

Pharmaceutical Organic Chemistry

Dr. Meenakshi N. Deodhar

Dr. Ashok Bhosale

Mrs. Jayashri R. Jagtap



PHARMACEUTICAL ORGANIC CHEMISTRY

for
B. Pharm Students
As per New Revised Syllabus

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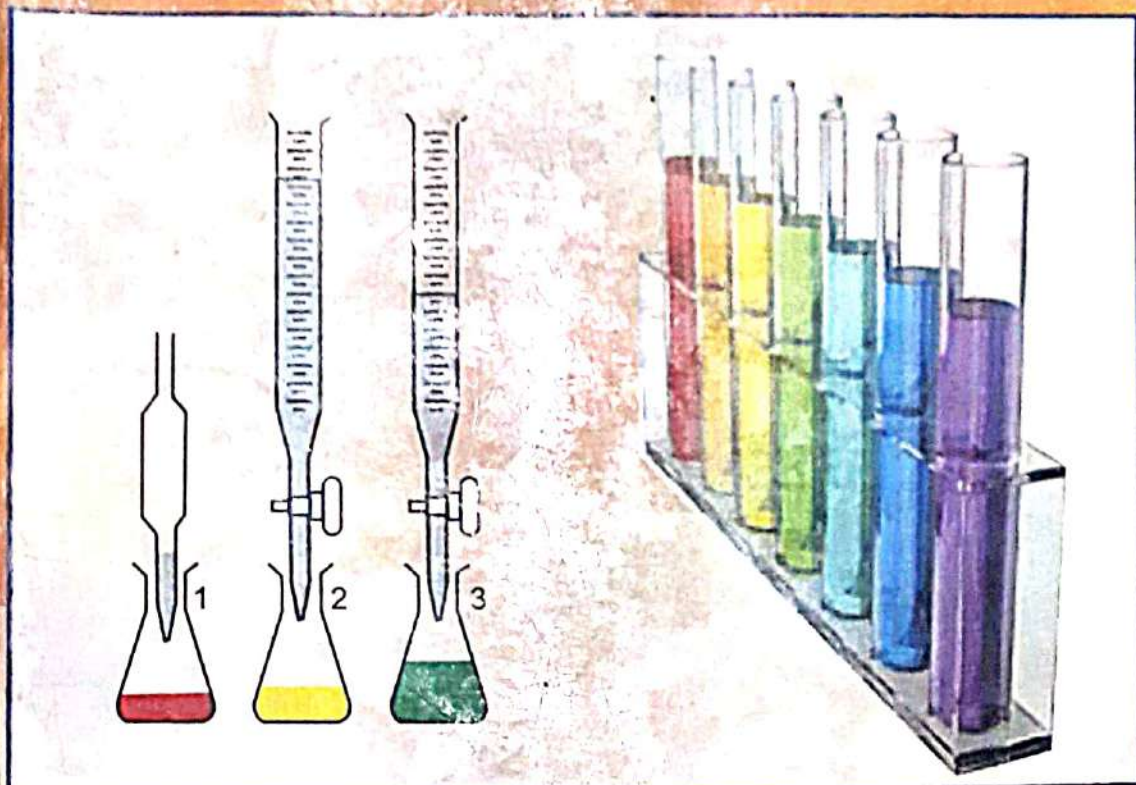
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PRACTICAL HANDBOOK OF PHARMACEUTICAL ORGANIC CHEMISTRY

