

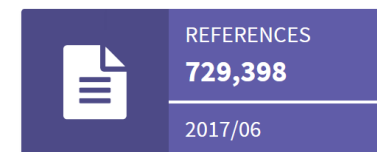
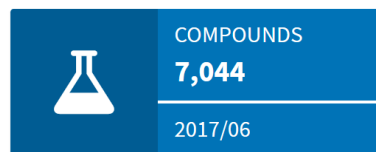
Approach to **Natural Product Archive**

An Effort to Target/Mechanism Predictions

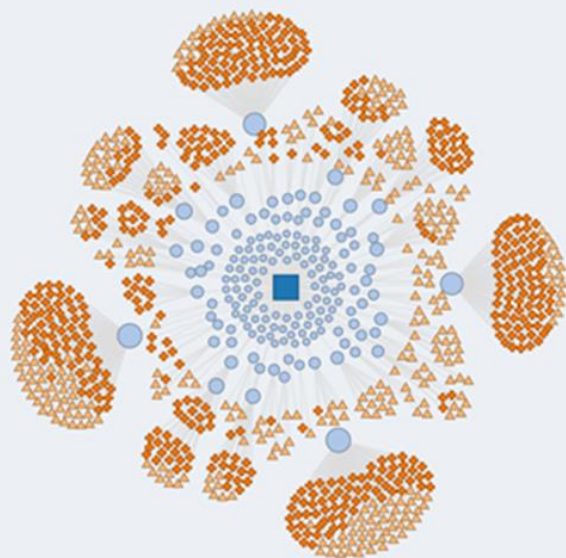
Ying-Ta Wu

Genomics Research Center, Academia Sinica

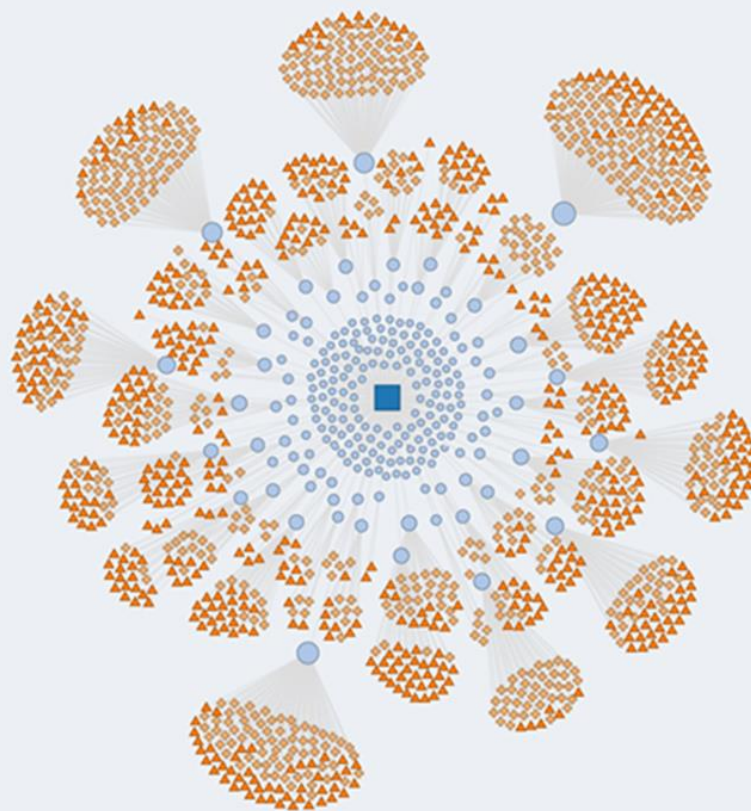
i Card Info.



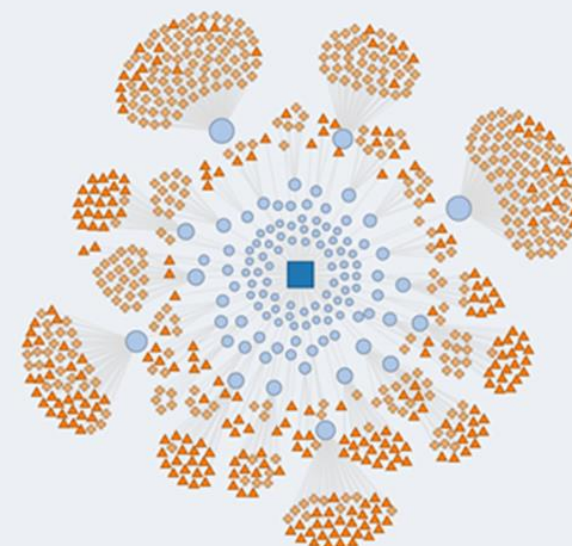
NAPA in sight



石菖蒲 (Acorus Rhizome)



丹参 (Red Sage Root and Rhizome)



肉苁蓉 (Desert-living Cistanche)

- : compound
- ⊕ : target
- ▲ : pathway

NAPA view

六味地黃丸 (Liu Wei Di Huang Wan)

