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Drug Design and Drug Discovery

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Abstract:- One of the key forces influencing the advancement of pharmaceuticals, biotechnology, and pharmacology is the drug industry. The process of finding and creating medications is known as drug discovery. It is a procedure designed to find a substance that has therapeutic value in treating and curing illness. The identification of candidates, synthesis, characterisation, screening, and tests for therapeutic efficacy are all steps in the drug discovery process.A chemical will start the drug development process before going through clinical trials if its efficacy in these tests has been demonstrated. Despite encouraging discoveries and billions dollar investments, the process of developing a new drug is a time-consuming and costly endeavor that is now experiencing a crisis. Currently, only roughly 400 distinct pharmacological targets are targeted by all of the available medicines combined. It is predicted that the number of possible therapeutic targets that could be used in future drug therapy is at least ten times higher.The process of finding a chemical that has therapeutic potential for treating and curing disease is known as drug discovery. Candidate identification, synthesis, characterisation, validation, optimization, screening, and tests for therapeutic efficacy are all steps in this process.Following a compound's demonstration of relevance in theseresearch, the drug discovery process will development before going through clinical trials. A treatment that satisfies all regulatory standards and is safe and effective must go through multiple stages of the new drug development process.Our article's overarching thesis is that the procedure is drawn out, costly, and complex enough that numerous biological targets must be taken into account before a new drug is finally approved for clinical usage, and new research instruments might be required to look into each one.

Keywords:- *Drug Discovery; Drug Development; Clinical Trials; Potential Drug Targets; Clinical Trial*

I. INTRODUCTION

The process of finding a molecule that can be used therapeutically to treat and cure an illness is known as drug discovery. A drug discovery project usually targets a biological target that has been demonstrated to have a part in the illness's progression or to have originated from a moleculewith intriguing biological properties.

The identification of candidates, synthesis, characterisation, screening, and tests for therapeutic efficacy are all steps in the drug discovery process.

Before going through with clinical trials, a molecule will start the medication development process if these studies have demonstrated its value.

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Because human clinical testing and research and development are expensive processes, drug discovery and development is a costly process. The range of the average total cost of drug development is US$ 897 million to US$ 1.9billion. Usually, development takes ten to fifteen years.

Although the majority of infectious disease cases occur in developing nations, there is a wide variety of medications available to treat various infectious diseasesis constrained. The majority of medications have previously been found either by chance discovery or by figuring out the active component from conventional treatments.

Currently, a novel strategy is being attempted to comprehend the molecular and physiological mechanisms governing illness and infection and to target particular entities according tothis understanding.

Drug development is a complex process that includes identifying a chemical compound that can be used therapeutically to treat and manage an illness state. New insights into a disease process often lead to the discovery of novel pharmaceuticals, which enable researchers to create medications that counteract or stop the consequences of the illness.

The identification of drug candidates, synthesis, characterisation, screening, and tests for therapeutic efficacy are all steps in the drug discovery process. Achemical will begin the process of medication development after clinical trials if it yields favorable results in these investigations.

The significant costs associated with clinical trials and research and development make drug discovery and development an expensive process. To create a single novel medicinal molecule, it takes between 12 to 15 years from the molecule from the moment of its discovery until the point at which it is sold for medical use Research and development expenses for each effective medication are estimated to range from $900 million to $2 billion on average.

The cost of the thousands of errors is included in this figure: In the end, just one compound out of every 5,000–10,000 that enter the pipeline for research and development is approved. These figures defy belief, but a quick review of the R&D process can help explain why so many compounds fail to reach the market and why it requires such a significant amount of time and money to develop one medication that actually helps patients.The greatest logical and scientific minds, advanced lab and technology, vast resources, and diversified project management are all necessary for success. It also requires luck and perseverance.

Eventually, billions of people experience relief, optimism, and faith thanks to the drug discovery process with a lengthy history, drug design is a sophisticated field of pharmaceutical research. Since Emil Fisher proposed at the close of the 1800s that the relationship between a drug and its receptor is similar to that between a key and a lock, a great deal of progress has been made in the field of drug design. Drug design has gradually evolved into a logical, well-structured science with a strong theoretical foundation and real-world applications. Currently, the most sophisticated method for drug discovery is drug design. In order to accomplish its primary objective—the creation of potent, targeted, safe, well-tolerated medications—it makes use of scientific and technological advancements and incorporates them into its extensive toolkit of techniques. One of the current disciplines that is developing the fastest is drug design, and its advancement is fueled by.

