

**THEORETICAL STUDY OF THE BIOLOGICAL ACTIVITY OF 1,6-BIS  
(4-BROMOPHENOXY) HEXA-2,4-DIENE**

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**Abstract:**

Today, in the process of studying the composition of each chemical compound, its biological activities are also fully studied. In recent years, many substituted diaryldipropargyl esters with different biological activities have been synthesized and their biological activities have been studied. In this study, it was found that some substituted arylpropargyl ester compounds have enzyme-inhibiting, hormone-stimulating, and skeletal muscle-relaxing properties that catalyze many biochemical reactions. It is known that today biological research requires a lot of money, therefore, in this study, the results of the study of the biological activities of 1,6-bis(4-bromophenoxy) hexa-2,4-diene through the PASS (online) program are presented.

**Keywords:** pharmacological activity, pharmacological inactivity, Pass (Prediction of activity spectra for substances), biological activity, inhibitor, diaryldipropargyl esters.

**Introduction**

Exchanged diaryldipropargyl ethers are an important type of compounds held by three bonds and an ether group. Biologically active substances are studied in bioorganic chemistry, pharmaceutical chemistry, biological chemistry, and other disciplines. The reason for the intensive development of this direction is the study of many important physicochemical life activities of modern inspection methods, conformational structures, molecular effects, fermentant and volatile state in chemical processes in complex mixtures. Most importantly, the mechanisms of action of bioactive substances at the molecular, cellular, and systems level are investigated. Biologically active substances play an important role in the normal course of all vital processes in the body. Exchanged diaryldipropargyl ethers are now widely used as inhibitory and anti-several agents in medicine and important chemical processes.

Due to these characteristics, interchangeable diaryldipropargyl ethers are used in the manufacturing of inhibitors with numerous properties in chemical processes. Also in medicine, the effect of the skin on itching, zinc deficiency, eye toxicity, diarrhea, embryotoxicity, sleep disturbance, respiratory failure, inflammation, swelling, itchy eyes, pulmonary edema, changes in the color of ulcers and urine have been shown [1-2].

Several online and offline platforms for the study of the bioactivity of relevant chemical compounds have also been launched, which are significant in that they provide preliminary information about the bioactivity of the object we are studying, processing data. In the PASS online program, more than 4,000 biological activities can be studied based on the structure of a substance. In this case, the Pa value for the substance is the pharmacological activity in relation to the particular disease, and the Pi value is the indicator value of the

pharmacologically inactive to that disease. Only  $P_a > 0.3$  is there a higher probability of higher pharmacological activity in relation to given diseases [1-2].

### ANALYSIS OF THE RESULTS OBTAINED

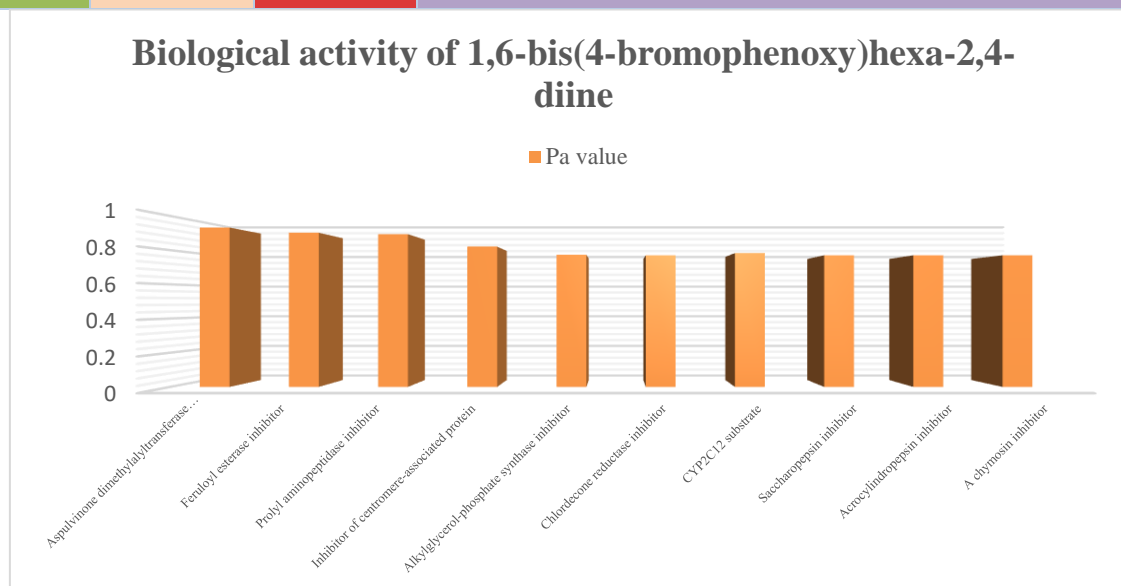
In scientific studies study of the biological activity of halogenated derivatives of exchanged diaryldipropargil ethers and their inhibitory and effects on human health in chemical reactions, it was revealed that 1,6-bis(4-bromophenoxy) hexa-2,4-diene has a number of beneficial properties, but the mechanism of their action is not yet fully understood.

