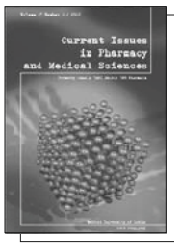

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Synthesis of new derivatives of 9-aryl-3-ethoxycarbonylmethyl-2,4,5(9H)-trioxo-7,8-dihydroimidazo[1,2-a][1,3,5]triazepine

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ABSTRACT

The series of new derivatives of 9-aryl -3-ethoxycarbonylmethyl-2,4,5(9H)-trioxo-7,8-dihydroimidazo [1,2-a][1,3,5]triazepines was obtained by condensation of 1-(1-arylimidazoline-2-ylidene)-3-ethylcarbonylurea with diethyl oxalic acid ester. Considering the structure of the obtained compounds it can be expected that these compounds can reveal pharmacological activity.

Keywords: 1-(1-arylimidazoline-2-ylidene)-3-ethylcarbonylureas derivatives, diethyl oxalic acid ester

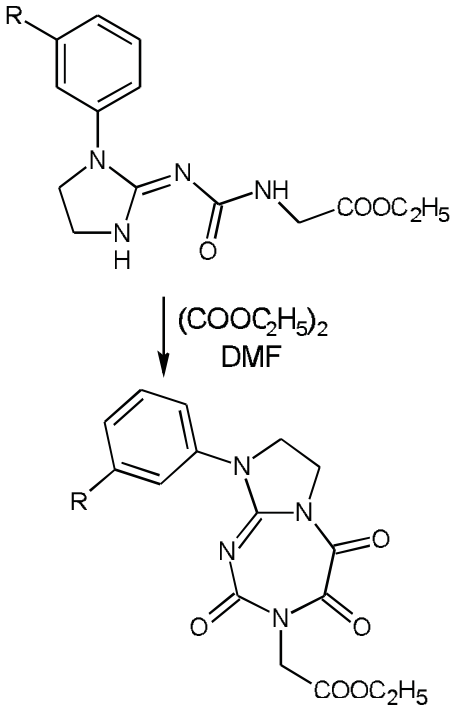
INTRODUCTION

The syntetic derivatives of triazepine form are various and important group of medicines.In the search for new derivatives with potential pharmacological activity received of new imidazo[1,2-a][1,3,5]triazepine was obtained. Some derivatives of imidazotriazepine show activity as muscule relaxants [1], have antifungal [8]anti-diabetic [3,9,10], antimicrobial [2,4], antiviral [7,12], anticancer [7] properties.This heterocyclic system was obtained in two-step reaction. It seemed worthwhile to syntesize new imidazo[1,2-a][1,3,5]triazepine derivatives and to estimate their pharmacological activity.

RESULTS AND DISCUSSION

New 9-aryl-3-ethoxycarbonylmethyl-2,4,5(9H)-trioxo--7,8-dihydroimidazo[1,2-a][1,3,5] triazepines were received as a result of condensation of 1-(1-arylimidazoline-2-ylidene)-3-ethylcarbonylureas [6,11] with diethyl oxalic acid ester.The reaction was conducted in the boiling temperature of the solvent.The reaction sequence leading to the formation of I-V is outlined in the Scheme

Melting points were determined on a Boetius apparatus and given uncorrected.The ^{1}HNMR spectra were recorded on AVANCE 300 MHz spectrometers stiffy Brucer in DMSO-d_6 with TMS as internal standard.The mass spectra were recorded using micr OT-Q II stiffy Brucer mass spectrometers. Elemental analyses were performed on a Perkin-Elmer analyzer .All the compounds were recrystallized from 2-propanol. Chemicals were purchased from Merck Co or Fluca Lab. And without purification.Purity was checked by TLC on Merck Co.TLC Was performed on commercial Merc SiO_2 Plates with chloroform-methanol (10:2) solvent system visualization with UV.



R= H, 4 -CH$_3$, 4 -OCH$_3$
3 -Cl, 4 -Cl

Fig. 1. Experimental Design

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The physical data of new compounds are shown in Table 1.

Table1. The physical data of new compounds

Comp.	R	Formula (mol. wt.)	M.p. (°C) Yield (%)	Analysies (calctd/found)				
				% C	% H	% Cl	% N	% S
I	H	$C_{16}H_{16}N_4O_5$ 344,34	251-53 36	55.81 55.23	4.68 4.80		16.27 16.60	
II	2-CH_3	$C_{17}H_{18}N_4O_52$ 358,37	243-43 40	56.98 56.59	5.06 5.36		21.68 21.82	
III	4-OCH_3	$C_{17}H_{18}N4O62$ 374,37	254-56 42	54.54 54.64	4.85 4.27		14.97 14.26	
IV	3-Cl	$C_{16}H_{15}N_4O_5Cl$ 378,79	283-85 32	50.73 50.80	3.99 3.17	9.36 9.38	14.79 14.00	
V	4-Cl	$C_{16}H_{15}N_4O_5Cl$ 378,79	218-20 40	50.73 50.52	3.99 3.37	9.36 9.12	14.79 14.80	

^{1}H NMR (DMSO-d_6); (ppm) for:
Comp. I: 6.65-6.90 (m.5H.CH_{arom}); 4.60-4.72 (m.5H.$COOC_2H_5$); 4.23 (t.2H.N-CH_2); 3.52-3.8 (m.4H.2CH_2)
Comp. III: 7.50-7.85 (m.4H.CH_{arom}); 4.62-4.76 (m.5H.$COOC_2H_5$); 4.17 (t.2H.N-CH_2); 3.33-3.60 (m .4H.2CH_2); 2.50-2.62 (s.3H.OCH_3)
Comp. IV: 7.10-7.30 (m.4H.CH_{arom}); 4.50-4.70 (m.5H.$COOC_2H_5$); 4.19 (t.2H.N-CH_2); 3.68-3.9 (m.4H.2CH_2)
Comp. V: 7.11-7.16 (m.4H.CH_{arom}); 4.58-4.70 (m.5H.$COOC_2H_5$)); 4.33 (t.2H.N-CH_2); 3.52-3.8 (m.4H.2CH_2)

EXPERIMENTAL

Synthesis of 9-aryl-3-ethoksycarbonylmethyl-2,4,5(9H)-trioxo-7,8-dihydroimidazo[1,2-a] [1,3,5] triazepines

The diethyl oxalic acid ester (0.01 mole) was added to 1-(1-arylimidazolidine-2-ylidene)-3 ethylcarbonylureas (0.01 mole) dissolved in 50 cm^3 of DMF. The mixture was heated under reflux for 10-12h.The solvend was evaported.The precipitate was filtered off and recrystallized.

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