DIALKYL ISOMERS OF BENZENESULFONAMIDPHENYLPYRIMIDINE-4(1*H*)-ONE: SYNTHESIS, STRUCTURE AND PHARMACOLOGICAL STUDIES

Denis S. Anenko[a]*, Ivan P. Kodonidi[b], Sergey D. Kirik[c,d], Tamara N. Glizhova[a] and Narzullo B. Saidov[e]

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ABSTRACT

Interaction of *N*-acetyl-2-phenylacetamide with sulfanilamide and *N*-(2-phenylacetyl)propanamide with sulfanilamide led to the preparation of the two isomeric benzenesulfonamidphenylpyrimidin-4(1*H*)-ones. In positions 2 and 6, the synthesized phenylpyrimidin-4(1*H*)-ones contained methyl and ethyl as substituents in the first case (IIa), and ethyl and methyl – in the second one (IIb), respectively. The crystal structures of the compounds have been determined by X-ray powder diffraction. It has been established that the positions of substituents significantly affect the conformation of molecules. In molecule IIa, the phenyl ring is rotated to the pyrimidine one by 84°; in IIb, the both rings lie in the same plane. Due to different conformations, the packing of molecules in the crystal lattice changes significantly. Pharmacological properties of isomeric pyrimidinones have been studied in relation to the anti-inflammatory and cerebroprotective activity in chronic traumatic encephalopathy. A comparative analysis of the drug similarity has been carried out. Screening of anti-inflammatory and cerebroprotective activities has shown that compound IIa surpassed its structural isomer in the pharmacological action, which was interpreted as a greater elasticity result of molecule IIa compared to IIb due to the less extended π-system.