II. MODERN DRUG DISCOVERY PROCEDURES

➢ *Step 1: Identifying the Target*

The first crucial step in the drug discovery process is target identification. In general, a drug target is the particular binding site that a drug binds to in vivo and uses to carry out its activity. A particular medication target may have the following traits:

- A biomolecule (or biomolecules), usually a protein, that may exist in an isolated or complex form is theis the therapeutic target.
- The unique places on biomolecules complement one another.
- When a biomolecule attaches to a tiny molecule, the structure of the biomolecule may change, but these changes are typically reversible.
- Different physiological reactions that result from the modification of the biomolecule's structure lead to the control of the state of the cell, organ, tissue, or body.
- The physiological reactions brought on by modifications in the structure of biomolecules are important for complicated control and can treat diseased diseases.
- Over the course of the pathogenic process, the biomolecule's expression, activity, and structure may alter.
- Drugs are small chemicals that bind to biomolecules.

A critical molecule participating in a specific metabolic or signal transduction pathway that is unique to a disease condition or disease is known as a therapeutic target, as the description abovemakes clear.

The phrase "drug target" is disputed in the pharmaceutical business and has many limits. There are a few things to remember in this regard.

To begin with, a pharmacological target is a relative term. To begin with, a drug target is a biomolecule that is a part of a transduction pathway, much like other biomolecules. There is just onedistinction between the two:

Location and function within the transduction pathway. Another feature is that each pharmacological target is specific to a particular spectrum of disorders, meaning that each target is dependent on the condition.

➢ *Second,*

There are obviously many distinct pharmacological targets with regard to a given disease because the majority of

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human diseases are very complex and involve numerous risk factors. There is no way that a particular disease might be cured by focusing on a particular target. But the presence of multiple targets in a disease does not imply that each target contributes equally to its pathophysiology.Illness, and as a result, medications that target these targets in the treatment of the illness would not work as well.

- *Third,*

Medication objectives are subject to alter, so as our understanding of biomolecules and their function in the aetiology of specific diseases advances, the significance of therapeutic targets may be overestimated or underestimated.In actuality, knowledge of the disease's pathophysiology serves asthe foundation for the identification of pharmacological targets.

- *Fourth,*

A single medicine may have several targets, and multiple drugs target the same target. A drug's relationship with its target is one-to-many or many-to-one, rather than one-to-one.

- *Fifth,*

Researchers often want to obtain more selective medications that target newly identified and verified pharmacological targets. Nonetheless, it's important to remember that the body is a complex entity, and taking a medication with more specific side effects could upset its equilibrium. Ropecoxib is a particular COX-2 inhibitor as opposed to aspirin.

However, research has indicated that rofecoxib raises the risk of cardiovascular disease; as a result, themedicine was taken off the market.

- *Sixth,*

One biomolecule is typically referred to as a therapeutic target. A drug target can be categorized into two kinds based on the availability of drugs: prospective drug targets and established drug targets. medication objectives. The former are those that have a strong body of research backing them up, covering topics such as how the target affects human pathology and how it behaves normally in physiology.

