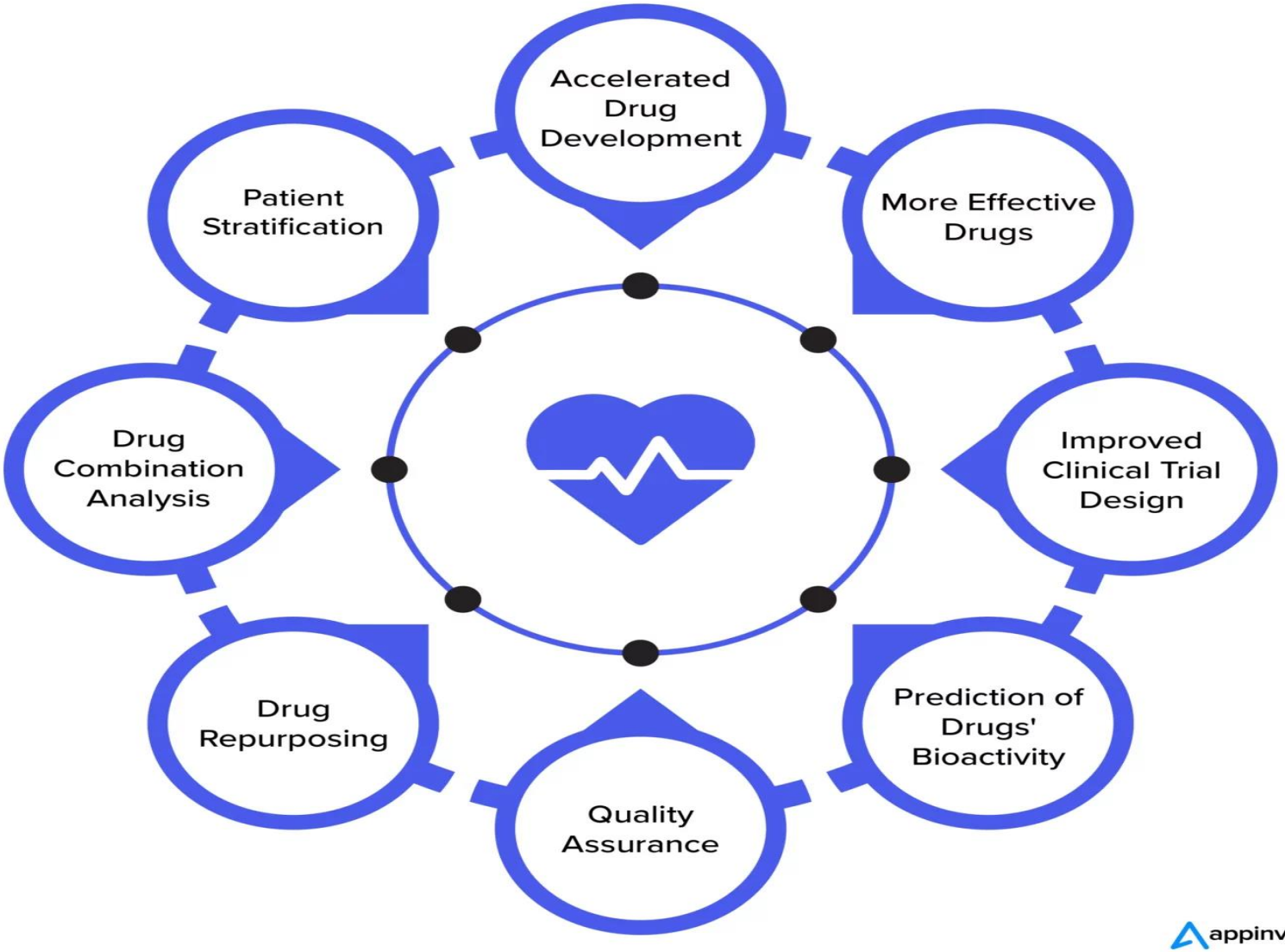
Artificial Intelligence can boost Pharmacognosy and Drug Discovery

Presenter:
Dr. Laleh Khodaie
Associate Professor of Pharmacognosy
Pharmacy faculty of Tabriz
Tabriz University of Medical Sciences
Tabriz, Iran.


یووال نوح هراری
۲۱ درس
برای قرن ۲۱

Ways in Which AI Transforms Drug Discovery



appinventiv

Introduction

- Artificial intelligence (AI) technology plays a role in various **medical fields**.
- It has the ability of the machine to **mimic** human **analytical reasoning**.
- Emergence of **data-based medicine** in the clinical Recent research has linked **health care** with **AI** to acquire the **proper knowledge** in **herb usage**.

Introduction

- Representation of **different networks** related to **symptoms** to **predict herb selection**.
- Facilitating the **discovery** of new drugs.
- The AI and learning tools facilitate **research**, **drug discovery**, and **decision-making** on **unclear** clinical evidence of **herbal therapies**.
- **AI** is currently used for **pattern diagnostics**.
- **Symptoms** classifications, **clinical data** of patients, and finding **drug candidate** substances in the **CAM** or **traditional medicine** fields.