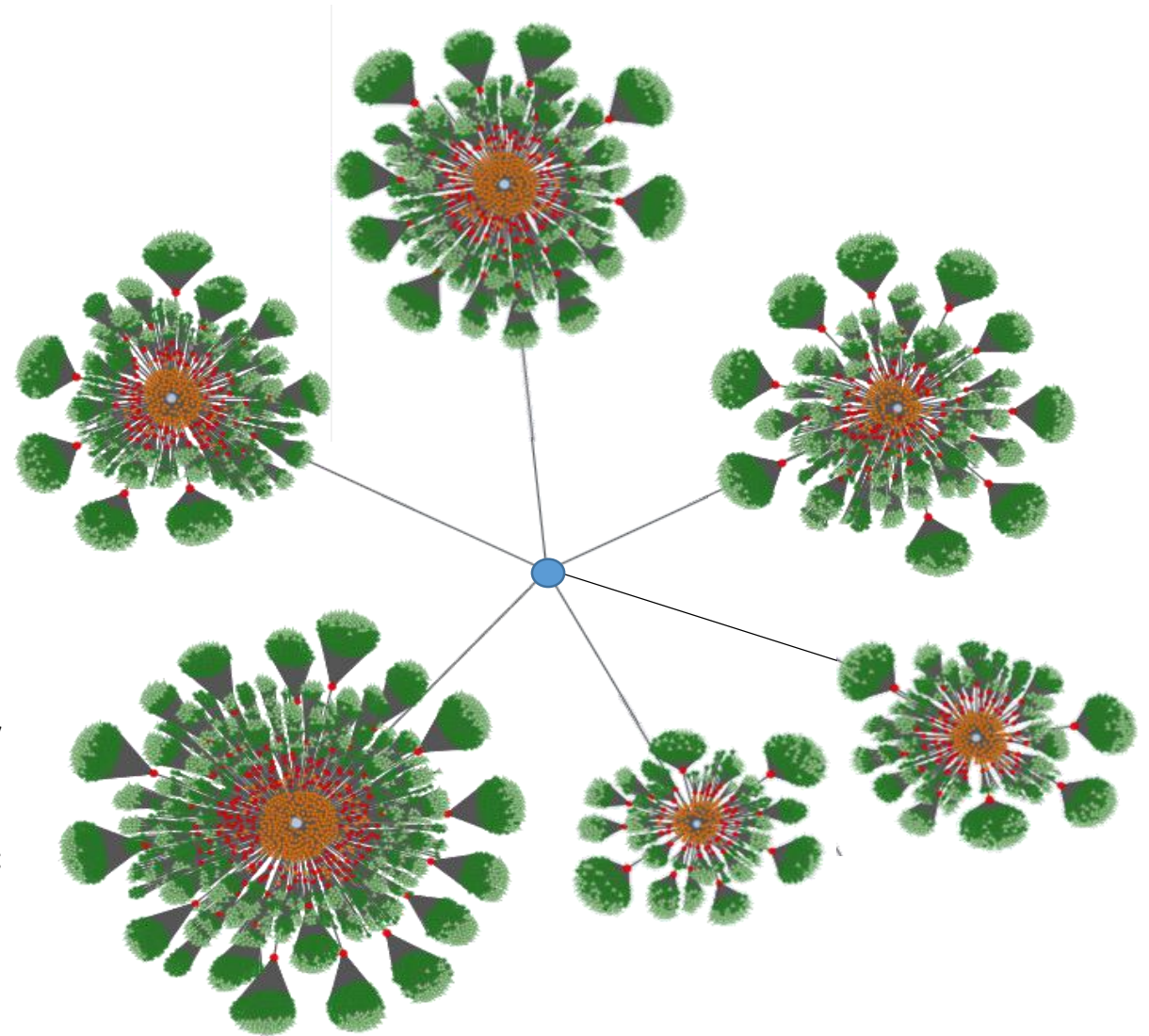
is one of the ten most famous classical Chinese herb formulae

Uses: shenyinxu (kidney yin deficient)

Syndromes:

Back pain, lack of strength in knees and legs, losing hair, bad gum and teeth, irregular menses, ringing the ears, red face, hot body, prefer cool, uneasiness, dry and cracked lips, dark red tongue with yellow fur, or even with cracks, or black and with spurs.

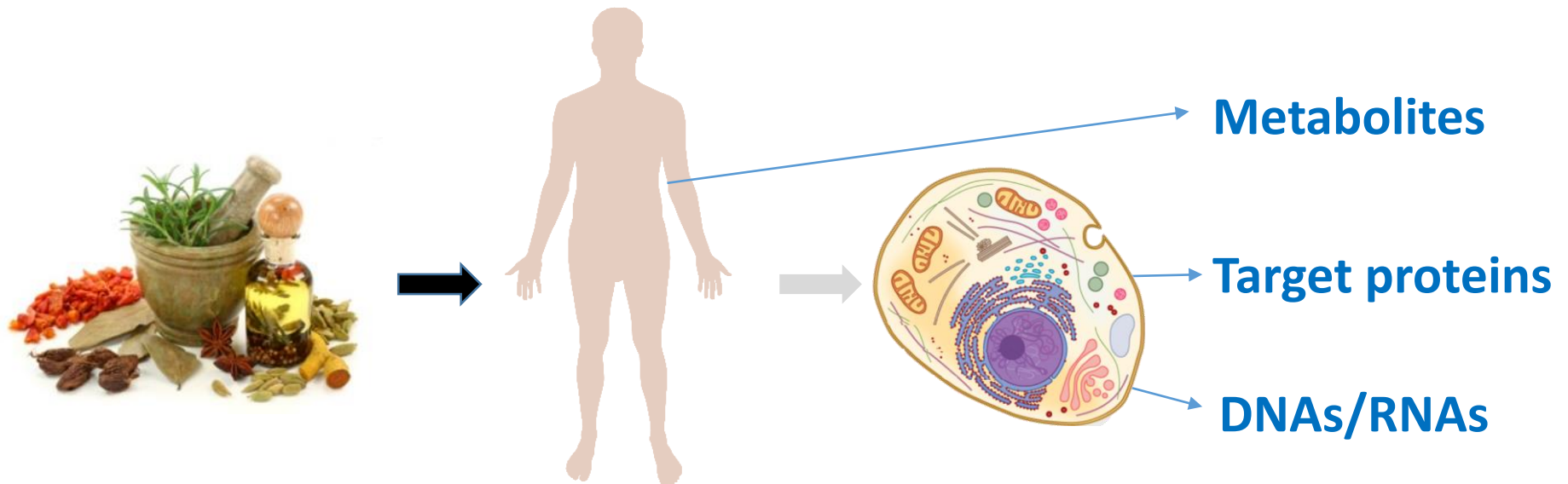
Modern day usage includes: as anti-oxidant[1], anti-inflammatory [1], anti- cancer, for prostate enlargement, geriatric dementia , and type II diabetes, together with the use of gui pi tang to improve white blood cell count caused by chemotherapy, chronic infection of the sinus area. Dr. Joe H. K. Chu, Complementary and Alternative Healing University
<http://alternativehealing.org>



Herbal medicines have often maintained their popularity for historical and cultural reasons.