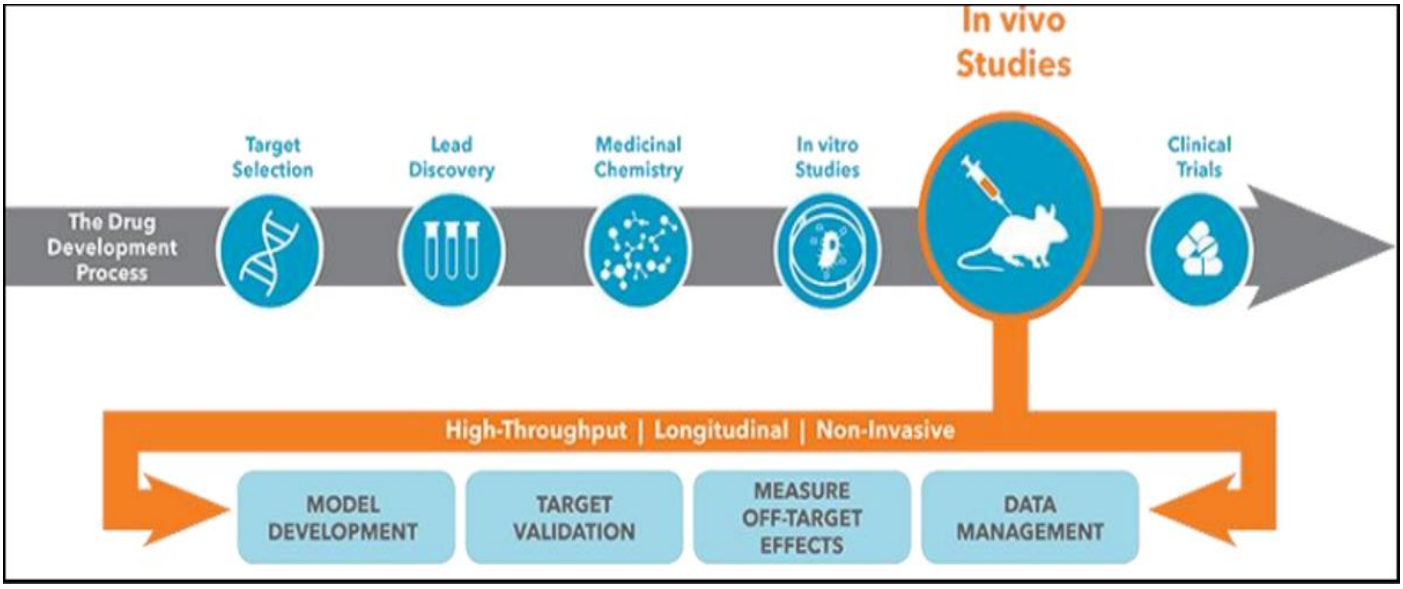

Fig 1 Stages of Drug Discovery and Development Process

The science of drug design has achieved significant strides that have elevated it to the forefront of drug discovery both now and in the future . First among these is knowledge of drug-receptor identification. Emil Fisher likened the relationship between a medication and its receptor to that between a key and a lock in the early 1890s. He reasoned that without altering their conformations, the medication and the receptor interact as solid bodies. Daniel Koshland recently proposed that throughout an encounter, both molecules go through conformational changes and take on the best configuration to bond with one another. X-ray structures and in silico simulations have repeatedly demonstrated the validity of this theory, and it is now established that ligands do, in fact, adopt conformations during interactions.

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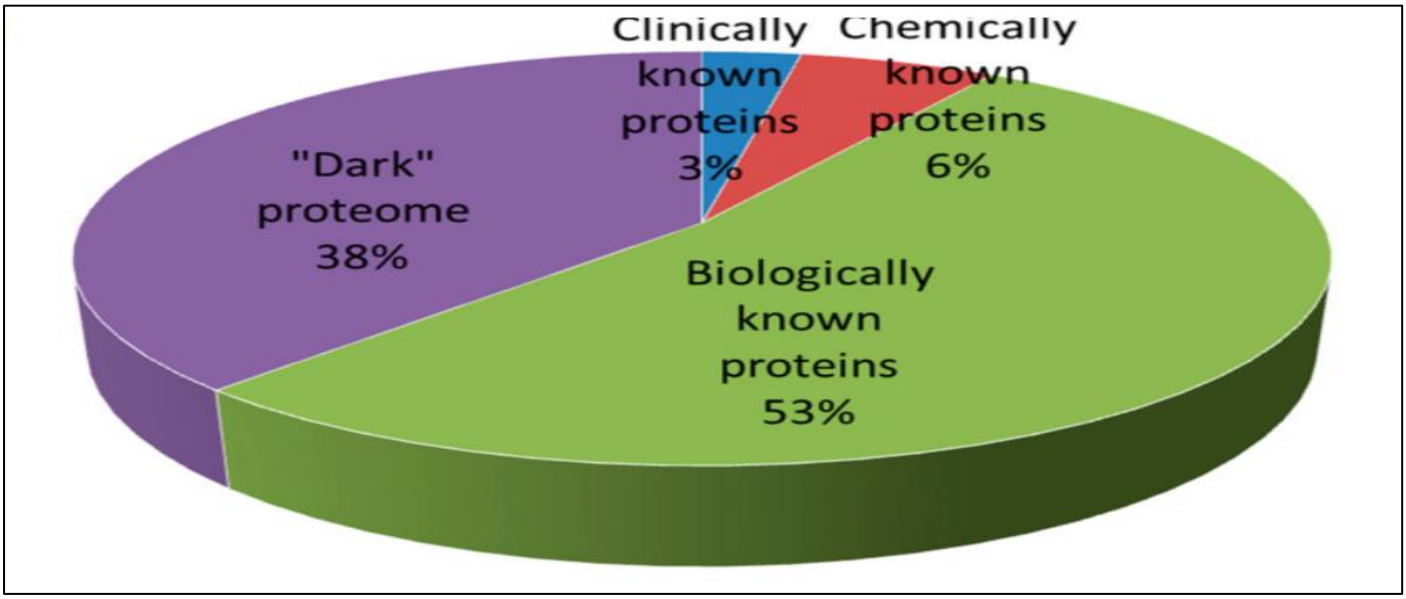

