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SYNTHESIS OF ACETYLENIC ALCOHOLS BASED ON CYCLOPROPYLACETYLENE, THEIR THEORETICAL ENERGETIC CHARACTERIZATION, AND MOLECULAR DOCKING ANALYSIS WITH NADPH OXIDASE (7U8G) PROTEIN

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Abstract. In this study, an efficient synthetic method for a series of novel aromatic acetylenic alcohols (1-6) was developed based on cyclopropylacetylene and various substituted benzaldehyde derivatives. The reaction was performed at room temperature in the presence of potassium tert-butoxide (*t*-BuOK), yielding the desired products in high yields of 85-91%. The chemical structures of the synthesized compounds were unambiguously characterized using ^{1}H, ^{13}C, and ^{19}F NMR spectroscopy. Furthermore, the energetic parameters of the compounds were investigated using HyperChem 7.0 software to theoretically substantiate their structural stability. The electronic characteristics were further analyzed using Density Functional Theory (DFT) at the B3LYP/6-31G level within the Gaussian software suite.

To evaluate their potential biological activity, molecular docking studies were conducted against the 7U8G (NOX2) target protein. Among the tested compounds, 3-cyclopropyl-1-(3-(trifluoromethyl)phenyl)prop-2-yn-1-ol exhibited the highest binding affinity with a docking score of -8.1 kcal/mol. This compound was found to form a stable hydrogen bond with the HIS A:209 amino acid residue of the protein. The obtained theoretical data were found to be in high correlation with the experimental and spectral results.

Keywords: aromatic acetylenic alcohols, benzaldehyde derivatives, cyclopropylacetylene, alkynylation reactions, *t*-BuOK, NMR spectroscopy, Gaussian (DFT), molecular docking, 7U8G protein (NOX2), binding energy.

Siklopropilatsetilen asosida atsetilen spirtlari sintezi, ularning nazariy energetik xarakteristikalari va nadfoksidaza oqsili (7U8G) bilan molekulyar birikish tahlili

Annotatsiya. Ushbu tadqiqotda siklopropilatsetilen va benzaldegidning turli hosilalari asosida bir qator yangi aromatik atsetilen spirtlari (1-6) sintez qilishning samarali usuli ishlab chiqilgan. Reaksiya xona haroratida kaliy uchlamchi butoksidi (t-BuOK) ishtirokida olib borildi, bu yuqori unumlar (85-91%) bilan maqsadli mahsulotlarni olish imkonini berdi. Sintez qilingan birikmalarning kimyoviy tuzilishi 1H, 13C va 19F YAMR spektroskopiya usullari yordamida aniq tasdiqlandi. Bundan tashqari, HyperChem 7.0 dasturiy ta’minoti yordamida birikmalarning strukturaviy barqarorligini nazariy asoslash uchun ularning energetik parametrlari o‘rganildi. Elektron xarakteristikalar Gaussian dasturiy paketida B3LYP/6-31G darajasida zichlik funksionallari nazariyasi (DFT) usulida qo‘shimcha tahlil qilindi.

Potensial biologik faollikni baholash uchun nishon - 7U8G (NOX2) oqsili bilan molekulyar doking tadqiqotlari o‘tkazildi. Tekshirilgan birikmalar orasida 3-siklopropil-1- (3- (triftormetil) fenil) prop-2-in-1-ol -8.1 kkal/mol doking energiyasi bilan

bog‘lanishga eng yuqori moyillikni ko‘rsatdi. Ushbu birikma oqsilning HIS A:209 aminokislota qoldig‘i bilan barqaror vodorod bog‘ hosil qilishi aniqlandi. Olingan nazariy ma’lumotlar eksperimental va spektral natijalar bilan yuqori darajada bog‘liq.

Kalit so‘zlar: aromatik atsetilen spirtlari; benzaldegid hosilalari; siklopropilatsetilen; alkinillash reaksiyalari; t-BuOK; YAMR-spektroskopiya; Gaussian (DFT); molekulyar doking; 7U8G (NOX2) oqsili; bog‘lanish energiyasi.

