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ABSTRACT

of the dissertation for the degree of Doctor of Philosophy

SYNTHESIS AND STUDY OF PYRAZOLE, N-BENZIL, N-ALLYLANILIN DERIVATIVES AND THEIR METAL COMPLEXES

Speciality:	2306.01 – Organic chemistry
Field of science:	Chemistry
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Baku – 2024

The work was performed at the Republic of Azerbaijan Ministry of Education and Sciences, Institute of Additive Chemistry, named after academician Ali Guliyev at the laboratory "Physiologically active organic compound" and at the Chemical Engineering Research Centre of the Baku Engineering University.

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Dissertation council ED 1.16 of Supreme Attestation Commission under the President of the Republic of Azerbaijan operating at institute of Petrochemical Processes named after Yusif Mammadaliyev

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GENERAL CHARACTERISTIC OF THE WORK

The relevance of the topic and degree of elaboration. Considering the recent expansion of the scope of many global diseases and the adaptation of bacteria, fungi, and viruses that often cause these diseases to the effect of existing drugs, scientists and researchers of the world have made one of the main goals of the development of the pharmaceutical industry by expanding the synthesis of medicinal substances, pharmacological preparations, and biological supplements that are more effective than their existing counterparts. whom they chose.

The analysis of the latest literature data shows that nitrogenous compounds[1], especially their heterocyclic derivatives, found in the composition of newly created medicinal substances, are widely used not only in pharmacology, but also in other fields: agrochemistry, engineering, and in the preparation of synthetic materials in the field of polymers. The effect of nitrogen atoms on the molecule causes the formation of hydrogen bonds and polarity in medicinal substances. Nitrogen atoms have a great influence on the physiological activity of medicinal substances, and for this reason, the presence of this atom in medicinal substances is considered very important. Considering all this, the nitrogen atom and its compounds are widely used in synthesizing various compounds.

It is possible to find enough scientific research in this direction in the world literature. Scientists of the Additives Chemistry Institute, taking into account the mentioned need, attach great importance to joint international research in this direction. As a result of their research conducted many years ago, they determined that many nitrogenous organic substances synthesized for additives improve the operational properties of lubricants and also have biological activity. For example, substances obtained based on aminothiol, amino alcohol, hetarylsulfonamide, and other compounds, in addition to being a high-

[1]Kaper, T. Stereoselective Synthesis of Tertiary Allylic Amines by Titanium-Catalyzed Hydroaminoalkylation of Alkynes with Tertiary Amines / T. Kaper, D. Geik, F. Fornfeist [et al.] // Chemistry – A European Journal, – 2022. v. 28, – p. 1-4.

quality additive for lubricants, as well as having disinfectant, antiseptic, antialcohol, numbing, and other properties, have been proven as a result of tests conducted in many organizations[2].

However, in this literature information, the acquisition of physiologically active pyrazole and other aromatic amine derivatives and their metal complexes based on dicyandiamide, as well as computer research of the theoretical-experimental mechanism of the synthesis reactions of these compounds, as well as antioxidant and enzyme-isoenzyme inhibitors[3] as separate functional properties the study of their activities are generally not encountered. Taking into account that, as we mentioned above, scientific research in the direction of obtaining and applying medicinal substances consisting of nitrogen-containing heterocyclic compounds is expanding, according to the topic of the dissertation, the synthesis of pyrazole and other aromatic amine-based compounds with physiological activity and their metal complexes[4], computer-experiment research, the creation of new, more effective physiologically active substances based on them is relevant, then the experiences obtained in these directions also provide a serious basis for the synthesis of antioxidants with different functional groups and new heterocyclic compounds with high biological activity. According to the above, it is important to develop and prepare the theoretical basis for the synthesis, research, and application of new heterocyclic compounds based on N-benzyl-, N-allyl aniline, triazine[5], pyrazole, which

[2]Hou, L. Trinuclear-based Copper(I) Pyrazolate Polymers: Effect of Trimer π-Acid·Halide/Pseudohalide Interactions on the Supramolecular Structure and Phosphorescence / L. Hou, W.-J. Shi, Y.-Y. Wang [et al.] //. Inorganic Chemistry, – 2011. v. 50, – p. 261-270.

[3]Pedrood, K. Design, synthesis, characterization, enzymatic inhibition evaluations, and docking study of novel quinazolinone derivatives / K. Pedrood, M. Sherafati, M. Mohammadi-Khanaposhtani, M.S. Asgari [et al.] // International Journal of Biological Macromolecules, – 2021. v. 170, – p. 1-12.

[4]Igashira-Kamiyama, A. Syntheses, Structures, and Magnetic Properties of Tetramanganese(III) and Hexamanganese(III) Complexes Containing Derivative of Biguanidate Ligand: Ferromagnetic Interaction via Imino Nitrogen /A. Igashira-Kamiyama, T. Kajiwara ,M. Nakano, [et al.] // Inorganic Chemistry, – 2009. v. 48, – p. 11388-11393

[5]Shixaliyev, N.Q. Halogen-bonded tris (2,4-bis (trichloromethyl)-1,3,5-triazapentadienato)-M (III)[M= Mn, Fe, Co] complexes and their catalytic activity in the peroxidative

are substances with high physiological activity and prevent the oxidation of lubricants. and with interdisciplinary (multidisciplinary) significance, it conditions the continuation of scientific research at a qualitatively new stage.

The work objective and subject. The object of research was various aliphatic halide derivatives, amines, benzaldehyde, cyano compounds, and transition metal salts. Based on these reactive compounds, binary amines with physiologically active effects, including heterocyclic substances containing a triazine ring and metal complexes containing a pyrazole ring in the molecule, were synthesized.

The role of non-covalent bonds, π-stacking interactions, and hydrogen bonding in the formation of the molecular structure of multifunctional compounds taken as the subject of research, as well as their biocidal properties against microbial damage and oxidation of hydrocarbons on the one hand, and on enzymes and their isoforms through molecular docking on the other hand inhibitory activities were studied.

The purpose of the work. Synthesis of new heterocyclic compounds consisting of pyrazole and other aromatic amines using the possibilities of sophisticated organic synthesis and modern computer software, the computer-experimental study of the mechanism of some of their reactions, their physiological activity - antioxidant, inhibitory effects on enzymes-isoenzymes, drug substances, and biological supplements based on them The main goal of the dissertation was to conduct purposeful and systematic research to develop the scientific basis of its creation. To achieve this goal, the following issues have been resolved:

- Development of a convenient synthesis method that leads to a substantial increase in the yield of N-benzyl-, N-allylanilin derivatives;
- 2-(4-amino-6-phenyl-1,2,5,6-tetrahydro-1,3,5-triazine-2(1H)-ylidene)-malononitrile based on one-step three-component synchronous condensation, as well as a new pyrazole-based synthesis of metal complexes, carrying out detailed structural analyzes of the obtained new substances with modern physicochemical analysis methods;

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oxidation of 1-phenylethanol to acetophenone / N.Q. Shixaliyev, A.V. Gurbanov, A.M. Maharramov [et al.] // New Journal of Chemistry, – 2014. v. 38, – p. 4807-4815.

- computer-chemical study of the theoretical-experimental mechanism of some reactions with Density Functional Theory (DFT) calculations;
- study of catalytic activity of all new metal complexes in peroxide oxidation of styrene to benzaldehyde;
- study of antioxidant properties of synthesized N-benzyl-, N-allylanilin derivatives in model reactions by kinetic method;
- studying the effect of some samples against microbiological damage in M-8 oil and coolants;
- Carrying out studies of high inhibitory effects of N-benzyl-, N-allylanilin derivatives on AChE enzyme, CA I, II isozymes in living organisms by molecular docking method.

