

EDUCATION AND SCIENCE IN THE PERIOD OF GLOBAL CRISES AND CONFLICTS IN THE 21st CENTURY



COLLECTIVE MONOGRAPH

**EDUCATION AND SCIENCE
IN THE PERIOD OF GLOBAL
CRISES AND CONFLICTS
IN THE 21st CENTURY**

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SOME ASPECTS OF THE INTERACTION OF THE CHEMICAL STRUCTURE AND BIOLOGICAL ACTIVITY OF THE MEDICINAL SUBSTANCE

It is known that the biological properties of medicinal substances completely depend on the peculiarities of their chemical structure. Diversity of biologically active substances is achieved by using the basic principles of the strategy of creating new substances. It is copying known physiologically active substances, chemical modification of the structure of known synthetic and natural medicinal substances, the introduction of a pharmacophoric group of a known medicinal substance into a molecule of a new substance, molecular modeling, the creation of combined drugs, the methodology of combinatorial chemistry (the technique of miniaturization of syntheses was created and biotested, allowing to synthesize up to several thousand new compounds per day), bioisostery, search for antimetabolites based on the study of drug metabolism, the strategy of pro-drugs¹.

For example, when creating a variety of sulfanilic acid amide derivatives, this is the main research scaffold *para*-aminobenzenesulfamide substituted by functional groups $-NHR$ and $-SO_2NHR(R')$. The formation of a substituted aromatic fragment of the main scaffold in sulfonamide molecules is carried out due to acetylation, halogenation, and amination reactions (fig.1):

¹ Hubsky, Y.I. & Velchynska, O.V. Synthesis and biological activity studies of new N-substituted [(phosphinothiadiazolyl) amino] succinimides. *Med. Khim*, 2008, V.10, p. 5–11; 2Welchinskaya, H.V., Pieczusak, B., Kovalenko, E.A., Sharykina, N.I., Getman, K.I. & Podgorsky, V.S. Biological activity of bacterial lectins and their molecular complexes with heterocyclic bis-adducts. *Mikrobiologichnyi Zhurnal*, 2003, V.65(5), p. 20–25.

Source: Author's research.

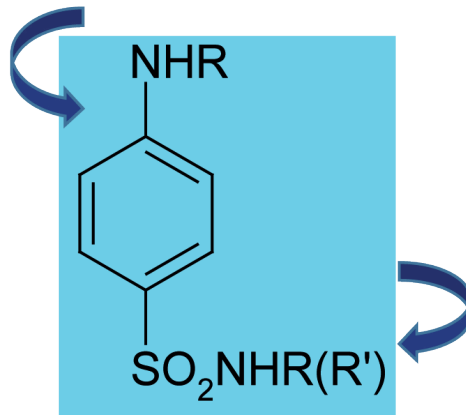


Figure 1. Basic scaffold of the sulfonamide molecule

The next stage is the structural functionalization of derivatives of sulfanilic acid amides by chemical modification in the positions of functional groups in the composition of molecules. Well-known drugs were synthesized in this way: sulfazine, sulfacyl sodium, phthalazole, biseptol and others (fig.2):

Source: Author's research.