Синтез ацетиленовых спиртов на основе циклопропилацетилена, их теоретические энергетические характеристики и молекулярный доккинг-анализ с белком nadph оксидазы (7U8G)

Аннотация. В данном исследовании разработан эффективный метод синтеза серии новых ароматических ацетиленовых спиртов (1-6) на основе циклопропилацетилена и различных производных бензальдегида. Реакция проводилась при комнатной температуре в присутствии трет-бутоксида калия (*t*-BuOK), что позволило получить целевые продукты с высокими выходами (85-91%). Химическая структура синтезированных соединений была однозначно подтверждена методами ЯМР ^{1}H, ^{13}C и ^{19}F спектроскопии. Кроме того, с помощью программного обеспечения HyperChem 7.0 были изучены энергетические параметры соединений для теоретического обоснования их структурной стабильности. Электронные характеристики были дополнительно проанализированы методом теории функционала плотности (DFT) на уровне B3LYP/6-31G в программном пакете Gaussian.

Для оценки потенциальной биологической активности были проведены исследования молекулярного докинга с мишенью - белком 7U8G (NOX2). Среди протестированных соединений 3-циклопропил-1-(3-(трифторметил)фенил)проп-2-ин-1-ол продемонстрировал наибольшее сродство к связыванию с энергией докинга -8.1 ккал/моль. Установлено, что данное соединение образует стабильную водородную связь с аминокислотным остатком HIS A:209 белка. Полученные теоретические данные находятся в высокой корреляции с экспериментальными и спектральными результатами.

Ключевые слова: ароматические ацетиленовые спирты; производные бензальдегида; циклопропилацетилен; реакции алкинилирования; t-BuOK; ЯМР-спектроскопия; Gaussian (DFT); молекулярный докинг; белок 7U8G (NOX2); энергия связывания.

Introduction. Compounds containing an acetylene group play a crucial role in organic synthesis, materials science, and pharmaceuticals [1]. Currently, the introduction of acetylene groups into target molecules via cross-coupling reactions of terminal alkynes is considered one of the most effective synthetic strategies [2, 3]. In this research, a direct cross-coupling reaction was performed between acetylenic alcohols and benzyl carbonates in the presence of a Pd catalyst to form a C*(sp)*–C*(sp^3)* bond. The uniqueness of this method lies in the simultaneous cleavage of C–C and C–O bonds. Unlike traditional Sonogashira reactions, stable and cost-effective acetylenic alcohols were utilized as alkylating reagents instead of unstable and volatile terminal alkynes. Reactions conducted using a $Pd(OAc)_2$ catalyst, a 1,4-bis(diphenylphosphino)butane ligand, and a K_2CO_3 base demonstrated high efficiency, with yields reaching up to 99%. The reactivity of various substituted benzyl carbonates and acetylenic alcohols was investigated, proving the methods versatility across a wide range of substrates and its practical efficiency in organic synthesis [4]. Studies conducted by Park and his research team proposed a

regioselective synthesis method for obtaining α-substituted acrylamides from terminal alkynes. This approach enabled the high-yield synthesis of α-substituted acrylamides, which serve as the structural backbone for bioactive substances, notably antidepressant drugs such as Levomilnacipran. The mechanism of this process is based on the regioselective attachment of the amide group to the α-position within a metallocatalytic cycle [5]. Furthermore, new palladium complexes based on sydnone and sydnone imine derivatives were synthesized, demonstrating high catalytic activity in Sonogashira-Hagihara reactions. The coupling reactions between aromatic bromides and acetylenic alcohols, such as 2-methylbut-3-yn-2-ol, resulted in yields of up to 100%. Once incorporated into the molecule, the hydroxyl group within the acetylenic alcohols can be subsequently converted into other functional groups or selectively removed. This characteristic makes them universal intermediates not only in Sonogashira reactions but also in the synthesis of complex pharmacological agents and heterocyclic systems [6]. Reactions were also carried out using terminal alkynes and various ketones in the presence of *n*-BuLi at -78ºC to synthesize corresponding acetylenic alcohols. Important organic compounds were then obtained through the hydration of these synthesized alcohols. Consequently, it has been proven that acetylenic alcohols possess significant practical value in the synthesis of complex molecules by reacting with compounds containing various functional groups [7-10]. Furthermore, nucleophilic addition reactions of alkynes containing two triple bonds with benzaldehyde and its various substituted derivatives were carried out in the presence of the $RuCl_2/Cy_2NH/EtOH$ catalytic system to synthesize the corresponding diynediols. Based on the composition and structure of the substituents in the aldehydes, relative efficiency series for the formation of diynediols were established [11]. Researchers from Xiamen University investigated the substitution reactions of secondary and tertiary acetylene alcohols with various nucleophiles, such as allyltrimethylsilane, alcohols, aromatic compounds, phenols, naphthols, thiols, and amides, in a MeCN (acetonitrile) solution. In this process, $BiCl_3$ was employed as a catalyst for the first time. New types of organic compounds were synthesized by forming C–C, C–O, C–S, and C–N bonds through the substitution of the hydroxyl group in acetylene alcohols with different functional groups. The research results indicated that the substitution of terminal acetylene alcohols with nucleophiles was challenging, resulting in low product yields [12, 13].

