IJPPR
INTERNATIONAL JOURNAL OF PHARMACY & PHARMACEUTICAL RESEARCH
An official Publication of Human Journals
ISSN 2349-7203
HUMAN

Human Journals
Review Article
June 2021 Vol.:21, Issue:3

Benzoxazole as Anticancer Agent: A Review

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HUMAN

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Submitted: 22 May 2021
Accepted: 29 May 2021
Published: 30 June 2021

Keywords: Cancer, Benzoxazole, Anticancer Agents

ABSTRACT

Despite tremendous efforts in the quest for successful anticancer drugs, cancer remains one of the leading causes of death in the world, with a long-term prognosis that is still unfavourable. New generations of Benzoxazoles with altered structure and biological profiles were found to be more potent and have higher biological activity. In light of all of this, we have put together this analysis.

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1. INTRODUCTION:

Cancer is a dynamic illness in which a large number of factors communicate over a wide range of spatial and temporal scales, resulting in massive datasets related to the various scales.[1] Cancer is the leading cause of death on the planet. Unfortunately, at the tissue level, it is a variety of illnesses, and this variety is a significant obstacle for its specific diagnosis, followed by treatment efficacy. Cancer, in general, disrupts cellular relationships and causes vital gene dysfunction. The cell cycle is disrupted, which results in abnormal proliferation.

In a recent study, it was discovered that good knowledge sharing increases patients' autonomy and participation in their treatment, reduces psychological distress, promotes improved adherence, and instill seasonable expectations. As a result, knowledge pro- vision is an important part of cancer care, serving not only ethical imperatives but also improving cancer care and treatment.[2]

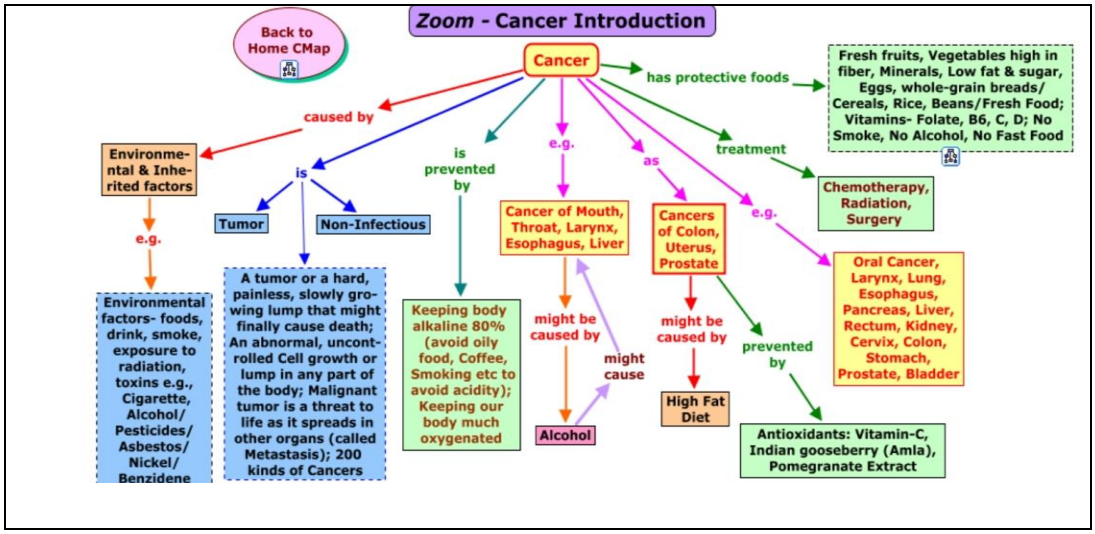


Figure no.1 Introduction of cancer

2. SIGN AND SYMPTOMS:

Cancer symptoms and signs vary depending on the form and grade of cancer; however, although general signs and symptoms are not very clear, patients with various cancers can experience the following: Fatigue, weight loss, nausea, skin changes, bowel or bladder function changes, irregular bleeding, constant cough or voice change, fever, lumps, or tissue masses. Most cancers are symptomatic until they are diagnosed, but the importance of lower-risk signs and clinical findings that may be seen in general practice is unknown. [3]

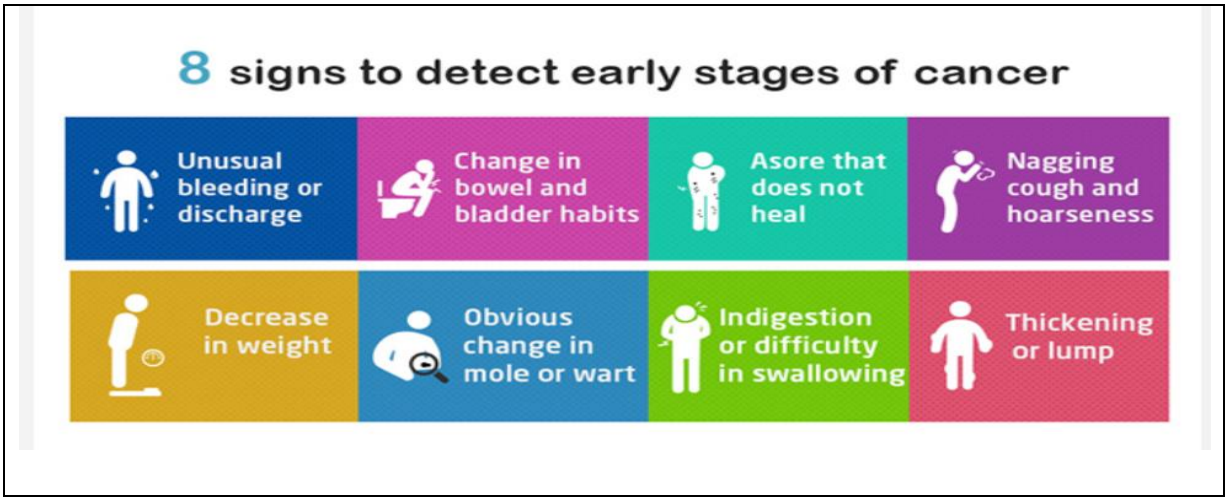


Figure No. 3: Stages of cancer

3. CAUSES OF CANCER:

There are several factors that can trigger cancer in various body sections, including tobacco usage (22% of deaths), poor diet (10% of deaths), obesity (10% of deaths), lack of physical activity (10% of deaths), excessive alcohol intake (10% of deaths), and other factors such as ionizing radiation, environmental contaminants, and infection. Cancer is caused by the interaction between genetic factors and 3 categories of agents which we consume externally including:

3.1 Physical Carcinogens: Ionizing radiation such as radon, ultraviolet rays from sunlight, uranium, radiation from alpha, gamma, beta, and X-ray-emitting sources.