The problem of herbal medicine

- An **enormous** amount of **herbal knowledge** has already been **published** in the form of **text** or **documents** for a long time.
- A primary factor of this investigation is the lack of experts to **classify** herbal usage and **pharmacological properties** and specified **targets.**
- It leads to **misinterpretations** about **herb usage**.
- Identification of Phytochemicals can help.
- **Isolation** and **Investigation** of **phytochemicals** is **costly** and **time-consuming**.

AI algorithms

- A simple example of an algorithm
- **The AI algorithm** is the **programming** that **tells the computer** how to learn to operate.
- **Types** of Artificial Intelligence Algorithms

1. Machine Learning (ML)

- Machine Learning is a subset of AI
- It focuses on developing algorithms that allow computers to learn from and make predictions based on data.

2. Deep Learning (DL)

- It's another subset of AI
- The device continues to gain knowledge to improve processes and run tasks more efficiently.

How AI algorithms can help?

- An **Artificial Intelligence Algorithm** makes it easier to go through **massive amounts of data.**
- It acts By Using **specialized software**.
- Researchers can process large amounts of **information** from **databases** to **find correlations**.
- That often leads to **cures**, **diagnosis**, **new treatments**, **drug repurposing**, **vaccine integration**, and more.

Databases

- **AI algorithms** analyze **extensive data** from **databases** providing **herbal medicine information**.
- There are well-developed **herbal medicine databases** from **several countries**.
- They help in **predicting** different **ingredients** and various **effects** for **various diseases** using **AI models**.
- They will assist **physicians** in helping patients and drug discovery.

Databases

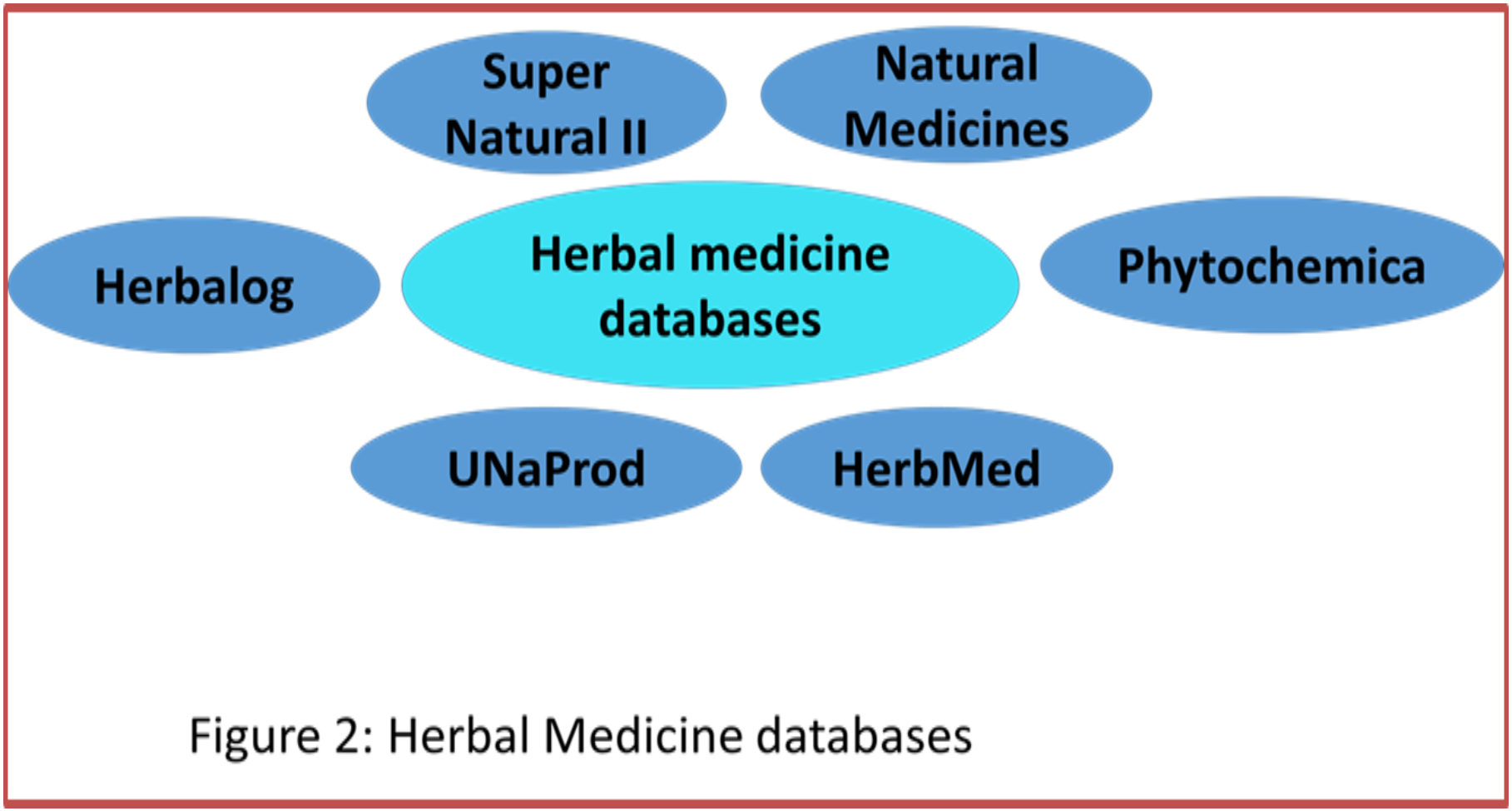


Figure 2: Herbal Medicine databases

Databases

600 **Table 1**. Comprehensive herbal databases to extract information for PHM.

