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Structure of a Nucleoside N_1-Analogue of Formycin B Exhibiting the 'mid-*anti*,C(3')-*endo*' Conformation

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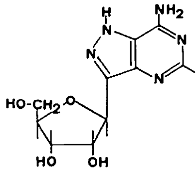
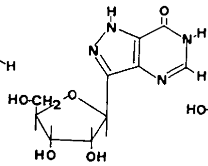
Abstract. 6-Benzyl-3-methyl-1-(β-D-ribofuranosyl)-7*H*-pyrazolo[4,3-*d*]pyrimidin-7-one, $C_{18}H_{20}N_4O_5$, $M_r = 372\cdot38$, orthorhombic, $P2_12_12_1$, $a = 5\cdot442$ (1), $b = 13\cdot387$ (2), $c = 23\cdot759$ (4) Å, $V = 1730\cdot9$ (6) Å^3, $Z = 4$, $D_x = 1\cdot43$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0\cdot71069$ Å, $\mu = 0\cdot10$ mm^{-1}, $T = 294$ K, $F(000) = 784$, final $R = 0\cdot039$ for 1154 observed reflections [$I > 2\sigma(I)$]. *N*-Nucleoside analogues of formycin A and B are studied as potential antiviral and antitumor agents. The conformational parameters of the present compound are: a C(3')-*endo* ($^3E/^3T_2$) ribose conformation, a mid-*anti* glycosidic bond rotation [$\chi = 66\cdot4$ (4)°] and a *gauche–trans* conformation around the ribose C(4')—C(5') bond. The hydrogen bonding in the crystal is analyzed in terms of graph formalism and it is found to correspond {according to the formalism of Kuleshova & Zorky [*Acta Cryst.* (1980), B**36**, 2113–2115]} to the $F_6{}^6(3,4,6)$ or $F_6{}^8(2,3,4,6)$ graphs according to whether the bifurcated hydrogen bonds are considered to be single or double bonds.

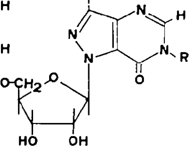
Introduction. The *C*-nucleoside formycin A (I) is an isomer of adenosine, where imidazole replaces the pyrazole ring. Both formycin A and its analogue and metabolite formycin B (II) have been identified in naturally occurring systems; it has been found that they have definite antiviral and antitumor properties and are generally thought to be able to substitute for adenosine in several enzymatic reactions occurring at the nucleotide level. For these reasons a number of studies have been undertaken both on *C*- and *N*-nucleosides, the latter differing from the former in the substitution position of the ribofuranosyl ring. In particular, crystal and molecular structures of several *C*-nucleosides [formycin A.H_2O (Prusiner, Brennan & Sundaralingam, 1973); formycin A.HBr (Koyama, Umezawa & Iitaka, 1974); formycin B and oxoformycin B (Koyama, Nakamura, Umezawa & Iitaka, 1976)] and *N*-nucleosides (Altona & Sundaralingam, 1972, and references therein; Sprang, Scheller, Rohrer & Sundaralingam, 1978; Srikrishnam, Parthasarathy, De & Chheda, 1983) have been determined.



Formycin A
(I)



Formycin B
(II)



Present compound
(R = $-CH_2Ph$)

(III)

We report here the structure of another *N*-nucleoside (III) as part of a systematic synthetic project under development in our University which is aimed at producing new compounds having increased antitumor and antiviral properties (Baraldi, Simoni, Periotto, Manfredini, Guarneri, Manservigi, Cassai & Bertolasi, 1984).

