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Computer Prediction of the Bioactivity of Potential Drugs of Biological/ Biotechnological Origin – Propargyl Ethers with Pharmacophore Group as a Stage of Drug Development

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Abstract. The aim of the study is to introduce the AI Tools toolkit into the process of developing new drugs that contain acetylene fragments as a scaffold. Propargyl organic substances differ from other compounds in their increased chemical and, accordingly, biological activity, since these molecules contain a terminal triple bond in a complex with a different set of pharmacophores. Propargyl compounds remain an interesting object in the search for new biologically active substances (BAS) for the creation of effective drugs in the future. The starting compound in the synthesis of propargylic compounds is propargylic alcohol, on the basis of which a range of biologically active substances have already been synthesized that have found their application in medicine and pharmacy. Propargyl molecules are actively used in bioisosteric substitution procedures, which opens up a wide field for the creation of new biologically active substances. However, to calculate the degree of biological effectiveness, physical parameters and chemical characteristics of the propargylic compounds that are planned to be synthesized, computer analysis, rational drug design in silico – targeted search for BAS, pharmacophore modeling, virtual screening helps. It is important to identify proteins and ligands that the synthesized compounds will act on, based on the results obtained by methods of biological and chemical predictive informatics. During the procedure for evaluating the structure and action of the synthesized molecule, the hypothesis of «molecular similarity» is used. A comparative analysis of the chemical structure features of new unannealed propargyl polyfluorosubstituted ethers and their structurally related compounds, as well as the relationship between their structure and biological activity, was conducted. Computer prediction of physicochemical parameters and potential biological properties and off-target effects of new unannealed propargyl alcohol derivatives and their related compounds was performed using the Swiss TargetPredictio program (SIB Swiss Institute of Bioinformatics).

Keywords: propargylic compounds, drugs of biological/biotechnological origin, scaffold, validation of methods, in silico, Swiss TargetPredictio.

INTRODUCTION

AI Tool (Artificial Intelligence Tool) is a program that uses artificial intelligence technologies to perform tasks that usually require human intelligence. AI Tool technologies provide forecasting and analytics and allow you to obtain tools that analyze data to predict future trends in the creation of original biologically active substances and medicines. Propargyl organic substances are characterized by high chemical and biological activity, since they contain a terminal triple bond in complex with pharmacophore groups. Propargyl compounds remain an interesting object in the search for new biologically active substances (BAS) for the creation of effective drugs in the future. The starting compound in the synthesis of propargyl compounds is propargyl alcohol. Functional derivatives of propargyl alcohol have found their application in medicine and pharmacy. Propargyl molecules are used in bioisosteric substitution procedures, which opens a wide field for the creation of new biologically active substances.

Biological drugs containing triple bonds are utilized for high reactivity or binding stability. For example, Erlotinib (EGFR inhibitor for lung cancer), Neratinib (tyrosine kinase inhibitor for HER2+ breast cancer), Rasagiline for Parkinson's disease. Erlotinib is used in Raman imaging to track cellular metabolism. Polyacetylenes are natural compounds with multiple triple bonds that show biological activity. Triple bonds are relatively rare in natural drugs because they can be highly reactive, but they are increasingly utilized in synthetic drug design and molecular probes. However, to calculate the degree of biological effectiveness, physicochemical parameters of propargyl compounds that are planned to be synthesized, computer analysis, rational drug design in silico – targeted search for BAS, pharmacophore modeling, virtual screening helps. It is important to identify biotargets of pharmacological and toxic effects of the studied compounds obtained by methods of biological and chemical predictive informatics. To assess the structure and action of the synthesized molecule, the hypothesis of “molecular similarity” is used.

A comparative analysis of the features of the chemical structure of new propargyl polyfluorosubstituted esters and their structurally related compounds was carried out. An analysis of the “structure-biological activity” relationship of propargyls was performed.