3.2 Chemical Carcinogens: Compounds like n-nitrosamines, asbestos, cadmium, benzene, vinyl chloride, nickel, and benzidine and contains about 60 known potent cancer-causing toxins or chemicals in cigarette smoking or tobacco consumption, a drinking water contaminant (arsenic), a food contaminant (aflatoxin).

3.3 Biological Carcinogens: Infections from certain bacteria, viruses, or parasites and Pathogens like human papillomavirus (HPV), EBV or Epstein-Barr virus, hepatitis B and C, Kaposi's sarcoma-associated herpes virus (KSHV), Markel cell polyomavirus, Schistosoma spp., and *Helicobacter pylori*. Aging is also the cause of cancer. Age is the common incidence of cancer, which dramatically rises.

3.4 Genetics: Genetic is the commonest cause for cancer or tumor-like Ovarian, breast, prostate, skin cancer, and colorectal cancer. Individuals that eat heaps of cooked meat can

also increase risk because of compounds fashioned at high temperatures. Proving that a substance doesn't cause or isn't associated with hyperbolic cancer risk is tough. When new epidemiological studies allowed improvements over original Comparative Risk Assessment project analyses for example, relative risks for site-specific cancers as a result of smoking with better adjustment for possible confounders and new exposure data sources for overweight and obesity new exposure data and epidemiological evidence on disease outcomes and relative risks were used.

4. MECHANISM OF SPREAD OF CANCER:

Malignant tumors capacity to metastasize is primarily responsible for their lethality. Despite the development of improved local treatments such as surgery and radiotherapy, as well as systemic chemotherapy, the clinical problem in oncology remains the prevention of metastatic spread.

The ability of malignant tumors to metastasis largely is responsible for their lethality. Thus, despite the advent of better local treatment in the form of surgery and radiotherapy and systemic chemotherapy, the clinical challenge in oncology remains that of combating metastatic spread. Any cells from primary cancer must break apart, migrate to another part of the body, and begin developing there in order to spread. Cancer cells do not adhere to each other as well as healthy cells. They can also create chemicals that encourage them to move about. The diagram below shows a tumor in the cells lining a body structure such as the bowel wall. The tumor grows through the layer holding the cells in place (the basement membrane).

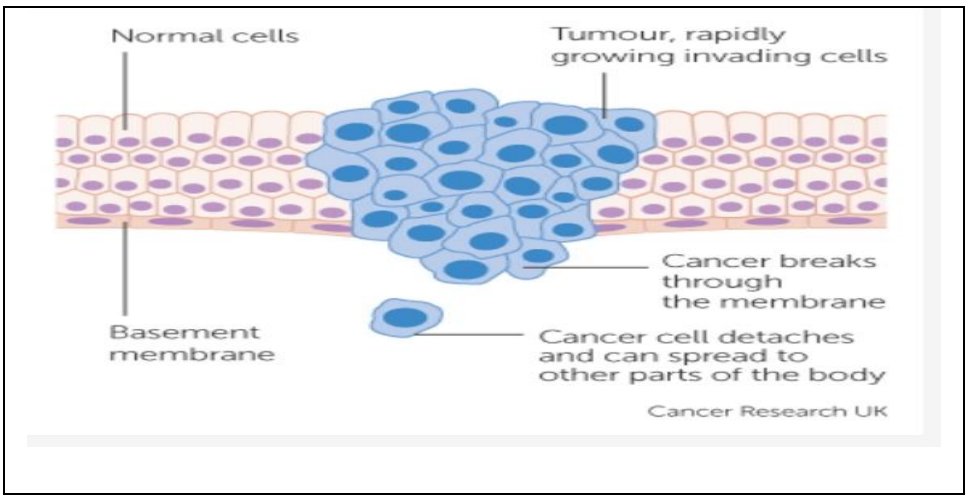


Figure no. 4: Spread of cancer

5 PATHOGENESIS OF TUMOR:

Nests of neoplastic cells in a connective tissue matrix are a common sight in invasive carcinoma. The number of aggregates of carcinoma cells seen as the tumor expands and covers greater areas of tissue increases.[7] here are a variety of mechanisms that can lead to a malignant phenotype in a single cell, but they all require several genetic and epigenetic change tumor development occurs when cells with a neoplastic phenotype gain additional characteristics that contribute to malignancy and metastasis. Tumor development begins clonally with a single neoplastically transformed cell, and the incipient tumor grows by clonal expansion of that cell. [8]

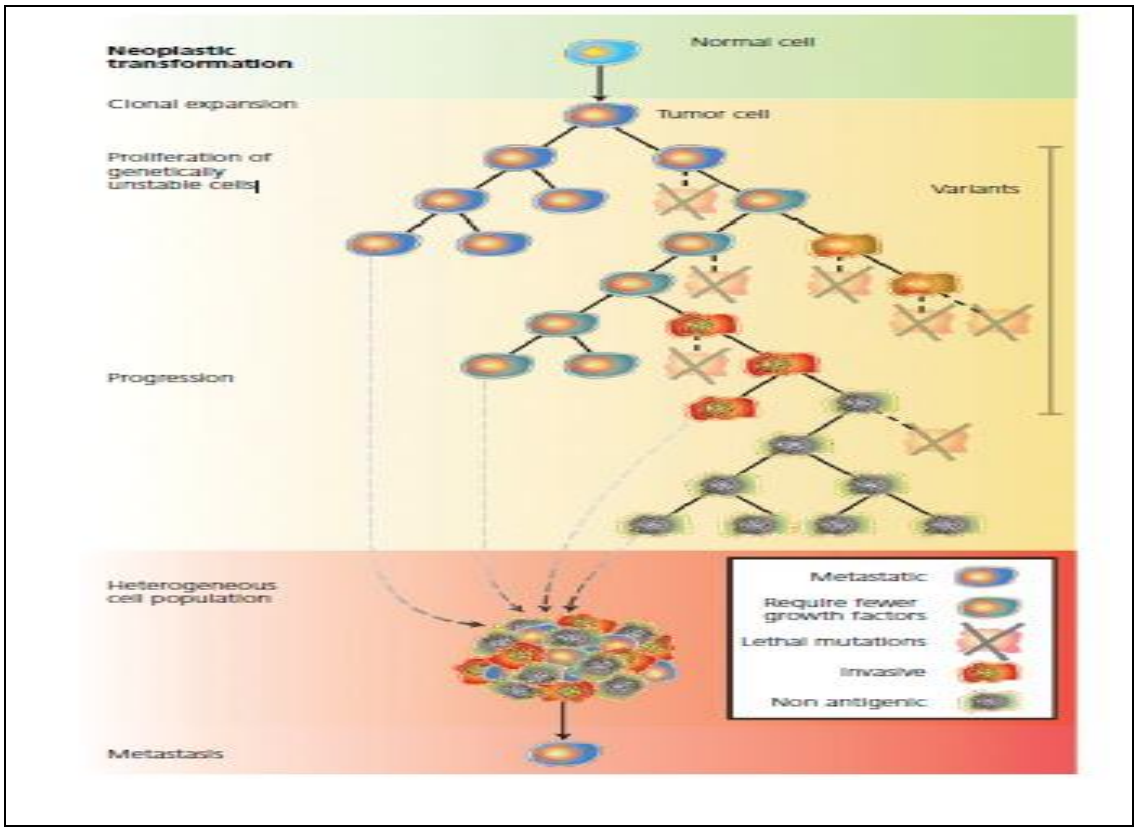


Figure no. 5: Tumor cell heterogeneity.

