## Reverse Pharmacognosy

M.M. Ahmadian-Attari Pharm.D., Ph.D.



### What is Pharmacognosy

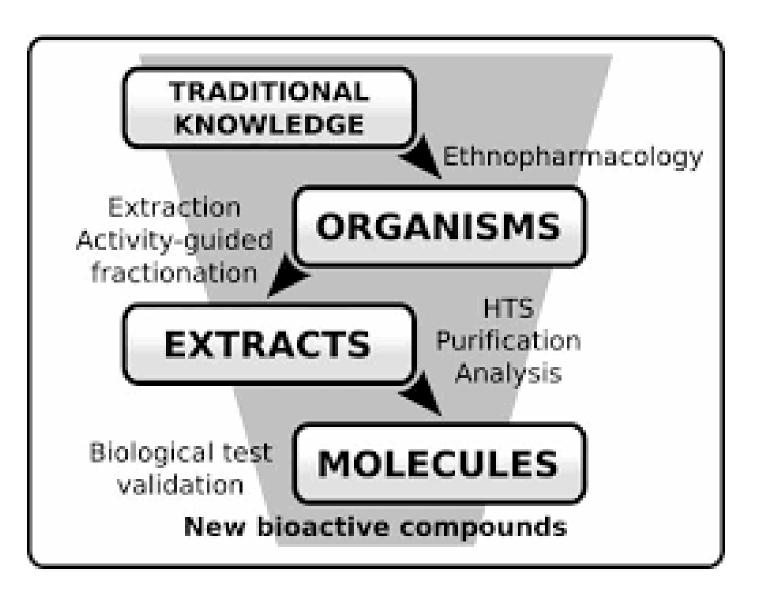
"the study of the physical, chemical, biochemical and biological properties of drugs, drug substances or potential drugs or drug substances of natural origin as well as the search for new drugs from natural sources".



## Blind screening











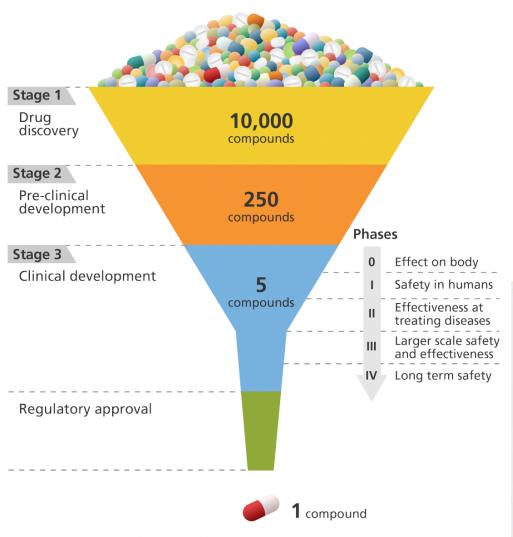
اقاب كارندا چهار وربه و آن شرخ امير و درسي مي فرد و اربار فيرس كلارند و با آب ركانا نول جب بند نديند ركنا ركوعي شري اربي خير مي بند في التنابي المين المين



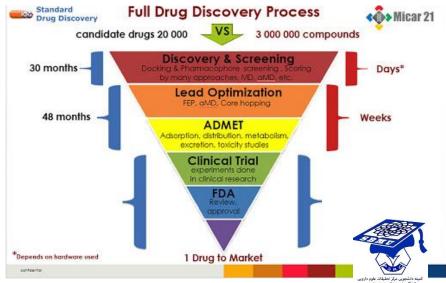




#### Virtual screening vs. Blind screening

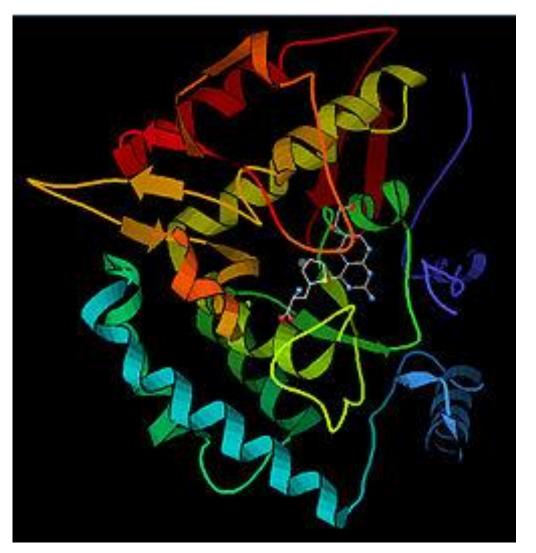


Computational drug discovery
(In silico methods)



Compound

Target





# Traditional knowledge and virtual screening

What is the exact pathology of Alzheimer's?