Research methods. The syntheses were mainly carried out by traditional elegant organic synthesis methods. The crystal structures of the obtained substances were confirmed by a Bruker APEX II CCD diffractometer. IR spectral analysis was performed with an Agilent Cary 630 FT-IR, 1H, 13C NMR spectra with a Bruker 300 MHz instrument. Mass spectra (ESI-MS) were recorded with an ion irradiation device (Varian 500-MS ion-mass spectrometer), and UV-absorption spectra were recorded with a Lambda 35 UV-vis spectrometer. Elemental analyses of carbon, hydrogen, and nitrogen were carried out at the Microanalytical Service Center of the Super Technical Institute of the University of Lisbon, Portugal.

Main points to defense. The theoretical bases of the dependence of the antioxidant and enzyme-isoenzyme inhibitory properties of N-benzyl- and N-allylanilin derivatives obtained with high yield and selectivity by an easy and economically efficient method were established.

2-(4-amino-6-phenyl-1,2,5,6-tetrahydro-1), containing a triazine ring and various functional groups in the molecule, whose theoretical-experimental mechanism was studied in detail by computer calculations and its structure by X-ray and Hirfeld surface analysis, For the first time, the possibility of carrying out one-step, three-component targeted synthesis of 3,5-triazin-2(1H)-ylidene)-malononitrile without the presence of a catalyst was determined.

A method of efficient synthesis of new metal complexes containing a pyrazole ring was developed and it was determined that the coordina-

tion environment and supramolecular chemistry of the obtained complexes depend on the nature of the metal atoms and the reaction conditions. When the catalytic activity of pyrazole-based complexes in peroxide oxidation of styrene to benzaldehyde was studied, it was found that, unlike traditional catalysts, the yield of benzaldehyde as a target product increases up to 80% due to the catalytic effect of 4 new complexes taken under optimal conditions. Taking into account the activity of these complexes, it is comparatively explained that they are related to the structures of more effective antioxidant and biocide properties.

The novelty of the work.

– Targeted and convenient synthesis methods of physiologically active N-benzyl-, N-allylanilin derivatives were developed, and optimal conditions were found for substantially increasing the yield and selectivity of the target compounds[6];

– 2-(4-amino-6-phenyl-1,2,5,6-tetrahydro-1,3), which retains a triazine ring and a different functional group in the molecule through a one-step three-component reaction using sophisticated organic synthesis methods and the latest possibilities of computer chemistry. 5-triazine-2(1H)-ylidene)-malononitrile was synthesized[7] and structural analyses by X-ray and Hirschfeld surface analysis were carried out and it was determined that monoclinic P21/ with two independent molecules (I and II) and one dimethylformamide solvent molecule in the asymmetric unit It crystallizes as a racemate in space group c. Both molecules (I and II) have stereo activity at the carbon atoms where the triazine rings are attached to the phenyl ring;

– for the first time, theoretical predictions were experimentally tested with DFT calculations for the synthesis reaction of tetrahydro-s-triazine with three-component condensation in one step without a

[6]Mahmudov, I. Synthesis and inhibition profiles of N-benzyl- and N-allyl aniline derivatives against carbonic anhydrase and acetylcholinesterase – A molecular docking study / I. Mahmudov, Y. Demir, Y. Sert [et al.] // Arabian Journal of Chemistry, – 2022. v. 15, – p. 103645.

[7]Mahmudov, I. Crystal structure and Hirshfeld surface analysis of 2-(4-amino-6-phenyl-1,2,5,6-tetrahydro-1,3,5-triazin-2-ylidene)malononitrile dimethylformamide hemisolvate / I. Mahmudov, Z. Atioglu, M. Akkurt [et al.] // Acta Crystallographica Section E, – 2022. v. 78, – p. 779-784.

catalyst, comprehensive theoretical-experimental studies were conducted in terms of simulating those chemical reactions with quantum chemical calculations, and important results were obtained. The importance of this work has been further enhanced by the fact that it was synthesized under milder conditions and by an atom-efficient method achieved by computer simulation;

– during the research, new metal complexes of pyrazole-based compounds with different substituted and ring sizes were synthesized, structural analyses were carried out with modern physicochemical analysis methods, and it was confirmed that they were not known in the world literature until now with international search programs. Successful use of 1,3,5-triazopentadienyl chelating ligand with 1H-pyrazole fragment to synthesize new tetranuclear Co(II/III) (IX) and mononuclear Ni(II) (X) and Cu(II) (XI and XII) complexes has been done[8]. Unlike most cases where the metal ion is bonded to the imine nitrogen atoms of both 1,3,5-triazopentadienyls, the cobalt and copper ions are bonded to one 1H-pyrazole nitrogen atom, and the central nitrogen atom of the 1,3,5-triazopentadienyl ring. It was determined that the coordination environment and supramolecular chemistry of the received complexes depend on the nature of metal atoms and reaction conditions;

– the catalytic activity of pyrazole-based complexes in the oxidation of styrene to benzaldehyde in the presence of peroxide was studied. From the study of oxidation type, mole ratio of styrene and catalyst, reaction temperature, time, and catalytic activity, it was found that under optimal conditions, the high yield of benzaldehyde as a target product increased up to 80% due to the catalytic effect of four new complexes;

– the antioxidant properties[9] of the synthesized compounds were investigated in model reactions using the kinetic method. It was found that the synthesized compounds are effective inhibitors of hydrocarbon

[8]Mahmudov, I. Co(ii/iii), Ni(ii) and Cu(ii) complexes with a pyrazole-functionalized 1,3,5-triazopentadiene: synthesis, structure and application in the oxidation of styrene to benzaldehyde / I. Mahmudov, A.V. Gurbanov, L.M.D.R.S. Martins [et al.] // New Journal of Chemistry, – 2023. v. 47, – p. 10826-10833.

[9]Махмудов, И.Г. Синтез и антиоксидантные свойства производных пиразола и их металлокомплексов // Journal of Baku Engineering University: Chemistry and Biology, – 2022. v. 6, – с.170-176.

oxidation. Also, during the research, it was found that some samples of N-benzyl-, N-allyl aniline derivatives show biocidal properties against microbiological damage in M-8 oil and coolants;

A new generation of inhibitors has been created that inhibit metabolic enzymes associated with some global diseases (Epilepsy, Alzheimer's, and other neurological diseases).

The theoretical and practical significance of the work. An efficient method for the synthesis of metal complexes of some pyrazole derivatives based mainly on cyandiamide, hydrochloric acid, and salts (copper (II) chloride dihydrate, copper (II) acetate monohydrate and cobalt (II) acetate tetrahydrate) was developed. The dependence of the physiological activity of the synthesized new compounds on antioxidant and inhibitory effects on enzyme-isoenzymes on the size of the ring in the molecule, functional substitution, or hetero atom effect was determined.

N-benzyl-, N-allylanilin derivatives have high inhibitory effects on acetylcholinesterase (AChE), Carbonic Anhydrase I and II (CA I, II) isoenzymes in the living organism, and as a result of numerous analyses, including "molecular docking" studies, it was found that in the future representatives of these inhibitors with separate functional groups can be used as potential drugs against epilepsy, diabetes, duodenal and stomach ulcers, glaucoma, Alzheimer's and neurological diseases.

Approbation and application. 15 scientific works have been published on the subject of the dissertation, 5 of them are articles (2 of which are single-authored articles), and the rest are theses. 3 of the articles were abstracted in the ISI Web of Knowledge search system of the Scientific Information Institute (ISI) of "Klariveit Analytics" company, included in the "Web of Science" and "Scopus" databases, with a high impact factor recommended by the High Attestation Commission under the President of the Republic of Azerbaijan (Arabian Journal of Chemistry, IF=6.212; New journal of chemistry, IF-3.925 and Acta Crystallographica Section E: Crystallographic Communications, 0.261) were published in foreign journals.