A herbal formula is a mixture of hundreds of chemical ingredients, which are referred to as botanical (or Herbal) Natural Products (or phytochemicals).

- Effectors in a herbal medicine ?
- Modes of action to cure diseases or “kill” invaders ?



Modern Medicine Aspect

Improvements are required for :

Drug Property

works for ADME/Tox, PK/PD

Secondary metabolites
have evolved to be bioactive

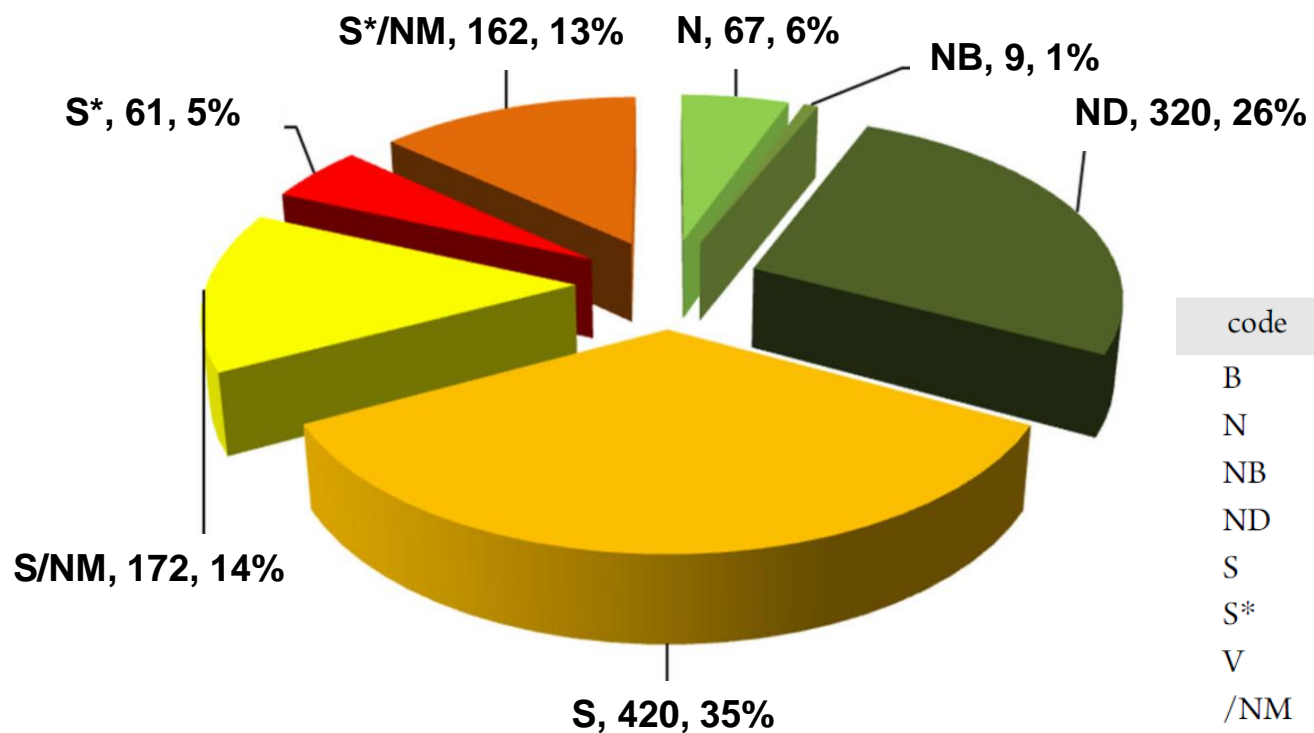
Potency and Selectivity

Plant vs Homo sapiens

And other necessity factors to turn a NP into a pharmaceutical drug.