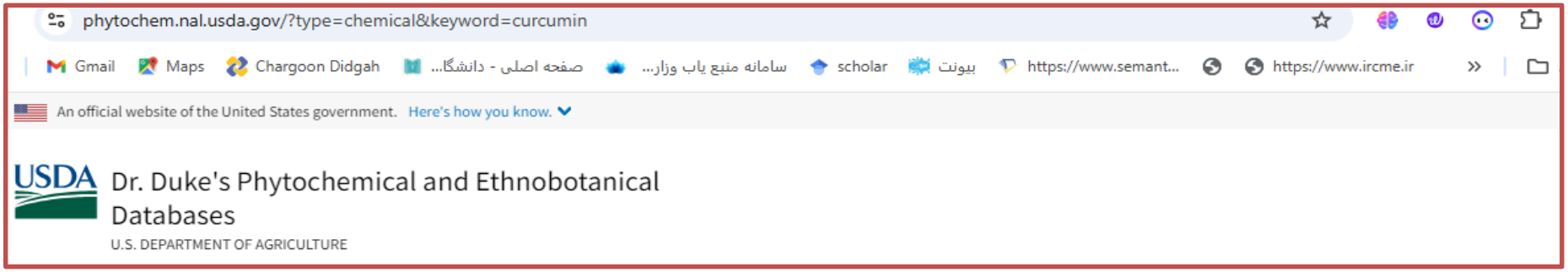
No.	Database	Dominant Features
1	Dictionary of Natural Products https://dnp.chemnetbase.com/chemical/ChemicalSearch.xhtml?dswid=4400	It is a Plant-metabolite database.

27

2	Traditional Chinese Medicine Integrated Database http://www.megabionet.org/tcmid/	Prescriptions, herbs by English, Chinese, and Latin names, Formulas or herbs could be searched by target proteins, and disease could be searched.
3	MPD3 http://bioinform.info	

ed States)

Databases



Search the Databases

Dr. Duke's Phytochemical and Ethnobotanical databases facilitate in-depth plant, chemical, bioactivity, and ethnobotany searches using scientific or common names. Search results can be downloaded in PDF or spreadsheet form. Of interest to pharmaceutical, nutritional, and biomedical research, as well as alternative therapies and herbal products.

Search

Filter by entity type

Chemical

Enter search terms

curcumin

Search | Clear

Displaying 1 - 20 of 20

Key:

A = Biological Activity | C = Chemical | E = Ethnobotany Plant | P = Plant | S = Syndrome | U = Ethnobotany Use

C 5-EPIHEXAHYDROCURCUMIN

C 5'-METHOXY-CURCUMIN

Databases

pubchem.ncbi.nlm.nih.gov/#query=curcumin&tab=pubmed

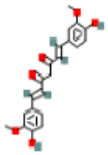
Gmail Maps Chargoon Didgah صفحه اصلی - دانشگا... سامانه منبع یاب وزار... scholar بیونت https://www.semant... https://www.ircme.ir

SEARCH FOR

curcumin

Treating this as a text search.

BEST MATCH



curcumin; 458-37-7; Diferuloylmethane; Natural yellow 3; Kacha haldi; Indian saffron; Curcuma; Gelbwurz; ...

