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Review Article

A Review Studies of Sulfonamide as Multifunctional Agents from Antibacterial Activity to Anticancer Application

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Abstract: Sulfonamide has medicinal properties and molecular mobility that serve as key synthetic bioactive molecules in pharmaceutical science. Since the discovery of Prontosil in the early 1900s, sulfonamides have been widely studied as antibacterial agents targeting folate biosynthesis. Recent modifications to structures using heterocyclic rings, electron-withdrawing substituents, and hybrid pharmacophores have improved their antibacterial, anticancer, anti-inflammatory, antiviral, and enzyme inhibitory activities. This review covers current breakthroughs in sulfonamide derivative production, biological activity, resistance mechanisms, and therapeutics. Microwave-assisted and green synthesis methods, molecular docking, ADMET prediction, and targeted therapeutics are prioritized. Through suppression of carbonic anhydrases, cyclooxygenases, histone deacetylases, and dihydropteroate synthases, sulfonamide derivatives were effective against multidrug-resistant infections and various human cancer cell lines. Many derivatives have good receptor-binding interactions and pharmacokinetics, according to computational studies. However, bacterial resistance, toxicity, and hypersensitivity responses remain clinical issues, and nanotechnology, AI-assisted drug discovery, and multitarget therapy design which that increase sulfonamide-based treatment selectivity and efficacy.

Keywords: Anticancer activity; Drug resistance; Sulfonamides; Therapeutic applications.

INTRODUCTION

Sulfonamides, among first and most significant synthetic antimicrobials, were essential to contemporary chemotherapy. Sulfonamide-based compounds have been extensively researched since the discovery of Prontosil in the early 20th century due to its broad-spectrum antibacterial efficacy and precise mechanism of blocking folate synthesis in microorganisms. Despite their effectiveness, traditional sulfonamides have been impeded by bacterial resistance, suboptimal physicochemical properties, and adverse effects [1].

To overcome these limitations, significant structural modifications of the sulfonamide scaffold have yielded several derivatives with improved pharmacological properties. The incorporation of heterocyclic systems and electron-donating or electron-withdrawing substituents has significantly enhanced their biological efficacy. Sulfonamide compounds now demonstrate antibacterial, antiviral, anti-inflammatory, carbonic anhydrase inhibitory, diuretic, and anticancer activities [2].

The sulfonamide, as shown in Figure 1, functional group ($-SO_2NH_2$) is a preferred pharmacophore in medicinal chemistry due to its hydrogen bonding capabilities and robust interactions with biological targets. This enables attachment to pathogenic enzymes and receptors, such as carbonic anhydrases and cyclooxygenases, which are associated with cancer [3]. Thus, recent studies have focused on generating new sulfonamide compounds with improved selectivity and efficacy for particular molecular targets. Due to the need for effective anticancer medicines, sulfonamide derivatives are being tested against MCF-7 tumor cells. In reasonable drug design, computations, such as molecular docking and ADMET

prediction, can identify potential compounds with good binding affinities and pharmacokinetics before experimental confirmation [4].

Synthesis, description, and biological function of novel sulfonamide compounds with antibacterial and anticancer activities are presented in this work. In addition, in silico evaluations confirm experimental results and supply mechanistic details about the compounds' interactions with cellular targets.

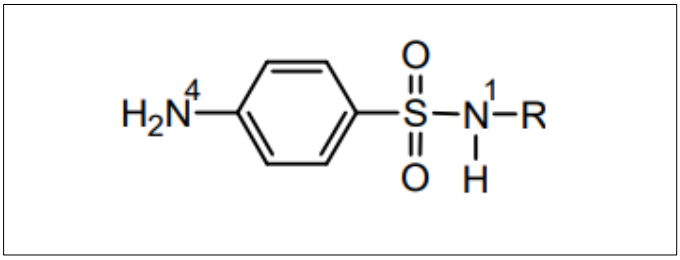


Figure 1: Structure of sulfonamides

This review analyses novel sulfonamide molecule production, biological function, medicinal uses, and molecular concepts. An improved antibacterial, anticancer, anti-inflammatory, and enzyme inhibitory pharmacological molecule is highlighted. Environmental chemistry, microwave-assisted synthesis, molecular docking, ADMET prediction for rational drug design, and new synthetic methods. Toxicity, microbial resistance, and clinical limits are also examined, and targeted treatment, nanotechnology, AI-assisted drug development, and combination therapy are promising with sulfonamide compounds.