Fig 2 The human druggable proteome divided according to the target development level [28]. Clinically known targets includes proteins linked to at least one approved drug. Chemically known targets includes proteins known to bind with high potency small molecules that are not yet drugs. Biologically known targets refer to proteins that have a link to any disease but have not been studied for binding to small molecules. The "dark" proteome includes the unstudied proteins.

III. COMPUTER-AIDED DRUG DESIGN

The use of computational technologies in drug design and discovery processes has grown. Drug-receptor complexes are frequently studied using computational chemistry techniques in atomic specifics and to compute the characteristics of potential small-molecule drugs. The massive chemical and biological activity databases that all pharmaceutical companies today own must be managed and organized, and these databases must be used to their fullest potential, which requires the application of tools from the information sciences and statistics.

Furthermore, computerized automation of the process of creating chemical derivatives is highly feasible. Using targeted structure-based combinatorial chemistry, libraries of derivative compounds are created from active site studies. This method's combinatorial nature opens up the possibility of many different potential structures. A computer is capable of producing and predicting. All possible derivatives can be generated and predicted by a computer quickly, yielding a list of the top choices. Essentially, a computer the chemist can concentrate on, create, and test only the most promising ligands by filtering out all weak binding molecules. Therefore, the most efficient way to use these capabilities is to help refine lead molecules by using the CADD program. In contemporary drug design, using computer modeling to refine structures has become common procedure.

➢ *Accordingly, the Current Function of computers in Drug Design is to:*

Information storage and retrieval (a)

- Experimentally determined structures for biological targets (enzymes) and pharmacological compounds using X-ray cryst allography.
- Activities and molecules to examine the effects of minute structural modifications.

➢ *Challenges in Computer-Aided Drug Design*

CADD requires highly intelligent individuals with interdisciplinary understanding of several scientific domains, most notably biology, chemistry and computation, which presents a significant obstacle. For this particular field. Accuracy and processing speed are crucial in scientific computing. Thus, a great deal of approximation, several algorithmic shortcuts, and a multitude of assumptions have to be employed in order to complete the computations in a limited amount of time. As a result, the estimated accuracy of any ligand-receptor interaction is significantly reduced. This continues to be the biggest obstacle in CADD. The production of an enormous amount of unwanted chemical structures because there are almost an endless number of possible atom combinations, and the majority of these are more hazardous, difficult to synthesize, or chemically unstable in the past ten years, better software has been developed with more user-friendly programs, faster and better computing facilities, and the ability to create synthetic chemical compounds that are stable and viable while also having a refining feature—all in response to the deficiencies of CADD.

➢ *Software used*

The following are some of the key aspects of software that is commonly used in drug design:

- *Gratitude*

✓ Finds the optimal ligand-receptor binding modes automatically by using the energy of the ligand/receptor complex (energy-driven method)
✓ Automated, flexible docking

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The three programs that make up AutoDock (Automated Docking of Flexible Ligands to Receptors) are as follows:

The process of docking the ligand to a series of grids that describe the target protein is carried out by AutoDock. AutoGrid computes these grids beforehand.