Compound CID: 969516

MF: $C_{21}H_{20}O_6$ MW: 368.4g/mol

IUPAC Name: (1E,6E)-1,7-bis(4-hydroxy-3-methoxyphenyl)hepta-1,6-diene-3,5-dione

SMILES: COC1=C(C=CC(=C1)/C=C/C(=O)CC(=O)/C=C/C2=CC(=C(C=C2)O)OC)O

InChIKey: VFLDPWHFBUODDF-FCXRPNKRSA-N

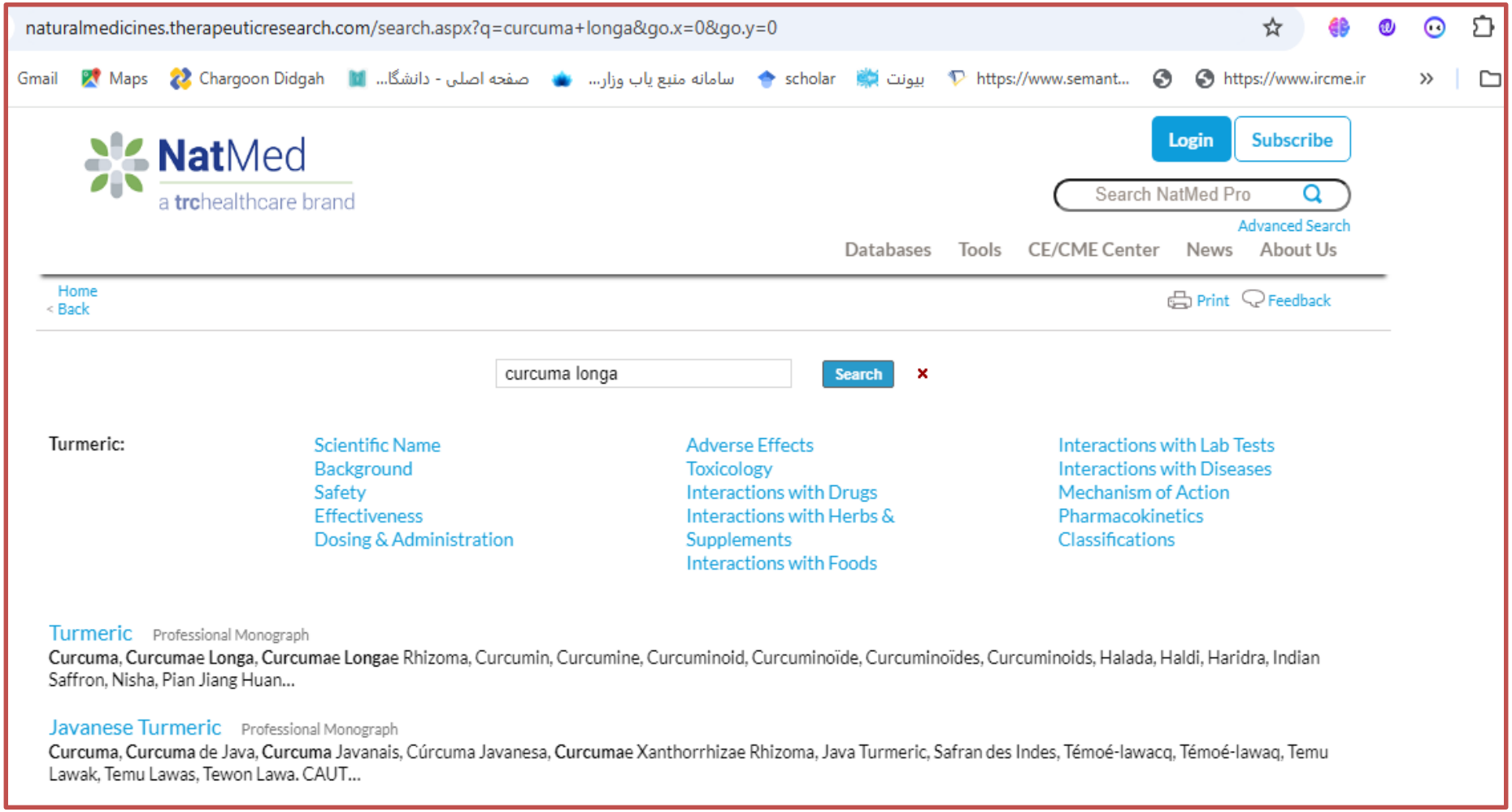
InChI: InChI=1S/C21H20O6/c1-26-20-11-14(5-9-18(20)24)3-7-16(22)13-17(23)8-4-15-6-10-19(25)21(12-15)27-2/h3-12,24-25H,13H2,1-2H3/b7-3+,8-4+

Create Date: 2004-09-16

Summary Similar Structures Search Related Records PubMed (MeSH Keyword)