Therefore, the synthesis of acetylenic alcohols, the modification of organic compounds containing various functional groups based on them, and the study of their catalytic properties represent one of the most urgent and promising scientific directions today. This field aligns with the principles of “green chemistry” and the development of effective methods for creating modern pharmaceuticals [14, 15].

Experimental part: IR spectra were recorded on a Perkin-Elmer Spectrum 2000 FT-IR spectrometer using KBr pellets. ^1H NMR (400.1 MHz) and ^{13}C NMR (100.6 MHz) spectra were obtained on a Bruker AMX spectrometer in $CDCl_3$ as the solvent, with TMS or GMDS as internal standards (δ-scale). Solvents were evaporated using Heidolph Hei-VAP Core and Expert rotary evaporators. Purification of the crude products was performed by flash or column chromatography on silica gel 60, using various organic solvents as eluents. Reaction progress and product purity were monitored by thin-layer chromatography (TLC).

The synthesis of aromatic acetylenic alcohols (1-6) bearing various substituents was carried out according to the following procedure. A 50 mL round-bottom flask was charged with cyclopropylacetylene (1.2 equiv.) and potassium *tert*-butoxide (*t*-BuOK, 1.5 equiv.) as a strong base under a nitrogen atmosphere. Subsequently, the corresponding substituted benzaldehyde (1 equiv.) was added to the mixture. The reaction mixture was stirred at room temperature (25°C) using a magnetic stirrer for 2-4 hours. The progress of the reaction was monitored by thin-layer chromatography (TLC). Upon completion, the reaction mixture was quenched and washed with distilled water. The organic layer was extracted three times with ethyl acetate (3x10 mL). The combined organic phases were washed with a saturated NaCl solution (brine) and dried over anhydrous Na_2SO_4. After the evaporation of the solvent using a rotary evaporator, the crude product was purified by column chromatography. The target acetylenic alcohols (1-6) were obtained in high yields, ranging from 85% to 91%.

Molecular docking. The molecular interactions between the synthesized acetylenic alcohol derivatives (1-6) and the human protein NADPH oxidase complex (7U8G, NOX2) were investigated using the AutoDock Vina algorithm. The 7U8G protein is a crucial enzyme involved in the generation of reactive oxygen species (ROS) in cells and serves as a primary target in drug design. For the

docking simulations, the Cryo-EM structure of the protein was retrieved from the Protein Data Bank (PDB). The structure was pre-processed by removing crystallographic water molecules and heteroatoms, followed by the addition of polar hydrogen atoms. The ligands were converted into stable, low-energy conformations and energy-minimized using Avogadro software. The docking calculations were performed within a grid box of 40 × 40 × 40 Å centered at the coordinates x = 51.504, y = 53.447, and z = –1.541. Visualization of the protein-ligand complexes and detailed interaction analysis were carried out using BIOVIA Discovery Studio.

Results and discussion. In this study, the synthesis of aromatic acetylenic alcohols (1–6) from various substituted aromatic aldehydes and cyclopropylacetylene was achieved through a nucleophilic addition reaction in the presence of a strong base, potassium *tert*-butoxide (*t*-BuOK). Based on existing literature and the experimental results obtained, the following reaction mechanism is proposed. The process begins with the in situ deprotonation of the terminal acetylene. The tert-butoxide anion from *t*-BuOK abstracts the acidic terminal proton of cyclopropylacetylene. This acid-base interaction results in the formation of *tert*-butyl alcohol and a highly nucleophilic cyclopropylacetylenide anion. In the subsequent step, the generated acetylenide anion performs a nucleophilic attack on the carbonyl carbon (C=O), which acts as the electrophilic center of the aromatic aldehyde. During this stage, the π-bond of the carbonyl group is cleaved, leading to the formation of a new carbon-carbon bond and an intermediate potassium alkoxide complex. This step defines the core framework of the molecule, as further supported by the bonding energy results obtained via HyperChem software. In the final stage of the reaction, the potassium alkoxide is protonated by proton sources in the medium. As a result, the target aromatic acetylenic alcohols are formed, and *t*-BuOK is regenerated or sequestered from the system as a salt. The general reaction scheme for the synthesis of these aromatic acetylenic alcohols and their structural formulas are proposed as follows:

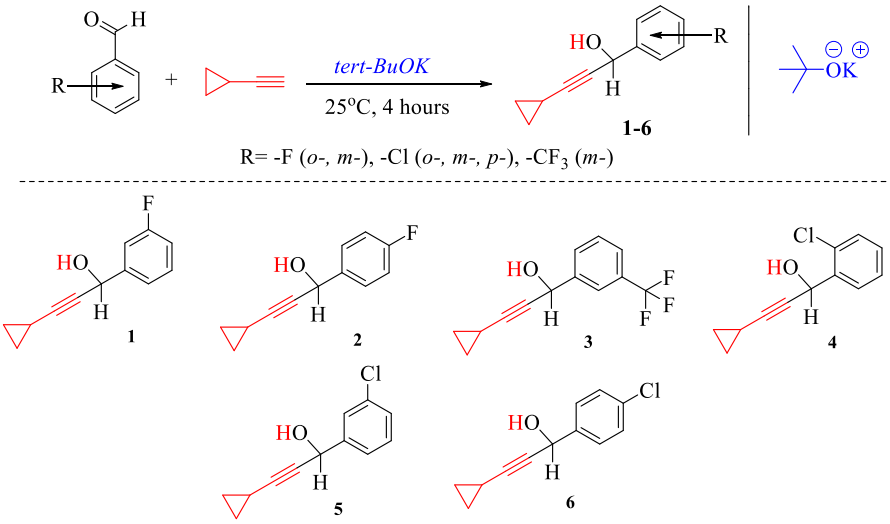

Figure 1. General reaction scheme for the synthesis of aromatic acetylenic alcohols and their structural formulas

A series of aromatic acetylenic alcohols were synthesized through the reaction of cyclopropylacetylene with various substituted benzaldehyde derivatives. During the investigation, the effects of temperature, reaction duration, molar ratios of substrates and reagents, as well as the structural characteristics of the aldehydes on the reaction progress and product yields were systematically evaluated.

Table 1

Optimization of reaction conditions

№	Base	Solvent	Temperature °C	Time (h)	Yield (%)
1	Et_3N	THF	20	4	15-20
2	K_2CO_3	THF	25	4	15
3	*i-Pr₂NEt*	CH_2Cl_2	25	6	25
4	KOtBu	THF	10	2	65

5	KOtBu	THF	25	4	91
6	KOtBu	THF	35	6	78
7	KOtBu	THF	40	4	58
8	KOtBu	Mezitilen	25	6	72

Among the bases screened for the studies, KOtBu was found to provide the highest efficiency. This is attributed to the fact that weaker bases, such as Et_3N or K_2CO_3, lack sufficient activity to deprotonate the terminal alkyne, leading to a sharp decrease in yield.

To evaluate the effect of temperature on the product yield, the reaction was conducted under conditions ranging from 10°C to 40°C. The optimal temperature was determined to be 25±1°C, at which the tert-butoxide anion completely deprotonates the alkyne, thereby minimizing side reactions. When investigating the influence of reaction duration on the yield, it was found that increasing the time from 2 to 4 hours led to a significant rise in product formation. Extending the process to 6 hours did not result in any notable change in yield. Furthermore, the effect of the molar ratio of starting materials (aldehyde:alkyne:base) was examined. It was observed that a slight excess of alkyne (1:1.2 mol) contributed to an increase in yield. This ensures a high concentration of the acetylenide anion, shifting the equilibrium toward the formation of the product. The results also revealed that the nature of the substituents on the benzaldehyde ring significantly affects the yield. Some physicochemical characteristics, yields, and chromatographic data of the synthesized aromatic acetylenic alcohols are summarized in table 2.