Experimental. Crystal $0\cdot07 \times 0\cdot17 \times 0\cdot21$ mm; recrystallization from methanol/diethyl ether (1:1); Enraf–Nonius CAD-4 diffractometer; graphite-monochromated Mo $K\alpha$ radiation; $\omega/2\theta$ scan ($2° \leq \theta \leq 26°$); cell parameters from 25 reflections in the range $10° \leq \theta \leq 14°$; 1986 reflections collected ($0 \leq h \leq 6$, $0 \leq k \leq 16$, $0 \leq l \leq 28$), 1154 having $I \geq 2\sigma(I)$ used; 2 standard reflections monitored every 2 h showed no significant variation during data collection; no correction for absorption or extinction; solution by direct methods (*MULTAN*82: Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982); refinement by full-matrix least squares on *F*; non-H atoms anisotropic, hydrogen-bond-implied H isotropic and remaining H atoms calculated; 256 parameters refined; final $R = 0\cdot039$ and $wR = 0\cdot041$; $1/w^2 = \sigma^2(I) + 0\cdot05|F_o|^2$; max. $\Delta/\sigma = 0\cdot13$; $S = 1\cdot1$; final difference-map peaks in the range $-0\cdot17$ to $0\cdot20$ e Å^{-3}. Identical results were obtained for both enantiomorphic structures and therefore the absolute configuration was not determined. Scattering factors from *International Tables for X-ray Crystallography* (1974); all calculations performed with the CAD-4 *SDP* system of programs (Frenz, 1978) and *PARST* (Nardelli, 1983).

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Discussion. Atomic parameters are given in Table 1.* Bond distances and angles and a selection of torsion angles are reported in Table 2. An *ORTEP* (Johnson, 1971) view of the molecule is shown in Fig. 1.

Bond distances and angles of the pyrazolopyrimidinone moiety agree within 3·5σ with those found in the same group in formycin B (Koyama *et al.*, 1976). The group is almost perfectly planar, the angle between the planes through the six- and five-membered rings being 1·6 (1)°.

The most important aspects of these molecules concern their conformations, the rotation around the N(4)—C(1′) *N*-glycosyl bond and the puckering of the ribofuranose unit being equally involved. Such a problem has been discussed from a general point of view by Altona & Sundaralingam (1972) and the pertinent nomenclature is given by Sundaralingam (1969). In the present case χ = N(3)—N(4)—C(1′)—O(4′) is 66·4 (4)° allowing us to classify the glycosyl conformation as mid-*anti* ($40 \le \chi \le 90°$). The puckering of the ribose ring can be described by the pseudorotation parameters P (phase angle) and τ_m (maximum puckering amplitude), respectively 12·2 (4) and 41·5 (4)°. This corresponds to a C(2′)-*exo*–C(3′)-*endo* conformation or, alternatively, to a 2:1 mixture of the ^3E and $^3T_2$ conformations [Altona & Sundaralingam (1972); note that for the last symbols

Table 1. *Positional* (×10⁴ *for non-*H *atoms,* ×10³ *for* H) *and thermal* (Å² ×10³) *parameters with e.s.d.'s in parentheses* (U_{eq} *according to Hamilton,* 1959)

	x	y	z	U_{eq}/U
C(1)	−881 (8)	1863 (3)	8912 (2)	36 (2)
C(2)	−1681 (9)	2839 (3)	8851 (2)	49 (2)
C(3)	−399 (11)	3612 (3)	9096 (2)	64 (3)
C(4)	1656 (10)	3429 (3)	9403 (2)	65 (3)
C(5)	2466 (9)	2460 (4)	9475 (2)	63 (3)
C(6)	1207 (9)	1683 (3)	9231 (2)	47 (3)
C(7)	−2251 (8)	1012 (3)	8630 (2)	42 (2)
C(8)	660 (9)	−319 (3)	8397 (2)	42 (2)
C(9)	2904 (7)	−340 (3)	7607 (2)	30 (2)
C(10)	1676 (8)	472 (3)	7396 (1)	30 (2)
C(11)	−240 (8)	973 (3)	7697 (2)	34 (2)
C(12)	4683 (8)	−611 (3)	7204 (2)	33 (2)
C(13)	6499 (9)	−1441 (3)	7216 (2)	43 (2)
C(1′)	2325 (8)	1552 (3)	6526 (1)	31 (2)
C(2′)	4680 (8)	2135 (3)	6445 (2)	36 (2)
C(3′)	5738 (8)	1665 (3)	5913 (2)	36 (2)
C(4′)	3442 (8)	1519 (3)	5561 (2)	32 (2)
C(5′)	3622 (10)	738 (3)	5108 (2)	51 (2)
N(1)	−623 (7)	496 (2)	8220 (1)	38 (2)
N(2)	2398 (7)	−765 (2)	8124 (1)	39 (2)
N(3)	4555 (7)	21 (2)	6770 (1)	37 (2)
N(4)	2686 (6)	671 (2)	6882 (1)	34 (1)
O(1)	−1419 (5)	1708 (2)	7563 (1)	45 (1)
O(4′)	1602 (5)	1236 (2)	5972 (1)	33 (1)
O(2′)	3994 (6)	3145 (2)	6333 (1)	45 (2)
O(3′)	7444 (6)	2292 (2)	5630 (1)	57 (2)
O(5′)	1554 (8)	694 (2)	4755 (1)	64 (2)
H(2′)	524 (8)	351 (3)	652 (2)	63 (13)
H(3′)	870 (7)	205 (2)	568 (1)	44 (11)
H(5′)	142 (12)	131 (4)	452 (3)	152 (25)

