

## Synthesis and study of new azo dyes based on functionally substituted derivatives of salicylic acid

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### Abstract

Three chromatographically pure azo dyes based on salicylic acid and para-nitroaniline were isolated in 60-64% yields. The structure of the synthesized compounds was proved by IR spectroscopy. The spectra of the compounds contain characteristic absorption bands associated with the vibrations of O–H, N–H, C=O, and N=N groups. The products precipitated as orange-brown powders, which corresponds to compounds with a short system of conjugated double bonds. The predominant tautomeric form of existence of the synthesized azo compounds was determined – 5,5'-(diazene-1,2-diyl)bis(2-hydroxybenzoic acid), 2-hydroxy-5-((4-nitrophenyl)-diazene)benzoic acid, 5-amino-2-hydroxy-4-((4-nitrophenyl) diazenyl) benzoic acid. It was shown that they all exist as azo-tautomers. To determine the dyeing power of potential dyes, a test cold dyeing was carried out on samples of a multichannel consisting of six main types of fabrics used in the textile industry, under conditions corresponding to dyeing with acid and reactive dyes. The ability of the compounds to act as acid dyes was established, coloring woolen, polyamide and acetate fibers in yellow-orange and beige-brown colors. The introduction of an amino group into the salicylic acid fragment weakens the color properties of the azo dye molecule. The calculation of the toxicity of compounds with intravenous and oral routes of administration, carried out according to the GUSAR program, shows their low toxicity (4-5 toxicity class). The introduction of an amino group into the azo dye molecule is accompanied by an increase in its toxicity. All isolated compounds comply with Lipinski's rule, which indicates their bioavailability. Prediction of the biological activity of the compounds, carried out using the PASS program, shows that with a probability of more than 90%, the synthesized compounds exhibit antiseptic properties without irritating the skin and mucous membranes. This allows the isolated compounds to be considered promising for use as dyes in cosmetics.

### References

- [1] K. Raghavendra, K. Kumar. Synthesis and their antifungal, antihelminthic and dyeing properties of some novel azo dyes. *Research journal of pharmaceutical, biological and chemical sciences*. **2013**. Vol.3. No.2. P.275-280.
- [2] D.S. Gusarov, M.A. Ryabov, Thi Ngok Anh Vu, and O.V. Kovalchukova. Quantum-chemical modeling of structure and properties of nitrogen derivatives of phloroglucinol. *Butlerov Communications*. **2019**. Vol.57. No.3. P.51-57. DOI: 10.37952/ROI-jbc-01/19-57-3-51
- [3] A. Teimouri, A. Chermahini, M. Ghorbani. The green synthesis of new azo dyes derived from salicylic acid derivatives catalyzed via baker's yeast and solid acid catalysis. *Chemija*. **2013**. Vol.24. No.1. P. 59-66.
- [4] C. Patil, C. Nehete. The azo derivatives of salicylic acid. *International journal of pharmaceutical sciences review and research*. **2015**. Vol. 33. No.2. P.248-256.
- [5] O.V. Kovalchukova, B.E. Zaitsev, and S.B. Strashnova. Features of coordination chemistry of polyfunctional N-containing heteroaromatic hydroxyl-compounds. *Butlerov Communications*. **2011**. Vol.24. No.1. P.76-83. ROI-jbc-01/11-24-1-76
- [6] O.V. Kovalchukova, O.V. Volyanskiy, P.V. Strashnov, O.V. Korolev, S.B. Strashnova, and T.A. Epiphanova. Electronic structure, ionic equilibria and complex formation of some derivatives of 1-phenyl-3-methylpyrazolone-5. *Butlerov Communications*. **2011**. Vol.24. No.1. P.84-89. ROI-jbc-01/11-24-1-84

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- [7] O.V. Kovalchukova, S.B. Strashnova, P.V. Strashnov, E.P. Romashkina, O.V. Volyanskiy, and K.I. Kobrakov. Spectral and quantum-chemical studies of tautomeric and ionic transformations of azo-dyes based upon methylfloroglucine. *Butlerov Communications*. **2011**. Vol.24. No.1. P.90-94. ROI-jbc-01/11-24-1-90
- [8] O.V. Kovalchukova, O.V. Volyansky, Al Tahan Rana Abdulillah Abbas, B.E. Zaitsev, D.N. Kuznetsov, and T.I. Berikashvili. Complex compounds of metals with some azo-derivatives of benzo[4,5]imidazo[1,2-c]quinazoline carboxylic acids. *Butlerov Communications*. **2014**. Vol.40. No.11. P.122-127. ROI-jbc-01/14-40-11-122