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BIOLOGICAL ASPECTS OF NOVEL BENZOTHIAZOLE DERIVATIVES

Alpa Verma [1], Arun Kumar [* 1], Syed Misbahul Hasan [1], Kuldeep Singh [1], Bhavana Dubey [1] and Parul Mishra [2]

Department of Pharmaceutical Chemistry [1], Department of Pharmaceutics [2], Integral University, Kursi Road, Lucknow - 226026, Utter Pradesh, India.

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Correspondence to Author:
Dr. Arun Kumar

Associate Professor, Department of Pharmaceutical Chemistry, Integral University, Kursi Road, Lucknow - 226026, Utter Pradesh, India.

E-mail: arun@iul.ac.in

ABSTRACT: The heterocyclic compounds are formed by the hetero atoms (O, S, N, *etc*.) in the cyclic ring system. These are mainly started from 3-membered to 10- membered heterocyclic rings. The compound containing heterocyclic molecules shows potent activity in various pharmacological targets. Benzothiazole is a fusion of a benzene ring with a 5-membered thiazole ring which is widely used in heterocyclic compounds. The benzothiazole pharmacophore and its derivatives are used for the development of novel drugs and have also shown different pharmacological and biological activities such as anticancer, antibacterial, antifungal, anti-inflammatory, analgesic, anti-HIV, antioxidant, anticonvulsant, antitubercular, antidiabetic, antileishmanial, antihistaminic, antimalarial activities. In previous years, few new benzothiazoles have been shown with different biological responses. In such a manner, this review illuminates the benzothiazole and its substituted product that possesses distinct biological activity. This article discovered a novel benzothiazole-based drug that has shown less toxic and more active effects.

INTRODUCTION: The chemical and biological research of compounds containing heterocyclic moiety plays an essential role in medicinal chemistry. Heterocyclic compound has the property to find more potent drug and less toxic effect. A different heterocyclic compound contains various pharmacological activities and thus can be used as a pharmacophore moiety in the discovery of new drug molecule. A heterocyclic compound containing a cyclic ring comprises more than one kind of atom. There are various kinds of heterocyclic systems: Monocyclic system, Fused Polycyclic system, Bridged heterocyclic system.

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The compound obtained from the heterocyclic moiety work as an essential part the current drug development like pyrrole, pyridine, furan, thiophene, benzimidazole, benzothiazole, benzoxazole *etc*., that are broadly useful in the discipline of medicinal chemistry having various pharmacological responses including antibacterial, antifungal, anti-viral, anti-tubercular, analgesic, anti-inflammatory, antidiabetic, anticancer, antihistaminic, antimalarial, antioxidant, *etc.*

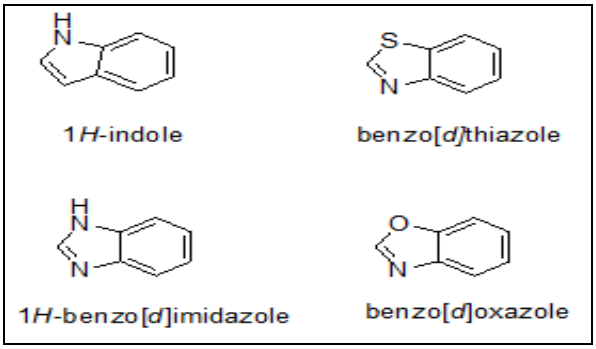


FIG. 1: FUSED HETEROCYCLIC COMPOUNDS

Benzothiazole: Benzothiazole (1,3-benzothiazole) is a fusion of a 6-membered benzene ring with a 5-membered thiazole ring which contains sulfur and nitrogen atoms having various pharmacological activities. The benzothiazole pharmacophore involved in research that main purpose is to evaluating novel drug that possess different biological responses like- antitubercular [1, 2], antimicrobial [3-5], antimalarial [6], anticonvulsant [7, 8], anthelmintic [9], analgesic & anti-inflammatory [10, 11], antidiabetic [12], antiglutamate [13] and antitumor [14, 15], neuron protective [16] actions. Benzothiazoles are beneficial for different diseases like neurodegenerative disorders, central muscle relaxants, anti-cancer activities, etc. Benzothiazoles is broadly useful in dyes like thioflavin [17].