In this study, the results of the study of some biological activity of 1,6-bis(4-bromophenoxy)hexa-2,4-diene using the PASS (online) program are presented.

The PASS online program works on the principle of structural and biological activity. In cases where the pharmacological activity is higher than the value of  $P_a > 0.7$ , the probability of a higher activity of the substance is observed in comparison with the given diseases.

**Table 1** Activity chart of 1,6-bis(4-bromophenoxy)hexa-2,4-diene, obtained in Pass Online

N <sub>o</sub>	P <sub>a</sub>	P <sub>i</sub>	Activity
1	0,932	0,004	Aspulvinone dimethylalyltransferase inhibitori
2	0,902	0,004	Feruloyl esterase inhibitor
3	0,893	0,004	Prolyl aminopeptidase inhibitor
4	0,821	0,004	Centromere-linked protein inhibitor
5	0,773	0,004	Alkylglycerone-phosphate synthase inhibitorium
6	0,770	0,026	Chlordecone reductase inhibitori
7	0,783	0,040	CYP2C12 substrate
8	0,770	0,027	Saccaropepsin inhibitor
9	0,770	0,027	Acrocyclopepsin inhibitor
10	0,770	0,027	Chymosine inhibitori



**Diagram 1.** Biological activities of 1,6-bis(4-bromophenoxy)hexa-2,4-diene as calculated in the PASS (online) program

Aspulvinone dimethylallyltransferase inhibitor. Aspulvinone is a dimethylallyltransferase inhibitor. In enzymology, aspulvinone dimethylallyltransferase (EC 2.5.1.35) is an enzyme that catalyzes a chemical reaction.

$2 \text{ dimethylallyl diphosphate} + \text{aspulvinone E} \rightleftharpoons 2 \text{ diphosphate} + \text{aspulvinone H}$

Thus, the two substrates of this enzyme are dimethylallyl diphosphate and aspulvinone E, and its two products are diphosphate and aspulvinone H [3].

Feruloyl esterase inhibitor. The enzyme feruloyl esterase (EC 3.1.1.73) catalyzes the reaction. feruloyl-polysaccharide + H<sub>2</sub>O  $\rightleftharpoons$  ferulate + polysaccharide

This enzyme belongs to the family of hydrolases, specifically enzymes that act on carboxylic ester bonds [4].

Prolyl aminopeptidase inhibitor. Prolyl aminopeptidase (EC 3.4.11.5, proline aminopeptidase, pro-X aminopeptidase, cytosol aminopeptidase V, proline iminopeptidase) is an enzyme. This enzyme catalyzes the following chemical reaction:

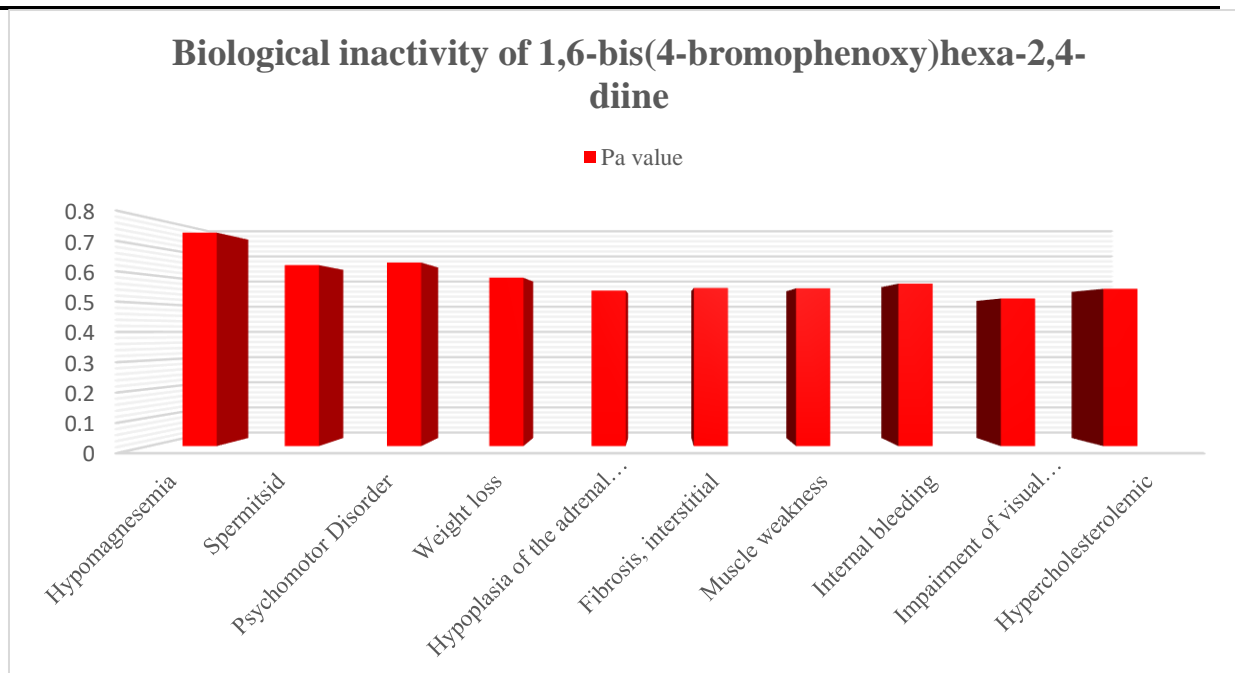
Separation of N-terminal proline from peptide