Computer prediction of the properties of synthesized fluorinated derivatives of propargyl alcohol and related compounds was performed using the Swiss program TargetPredictio (Swiss Institute of Bioinformatics SIB) using the following tools: SwissDock, SwissParam, SwissADME, SwissBioisostere, SwissSimilarity. The analysis performed paves the way for understanding the molecular mechanisms underlying a particular phenotype or bioactivity, rationalizing possible beneficial or adverse side effects, predicting off-target effects of known molecules, and opening the way for drug repurposing.

LITERATURE REVIEW

The basic compound in a series of propargylic compounds is propargylic alcohol. It is synthesized from acetylene by reaction with formaldehyde through ethynylation (Reppe synthesis). By iodocyclization of propargylic alcohol with various reagents, derivatives were synthesized, in the chemical structure of which the free alcohol group, or its oxidized form – the carbonyl group, is preserved. This allows to preserve the reactivity of the synthesized molecules for further chemical transformations of the synthesized products (Daina et al., 2019; Akmalayuly et al., 2020; Faizullaev et al., 2020; Omanov et al., 2020; Calogero et al., 2021; Fernández et al., 2022; Freitas et al., 2020).

Vinylacetylene is an important monomer in the synthesis of acetylene compounds with a high molecular weight. It has high adhesion and elasticity parameters. Vinylacetylene is obtained from olefins, alkanes, acetylene by oxidation in the presence of catalysts (Au/Pd). According to the Moiseev reaction, vinylacetylene is synthesized by esterification of ethylene. Acetic acid is used as an etherifying agent. Acetylene remains the main source for the synthesis of vinylacetene. Zinc acetate catalysts are used as catalysts. To increase their activity and stability, a change in the mode of applying the catalyst to the substrate under the conditions of ultrasound flow on the solution-carrier system is used. Salt catalysts are applied to activated carbon and become adsorptive (Faizullaev et al., 2020; Abonia et al., 2023; Horino et al., 2019; Jolly et al., 2021; Grzelakowska et al., 2019; Guo et al., 2019; Qian et al., 2019).

Previously, propargyl ethers were synthesized, the molecules of which contain the pharmacophore group – $\text{OCF}_2\text{CHBrCl}$. For the synthesis of these compounds, fluorothane was used as a source of pharmacophore group. For the reactions, a two-phase water-benzene system was used, and technical benzyltrimethylammonium chloride was used as an interphase carrier. Other synthesis conditions were also proposed: solvent – benzene, potassium hydroxide (dust), catalyst dibenzo-18-crown-6-ether (Tsekhmister & Welchinska, 2016; Welchinska et al., 2024; Welchinska & Vilchynska, 2016; Velchinskaya et al., 2007; Velchinskaya et al., 1999; Welchinska et al., 1997).

The formation of complexes of crown compounds with cations makes it possible to provide solubility to both inorganic and organic compounds. In this case, the interaction of the cation with the anion is weakened during the complexation of the cation and the lipophilicity of the crown compound groups. The concentration of the solution is determined by the nature of the solvent, the level of lipophilicity of the crown compound, the nature of the cations and the counterion. In nonpolar media, anions are not solvated, therefore, their reactivity increases, if compared with the reactivity in aqueous, alcoholic solutions. Cations in such solutions are separated from anions by the crown compound (Kuzmenko et al., 1995; Welchinska et al., 2025; Welchinska et al., 2026).