Table 2

Physicochemical characteristics and yields of the synthesized aromatic acetylenic alcohols (1-6)

№	Compound name	Molecular formula	Molecular weight (g/mol)	Yield (%)	System	R_f value
1	3-cyclopropyl-1-(3-fluorophenyl)prop-2-yn-1-ol	$C_{12}H_{11}OF$	190.214	91.3	Hex:EtOAc (14:1)	0.44
2	3-cyclopropyl-1-(4-fluorophenyl)prop-2-yn-1-ol	$C_{12}H_{11}OF$	190.214	85.6	Hex:EtOAc (14:1)	0.54
3	3-cyclopropyl-1-(3-(trifluoromethyl)phenyl)prop-2-yn-1-ol	$C_{13}H_{11}OF_3$	240.214	86.4	Hex:EtOAc (14:1)	0.45
4	1-(2-chlorophenyl)-3-cyclopropylprop-2-yn-1-ol	$C_{12}H_{11}OCl$	206.668	87.1	Hex:EtOAc (14:1)	0.37
5	1-(3-chlorophenyl)-3-cyclopropylprop-2-yn-1-ol	$C_{12}H_{11}OCl$	206.668	90.2	Hex:EtOAc (14:1)	0.39
6	1-(4-chlorophenyl)-3-cyclopropylprop-2-yn-1-ol	$C_{12}H_{11}OCl$	206.668	86.3	Hex:EtOAc (14:1)	0.31

As evidenced by the results presented in the table, the position and nature of the substituents on the aromatic ring significantly influenced the product yields. Aldehydes containing fluorine or chlorine atoms at the *m*-position provided higher yields, as seen in the synthesis of 3-cyclopropyl-1-(3-fluorophenyl)prop-2-yn-1-ol (1) at 91.3% and 1-(3-chlorophenyl)-3-cyclopropylprop-2-yn-1-ol (5) at 90.2%. In contrast, a slight decrease in yield was observed for the *p*-substituted analogs, specifically 3-cyclopropyl-1-(4-fluorophenyl)prop-2-yn-1-ol (2) at 85.6% and 1-(4-chlorophenyl)-3-cyclopropylprop-2-yn-1-ol (6) at 86.3%. Furthermore, the derivative containing a strong electron-withdrawing group, 3-cyclopropyl-1-(3-(trifluoromethyl)phenyl)prop-2-yn-1-ol (3), was synthesized with a yield of 86.4%.

The structural identities of the resulting aromatic acetylenic alcohols were confirmed by spectroscopic methods, including ^1H, ^{13}C NMR, and IR spectroscopy.

Physicochemical characterization: The structures of the synthesized aromatic acetylenic alcohols were confirmed using modern ^1H and ^{13}C NMR spectroscopy. As a representative example, the ^1H and ^{13}C NMR spectra of 3-cyclopropyl-1-(3-fluorophenyl)prop-2-yn-1-ol (1) are presented in figure 2.

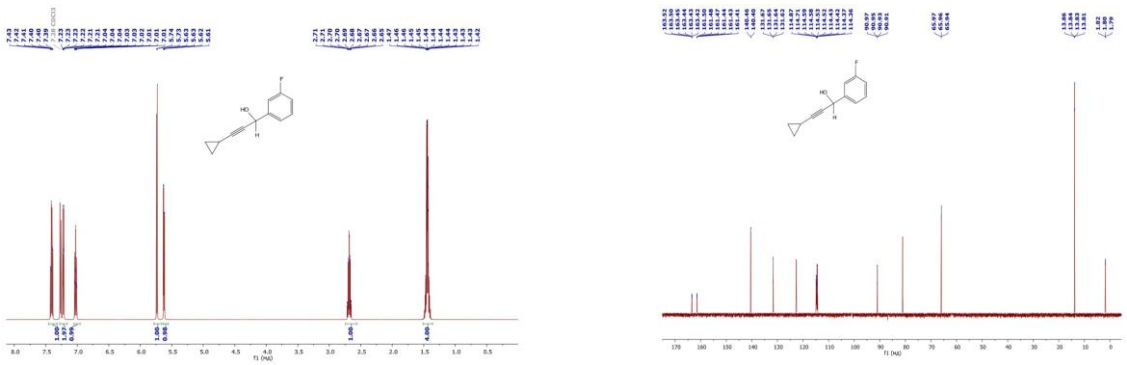

Figure 2. 3-cyclopropyl-1-(3-fluorophenyl)prop-2-yn-1-ol (^{1}H, ^{13}C) NMR spectroscopy

3-cyclopropyl-1-(3-fluorophenyl)prop-2-yn-1-ol (1). ^{1}H YaMR (400 MHz, $CDCl_3$) δ: 7.41 (td, J=7.5, 5.0 Hz, 1H, Ar.), 7.22 (dt, J=8.0, 1.5 Hz, 2H, Ar.), 7.03 (tt, J=7.8, 1.6 Hz, 1H, Ar.), 5.74 (d, J=6.7 Hz, 1H, CH=), 5.62 (dd, J=6.7, 2.5 Hz, 1H, CH=), 2.68 (m, J=7.1, 2.6 Hz, 1H, CH-cyclopropyl), 1.51-1.36 (m, 4H, CH_2-cyclopropyl).