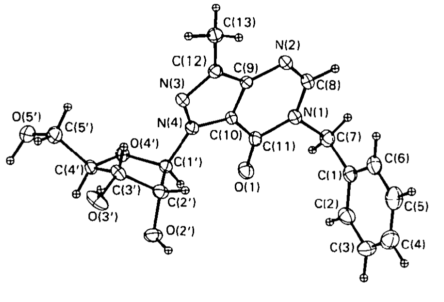

Fig. 1. An *ORTEP* view of the molecule, showing the thermal ellipsoids at 40% probability.

Table 2. *Bond distances* (Å), *bond angles* (°) *and torsion angles* (°) *with e.s.d.'s in parentheses*

C(1)—C(2)	1·385 (6)	C(12)—C(13)	1·487 (6)
C(1)—C(6)	1·387 (7)	C(12)—N(3)	1·336 (5)
C(1)—C(7)	1·518 (6)	C(1′)—C(2′)	1·513 (6)
C(2)—C(3)	1·377 (7)	C(1′)—N(4)	1·465 (4)
C(3)—C(4)	1·358 (8)	C(1′)--O(4′)	1·438 (4)
C(4)—C(5)	1·381 (7)	C(2′)—C(3′)	1·525 (7)
C(5)—C(6)	1·374 (7)	C(2′)—O(2′)	1·428 (5)
C(7)—N(1)	1·487 (5)	C(3′)—C(4′)	1·516 (6)
C(8)—N(1)	1·362 (5)	C(3′)—O(3′)	1·421 (5)
C(8)—N(2)	1·293 (6)	C(4′)—C(5′)	1·504 (6)
C(9)—C(10)	1·371 (6)	C(4′)—O(4′)	1·449 (5)
C(9)—C(12)	1·409 (6)	C(5′)—O(5′)	1·405 (6)
C(9)—N(2)	1·382 (5)	N(3)—N(4)	1·365 (5)
C(10)—C(11)	1·431 (6)	O(2′)—H(2′)	0·94 (4)
C(10)—N(4)	1·366 (4)	O(3′)—H(3′)	0·76 (4)
C(11)—N(1)	1·413 (5)	O(5′)—H(5′)	1·00 (6)
C(11)—O(1)	1·217 (5)		