History and Epidemiology

In 1939, Gerhard Domagk earned the Nobel Prize for discovering prontosil, demonstrating sulfonamides' relevance in antimicrobial chemotherapy [5]. Penicillin's antibacterial properties were discovered by Alexander Fleming, but mass manufacture wasn't possible until the 1940s. Despite new antibiotic classes, sulfonamides remain effective, particularly in combination regimens like trimethoprim–sulfamethoxazole, which disrupt folate metabolism synergistically to kill bacteria. Since sulfonamides are the most common drug-induced hypersensitivity, their therapeutic usage might generate side effects [6].

Synthetic sulfonamides have a broad spectrum of antibacterial activity, targeting most Gram-positive and Gram-negative pathogens. Sulfonamide, known as Prontosil, as shown in Figure 2, was initially a prodrug. Prontosil experiments started in 1932 at Bayer AG, a division of IG Farben. The Bayer researchers proposed using coal-tar colors that bind to bacteria and parasites to target dangerous organisms in the body. A team led by Gerhard Domagk worked under Farben executive Heinrich Hörlein to find a red dye synthesized by Bayer chemist Josef Klarer that effectively stopped bacterial infections in mice after years of unsuccessful efforts. Bayer had developed Prontosil, the first medication to treat various bacterial infections in the body [7].

It strongly protected against illnesses caused by streptococci, such as blood infections, childbed fever, and erysipelas, with little impact on other cocci illnesses. It had no impact in the test tube but showed antibacterial activity only in real animals. However, Bovet noticed it later [8].

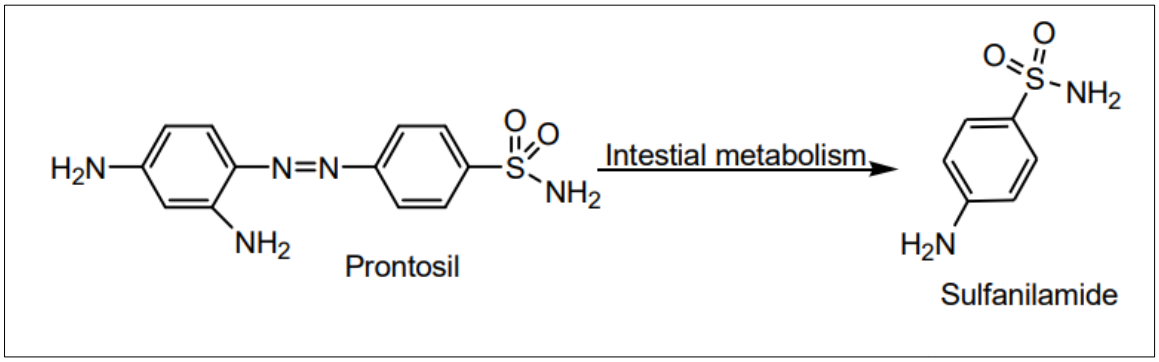


Figure 2: Synthesis of sulphanamide from prontosil [8]

Sulfonamides are formed from sulfonic acid, using sulfonyl chloride as a mediator. Using microwave irradiation, this synthesis is simple and yields high yields with acceptable functional group tolerance [9], as shown in Figure 3.