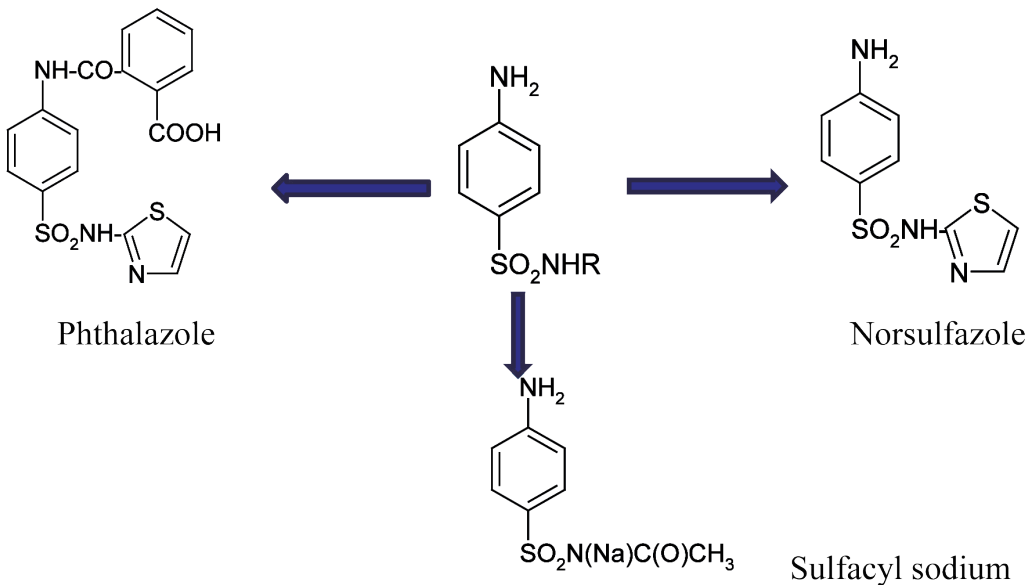


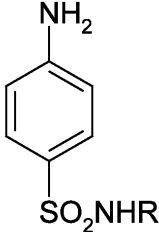
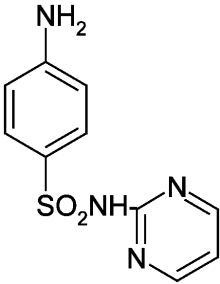
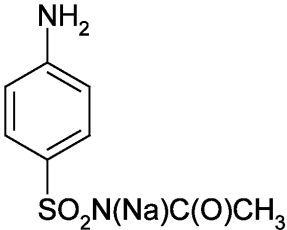
Figure 2. The sulfonamides

Let's consider the features of the chemical structure of sulfanilic acid amide derivatives (tabl.1):

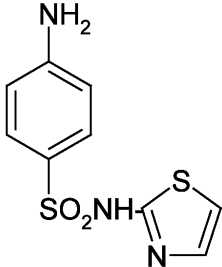
Table 1.

Chemical characteristics of the sulfanilic acid amide derivatives structure

Source: Author's research.

1	2
	<ul style="list-style-type: none"> – amphoteric molecule: the main properties are due to the presence of an aromatic NH_2 group, acidic properties are due to the presence of a hydrogen atom in the sulfamide $-\text{SO}_2\text{NHR}$ group aromatic ring – unsaturated aromatic system three double bonds and a coupled system – Carbon atoms of the aromatic ring in the state of sp^2-hybridization – Nitrogen atom in the amino group has an unshared pair of electrons and participates in conjugation – high stability of «aromaticity» of the cycle, cyclic delocalization energy
 <p>Sulfazine, 2-(<i>p</i>-aminobenzene-sulfamido)-pyrimidine</p>	<ul style="list-style-type: none"> – the presence of a pyrimidine heterocyclic fragment – amphoteric molecule: the main properties are due to the presence of an aromatic NH_2 group, acidic properties are due to the presence of a hydrogen atom in the sulfamide $-\text{SO}_2\text{NHR}$ group aromatic ring – unsaturated aromatic system three double bonds and a coupled system – Carbon atoms of the aromatic ring in the state of sp^2-hybridization – Nitrogen atom in the amino group has an unshared pair of electrons and participates in conjugation – high stability of «aromaticity» of the cycle and delocalization energy
 <p>Sulfacyl sodium, sodium <i>p</i>-aminobenzene-sulfonylacetamide</p>	<ul style="list-style-type: none"> – electronegative aceto-group – amphoteric molecule: the main properties are due to the presence of an aromatic NH_2 group, acidic properties are due to the presence of a hydrogen atom in the sulfamide $-\text{SO}_2\text{NHR}$ group aromatic ring – unsaturated aromatic system three double bonds and a coupled system – Carbon atoms of the aromatic ring in the state of sp^2-hybridization – Nitrogen atom with an unshared pair of electrons and participates in conjugation – high stability of «aromaticity» of the cycle and delocalization energy

Continuation of table 1

1	2
 <p data-bbox="135 555 354 627">Norsulfazol, 2-(<i>p</i>-aminobenzene- sulfamido)-thiazole</p>	<ul style="list-style-type: none"> – the presence of a thiazole heterocyclic ring – amphoteric molecule: the main properties are due to the presence of an aromatic NH₂ group, acidic properties are due to the presence of a hydrogen atom in the sulfamide -SO₂NHR group aromatic ring – unsaturated aromatic system three double bonds and a coupled system – Carbon atoms of the aromatic ring in the state of sp²-hybridization – Nitrogen atom with an unshared pair of electrons and participates in conjugation – high stability of «aromaticity» of the cycle and delocalization energy

Pharmacological properties of Sulfazine: bacteriostatic effect; in infections caused by hemolytic streptococcus, pneumococcus, staphylococcus; with malaria.