Which bonds in the ligand are designated as rotatable is determined by AutoTors Offer an automated process to anticipate how ligands will interact with bio molecular targets, assist in reducing the range of conformational possibilities, and identify the most.

- *Appropriate Arrangement*

✓ Employs a grid-based molecular affinity potentials-based Monte Carlo (MC) simulated annealing (SA) technique for configurational exploration and quick energy evaluation.
✓ It has applications in X-ray crystallography, SBDD, lead optimization, virtual screening, combinatorial library design, protein-protein docking, and chemical mechanism research.
✓ It is a potent solution to the challenge of docking a flexible substrate into the binding site of a static protein.

➢ *Molecular Docking and Virtual Screening:*

- AutoDock
- AutoDock Vina
- FlexX
- GOLD
- MOE-Dock

➢ *Pharmacophore Modeling and QSAR:*

- Pharmer
- Phase
- QSAR+
- Molinspiration

➢ *Molecular Dynamics Simulations:*

- Desmond
- GROMACS
- LAMMPS
- NAMD

➢ *Quantum Mechanics and Molecular Mechanics (QM/MM):*

- Gaussian
- ORCA
- QMERA
- Jaguar

➢ *Machine Learning and Artificial Intelligence:*

- DeepChem
- ChemML
- TensorFlow
- PyTorch

➢ *Cheminformatics and Data Analysis:*

- RDKit
- ChemPy
- Pybel
- CDK (Chemistry Development Kit)

➢ *Visualization and Graphics:*

- PyMOL
- Chimera
- VMD (Visual Molecular Dynamics)
- Molscript

➢ *Drug Discovery and Development:*

- Pipeline Pilot
- Knime
- Chemaxon
- CambridgeSoft

➢ *Molecular Modeling and Simulation:*

- CHARMM
- AMBER
- GROMOS
- OPLS

➢ *Computational Chemistry and Physics:*

- GAMESS
- Gaussian
- ORCA
- QMERA

- Note: This list is still not exhaustive, as new software and tools are being developed and released regularly.

IV. METHODOLOGY

A. The Methodology for Drug Design and Drug Discovery Typically Involves the following Steps:

➢ *Target Identification:*

- Identify a biological target (protein, receptor, enzyme) involved in a disease or condition.
- Validate the target through experimental and computational methods.

➢ *Lead Identification:*

- Use various methods such as:
- High-throughput screening (HTS)
- Virtual screening (VS)
- Fragment-based lead discovery (FBLD)

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- Identify small molecules or fragments that bind to the target.

➢ *Lead Optimization:*

- Use structure-based drug design (SBDD) and ligand-based drug design (LBDD) techniques.
- Optimize lead molecules through:
- Chemical modifications
- Molecular modeling and simulations
- Experimental testing

➢ *Preclinical Testing:*

- In vitro assays (cell-based, biochemical)
- In vivo studies (animal models)
- Evaluate efficacy, toxicity, and pharmacokinetics (PK).

➢ *Clinical Testing:*

- Phase I: Safety and PK in healthy volunteers
- Phase II: Efficacy and safety in patients
- Phase III: Large-scale efficacy and safety trials

➢ *Computational Tools and Methods:*

- Molecular modeling and simulations
- Docking and scoring
- Pharmacophore modeling
- Quantitative structure-activity relationships (QSAR)

➢ *Experimental Methods:*

- X-ray crystallography
- Nuclear magnetic resonance (NMR) spectroscopy
- Mass spectrometry (MS)
- Biochemical and cellular assays

➢ *Data Analysis and Interpretation:*

- Use statistical and machine learning methods
- Analyze and interpret data from experimental and computational methods

➢ *Iterative Cycle:*

- Refine and repeat the process based on results and new information

- Note: This is a general outline, and the specific methodology may vary depending on the project and the organization.

➢ *Some of the Computational Tools and Software used in Drug Design and Discovery Include:*

- Molecular modeling: MOE, SYBYL, PyMOL
- Docking and scoring: GOLD, DOCK, GLIDE
- Pharmacophore modeling: PHASE, MOE
- QSAR: MOE, SYBYL, R
- Molecular dynamics simulations: GROMACS, AMBER, NAMD

➢ *Some of the Experimental Methods and Techniques used in Drug Design and Discovery Include:*

- X-ray crystallography: Rigaku, Bruker
- NMR spectroscopy: Bruker, Varian
- Mass spectrometry: Thermo Fisher, Agilent
- Biochemical and cellular assays: ELISA, Western blot, cell-based assays.