Chemistry: Benzothiazole is an organic heterocyclic compound consisting of benzene and thiazole rings (it contains a 5-membered ring with 1 nitrogen and sulfur atom). The molecular weight of benzothiazole is 135.19 g/mol. This is colorless liquid that is soluble in water, and the boiling point is 227 °C. This article has studied a different type of benzothiazoles' derivatives.

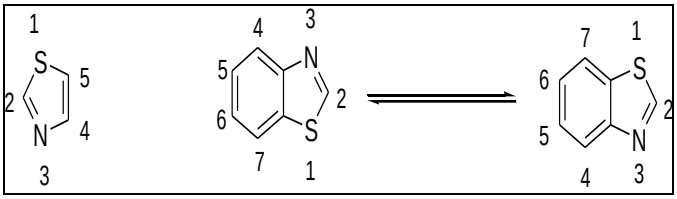


FIG. 2: NUMBERING OF ATOMS IN BENZOTHIAZOLES

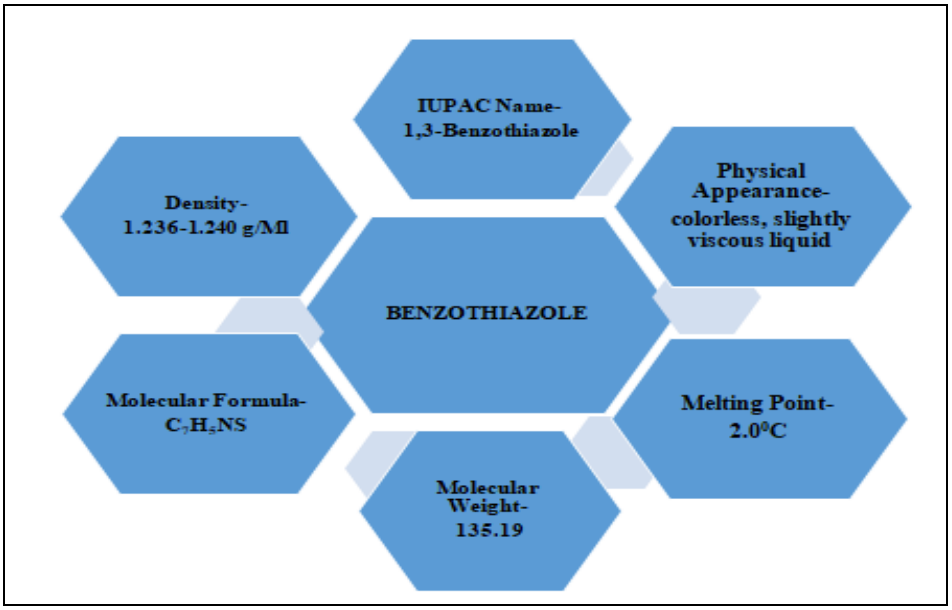
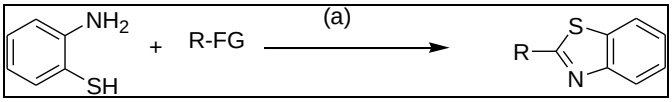


FIG. 3: PROPERTIES OF BENZOTHIAZOLES

Conventional Methods of Benzothiazole: A.W. Hofmann synthesized a compound named mercaptobenzothiazole in 1887 by the reactions between carbon disulfide and *o*-amino thiophenol. In this reaction, simple cyclization was done, so various method has been reported and applied with various catalysts and reaction conditions.