C(2)—C(1)—C(6)	118·6 (4)	N(4)—C(1′)—O(4′)	109·2 (3)
C(2)—C(1)—C(7)	120·5 (4)	C(1′)—C(2′)—C(3′)	102·3 (3)
C(6)—C(1)—C(7)	120·9 (4)	C(1′)—C(2′)—O(2′)	106·9 (3)
C(1)—C(2)—C(3)	120·4 (4)	C(3′)—C(2′)—O(2′)	109·6 (3)
C(2—C(3)—C(4)	120·6 (4)	C(2′)—C(3′)—C(4′)	101·5 (4)
C(3)—C(4)—C(5)	119·9 (5)	C(2′)—C(3′)—O(3′)	113·3 (3)
C(4)—C(5)—C(6)	120·0 (5)	C(4′)—C(3′)—O(3′)	110·7 (4)
C(1)—C(6)—C(5)	120·5 (4)	C(3′)—C(4′)—C(5′)	115·5 (4)
C(1)—C(7)—N(1)	110·2 (3)	C(3′)—C(4′)—O(4′)	103·4 (4)
N(1)—C(8)—N(2)	126·2 (4)	C(5′)—C(4′)—O(4′)	110·2 (3)
C(10)—C(9)—C(12)	106·9 (4)	C(4′)—C(5′)—O(5′)	113·9 (4)
C(10)—C(9)—N(2)	123·7 (4)	C(7)—N(1)—C(8)	118·4 (3)
C(12)—C(9)—N(2)	129·4 (4)	C(7)—N(1)—C(11)	117·0 (3)
C(9)—C(10)—C(11)	123·0 (3)	C(8)—N(1)—C(11)	123·9 (4)
C(9)—C(10)—N(4)	106·6 (4)	C(8)—N(2)—C(9)	113·7 (3)
C(11)—C(10)—N(4)	130·4 (4)	C(12)—N(3)—N(4)	107·0 (3)
C(10)—C(11)—N(1)	109·6 (4)	C(10)—N(4)—C(1′)	128·3 (3)
C(10)—C(11)—O(1)	129·2 (4)	C(10)—N(4)—N(3)	110·5 (3)
N(1)—C(11)—O(1)	121·2 (4)	C(1′)—N(4)—N(3)	120·1 (3)
C(9)—C(12)—C(13)	129·5 (4)	C(1′)—O(4′)—C(4′)	110·6 (3)
C(9)—C(12)—N(3)	109·0 (4)	C(2′)—O(2′)—H(2′)	103 (3)
C(13)—C(12)—N(3)	121·5 (4)	C(3′)—O(3′)—H(3′)	106 (3)
C(2′)—C(1′)—N(4)	112·1 (3)	C(5′)—O(5′)—H(5′)	111 (4)
C(2′)—C(1′)—O(4′)	105·5 (3)		

	Symbol*	
N(3)—N(4)—C(1′)—O(4′)	χ	66·4 (4)
N(3)—N(4)—C(1′)—C(2′)		−50·1 (4)
C(1′)—C(2′)—C(3′)—C(4′)	θ_0, τ_2	39·7 (4)
C(2′)—C(3′)—C(4′)—O(4′)	θ_1, τ_3	−37·4 (4)
C(3′)—C(4′)—O(4′)—C(1′)	θ_2, τ_4	21·1 (4)
C(4′)—O(4′)—C(1′)—C(2′)	θ_3, τ_0	4·3 (4)
O(4′)—C(1′)—C(2′)—C(3′)	θ_4, τ_1	−27·7 (4)
O(4′)—C(4′)—C(5′)—O(5′)	ψ_1	69·4 (5)
C(3′)—C(4′)—C(5′)—O(5′)	ψ_2	−173·9 (4)

* For symbols see Altona & Sundaralingam (1972).

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42308 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

the numbering scheme is 1,2...5 for C(1′),...,C(4′), O(4′)]. Finally, the torsion angles ψ_1 = O(4′)—C(4′)—C(5′)—O(5′) and ψ_2 = C(3′)—C(4′)—C(5′)—O(5′) are 69·4 (5) and −173·9 (4)°, defining the conformation around C(4′)—C(5′) as *gauche–trans*. Values of χ in the range −10 to 40° (normal-*anti*) have been found to be associated with the C(3′)-*endo* ribose conformations, while χ values in the range 40 to 120° (mid-*anti* and high-*anti*) with C(2′)-*endo* conformations (Sprang *et al.*, 1978). The present compound, therefore, is atypical as it displays a mid-*anti*, C(3′)-*endo* conformation. This can be tentatively imputed to the repulsion effect of the added O(1) ketonic O in position 7 of the heterobicycle – otherwise the conformation would be normal-*anti*.

The molecular packing along **a** is shown in Fig. 2. All hydrogen bonds are intermolecular and are reported in Table 3. The asymmetric unit accepts four hydrogen bonds to N(2),O(4′),O(2′) and O(3′) [the last two being donated by the same atom H(5′)] and is donor of two hydrogen bonds from O(2′)—H(2′) and O(3′)—H(3′) and of a bifurcated one from O(5′)—H(5′). It has been reported that the hydrogen bond accepted by O(4′) is rather unusual in normal nucleosides or nucleotides and seems to be more often a feature of modified nucleosides (Srikrishnam *et al.*, 1983, and references therein).