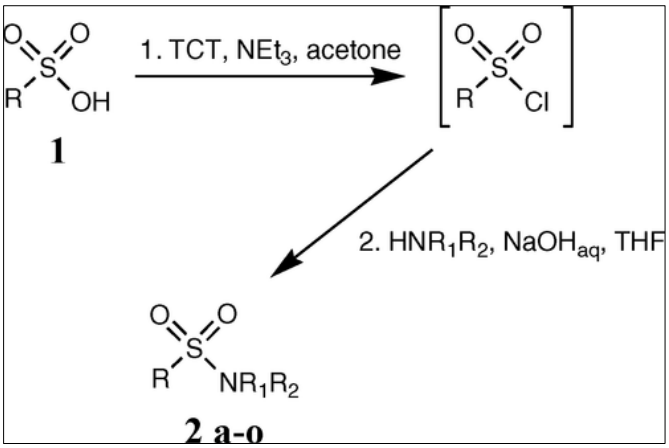
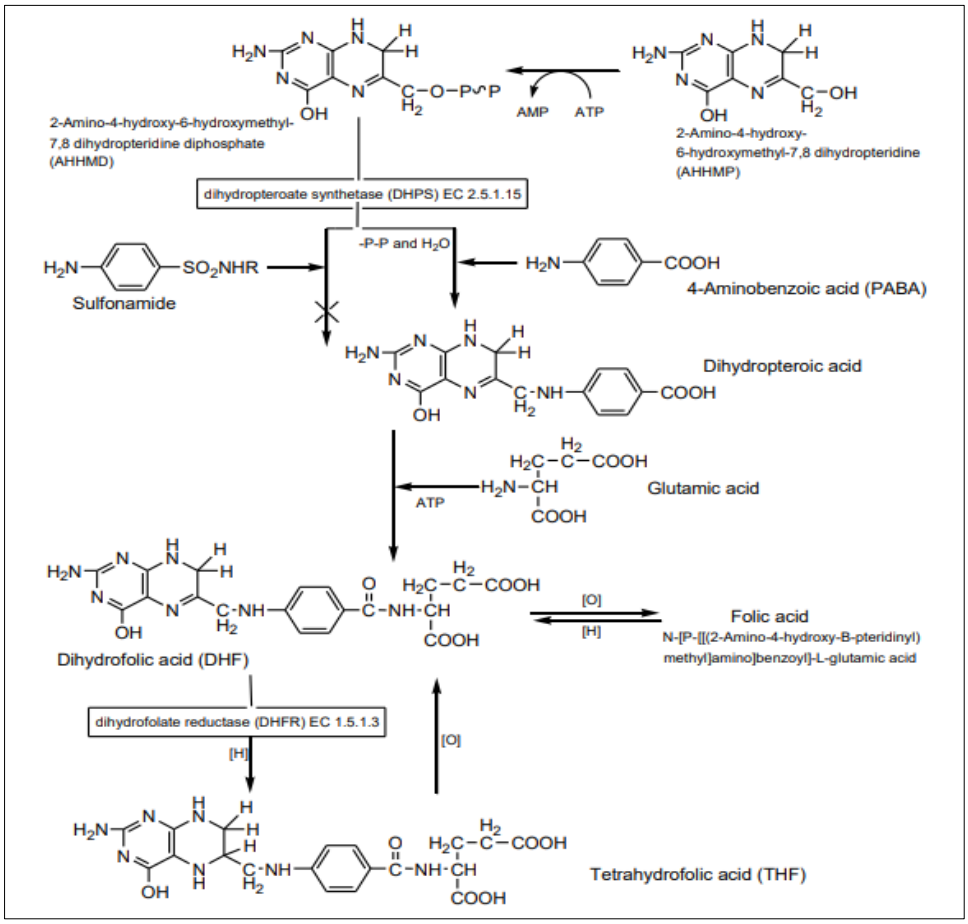


Figure 3: Synthesis of sulfonamides with using microwave irradiation [9]

Action of sulfa drugs

The action of sulfa medicines has been thoroughly investigated and described as follows. Bacteriostatic dosages of sulfonamides are often used to prevent or restrict bacterial proliferation. Sulfonamides block folic acid production in bacteria, resulting in bacteriostatic effects. Bacteria synthesize folic acid using natural compounds and enzymes. Sulfonamides inhibit the enzyme dihydropteroate synthetase, which converts PABA and dihydropteroate diphosphate to folic acid.dihydropteroic acid, folic acid and DNA precursor. In the dihydropteroate synthtase, sulfonamides compete with PABA for the "active site."They are "competitive inhibitors" of this enzyme [10].

Sulfonamides' structural resemblance to PABA fools the enzyme into interacting with the drug instead of the endogenous molecule. Sulfonamide displacement of PABA results in the creation of a "false" metabolite in folic acid synthesis, preventing continuation of the cycle [10].



Scheme 1: Mechanism of sulfonamides action [10]

Green Synthesis of Sulfonamide Compounds

Green synthesis of sulfonamide compounds is ecologically friendly, and traditional synthetic methods use hazardous solvents, dangerous chemicals, and extensive reaction periods, which at first harm the environment. Thus, recently published studies have employed plant extracts, water-based medium, biocatalysts, and solvent-free conditions for eco-friendly methods. Flavonoids and phenolic substances from plants promote catalytic transformations and reaction efficiency. Green synthesis improves product quality, saves energy use, and reduces waste. Due to bioactive natural substances, biologically produced sulfonamide derivatives have better antibacterial and anticancer activities. Green chemistry solutions are promise for sustainable medicinal chemistry and help industrialize safer and more effective sulfonamide-based therapies [11].

Microwave-Assisted Sulfonamide Synthesis

Sulfonamide derivatives produced quickly and efficiently via microwave-assisted synthesis. Instead of heating the reaction mixture, microwave irradiation evenly distributes energy, speeding molecular bonds and enhancing synthesis performance. This method is ecologically friendly since it reduces solvent usage and adverse reactions. Recent studies showed that microwave-assisted processes create sulfonamide compounds in minutes, with high yield and selective [12]. The approach also works with many heterocyclic systems and functional groups, making bioactive chemical production easier. These benefits have made microwave-assisted synthesis popular in pharmaceutical chemistry, especially for the quick manufacture of pharmacological antibacterial, anticancer, and anti-inflammatory sulfonamide derivatives [13].

