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GOSPODARKA I INNOWACJE

LABORATORIUM WIEDZY Artur Borcuch

Volume: 37 | 2023

Economy and Innovation
ISSN: 2545-0573

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TESTING THE BIOLOGICAL ACTIVITY OF SOME PROPERTIES OF PHENYLCHLORACETATE IN THE PASS ONLINE PROGRAM

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A R T I C L E I N F O.

Key words: Pass online, biological, phenyl chloroacetate, synthesis, phenyl phenoxy acetate. Activity, pharmacological, toxic, metabolic, enzyme, gene, expression, solvent, time, vacuum, chloroacetyl chloride.

Annotation

This article uses the PASS (online) program to study the biological activity of phenyl chloroacetate and phenyl phenoxy acetate. In this program, two new organic substances were found to have different biological activity. Relying on this data, the method of synthesis of phenyl chloroacetate and phenyl phenoxy acetate. It was first found by experiment. Research then synthesized phenyl phenoxy acetate.

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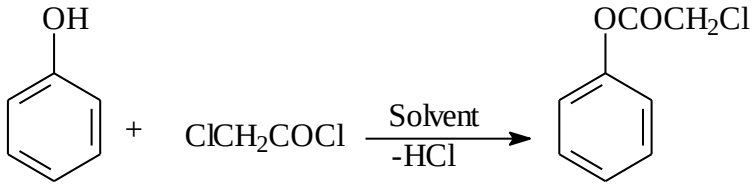
The study of the biological activity of substances often requires complex studies, a long time and large costs. But through the Pass online program, it is possible to theoretically study the biological activity of substances in a short time. During our study, there is an opportunity to consider the biological activity of the substance phenyl chloroacetate. We have developed a technique for synthesizing phenyl chloroacetate to obtain a biologically active substance.



Continuing scientific research, we worked on the synthesis of phenyl phenoxy acetate. and continued the method of its synthesis. The reaction follows:

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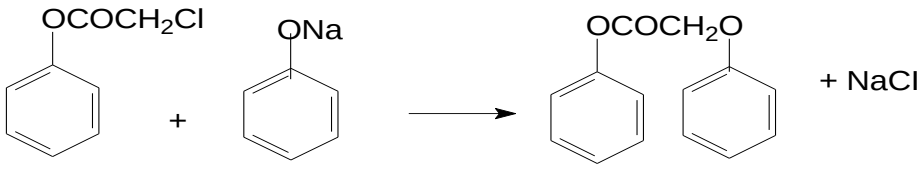

When the phenol O- chloracetylation reaction was conducted in a benzene solution, sodium phenolate was initially obtained and phenyl phenoxy acetate was synthesized by exposure to phenyl chloroacetate.

One of the pressing problems of today is the synthesis of biologically active compounds. It will take a long time. The purpose and mission of the scientific study is to identify biologically active compounds in their activities in the Pass online program and to carry out targeted syntheses from the prediction of unknown organic matter. Pass online predicts more than 3,800 biological activities, pharmacological effects, toxicity of mechanisms of action, and additional effects, interactions with metabolic enzymes and carriers, effects on gene expression, and more. Thus, it can predict compounds that have been developed on a computer but have not yet been synthesized. PASS (online) predicts more than 3,500 types of biological activity. For example, pharmacological effects, mechanisms of action, toxic and negative effects, interactions of metabolic enzymes and carriers, effects on gene expression, etc. The structure of the substance will be sufficient to predict the biological activity of the substance. Thus, it can even be predicted for a compound that has been developed on a computer but has not yet been synthesized. Prior registration is required to use the PASS (Online) service, which is free.

At the time of the analysis of the results obtained, it was found that chlorinated derivatives of phenyl chloroacetate have different biological activity. This is dominated by the same activity in different compounds, which is due to their chemical structure. The results of predicting some biological activity are given in the table below.

We used the PASS (online) program to study the biological activity of phenyl chloroacetate. Results are from the PASS (online) program.

The results obtained are presented in the table below.

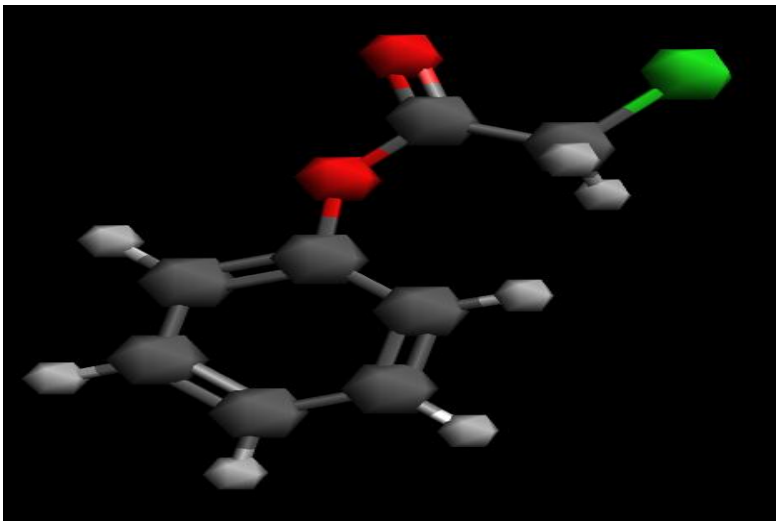

Figure 1. Table 1. PA > 0.7 biological activity obtained using the pass (online) program of phenyl chloroacetate