If any substitution at C-2 position of benzothiazoles that synthesized through a condensation reaction of *o*-amino thiophenolusing substituted COOH, CHO, nitriles or acid chlorides by the help of different cyclization reagents like I_2, $ZrOCl_2 \bullet 8H_2O$, Trimethyl silyl chloride, Pyridinium Chloro Chromate (PCC), Br_2, Trifluoride Etherate, Cerium Ammonium Nitrate (CAN) *etc* [18].



R-COOH, CHO, CN and *o*-esters, *etc*.

(a)-represents Strong acids or milder or oxidative reagents or various catalysts

FIG. 4: SYNTHESIZED MERCAPTO BENZO-THIAZOLE DERIVATIVES

According to Cuputo*et al.* [19] the synthesis of benzothiazole derivatives contains aryl amide or aryl urea substitution atposition-2 carbon atom in which some of the compounds represent *in-vitro* anticancer activity. 6-Trifluoro methoxy and *para*-substituted compound & *p*-cyano bearing moiety marked for the enhanced activity against Leukemia & Melanoma cell lines at 10-5 M concentration.

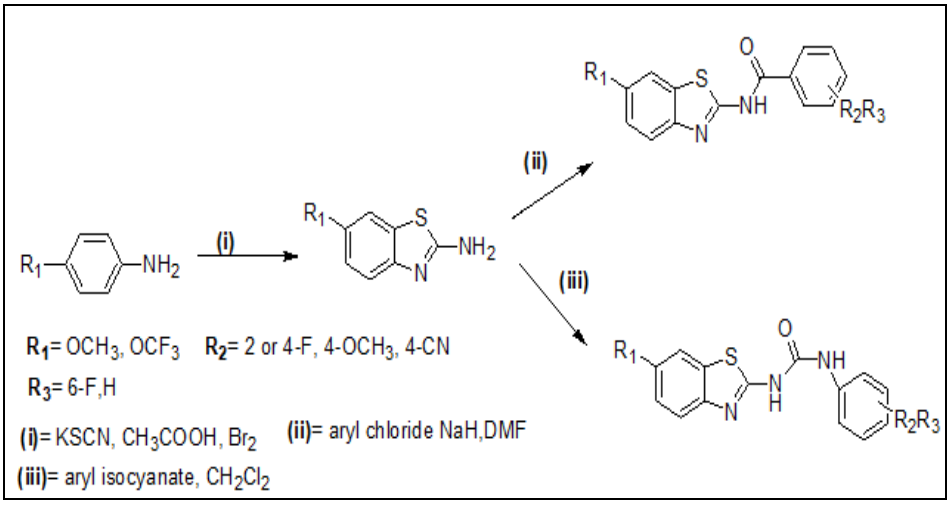


FIG. 5: BENZOTHIAZOLES DERIVATIVES SYNTHESIZED BY SUBSTITUTED ANILINE

Synthesis for 2-substituted Benzothiazole Derivatives: The procedure for the synthesis of benzothiazole derivatives is stated through Kenny and Mashelkar [20]. According to them, they found if 7 ml of acetic acid is taken with different benzaldehydes (2, 5.5 mmol) and 2-Aminobenzenethiol (1, 5 mmol) in an RB flask and refluxed it for 5–6 h **Fig. 5** that TLC observes. After that, the reaction mixture was cooled at room temperature and decomposed, and filtration was done. So, the crude product is obtained and purified through crystallization method with ethanol or through column chromatography via hexane: ethyl acetate act as a solvent. The Spectroscopic method is used for the characterization of synthesized compounds.

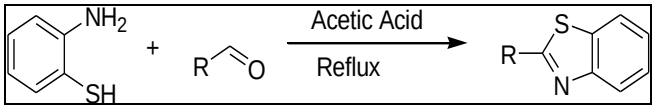


FIG. 6: SYNTHESIS OF BENZOTHIAZOLES DERIVATIVES BY DIFFERENT BENZALDEHYDE

Benzothiazole guanidine propanoic acid derivatives and their Schiff's bases were synthesized by Venkatesh & Tiwari [21] and estimated the cytotoxicity against the HeLa cell lines anti-microbial activity.