V. RESULT AND DISCUSSION

- Using molecular docking studies and virtual screening to identify possible lead chemicals
- Structure-based design and molecular modeling optimization of lead compounds
- Synthesis and biological assessment of optimized compounds
- Testing specific substances both in vitro and in vivo
- Finding a possible medication option with the appropriate toxicity profile and desired pharmacological activity

➢ *The Study's Findings show the value of Combining an Experimental and Computational Approach to Drug Design and Discovery: -*

Virtual screening and molecular docking studies allowed for the quick identification of possible lead compounds; - Structure-based design and molecular modeling optimization produced compounds with improved potency and selectivity; - Synthesis and biological evaluation of optimized compounds validated the expected activity and selectivity; - The identified drug candidate shows promise for further development and possible clinical application The study emphasizes the value of using computational tools in conjunction with experimental validation to provide an integrated strategy to drug design and discovery.

VI. CONCLUSION

The results of this study contribute to the development of new drugs and therapies and highlight the potential of computational tools in drug discovery. This study demonstrates the successful application of drug design and discovery methodologies in identifying a potential drug candidate. The combined use of computational and experimental approaches accelerated the discovery process and improved the efficiency of lead optimization.One of the most intricate and challenging processes in the pharmaceutical industry is the discovery of novel medications with potential therapeutic uses. Man-hours and millions of dollars are committed to finding novel therapeutic agents. Since a medication's efficacy depends on a wide range of variables, including its metabolism, toxicity, and bioavailability, rational drug design has long been a pipe dream. Reasonable medication design is now possible thanks to recent, remarkable scientific advancements in fields like molecular biology, computer sciences, and structural

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characterisation of biomacromolecules. CADD is now more than just a promising method. It is a realistic and useful method of supporting medicinal chemists. Although it is unlikely to produce pharmaceutical innovations on its own, it has grown to be a substantial