The disruption to the genetic apparatus of cells is the pathogenesis of cancer (mutation, disturbance of gene expression, activation of tumor promoter gene, inactivation of tumor suppressor genes, etc.). Based on this, the only pathogenesis cancer therapy is the application of methods of cancer gene therapy (RNA approaches, drug resistance, hematopoietic progenitor cell gene transfer, cancer stem cells, homologous recombination, ribosome technology, antisense technology, tumor suppressors, gene delivery systems—viral and non-

viral, anti-gene therapy—antisense, RNA &ribosome's; apoptosis, DNA synthesis and repair), aimed to eliminating the genetic damage and control over cancer cells. However, the methods of cancer gene therapy are only being developed and their use in clinical practice is the matter of the future.[9]

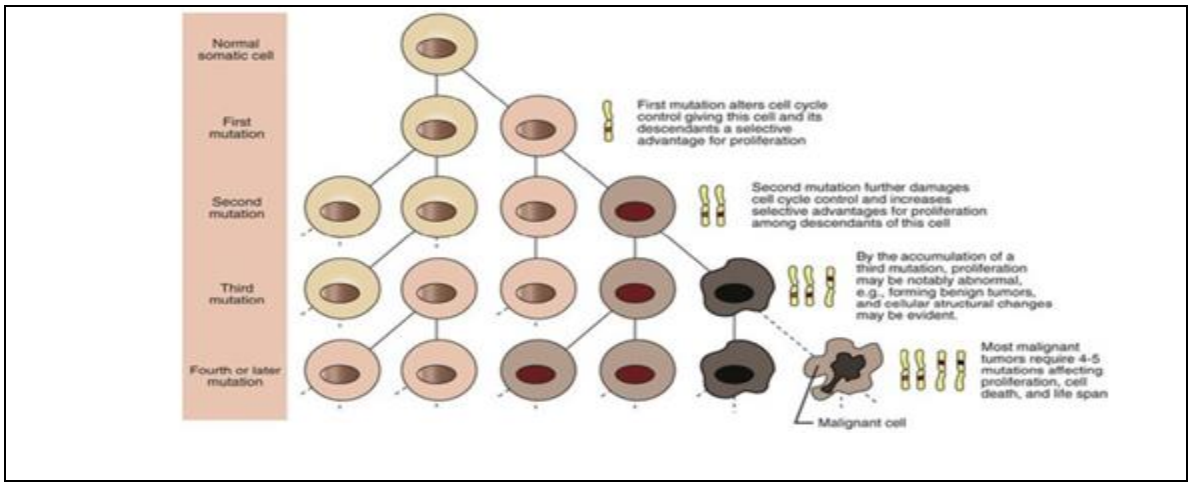


Figure no. 6: **Clonal Basis of Cancer**

6 DIAGNOSIS OF CANCER:

6.1 Chemotherapy uses drugs that target rapidly dividing cells to kill cancerous cells. The drugs can also help reduce tumors, but they can have serious side effects.

6.2 Hormone therapy entails taking drugs that alter the way those hormones function or prevent the body from producing them. This is a comma-separated list of cancers in which hormones play a major role, such as prostate and breast cancers.

6.3 Chemotherapy aims to kill cancerous cells with medications that target rapidly dividing cells. The drugs can also help shrink tumors, but the side effects can be severe.

6.4 Hormone therapy involves taking medications that change how certain hormones work or interfere with the body's ability to produce them. When hormones play a significant role, as with prostate and breast cancers, this is a common approach.

6.5 Immunotherapy is a form of treatment that boosts the immune system and encourages it to battle cancerous cells by using drugs and other treatments. Checkpoint inhibitors and adoptive cell transfer are two examples of these therapies.

6.6 Precision medicine, also known as personalised medicine, is a relatively recent concept. It entails using genetic testing to decide the best therapies for a person's specific case of cancer. Researchers have yet to show that it can effectively treat all types of cancer. (10)

6.7 Radiation therapy kills cancerous cells by exposing them to heavy doses of radiation. A doctor may also suggest that radiation be used to shrink a tumor before surgery or to alleviate tumor-related symptoms.

Affinity for malignant tissue has recently been discovered in many radiopharmaceuticals. Both radiopharmaceuticals that are used to find tumors Nonspecific is currently in use and can be detected by benign tumors and infectious processes, such as abscess and granuloma. The sensitivity of the tumor-imaging technique is determined by the radiopharmaceutical used, the type of tumor, and the size of the tumor.[11]