Natural Products as rich sources for drug

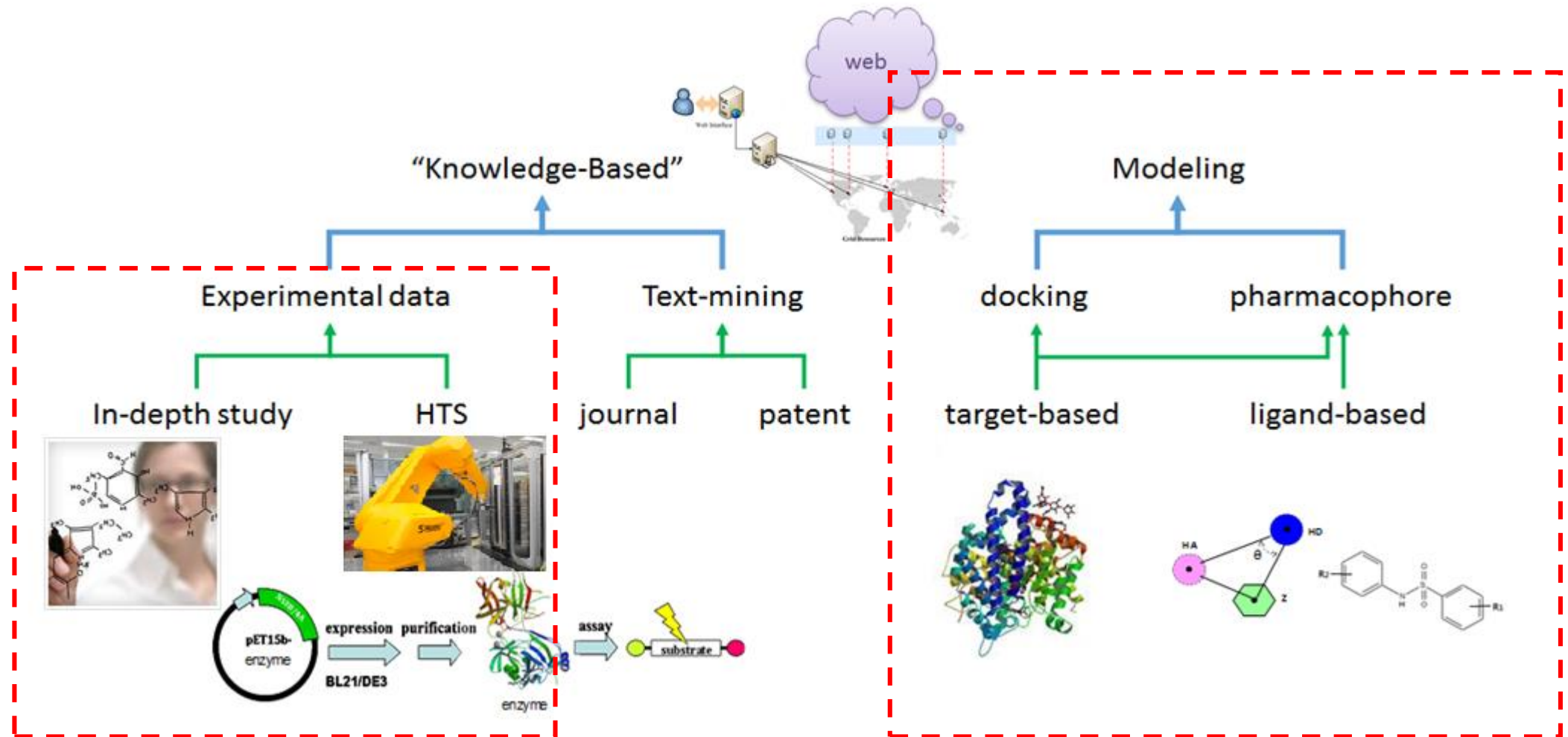
From 1981 to 2014



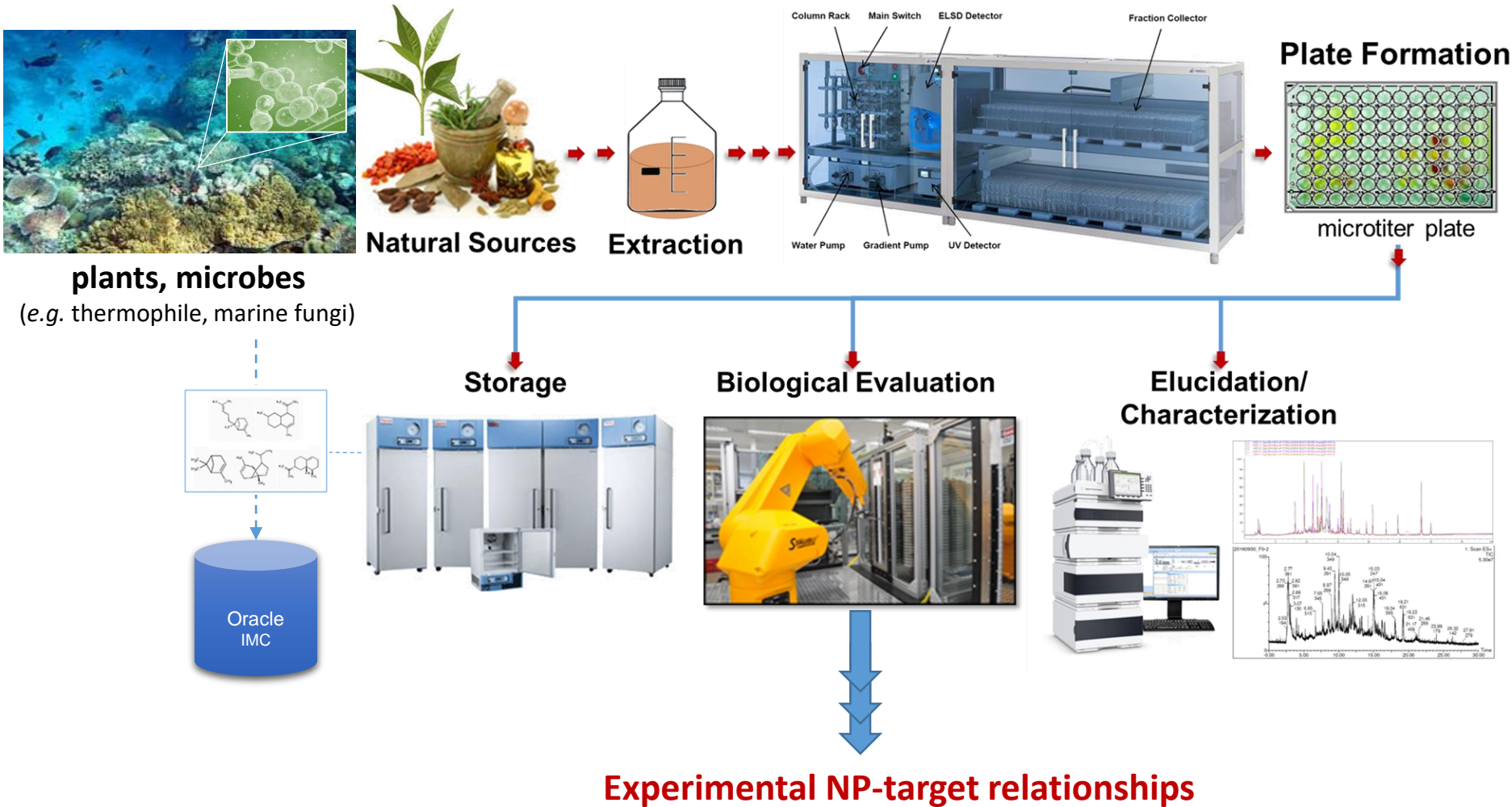
code	brief definition/year
B	Biological macromolecule, 1997
N	Unaltered natural product, 1997
NB	Botanical drug (defined mixture), 2012
ND	Natural product derivative, 1997
S	Synthetic drug, 1997
S*	Synthetic drug (NP pharmacophore), 1997
V	Vaccine, 2003
/NM	Mimic of natural product, 2003