Targeted and photodynamic therapy

Sulfonamide compounds are gaining popularity in photodynamic and targeted cancer treatment. Sulfonamide-based chemicals photosensitizers or targeting ligands that preferentially accumulate in tumor tissues in photodynamic treatment. Photoactivated reactive oxygen species cause cancer cell oxidative injury and apoptosis. Sulfonamide moieties also preferentially bind hypoxic tumor-overexpressed carbonic anhydrase isoforms, CA IX and CA XII. This selectivity improves medicine delivery to cancerous areas while lowering healthy cell toxicity. Recently, sulfonamides have been coupled with nanoparticles, antibodies, and fluorophores to enhance imaging and therapy. Precision oncology using sulfonamide-mediated specific treatment enhance treatment results for resistant and aggressive malignancies including breast and lung tumors [14].

Sulfonamide Combination Therapy

Sulfonamide derivative combination treatment is beneficial for overcoming microbial resistance and improving anticancer effectiveness. Inhibiting folate metabolism and improving antibacterial action, sulfonamides and trimethoprim are often used together. Recent research have examined co-administration of sulfonamides with anticancer medicines, kinase inhibitors, or metal-based medications to improve selectivity and diminish drug resistance. Drug dosages reduced in combination regimens, reducing side effects and toxicity. Sulfonamide derivatives and chemotherapeutic drugs promote apoptosis and decrease tumor development in cancer treatment. Additionally, nanocarrier systems can deliver sulfonamides and other medications to specified regions. Combination treatment maximizes the therapeutic potential of sulfonamide-based drugs [15].

ADMET/Molecular Docking Studies

Molecular docking and ADMET modeling are crucial to rational sulfonamide compound design, and molecular docking evaluates ligand-receptor interactions and predicts the binding affinity of manufactured molecules to target organisms such as DHPS, CA, COX-2, and HDACs. Many sulfonamide compounds showed significant binding energies via hydrogen bonding, π-π stacking, and hydrophobic interactions in active binding pockets. Electron-withdrawing substituents, heterocyclic systems, and aromatic moieties increased receptor affinity and biological activity. ADMET prediction also helps assess pharmacokinetic features including absorption, distribution, metabolism, excretion, and toxicity. Several prospective sulfonamide compounds followed Lipinski's rule of five and had good bioavailability, moderate lipophilicity, and low toxicity. Thus, molecular docking and ADMET analysis speed drug development and identify safer and more selective sulfonamide-based medicinal medicines [16-18], as shown in Table 1.

Table 1: Molecular Docking and ADMET results of Sulfonamide compounds

Compound Type	Docking Target	Key Molecular Interactions	ADMET Features
Heterocyclic sulfonamides	DHPS	Hydrogen bonding with active site residues	Good oral absorption
Benzene sulfonamides	COX-2	Hydrophobic and π–π interactions	Moderate lipophilicity
Sulfonamide–triazole hybrids	HDAC	Zinc-binding interactions	Acceptable bioavailability
Sulfonamide Schiff bases	Carbonic anhydrase	Hydrogen bonding and electrostatic interactions	Low predicted toxicity
Sulfonamide nanoparticles	Multiple targets	Enhanced cellular uptake	Improved drug delivery

Sulfa drugs as therapeutic agents

Sulfonamides with anti-carbonic anhydrase activity

Sulfonamides block the enzyme carbonic anhydrase (CA), which hydrates carbon dioxide and dehydrates bicarbonate at physiological pH (CO2+H2O→HCO3-+H+). This enzyme is found in red blood cells and kidneys. Bicarbonate production is crucial for carboxylation in metabolic pathways, including gluconeogenesis, lipogenesis, ureagenesis, and the biosynthesis of amino acids and pyrimidines. CA regulates CO2 release by transferring it from tissue to blood and lungs. CA, important for electrolyte secretion and balance, is a common target for inhibitors in illness therapy due to its widespread presence [19].

Since sulfonamides suppress CA, they have been used for over 50 years to treat disorders including heart failure, glaucoma, epilepsy, and even cancer by lowering blood pressure. Acetazolamide, methazolamide, ethoxzolamide, and dichlorophenamide are four sulfonamides used as systemic CA inhibitors since the 1950s (Figure 4). Since the 1990s, dorzolamide and brinzolamide have been introduced as topically active antiglaucoma medications (Fig 4).

