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# Insilico-Innovative Tool for Drug Design and Development

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***Abstract:***
*Discovery and development of a new drug is generally known as a very complex process which takes a lot of time and resources. So now a day's computer aided drug design approaches are used very widely to increase the efficiency of the drug discovery and development course. Various approaches of CADD are evaluated as promising techniques according to their need, in between all these structure-based drug design and ligand-based drug design approaches are known as very efficient and powerful techniques in drug discovery and development. These both methods can be applied with molecular docking to virtual screening for lead identification and optimization. In the recent times computational tools are widely used in pharmaceutical industries and research areas to improve effectiveness and efficacy of drug discovery and development pipeline. In this poster I am going to overview of innovative tool in the process of drug discovery and development research.*

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## I. INTRODUCTION:

The drug is most many times a natural small molecule that activates or inhibits the feature of a biomolecule such as a protein, which in flip results in a therapeutic gain to the patient. In the most fundamental sense, drug diagram entails the graph of small molecules that are complementary in form and cost to the biomolecular goal with which they engage and consequently will bind to it. Drug sketch often but now not necessarily relies on laptop modeling techniques. This kind of modeling is frequently referred to as computer-aided drug design. Finally, drug layout that relies on the expertise of the three-D structure of the biomolecular target is acknowledged as structure-based drug design. They involve, drug which bind to a target (e.g., protein, nucleic acid).

**REQUIREMENTS:**

❖ ***Selected/designed molecule should be:***

1. organic small molecule,
2. complementary in shape to the target,
3. oppositely charge to the bio-molecular target.

❖ ***The molecule will:***

- interact with target,
- bind to the target,
- Increase or decrease the effects of biomolecules.

❖ **Novel drug approaches like:**

- CADD (Computer Aided Drug Design),
- Molecular Modeling,
- Structure based drug design,
- Analog drug design,
- Combinatorial chemistry,
- Computational chemistry,
- Array technology,
- Pharmacogenomics,
- Combinatorial Chemistry,
- Proteomics,
- Recombinant DNA technology, etc.

## II. METHODS:

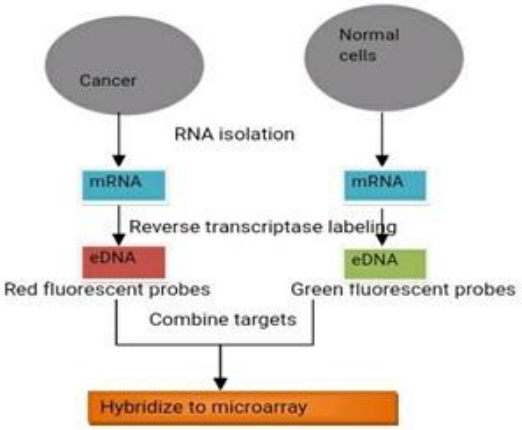
1. Array technology
2. Pharmacogenomics
3. Combinatorial Chemistry
4. Proteomics
5. Recombinant DNA technology.

**1. Array technology**

- Based on RNA & DNA hybridization reaction.
- Simultaneously several of gene can be analyzed.

**Advantages:**
- Miniaturization,
- Development of fluorescent labeled nucleotides, which is detected by laser screening.

**Methods used:**
- Chips located with synthetic oligonucleotides.
- Chip attached with DNA fragment.




**FLOWCHAT 1**: *Array Technology between Normal Cells & Cancer Cells*

**Types:**
1. DNA microarray
2. RNA microarray
3. Protein microarray
4. Antibody microarray
5. Tissue microarray

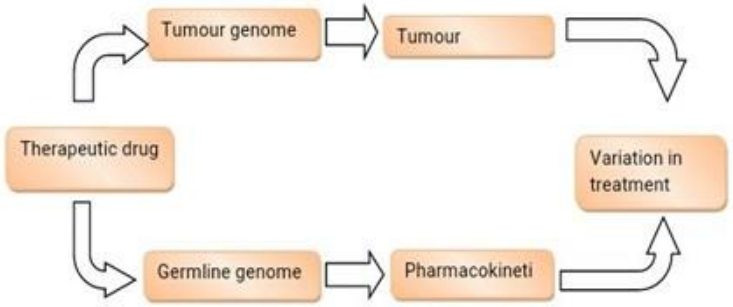
**Application of microarray:**
- *Monitor gene expression*
- Study regulatory networks,
- Drug discovery – mechanism of action
- Diagnostics – tumor diagnosis

- *Genomic DNA hybridizations*
- Explore microbial diversity
- Whole genomic comparisons – genome evolution
- Identify DNA biding sites
- Diagnostics – tumor diagnosis

**2. Pharmacogenomics**

Pharmacogenomics is the study of the role of the genome in drug response. It identifies reflects its combining of pharmacology and genomics. It analyzes genetic makeup individual affects response to drugs. Several genes which are responsible for variances in drug metabolism and response.