Pa	***Pi***	***Activity results of phenyl phenoxy acetate***
0,912	0,004	Antiallergic
0,849	0,005	Antiasthmatic

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0,835	0,001	Phospholipase A1 inhibitor
0,812	0,006	Antiinflammatory
0,789	0,028	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
0,783	0,025	CYP2J substrate
0,758	0,019	Nicotinic alpha6beta3beta4alpha5 receptor antagonist
0,748	0,020	Acylcarnitine hydrolase inhibitor
0,722	0,003	Rhinitis treatment
0,751	0,050	Ubiquinol-cytochrome-c reductase inhibitor
0,729	0,028	Sugar-phosphatase inhibitor
0,703	0,008	Dermatologic
0,701	0,009	Glucan 1,4-alpha-maltotriohydrolase inhibitor

Depending on the data of the PASS (online) program, we can see that phenyl chloroacetate has biological activity against most diseases. Antioxidant activity, for example: the results of predictions using the PASS program reveal additional medical-biological capabilities of compounds.

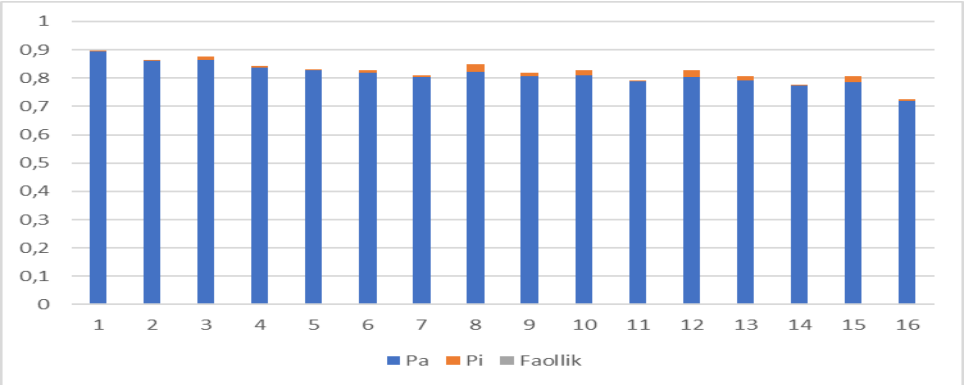

Figure 1. Graphics obtained using Pass online software.

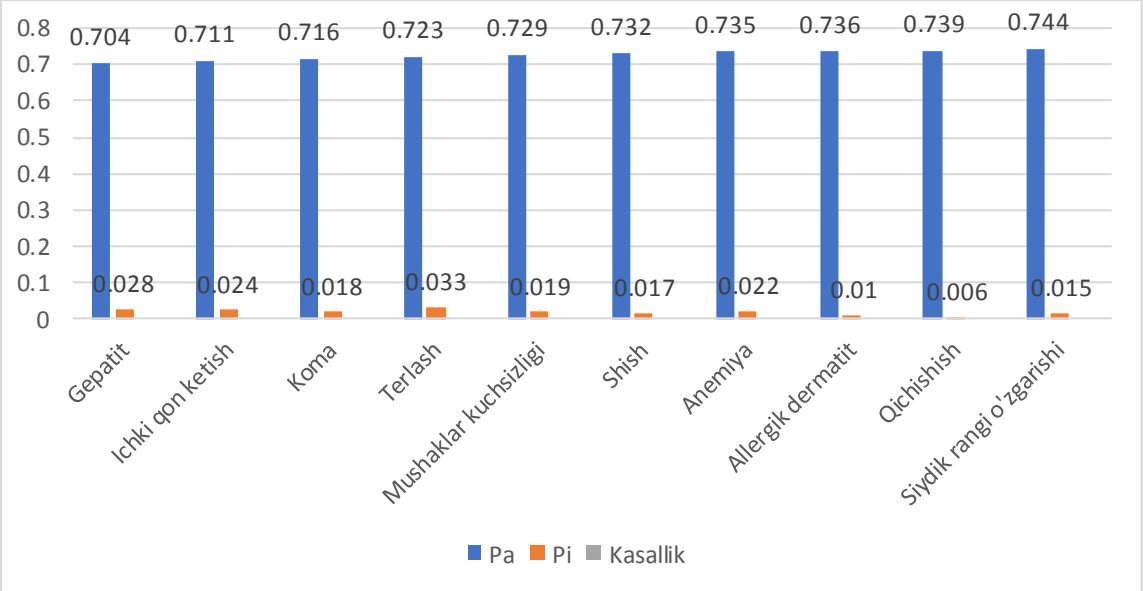

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Figure 2. Graphics obtained using Pass online software.

