

## REGIOISOMERS OF PYRAZOLO[1,5-a]PYRIMIDINES DETERMINATION BY <sup>15</sup>N NMR SPECTROSCOPY

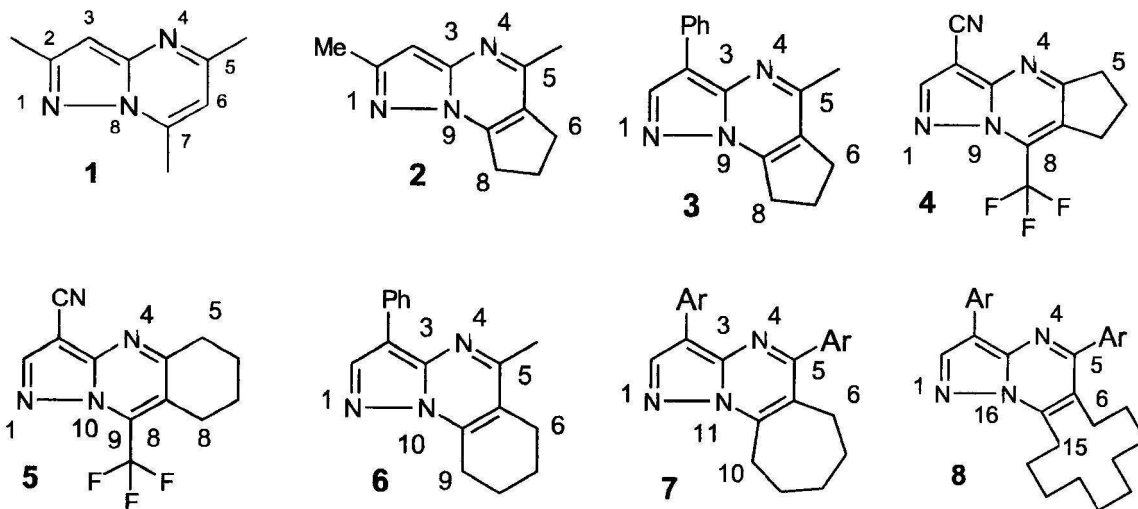
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Derivatives of pyrazolo[1,5-a]pyrimidines are an important type of fused heterocycles, which possess a wide field of pharmacological activities depending on their nature and substitution position in molecule. Different problems often appear under synthesis of these compounds which are connected with regioselectivity of such reactions and correct identification of isomer products. The formation of several isomers is a result of the attack by nucleophilic centers of 3(5)-aminopyrazol (NH<sub>2</sub>, N<sup>1</sup>) on electrophilic centers of polyfunctional compounds.

Produced pyrazolo[1,5-a]pyrimidines contain two isolated spin systems of magnetic nuclei <sup>1</sup>H и <sup>13</sup>C between which neither direct nor indirect coupling exist. Long-range scalar interactions of aromatic and methyl (or methylene) protons with knot nitrogen-15 atom and the same one in position 4 in pyrazolopyrimidine fragment produced by <sup>1</sup>H-<sup>15</sup>N HMBC spectra prove to be the exact structure of these products. By this approach we have studied the following compounds:



There are the results of some of them by using NMR spectrometer Jeol ECX-400A:

**Compound 1:**  $\delta N^8 = -156.6$  ppm,  $\delta N^4 = -111.9$  ppm and  $\delta N^1 = -110.7$  ppm relative to nitromethane.  $^3J(2-CH_3-N^1) = 11.5$  Hz;  $^3J(5-CH_3-N^4) = 11.7$  Hz;  $^3J(7-CH_3-N^8) = 13.8$  Hz;  $^3J(H^3-N^8) = 13.4$  Hz;  $^3J(H^6-N^8) = 12.2$  Hz.

**Compound 4:**  $\delta N^9 = -167.5$  ppm,  $\delta N^4 = -102.3$  ppm and  $\delta N^1 = -99.3$  ppm. Cross-peaks  $N^1/H^2$ ,  $N^9/H^2$  and  $N^4/C^5H_2$  are observed in <sup>1</sup>H-<sup>15</sup>N HMBC spectrum.

**Compound 8:** (Ar = 4-ClC<sub>6</sub>H<sub>4</sub>):  $\delta N^{16} = -152.5$  ppm,  $\delta N^1 = -107.3$  ppm. Cross-peaks  $N^1/H^2$ ,  $N^{16}/H^2$  и  $N^{16}/C^{15}H_2$  are observed in <sup>1</sup>H-<sup>15</sup>N HMBC spectrum.

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