The main scientific and practical innovations of the dissertation work and important scientific results obtained were reported and discussed at scientific conferences, forums, and scientific symposia. Including:

- XXXII International scientific and technical conference "Chemical

reagents, reagents and processes of low-tonnage chemistry" "Reactive – 2019", dedicated to the 80th birthday of Academician of Bashkortostan D.R.Rakhmankulov (Ufa, Russia, September 5-6, 2019);

- II International Scientific Conference of the Council of Young Scientists and Specialists dedicated to the 75th anniversary of the Azerbaijan National Academy of Sciences entitled "Multidisciplinary approach in solving modern problems of fundamental and applied sciences" (Baku, Azerbaijan, March 03-06, 2020);
- V International Scientific Conference of Young Researchers dedicated to the 98th anniversary of the birth of national leader Heydar Aliyev (Baku, Azerbaijan, April 29-30, 2021);
- Second international bilateral Workshop on science between Dokuz Eylul University and Azerbaijan National Academy of Sciences (Baku, Azerbaijan, November 18, 2022);
- Republican scientific conference dedicated to the 110th anniversary of Academician Ali Guliyev on "Organic substances and composition materials of various purposes" (Baku, Azerbaijan, June 1-2, 2022);
- II Republican scientific conference "Chemistry and chemical technology" dedicated to the 100th anniversary of the birth of National Leader Heydar Aliyev for doctoral students, masters, and young researchers (Baku, Azerbaijan, May 4-5, 2023);
- VII International Scientific Conference of young researchers dedicated to the 100th anniversary of the birth of National Leader Heydar Aliyev (Baku, Azerbaijan, April 28-29, 2023);
- Republican scientific conference on "Modern approaches in chemistry and chemical technology" dedicated to the 80th anniversary of the Department of Petrochemistry and Chemical Technology of Baku State University (Baku, Azerbaijan, December 14, 2023).

The name of the organization the work dissertation carried out. The dissertation work was part of the main research plan of the Institute of Chemistry of Additives named after academician A.M. Guliyev of the Ministry of Science and Education of the Republic of Azerbaijan and was carried out under the priority directions of the laboratory "Physiologically active organic compounds".

The applicant's contribution to the research conducted. In the thesis work, setting the issues, conducting experiments, and analyzing

and summarizing the obtained results were carried out with the personal participation of the author.

The total volume of the dissertation with a sign indicating the volume of the structural sections of the dissertation separately. The dissertation consists of 176 computer-printed pages including figures and tables, "Introduction", 3 chapters, "Results", "Referenced literature list", "Appendices" and "Abbreviations", which includes 315 named sources cited in the dissertation. and a list of conventional symbols. Excluding tables, pictures, bibliography, and appendices, the total volume of the dissertation is 166627 characters, including the Introduction – 15877 characters, the first chapter – 45264 characters, the second chapter – 82721 characters, the third chapter – 18231 characters, and the conclusion – 4534 characters contained.

The relevance, purpose and tasks, scientific novelty, and practical importance of the work and approval of the results are reflected in the Introduction.

In the first chapter, a comparative analysis of modern literature data, mainly devoted to pyrazoles and their metal complexes, was reflected.

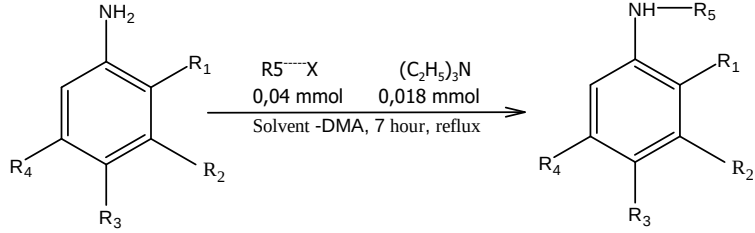
In the second chapter, development of a convenient synthesis method that leads to a substantial increase in the yield of N-benzyl-, N-allylanilin derivatives; new metal complexes based on 2-(4-amino-6-phenyl-1,2,5,6-tetrahydro-1,3,5-triazin-2(1H)-ylidene)-malononitrile and pyrazole based on one-step three-component reaction synthesis, detailed structural analysis of the obtained new substances with modern physico-chemical analysis methods; DFT analysis of the theoretical-experimental mechanism of some reactions; study of catalytic activity of all new complexes in peroxide oxidation of styrene to benzaldehyde; Study of antioxidant properties of N-benzyl, N-allylanilin derivatives in model reactions by kinetic method; the study of the effect of some samples against microbiological damage in M-8 oil and cooling liquids and finally the study of the high inhibitory effects of N-benzyl-, N-allylanilin derivatives on AChE enzyme, CA I, II isoenzymes in the living organism by the molecular docking method is written in detail.

In the third chapter, there is a place for the experimental part of the research work, and a broad description of the materials and methods used.

In the results section, the main results obtained from the dissertation research are presented.

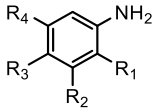
BASİC CONTENT OF THE WORK

Synthesis and study of N-benzyl- and N-allylaniline derivatives. A convenient synthesis method has been developed, which provides a significant increase in the yield and selectivity of N-benzyl and N-allylanilin derivatives, which are important products from the point of view of pharmaceuticals and industry. The synthesis process of these compounds was carried out according to the given reaction according to the scheme. (Scheme 1) Alkyl bromide and benzyl chloride were taken as substrates for the alkylation reaction, and triethylamine was used as a scavenger of halogen ions in the counter-cooling state of DMA. Substituted triazine derivatives can be synthesized in a variety of ways. The most common methods are nucleophilic aromatic substitution of cyanuric chloride, cycloaddition reactions to form the triazine ring, cyclotrimerization of organic cyanamides and nitriles, etc.



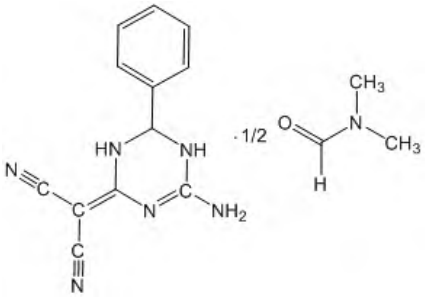
0,012 mmol

73-92 %

№			Compounds	Yield (%)
I	R_1, R_2, R_4=H, R_3=Cl	R_5=Allyl, X=Br	I	92
II	R_1, R_3, R_4=H, R_2=Cl		II	88
III	R_2, R_3=H, R_1, R_4=Cl		III	78
IV	R_2, R_3, R_4=H, R_1=Cl		IV	81
V	R_1, R_2, R_4=H, R_3=Cl	R_5=Benzyl, X=Cl	V	76
VI	R_1, R_3, R_4=H, R_2=Cl		VI	73

Scheme 1. Synthesis of N-benzyl- and N-allylanilin derivatives

Synthesis, crystal structure, and Hirshfeld surface analysis of 2-(4-amino-6-phenyl-5,6-dihydro-1,3,5-triazin-2(1H)-ylidene)-malononitrile. In particular, the one-step multicomponent reaction used is both efficient and facile, allowing for the simultaneous acquisition of targeted compounds. By such method 2-(4-amino-6-phenyl-5,6-dihydro-1,3,5-triazin-2(1H)-ylidene)malononitrile (VII) (E)-1-(amino(1H-synthesized by a one-step multicomponent reaction of pyrazol-1-yl)methylene)guanidinium chloride in the presence of benzaldehyde and malononitrile (Scheme 2):