Compounds Substances Genes Proteins Pathways BioAssays **Literature** Patents

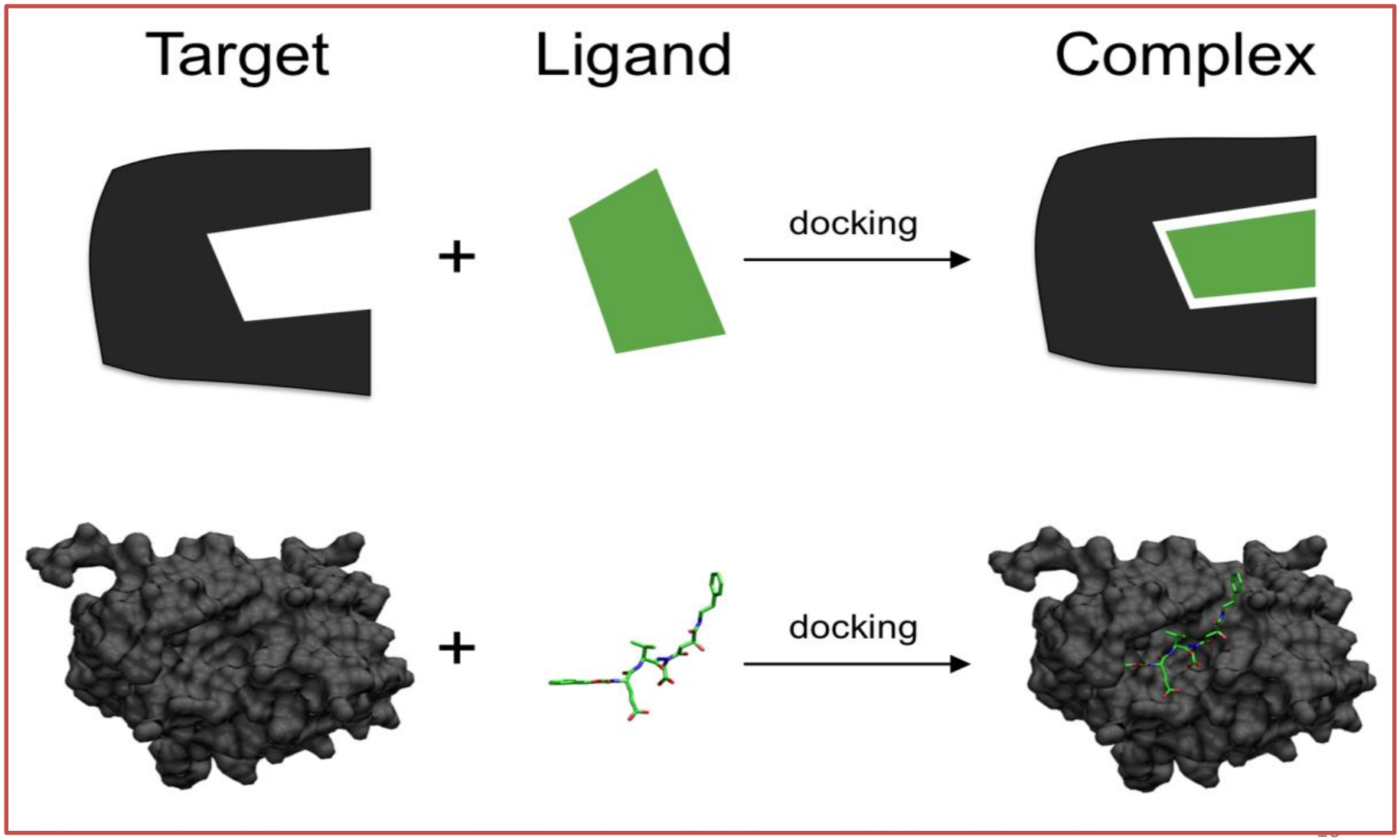
Databases


naturalmedicines.therapeuticresearch.com/search.aspx?q=curcuma+longa&go.x=0&go.y=0
Gmail
Maps
Chargoon Didgah
scholar
https://www.ircme.ir
NatMed
a trchealthcare brand
Login
Subscribe
Search NatMed Pro
Advanced Search
Databases
Tools
CE/CME Center
News
About Us
Home
< Back
Print
Feedback
curcuma longa
Search
Turmeric:
Scientific Name
Background
Safety
Effectiveness
Dosing & Administration
Adverse Effects
Toxicology
Interactions with Drugs
Interactions with Herbs & Supplements
Interactions with Foods
Interactions with Lab Tests
Interactions with Diseases
Mechanism of Action
Pharmacokinetics
Classifications
Turmeric Professional Monograph
Curcuma, Curcumae Longa, Curcumae Longae Rhizoma, Curcumin, Curcumine, Curcuminoid, Curcuminoïde, Curcuminoïdes, Curcuminoids, Halada, Haldi, Haridra, Indian Saffron, Nisha, Pian Jiang Huan...
Javanese Turmeric Professional Monograph
Curcuma, Curcuma de Java, Curcuma Javanais, Cúrcuma Javanesa, Curcumae Xanthorrhizae Rhizoma, Java Turmeric, Safran des Indes, Témoé-lawacq, Témoé-lawaq, Temu Lawak, Temu Lawas, Tewon Lawa. CAUT...

Traditional computational methods

- The approach based on **molecular docking** is a basic tactic.
- It is capable of analyzing **compound–protein interactions.**
- It can analyze **binding affinity by computational simulation.**
- Flexible docking programs are **DOCK, AutoDock, FlexX,** and **GOLD**
- They can predict **protein-ligand complex structures** with reasonable accuracy and speed.

