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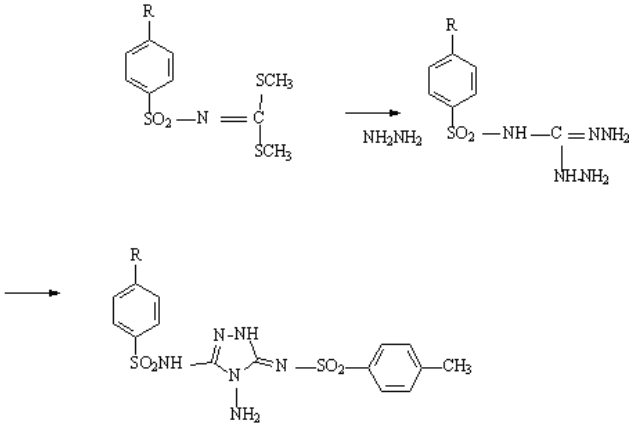
Synthesis of new derivatives of 4-amino-1,2,4-triazole

Synteza nowych pochodnych 4-amino-1,2,4-triazolu

Compounds containing 4-amino- 1,2,4-triazole moiety have received considerable attention among medicinal chemists because molecules with these structural features have been found to display a wide range of potent biological activities, such as antibacterial,antimicrobial [1-4,9], antifungal [4,5], antituberculosis [6].Synthesis and determination of the structure of five derivatives of this ring [7,8] system was aimed towards investigatig their potential pharmacological activity. Results of pharmacological screenings will be published elsewhere.

RESULTS AND DISCUSION

We applied a two-step reaction in the synthesis of the required 4-amino-1,2,4-triazole.The reaction of dimethyl N-phenylsulfonyliminodithioic acid esters with hydrazine hydrate afforded the phenylsulfonyl derivatives of diamino guanidine (imidocarbonic acid hydrazide).Then in the reaction of dimethyl N-tosyliminodithioic acid ester the novel group of 4-amino-1,2,4-triazole derivatives was obtained. The reaction sequence leading to the formation of I-V is outlined in the Scheme.



R=H, CH_3, Cl, $NHCOCH_3$

The physical data of new compounds are shown in Table:

Comp.	R	Formula (mol.wt.)	M.p. (°C) Yield (%)	Analysies (calctd/found)				
				% C	% H	% Cl	% N	% S
I	H	$C_{15}H_{16}N_6O_4S_2$ 408.47	224-26 36	44.11 44.23	3.95 3.80		20.58 20.60	15.70 15.63
II	2-CH_3	$C_{16}H_{18}N_6O_4S_2$ 421.49	263-64 40	45.60 45.59	4.30 4.36		19.94 19.82	15.22 15.33
III	4-CH_3	$C_{16}H_{18}N_6O_4S_2$ 421.49	251-53 42	45.60 45.64	4.30 4.27		19.94 19.26	15.22 15.20
IV	NHAc	$C_{17}H_{19}N_7O_4S_2$ 465.53	257-59 32	43.86 43.80	4.11 4.17		21.06 21.00	13.78 13.90
V	4-Cl	$C_{15}H_{15}N_6O_4S_2Cl$ 442.92	266-68 40	40.68 40.52	3.41 3.37	8.00 8.12	18.98 18.80	14.48 14.50

^{1}H NMR (DMSO-d_6); (ppm) for:
Comp.I : 11.17 (m,2H,2NH); 7.29-7.83 (m,9H,CH_{arom}); 5.43 (s,2H,NH_2); 2.75 (s,3H,CH_3)
Comp.III:11.11 (m,2H,2NH); 7.12-7.20 (m,8 H,CH_{arom}); 5.44 (s,2H,NH_2); 2.64-2.68 (m,6H,2CH_3)
Comp.IV: 13.20 (s,1H,NH); 11.21(m,2H,2NH); 7.10-7.30 (m,8H,CH_{arom}); 5.43 (m,2H,NH_2); 2.7-2.73 (m,6H,2CH_3)
Comp.V: 11.24 (m,2H,2NH); 7.11-7.16 (m,8H,CH_{arom}); 5.40 (s,2H,NH_2); 2.73 (s,3H,CH_3)

EXPERIMENTAL DESIGN

M.p.s were determined on Boetius apparatus and uncorrected. ^{1} HNMR spectra chemical shifts were measured on a Tesla BS 567 A in $CDCl_3$ with as internal standard. Elemental analysis and spectral data are on request from the author. All compounds were recrystallized from isopropanol (propan-2-ol).

SYNTHESIS OF 1H-3-ARYLSULFONYLAMINO-4-AMINO-5-TOSYLIMINO-1,2,4-TRIAZOLES

The dimethyl N-tosyliminodithioic acid ester (0.01 mole) was added to 1-arylsulfonylamino-2,3-diaminoguanidine (0.01 mole) dissolved in 50 cm^3 of DMF. The mixture was heated under reflux for 10–12 h. The solvent was evaporated. The precipitate was filtered off and recrystallized.

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SUMMARY

The series of new derivatives of 1H-3-arylsulfonylamino-4-amino-5-tosylimino-1,2,4-triazole was obtained by condensation of 1-arylsulfonylamino-2,3-diaminoguanidyny with dimethyl N-tosyliminodithioic acid ester.Considering the structure of the obtained compounds it can be expected that these compounds can reveal pharmacological activity.

STRESZCZENIE

Otrzymano szereg pochodnych 1H-3-arylosulfonylo-4-amino-5-tosylimino-1,2,4-triazolu w reakcji kondensacji 1-arylosulfonyloamino-2,3-diaminoguanidyny z estrem dimetylowym kwasu N-tosyliminoditiowęglowego. Pochodne te mogą wykazywać działanie farmakologiczne.Zostaną przekazane do badań mikrobiologicznych.