^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 142.8 (Ar, C), 132.5 (CH=), 128.6 (2CH, Ar), 127.4 (CH, Ar), 126.3 (2CH, Ar), 124.8 (=CH), 78.5 (C-OH yoki C≡C), 31.2 (CH-cyclopropyl), 5.4 (CH_2-cyclopropyl).

^{19}F NMR (376 MHz, $CDCl_3$) δ: -113.4 (s, 1F, Ar-F).

3-cyclopropyl-1-(4-fluorophenyl)prop-2-yn-1-ol (2). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.68-7.56 (m, 2H), 7.33-7.22 (m, 2H), 5.84 (d, J=6.7 Hz, 1H), 5.78 (dd, J=6.7, 2.5 Hz, 1H), 2.84 (pd, J=7.1, 2.5 Hz, 1H), 1.69-1.46 (m, 4H).

^{13}C NMR (100.6 MHz, $CDCl_3$) δ; 162.5 (d, J=245.2 Hz, C_{ar}-F), 136.8 (d, J=3.1 Hz), 128.4 (d, J=8.2 Hz, 2C), 115.3 (d, J=21.4 Hz, 2C), 88.2 (C≡C), 76.5 (C≡C), 63.8 (CH-OH), 8.4 (CH, cyclopropyl), -0.4 ($2CH_2$, cyclopropyl).

3-cyclopropyl-1-(3-(trifluoromethyl)phenyl)prop-2-yn-1-ol (3). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.59 (t, J=1.4 Hz, 1H), 7.49 (dt, J=7.5, 1.6 Hz, 1H), 7.30 (t, J=7.5 Hz, 1H), 7.21 (dt, J=7.5, 1.5 Hz, 1H), 5.62 (d, J=6.6 Hz, 1H), 5.50 (dd, J=6.7, 2.5 Hz, 1H), 2.47 (pd, J=7.0, 2.5 Hz, 1H), 1.51-1.18 (m, 4H).

1-(2-chlorophenyl)-3-cyclopropylprop-2-yn-1-ol (4). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.61-7.38 (m, 2H), 7.34-7.18 (m, 2H), 5.83 (dd, J=7.0, 2.5 Hz, 1H), 5.49 (d, J=7.0 Hz, 1H), 2.62 (m, J=7.0, 2.6 Hz, 1H), 1.49-1.21 (m, 4H).

1-(3-chlorophenyl)-3-cyclopropylprop-2-yn-1-ol (5). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.50-7.32 (m, 2H), 7.26 (tt, J=7.1, 1.5 Hz, 2H), 5.95-5.12 (m, 2H), 2.61 (m, J=7.0, 2.2 Hz, 1H), 1.60-0.96 (m, 4H).

1-(4-chlorophenyl)-3-cyclopropylprop-2-yn-1-ol (6). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.46 (d, J=8.4 Hz, 2H, Ar-H), 7.33 (d, J=8.4 Hz, 2H, Ar-H), 5.42 (s, 1H, CH-OH), 2.24 (s, 1H, OH), 1.32-1.24 (m, 1H, CH), 0.82-0.65 (m, 4H, 2CH).

^{13}C NMR (100.6 MHz, $CDCl_3$) δ:139.6 (Ar, C-CH), 133.8 (Ar, C-Cl), 128.6 (2CH, Ar), 127.9 (2CH, Ar), 90.1 (C≡C), 75.8 (C≡C), 63.9 (C-OH), 8.5 (CH-cyclopropyl), 1.5 ($2CH_2$-cyclopropyl).