Traditional computational methods



Traditional computational methods

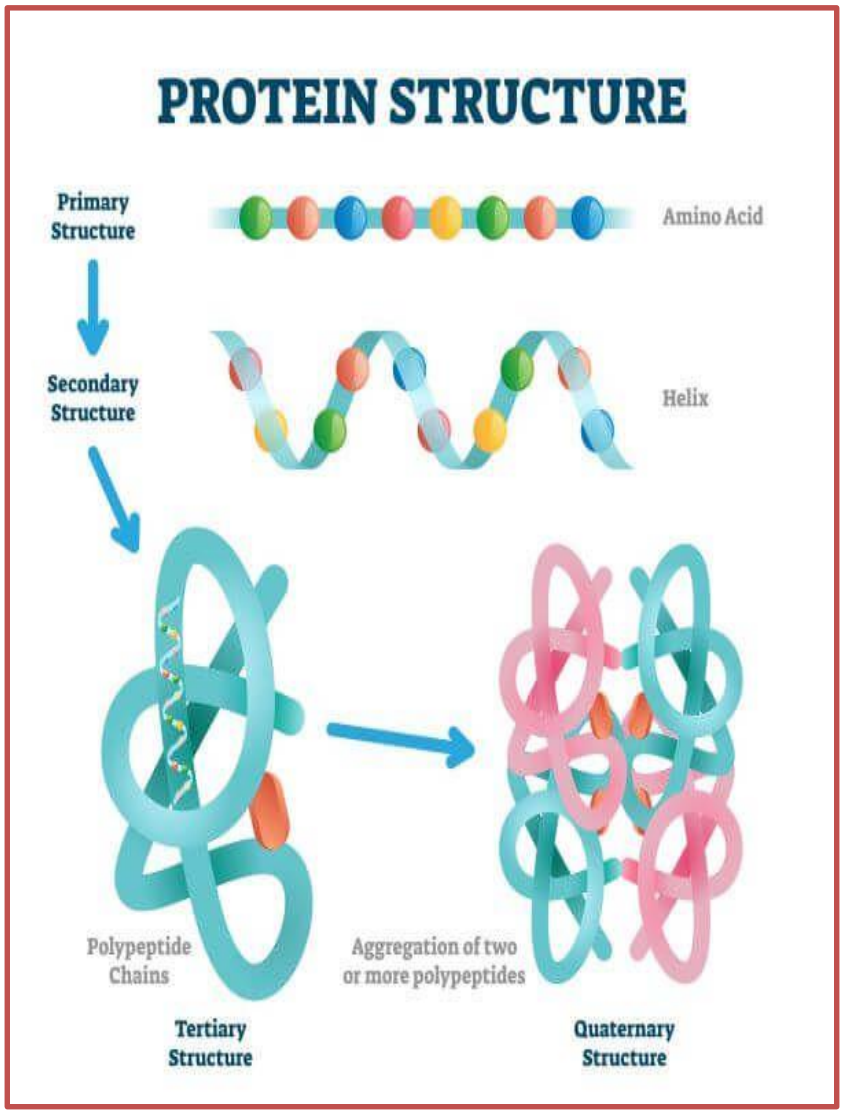
- **Atom sequences** and **amino acid residues** can be used to express both the medicine as well as the target.
- **Descriptors** based on **sequences** were selected.
- **log P** is the logarithm of the partition coefficient.
- LogP > 0, states the drug is lipophilic
- LogP < 0 states the drug is hydrophilic.
- **log D** is the logarithm of the distribution coefficient.
- **log D** interprets the distribution of a compound between water and oil phases.

Traditional computational methods

- **ΔG** (Kcal/mol) or **Gibbs free energy**
- It represents the **change** in **energy of a system** during a **chemical reaction** at **constant temperature** and **pressure**.
- It is measured in kcal/mol.
- A **negative ΔG** (< 0) indicates that the **reaction** is **spontaneous**.
- While a **positive ΔG** (> 0) means the **reaction** is **non-spontaneous**.

Traditional computational methods

- For having true indicators we need to **target proteins' 3D structures.**
- Some target proteins' 3D structures aren't available.
- Then the **effectiveness** of **molecular docking** is **limited**.



AI overcomes the limitations

- Sometimes, there are only **a few** known **binding molecules** for a target
- AI technologies **overcome** the **restrictions** of the high-dimensional structure of the **drug and target protein.**
- By using **unstructured-based** approaches which do **not** need **3D structural data** or docking for DTI (drug-target interaction) **prediction**.