With the Pass online program, it is possible to simultaneously test a large number of compounds, save valuable reagents, prevent the waste of reagents, increase the speed and efficiency of scientific work on time. Currently, scientists from scientific laboratories of developed countries of the world are effectively working on the synthesis of new substances through theoretical calculations on the principle of "structure-biological activity". Scientific laboratories have special sections that predict the biological activity of substances, through the conclusion given by them, a biologically active drug is synthesized against a particular disease.

2.4 Testing the biological activity of some properties of phenyl phenoxy acetate in the Pass online program

We used the PASS (online) program to study the biological activities of phenyl phenoxy acetate. Results were obtained from the PASS (online) program.

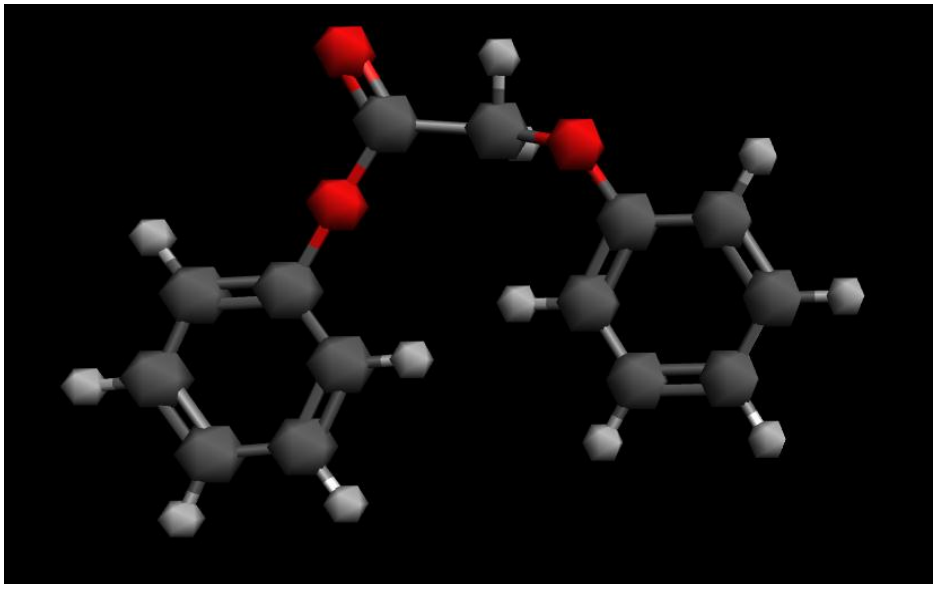

Figure 2. Table 2. Biological activity of phenyl phenoxy acetate

Pa	*Pi*	Activity results of phenyl phenoxy acetate
0,912	0,004	Antiallergic
0,849	0,005	Antiasthmatic
0,835	0,001	Phospholipase A1 inhibitor
0,812	0,006	Antiinflammatory
0,789	0,028	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
0,783	0,025	CYP2J substrate
0,758	0,019	Nicotinic alpha6beta3beta4alpha5 receptor antagonist
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0,722	0,003	Rhinitis treatment
0,751	0,050	Ubiquinol-cytochrome-c reductase inhibitor

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EXPERIMENTAL PART

Experience №. 1. Synthesis of phenyl chloroacetate. 9.4 g (0.1 g-mol) of phenol was dissolved in a 30 ml pyridine reversible refrigerant-mounted bottom round flask and 11.3 g (0.1 g-mol) chloroacetyl chloride was added. The reaction mixture is boiled and turns dark red during boiling. A solution of 10 ml of diluted sulfuric acid is added to it and cooled with ice water. The reaction product is isolated as an oily substance. To separate pyridine from the mixture, a solution of diethyl ether and dilute acid was released. The ether part is separated and dried with $CaCl_2$.After the release of the solvent, phenyl chloroacetate was released in vacuum. The reaction yield is 10.2 g (60%). T. boil. 120-122^{0}C / 20mm. Mercury. column.

Experience № 2. Synthesis of phenyl phenoxy acetate. 50 ml of absolute benzene and 3.57 g (0.038 g-mol) of phenol were dissolved in a double-mouthed flask with a return cooler and Mixer installed. It was topped with sodium metal, which was slightly purified from the oxide curtain of 0.9 g (0.038 G-atom). After the formation of sodium phenolate slowed down, the reacting mixture was heated in a water bath for 8 hours. Then, slowly, 6.48 g (0.038 g-mol) of chloracetyl chloride was released and the reacting mixture was boiled for 10 hours. The reaction was detected by a Belshtein sample. The reaction mixture was washed in alkaline water, extracted three times in benzene and dried with $CaCl_2$. The product was driven in a vacuum after benzene was driven in a water pump. Phenyl phenoxy acetate yield 5.36 g (67%). T. boil. 205-210^{0}C 18 mm. Mercury. column. T. cold. 49-500C (alcohol).

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