Crown compounds prevent the approach of cations and anions, reduce the effective charge of cations. However, this increases the reactivity of anions. These factors allow organic reactions to be carried out with the participation of inorganic bases and salts in non-polar and polar organic solvents. The use of crown compounds in synthesis increases the rate of reactions and the final yield of reaction products. Crown compounds are able to increase the solubility of alkali metals in ethers, aromatic substances, amines. Complexes of crown compounds with salts are used to separate racemates of ethers and amines, individual optical isomers. The stability constant K of complexes of metal cations with crown esters is much higher in the case of close values of the diameters of the ion and the crown cavity. The value of K of complexes with crown esters is higher than that of noncyclic complexes (glymes). The value of K depends on the solvent in which the complexation occurs. The values are much higher in methanol than in water. During complexation, the solvation shells of cations are destroyed. Such shells are more stable in aqueous solutions, but not in alcoholic solutions (methanol). In the presence of crown esters and cryptands, the solubility of alkali metals in amines, in ethers, in benzene and toluene, in mesitylene increases. Known crown esters include tetramethyl-12-crown-4; dicyclohexyl-14-crown-4; cyclohexyl-15-crown-5; 18-crown-6; cyclohexyl-18-crown-6; dicyclohexyl-18-crown-6 (two isomers); dibenzo-18-crown-6; 21-crown-7; dibenzo-21-crown-7; 24-crown-8; pentaglyme, etc. (Yamamoto et al., 2014; Zhang et al., 2020; Zhang et al., 2022).

We have investigated the effect of complexation of DBZ-18-crown-6 with potassium chlorides and calcium deposited on the surface of silica gel on gas-phase reactions of exchange of bromine or iodine for chlorine, cleavage of hydrohalides from alkyl halides. To improve the dissolution of potassium hydroxide in an organic solvent in benzene, we used dibenzo-18-crown-6-ester, since the hydroxy group under such conditions becomes more active than in water or methanol. A donor-acceptor bond is formed: $O: - K^+$ (Kuzmenko et al., 1995; Welchinska et al., 2025; Welchinskaya et al., 2003).

OBJECTIVES

To analyze the features of the chemical structure of new unannealed derivatives of propargylic alcohol and their related compounds; to perform computer prediction of physicochemical and biological properties and off-target effects using the Swiss TargetPredictio program (SIB Swiss Institute of Bioinformatics) of synthesized derivatives of propargylic alcohol; to interpret the obtained data and draw conclusions regarding the feasibility of synthesizing new unannealed derivatives of propargylic alcohol and their related compounds.

METHODOLOGY

One of the first stages of developing a new drug is forming an idea about the structure of the compound to be synthesized, and initial computer screening – a search for lead compounds, among which the most promising molecule is selected. Computer prediction allows you to predict not only the physicochemical characteristics of the synthesized molecule, but also its pharmacological properties and toxicity. A drug has a targeted and positive effect on certain biological targets in the body. Thus, it is important to predict the biological targets and specific pharmacological activity of a future drug. The most difficult is to predict the properties of pharmaceutical compositions of biological and biotechnological origin. Chemical-biological compositions contain components of natural origin – a biological component and a chemical component. Potential chemical components of medicinal products of biological/biotechnological origin include molecules with a triple bond, for example, propargyl ether derivatives.

RESULTS AND DISCUSSION

To work in the program Swiss TargetPredictio, we execute the program menu using the CADD online toolkit (SIB Molecular Modeling Group). Compatibility icons are used. CADD is a structural drug discovery method. This method determines biological/chemical properties, regardless of static properties (chemical composition) or dynamic changes (DNA conformational changes), which are fundamentally determined by molecular structure, taking into account the study of “structure-activity” relationships. The probability values of the prediction results are calculated based on a combination of indicators of similar compounds (2D and 3D), for which activity on a given protein is described. Information is obtained about the biological activity of the molecule on the biotarget – protein, or the absence of biological activity. EEG «by homology» confirms the prediction of the similarity of the molecule with similar molecules that are active on the specified proteins.

We investigated unsaturated polyfluorosubstituted ethers with pharmacophore groups (I-III) (Tab. 1).

