an intermediate in the synthesis of γ-dipeptides of the neuroexcitatory amino acid kainic acid.

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Structure of *N*-Triphenylmethyl-2-oxa-5-azabicyclo[2.2.1]heptan-3-one

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Abstract. $C_{24}H_{21}NO_2$, $M_r = 355{\cdot}42$, orthorhombic, $P2_12_12_1$, $a = 9{\cdot}503\ (2)$, $b = 12{\cdot}853\ (3)$, $c = 15{\cdot}601\ (4)$ Å, $V = 1905{\cdot}5\ (8)$ Å^3, $Z = 4$, $D_x = 1{\cdot}24$ g cm^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 0{\cdot}85$ cm^{-1}, $F(000) = 752$, room temperature, $R = 0{\cdot}039$ for 1079 unique observed reflections. The atoms C(24), N(20), C(21) and C(22) of the proline ring [O$_2$C—C(24)—N(20)—C(21)—C(22)—C(23)] lie in a plane to within ±0·06 Å while C(23) is out of the plane by 0·85 Å. The two planes of the six-membered ring [C(24)—N(20)—C(21)—C(22) and C(24)—C(25)—O(26)—C(22)] form a dihedral angle of 55 (1)°. The dihedral angles between the plane of the three C atoms C(22), C(23) and C(24) and the two planes of the six-membered ring are 126 (1) and 71 (1)° respectively. Other bond lengths and angles are normal.

Experimental. Recrystallization from acetone, m.p. 503–508 K, $[\alpha]_D^{25°C} = +104{\cdot}6°$ [$CHCl_3$, 1 g dm^{-3}]. Plate crystal 0·48 × 0·48 × 0·08 mm, Enraf–Nonius CAD-4 diffractometer, ω–2θ-scan technique for data collection, lattice parameters from 25 reflections in range $7 < \theta < 10°$. Index range $0 < h < 12$, $0 < k < 14$, $-19 < l < 19$ for 5092 measured reflections up to $2\theta_{max} = 54°$. Averaged 2391, mean discrepancy on I 1·7% (for 4890 reflections); ω-scan width (0·7 + 0·3tanθ)°, scan rate 1·03–5·49° min^{-1}; horizontal aperture (2·4 + 0·9tanθ) mm, max. scan time 60 s; intensities of 00$\bar{4}$, 10$\bar{2}$ and 02$\bar{3}$ remeasured every 2 h, intensity decrease 2·5%, orientation-control reflections (13$\bar{4}$, 24$\bar{3}$, 22$\bar{7}$) every 500 reflections. 1079 unique observed reflections with $I > 1{\cdot}5\sigma(I)$ used for refinement. Final $R = 0{\cdot}039$, $wR = 0{\cdot}043$, $\sum w(\Delta F)^2$ minimized, $w = 0{\cdot}1307/[\sigma^2(F) + 0{\cdot}010869(F)^2]$, max. $\Delta/\sigma < 0{\cdot}7$ in final cycle (for non-H atoms); residual electron density in final difference synthesis between +0·12 and −0·18 e Å^{-3}, atomic scattering factors from *SHELX76* (Sheldrick, 1976); no absorption correction applied; heavier atoms refined with anisotropic temperature factors; H atoms positioned geometrically, riding model [C—H = 1·08 Å, overall U(H) = 0·069 (4) Å^2]. Computer programs used: *MULTAN87* (Debaerdemaeker, Germain, Main, Tate & Woolfson, 1987), *SHELX76* (Sheldrick, 1976) and *PLUTO* (Motherwell & Clegg, 1978). Atomic parameters are given in Table 1,* bond distances and angles in Table 2. Fig. 1 shows the atom numbering of the molecule.

Related literature. For the synthesis of the title and related compounds see Papaioannou, Stavropoulos & Karagiannis (1988), Bowers-Nemia & Joullie

