SYNTHESIS OF 5-ARYLIDENE-2,4,6(1*H*,3*H*,5*H*)PYRIMIDINETRIONE DERIVATIVES

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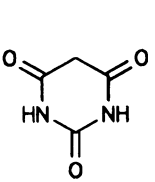
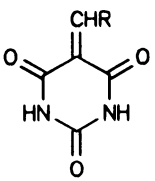
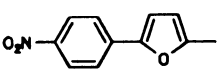
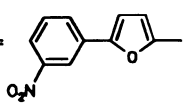
From the synthetic viewpoint, barbituric acid (*I*) and its derivatives serve most often in preparation of arylidene condensation products[1-3], i.e. compounds that have a strongly polarized double bond. Both aliphatic and aromatic aldehydes have been used. We have now synthesized new derivatives *II* by reaction of barbituric acid (*I*) with the corresponding heterocyclic aldehydes RCH=O. In all cases dimethylformamide was used as a reaction solvent without catalyst.

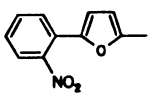
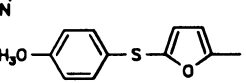


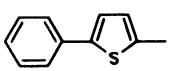
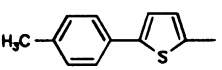
I

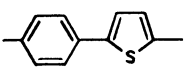
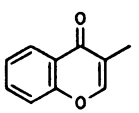


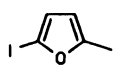
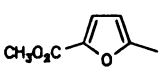
II

In formula *II* : *a*) R =  *b*) R = 

c) R =  *d*) R = 

e) R =  *f*) R = 

g) R =  *h*) R = 

i) R =  *j*) R = 

EXPERIMENTAL

Melting points were measured on a Kofler block and are uncorrected. IR spectra (cm^{-1}) were measured by the KBr technique.

5-Arylidene-2,4,6(1*H*,3*H*,5*H*)pyrimidinetriones (*IIa – IIj*)

A stirred solution of *I* (0.128 g, 0.001 mol) and the corresponding aldehyde (0.001 mol) in dimethylformamide (3 – 5 ml) was heated (80 °C) for 30 min. After this time, the reaction mixture was cooled and set aside overnight. The separated precipitate of compound *II* was collected, washed with cold ethanol, dried and purified by crystallization from dimethylformamide (Table I). IR spectra are presented in Table II.

TABLE I
5-Arylidene-2,4,6(1*H*,3*H*,5*H*)pyrimidinetriones *IIa – IIj*

Compound	Formula (M.w.)	M.p., °C Yield, %	Calculated/Found			
			% C	% H	% N	% S
IIa	$C_{15}H_9N_3O_5$	375 (decomp.)	57.88	2.91	13.50	
	(311.2)	89	57.81	2.90	13.45	
IIb	$C_{15}H_9N_3O_5$	330 – 332	57.88	2.91	13.50	
	(311.2)	96	57.79	2.88	13.52	
IIc	$C_{15}H_9N_3O_5$	271 – 272	57.88	2.91	13.50	
	(311.2)	93	57.91	2.90	13.46	
IId	$C_{16}H_{12}N_2SO_5$	268 – 269	55.80	3.51	8.14	9.31
	(344.3)	87	55.91	3.58	8.20	9.34
IIe	$C_{15}H_{10}N_2SO_3$	350 – 352	60.39	3.38	9.39	10.75
	(298.3)	61	60.45	3.41	9.27	10.70
IIf	$C_{16}H_{12}N_2SO_3$	370 (decomp.)	61.52	3.87	8.97	10.27
	(312.3)	71	61.61	3.90	8.89	10.32
IIg	$C_{15}H_9ClN_2SO_3$	370 (decomp.)	54.14	2.73	8.42	9.63
	(332.8)	53	54.14	2.85	8.62	9.64
IIh	$C_{14}H_8N_2O_5$	296 – 298	59.16	2.84	9.86	
	(284.2)	79	59.00	2.90	9.78	
IIi	$C_9H_5IN_2O_4$	365 (decomp.)	32.55	1.52	8.44	
	(332.1)	60	32.67	1.49	8.25	
IIj	$C_{11}H_8N_2O_6$	311 – 313	50.00	3.05	10.60	
	(264.2)	87	49.67	3.10	10.51	

TABLE II
IR spectral data for synthesized compounds

Compound	IR spectra, cm^{-1}
IIa	3 326, 3 193, 3 084, 1 732, 1 689, 1 574, 1 549, 1 524, 1 419, 1 381, 1 372, 1 335, 1 300, 1 275, 1 213, 1 042, 968, 854, 808, 754, 559
IIb	3 198, 3 140, 3 071, 1 746, 1 713, 1 665, 1 649, 1 645, 1 566, 1 536, 1 512, 1 431, 1 387, 1 354, 1 323, 1 300, 1 262, 1 231, 1 098, 1 042, 963, 509
IIc	3 200, 3 073, 1 746, 1 711, 1 665, 1 645, 1 565, 1 530, 1 429, 1 377, 1 319, 1 264, 1 227, 1 096, 1 055, 957, 509
IId	3 195, 3 079, 1 752, 1 703, 1 671, 1 595, 1 565, 1 497, 1 437, 1 420, 1 366, 1 310, 1 260, 1 254, 1 213, 1 171, 1 034, 949, 828, 787, 554, 505
IIf	3 193, 3 063, 1 742, 1 669, 1 568, 1 455, 1 449, 1 445, 1 431, 1 416, 1 401, 1 397, 1 341, 1 327, 1 264, 1 238, 812, 797, 538
IIg	3 191, 3 065, 1 742, 1 680, 1 669, 1 568, 1 449, 1 431, 1 406, 1 395, 1 341, 1 325, 1 262, 1 240, 1 090, 806, 802, 550
IIh	3 548, 3 376, 3 233, 3 087, 1 746, 1 688, 1 628, 1 564, 1 535, 1 464, 1 437, 1 406, 1 365, 1 348, 1 312, 1 265, 1 221, 1 192, 1 026, 853, 777, 758, 515
IIi	3 123, 3 040, 2 847, 1 740, 1 705, 1 653, 1 559, 1 426, 1 372, 1 319, 1 035, 945, 851, 812, 793, 552, 515
IIj	3 233, 3 177, 3 061, 1 740, 1 721, 1 705, 1 674, 1 586, 1 437, 1 393, 1 321, 1 298, 1 217, 1 024, 866, 798, 766, 563

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