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# CHEMISTRY IN DRUG DISCOVERY & DESIGNING

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### Contemporary drug discovery and design

The current scenario of development of new drugs needs no emphasis in light of the current global situation of health and disease. The conventional random screening method of drug discovery and design is time consuming and laborious with a long design cycle. It is a multidisciplinary, complex, costly and intellect intensive process. Rational drug design techniques can make drug discovery process more fruitful. Knowledge management and technique specific expertise can save time & cost, which is a paramount need of the hour. Drug discovery in the late 20<sup>th</sup> century was focused on the definition and characterization of the macromolecular substrates that serve as targets for drug design. The advent of genomics and the molecular biology revolution has permitted both the definition of new targets and the characterization of the genetic basis of disease states. Variety of concepts came up like pharmacogenomics, drug repurposing, polypharmacology, chemogenomics, phenotypic screening and high-throughput *in vivo* testing of mixture-based libraries in an integrated manner. These fields offer alternatives to the current paradigm of drug discovery, from a one target–one drug model to a multiple-target approach. Furthermore, the goals of lead identification are being expanded accordingly to identify not only ‘key’ compounds that fit with a single-target but also ‘master key’ compounds that favorably interact with multiple targets.

CADD is no longer merely a promising technique. It is a practical and realistic way of helping the medicinal chemist. It has become a significant tool, an aid to thought and a guide to synthesis. Remarkable progress has been made during the past few years in drug design and discovery. An improved generation of softwares with easy operation and superior computational tools to generate chemically stable and worthy compounds with refinement capability has been developed. These powerful new technologies should greatly accelerate the pace of new drug discovery.

### Recent Publications

1. Chaudhari R Y, Bhise S B, Yadav A S, Sonawane T (2016) QSAR, Synthesis and Docking Study of 1,4-DHP as Novel Antitubercular Agents JPRCP (6).
2. Ghodke Yogita Deepak\* & Yadav Anita Shashikant (2014) Extraction And Pharmacological Screening Of Carvone And It's Derivatives, Ijpa- 3(1).
3. Yadav Anita \*, Magdum C. S. (2014) Synthesis And Biological Activity Of 1, 6-Dihydropyridine Derivatives. Ijpa (3).
4. Yadav Anita Shashikant And Ghodke Yogita Deepak (2013) Kajal: Cosmeceutical, Ijpa 2(9).

### Biography

Anita Yadav has her expertise in computer aided drug designing. She has worked on Structure Based Drug Designing, Ligand Based Drug Designing, 2D, 3D and Group QSAR based Drug Designing, De-Novo Designing, Homology Modelling, Pharmacophore modelling, Lead Identification and QSPR Designing. She can design any agonist and antagonist for the resistant bacterial strains. She has worked on Synthesis, Purification, and Structural Elucidation & Pharmacological Evaluation of following classes of compounds: Anti-tubercular, Anti-diabetic, Anti-malarial, Anti-inflammatory and Antibacterial agents..She is Working as “Assistant Professor in Pharmaceutical Chemistry” at Dr. L. H. Hiranandani College of Pharmacy, Ulhasnagar (Affiliated to Mumbai University).

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