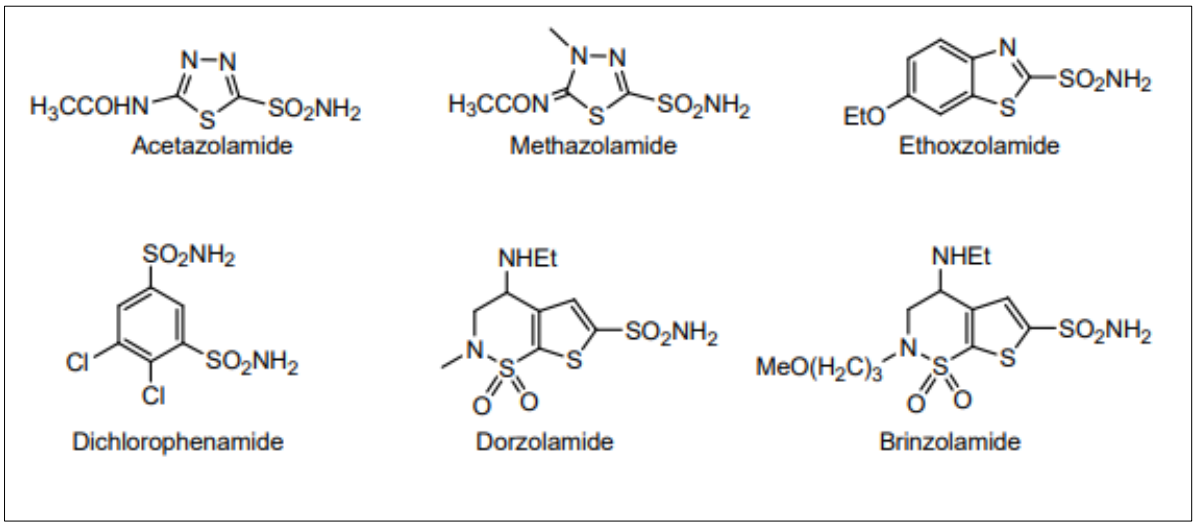


Figure 4: Some important Sulfonamides used as carbonic anhydrase inhibitors [19]

Sulfonamides with anticancer activity

Chloroquinoxaline, a sulfanilamide derivative, is in Phase II clinical studies (Figure5). (Chloroquinoxaline suppressed solid tumor development in breast, lung, ovarian, and skin cancer, with an uncertain method of action that did not influence folate metabolism, in contrast to the typical sulfonamide activity. Lack of progress in phase II clinical trials for nonsmall cell lung cancer led to the suspension of its development as a therapeutic candidate [20].

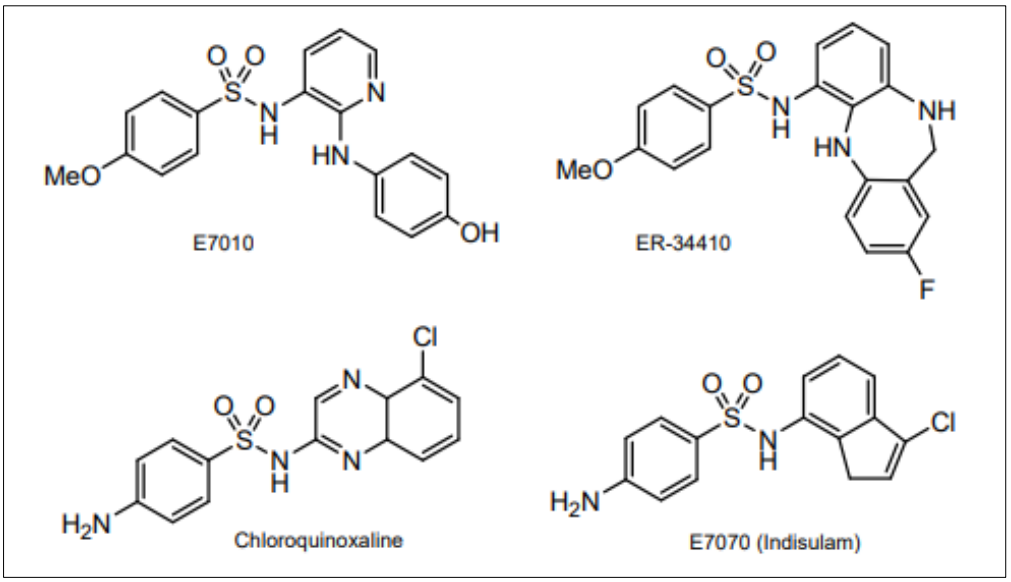


Figure 5: Some important sulfonamides used asanticancer agents [21]

COX inhibition by sulfonamides

Sulfonamides have been routinely used as selective COX-II inhibitors since 1999. Arachidonic acid is converted to prostaglandins by COX enzymes, which alter platelet aggregation, renal function, vasodilation, and pain perception [22].

