

A n n o t a t i o n

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„Synthesis and prediction biological activity of some derivatives of N-(4-carboxyphenyl)-2,3,4,6-tetra-O-acetyl- β -D-glucopyranosylamine“

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The N- β -glycosidic bond is widely represented in a large number of natural compounds, primarily in nucleic acids and glycoproteins, some coenzymes, as well as synthetic analogues of nucleotides, the antimetabolites, which are used in the treatment of tumor diseases and viral infections. The development of efficient synthetic methodologies for various N-glycosides and their derivatives will be useful in designing and preparing synthetic natural product analogues.

The goal of our work was to synthesize of glucoconjugates of N-(4-carboxyphenyl)-2,3,4,6-tetra-O-acetyl- β -D-glucopyranosylamine (III) and prediction of their biological activity.

N-(4-carboxyphenyl)-2,3,4,6-tetra-O-acetyl- β -D-glucopyranosylamine has been synthesized from D-glucose and 4-aminobenzoic acid by refluxing in 95% methanol in the presence of a NH_4Cl catalyst and by the further acetylation of synthesized N-(4-carboxyphenyl)- β -D-glucopyranosylamine. By condensation of N-(4-carboxyphenyl)-2,3,4,6-tetra-O-acetyl- β -D-glucopyranosylamine with H-L-Gly ethyl ester hydrochloride and H-L-His methyl ester dihydrochloride in the presence of dicyclohexylcarbodiimide and triethylamine at 0°C temperature, the corresponding derivatives have been obtained for the first time.

The structures of obtained compounds were established by physical-chemical methods of analysis.

With the help of computer program PASSO online based on the analysis of structure activity-relationships wide range of the prediction data of possible biological activity and toxic/side effects for synthesized compounds has been predicted.