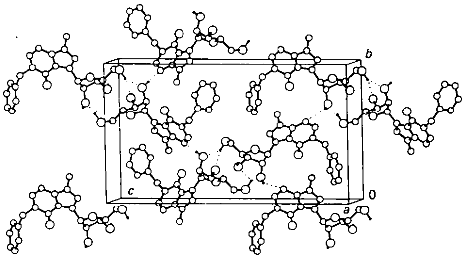

Fig. 2. The crystal packing along **a**. The two bifurcated hydrogen bonds are donated and accepted by the asymmetric unit (bottom-left molecule in the cell) by two molecules shifted by the vector (1,0,0). They appear to be superposed owing to the projection along **a**.

Table 3. *Hydrogen-bond lengths* (Å) *and angles* (°) (*e.s.d.'s in parentheses*)

A—H···B	Symmetry operation	A—H	A···B	H···B	A—H···B
O(2′)—H(2′)···N(2)	$1-x, \frac{1}{2}+y, \frac{3}{2}-z$	0·95 (4)	2·766 (4)	1·82 (4)	179 (4)
O(3′)—H(3′)···O(4′)	$1+x, y, z$	0·76 (4)	2·789 (4)	2·05 (4)	165 (4)
O(5′)—H(5′)···O(2′)	$x-\frac{1}{2}, \frac{1}{2}-y, 1-z$*	1·00 (6)*	3·323 (4)	2·52 (6)	136 (5)
O(5′)—H(5′)···O(3′)	$x-\frac{1}{2}, \frac{1}{2}-y, 1-z$*	1·00 (6)*	2·889 (4)	1·98 (6)	149 (5)

* Bifurcated hydrogen bond.

A complete graph representation of the hydrogen bonding inside the crystal is given in Fig. 3, where the points represent single molecules and the net of hydrogen bonds has been topologically distorted in such a way as to obtain the maximum interconnection net symmetry. The graph consists of infinite equivalent strips A,A',B,B', where the points are interconnected by a contiguous net of triangles and where all the zigzag interconnections are actually bifurcated hydrogen bonds (this is not shown in Fig. 3 for the sake of simplicity). Each strip is connected on both sides to two other strips lying at different levels by a net of rectangles so that a three-dimensional packing of hexagonal prisms is finally obtained. The prisms are oriented along the a axis in the crystal structure. The graph of Fig. 3 can be classified as F_6^6(3,4,6) according to Kuleshova & Zorky (1980); F_6^6 indicates that the graph has a three-dimensional framework, where each molecule is connected by 6 hydrogen bonds to 6 other molecules and (3,4,6) indicates the closed rings present in the graph. If the second component of the bifurcated hydrogen bond is also taken into account the symbol changes to F_6^8(2,3,4,6) (each molecule forms 8 hydrogen bonds with 6 neighbors, closing rings of 2,3,4 and 6 elements).

It should be noted that these particular graphs are probably rather uncommon as they have not been found by these authors in spite of the fact that they analyzed as many as 776 homonuclear hydrogen-bonding-containing molecular crystals.

The authors are indebted to Mr G. Bertocchi for skillful technical assistance.

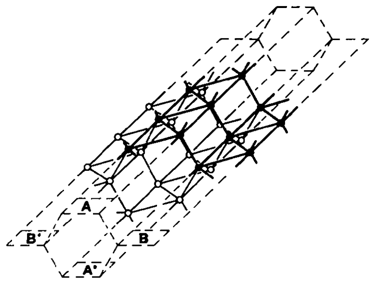

Fig. 3. Graph representation of the hydrogen-bonding connections inside the crystal. Each point represents a molecule and the net of interconnections is topologically deformed in such a way as to obtain the maximum net symmetry. The resulting graph can be classified as F_6^6(3,4,6), according to Kuleshova & Zorky's (1980) nomenclature. For the sake of clarity only molecules represented by full points show all the bonds starting from them.