Scheme 2. Graphical formula of 2-(4-amino-6-phenyl-5,6-dihydro-1,3,5-triazin-2(1H)-ylidene)malononitrile

The studied compound consists of two independent molecules in the asymmetric unit (molecule I with N1 and molecule II with N7) and one dimethylformamide solvent molecule. Figures 1 and 2 show the overlap of molecules I and II in the asymmetric unit with a difference of 0.173 Å:

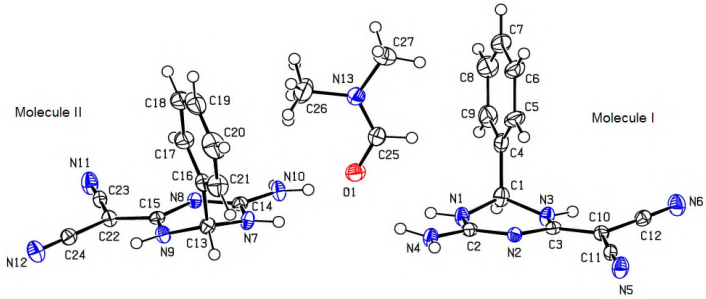


Fig. 1. Molecular structure of compound (VII).

Rings I and II of both molecules form dihedral angles of 86.8 (2)° and 86.63 (9)° at C4-C9 for the phenyl ring (I) and C16-C21 for the triazine midplane (II) respectively. Both racemic molecules I and II

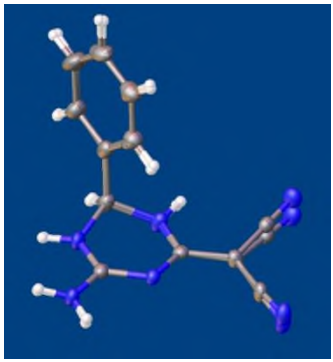


Fig. 2. Form of overlap of two independent molecules (I and II) in the asymmetric unit of the compound.

have a stereogenic center, and the chirality center is the selected asymmetric unit with respect to C1 for atoms (I) and C13 for atoms (II). Molecules I and II have normal geometric parameter values.

In the crystal, I and II are connected in parallel layers by intermolecular N—H···N and N—H···O hydrogen bonds through the solvent dimethylformamide molecule.

Hirshfeld surfaces for both molecules I and II were generated using Crystal Explorer 17. Figure 3 a,b for I and Figure 4 c,d for II). N—H···N and N—H···O interactions also produce red spots on Hirschfeld surfaces:

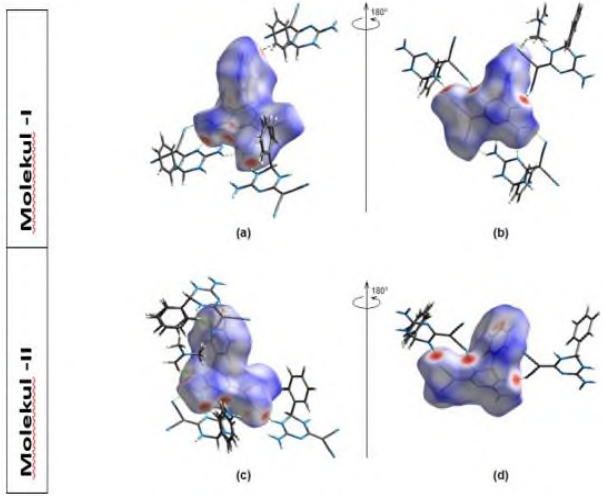


Fig. 3. Front and back views of three-dimensional Hirshfeld surfaces of compound I (a, b) and II (c, d) molecules.

Figure 4 shows the complete two-dimensional fingerprint plots for molecules I and II of the compound. N···H/H···N interactions (Fig. 4 b; 38.4% for I; 35.1% for II) are the main factor in crystallization with H···H (Fig. 3 c; 28.1% I; 26.9% for II) and C···H/H···C (figure 3 d; 23.4% for I; 26.3% for II) interactions representing the next highest parameters. The percentages of relatively weak interactions of molecules I and II are N···C/C··N (3.7% for I; 5.5% for II), N···N (2.6% for I; 1 for.9%). II), O···H/H···O (2.3% for I; 2.7% for II), C···C (1.3% for I; 1.3% for II and O···N/N ···O (0.2% for I; 0.2% for II). A comparison of the data shows that molecules I and II are quite similar:

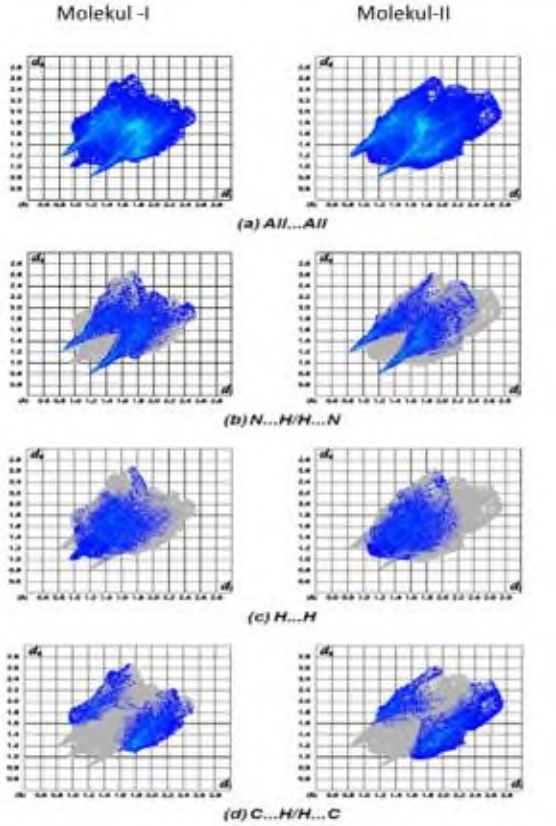


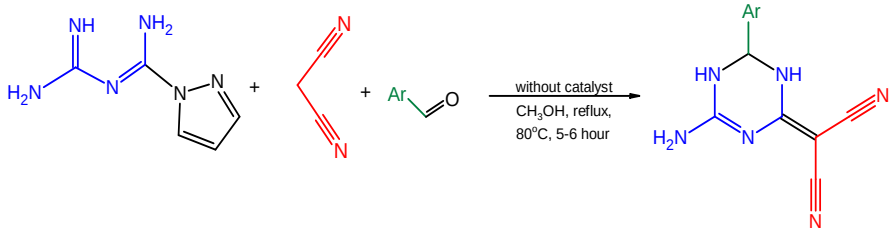
Fig. 4. (VII) Full two-dimensional fingerprint plots for molecules I and II of compound. (a) showing all interactions and (b) N···H / H···N, illustrated in (c). H···H and (d) C···H / H···C interactions. Values are the closest inner and outer distances (in Å) from given points on the Hirshfeld surface.

Two related compounds with a 1,2,3,4-tetrahydro-1,3,5-triazine unit are as follows. 3-(p-chlorophenyl)-4-[(dimethyl-4,6-pyridyl-2)methyl]-4,6-diphenyl-2-oxo-1,2,3,4-tetrahydro-1,3,5 -triazine and l-[(3,4-dichlorophenyl)methoxy]-1,6-dihydro-6,6-dimethyl-1,3,5-triazine-2,4-diamine hydrochloride 0,29-hydrate (B).

In crystal (A), the 1,2,3,4-tetrahydro-1,3,5-triazine ring exhibits a specific conformation. The intermolecular N–H···O hydrogen bond connects the pairs of molecules connected by the center of symmetry and forms an octagonal outline.