In the synthesized compounds, 3- [3-(6-hydroxy benothia-zoleguauidino] propanoic acid showed remarkable HeLa cytotoxicity activity. Sulfonamide &Bromo substituted compound showed MIC up to for anti-microbial activity.

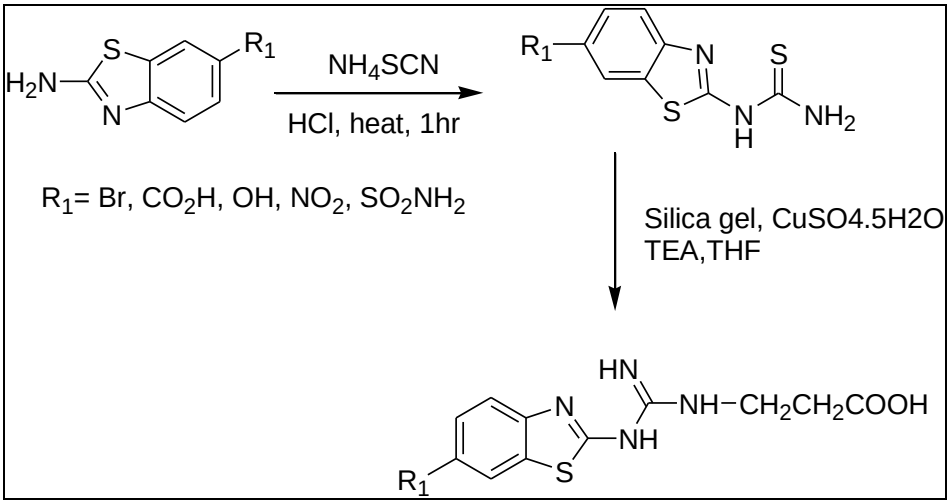


FIG. 7: SYNTHESIS OF BENZOTHIAZOLES BY USING SCHIFF'S BASE

Chauhan *et al.* [22] synthesized a series 4-formyl pyrazole substituted 6-chloro benzothiazole by Vilsmeier Haack cyclization reaction. The synthesized compounds exhibited anti-microbial activity and *p*-hydroxy substituted compounds had up to 94% inhibition ability compared to the standard.