David J. Newman, and Gordon M. Cragg
 J. Nat. Prod. 2016, 79, 629–661

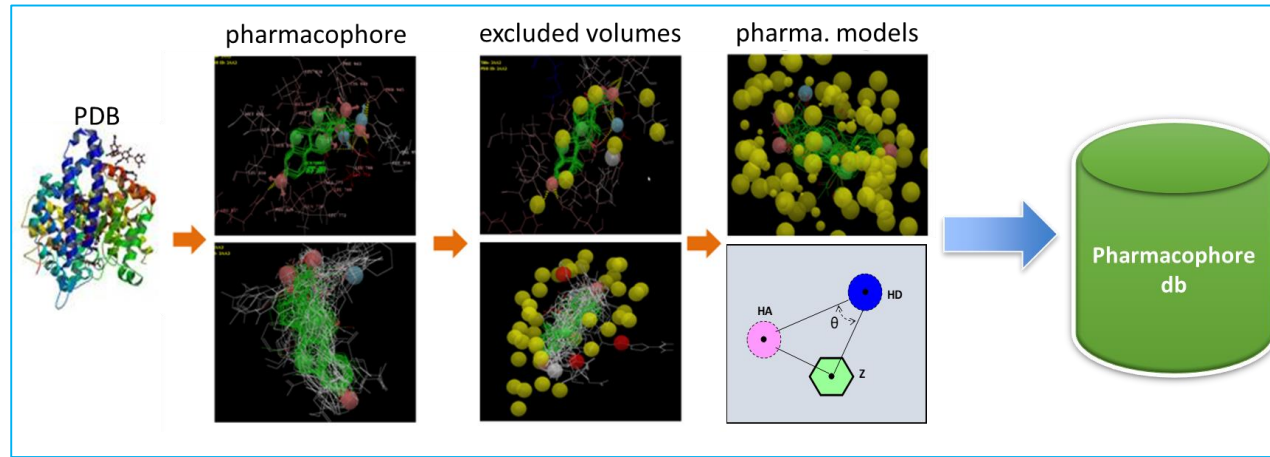
Drug-Target Relationships



Natural Product Library

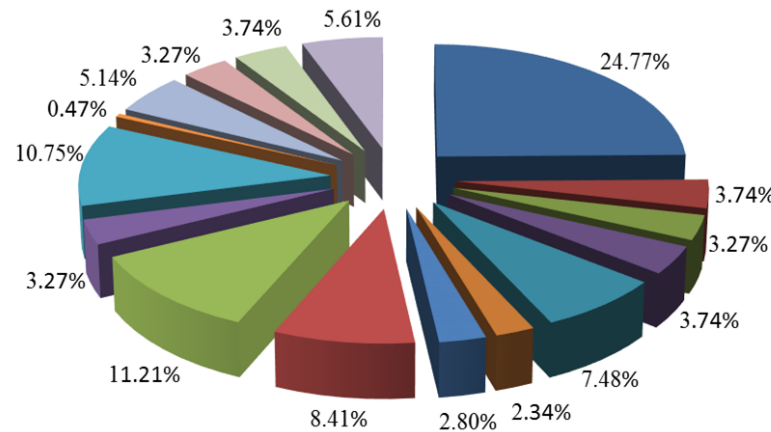
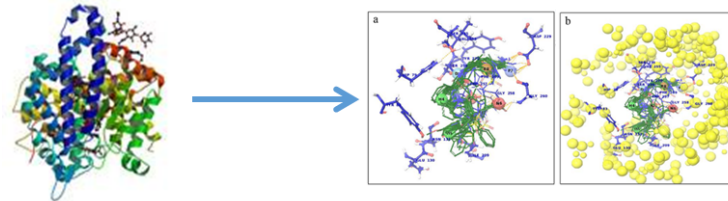