The structures of the synthesized compounds were fully confirmed by ^{1}H, ^{13}C, and ^{19}F NMR spectroscopy. To evaluate the pharmacophoric properties and potential biological activities of these derivatives, systematic *in silico* studies were conducted. In the subsequent stage of the research, comprehensive molecular docking analyses were performed to determine the relationship between the chemical structures of the newly synthesized derivatives and their theoretical pharmacological properties. In this process, the potential biological activities of the compounds and their interaction mechanisms with various protein targets were investigated using computational modeling methods. Molecular docking allows for the evaluation of the thermodynamic stability of the ligand and its binding affinity to the protein. The stability of the complex is reflected in the binding free energy (ΔG_{binding}) value. A more negative value indicates a stronger binding interaction. The binding energies with the 7U8G target protein are summarized in table 3.

Table 3

Molecular docking results of the synthesized compounds against 7U8G (NOX2) protein

№	Names of acetylene alcohols	7U8G (NOX2) Binding Energy (kkal/mol)
1	3-cyclopropyl-1-(3-fluorophenyl)prop-2-yn-1-ol	-7.2
2	3-cyclopropyl-1-(4-fluorophenyl)prop-2-yn-1-ol	-7.1
3	3-cyclopropyl-1-(3-(trifluoromethyl)phenyl)prop-2-yn-1-ol	-8.1
4	1-(2-chlorophenyl)-3-cyclopropylprop-2-yn-1-ol	-7.2
5	1-(3-chlorophenyl)-3-cyclopropylprop-2-yn-1-ol	-7.2
6	1-(4-chlorophenyl)-3-cyclopropylprop-2-yn-1-ol	-7.1

The analysis of the results revealed that 3-cyclopropyl-1-(3-(trifluoromethyl)phenyl)prop-2-yn-1-ol (3) exhibited the strongest binding affinity, with a binding energy of -8.1 kcal/mol. This indicates that compound 3 forms the most energetically favorable and stable complex within the active site of the 7U8G protein. In addition to the lead compound, 3-cyclopropyl-1-(3-fluorophenyl)prop-2-yn-1-ol (4) and 1-(3-chlorophenyl)-3-cyclopropylprop-2-yn-1-ol (5) were also identified as high-affinity ligands, both showing a binding energy of -7.2 kcal/mol. It was observed that the presence of halogen substituents (F, Cl) on the phenyl ring maintains the binding energy within the range of -7.1 to -7.2 kcal/mol. This consistency confirms that all synthesized derivatives possess a high degree of complementarity and suitability for the NOX2 protein target.To gain a detailed insight into the binding mechanism, the orientation and conformational positioning of 3-cyclopropyl-1-(3-(trifluoromethyl)phenyl)prop-2-yn-1-ol (3) within the active site of the protein were thoroughly analyzed.

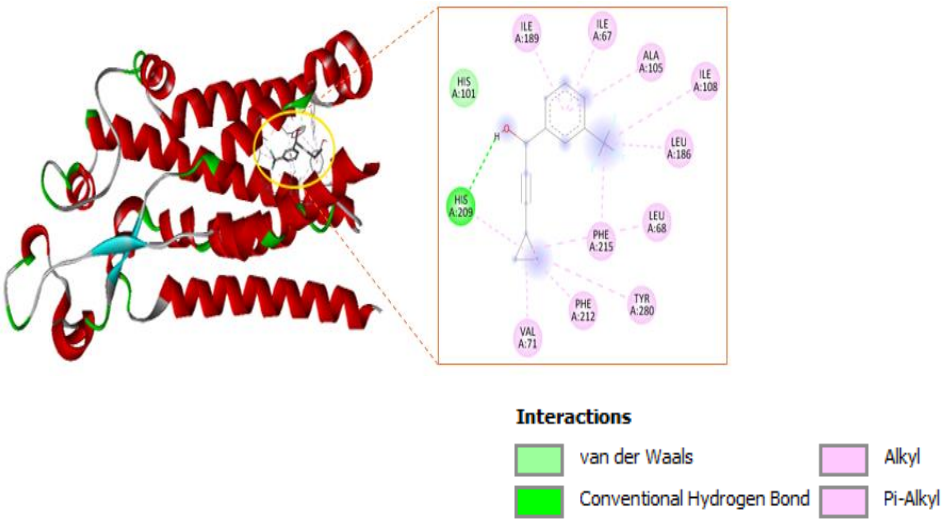

Figure 3. Binding mode and molecular interactions of 3-cyclopropyl-1-(3-(trifluoromethyl)phenyl)prop-2-yn-1-ol within the active site of the 7U8G protein

As illustrated in the figure, the hydroxyl group (-OH) of the compound forms a stable hydrogen bond with the HIS A:209 residue of the protein. The trifluoromethyl ($-CF_3$) moiety establishes multiple interactions with a cluster of hydrophobic amino acids, including ILE A:67, ILE A:189, ALA A:105, ILE A:108, and LEU A:186, which significantly contributes to the overall stability of the complex.

