SYNTHESIS AND PREDICTED BIOLOGICAL ACTIVITY OF ALICYCLIC AND AROMATIC DERIVATIVES β-ALANINE AND BENZIMIDAZOLES ON THEIR BASIS

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The products of accession of different amines with acrylic, methacrylic, crotonic acids and their derivatives are of great interest because they find application as intermediates in organic synthesis. The preparation of *N*-substituted β-aminopropionic acid derivatives was carried out by reacting equimolar amounts of morpholine, benzylamine, azepane and 4-aminopridine with methyl ester acrylic acid in a solution of isopropyl alcohol at room temperature for 24 hours. Received new β-alanine derivatives methyl-3-(azepan-1-yl)propanoate, methyl-3-(morpholin-4-yl)propanoate and methyl-3-benzylaminopropanoate were isolated by vacuum distillation with yields of 70 %, 90 %, 29 %, and methyl-3-(pyridinyl-4-amino)propanoate was isolated by recrystallization from isopropyl alcohol in 24 % yield. All the β-alanine derivatives was predicted on possible neurotropic biological activity by the PASS Online program. Azepane, benzylamine and 4-aminopyridine derivatives are showing possible activity "phobic disorders treatment", with a probability of 90 %, 83 % and 81 %, respectively. For the morpholine derivative, in addition to the possible activity of "treatment of phobic disorders" with a probability of 95%, an "antineuritic effect" was also detected with a probability of 80 %. A series of benzimidazoles of an aminocyclic and aromatic nature have been synthesized on the basis of the corresponding β-alanine esters by condensation with *o*-phenylenediamine in the presence of hydrochloric acid. The yields of the resulting 2-(2-azepan-1-ylethyl)-, 2-(2-morpholin-4-ylethyl)-, 2-(*N*-benzyl-2-aminoethyl)- and 2-(*N*-pyridin-4-yl-2-aminoethyl)-1*H*-benzimidazoles were 29 %, 52 %, 44 % and 18 %, respectively. Structures of all benzimidazoles are confirmed by ^{1}H NMR spectroscopy. The PASS Online program was used to calculate the possible biological activity. The PASS Online program presented for the all benzimidazoles possible biological activity: for azepan derivative – "treatment of acute neurological disorders" with a probability of 74 %, for morpholine derivative – "treatment of phobic disorders", with a probability of 84 %, "antineuritic effect" with a probability of 76 % and a "cerebral anti-ischemic" effect with a probability of 73 %, for

benzylamine derivative – "cerebral anti-ischemic" with a probability of 71 %. For the benzimidazole derivative of 4-aminopyridine, the PASS Online program did not reveal the desired possible activities with a probability of more than 70 %.

Keywords: benzimidazoles, β-alanine, PASS Online program.

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