Pharmacophore Database



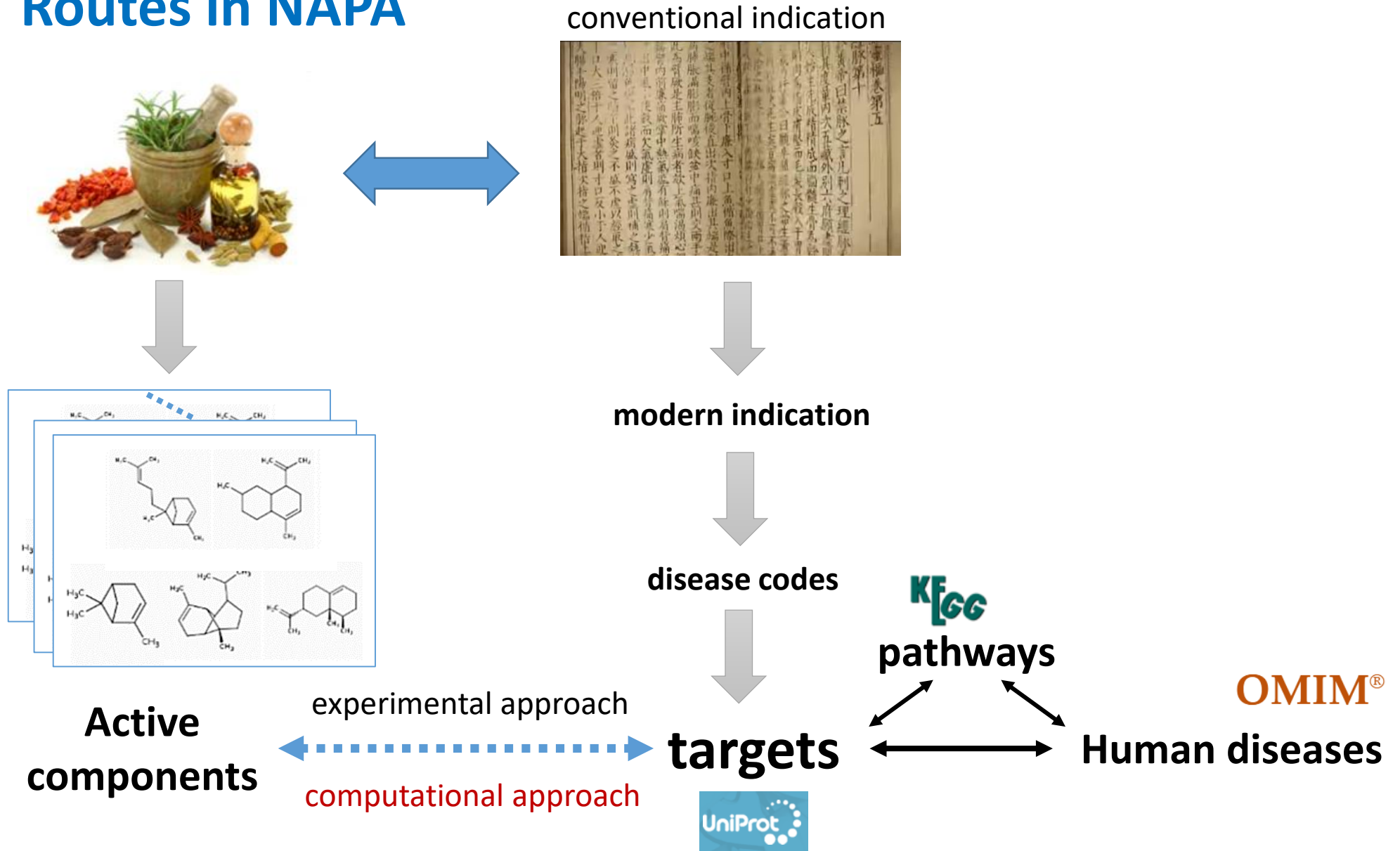
480 disease targets

- enzyme
- receptor
- Factors/regulators/hormones
- binding proteins
- transport proteins
- nuclear receptor
- signaling protein
- Lipid binding proteins
- drug binding proteins
- transcriptional factors
- DNA binding
- Cell cycles, DNA repair
- nucleoside metabolism
- transcriptional regulation



- Neoplastic diseases
- Hormone (and hormone antagonist)
- Blood pressure
- Blood homeostasis
- Immune response
- Viral infections
- Bacterial infections
- Renal and cardiovascular functions
- Synaptic and neuro effector
- Parasitic infectious disease
- Inflammation
- Gastrointestinal functions
- Metabolic disease
- Bone remodeling and resorption
- Glucose homeostasis
- Others

Routes in NAPA



細辛 Xi Xin

(1) Asari Radix (2)Asarum Root (3)Herb of Manchurian wild ginger



42

Formal Charater(UTF-8)	Hanyu PinYin	Name
中文	拼音	學名
細辛	Si-Sin	Radix Asari
細辛	Xi Xin	Asari Radix Radix et Rhizoma Asari

Source

馬兜鈴科(Aristolochiaceae)細辛屬(Asarum)

Properties (characteristics) 性味：

acid, warm, toxic to kidney
辛，溫，對腎臟有毒。

Channels (meridians) entered 歸經：

heart, kidney, lung, liver
心、腎、肺、肝

Actions & Indications 功效：

promotes sweating and disperse cold,
Reduce pain, warms lungs rid of phlegm
祛風散寒，通竅，止痛，溫肺化飲。

Radix et Rhizoma

1404



[Compound]

Asarinin

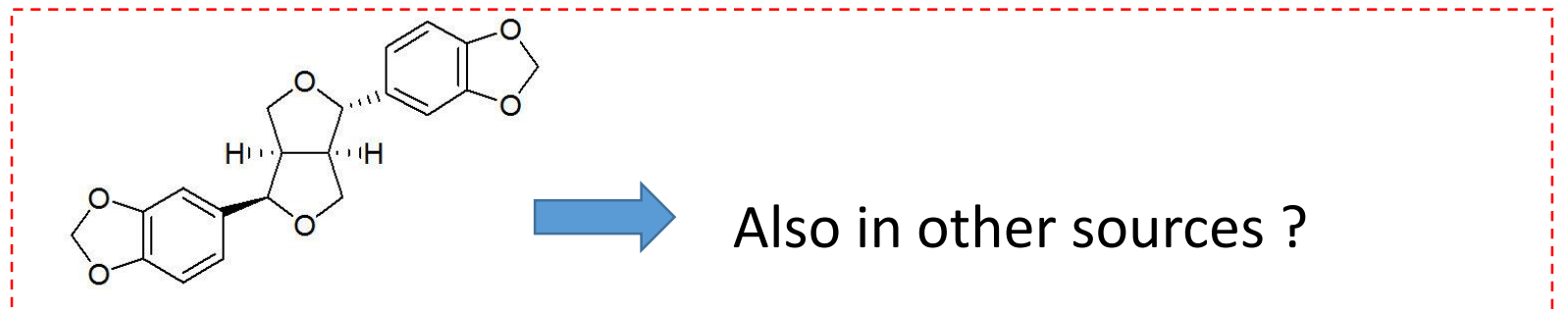


[Target]