In crystal (B), the dihydrotriazine nucleus is protonated at N(5), where the positively charged delocalization is maximal. Except for one H on N(4), all H atoms on N participate in either H···N or H···CI interactions.

DFT study of the cyclocondensation of (E)-1-(amino(1H-pyrazol-1-yl)methylene)guanidine to tetrahydro-s-triazine derivatives with aldehydes and malononitrile. A three-component synthesis was carried out in one step using tetrahydro-s-triazines according to the scheme shown below (Scheme 3):

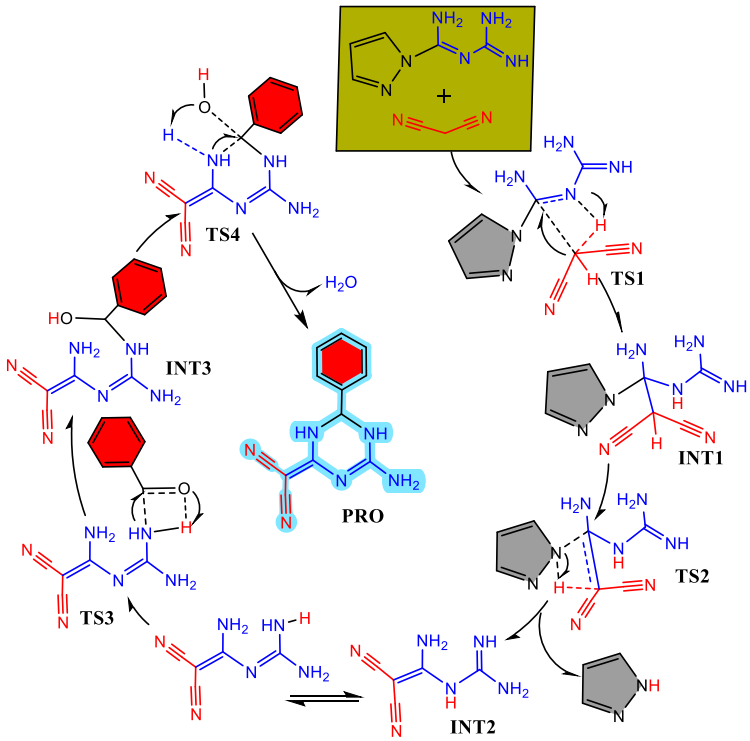


Scheme 3. Preparation reaction of tetrahydro-s-triazine.

The reaction mechanism calculated by DFT is shown in the following scheme (Scheme 4).

The ring formation resulting from X-ray analysis of the pyrazole group is the main reason to start the DFT calculation with the interaction between the carbon atom adjacent to the pyrazole and the malononitrile. As can be seen from the TS1 structure, the activated (acidic) proton of malononitrile is accepted by the nitrogen atom of the central imine adduct.

As a result, the increase in electrophilicity of the neighboring carbon of pyrazole (its electron density increases due to the loss of its



Scheme 4. Mechanism of synthesis of tetrahydro-s-triazine (PRO) based on pyrazole derivative and malononitrile confirmed by quantum chemical calculations.

proton) results in the attack of the malononitrile carbon and the formation of INT1. As can be seen from the structure of TS2, the attraction of the next proton of malononitrile by the nucleophilic pyrazole nitrogen results in the separation of the pyrazole molecule from the complex, as well as the acquisition of INT2. According to the scheme 3 the energies for DFT calculations are shown in the Table 1.

As a result of intramolecular proton migration (tautomerism) of the INT2 structure, the displacement of the proton and the double bond leads to better electron delocalization of the molecule and its stabilization by falling into the minimum energy state. The interaction of benzaldehyde with INT2 results in the attack of one of the terminal amine groups on the electrophilic carbon (benzaldehyde) and the spontaneous acceptance of the amine proton by the oxygen atom. The resulting intermediate (INT3) undergoes intramolecular dehydration as shown in

the structure of TS4, resulting in the formation of the same X-ray elucidated structure (PRO). This confirms that the calculated mechanism is quite logical.

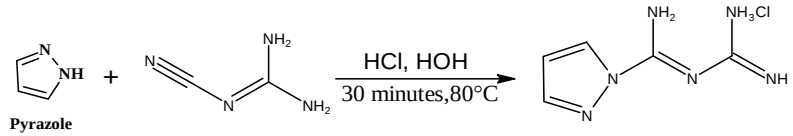
Table 1

The energies for DFT calculations

States	Energy, kcal/mol
Transition 1	30,2
Intermediate 1	10,5
Transition 2	25,2
Intermediate 2	8,2
Transition 3	12,2
Intermediate 3	-2,5
Transition 4	2,7
Product	-8,4

Co(II/III), Ni(II) and Cu(II) complexes of 1,3,5-triazopentadiene with a pyrazole ring: synthesis, structure and application in the oxidation of styrene to benzaldehyde. Research in this direction has several objectives: a) (E)-1-(amino(1H-pyrazol-1-yl)methylene) guanidinium chloride (H5L·HCl) metal complexes (Co(II/III), Ni(II) and Cu(II)) to synthesize; b) Metal complexes of 1,3,5-triazopentadienates are used as catalysts in the catalytic oxidation of styrene to benzaldehyde under mild conditions.

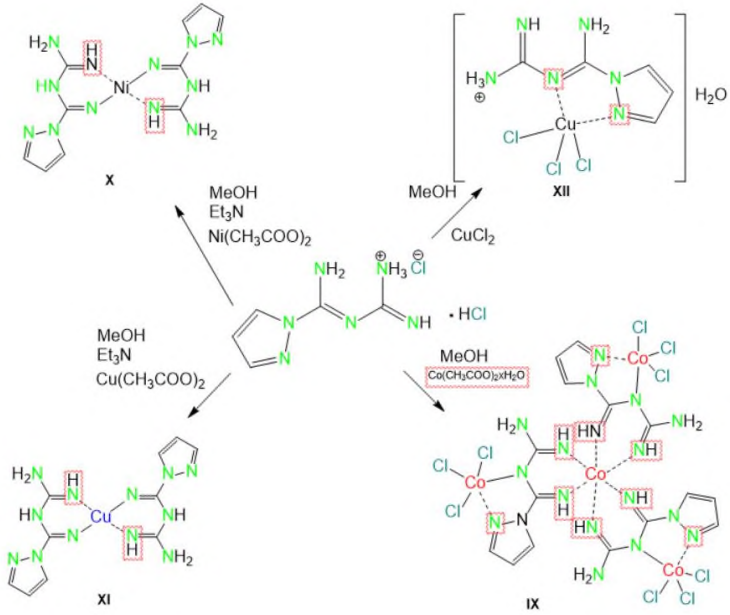
Synthesis of (E)-1-(amino(1H-pyrazol-1-yl) methylene)guanidinium chloride (H5L·HCl). Taking into account the importance of pyrazole-containing structures as biologically active substances, we synthesized a ligand based on cyanoguanidine and 3,5-dimethylpyrazole according to scheme 5:



Scheme 5. Synthesis of H5L·HCl ligand (VIII).

The synthesized ligand was used in the formation of metal, i.e., copper, nickel, and cobalt complexes, and these complexes can be used as catalysts for C(sp^3)-H activation and CO_2 conversion.