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Détermination Structurale à 205 K du Poly{bis[(*p*-bromophénylcarbamoyloxy)-4 butyl]-1,2 butène-1 yne-3 ylène}, $(C_{26}H_{26}Br_2N_2O_4)_n$

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Abstract. $M_r = (588)_n$, non-melting compound, triclinic, $P\bar{1}$, $a = 5{\cdot}670\,(3)$, $b = 22{\cdot}47\,(2)$, $c = 4{\cdot}864\,(3)$ Å, $\alpha = 97{\cdot}40\,(1)$, $\beta = 98{\cdot}98\,(5)$, $\gamma = 83{\cdot}26\,(6)°$, $V = 604\,(2)$ Å^3, $Z = 1$, $D_x = 1{\cdot}62$ Mg m^{-3}, $\lambda(\text{Cu }K\alpha) = 1{\cdot}54178$ Å, $\mu = 4{\cdot}52$ mm^{-1}, $F(000) = 298$, $T = 205$ K, $R = 0{\cdot}08$ for 1118 reflections with $F_o \geq 3\sigma(F_o)$. The polymer molecule of the title compound poly(4_pBPU) has a good planarity; the molecular conformation and structural stacks of the polymer ribbons are compared with those of the unsubstituted polymer compound poly(4PU); no difference in the atomic environment can explain the difference observed between the acetylene electronic structure of the poly(4_pBPU) backbone [C≡C $1{\cdot}16\,(1)$ Å] and the butatriene structure of poly(4PU).

Introduction. Les cristaux de poly{bis[(*p*-bromophénylcarbamoyloxy)-4 butyl]-1,2 butène-1 yne-3 ylène} sont obtenus par photopolymérisation à l'état solide (irradiation X, γ ou UV) du monomère diacétylénique R—C≡C—C≡C—R [$R = (CH_2)_n$COONHC$_6$H$_4$Br, $n = 4$] communément appelé DDD$_p$BPU (ou 4_pBPU) selon la nomenclature dodecadiyne-5,7 bis(*p*-bromophényluréthane)-1,12. Le monomère 4_pBPU cristallise sous deux formes polymérisables: l'une orange (recristallisation dans l'acétone), l'autre bleue (acétone/hexane ou tétrahydrofuranne), et ce, dès l'apparition de quelques dix millièmes de molécules polymère (Patel & Miller, 1981; Patel, 1980). Le polymère étudié ici est obtenu par irradiation X d'un monocristal de monomère forme 'orange'. Après vingt minutes d'irradiation [λ(Cu $K\alpha$), 3 mA, 50 kV], ce dernier éclate en fragments hétérogènes oranges (monomère très partiellement polymérisé) et noirs (polymère total); les clichés de poudre de chacune de ces parties témoignent de réseaux cristallins totalement différents. Le monomère 4_pBPU orange est donc très réactif sous irradiation; il présente toutes les caractéristiques d'un mécanisme de polymérisation selon un processus de croissance hétérogène, avec apparition de cristallites polymères au sein du cristal monomère, tel que le décrivent Wegner (1977) et Kaiser, Wegner & Fisher (1972) pour le HDPU 'forme II' [ou 1PU, $R = (CH_2)_n$COONHC$_6$H$_5$, $n = 1$], dès que ce dernier atteint un taux de polymérisation supérieur à 10%. Ceci différencie donc le 4_pBPU des autres monomères phényluréthane, tels que le composé chloré HD$_p$CPU [1_pCPU, $R = (CH_2)_n$COONHC$_6$H$_4$Cl, $n = 1$, forme rose] et le composé non substitué DDDPU [4PU ou TCDU, $R = (CH_2)_n$COONHC$_6$H$_5$, $n = 4$], qui tous deux polymérisent suivant un processus de solution-solide continue monomère–polymère, les molécules polymères se substituant progressivement et de façon aléatoire aux molécules monomères dans le réseau cristallin du monomère (Gross, Sixl, Kröhnke & Enkelmann, 1980; Brouty, Spinat & Whuler, 1984).

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