Dr. M. N. DEODHAR
Mrs. J. R. JAGTAP



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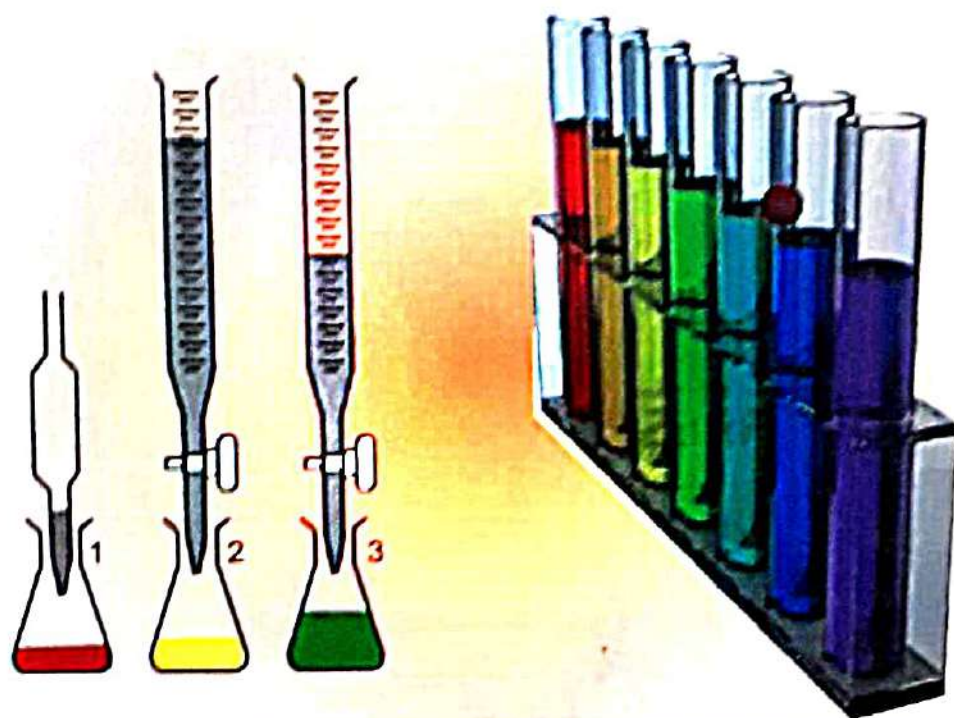
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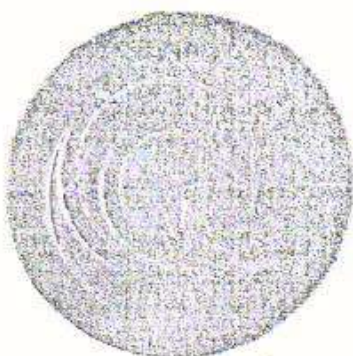
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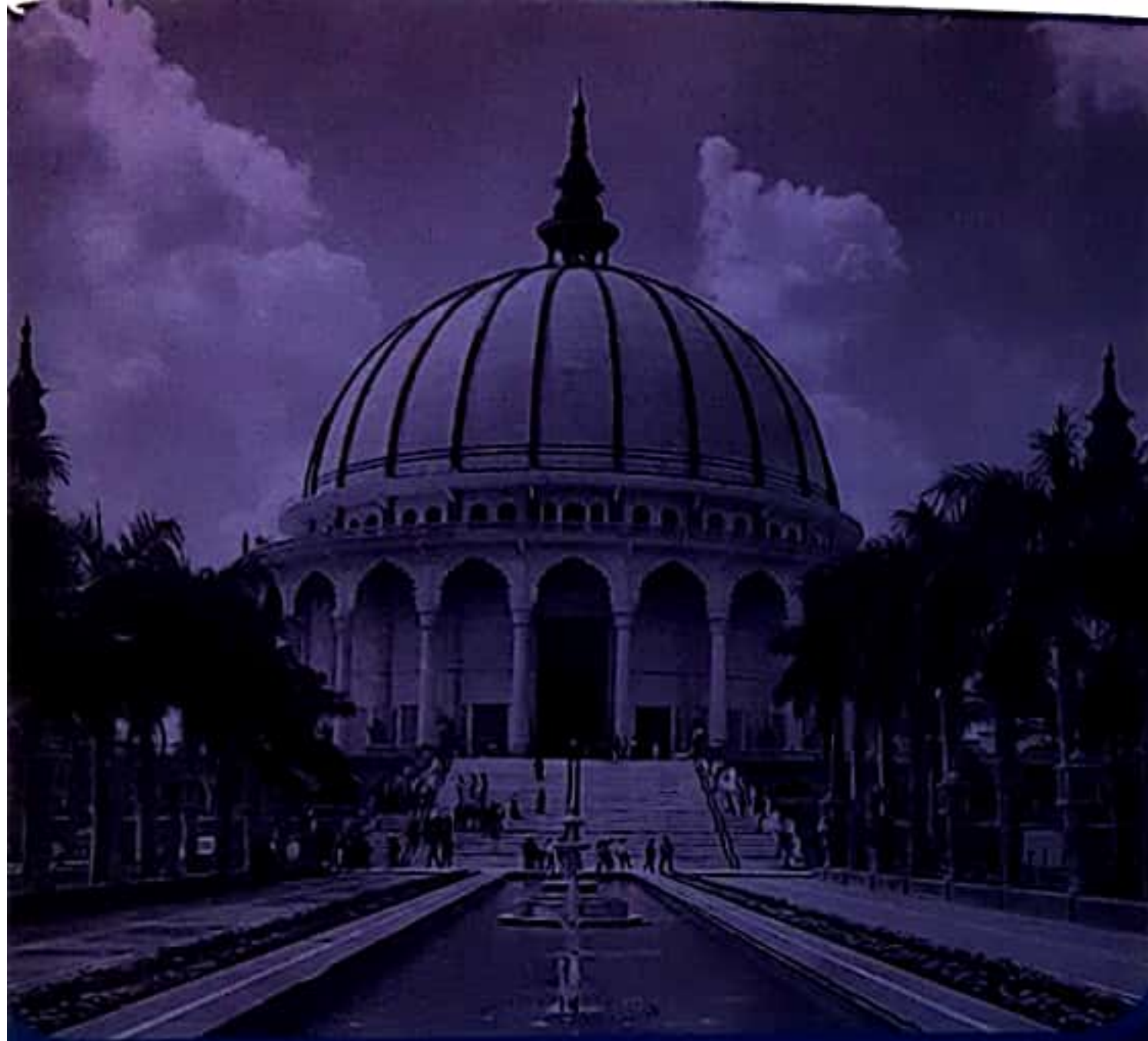
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**Title :** Docking studies of Indole derivatives as selective COX-2 inhibitors