EGFR

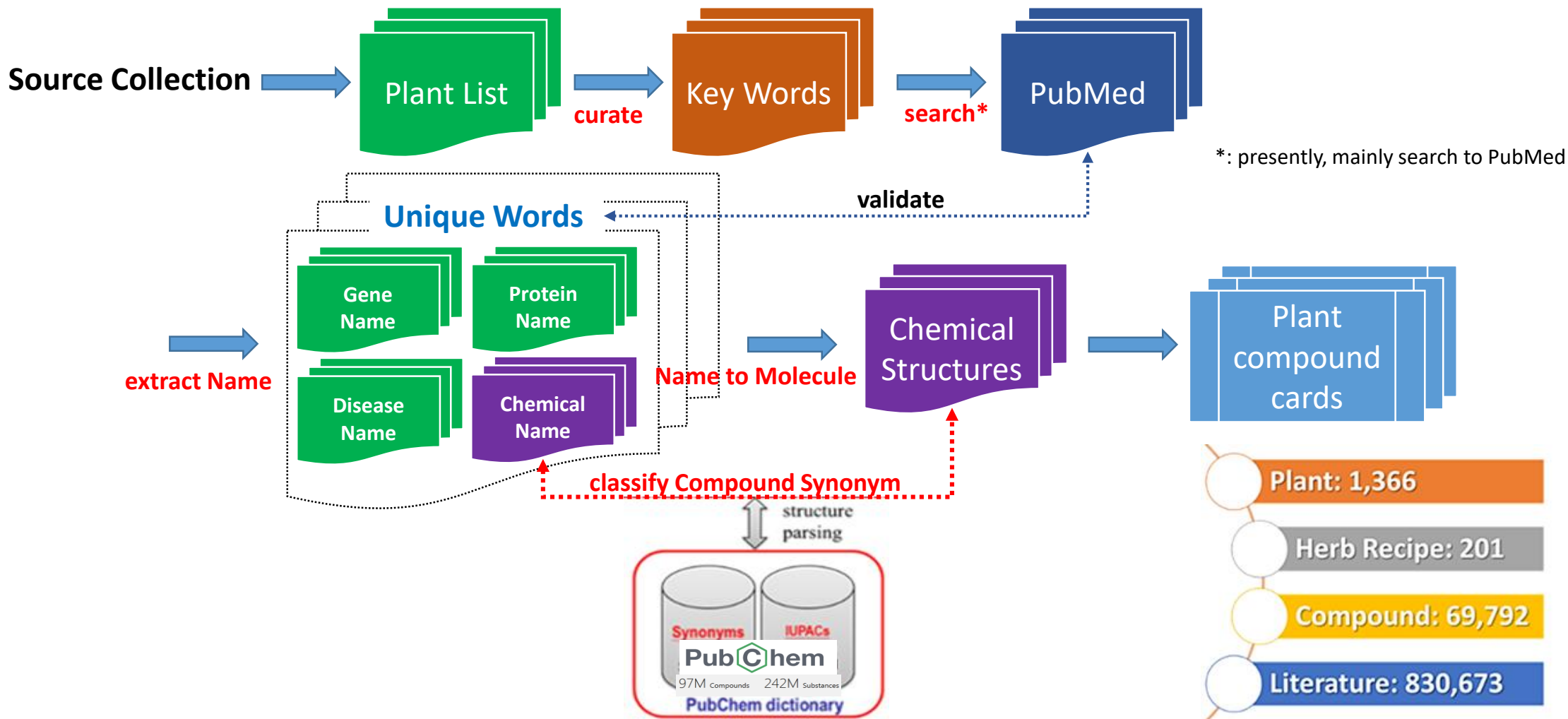
[Disease]