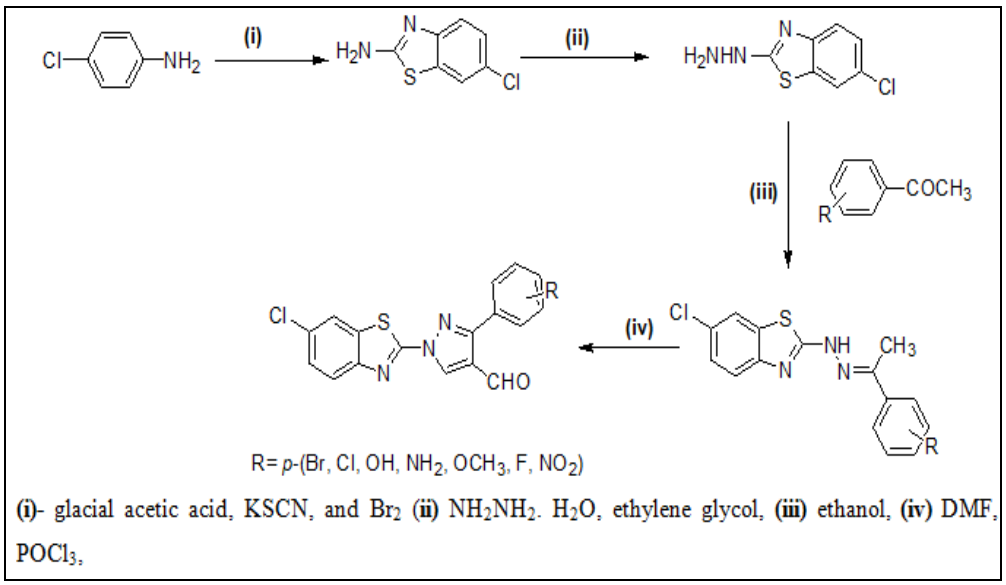


FIG. 8: VILSMEIER HAACK CYCLIZATION REACTION

By Condensation Reaction: Guo and co-authors [23] synthesized the different benzothiazole derivatives using various substituents after the condensation of 2-Aminobenzenethiolwith aldehydes *via* H_2O_2/HCl in ethanol which acts as a catalyst and keep it for 1 hrsat room temperature. Basically, 2-aminothiophenol/aromatic aldehyde / H_2O_2/HCl (1:1:6:3) has shown the maximum coupling activity. By this method, aldehydes contain e-donating and e-withdrawing substituents to get selective benzothiazoles with outstanding yields that show less product-reactive time.

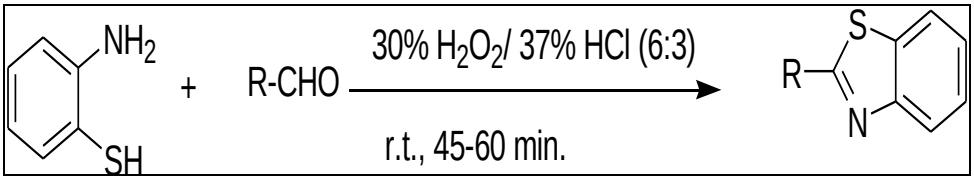


FIG. 9: CONDENSATION REACTION OF BENZOTHIAZOLE DERIVATIVES

Biological Aspects: Singh *et al.* [24] introduced different pharmacological as well as biological action like anti-microbial and anti-fungal activities. Musser *et al.* [25] also show anti-diabetic.

Anti-allergic activity is also found in benzothiazoles nucleus, and Patta*net al.* [26] shows anti-cancer orantitumor, Yoshida *et al.* [27] represent anti-inflammatory, anti-helminthic agents. The substitution of aryl group at 2nd position in benzothiazoles nucleus indicates antitumor activity and pyrimido-benzothiazoles and benzothiazolo-quinazolines obtained by the condensation reaction which exhibited anti-viral activity.

Antimicrobial Activity: Bronchopneumonia, Amoebic dysentery, typhoid, malaria, cough & cold and other infectious diseases, include tuberculosis, influenza, syphilis and AIDS are mainly lead to and spread through microbes. Gopkumar *et al.* [28] determined the antimicrobial activity of 2 - substituted – aryl -sulfonamido-5-substituted-benzothiazole (1, figure- ix) and another derivative like N-(2-amino-6-fluorobenzo [d] thiazol-7-yl) benzene sulfonamide (2, **Fig. 9** evaluates for the antibacterial as well as antifungal activities against some bacteriaslike *Bacillus subtilis, Salmonella typhi*as well as *S. dysentery* and also shown *C. albicans, S. aureus etc*. Various benzothiazolyl carboxamido pyrazoline derivatives has been prepared and studied for their anti-microbial activity.

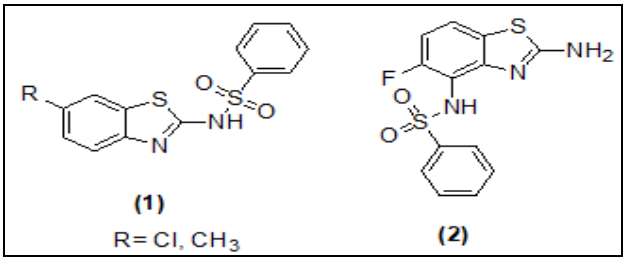


FIG. 10: BENZOTHIAZOLE DERIVATIVES ASANTIMICROBIAL ACTIVITY

Antitumor & Anticancer Activity: The benzothiazole pharmacophore having different substitutions indicates antitumor and anticancer activity.

The amino methyl phenyl derivatives 1, **Fig. 10** and 4, 7-dimethoxy benzothiazole 2, **Fig. 11** act as selective growth inhibitors against human cancer cell lines.

