 (1)	518 (5)
C(3)	1092 (3)	485 (2)	1847 (1)	485 (5)
C(4)	−217 (2)	1475 (1)	1343 (1)	385 (4)
C(5)	481 (3)	2947 (1)	1054 (1)	460 (5)
C(6)	−1078 (2)	4589 (1)	2534 (1)	379 (4)
C(7)	−3022 (2)	5623 (1)	2818 (1)	364 (4)
C(8)	−4732 (2)	5982 (1)	1884 (1)	395 (4)
C(9)	−3092 (2)	6136 (1)	3950 (1)	402 (21)
C(10)	−4738 (2)	7092 (1)	4461 (1)	402 (5)
C(11)	−4888 (3)	7515 (2)	5618 (1)	519 (5)
C(12)	−6875 (3)	8448 (2)	5668 (1)	581 (6)
C(13)	−7792 (3)	8518 (2)	4552 (1)	568 (6)
O(1)	−2579 (2)	916 (1)	965 (1)	513 (4)
O(2)	561 (2)	4325 (1)	3273 (1)	532 (4)
O(3)	−6515 (2)	7717 (1)	3787 (1)	506 (4)
N(1)	−1277 (2)	3975 (1)	1428 (1)	429 (4)
N(2)	−5982 (3)	6201 (1)	1071 (1)	539 (5)

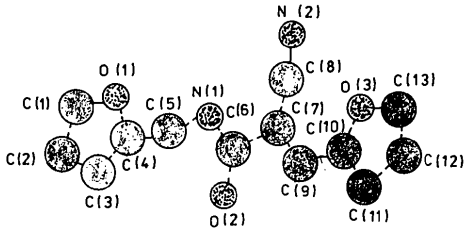

Fig. 1. A perspective view of the title compound, with the numbering scheme.

ties. The molecular structure described here should aid the interpretation of spectroscopic investigations and the elucidation of the bioactivity data.

Table 2. *Bond distances* (Å), *bond angles* (°) *and selected torsion angles* (°)

C(1)—C(2)	1.328 (3)	C(7)—C(8)	1.429 (2)
C(1)—O(1)	1.365 (2)	C(8)—N(2)	1.145 (2)
C(2)—C(3)	1.422 (3)	C(7)—C(9)	1.354 (2)
C(3)—C(4)	1.343 (3)	C(9)—C(10)	1.421 (3)
C(4)—C(5)	1.488 (3)	C(10)—C(11)	1.364 (2)
C(4)—O(1)	1.360 (2)	C(10)—O(3)	1.369 (2)
C(5)—N(1)	1.453 (3)	C(11)—C(12)	1.420 (3)
C(6)—N(1)	1.350 (2)	C(12)—C(13)	1.343 (3)
C(6)—O(2)	1.221 (2)	C(13)—O(3)	1.360 (3)
C(6)—C(7)	1.502 (2)		

C(2)—C(1)—O(1)	110.7 (2)	C(8)—C(7)—C(9)	123.7 (1)
C(1)—C(2)—C(3)	106.1 (1)	C(7)—C(8)—N(2)	174.0 (1)
C(2)—C(3)—C(4)	107.0 (1)	C(7)—C(9)—C(10)	129.8 (1)
C(3)—C(4)—O(1)	109.6 (1)	C(9)—C(10)—O(3)	121.4 (1)
C(3)—C(4)—C(5)	132.9 (1)	C(9)—C(10)—C(11)	128.6 (1)
C(5)—C(4)—O(1)	117.2 (1)	C(11)—C(10)—O(3)	109.9 (1)
C(4)—C(5)—N(1)	114.1 (1)	C(10)—C(11)—C(12)	106.6 (1)
O(2)—C(6)—N(1)	122.8 (1)	C(11)—C(12)—C(13)	105.9 (2)
C(7)—C(6)—N(1)	115.9 (1)	C(12)—C(13)—O(3)	111.7 (2)
C(7)—C(6)—O(2)	121.3 (1)	C(1)—O(1)—C(4)	106.6 (1)
C(6)—C(7)—C(9)	118.0 (1)	C(10)—O(3)—C(13)	105.9 (1)
C(6)—C(7)—C(8)	118.2 (1)	C(5)—N(1)—C(6)	120.9 (1)

C(2)—C(3)—C(4)—C(5)	−174.1 (1)	C(8)—C(7)—C(9)—C(10)	−0.3 (2)
C(3)—C(4)—C(5)—N(1)	−131.7 (2)	C(7)—C(9)—C(10)—C(11)	174.8 (2)
C(6)—C(7)—C(9)—C(10)	−178.7 (1)	C(9)—C(10)—C(11)—C(12)	−178.6 (2)

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Structure of Ethyl 5-(2,2,2-Trichloro-1-hydroxyethyl)furan-2-carboxylate

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Abstract. $C_9H_9Cl_3O_4$, $M_r = 287.5$, orthorhombic, *Pbca*, $a = 23.01$ (4), $b = 13.91$ (1), $c = 7.58$ (4) Å, $V = 2426$ (14) Å^3, $Z = 8$, $D_x = 1.57$ (1) g cm^{-3}, graphite-monochromated Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å, $\mu = 7.516$ cm^{-1}, $F(000) = 1168$, room temperature, $R = 0.034$ for 460 observed reflections

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