For this enzyme to work, the Mn<sup>2+</sup> ion is needed [5].

According to the program data, the activities of aspulvinone dimethylaltransferase and feruloyl esterase inhibitors within the studied activities of 1,6-bis(4-bromophenoxy)hexa-2,4-diine had higher Pa values than those with Pa values higher than 0.9, and Pa values of both the remaining inhibitors as well as the CYP2C12 and CYP2B5 substrates recorded values higher than 0.7 [3–4].

**Table 2** Toxicity table of 1,6-bis(4-bromophenoxy)hexa-2,4-diine obtained in PassOnline

No	Pa	Pi	Faoligi
1	0,748	0,011	Hypomagnesemia
2	0,634	0,011	Spermitsid
3	0,643	0,044	Psychomotor Disorder
4	0,590	0,043	Weight loss
5	0,545	0,030	Hypoplasia of the adrenal cortex
6	0,554	0,044	Fibrosis, interstitial
7	0,553	0,046	Muscle weakness
8	0,569	0,065	Internal bleeding
9	0,517	0,034	Impairment of visual sharpness
10	0,551	0,090	Hypercholesterolemic



**Figure 2.** Biological inactivity of 1,6-bis(4-bromophenoxy)hexa-2,4-diine as calculated in the PASS (online) program

**Hypomagnesemia.** Hypomagnesemia is a medical condition characterized by abnormally low levels of magnesium in the blood. Magnesium is an essential mineral that plays a crucial role in various functions in the body, including muscle and nerve function, energy production, and bone health. Hypomagnesemia can be caused by factors such as an improper diet, gastrointestinal disorders that affect magnesium absorption, or certain medications that reduce magnesium levels [6].

**Spermicide.** A spermicide is a contraceptive substance that destroys sperm that is inserted vaginally before intercourse to prevent pregnancy. A spermicide can be used alone as a contraceptive. However, couples who used only spermicide experienced a higher pregnancy rate than couples who used other methods. Usually, spermicides are combined with barrier methods of contraception such as diaphragms, condoms, cervical caps, and sponges. Combined methods have a lower pregnancy rate than either method alone. Spermicides are usually odorless, transparent, tasteless, non-staining and lubricating [7].

**Psychomotor disorder.** Psychomotor impairment involves a person's slowing down of thinking and reduced physical movements. This can cause significant slowing of physical and emotional reactions, including speech and affect. Psychomotor retardation is often seen in people with severe depression and in the depressive phase of bipolar disorder; it is also associated with adverse effects of certain drugs such as benzodiazepines [8].

## EXPERIENCE SECTION

The structure of the exchanged diaryldipropargil ethers, including 1,6-bis(4-bromophenoxy)hexa-2,4-diine, was plotted in the mole file in the ChemDraw Ultra section of the Chem Office program, and their pharmacological activity against certain diseases was studied using the PASS (online) program.

## CONCLUSION

When the biological activities of 1,6-bis(4-bromophenoxy)hexa-2,4-diene were studied in the Pass (online) program, it was found that compared to all inhibitors, aspulvinone dimethylallyltransferase and feruloyl esterase inhibitors were significantly more biologically active, with biological effects on hypomagnesemia, saliva, psychomotor impairment, weight loss, muscle weakness, internal bleeding, and visual acuity disorders, i.e., biological inactivity in relation to similar medical diseases. It has been theorized that the introduction of different functional groups into the molecule of exchanged diaryldipropargil ethers may lead to an increase in its activity as well as an exchange rate decrease [1].

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