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Pyrimidine-Sulphone Ligands (Formation, Characterization, Bio

Evaluation) as **Bio-Compounds**

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Abstract

In view of the great importance of the pyrimidine ring and its entry into many aspects of life, including aspects of medical and vital importance, where it was known to be a part of the synthesis of the amino acid histidine, in addition to its entry into the composition of many treatments such as anti-tumor, inflammatory and anti-fungal. Including that the electronic density of this ring is concentrated in the two sites containing the two nitrogen atoms, and then it becomes clear that when a suitable electrophile is available, it can bind with the imidazole ring in one of the two mentioned sites. It has been customary to prove the structures and specificity of the prepared ligands through chemical automated means to diagnose ligands, and then conduct vital studies for them to evaluate their effectiveness and all ligands are multi dentate. The synthesized ligands are type (Imidazole, pyrimidine, sulphone) that have high effect on DNA of bacteria, we noted that Ligands [6, 4] have high activity towards resistance of bacteria due to their ability to inhibition wall of bacterial cell then kill it for this reasone these ligands have more activity, also these ligands involved sulphone group in its structure.

Keyword: ligand ; pyrimidine; azo; sulpho; derivative; biocompounds; bio evaluation; bacteria.

1. Introduction

The pyrimidine derivatives are colored compounds due to the occurrence of electronic transitions that cause bright colors in their structures, including red, purple, black, orange and blue. It depends on the structures of the derivatives to which this color belongs [1-4]. It has wide uses, as a ligands are used in inorganic chemistry and as a textile dye, whether in industry or the field of Pathological analyzes [5-9] . Micro -organisms are the causes of many diseases, so we find a lot of research in the field of studying the biological activity of compounds [10-15] containing pyrimidine rings on various types of pathogenic bacteria: Spherical and helical. Nowadays there are increasing numbers of infections caused by bacteria that are resistant to most of the antibacterial treatments currently available. In some experiments conducted on mice, results were given that the association of pyrimidine [16-20] with some compounds used as chemotherapy for tumors improves its effectiveness and reduces the spread of the tumor as well as reduces the toxic effects that result from the chemotherapy itself. In reducing the spread of breast cancer in mice., The pyrimidine substitutes have similar efficacy to the pharmaceutical-pharmaceutical compounds [21-27] used in the treatment of ulcers and infections, nerve paralysis, ulcers, and they are also used as lipid oxidation inhibitors in experiments conducted on rats. The pyrimidine substitutes are effective in the industrial field [28-32]. Pyrimidine derivatives have been used in the manufacture of dyes for fabrics that contain nylon to give colors [33-37] between yellow and coffee.

EXPERIMENTAL PART:

The pyrimidine derivatives that contain the sulfone or sulfur group in their composition have high biological activity, high absorption in the body, and low toxicity, so they are widely used in the pharmaceutical industry, so they are characterized by being highly sensitive, so high purity materials were

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used to prepare them. Spectrophotometers with extremely high accuracy for its diagnosis and measurement from the University of Isfahan in the Chemical Research Center.

Production of Pyrimidine-Anile Ligand {1}:

2-methyl-4-formal mercaptophenyl (0.01 mole) condensed with aminopyrimidine (0.01 mole) in occurrence of acid-drops in refluxing step (2 hrs), then separation ,desiccating ,manifestation with absolute ethanol to Pyrimidine- Anile Ligand {1} appreciative to studies [4,6] .This reaction carried out via folloeing imination reaction of (Hugo-Schiff) that accurs between carbonyl of aldehyde and aromatic amine.

Production of Pyrimidine-Imidazole Ligand {2}:

Pyrimidine- Anile Ligand {1}(0.01 mole) condensed with amino acetic acid (0.01 mole) in occurrence of benzene as a solvent in refluxing step (5 hrs), then separation ,desiccating ,manifestation with absolute ethanol to Pyrimidine- Imidazole Ligand {2} appreciative to studies[4,6] .By following Ring clousure reaction with compound involving di terminal (neucleophile and electrophile) in condensation step to yiels cyclic compound.

Production of Pyrimidine-Imidazole Sulfide Ligand {3}:

Pyrimidine- Imidazole Ligand {2} (0.01 mole) condensed with p-nitro benzoyl chloride (0.01 mole) in occurrence of potassium carbonate in refluxing step (3 hrs), then separation ,desiccating ,manifestation with absolute ethanol to Pyrimidine-Imidazole Sulfide Ligand {3} appreciative to studies [4,6]

Production of Pyrimidine-Imidazole Sulfide Ligand {4}:

Pyrimidine- Imidazole Ligand {2} (0.01 mole) condensed with p-chloro ethylbenzoate (0.01 mole) in occurrence of acetone as a solvent (more favorable in this step) in refluxing step (2 hrs), then separation ,desiccating ,manifestation with absolute ethanol to Pyrimidine- Imidazole Sulfide Ligand {4} appreciative to studies [4, 6].

Production of Pyrimidine-Imine Ligand {5} :

4-Formal benzaldehyde (0.01 mole) condensed with aminopyrimidine (0.02 mole) in occurrence of acid-drops in refluxing step (2 hrs), then separation ,desiccating ,manifestation with absolute ethanol to

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Pyrimidine-Imine Ligand {5} appreciative to studies [4, 6].