COX-I and COX-II cause inflammation, but COX-II is the main culprit. Since 1991, COX-II has been inhibited to treat rheumatoid and osteoarthritis pain. Celecoxib and vadecoxibin 2002 are selective aryl sulfonamides. Figure 6. COX-II inhibitors.Both treat pain and inflammation, and as selective COX-II inhibitors, they don't have the side effects of NSAIDs like aspirin [23].

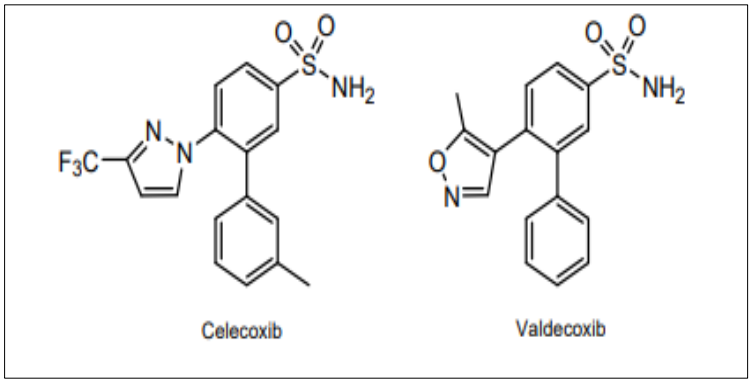


Figure 6: Some important sulfonamides used asCOX inhibitor [23]

Sulfonamide Resistance Mechanisms

Sulfonamide medication resistance is a worldwide health issue that reduces their therapeutic effectiveness, and the binding affinity and inhibitory action of this drug and its compounds are reduced by dihydropteroate synthase (DHPS) enzyme mutations, a major resistance mechanism [24]. Multiple bacterial species have plasmid-mediated resistance genes that encode drug-resistant target enzymes. Efflux pump overexpression reduces intracellular drug concentration by aggressively eliminating sulfonamide molecules from bacterial cells, contributing to resistance. Biofilm development helps multidrug-resistant bacteria like MRSA and Pseudomonas aeruginosa survive and resist antibiotics. Directional DNA transfer and reduced the permeability of membranes enhance bacterial resistance spread. A major difficulty in current medicinal chemistry is developing innovative sulfonamide compounds with increased target selectivity and resistance-overcoming abilities [25].

Sulfonamides as HIV inhibitors

Sulfonamides inhibit HIV proteases. HIV-protease is a homodimer with aspartyl active sites (Asp25 and Asp125) that can break complex bonds like Tyr-Pro and Phe-Pro. There are various HIV protease inhibitors available in clinical usage, commonly combined alongside reverse transcriptase inhibitors for Highly Active Anti-Retroviral Therapy (HAART). Research indicates that nonpeptidic protease inhibitors have greater bioavailability and slower excretion rates than peptide-base inhibitors. Protease inhibitors Amprenavir and Tipranavir are sulfonamide-derived medicines [26].

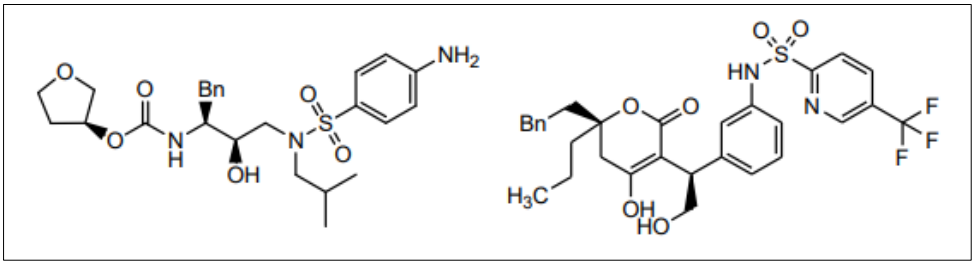


Figure 7: Some important sulfonamides used asHIV inhibitors [26]

Pathogenic bacteria

The pathogenesis of bacterial infection involves the commencement of the infectious process and the processes that cause illness symptoms. The characteristics of pathogen bacteria include transmissibility, adhesion to host cells, and invasion of host cells and tissues. It is toxic and elude the host's immune system.

Many infections caused by pathogen microorganisms are asymptomatic or not visible. Disease arises when microorganisms or their immune responses injure the body [27].

Staphylococcus, a genus of Gram-positive bacteria, forms grape-like clusters with individual cocci dividing in many planes with sizes of 0.5-1.5 µm.These non-motile, nonspore-forming facultative anaerobes have complicated dietary needs for development. A low DNA G+C content, strong salt tolerance, and heat resistance are seen. The most pathogenic S. aureus species Staphylococcus for community-acquired and nosocomic diseases. Healthy persons have asymptomatic colonization of the skin and mucous membranes, particularly the anterior nares. Approximately 20-30% of the population are permanently colonized by the bacteria, whereas the other 30% are transitory carriers. Colonization increases infection risk by providing a reservoir for germs when host defenses are impaired. Due to its role in infections and the rise of antibiotic-resistant strains, S.aureus is the most investigated staphylococcal species [28].