Synthesis and characterization of pyrazole-based metal complexes (IX-XII). The synthesis and characterization of (E)-1-(amino (1H-pyrazol-1-yl)methylene)guanidinium chloride ($H_5L{\cdot}HCl$) has been previously studied. In the presence of transition metals $Co(CH_3COO)_2 \cdot 4H_2O$, $Ni(CH_3COO)_2{\cdot}4H_2O$ (in the presence of triethylamine), $Cu(CH_3COO)_2{\cdot}H_2O$ (in the presence of triethylamine) and $CuCl_2{\cdot}\ 2H_2O$ in the presence of $H_5L{\cdot}HCl$ in methanol medium, different four-various-1, 3,5-triazopentadienates, [CoIII2{(CoIICl($H_4$4L)(H_2O)3}3 {(CoII(CH_3COO)(H4L)(H_3O)2-}3]6+(Cl−)6·H_2O (IX), [Ni(H4L)2] (X), [Cu(H4L)2] (XI) and [(H6L)$CuCl_3$]·H_2O (XII) were synthesized (Scheme 6): (IX-XII) In the IR spectra of complex compounds, the broad and strong ν(N−H) bonds are at 2952, 3347, 3377 and 3217 cm^{-1}, respectively, and the absorption of the ν(C=N) bond is at the wavelengths of 1587, 1595, 1592 and 1651 cm^{-1}, respectively. observed. In the H5L·HCl compound, it was observed at 1646 cm^{-1}, respectively. For the compound (IX), the band characteristic of the functional carboxyl (−COOH) group is found at the wavelength of 1700 cm^{-1}, which indicates the participation of the acetate carboxyl group in the coordination. proves.



Scheme 6. Synthesis of complex compounds (IX-XII).

UV/Vis spectra of compounds (IX-XII) in acetonitrile solution were observed with strong absorption from 283 to 312 nm and weak absorption from 418 to 481 nm.

The structures of all complexes were confirmed by X-ray crystallography, and they are summarized in Figure 5.

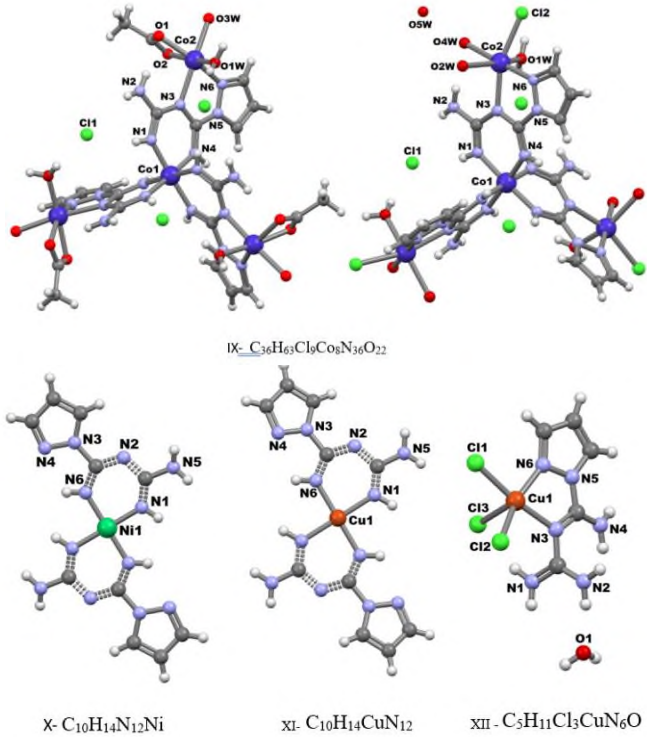


Fig. 5. Scheme of complexes (IX-XII) with some atomic numbers. Hydrogen atoms O2w, O3w, O4w and O5w are not shown in this structure.

As can be seen from Scheme 6, we synthesized new tetranuclear Co(II/III) (IX), mononuclear Ni(II) (X) and Cu(II) (XI and XII) complexes were synthesized. In other situations, a rare case was observed. Thus, cobalt in complex (IX) and copper atoms in complex (XII) coordinated with nitrogen atom of 1H-pyrazole and nitrogen atom of imine in 1,3,5-triazopentadienyl group.

The coordination environment of the obtained complexes and the chemical properties of the large molecule depend on the nature of the metal and the reaction conditions.

In the complex of compound (IX), the irregular coordination sphere Co was determined in cobalt (acetate anion and water molecule were displaced by chloride and two water molecules and partial eclipse occurred). The hydrogen atoms of these water molecules, including the last water molecule (Ow5), are unoccupied, which are defined by an eclipse of 0.5.

In both cations, the central Co^{3+} ion forms octahedral coordination with six donor nitrogen atoms of three 1,3,5-triazopentadienyl ligands. In the cation [CoIII{(CoII(CH3COO)(H4L)(H2O)2}3]3+, each Co^{2+} has two oxygen atoms of the carboxyl group of the central acetate ligand, two nitrogen atoms of the 1,3,5-triazopentadienyl ligand, and two oxygen atoms of the water molecules forms weak octahedral coordination with. Similarly, the CoII center in the [CoIII{(CoCl(H4L)(H_2O)3}3]3+ cation formed octahedral coordination with two nitrogen atoms, one chlorine atom, and three water molecules of the 1,3,5-triazopentadienyl ligand. 1 ,3,5-triazopentadienyl, chloride ligands, water molecules and chloride anions are included in intramolecular noncovalent bonds, resulting in a 3D macromolecular lattice (Figure 6): the complexes of compounds (X and XI) are structurally similar.

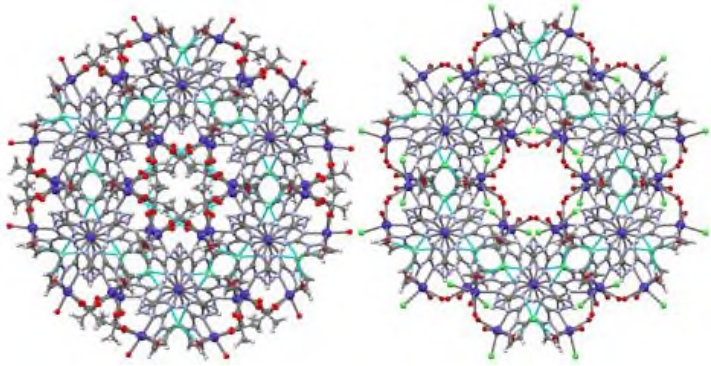
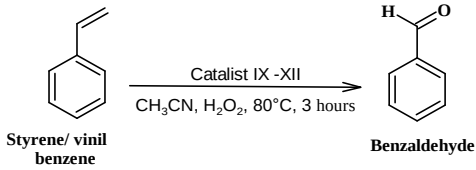


Fig. 6. (IX) intermolecular hydrogen bonds in the crystal formation of the compound.

STUDY OF THE FUNCTIONAL PROPERTIES OF THE SYNTHESIZED COMPOUNDS

Catalytic activity of pyrazole-based complexes in the catalytic oxidation of styrene to benzaldehyde. The activity of complexes (IX-

XII) in peroxide oxidation of styrene to benzaldehyde was studied (Scheme 7):



Scheme 7. Catalytic oxidation of styrene to benzaldehyde in the presence of complexes (IX-XII).

In general, styrene, catalyst, oxidant, and solution were introduced into the test tube of the reactor and heated for the desired time and duration. Selected results are reflected in Table 2.

Both tetranuclear Co(II/III) (IX) and mononuclear Ni(II) (X) complexes play a more selective catalytic role than Cu(II) complexes (XI and XII) in the peroxide oxidation of styrene to benzaldehyde. Compared to quaternary butyl hydroperoxide (TBHP) and non-solvent conditions, the catalytic activity was better in H_2O_2 and acetonitrile media. The higher catalytic activity of complex (XII) than the other complex (XI) is due to the fact that the chloride group is easily substituted and the synthetic transformation occurs as a result.