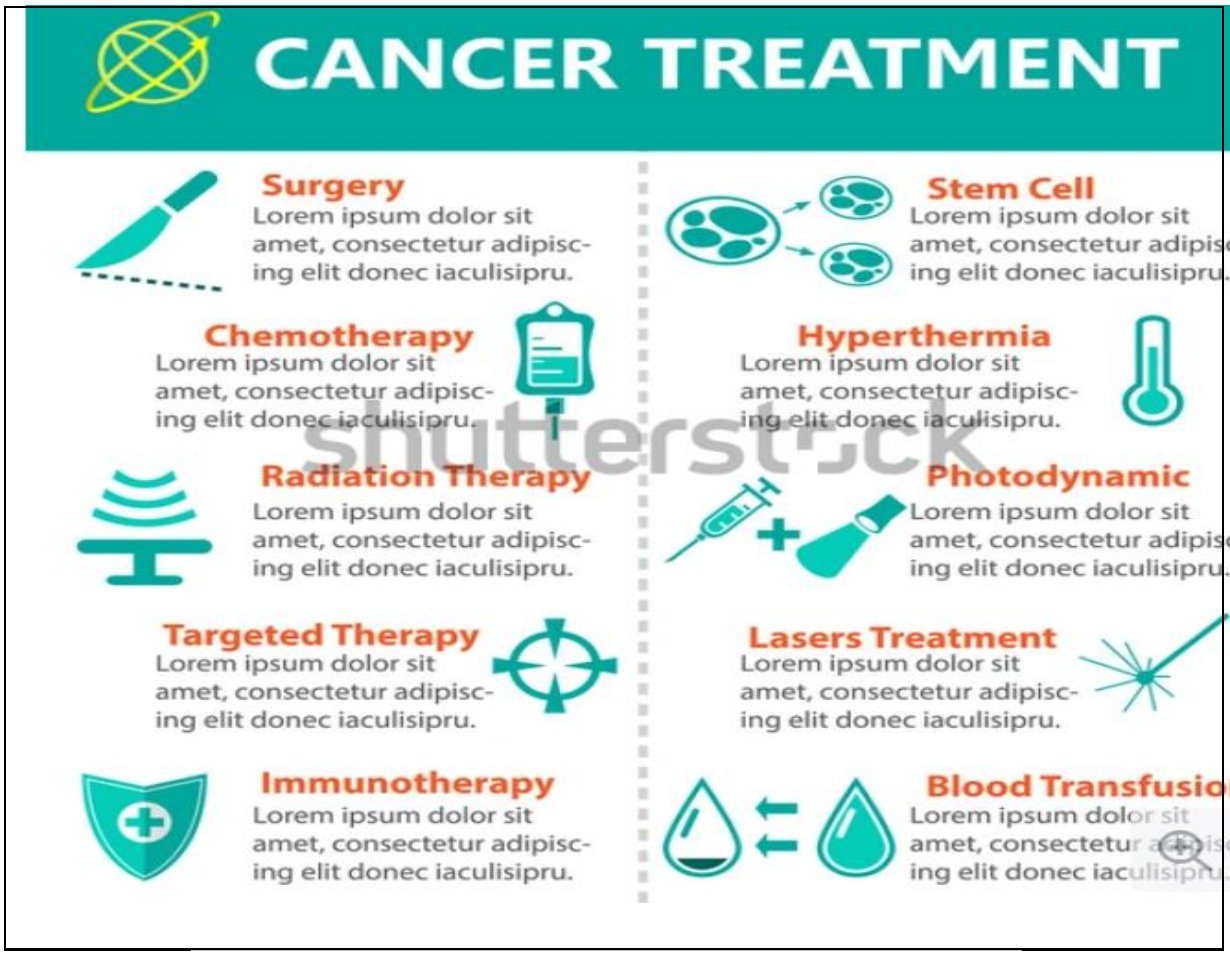


Figure no. 7: Treatment of cancer

7 CANCER WORLDWIDE:

Cancer is the world's second leading cause of death. Overall, cancer has become more common; in the United States alone, nearly 1,665,540 people were diagnosed with cancer in 2014, with 585,720 of them dying as a result of the disease. As a result, cancer is a significant issue that has an impact on the welfare of all human communities. Unfortunately, at the tissue level, it is a variety of illness, and this variety is a significant obstacle for its specific diagnosis, followed by treatment efficacy The prostate, lung and bronchus, colon and rectum, and urinary bladder all have the highest percentages of cancer forms in men. Prostate, lung and bronchus, colon and rectum, and urinary bladder cancers account for the highest concentrations of cancer forms in men. Breast cancer, lung and bronchus cancer, colon and rectum cancer, uterine corpus cancer, and thyroid cancer are the most common cancers in women. According to the data, prostate and breast cancer account for a significant portion of cancer in men and women, respectively Blood cancer, as well as cancers of the brain and lymph nodes, account for the highest number of cancer cases in children. [12]