Substitution of chlorine and fluorine of the derivatives on this moiety shows better cytotoxic activity. Substituted 2-(p-Aminophenyl) benzo-thiazole was observed to have an *in-vitro* antitumor effect for human cell line carcinoma on ovarian, lung, renal and colon.

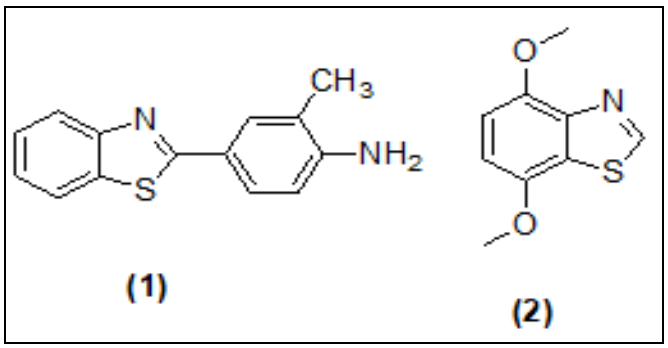


FIG. 11: BENZOTHIAZOLE DERIVATIVES ASANTITUMOR & ANTICANCER ACTIVITY

Wang *et al.* [29] synthesized a new benzothiazolyl mercaptan derivatives **Fig. 11** -1 and examinedthe anti-proliferative effect on HepG2 and MCF-7 cells. Several benzothiazoles products inhibits the cell growth and some derivatives have more efficient activity rather than cisplatin. Kumbhare *et al.* [30] synthesized benzothiazolyl thiocarbamides **Fig. 11**-2 with a catalytic extent of 4- dimethyl amino pyridine through oxidative cyclization using1-Butyl-3-methylimidazolium tribromide to give the N-bis-benzothiazole products.

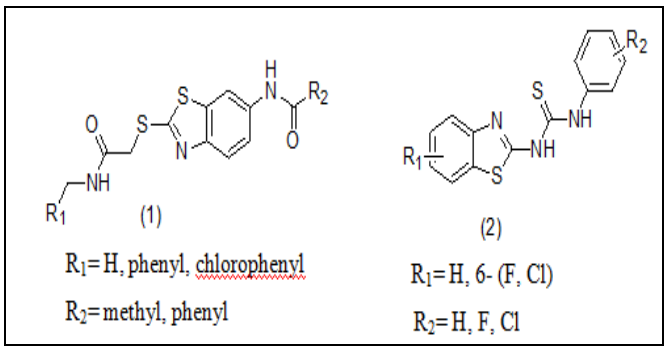


FIG. 12: BENZOTHIAZOLE DERIVATIVES ASANTI-PROLIFERATIVE ACTIVITY

Anticonvulsant Activity: Several benzothiazole derivatives are estimated and initiated to produce an important actionbeside different types of seizure's. Amit, B. N. *et al.* [31] synthesized a newer class of substituted-2-benzothiazolamines derivatives, which act as anticonvulsant agents. 2-(-4-aryl thiosemicar - bazidocarbonylthio) benzothiazoles and various benzothiazoles having sulphonamide derivatives, benzo-thiazolamines have been synthesized and evaluated against pentylenetetrazole which is firstly observed in 1978 that is active against electroshock and seizure's in anticonvulsive agents.