- Cytochrome P450s
- VKORC1
- TPMT




**FLOWCHAT 2***: Pharmacogenomics of Genomes in Drug Response*

Example case studies:

- Case A – Antipsychotic adverse reaction
- Case B – Pain Management
- Case C – FDA Warning on sedative drugs.

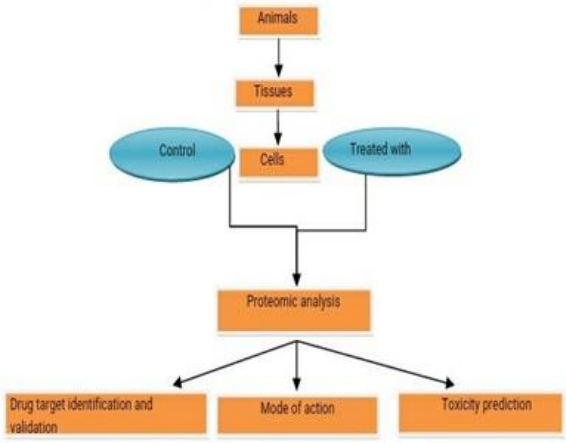
**3. Proteomics**

Proteomics involves study of large amounts of proteins. It's playeda vital role in living organism with many functions. In this process, proteome is an entire set of protein, which produced or modified by organism. It enables identification of ever-increasing number of proteins.

**Methods:**

There are three methods of separating protein complex

- Denaturing polyacrylamide gel electrophoresis (PAGE) or sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE),
- two-dimensional gel electrophoresis, and
- high-performance liquid chromatography (HPLC).




**FLOWCHAT 3**: *Steps Involved in Proteomics*

**Application:**

- New Drug Discovery
- Interaction proteomics and protein networks,
- Expression proteomics,
- Biomarkers,
- Proteogenomics,
- Structural proteomics.
- system biology,
- Human plasma proteome.

## III. RESULTS:

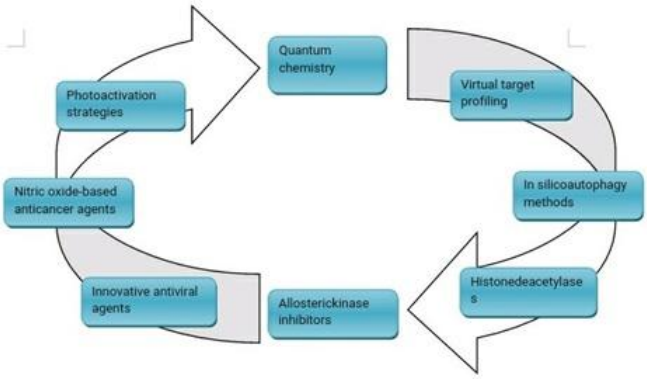
- Randomly screening of synthetic compounds,
- Novel compounds preparation from plants and animal origin(lead skeleton),
- Preparation of structural analogs & increase biological activity,
- Functions of isosteric principle.

## IV. DISCUSSION:

The rate of extent of drug design and discovery is dependent on ability to identify new target drug molecules, is also known as new chemical entities. It essentially possesses the inherent capability and control of a specific disease/ailment. Besides, being efficacious and safer in character, new chemical entities possess absolute position and functions of biological target, by making more or less core element of the entire drug design & discovery process.

**Modern techniques in drug design & discovery:**

- Quantum chemistry,
- Virtual target profiling
- In silicoautophagy methods
- Histonedeacetylases
- Allosterickinase inhibitors
- Innovative antiviral agents
- Nitric oxide-based anticancer agents
- Photoactivationstrategies.




**FLOWCHAT4**: *New Techniquesand Strategies in Drug Discovery*

## V. CONCLUSION:

Novel approaches in drug design is a creative process of finding new chemical entity based on knowledge of biological target. Bio-isosteres is an important lead modification, plays a vital role in alteration of pharmacokinetics of lead. In general, drug discovery in laboratory experiments is time consuming and expensive methods as compared to computational methods and it plays a vital role in pharmaceuticaldevelopment of new drug for therapeutic efficacy.

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