* Lists of structure factors, anisotropic thermal parameters, bond lengths and angles, details of least-squares planes and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51889 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Final positional parameters* ($\times 10^4$) *and their e.s.d.'s and equivalent isotropic temperature factors* ($Å^2$)

$$B_{eq} = \tfrac{4}{3}\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	*y*	*z*	B_{eq}
C(1)	1826 (5)	5135 (4)	3492 (3)	2·72
C(2)	830 (5)	5646 (4)	4151 (3)	3·02
C(3)	−481 (5)	5189 (5)	4334 (3)	3·83
C(4)	−1279 (7)	5550 (5)	5016 (4)	5·22
C(5)	−821 (7)	6344 (6)	5527 (4)	5·14
C(6)	458 (6)	6807 (4)	5344 (3)	4·20
C(7)	1272 (6)	6459 (4)	4664 (3)	3·30
C(8)	1042 (5)	4665 (4)	2721 (3)	2·69
C(9)	−170 (6)	5150 (4)	2407 (3)	3·51
C(10)	−812 (6)	4787 (5)	1668 (3)	4·26
C(11)	−286 (6)	3936 (4)	1242 (3)	4·00
C(12)	923 (6)	3466 (4)	1534 (3)	3·92
C(13)	1601 (6)	3831 (4)	2268 (3)	3·40
C(14)	2857 (5)	5926 (4)	3084 (3)	2·68
C(15)	4264 (6)	5669 (4)	2924 (4)	4·06
C(16)	5125 (7)	6380 (5)	2494 (4)	5·36
C(17)	4616 (7)	7307 (5)	2205 (4)	4·65
C(18)	3222 (7)	7554 (4)	2343 (4)	4·44
C(19)	2354 (6)	6875 (4)	2781 (3)	3·34
N(20)	2668 (4)	4310 (3)	3923 (3)	2·80
C(21)	1937 (6)	3329 (4)	4211 (3)	3·90
C(22)	2615 (6)	3145 (4)	5081 (3)	4·11
C(23)	2621 (6)	4221 (4)	5469 (3)	3·71
C(24)	3457 (5)	4656 (4)	4710 (3)	3·00
C(25)	4675 (7)	3899 (4)	4707 (4)	3·79
O(26)	4127 (4)	2960 (3)	4925 (2)	4·56
O(27)	5897 (4)	4025 (3)	4523 (3)	5·33

Table 2. *Bond distances* (Å) *and angles* (°)

N(20)—C(21)	1·508 (6)	C(21)—N(20)—C(24)	103·5 (4)
C(21)—C(22)	1·522 (7)	N(20)—C(21)—C(22)	101·6 (4)
C(22)—C(23)	1·509 (7)	C(21)—C(22)—C(23)	102·5 (4)
C(23)—C(24)	1·532 (7)	C(22)—C(23)—C)24)	91·5 (4)
C(24)—N(20)	1·506 (6)	N(20)—C(24)—C(23)	105·3 (4)
C(24)—C(25)	1·512 (7)	C(23)—C(22)—O(26)	102·1 (4)
C(25)—O(26)	1·357 (6)	C(22)—O(26)—C(25)	105·7 (4)
O(26)—C(22)	1·477 (6)	O(26)—C(25)—C(24)	106·1 (5)
C(25)—O(27)	1·208 (6)	C(25)—C(24)—C(23)	99·4 (4)

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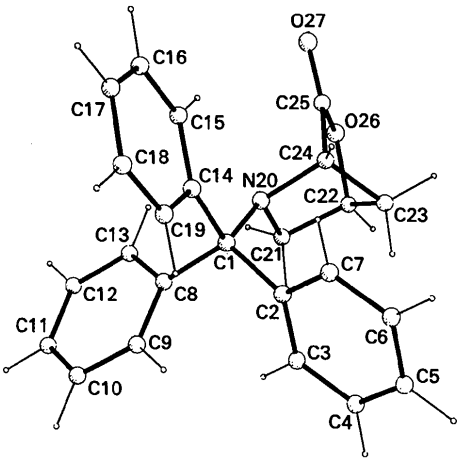

Fig. 1. The atom numbering of the molecule.

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Structure of 5-Methyl-2′-deoxycytidine 5′-Monophosphate Dihydrate

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Abstract. $C_{10}H_{16}N_3O_7P.2H_2O$, $M_r = 357·2$, triclinic, $P\bar{1}$, $a = 4·8520$ (8), $b = 8·3703$ (8), $c = 10·0199$ (12) Å, $\alpha = 104·578$ (9), $\beta = 102·332$ (13), $\gamma = 93·670$ (11)°, $V = 381·75$ Å^3, $Z = 1$, $D_x = 1·55$, $D_m = 1·53$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 2·01$ mm^{-1}, $F(000) = 188$, $T = 290$ K, $R = 0·049$ for 1568 unique reflections.

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