Osteoarthritis

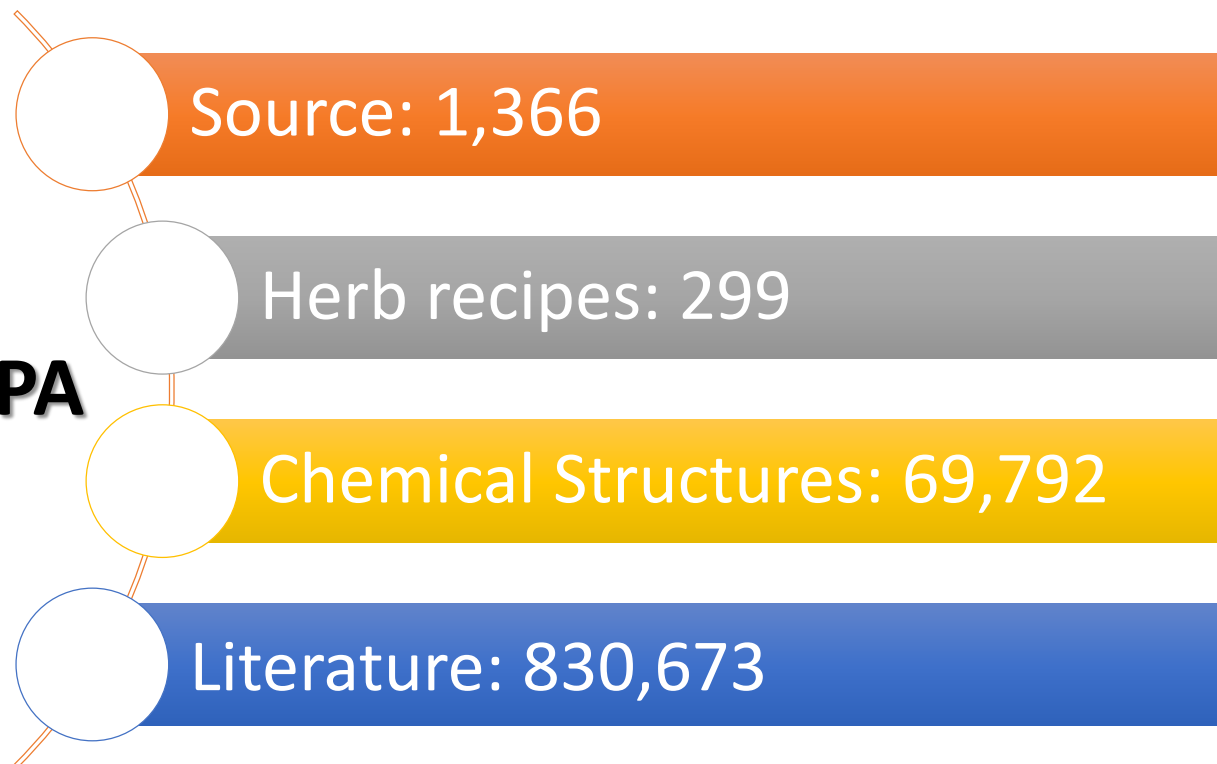


Workflow

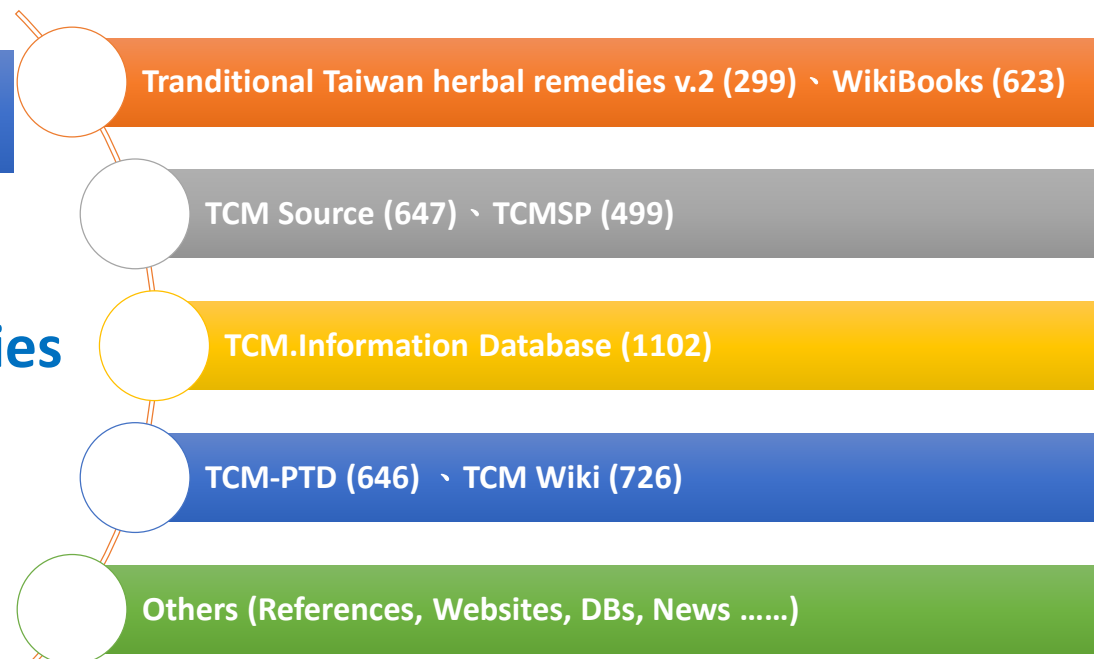
Ping Yin	Latin Name (Pharmaceutical Name)	English Name (Common Name)
石菖蒲	ACORI GRAMINEI RHIZOMA	Acorus Rhizome
猪苓	POLYPORUS	Agaric
藿香	AGASTACHIS HERBA	Agastache Herb
⋮	⋮	⋮



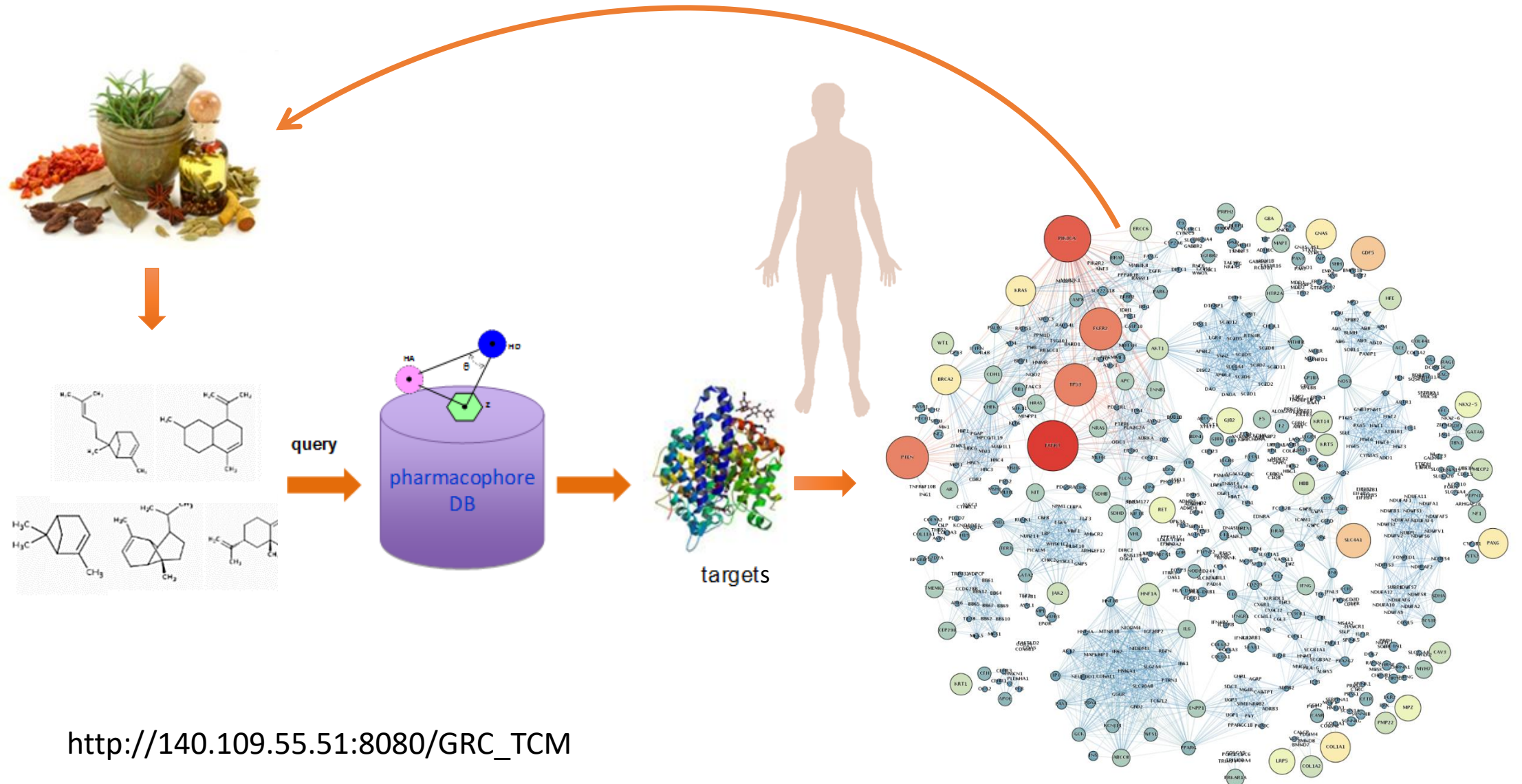
NAPA



1,366 Entries



A use of NAPA



Acknowledgement

Credits:

Jiraporn Nawarak 林力雯

Chun-Hung Su 蘇俊宏

Hua-Ting Hsu 許華亭

Thank YOU

感恩

Funding Supports:



中央研究院--登峰科技計畫

謝謝