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LETTERS
TO THE EDITOR

Reaction of 6-Aminouracils with Hydrazide Nucleophiles

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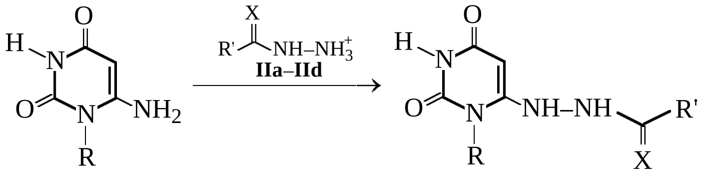
Searching for approaches to varying nitrogen-containing functional groups in uracils, we found that 6-aminouracils **Ia** and **Ib** [1] undergo acid-catalyzed substitution of the exocyclic amino group by hydrazides **IIa** and **IIb**, semicarbazide (**IIc**), and thiosemicarbazide (**IId**).



Ia, Ib **IIIa–IIIh**

I, R = H (**a**), CH_3 (**b**). **II**, R' = CH_3, X = O (**a**); R' = C_6H_5, X = O (**b**); R' = NH_2, X = O (**c**); R' = NH_2, X = S (**d**). **III**, R = H, R' = CH_3, X = O (**a**); R = CH_3, R' = CH_3, X = O (**b**); R = H, R' = C_6H_5, X = O (**c**); R = CH_3, R' = C_6H_5, X = O (**d**); R = H, R' = NH_2, X = O (**e**); R = CH_3, R' = NH_2, X = O (**f**); R = H, R' = NH_2, X = S (**g**); R = CH_3, R' = NH_2, X = S (**h**).

The reaction was performed in water (50 ml per 0.01 mol of **Ia** or **Ib**) under reflux for 2 (uracil **Ia**) or 4 h (uracil **Ib**). Reagents **IIa** and **IIb** were taken in a double excess with respect to uracils **Ia** and **Ib**, as a mixture of acetate and hydrochloride. Compounds **IIIa**–**IIIf** precipitated and were recrystallized from water. Compounds **IIIg** and **IIIh** were first neutralized with ammonia solution to pH 7 and washed with boiling ethanol to remove excess thiosemicarbazide.

2-(2,6-Dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)-acetohydrazide (IIIa), yield 52%, mp >300°C. Found, %: C 39.10; H 4.33; N 30.40. $C_6H_8N_4O_3$. Calculated, %: C 39.13; H 4.35; N 30.43. **2-(3-Methyl-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)-acetohydrazide (IIIb),** yield 40%, mp >300°C. Found, %: C 42.40; H 5.00; N 28.30. $C_7H_{10}N_4O_3$. Calculated, %: C 42.42; H 5.05; N 28.28. **2-(2,6-Dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)benzohydrazide (IIIc),** yield 73%, mp >300°C. Found, %: C 53.63; H 4.06; N 22.78. $C_{11}H_{10}N_4O_3$. Calculated, %: C 53.66; H 4.07; N 22.76. **2-(3-Methyl-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)benzohydrazide (IIId),** yield 42%, mp >300°C. Found, %: C 55.40; H 4.60; N 21.53. $C_{12}H_{12}N_4O_3$. Calculated, %: C 55.38; H 4.62; N 21.54. **2-(2,6-Dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)hydrazinocarboxamide (IIIe),** yield 82%, mp 270–272°C. Found, %: C 32.40; H 3.80; N 37.82. $C_5H_7N_5O_3$. Calculated, %: C 32.43; H 3.78; N 37.84. **2-(3-Methyl-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)hydrazinocarboxamide (IIIf),** yield 47%, mp 260–264°C. Found, %: C 36.20; H 4.50; N 35.20. $C_6H_9N_5O_3$. Calculated, %: C 36.18; H 4.52; N 35.18. **2-(2,6-Dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)hydrazinocarbothiamide (IIIg),** yield 45%, mp 240–243°C. Found, %: C 29.90; H 3.50; N 34.80. $C_5H_7N_5O_2S$. Calculated, %: C 29.85; H 3.48; N 34.83. **2-(3-Methyl-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)hydrazinocarbothiamide (IIIh),** yield 34%, mp 277–280°C. Found, %: C 33.50; H 4.20; N 32.55. $C_6H_9N_5O_2S$. Calculated, %: C 33.49; H 4.19; N 32.56.

Earlier compounds like **IIIa**–**IIIh** were prepared in three stages from *N*-alkylbarbituric acids [2].

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Purity control was performed by TLC on Silufol UV-254 plates, eluents CH_3OH–$CHCl_3$, 1:2 (**IIIa**, **IIIb**, **IIIe, IIIh**) or CH_3OH–$CHCl_3$–C_6H_{14}, 1:4:1 (**IIIc**, **IIId**).

The structure of compounds **IIIa**–**IIIh** was proved by means of mass spectrometry and IR spectroscopy. The mass spectra were obtained on a Varian MAT-112 instrument, ionizing energy 70 eV, ion source temperature 220°C. The IR spectra were measured in mineral oil on a Specord-80 instrument.

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