Table 1. Chemical formulas of unsaturated polyfluorosubstituted ethers with pharmacophore groups (I-III)

Features of the chemical structure	Chemical formula
Ethyl radical, pharmacophoric group -CF ₂ CHBrC	$C_2H_5C \equiv C-CH_2OCF_2CHBrCl$ I
Phenyl radical, pharmacophore group -CF ₂ CHBrC	$C_6H_5C \equiv C-CH_2OCF_2CHBrCl$ II
Fluoroheptoxymethylene radical, pharmacophoric group -CF ₂ CHBrC, two methylene groups	$H(CF_2)_6CH_2OCH_2C \equiv C(CH_2)_2OCF_2CHBrCl$ III

Source: Compiled by the author based on Radchenko et al. (1991) and Kuzmenko et al. (1995).

The synthesized molecules are characterized by a special combination of functional groups and unique molecular fragments. Electron-donating methyl and phenyl radicals are present, which saturate the system with electron density, but are located at such a distance that they do not significantly affect the reactivity of the triple bond, which is electron-unsaturated and chemically active as a result.

The dodecafluoromethyleneoxy group, on the other hand, is electron-withdrawing, as it contains an electronegative oxygen atom and 12 fluorine atoms. These atoms pull the electron density away from the triple bond and thus deplete it, increasing its reactivity. The difluorobromochloroethoxy group is also electronegative, is an acceptor, and further depletes the triple bond density and increases its reactivity. However, the presence of the -(CH₂)₂- electron-donating fragment, on the contrary, quenches the deficiency of electron density on the triple bond, so compound III will differ in chemical properties from the chemical activity of compounds I and II.

Such a set of simultaneously present electron donors, electron acceptors, electropositive and electronegative groups in combination with a triple bond and the presence of three types of halogens with mesomeric and inductive effects characterizes the molecules as promising biologically active compounds, which is subject to additional research.

The synthesized molecules were studied during the initial laboratory screening (laboratory of the Institute of Organic Chemistry of the National Academy of Sciences of Ukraine, Kyiv). It was found that the synthesized compounds (I-III) exhibit bactericidal activity when exposed to phytopathogenic microorganisms.

Using spectral methods of IR spectrometry, ¹H NMR, ¹⁹F NMR, the chemical structure of the synthesized compounds (I-III) was proven. IR spectra were recorded on UR-20, Specord M-80 spectrometers. NMR spectra were recorded on a Gemini-200 instrument with an operating frequency of 200 MHz. DMSO-d₆, CD₂Cl₂ were used as solvents for sample preparation; HMDS is an internal standard.

The results of the prediction of physicochemical characteristics, topological polar surface area (tPSA), iLOGP (physical model of lipophilicity), analysis data using the physicochemical filters Lipinski, Veber, Egan; Bioavailability platform data for compounds I-III are presented in Tab. 2-4.

Table 2. Physicochemical characteristics, iLOGP, Bioavailability, pharmacokinetic properties, drug affinity of compound I

$C_2H_5C \equiv C-CH_2OCF_2CHBrCl$ I	
Number of return bonds	3
Number of H-bond acceptors	3
Number of H-bond donors	0
Molar refraction	47.82

Continuation of Table 2

Lipophilicity Log P _{o/w} (iLOGP) Log P _{o/w} (XLOGP3) Log P _{o/w} (WLOGP) Consensus Log P _{o/w}	2.82 3.42 3.89 3.21
Pharmacokinetics	GI absorption – high, Blood-brain barrier (BBB) – Yes
Affinity to medicinal substances	Lipinski Yes; 0 violation Ghose Yes Veber Yes
Bioavailability assessment	0.55

Source: Authors.

Table 3. Physicochemical characteristics, iLOGP, Bioavailability, pharmacokinetic properties, drug affinity of compound II

$C_6H_5C \equiv C-CH_2OCF_2CHBrCl$ II	
Number of return bonds Number of H-bond acceptors Number of H-bond donors Molar refraction	3 3 0 73.12
Lipophilicity Log Po/w (iLOGP) Log Po/w (XLOGP3) Log Po/w (WLOGP) Consensus Log Po/w	3.48 4.84 5.31 4.25
Pharmacokinetics	GI absorption – high, BBB – absent
Affinity to medicinal substances	Lipinski Yes; 0 violation Ghose Yes Veber Yes
Bioavailability assessment	0.55

Source: Authors.