Investigation of antioxidant properties of pyrazole-based metal complexes. In order to determine the mechanism of antioxidant action of the synthesized compounds, we studied the kinetics of their reaction with cumyl peroxide radicals and cumyl hydroperoxide.Studies have shown that the investigated inhibitors effectively degrade cumyl hydroperoxide.At the same time, one molecule of the investigated inhibitors is capable of breaking down several thousand molecules of hydroperoxide, which means that the reaction is catalytic. Table 3 lists the values of the kinetic parameters of the reaction of the synthesized compounds with cumyl peroxide radicals and cumyl hydroperoxide.

Analysis of the kinetic parameters of the reaction of pyrazole-based metal complexes with cumylperoxide radicals and cumylhydroperoxide in the table shows that compound (XI) is the most effective inhibitor of oxidation. In terms of effectiveness of terminating oxidation chains by reaction with cumyl peroxide radicals, the indicated inhibitor is at the level of an inhibitor of ionol oxidation widely used in practice.

Table 2

(IX-XII) effect of catalytic activity of complexes on reaction conditions (*chosen results*)

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Entry	Catalyst	Solvent	Oxidant	T, °C	t, hour	n (styrene)/ n (cat)	Yield, % [a]	Conversion, %
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
1	-	NCMe	H_2O_2	80	3	1 mmol/ 5 μmol	-	-
2	$Co(CH_3COO)_2 \cdot 4H_2O$						6.9	33
3	$Ni(CH_3COO)_2 \cdot 4H_2O$						5.8	17
4	$Cu(CH_3COO)_2 \cdot H_2O$						10.6	56
5	$CuCl_2 \cdot 2H_2O$						9.4	47
6	**IX**	NCMe	H_2O_2	80	3	1 mmol/ 5 μmol	39.6	99
7	**X**						37.1	57
8	**XI**						57.0	77
9	**XII**						80.0	83
10	**IX**	—	H_2O_2	80	3	1 mmol/ 5 μmol	2.0	6
11	**X**						3.6	18
12	**XI**						11.0	22
13	**XII**						16.4	26
14	**IX**	NCMe	TBHP	80	3	1 mmol/ 5 μmol	16.0	>99
15	**X**						14.4	72
16	**XI**						19.1	91
17	**XII**						35.3	98
18	**IX**	NCMe	H_2O_2	60	3	1 mmol/ 5 μmol	21.5	50
19	**X**						17.6	27
20	**XI**						29.1	41
21	**XII**						39.2	40
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
22	**IX**	NCMe	H_2O_2	80	2	1 mmol/ 5 μmol	23.0	64
23	**X**						19.8	33
24	**XI**						45.8	52
25	**XII**						53.4	58
26	**IX**	NCMe	H_2O_2	80	3	1 mmol/ 10 μmol	19.0	>99
27	**X**						23.0	72
28	**XI**						37.4	89
29	**XII**						43.7	93

[a]value were collected based on GC analyses. (by internal standard method).

However, unlike ionol, this inhibitor can catalytically degrade cumylhydroperoxide. At the same time, among the investigated compounds, this inhibitor has the highest value of the catalytic coefficient (ν) – 12000.

Table 3

Cumyl peroxide radicals of synthesized compounds (IX, XI, XII) and kinetic parameters of the reaction of cumin with hydroperoxide.

№	Structure of metal complexes	Induction cycle of cumene autoxida-tion (T=110°C), τ, minutes.	Reaction with RO_2^* (T=60°C)		Reaction with CHP (T=110°C)	
			f	$k_7 \cdot 10^{-4}$ l/mol·s	K, l/mol.s	*ν*
IX	$[Co^{III}_2\{(Co^{II}Cl(H_4L)(H_2O)_3\}_3\{(Co^{II}(CH_3COO)(H_4L)(H_2O)_{2-}\}_3]^{6+}(Cl^-)_6 \cdot H_2O$	100	0.5	2.01	11	10000
XI	$[Cu(H_4L)_2]$	180	1.58	2.6	14.5	12000
XII	$[(H_6L)CuCl_3] \cdot H_2O$	120	1.056	2.24	13	6000
Ionol		150	2.10	2.00	-	-

Inhibitory activities of N-benzyl- and N-allylanilin derivatives on enzyme-isoenzymes. N-benzyl and N-allylanyl derivatives also show physiological activity. Taking into account the relevance of the study of synthesized antioxidants as physiologically active substances, the effects of these compounds on acetylcholinesterase (AChE) and carbonic anhydrase I, II (hCA I, II)) were determined.

In recent studies, N-benzyl- and N-allylanilin derivatives synthesized by new methods inhibited hCA I isoenzyme. Based on the results, it was determined that both N-allyl- and N-benzyl compounds increased hCA I inhibition capacity depending on the chlorine group in the para position. N-allyl group showed better inhibition property than N-benzyl group. A similar situation was observed in the meta state of the chlorine atom. The inhibitory effect of hCA I changed in the para->meta->ortho direction depending on the position of the chlorine atom in N-allylanilin derivatives. A similar situation was observed in N-benzyl derivatives.

The addition of a chlorine atom to the ortho-position of the aniline fragment in N-allyl-2-chloroaniline (IV) led to a certain decrease in the inhibition ability.

Among N-benzyl and N-allylaniline derivatives, N-benzyl-4-chloroaniline (V) shows the best inhibitory effect. As can be seen from the results, for hCA I, the presence of the chlorine atom in the para position in N-benzylaniline shows a more effective inhibition property than in

the meta position.

The chlorine atom in the N-allyl group acts on the aniline in the meta position and has a better inhibition effect on hCA I. Depending on the position of the chlorine atom, it affects N-allylanilin, depending on its position (meta- > para- > ortho direction) the inhibitory effect of hCA II isoenzyme is strengthened. By adding a chlorine atom to the ortho position, the inhibitory effect of the aniline molecule in compound (IV) is reduced, but this hCA is also completely different.

It was determined that N-benzyl-4-chloroaniline (V) from N-benzyl- and N-allylanilin compounds has a good inhibitory effect on AChE as a cholinergic enzyme.

Summarizing the above, it was concluded from the comparative analysis that in the near future, representatives of these inhibitors with separate functional groups can be used as potential drugs against epilepsy, Alzheimer's and other neurological diseases.

Molecular docking studies. During the study, the in silico molecular relationships of compounds (I-VI) with both hCA I and II isoenzymes and AchE receptors were studied using the AutoDock Vina program. First, the structure of each molecule or ligand (I-VI) in the gas phase was determined based on Density Functional Theory (DFT) method B3LYP functional and 6-311++G (d, p) with Gaussian 09 W package program.

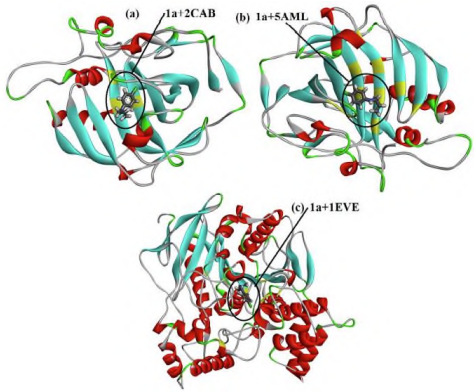

Fig. 7. 2CAB, 5AML three-dimensional structure and 1EVE proteins with combination (I)

When evaluating the results, it was determined that the molecule (I) shows a fairly high inhibitory property. (I) It exhibits good inhibitory

activity when interacting with hCA I/PDB: 2CAB, hCA II/PDB: 5AML and AchE/PDB. The energies of 1 EVE are 9.1, 8.8 and 9.3 kcal/mol, respectively. For this reason, the evaluation of relations is only noted as (I) + 2CAB, (I) + 5AML, (I) + 1EVE**.** Summarizing the above, it can be concluded that the molecule (I) shows a potential inhibitory property for all three enzymes and shows a rather strong inhibitory property for the AchE enzyme in particular. Additionally, Figure 7 shows the active part of the molecule (I) and the internal position of the enzyme.