Furthermore, the cyclopropyl and phenyl rings form hydrophobic (pi-alkyl) contacts with the PHE A:212, PHE A:215, and VAL A:71 residues. These synergistic interactions ensure the tight binding of the ligand within the active site of the NOX2 protein.

To investigate the geometric and energetic parameters of the synthesized aromatic acetylenic alcohols, semi-empirical calculations were performed using the HyperChem 7.0 software package.

The thermodynamic and structural energy indicators obtained from these calculations, including thermal energy, Van der Waals energy, and bond energy, are summarized in table 4.

Table 4

Calculated energy parameters of the synthesized aromatic acetylenic alcohols (1-6)

Aromatic acetylene alcohols	Thermal energy, kcal/mol	Van der Waals energy, kcal/mol	Coulomb energy, kcal/mol	Torsion energy, kcal/mol	Valence angle energy, kcal/mol	Bond energy, kcal/mol
1	3.2833	2.9637	1.3050	-3.1351	0.2874	1.8622
2	3.2491	2.9955	1.2681	-3.1279	0.2822	1.8313
3	8.8165	3.9246	1.3850	0.7888	0.416	2.3022
4	-0.4868	0.1116	-0.0390	-2.9379	0.4655	1.9132
5	2.4977	2.9276	0.9284	-3.2152	0.2862	1.5708
6	2.6468	3.0885	0.8892	-3.2089	0.2881	1.5899

The obtained theoretical results indicate that compound 3-cyclopropyl-1-(3-(trifluoromethyl)phenyl)prop-2-yn-1-ol (3), which formed the most stable complex with the 7U8G protein, significantly differs from the other derivatives in terms of its energetic parameters. Specifically, the calculated thermal energy (8.8165 kcal/mol) and Van der Waals energy (3.9246 kcal/mol) for 3-cyclopropyl-1-(3-(trifluoromethyl)phenyl)prop-2-yn-1-ol (3) reached the highest values among the series.

This confirms the positive impact of the trifluoromethyl ($-CF_3$) moiety on the overall molecular energy profile and its enhanced ability to engage in hydrophobic interactions within the protein's active site. Such energetic characteristics align with the docking data, emphasizing the role of the trifluoromethyl substituent in stabilizing the ligand-protein complex.

At the same time, the positive torsion energy value for 3-cyclopropyl-1-(3-(trifluoromethyl)phenyl)prop-2-yn-1-ol (3) (0.7888 kcal/mol) indicates that its spatial structure exists in a slightly strained conformation. In comparison with docking analyses, this specific conformational feature provides the energetic basis for the ligand to form a stable hydrogen bond with HIS A:209 and other robust interactions with hydrophobic amino acids within the active site of the 7U8G protein.

Conclusion. A series of acetylenic alcohols (1-6) were synthesized starting from cyclopropylacetylene and aromatic aldehydes with varying electronic natures. The reaction was optimized at room temperature (25°C) for 4 hours using potassium tert-butoxide (*t*-BuOK) with a molar ratio of 1:1.2:0.2 (aldehyde:alkyne:base).

It was demonstrated that the substituent nature significantly influences the yield, with the highest yields obtained for m-substituted halogenated derivatives 1 (91.3%) and 5 (90.2%), attributed to the activation of the carbonyl center by electron-withdrawing effects.

Theoretical calculations via HyperChem 7.0 confirmed the high stability of the derivatives, specifically highlighting compound 3 with the highest thermal (8.8165 kcal/mol) and Van der Waals (3.9246 kcal/mol) energies.

Molecular docking studies revealed a high binding affinity of these acetylenic alcohols toward the NADPH oxidase (7U8G) protein. Notably, compound 3 exhibited a binding energy of -8.1 kcal/mol and formed a stable hydrogen bond with HIS A:209, suggesting its potential as a bioactive lead compound. These findings provide a robust theoretical and practical framework for the targeted synthesis and pharmacological prediction of novel acetylenic alcohols.

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