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REFERENCES

[1]. Shayne CG. Introduction: drug Discovery in the 21stCentury. Drug Discovery Handbook, Wiley Press, 2005; 1-10.
[2]. Smith GC, OíDonnel JT. The Process of New Drug Discovery and Development, Eds., 2nd edition, Informa Healthcare, New York 2006.
[3]. Moffat J, Vincent F, Lee J, Eder J, Prunotto M. Opportunities and Challenges in phenotypic drug discovery: an industry perspective. Nature Reviews Drug Discovery, 2017; 16(8):531-543.
[4]. DiMasi JA, Hansen RW, Grabowski HG. The price of innovation: new Estimates of drug development costs. Journal of Health Economics, 2003; 151-185.
[5]. Gashaw I, Ellinghaus P, Sommer A, Asadullah K. What makes a good Drug target. Drug Discovery Today, 2012; 17:S24-S30.
[6]. Lindsay MA. Target discovery. Nature Reviews Drug Discovery, 2003; 2:831–838.
[7]. Terstappen G, Schlüpen, C, Raggiaschi R, Gaviraghi G. Target Deconvolution strategies in drug discovery. Nature Reviews Drug Discovery, 2007; 6(11):891-903.
[8]. Peet NP. What constitutes target validation? Targets. 2003; 2:125–127.
[9]. Imming P, Sinning C, Meyer A. Drugs, their targets and the nature and Number of drug targets. Nature Reviews Drug Discovery, 2006; 5:821-834.
[10]. Odilia Osakwe. Social Aspects of Drug Discovery, Development and Commercialization. Chapter 6 Preclinical In Vitro Studies: Development and Applicability. Elsevier. 2016.
[11]. Croston G. The utility of target-based discovery. Expert Opinion on Drug Discovery, 2017; 12(5):427-429.
[12]. Henning SW, Beste G. Loss-of-function strategies in drug target Validation. Current Drug Discovery Technology, 2002; 17–21.
[13]. John GH, Martyn NB, Bristol-Myers S. High throughput screening for Lead discovery. Burger_s Medicinal Chemistry and Drug Discovery, 6Th Edition, Drug Discovery and Drug Development, Wiley Press, 2002; 2:37-70.
[14]. Patidar AK, Selvam G, Jeyakandan M, Mobiya AK, Bagherwal A, Sanadya G, Mehta R. Lead Discovery and lead optimization: A useful Strategy in molecular modification of lead compound in analog design. International journal of drug design and discovery. 2011; 2(2):458-463.
[15]. Huber W. A new strategy for improved secondary screening and lead Optimization using high-resolution SPR characterization of compound– Target interactions. J Mol. Recogn. 2005; 18:273–281.
[16]. Lofas S. Optimizing the hit-to-lead process using SPR analysis. Assay Of Drug Development Technologies, 2004; 2:407-416.
[17]. Barile FA. Pri. Nciples of Toxicological Testing. CRC Press, USA, 2008.
[18]. Friedman LM, Furberg CD, Demets DL. Fundamentals of clinical Trials. 4th ed. New York: Springer Science and Business Media LLC; 2010.
[19]. Faqi AS. A comprehensive guide to toxicology in preclinical drug Development. Waltham, MA: Elsevier; 2013.
[20]. Vogel HG. Drug Discovery and Evaluation 2nd edition. Springer, USA, 2002.
[21]. Karara AH, Edeki T, McLeod J, et al. PhRMA survey on the conduct Of first-in-human clinical trials under exploratory investigational new Drug applications. Journal of ClinicalPharmacology, 2010; 50:380–391.
[22]. Fitzpatrick S. The clinical trial protocol. Buckinghamshire: Institute of Clinical Research; 2005.
[23]. Kinders, Robert, et al. Phase 0 Clinical Trials in Cancer Drug Development: From FDA.
[24]. DiMasi J. Risks in New Drug Development: Approval success Rates For Investigational Drugs. Clinical Pharmacology & Therapeutics, 2001; 297-307.
[25]. Friedhoff L. New Drugs: An Insider‘s Guide to the FDA‘s New Drug Approval Process for Scientists, Investors and Patients. New York, NY: PSPG Publishing; 2009.
[26]. FDA, The FDA and the Drug Development Process: How the FDA Insures that drugs are safe and effective, FDA Fact sheet, 2002.
[27]. Adams CP, and Brantner VV. New Drug Development: Estimating Entry from human clinical trials. Bureau of Economics Federal Trade Commission. 2003.
[28]. Lipinski CA, Lombardo F, Dominy BW, Feeney PJ. Experimental and Computational approaches to estimate solubility and permeability In drug discovery and development settings. Adv Drug Deliv Rev 2001;46:3-26.

ISSN No:-2456-2165 https://doi.org/10.38124/ijisrt/IJISRT24SEP329

[29]. Luscombe NM, Greenbaum D, Gerstein M. What is bioinformatics? A proposed definition and overview of the field. Methods Inf Med 2001;40:346-58.
[30]. Manly CJ, Louise-May S, Hammer JD. The impact of informatics and Computational chemistry on synthesis and screening. Drug Discov Today 2000;6:1101-10.
[31]. Meyer AY, Richards WG. Similarity of molecular shape. J Comput Aided Mol Design 1991;5:427-36.
[32]. Meyer EF, Swanson SM, Williams JA. Molecular modelling and drug Design. Pharmacol Ther 2000;85:113-21.
[33]. Mulholland AJ, Grant GH, Richards WG. Computer modelling of enzyme Catalysed reaction mechanisms. Protein Eng 1993;6:133-9.
[34]. Oprea T.I., Bologa C.G., Brunak S., Campbell A., Gan G.N., Gaulton A., Gomez S.M., Guha R., Hersey A., Holmes J., et al. Unexplored therapeutic opportunities in the human genome. Nat. Rev. Drug Discov. 2018;17:317–332. Doi: 10.1038/nrd.2018.14. [PMC free article] [PubMed] [CrossRef] [Google Scholar]

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CERTIFICATE

This is to certify that **GROUP 2** of Department Pharmaceutical Science and Technology of Madan Mohan Malaviya University of Technology, Gorakhpur has carried out the project work presented in this report entitled "**DRUG DESIGN AND DRUG DOSCOVERY**". The report embodies results of their works and studies carried out by the student themselves and the content of report does not form the part of any other degree to this candidate or to anybody else.

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