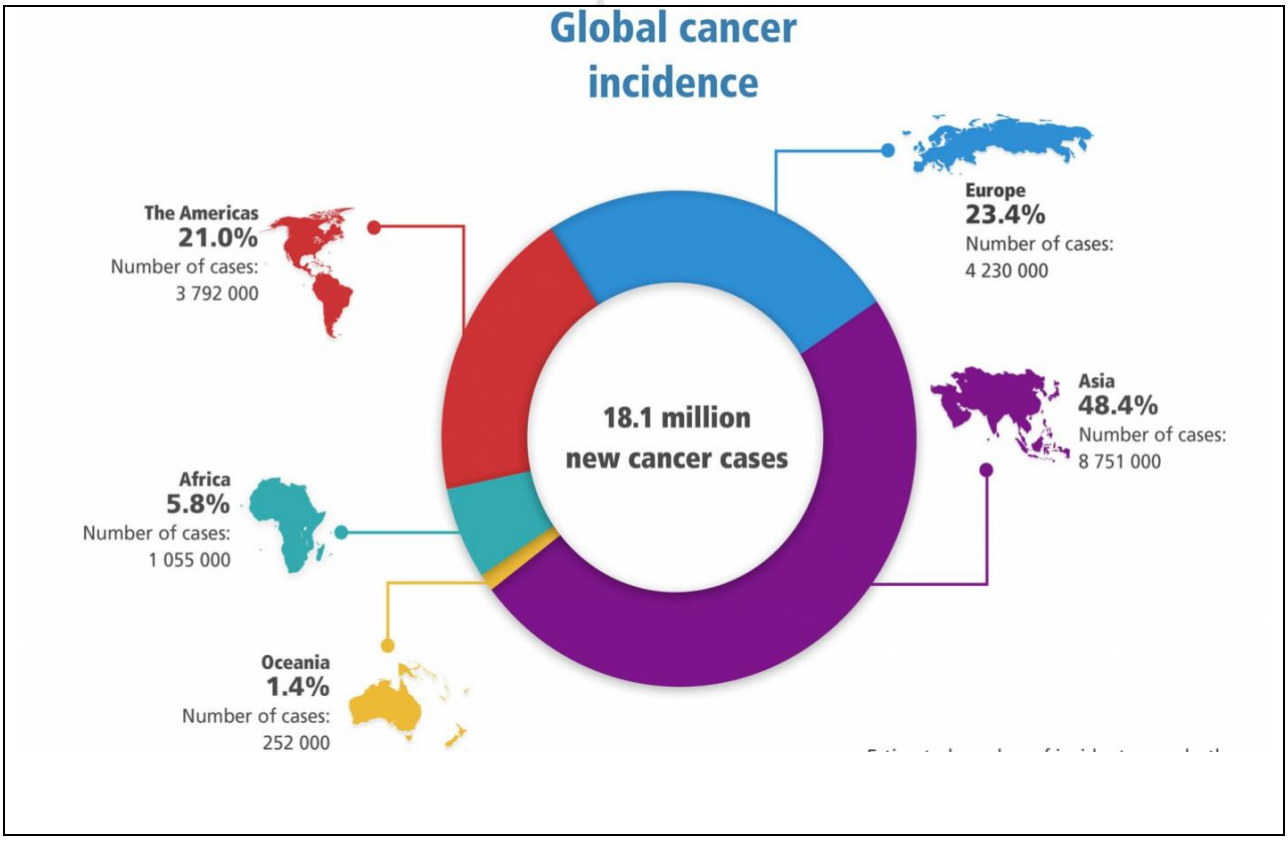


Figure no. 8: Global cancer incidence

8 LIFE CYCLE OF CANCER:

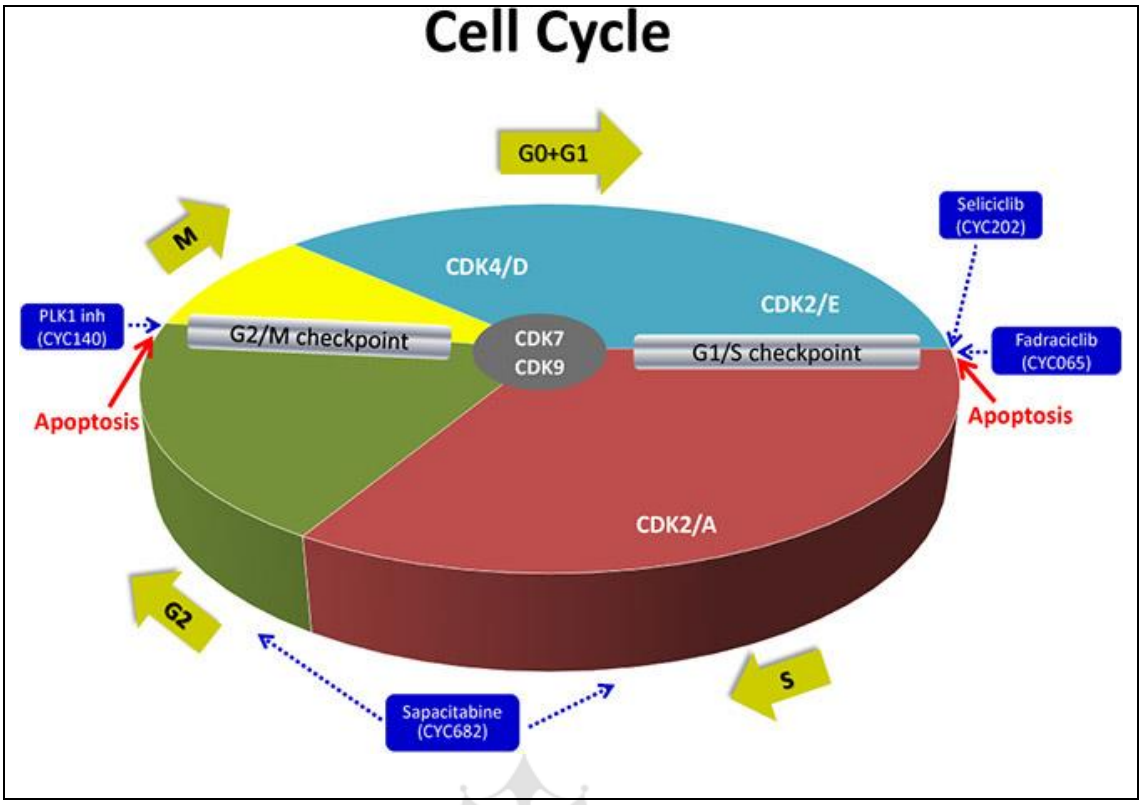


Figure no. 9: Cancer Cell Cycle

Cancer is caused by the cell cycle, which is the mechanism by which cells progress and divide. The cell cycle, which governs how a cell grows, replicates its DNA, and divides in normal cells, is governed by a complex network of signalling Pathways. This procedure also requires mechanisms to ensure that mistakes are corrected and that if they are not, the cells will commit suicide (apoptosis). As a result of genetic mutations, cancer develops this regulatory process malfunctions, resulting in uncontrolled cell proliferation. Abnormal cell cycle activity is a hallmark of cancer. Mutations in upstream signalling pathways or genetic lesions within genes encoding cell cycle proteins may cause this [13]. Checkpoint control is a more supervisory method of cell cycle regulation. It isn't a necessary component of the cycle progression system. Cell cycle checkpoints sense flaws in critical events such as DNA replication and chromosome segregation. [14]

8.1 The Cell Cycle Biology:

Cell division is triggered by a complex network of molecular and biochemical signals. The cell division mechanism, also known as mitosis, has four stages:

1. The G1 or gap period, during which the cell develops and prepares to synthesize DNA;

2. The S, or synthesis, phase, during which the cell synthesizes DNA;

3. The G2 (second gap) phase, during which the cell prepares to divide; and

4. The M (mitosis) phase, during which the cell divides.

9 BENZOXAZOLE:

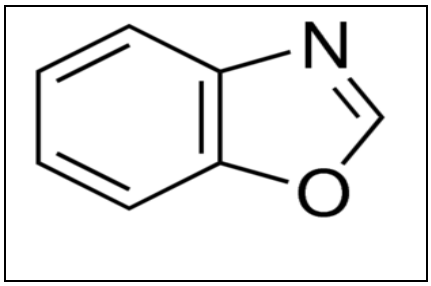


Figure No. 10: Structure of benzoxazole

The central structure of most biologically active compounds is made up of a sequence of benzoxazole and heterocyclic derivatives bearing nitrogen, oxygen, and oxazole moieties. [15]Benzoxazoles have been shown to have a wide range of biological effects[16] .A series of benzoxazole and derivatives of heterocyclic bearing nitrogen, oxygen and oxazole moieties constitutes the core structure of a several biological active compounds. Benzoxazoles have been reported to show a broad spectrum of biological activities. Recent observations suggest that substituted benzoxazoles and related heterocycles possess potential activity with lower toxicities in the chemotherapeutic approach in man. Careful literature survey revealed that targets containing benzoxazole moiety, either isolated from plants or accessed by total synthesis, have remarkable biological activities.[17]antiviral, antimicrobial, antibacterial, antifungal, anticancer, antidepressant, and anti-inflammatory properties.[18]

It was tested on human A-549 lung carcinoma cells with benzoxazole bound to piperazine derivatives. The preliminary findings were unsatisfactory, and the results were poor due to the aryl piperazine compounds' low solubility. Benzoxazoles in combination with oxadiazoles have been shown to have anticancer properties.[19]The cytotoxic effects of the synthesized benzoxazole compounds were tested on four human cancer cell lines. Natural products containing benzoxazoles [20] were tested against the lung cancer cell line A549 and the breast cancer cell line MCF-7 [21]. The chemical, agrochemical dye-stuff, polymer, and pharmaceutical industries all depend heavily onBenzoxazole [22]In continuation of such

investigations and in a search for less toxic and pharmacologically more potential Benzoxazole derivatives. [23]

9.1 Chemistry of Benzoxazole:

Benzoxazole is an aromatic molecule with a planar structure,[19] the organic compound benzoxazole has a benzene ring fused to an oxazole ring. Oxazole (2) is a five-membered azole with an oxygen atom and a pyridine form nitrogen atom at the 3-position. The pharmacological activity of benzoxazoles differs significantly depending on the substitution pattern of the nucleus. [14] Benzoxazole is a 1-oxa-3-aza-1H-indene with the molecular formula C7H5NO and melting and boiling points of 29-30°C and 182°C, respectively. It has a pyridine-like odour and is white to light yellow in color.

