SYNTHESIS OF ACETALS OF PURIN-9-YLPROPIONALDEHYDES AND PURIN-9-YL-α-AMINOBUTYRIC ACIDS

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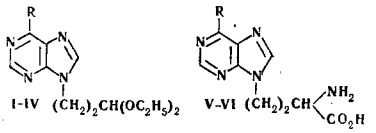
6-Chloro-, 6-mercapto-, 6-methylthio-, and 6-amino-9-(3',3'-diethoxypropyl)purines, γ-(6-mercaptopurin-9-yl)-α-aminobutyric acid, and γ-(6-methylthiopurin-9-yl)-α-aminobutyric acid have been synthesized.

In analogy with previous work [1, 2], by the alkylation of 6-chloropurine and 6-methylthiopurine with 1-chloro-3,3-diethoxypropane we have obtained diacetyls of 6-substituted purin-9-ylpropionaldehyde (I, II). By the nucleophilic replacement of the chlorine in I by means of thiourea and of ammonia we have obtained 6-mercapto- and 6-amino-9-(3',3-diethoxypropyl)purines (III, IV).



I R = Cl; II R = SCH_3; III R = SH;
IV R = NH_2; V R = SH; VI R = SCH_3

By hydrolysis and subsequent cyanohydrin synthesis, for III we have obtained γ-(6-mercaptopurin-9-yl)-α-aminobutyric acid (V). The alkylation of V with methyl iodide in an alkaline medium has given γ-(6-methylthiopurin-9-yl)-α-aminobutyric acid (VI). The purinyl-α-aminobutyric acids obtained are characterized by high solubility in water.

Table 1. Characteristics of the Compounds Obtained

Compound	Mp, °C*	R_f in system†		UV spectra					
				pH 1		pH 7		pH 13	
		1	2	λ_{max}, nm	lg ε	λ_{max}, nm	lg ε	λ_{max}, nm	lg ε
I	43[a]	0,95	0,96	265	3,60	265	3,64	265	3,65
II	34—35[a]	0,95	0,96	295	4,21	286	4,24	287	4,31
III	298—300[b]	0,92	0,93	323	4,27	320	4,53	309	4,27
IV	127[c]	0,78	0,80	258	3,48	258	3,52	261	3,54
V	258—259[d]	0,33	0,20	322	3,30	321	3,29	310	3,28
VI	231—232[d]	0,71	0,65	294	3,47	286	3,52	285	3,99

(continued)

Empirical formula	Found, %				Вычислено, %			
	C	H	N	S	C	H	N	S
$C_{12}H_{17}ClN_4O_2$	50,54	6,14	19,92	—	50,61	6,02	19,68	—
$C_{13}H_{20}N_4O_2S$	52,49	6,71	19,19	10,74	52,68	6,80	18,89	10,82
$C_{12}H_{18}N_4O_2S$	51,19	6,51	19,61	11,28	51,04	6,64	19,84	11,35
$C_{12}H_{19}N_5O_2$	54,47	7,34	26,50	—	54,32	7,22	26,40	—
$C_9H_{11}N_5O_2S \cdot 1/2H_2O$	41,11	4,73	26,45	12,38	41,21	4,57	26,66	12,23
$C_{10}H_{13}N_5O_2S \cdot H_2O$	42,00	5,46	24,39	11,40	42,09	5,33	24,55	11,24

*[a]From hexane; [b]from propanol; [c]from ethanol; [d]from water.
†System 1: n-C_3H_7OH—NH_4OH—H_2O (6:3:1); system 2: iso-C_3H_7OH—NH_4OH—H_2O (7:1:2). Paper: FN-11.

The positions of the substituents at $C_{(6)}$ and $N_{(9)}$ of the purine ring in the compounds obtained were confirmed by comparing their UV spectra with the known spectra of the diacetals of 6-substituted purin-9-ylacetaldehydes and 6-substituted purin-9-yl-α-alanines.

Some constants of these compounds and analytical information are given in Table 1.

REFERENCES

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