**Aim and Objectives :** An area of design and synthesis of novel COX-2 inhibitors is being explored for drugs with better efficacy and safety profile. Novel indole derivatives were synthesized, purified and characterized. The compounds showing comparable analgesic and anti-inflammatory activities were selected for docking studies.

**Materials and Methods :** In the present work, docking studies were carried out using CYCLOOXYGENASE-2 complexed with a selective inhibitor, SC-558. The docking studies were carried out in VLife Molecular Docking Suite 3.5 by using Biopredicta. Twenty four molecules from six series were studied by docking with an aim to further confirm the binding affinities of synthesized molecules (ligands) to COX-2 enzyme and also to reveal their binding interactions with the enzyme.

**Results and Discussion :** The results of docking studies indicate that the compound IIB17 with highest docking score, was found to be involved in the hydrogen bonding with a residue Lys 97. The hydrogen bonding distance between NH group of IIB17 with NH of lysine97A was found to be 1.599 Å (N-----H). The pyrimidine ring at 3 position was surrounded by active site amino acid residues His 356A, Gly 350A, His 351A, and Asn 581A. The indole ring found to interact with residues His 356A, Lysine97A. The benzene ring on pyrimidine nucleus was found to interact with Asn581A and Gly 192A.

**Conclusion :** Compounds IIB17, IIB11, IIB2, IIA2, IIB4, IIA4, IIB3, IIA5, IIB5 and IIB7 have shown good docking scores comparable to SC558 promoting us to conduct enzyme inhibition assays.

**Keywords :** COX-2 enzyme, docking, indole derivatives.



**Presenting Author :** Smita Pawar

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**Title :** In silico design, synthesis, and biological evaluation of some quinazolinone derivatives as potential antimicrobial agents

**Aim and Objectives :** Development of resistance to antimicrobial agent by microorganisms is causing the decrease in efficiency of existing antimicrobial agents. Ignoring this problem today can create a serious hazard to life. Hence there is urgent need for development of newer antimicrobial agents which will help in curing the infections. Quinazolinone derivatives also showed antimicrobial activity through DNA gyrase and topoisomerase inhibition. So, present work aims at synthesizing the benzothiazole derivatives with quinazoline-4-one and to evaluate it for antimicrobial activity. So we have designed a new series of benzothiazole derivatives. Docking studies have been carried out on DNA gyrase enzyme to check the probable interactions of synthesized compounds. So our aim is to design the newer antimicrobial analogue of benzothiazole.

**Materials and Methods :** 3-(substituted-benzo[d]thiazol-2-yl)-2-substituted-quinazolin-4(3H)-one S(1-7) were synthesized by reaction of substituted 2-aminobenzothiazole B(1-7) with benzoxazin-4-one. The physical properties and spectral characteristic of synthesized compounds were identified with the help of, M.P. and FTIR, NMR respectively. The completion of reaction was monitored by TLC. The compounds S (1-7) were evaluated for antimicrobial activity. The designed compounds were docked in 3G75 protein molecule and interactions were recorded.

**Results and Discussion :** Compound S3 was found to be significant and also compound S4 and S5 significant antimicrobial activity. Compounds S1, S2, S6, and S7 showed moderate activity.

**Conclusion :** Thus, we conclude that the synthesized compounds have a potential for further development as novel antimicrobial agents.

**Keywords :** Benzothiazole, quinazolinone.



# Certificate of Recognition

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