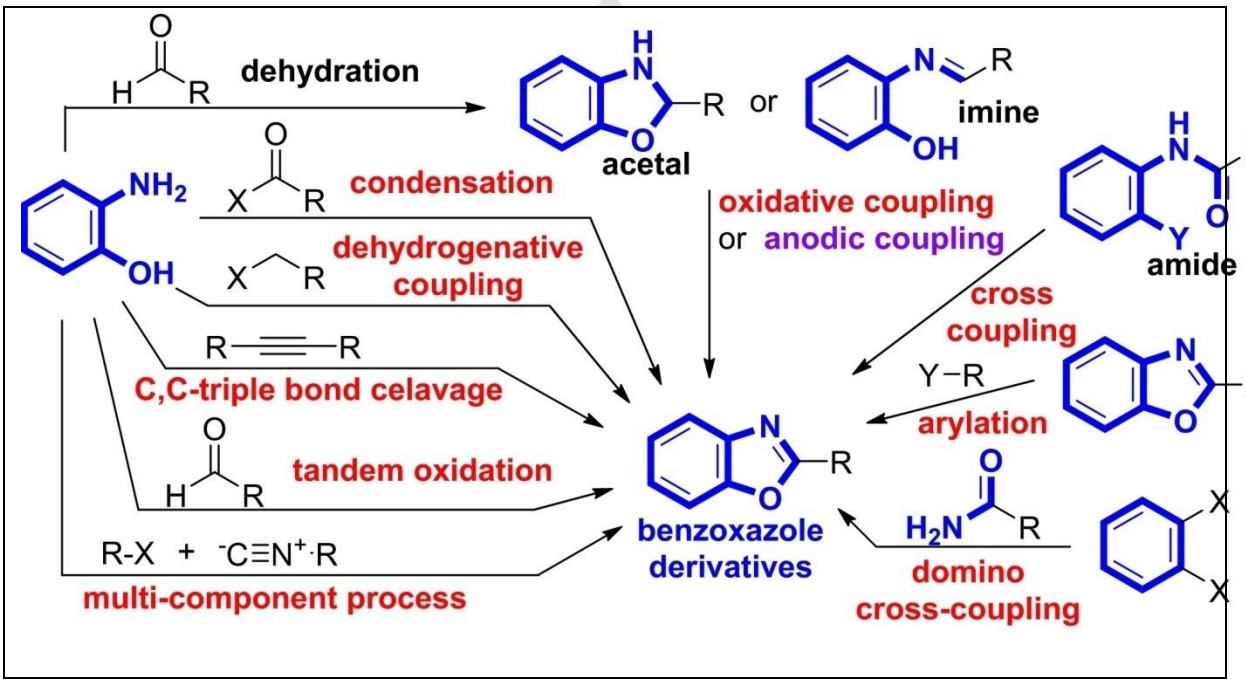
In cyclic systems, benzoxazole is a planar molecule with conjugated electron sextets. Weakly simple properties are conferred by the lone pair of electrons on nitrogen, which is co-planar with the heterocyclic ring and thus not involved in delocalization. [24]. Because of their structural resemblance to nucleic bases like adenine and guanine, benzoxazole moieties have gotten a lot of attention in chemistry and biochemistry. This helps them to interact easily with biopolymers in living systems. [25]

In general, new drugs are discovered in the pharmaceutical field through molecular modification of a lead compound with known activity. By removing, substituting, or adding a new moiety to the parent lead compound, molecular modification may potentially result in augmenting the activity, which includes combining different groups with identical activity in one compound. According to a review of the literature, drug design through molecular modification is a productive source of new drugs. As a result, the need to synthesize new molecules as potential therapeutic agents has become more important in recent years. Benzoxazole derivatives are a significant subclass of the compounds studied. Benzoxazole is a planar molecule with aromatic chemical properties [19] Benzoxazole is an organic compound, which has benzene fused with an Oxazole ring Oxazole is 1, 3 azole having oxygen atom and a pyridine type nitrogen atom at the 3-position in a five member ring. A slight change in the substitution pattern of benzoxazole nucleus causes distinguishable difference in their pharmacological activity. Benzoxazole is 1-oxa-3-aza-1H-indene, having molecular formula of C_7H_5NO with melting point and boiling point of 29-30°C and 182°C. It is white to light yellow in color with odour similar to pyridine. Benzoxazole is a planar molecule with conjugated π electrons sextets in the cyclic systems. The lone pair of electrons on nitrogen,

which is co-planar with heterocyclic ring and therefore not involved in delocalization, confers weakly basic properties.[24]

Benzoxazole moieties have attracted special attention in chemistry and biochemistry because of their structural similarity with nucleic bases, such as adenine and guanine, which allows their easy interaction with the biopolymers in living system.[25]Generally in the pharmaceutical field, new drugs are continuously discovered by molecular modification of lead compound of established activity. Molecular modification can possibly result in augmenting the activity which involves combination of separate group having similar activity in one compound by eliminating, substituting or adding new moiety to parent lead compound. In the survey of literature, it is seen that drug design by molecular modification is a productive source of new drug. Therefore, the need to synthesize new molecules as potential medicinal agents is more relevant today. Among the variety of compounds studied, benzoxazole derivatives form an important class. [26]

9.2 synthesis of benzoxazole derivative:



10. Pharmacological Activity of Benzoxazole.

Benzoxazole derivatives have a wide range of pharmacological effects. As a result, benzoxazole has a special place in the field of medicinal chemistry. The benzoxazole ring

system can be found in nature on rare occasions. In science, benzoxazole is used as a starting material for the development of larger, normally bioactive structures.

a) Anti-inflammatory activity:

b) Inflammation as a symptom of many diseases is a huge source of concern for doctors all over the world. The aggregation of a large number of phagocyte cells at the site of inflammation is the single most important event in this process. Inflammation is triggered by tissue damage caused by the introduction of a foreign antigen, trauma, or local exposure to certain chemicals. This may consist of a fluid stasis as well as the accumulation of several cellular and no cellular elements of the immune response. In most of these cases, it has been proved that the 5-substituted benzoxazole, substituted sulfonyl derivatives and carbohydrazides, have promising anti-inflammatory activity. Also, benzoxazole at its 5th position is more prone for its lipophilic action and therefore we go the substitution at 5th position of benzoxazole. Hence, it was planned to synthesize the *N*`[substituted sulfonyl]-1,3-benzoxazole-5-carbohydrazide to get good anti-inflammatory activity.