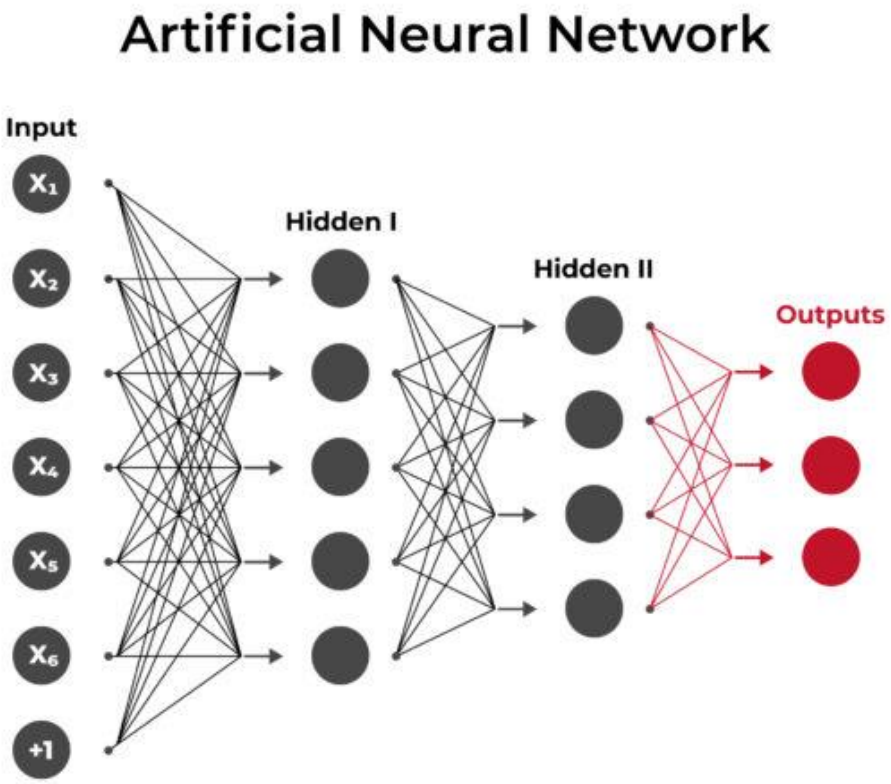
AI algorithms generate forecast

- We want to assess drugs behavior in the human body.
- **Databases** give information regarding **properties** and **biological activities** of the **drug molecule**.
- Biological activities are:
- **Absorption**, **distribution**, **metabolism**, and **excretion** (ADME)
- ADME is strongly influenced by **physicochemical parameters** of drugs.
- ADME and physicochemical parameters of drugs produce **molecular input line in** entry system

AI algorithms generate forecast

- Generally, the data used here include:
- **Molecular descriptors** (e.g., physicochemical properties)
- **Molecular fingerprints** (in molecular structure)
- To produce molecular **input line** entry system for Neural Networks (NNs).

AI algorithms generate forecast



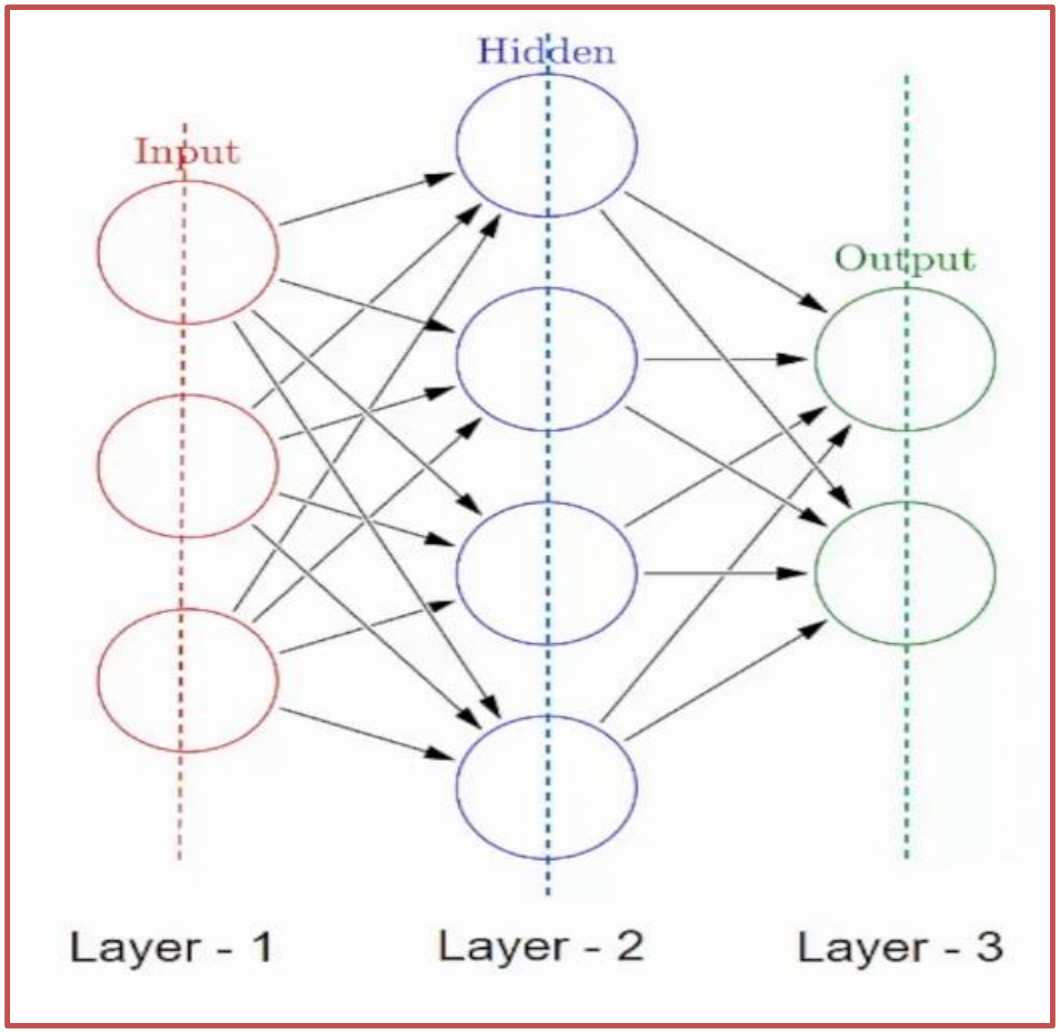
Libraries of chemical and biological data

- In recent years, several libraries of **chemical** and **biological data** including **ChEMBL** and **PubChem** have become available.
- For storing information on **millions of molecules** for .
- These libraries are **machine-readable**.
- They are used to build **machine-learning models** for drug discovery.
- For instance, **NNs** have been used to **generate molecular fingerprints** from a large set of **molecular graphs** with information about **each atom** in the molecule.