Table 4. Physicochemical characteristics, iLOGP, Bioavailability, pharmacokinetic properties, drug affinity of compound III

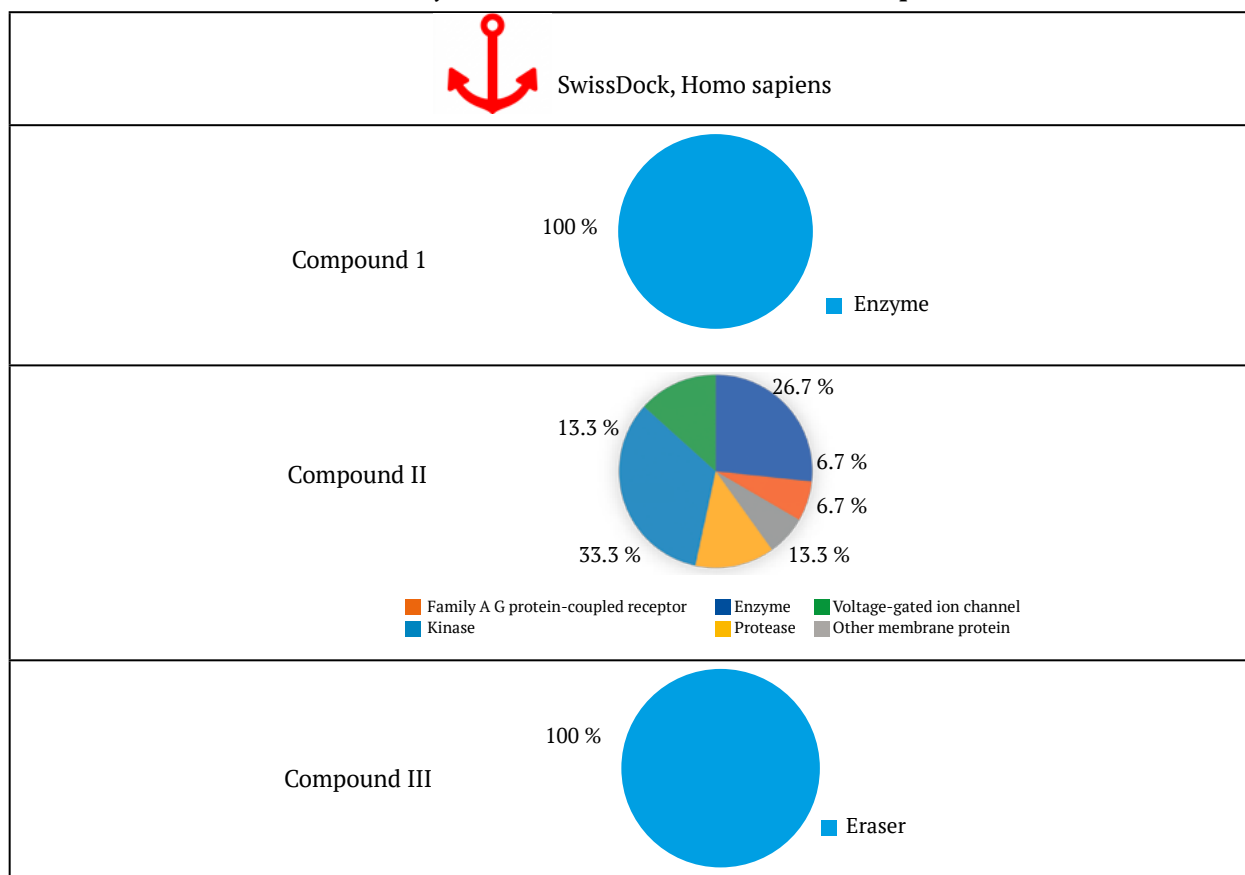
$H(CF_2)_6CH_2OCH_2C \equiv C(CH_2)_2OCF_2CHBrCl$ III	
Number of return bonds Number of H-bond acceptors Number of H-bond donors Molar refraction	12 16 0 90.27
Lipophilicity Log Po/w (iLOGP) Log Po/w (XLOGP3) Log Po/w (WLOGP) Consensus Log Po/w	0.00 7.59 13.01 6.76
Pharmacokinetics	GI absorption – low, BBB – absent
Affinity to medicinal substances	Lipinski No; 0 violation Ghose 2: MW>480 Veber No, Rotors>10
Bioavailability assessment	0.17