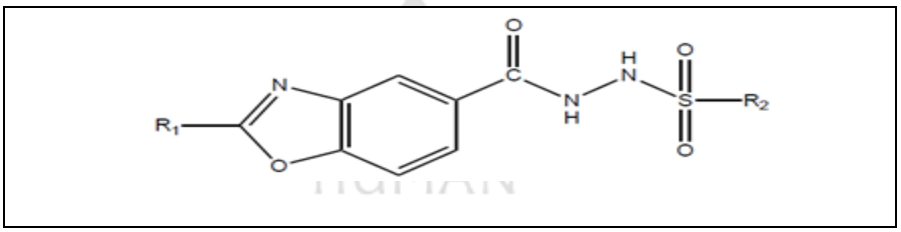


Figure No. 11: *N*`[substituted sulfonyl]-1,3-benzoxazole-5-carbohydrazide

c) Antibacterial activity:

Design, Facile Synthesis, and Antibacterial Activity of Hybrid 1,3,4-thiadiazole-1,3,5-triazine Derivatives by Vaibhav Dubey et al–S– Bridge tethering with the help of spectroscopic and elemental analysis, some hybrid 1,3,4-thiadiazole-1,3,5-triazine derivatives tethered via –S– bridge was synthesized and characterized.

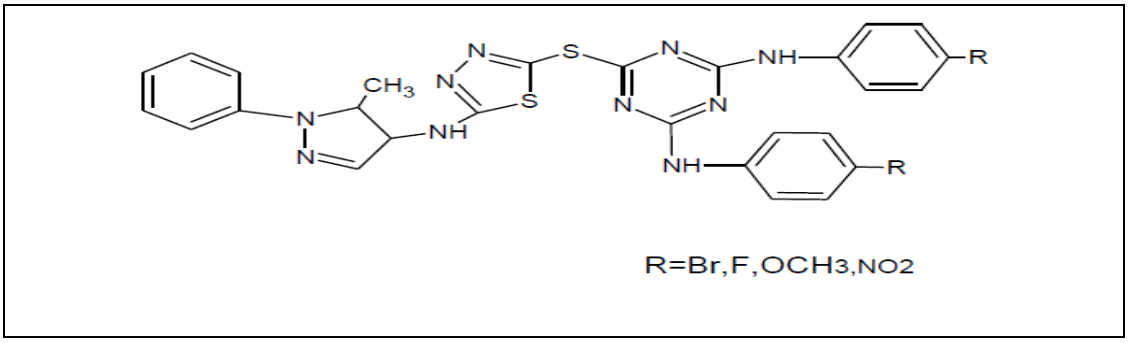


Figure No. 12: 1,3,4-thiadiazole-1,3,5-triazine derivatives tethered

d) Antitubercular activity: Tuberculosis (TB) is a bacterial infection caused primarily by Mycobacterium tuberculosis (MTB). The rising prevalence of multidrug-resistant tuberculosis necessitates the discovery and creation of new tuberculosis drugs with a different mechanism of action. Several benzoxazole derivatives have been synthesised and tested for biological activity in recent years.

Surprisingly some of them showed antitubercular potential. Despite this, no benzoxazole derivatives have progressed to the preclinical hit-to-lead optimization stage of anti-TB study. In this study, we summarise recent articles that assess the efficacy of the benzoxazole heterocycle in the production of novel anti-TB agents, as well as discuss the potential prospects.[29]Synthesis of novel pyrazoline and benzoxazole compound combinations (K). Microplate Alamar Blue Assay (MABA) is used to test the anti-TB activity of strains H37RV.

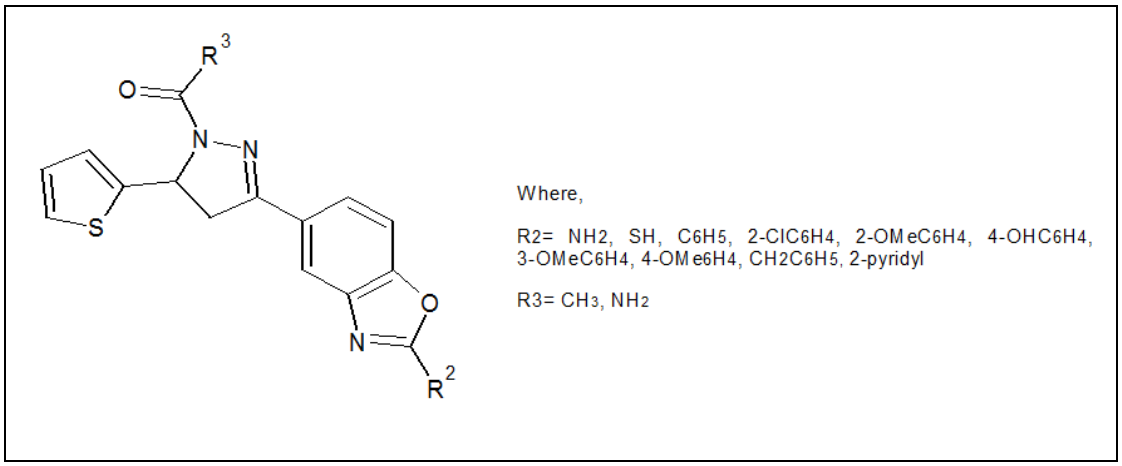


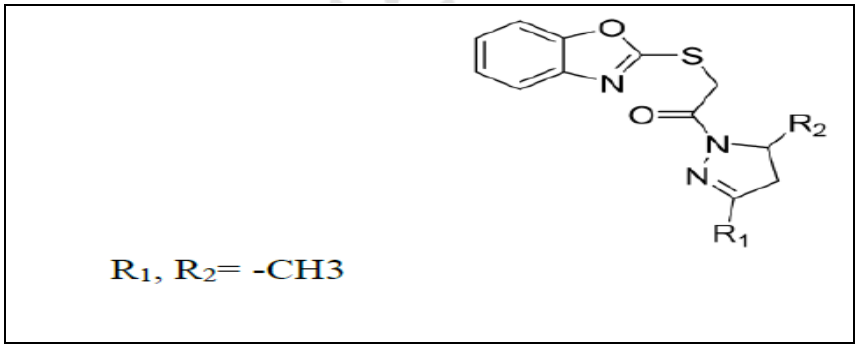
Figure No. 13: Novel pyrazoline and benzoxazole compound

