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1(1,2,4 TRIAZOLE 3-AZO)NAPHTHOL-2

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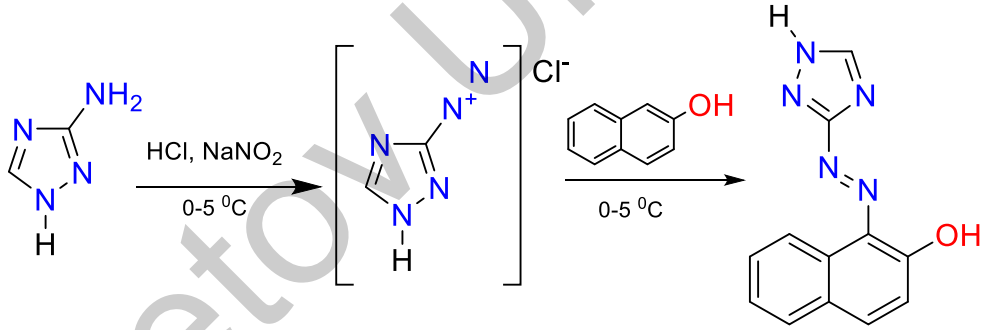
Aromatic azo compounds are structurally versatile compounds widely used in the production of dyes, pigments, food additives, sensors, and materials with unique photophysical properties. Their high practical significance in pharmaceuticals, optics, electronics, and polymer chemistry has led to sustained interest in the development of new methods for their synthesis. Azo dyes have a nitrogen and nitrogen double bond as chromophores. These dyes are formed by taking a diazonium salt and attaching it to a strongly activated aromatic ring[1]. In addition to dyes, they can be used as pigments, food additives, indicators, in the textile industry, pharmaceuticals, cosmetology and medicine. [2-3] Azo dyes are compounds with intense color. They are also used in analytical chemistry for the detection of metals. The chemical stability, toxicity and resistance to biodegradation of azo compounds pose a serious problem for the environment. Therefore, in-depth study of the molecular structure, electronic properties and reaction activity of azo dyes through theoretical approaches has become a pressing issue[4].

Azo compounds have a variety of biological activities, including antimicrobial, antioxidant, antitumor, and antiviral effects. Studies have shown that derivatives of heterocyclic azo compounds are active against pathogens such as Staphylococcus aureus, Escherichia coli, and others, and azo-metal complexes demonstrate antibacterial efficacy, making them promising candidates in the fight against resistant strains. In silico methods (PASS) are also helpful in this, allowing one to predict types of activity based on the structure of the molecule and expand the pharmacological spectrum of possible applications [5].

The synthesis involved the formation of a 3-amino 1,2,4-triazole diazonium salt at low temperature, followed by reaction with 2-naphthol in alkaline medium, which resulted in a color change from colorless to red-yellow. The resulting product was neutralized, filtered, washed, and purified by recrystallization from ethanol (yield: 72%). The structure of the resulting ligand 1(1,2,4 triazole 3-azo)naphthol-2 was characterized by Fourier transform infrared spectroscopy (FTIR), HPLC, nuclear magnetic resonance (1H-NMR and 13C-NMR), mass spectroscopy (MS), and elemental analysis. The biological activity was determined using the PASS ONLINE program.



When checking the purity of the obtained azo compound in HPLC, we see that the product was obtained with a purity of 89.8% at 3.476 min. The azo compound was then recrystallized and purified in ethanol.

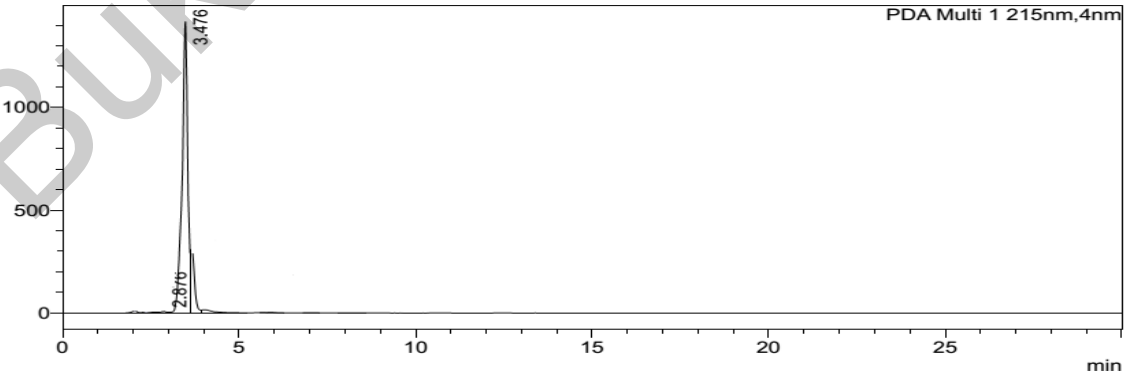


Figure 3. – Checking the purity of the obtained azo dye

Ik spectroscopy analysis

In the azo compound, the absorption at 3122 cm^{-1} belongs to the O-H group, 3063 cm^{-1} belongs to the C-H of the aromatic ring, the absorption at 1537 cm^{-1} belongs to the N=N (azo group), 1249 cm^{-1} is characteristic of the C–O bond, 740 cm^{-1} is characteristic of the C–H bond in the aromatic ring (strong absorption at 1600–1622 cm^{-1}) belongs to the NH group