Pharmacological properties Sulfacyl sodium: bacteriostatic action; antibacterial agent for ophthalmology, a wide spectrum of action.

Pharmacological properties of Norsulfazol: bacteriostatic action; in infections caused by streptococcus, staphylococcus; with pneumonia and meningitis.

Pharmacological properties of Sulfamethoxazole: bacteriostatic action; chemotherapeutic activity (malarial plasmodium, toxoplasma, staphylococci, streptococci).

Pharmacological properties of Fthalazol: an antibacterial agent, it is a pro-drug of norsulfazol (dysentery, colitis, other acute intestinal diseases).

Toxicological properties of the sulfanilic acid amide derivatives:

From the blood and lymphatic system: leukopenia, hemolytic anemia, thrombocytopenia.

From the cardiovascular system: tachycardia, myocarditis.

From the side of the nervous system: depression, visual disturbances, psychosis, convulsions.

From the respiratory system: pulmonary infiltrates.

From the gastrointestinal tract: increased activity of liver enzymes, cholestatic hepatitis.

Allergic reactions: toxic epidermal necrolysis (Lyell's syndrome), systemic lupus erythematosus, anaphylactic shock, Quincke's edema.

Regularities of structure-activity dependence of sulfonamides:

- the *p*-aminophenyl group is a carrier of antimicrobial properties;

- substitution of hydrogen atoms in the aromatic ring (phenyl radical) - decrease in antimicrobial activity;
- replacement of hydrogen atoms in the $-NH_2$ group by R - disappearance of antimicrobial properties;
- substitution of hydrogen atoms in $-NH_2$ by R – antimicrobial properties do not disappear if R in the body is subject to elimination (hydrolysis) example, Phthalazol (where R is a phthalic residue acids) (fig.3):

Source: Author's research.

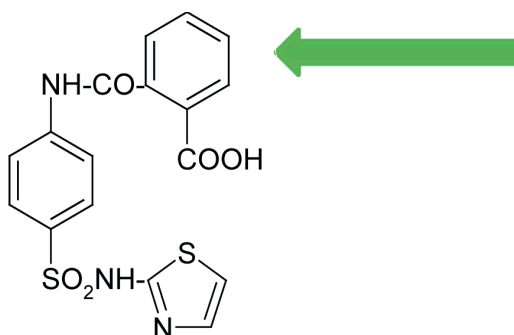


Figure 3. Phthalazol structure.

The level of toxicity increases when present electron acceptor groups, oxygen-containing groups, aromatic radicals (fig.4).

Source: Author's research.

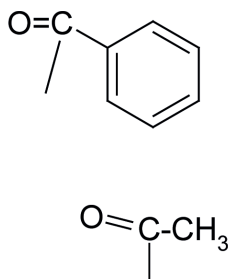


Figure 4. Electron acceptor groups.

Thus, it can be argued that the chemical structure of the molecule is a matrix that ensures the biological activity of the substance. When creating substances with predicted biological activity, we repeatedly used specific synthetic approaches to achieve the set goal of the experiment².

2 Elena Welchinska & Valeriia Vilchynska. New Compound N1, N1'-(2''-Bromo-2''-Chloroethenyl)-Bis-(5-Fluorouracil) As The Active Antitumor Agent For Sarcoma 180. CBU International Conference Proceedings. 2016, V. 4, p.740-743. DOI: <https://doi.org/10.12955/cbup.v4.842>; Welchinska, O.V., Sharikina, N.I., Kovalenko, E.Ö. Finding of anticancer medical drugs by way of creation of new ant metabolites of pyrimidin's change-bis-derivatives of 5 (6)-substituted uraciles and their molecular complexes with bacterial lectines. Naukovy zapyski Ternopolskogo natsionalnogo pedagogichnogo universitetu imeny V. Hnatuka. Seria: biology. 2008, V.1(35), p. 62–68.