e) Anti-microbial activity

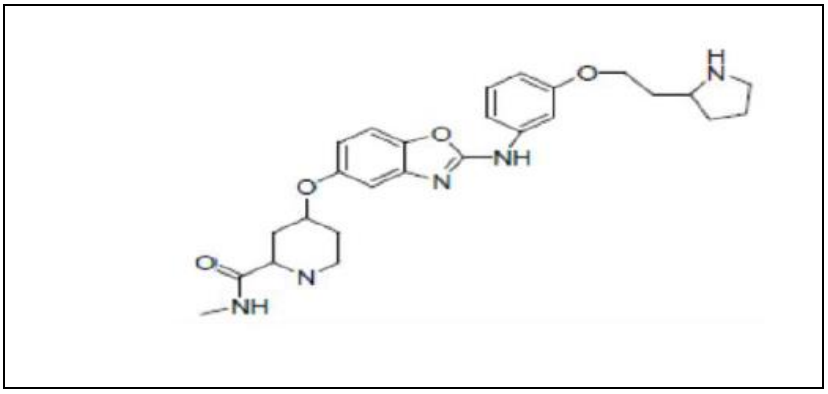
2-(1,3-benzoxazol-2-yl)-5-(diethylamino)phenol,2-(1,3-benzothiazol-2-yl)-5-(diethylamino)phenol and their derivatives were synthesized starting from p-N,N-diethyl amino salicylaldehyde with various substituted o-phenylenediamine, o-aminophenol, or o-aminothiophenol. Using the serial dilution process, both compounds were tested for in vitro antibacterial activity against Escherichia coli and Staphylococcus aureus strains, as well as in vitro antifungal activity against *Candida albicans* and *Aspergillus niger* Strains. The minimum inhibitory concentration (MIC) in lg/mL was used to measure antibacterial activity. [30]

f) Anti-convulsant activity:

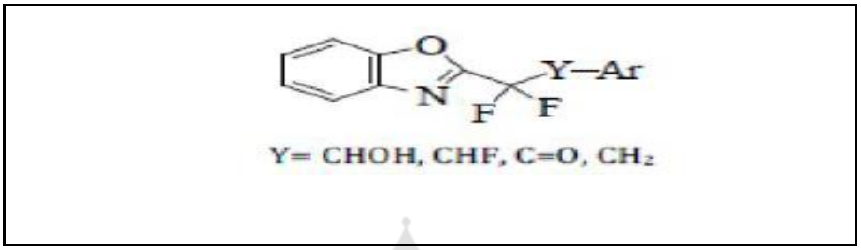
PTZ-induced convulsions in albino mice were used to screen 2-mercapto benzoxazole and 2-mercapto benzimidazole for in vivo anticonvulsant activity. The majority of the compounds were found to be effective in preventing convulsions caused by pentylenetetrazol. As compared to a regular drug, certain compounds showed the most activity.



g) Miscellaneous: A series of 2-aminobenzoxazoles with a strong pharmacokinetic profile are tested for their selective vascular endothelial growth factor-2 receptor kinase inhibitor activity.



They're also being tested as imaging agents for Alzheimer's disease (AD)-related amyloid plaque in vitro and *In-vivo*. For use in AIDS therapy, certain fluorine-containing benzoxazole derivatives are screened for activity against HIV-I.



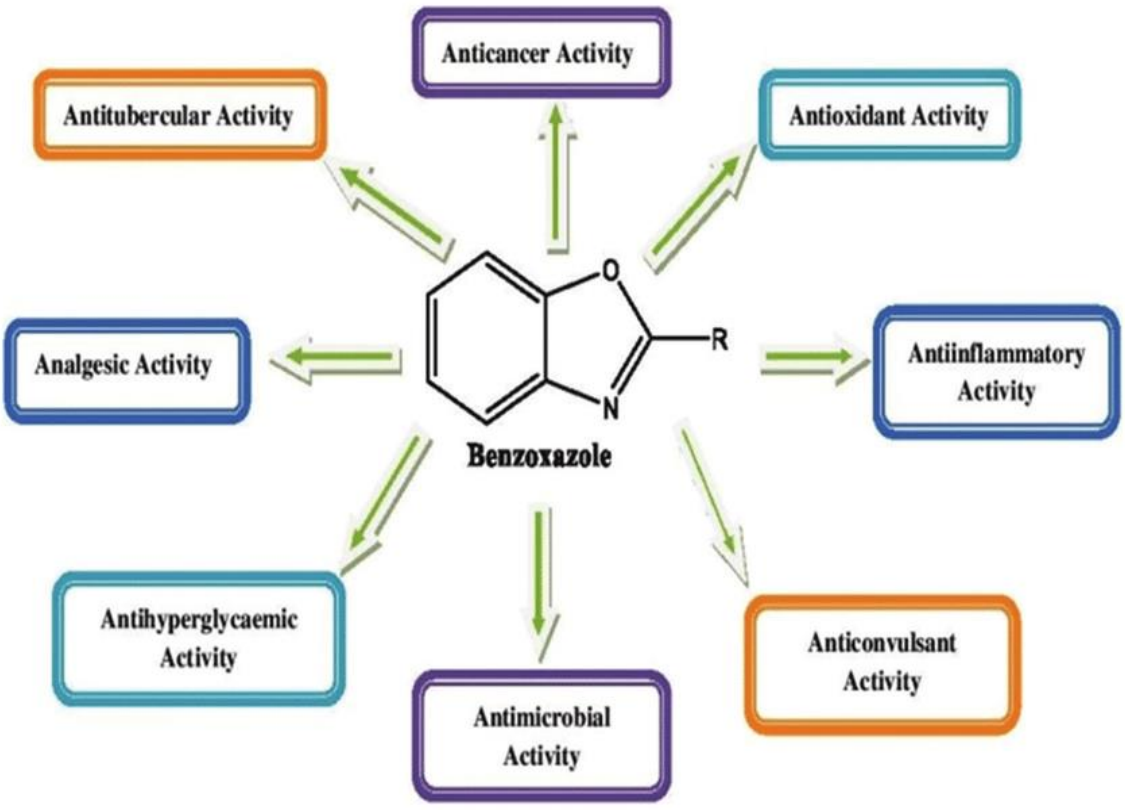


Figure no. 2 Different activities of benzoxazole

11 CONCLUSION:

The synthesis methodologies and importance of benzoxazoles were explored and reviewed in this paper, given the biological and pharmacological value of these compounds.

Acknowledgments:

The authors of this review article are thankful to the Principal, Government College of Pharmacy, Karad for allowing us to present this paper. We are also thankful to AICTE for providing research fellowship to complete our research work and convert our research work into publications.

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