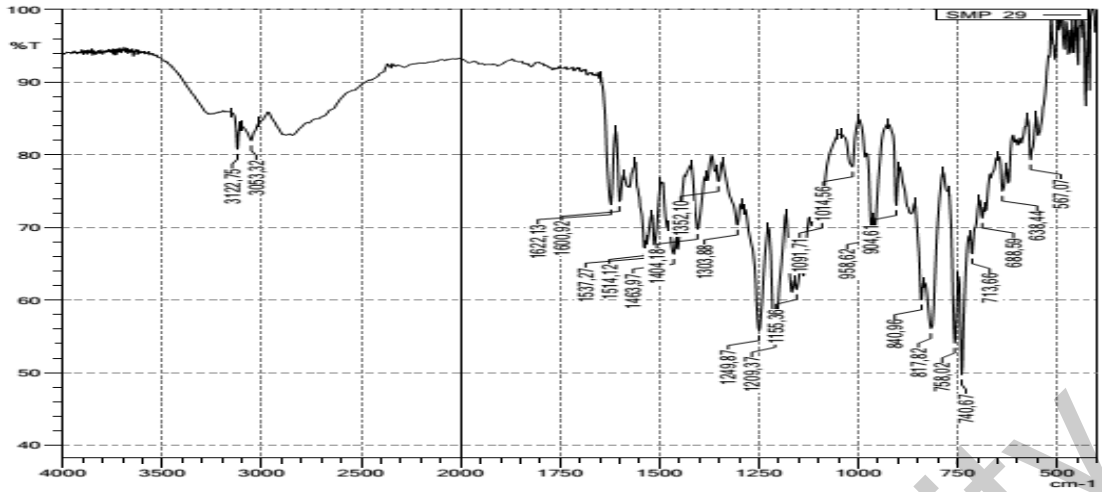
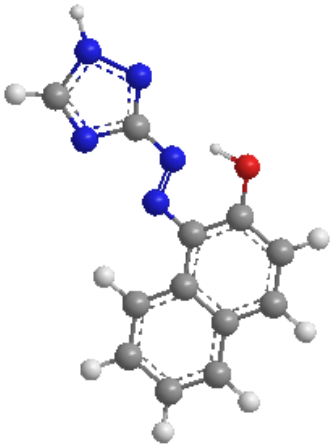


Figure 2. – IR spectra of azo compounds



All Pa>Pi Pa>0,3 Pa>0,7 ok

Pa	Pi	Activity
0,692	0,066	Aspulvinone dimethylallyltransferase inhibitor
0,611	0,005	Thiol protease inhibitor
0,575	0,001	Azobenzene reductase inhibitor
0,563	0,021	HMGCS2 expression enhancer
0,542	0,006	Ferredoxin hydrogenase inhibitor
0,513	0,013	CDK9/cyclin T1 inhibitor
0,520	0,037	Aminobutyraldehyde dehydrogenase inhibitor
0,493	0,011	ATP phosphoribosyltransferase inhibitor
0,520	0,039	Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
0,519	0,046	Glucose oxidase inhibitor

Figure 3. - In silico prediction using PASS Online

"In silico prediction using PASS Online revealed that the synthesized compound has a high probability of inhibiting aspulvinone dimethylallyltransferase (Pa = 0.692), thiol protease (Pa = 0.611), and azobenzene reductase (Pa = 0.575). In addition, inhibitory effects on ferredoxin hydrogenase, CDK9/cyclin T1, and a number of other enzymes are predicted with a probability higher than 0.5. This indicates a possible multi-target biological activity of the molecule and the need for further experimental studies."

"In silico prediction using PASS Online revealed that the synthesized compound has a high probability of inhibiting aspulvinone dimethylallyltransferase (Pa = 0.692), thiol protease (Pa = 0.611), and azobenzene reductase (Pa = 0.575). Moreover, additional activities such as ferredoxin hydrogenase inhibition and CDK9/cyclin T1 inhibition were predicted with Pa > 0.5, suggesting a potential multitarget biological profile and highlighting the need for experimental validation."

Conclusion:

Azodecompounds are one of the most important compounds in the synthesis of metallocomplexes, in addition to dyes. The structure of the obtained azocompound was determined using modern physical research methods. Its biological activity was theoretically determined using the PASS ONLINE program. Although its biological activity did not give a very high result, it can be analyzed as a biologically active substance.

References:

1.Valiulin R. Organic Chemistry: 100 Must-Know Mechanisms // Organic Chemistry: 100 Must-Know Mechanisms. – De Gruyter, – 2020. – P. 97-98.

2.A.J. Jarad, I.Y. Majeed, A.O. Hussein, Synthesis and spectral studies of heterocyclic azo dye complexes with some transition metals, J. Phys. Conf. Ser., 2018, doi: 10.1088/1742-6596/1003/1/012021.

3.R. Zhao, C. Tan, Y. Xie, C. Gao, H. Liu, Y. Jiang, One step synthesis of azo compounds from nitroaromatics and anilines, Tetrahedron Lett. 52 (2011) 3805–3809, doi: 10.1016/j.tetlet.2011.05.054 .

4.Kalaycı T. et al. Quantum chemical calculations of m-toluidine and investigation of its adsorption on eggshells //Erzincan University Journal of Science and Technology. – 2023. – Т. 16. – №. 1. – С. 169-183.

5.Yilmaz, M., Özdemir, A., & Gokce, H. (2024). Azo dyes and their metal complexes: Promising antimicrobial agents. Journal of Molecular Structure, 1290, 136965. https://doi.org/10.1016/j.molstruc.2024.136965