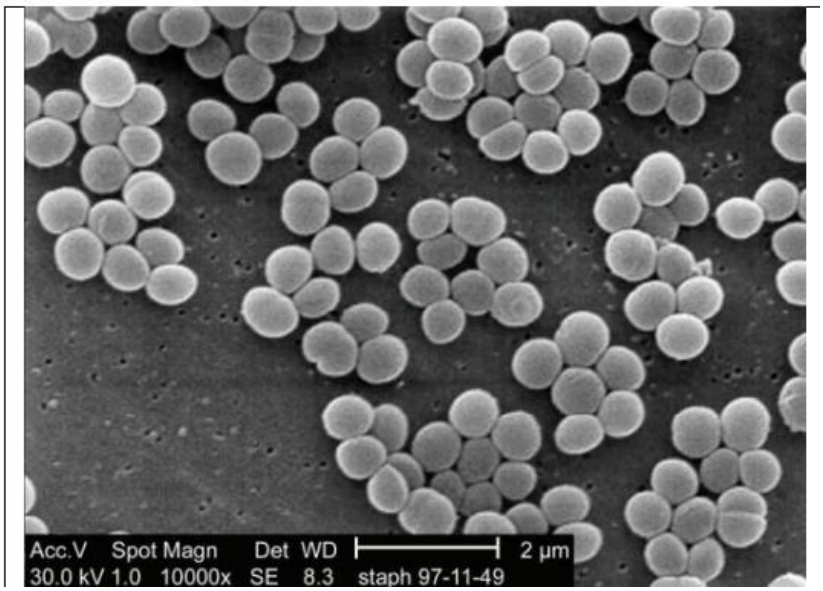


Figure 8: scanning electron microscopy of staphylococcus aureus [28]

The Gram-negative rod Pseudomonas aeruginosa (P.aruginosa) is non-fermentative and aerobic, measuring 0.5 to 0.8 µm by 1.5 to 3.0 µm. Most strains are able to move using a single polar flagellum. This species thrives in damp settings and utilizes various organic molecules for development, enabling it to thrive in nutrient-limited ecological niches, including water, soil, and plant/animal tissues [29].

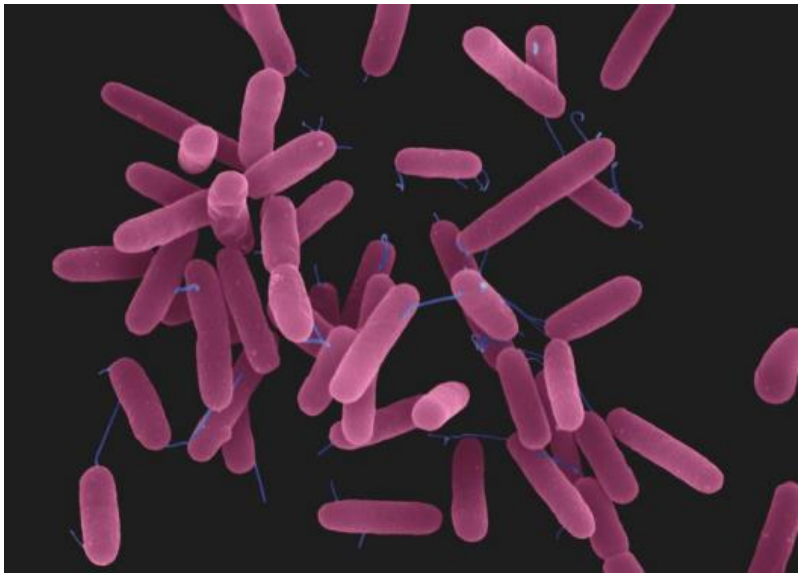


Figure 9: Structure of *Pseudomonas aeruginosa* [29]

Common biochemical characteristics of *P. aeruginosa* isolates include positive oxidase test, growth at 42 °C, arginine and gelatine hydrolysis, and nitrate reduction. *P. aeruginosa* strains produce soluble pigments, *pyoverdin* and *pyocyanin*.

In clinical practice, *Pseudomonas aeruginosa* can cause various infections, including acute septicemia, urinary tract infections, corneal ulceration, endocarditis, and pneumonia, in addition to chronic CF lung infection [30].