Source: Authors.

Bioavailability is a measure of how well a substance is absorbed and utilized by the body after oral administration, acting as a rapid screening tool for drug candidates. Measures such as the Abbott score indicate the probability (e.g., 85 %, 56 %, 11 %) based on molecular properties (polar surface area – PSA) of potential success ($F > 10$ %). It is a crucial measure in drug development that estimates the fraction that reaches the bloodstream, often using computational models that estimate factors such as size, charge, and polarity.

The results of the analysis of the SwissDock toolkit (based on EADock DSS) for predicting molecular interactions that may occur between a target protein and a small molecule were obtained; the SwissParam toolkit – an approximation of the free energy of ligand binding to the target, is used to compare different target/ligand combinations (human organism) (Tab. 5).

Table 5. The results of the analysis of the SwissDock toolkit for compounds I-III



Source: Authors.

Predicted potential biological targets (by homology): compound I – Enzymes; compound II- Protease (Cathepsin K, gamma-secretase), Kinase (protein tyrosine JAK1, JAK3), Cytochrome P450, Phosphodiesterase, Phosphatase (protein tyrosine phosphatase 1B), Oxidoreductase, Transferase; compound III – Eraser – Histone deacetylase 6.

Predicted pharmacological properties: compound I (anxiolytic, anticonvulsant, sedative effects); compound II (phosphodiesterase-4 (PDE4) inhibitor), antiparasitic effect (protozoal infections, trypanosomiasis).

CONCLUSIONS

A comparative analysis of the features of the chemical structure of new propargyl polyfluorosubstituted ethers and their structurally related compounds, the relationship between their structure and biological activity was carried out.

Computer prediction of pharmacological properties and off-target effects of synthesized propargyl polyfluorosubstituted ethers was performed using the Swiss TargetPredictio program based on physicochemical and biological parameters.

The results of predicting the properties of compounds I-III were obtained: the number of reversible bonds (3), H-bond acceptors (3), H-bond donors (none), molar refraction values (47.82-90.27);

lipophilicity (Log Po/w: iLOGP from 0.00 (III) to 3.48 (II); XLOGP3 from 3.42 (I) to 7.59 (III); WLOGP from 3.21 (I) to 6.76 (III); pharmacokinetic parameters (GI absorption – high (for compound I), low (for compounds II, III); BBB – high (for compound I), absent (for compounds II, III); bioavailability (0.55 – for compounds I, II; 0.17 – for compound III); predicted potential biodegradation effects of compounds (Protease (Cathepsin K, gamma-secretase), Kinase (tyrosine-protein JAK1, JAK3), Cytochrome P450. Phosphodiesterase. Phosphatase (protein-tyrosine phosphatase 1B), Oxidoreductase, Transferase, Enzymes, Eraser – Histone deacetylase 6); predicted pharmacological properties: compound I (anxiolytic, anticonvulsant, sedative effects); compound II (phosphodiesterase-4 (PDE4) inhibitor), antiparasitic effect (protozoal infections, trypanosomiasis).

DECLARATION

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