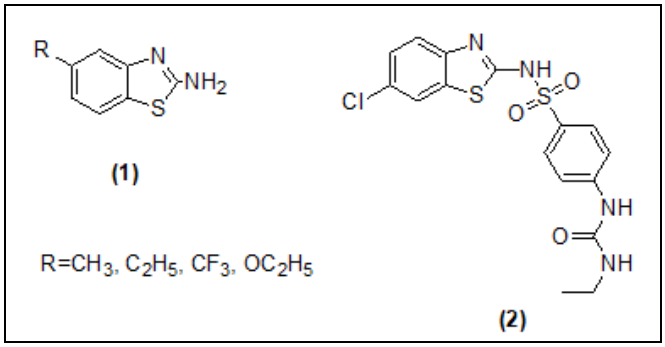


FIG. 13: BENZOTHIAZOLE DERIVATIVES ASANTICONVULSANT ACTIVITY

Antileishmanial Activity: According to Delmas*et al.* [32] synthesized 1,3-Benzothiazol-2-yl-amino-9-(10*H*)-acridinone substituents by *in-vitro* antileishmanial activity **Fig. 13**. Although the development of amphotericin B formulation that is easy to minimize toxicity and maximize the antileishmanial effect.

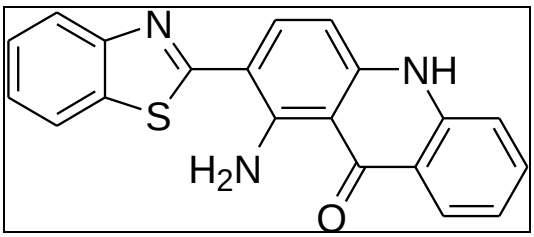


FIG. 14: BENZOTHIAZOLE DERIVATIVES ASANTILEISHMANIAL ACTIVITY

Antioxidant Activity: As per Tzanova *et al* [33] synthesized of 3 novel diphenyl methanone having thiazol pharmacophore 1, **Fig. 14** and also find antioxidant properties. Derivatives of 5 - (2, 5 - dihydroxybenzoyl) – 2 (3*H*)-Benzothiazolol shown the essential antioxidant properties and less toxic effect on cells as well as action of oxygen radical is also minimize and may produce 2-Methylpropane-2-peroxolforentirely 3- cell lines and estimated by

in-vitro Cressier *et al.* [34] synthesized and characterized of noval derivatives of benzothiazoles and thiadiazoles 2, **Fig. 14.**

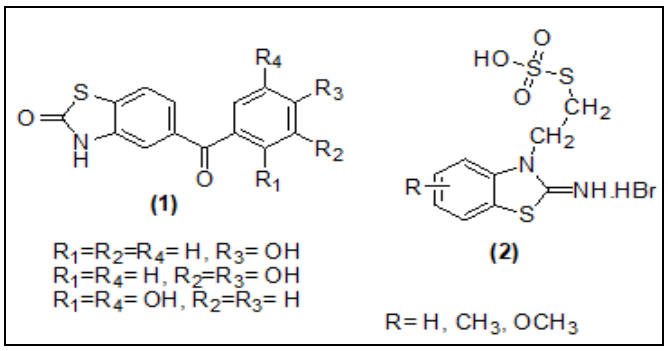


FIG. 15: BENZOTHIAZOLE DERIVATIVES ASANTIOXIDANT ACTIVITY

Anti-inflammatory Activity: Viegas-Junior *et al* [35] reported in the recent year, several benzothiazoles derivatives based on anti-inflammatory has been synthesized and a few novel2-(tert-butyl-3',5'-dimethylpyrazol-1'-yl) -6-substituted benzothiazoles as well aspyrazoline-3, 5-dione structure which have shown major anti-inflammatory and also non-steroidal anti-inflammatory agents are shown by pyrazolones and pyrazolinones. Most of the novel derivative has been produces important anti-inflammatory activity. Xie *et al.* [36] also synthesized 2-(2-pentadecy l-4, 5-dihydro-1, 3-oxazole) methylthio -1 *H*-Benzimidazoles / Benzothiazoles and benzoxazoles obtained from 2-Hydroxy-6-pentadecylbenzoic acid (anacardic acid)which prevent human (COX-2) cycloxygenase-2-enzyme.