Production of Pyrimidine-Sulphone Ligand {6}:

Pyrimidine-Imine Ligand {5} (0.01 mole) condensed with p-toluine sulphonyl chloride (0.02 mole) in occurrence of benzene as a splvent in refluxing step (2 hrs), then separation ,desiccating ,manifestation with absolute ethanol to Pyrimidine-Imidazole Sulphone Ligand {6} appreciative to studies[4,6] .

RESULTS AND DISCUSSION:

The multi-biological activity of these compounds prompted us to prepare new derivatives of them and encouraged us to do so because their derivatives have benign effects. All the prepared compounds have pharmacological qualities, that is, they have biological activity, and accordingly, the opinion settled on the preparation of derivative compounds, some of which are cyclic and others are noncyclic. Based on the foregoing, the organic compounds prepared in this study were diagnosed using wellknown diagnostic methods, including:

Ultraviolet-Visible Spectroscopy:

The prepared ligands were distinguished by their bright colors because they absorb light in the visible region of the spectrum, as they are accompanied by other absorptions [38-42] in the near regions of both the infrared and ultraviolet-visible region, which is a result of the magnetic and color properties of those ligands containing color-deep groups that increase the wavelength of the ligands.



Configuration.1:U V.Vis Pyrimidine Ligands{1-6}

FT.IR- Revealing:

The bands in the spectra of the ligands suffered from the difference in the intensity of the bands compared to the bands of the ligands [43-47], as well as the occurrence of varying displacements for most of these bands., We noted appearance bands at [(2410) (2398)]cm⁻¹ for (SH-) thiol group in Ligands {1,2} respectively, while it disappeared in Ligands {3,4} as a result to formation (S-CO-) groups, also new bands represented by [(3289) (3241)] cm⁻¹ for (NH-) amine group for endocylce -imidazole ring in Ligands {3, 4}., But in ligand {5} appeared band at (1619) cm-1 for (CH=N-) anile group that disappeared in ligand {6} as a result to formation Sulphone group [48-52] (-SO₂-) at (1205) cm⁻¹ ,also other band at (1688) for carbonyl of amide (CO-N), new band [53-57] at (1652) for (C=N) endocycle of pyrimide ring in most of ligands, all spectral revealing approving to investigation reference [14], some of spectra:



Configuration.2: I.R Pyrimidine Ligand {3}



Configuration.2: I.R Pyrimidine Ligand {6}

Mass - Revealing:

The illuminating of pyrimidine Ligands subsidized another indication of prepared ligands {1-6} that acted by fractions of practical groups [58-61] in matching molecular weight that pointed to structure of measured ligands in mass- figures which idicated to improving structures of prepared ligands., all spectral revealing approving to investigation reference [14], some figures(4, 5):



Configuration.4 : Mass –Spect. of Pyrimidine Ligand{2}

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Configuration.5: Mass-Spect. of Pyrimidine Ligand {6}



Photo.1: Inhibition of Ligands on Streptococcus Pneumonia

Bio- Studies [3, 5]

In previous studies, some researchers have used several biological studies in the treatment of types of cancer (leukemia, lung, colon, skin, ovary, kidney and central nervous system cancer), as well as the use of pyrimidine derivatives as anti-bacterial and antifungal agents, so we completed this study with tests for the efficiency of prepared derivatives against microbes [4, 5]. These germs were chosen because of their importance in the medical field, as they cause many different diseases, as well as differ in the nature of their resistance to antibiotics and therapeutic chemicals [62-66]. The results in the table indicate that all the tested compounds have the ability to inhibit the bacteria used, and it was noted that with the increase in the concentration of the substance, the diameter of the area free of bacterial growth increased., we noted that Ligand [6,4] have high activity towards resistance of bacteria due to their ability to inhibition wall of bacterial cell then kill it for this reason these ligands have more activity, also these ligands involved sulphone group in its structure.



Photo. 2: Inhibition of Ligands on Escherichia. Coli

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Table 1

Influence of resistance of Pyrimidine Ligands against Bacteria in Conc. (60 micro gram)

Pyrimidine	Staphylococcus	Streptococcus pneumonia	Escherichia. Coli
Ligands	aureus		
Pyrimidine {1}	+	++	+
Pyrimidine {2}	++	++	++
Pyrimidine {3}	++	++	++
Pyrimidine {4}	+++	+++	+++
Pyrimidine {5}	++	+	++
Pyrimidine {6}	+++	+++	+++

(+): inhibition (2-6) mm

(++): inhibition (7-10) mm

(+++) : inhibition (11-16) mm



Configuration.6: Production of Pyrimidine Ligands {1-6}

Conclusions:

The bands in the spectra of the ligands suffered from the difference in the intensity of the bands compared to the bands of the ligands, as well as the occurrence of varying displacements for most of these bands., Also the results indicated that Ligand [6,4] have high activity towards resistance of bacteria due to their ability to inhibition wall of bacterial cell then kill it for this reasone these ligands have more activity, also these ligands involved sulphone group in its structure

Conflict of interest: The authors declare that there is no conflict of interest.

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