Libraries of chemical and biological data

- This database also contains information on **accurate mass**, **molecular formula**, **metabolite name**, and **mass spectra** in several ionization mode.
- (ChEBI) database contains molecular entities focusing on small chemical compounds.

Neural Network Model



Phytochemicals and chromatographic conditions

- Bioactivity assessment of medicinal plants requires determination of their active ingredients.
- Natural extracts are multicomponent and complex.
- Thus, phytochemical studies are challenging and time-consuming.
- Various AI strategies could be applied to facilitate prediction and determination of phyto-constituents.
- **Computational phytochemistry** is about using computational approaches, to predict herbal ingredients, metabolomics for **chemical fingerprinting**, and **taxonomy**.
- **Previously** obtained **spectroscopic data** could be applied to obtain **structure determination** of phyto-constituents.

Pharmaco-therapeutic effects

- Herbal products and medicinal plants form the major part of the prescriptions
- Therapeutic effects are yet to be confirmed by modern science.
- We require discovering rational usage patterns and refining the massive number of prescriptions.
- AI approaches could assist in analyzing large-scale biomedical information to recognize potential therapeutic applications of existing herbs for other ailments.
- New indications could be allocated for approved herbal medicine, which is cost-effective
- It opens up new avenues for the drug discovery process

Drug repurposing attempts

- AI-assisted drug repurposing involves utilizing artificial intelligence algorithms and techniques to identify potential new uses for existing drugs.
- To uncover new uses for drugs that are already on the market and have been approved.
- It has attracted much attention since it takes less time, costs, and less money.

Drug–drug interactions (DDIs) side effect prediction

- In the laboratory, to determine whether the medications have any **unfavorable side effects**, **several tests** are conducted on them.
- However, these examinations are both **pricey** and additionally **lengthy**.
- Recently, many **computational algorithms** for detecting medication adverse effects have been created.
- **Computational methodologies** are replacing **laboratory experiments**.

Drug–drug interactions (DDIs) side effect prediction using DL

- Even though a medication has a **strong affinity** for binding to **one target**, it binds to **several proteins** as well with **varied affinities**, which might cause **adverse consequences.**
- Predicting DDIs can assist in **reducing** the **likelihood of adverse reactions** and **optimizing** the **medication development** and **post-market monitoring processes.**

Predicting toxicity

- Toxicity prediction forms a **crucial stage** in **drug discovery**.
- Types of toxicity
- This study **guarantees safe** and **effective** use and **decreases late-stage failures**.
- AI-based drug toxicity assists in **predicting** herbal toxicity.
- **ML algorithms** and **DL architectures** assist in identifying **potentially toxic phytochemicals** and **herbal extracts**
- **This happens** before being examined in **preclinical** and **clinical trials**.

Identification

- Identification, taxonomic evaluation, and authentication of herbal species are challenging.
- One branch of **quality maintenance** is related to the **authentication** of herbs.
- Botanists and taxonomists assign the identity of medicinal plants based on organoleptic properties.
- Previously, various species of herbs were identified by traditional methods or the **visual** and **manual approaches.**
- **AI technology** could assist in developing a **novel system without** human interference.
- Such as **image processing approaches**.

Natural Drug Discovery

- Drug discovery is **defined** as the introduction of **novel drugs** against ailments.
- **Herbs** and **herbal medicine** have the potential to be used as **alternative** and **preventive** agents.
- Many **conventional** and **chemical** therapeutic agents **cannot** confront **malignant** and **chronic** diseases.
- Herbs with a myriad of **phytochemicals** can be used to isolate **lead compounds**.
- **AI** and **ML** are increasingly being used to discover **new herbal drugs.**
- These technologies can analyze **molecular structures**.
- They help **predict potential pharmacological activities**, and **clinical use** to streamline drug discovery.

Standardization

- **Quality** and **quantity** control of herbal drugs play a crucial role in **guaranteeing** their clinical efficacy.
- **Herbal quality control** is categorized into **several** classifications.
- Including the **detection of contaminants**, **authentication** of herbal ingredients, and the **amount** of **bioactive phytochemicals**, **moisture**, **ash**, **impurities**, or **contaminants**.
- Standardization of herbal medicine by conventional attributes requires the **isolation of active compounds**, which is **time-consuming** and needs **high cost**.
- AI systems facilitate **digital detection**,


Thank you