Multiple sclerosis?

Epilepsy?

ALS?

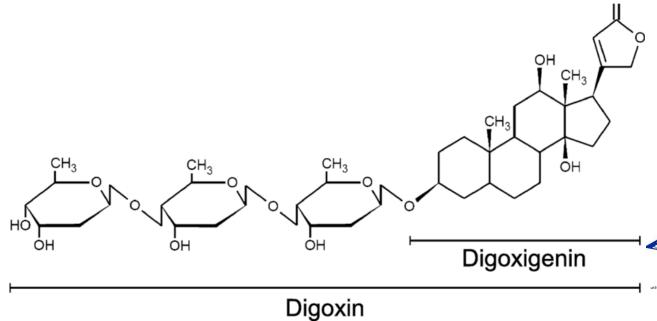
etc.



## Finding lead compounds

Galantamine

Digoxin



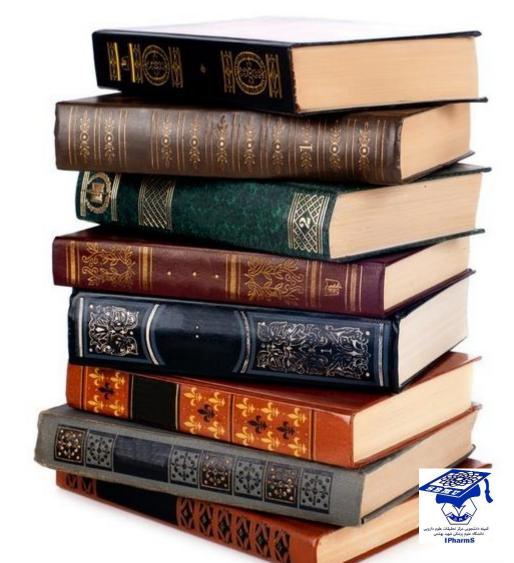
Galegine → Metformin

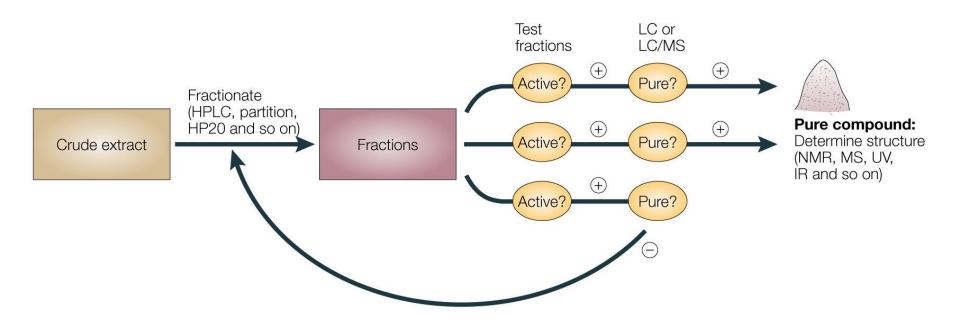


Podophyllotoxin → Etoposide



- Traditional medicine
- Ethnic knowledge

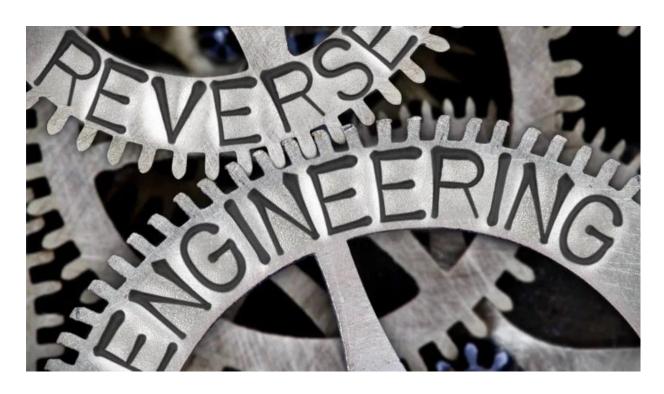






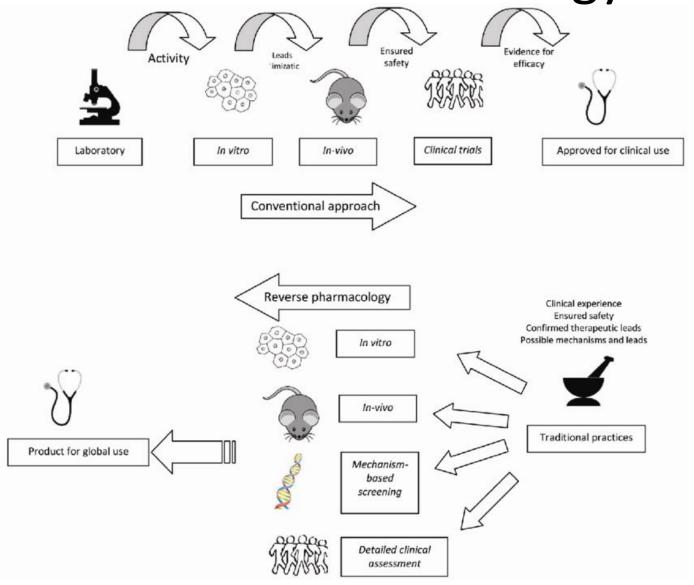
#### "Reverse"

Reverse engineering





Reverse Pharmacology





## **Reverse Pharmacognosy**

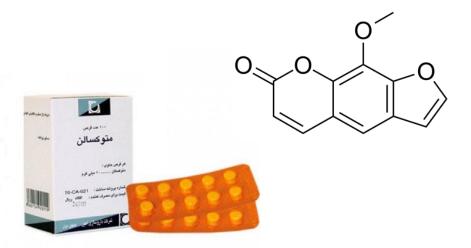


#### Reverse Pharmacognosy Pharmacognosy Vegetal realm Natural compounds Ethnopharmacological Druglikeness criteria & botanical selection selection Greenpharma Diversity selection criteria selection Plants Molecule Database