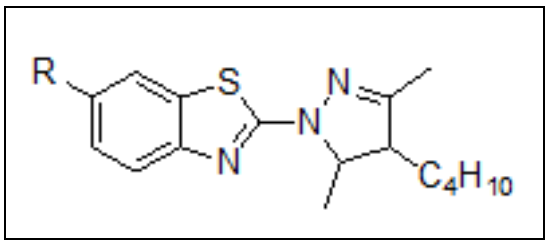


FIG. 16: BENZOTHIAZOLE DERIVATIVES ASANTI-INFLAMMATORY ACTIVITY

Antidiabetic Activity: Metabolic disorder identified through hyperglycaemia, glycosuria, hyperlipidemia, nitrogen imbalance that is known as Diabetes. Moreno-D´ıaz *et al.* [37] synthesized N-(6-substituted- 1,3-benzothiazol-2-yl) benzene sulfonamide-substituents (1) use for the checking antidiabetic activity on noninsulin-dependent diabetes mellitus rat model by *in-vivo* methods which is estimated by the help of 11-HSD1 and PTP-1B enzymes. Patil *et al.* synthesized and evaluated substituted (*E*)- 3-(2-Benzo[*d*] thiazolyl-amino) phenyl prop-2-en-1-ones (2) for antidiabetic activity through Selective inhibitors of 11*β*-hydroxysteroid dehydrogenase type-1 (11*β*-HSD1) have treatments used for diabetes mellitus type-2 or obesity.

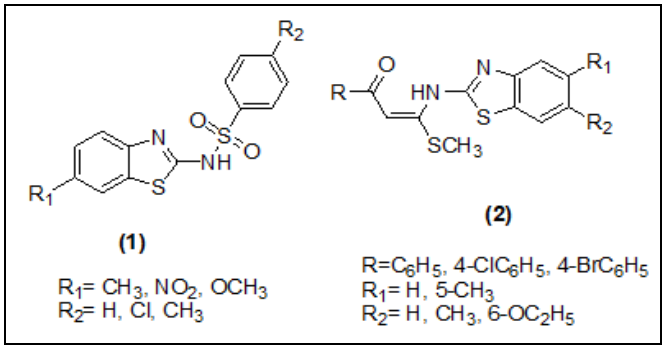


FIG. 17: BENZOTHIAZOLE DERIVATIVES ASANTIDIABETIC ACTIVITY

Antitubercular Activity: Pereira *et al.* [38] reported to synthesized the two novel metal complexes of 2-(2 thienyl) benzothiazoles-BTT (1). These complexes represent the maximum action against *Mycobacterium tuberulosis*. Telvekar *et al.* [39] synthesized the newbenzothiazoles, substituted 2-(2-(4-aryloxybenzylidene) hydrazinyl) derivatives designed incorporate with 2-hydrazino-benzothiazole and 4-(aryloxy) benzaldehyde (2).

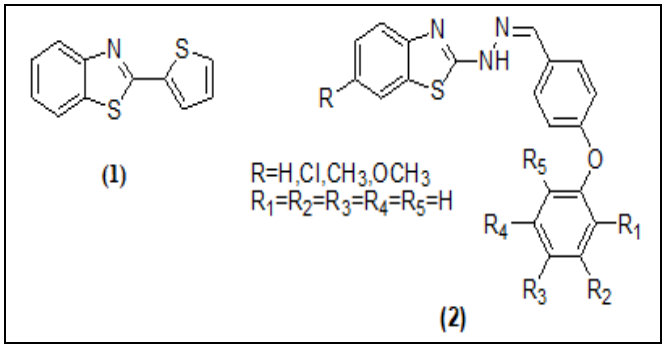


FIG. 18: BENZOTHIAZOLE DERIVATIVES ASANTITUBERCULAR ACTIVITY

CONCLUSION: This review mainly deals with lead compounds in the discovery of novel drug molecules of benzothiazole derivatives by different methods like condensation and cyclization reaction, synthesis and biological action for various benzothiazole moieties mentioned in the different articles and journals. Several reviews have reported that benzothiazole moiety produces a large number of pharmacological as well as a biological applications like antimicrobial, antitumor,

anticonvulsant, antileishmanial, antioxidant, anti-inflammatory, antidiabetic and antitubercular activity.

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