Sulfonamide Research Bibliometric Analysis

Bibliometric evaluation quantifies sulfonamide studies and reveals pharmaceutical chemistry trends. Sulfonamide derivative articles increased during the last decade, notably in antibiotic resistance, anticancer treatment, and enzyme inhibition, according to bibliometric research, and China, the US, and India contribute heavily to global research. Most referenced papers concentrate on sulfonamide-based carbonic anhydrase inhibitors, heterocyclic hybrids, and molecular docking; Furthermore, institutional and researcher collaborative networks have grown, boosting medication design innovation. The integration of computational and nanotechnological methodologies into sulfonamide research has led to the rise of keywords such as molecular docking, ADMET, nanoparticles, and targeted therapy. The bibliometric assessment helps identify research gaps and future scientific objectives [31].

Sulfonamide Development Timeline

The development of sulfonamides was a major milestone in pharmaceutical chemistry and antibacterial medicine. The 1930s discovery of Prontosil began the sulfonamide era and delivered the first clinically viable manufactured antibacterial medications. Prior penicillin and other antibiotics, sulfonamides were frequently used to treat bacterial illnesses in the 1940s and 1950s. Later structural alterations produced several compounds with improved pharmacological characteristics and wider medicinal uses. Sulfonamide molecules became diuretics, carbonic anhydrase inhibitors, COX-2 inhibitors, and antidiabetics in subsequent decades. Recent research has concentrated on sulfonamide-based anticancer drugs, molecular targeting, and nanotechnology-assisted delivery. Improved sulfonamide compounds with higher selectivity and therapeutic effectiveness have been discovered faster using computational drug design, molecular docking, and AI [32].

Sulfonamide Therapeutics SWOT Analysis

SWOT analysis helps assess sulfonamide compound medicinal potential, and these compounds inexpensive, biologically active, structurally diverse, and easy to synthesize. Sulfonamide scaffolds are compatible with molecular changes, allowing the synthesis of antibacterial, anticancer, anti-inflammatory, and enzyme inhibitory medicines. Bacterial resistance, hypersensitivity responses, and poor therapeutic selectivity persist. Sulfonamide research opportunities include nanotechnology-based medication delivery, AI-assisted drug development, targeted cancer therapy, and combo treatments. Additionally, molecular docking and ADMET prediction help find safer and more effective options, and multidrug resistance, regulatory issues, and toxicity still hinder clinical translation. Future sulfonamide medication development requires continual optimization and mechanistic studies [32].

Proposed Sulfonamide Activity Mechanism

A hypothesized sulfonamide activity mechanistic model incorporates different biochemical pathways depending on biological target and therapeutic use. In antibacterial therapy, sulfonamides compete with dihydropteroate synthase to inhibit folic acid and DNA synthesis. Sulfonamide compounds activate apoptosis and reduce tumour growth by inhibiting carbonic anhydrases, histone deacetylases, and cyclooxygenases. In molecular docking, hydrogen bonding, hydrophobic interactions, and conductive interactions greatly impact biological receptor binding affinity. Electron-withdrawing substituents increase object selectivity and effectiveness. Sulfonamide compounds may induce oxidative stress, mitochondrial dysfunction, and cancer cell cycle arrest, according to recent studies. Thus, enzyme inhibition, molecular recognition, and intracellular signalling control seem to be sulfonamides' biological effects [33].

Future Perspectives

Study on sulfonamide molecules increases selectivity, drug resistance, and negative effects. Predictive modelling and virtual screening utilising machine learning and artificial intelligence might accelerate sulfonamide medication development. Delivery strategies based on nanotechnology reduce systemic toxicity, increase bioavailability, tailored administration, and therapeutic efficacy Heterocyclic or metal-based hybrid chemicals and drug scaffolds may cure resistant bacteria and aggressive cancers. Despite experimental confirmation, molecular docking, molecular dynamics simulations, and ADMET prediction will uncover exceptionally potent candidates, and personalised medicine and biomarker-guided medications will increase cancer therapeutic selectivity. Integrating computational chemistry, nanomedicine, and molecular biology expands sulfonamide-based therapeutic applications [34].

CONCLUSION

The biological roles and therapeutic applications of sulfonamide molecules make them significant drug chemistry frameworks. Heterocyclic structures, electron-withdrawing substituents, and hybrid molecular frameworks improve antibacterial, anticancer, and enzyme inhibitory actions. New green synthesis and microwave-assisted technologies make structurally diverse sulfonamide compounds with better biological activity quickly and ecologically. To overcome multidrug resistance, novel medications are required, and nanotechnology, customized delivery, AI-assisted drug design,

and combination therapy may improve sulfonamide-based therapies' selectivity and efficacy. Future research should combine computational chemistry, molecular biology, and advanced pharmaceutical manufacturing to enhance medical translation and drug results.

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