In this case, the experimental results support the theoretical results and show promise for future drug design.

RESULTS

1. An efficient synthesis method of N-benzyl- and N-allylanilin derivatives has been developed. In the presence of 0.018 mmol of triethylamine catalyst and N,N-dimethylacetamide as a solvent, as a result of the reaction of alkyl and aryl derivatives of aniline with allyl bromide and benzyl chloride in the ratio of 0.012:0.04 mmol for 7 hours, the yield of targeted substances was increased to 72-92% [4].

2. Using sophisticated organic synthesis methods and the latest possibilities of computer chemistry, (E)-1-[amino(1H-pyrazol-1-yl)methylene]guanidine chloride with benzaldehyde and malononitrile in a 1:1:1 mmol ratio for 5 hours in the presence of methanol 2-[4-amino-6-phenyl-5,6-dihydro-1,3,5-triazin-2(1H)-ylidene]malononitrile 47, which is a targeted substance by a one-step three-component reaction without the presence of a catalyst for the first time synthesized in % yield. X-ray structural analysis of the obtained new substance determined that it has stereo activity at carbon atoms where triazine rings are attached to phenyl in each independent molecule that crystallizes in the form of a monoclinic racemate together with the dimethylformamide molecule. According to the Hirschfeld surface analysis, the Van der Waals interaction forces, which ensure the stability of the molecular structure, contribute significantly to the formation of a single crystal [6].

3. 1:1 of (E)-1-[amino(1H-pyrazol-1-yl)methylene]guanidine chloride (H5L·HCl) with the corresponding salts of Co, Ni and Cu in methanol medium in the presence of triethylamine catalyst and New metal complexes were synthesized with 57-80% yield of interaction in 1:0.5

mmol ratios, their structure was confirmed by modern physico-chemical analysis methods, and their novelty was confirmed by "SciFinder" international scientific search system. It was determined by X-ray diffraction of the structures of the complexes that the H5L·HCl compound is a potential N-donor ligand and coordinates as an N4 donor for cobalt and as an N2 donor for nickel and copper. In the tetranuclear cobalt complex, the coordination geometry around CoIII or CoII atoms is octahedral, in [Ni(H4L)2] and [Cu(H4L)2] complexes, it is planar around Ni and Cu atoms, and in the [(H6L)CuCl3]·H2O complex, it has a pyramidal planar structure around Cu. . The rectangular plane has two chlorine atoms strongly bonded to the copper atom, two nitrogen atoms of the bidentate, and a third chlorine atom in the apical position, which forms an apical weak bond. Since the nitrogen atom of the free imine group is protonated, the complex is neutral. The mentioned gives catalytic activity to the complexes [10].

4. The study of the mechanism of the three-component reaction of (E)-1-(amino(1H-pyrazol-1-yl)methylene)-guanidine chloride with benzaldehyde and malononitrile by DFT calculations using the capabilities of modern computer software theoretically confirmed that this reaction is one-step [14].

5. All 5. From the study of the catalytic activity of the synthesized pyrazole metal complexes in the peroxide oxidation of styrene to benzaldehyde, it was found that both Cu(II) complexes play the role of a selective catalyst for this process compared to the tetranuclear Co(II/III) and mononuclear Ni(II) complexes. Better catalytic activity is observed when H_2O_2 and acetonitrile are used instead of tetrabutylhydroperoxide and in solvent-free conditions. The higher catalytic activity of the $[(H_6L)CuCl_3]\cdot H_2O$ complex compared to $[Cu(H_4L)2]$ can be attributed to the presence of chloride ligands that can undergo easy displacement and consequently accelerate this synthetic transformation. Overall, the catalytic effect of these four new pyrazole-based complexes increases the yield of benzaldehyde as the target product by to 80% [10].

6. By studying the antioxidant properties of the synthesized compounds in model reactions using the kinetic method, it was determined that the relevant metal complexes are effective inhibitors of hydrocarbon oxidation, and the mechanism of antioxidant action consists of the breaking of oxidation chains as a result of the reaction with peroxide

radicals, and for some, the catalytic decomposition of hydroperoxides into molecular products. The analysis of the kinetic parameters of the reaction of pyrazole-based metal complexes with cumylperoxide radicals and cumylhydroperoxide shows that the nickel complex of pyrazole is the most effective inhibitor of oxidation. This inhibitor has the highest value of the catalytic coefficient (ν) – 12000 [9].

7. The study of the effect of some samples of N-benzyl- and N-allylanilin derivatives against microbiological damage in lubricating-coolant fluids showed that these compounds are much higher than the widely used 8-oxyquinoline due to their biocide properties [9].

8. It was determined that N-benzyl-, N-allylanilin derivatives have high inhibitory effects on AChE enzyme, CA I, II isoenzymes in the living organism, including as a result of "molecular docking" studies, it was found that N-benzyl and N-allylanilin derivatives IC50 have effective inhibitory activity in the range of 182.45 to 520.21 nM and Ki in the range of 149.24 ± 15.59 to 519.59 ± 102.27 nM. Among these compounds, N-benzyl-4-chloroaniline shows the highest inhibitory property on AChE. As a result, it was concluded from the comparative analysis that soon representatives of these inhibitors with separate functional groups can be used as potential drugs against epilepsy, Alzheimer's and other neurological diseases [6].

The following scientific works have been published on the dissertation materials

1. Mahmudov, I.H., Safarov, B.E., Aliyeva, L.N, Isakov, M.E., Abdullayev, Y.A., Sujayev, A.R. Creation of new and combined effects of antioxidants // XXXII International Scientific and Technical Conference "Chemical reagents, reagents and processes of small-scale chemistry", – Ufa, Bashkortostan: – 5 – 6 september, –2019, – p.80.

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3. Mahmudov, I.H., Sujayev, A.R., Abdullayev, Y.A. Synthesis

of aromatic thioamides by green method // Materials of the 5th International Scientific Conference of Young Researchers dedicated to the 98th anniversary of the birth of national leader Heydar Aliyev, – Khirdalan, Azerbaijan: – 29 – 30 April, – 2021, – p.354.

4. Mahmudov, I.H. Synthesis and Inhibition Profiles of N-Benzyl-and N-Allyl Aniline Derivatives against Carbonic Anhydrase and Acetylcholinesterase – A Molecular Docking Study / Ibadulla Mahmudov, Yeliz Demir, Yusuf Sert, Yusif Abdullayev, Afsun Sujayev, Saleh H Alwasel, Ilhami Gulcin // Arabian Journal of Chemistry, – 2022. v. 15, №3, – p.103645-103655.

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8. Mahmudov, I.H. Investigation of N-benzyl- and N-allylanyline derivatives as biocidal additives to prevent microbiological damage to hydrocarbons, /Journal of Baku Engineering University Chemistry and Biology, – 2022. v. 6, №1, – p.11-18.

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The defense will be held on 24 June 2024 at 14^{00} at the meeting of the Dissertation council ED 1.16 of Supreme Attestation Commission under the President of the Republic of Azerbaijan operating at the Institute of Petrochemical Processes named after acad. Y.H.Mammadaliyev of the Ministry of Science and Education Republic of Azerbaijan

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Abstract was sent to the required addresses on 14 May 2024.

Signed for print: 08.05.2024
Paper format: A5 (60×90 1/16)
Volume: 37 437
Number of hard copies: 20