Molecule Library Extracts Virtual screening with Selnergy™ and/or Biological tests Biological tests Knowledge-base Biq-guided identification identification Bio-active molecule(s) Plant(s)



#### Ammi majus

Furanochromone:Methoxsalen



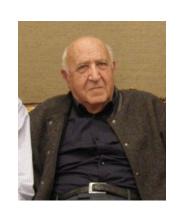




#### Ammi majus

- Native to Egypt
- Methoxsalen content in the seed =1%



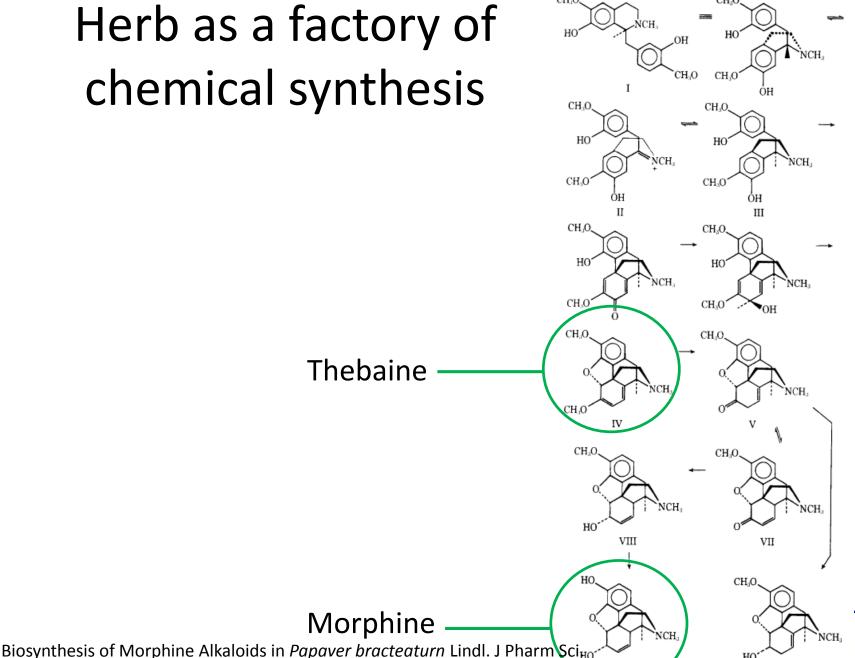




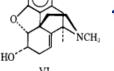


- Diplotenia damavandica
- Native to Iran
- Methoxsalen content in the seed = 5%

## Herb as a factory of chemical synthesis

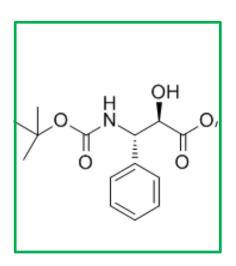


1978; 67(1):103-6.





#### taxol



docetaxel



- Different biosynthesis pathways
- Different precursors
- New chemical entity



corylus avellana