KSBi-BIML 2026

Bioinformatics & Machine Learning(BIML) Workshop for Life Scientists

생명정보학 & 머신러닝 워크샵 (온라인)

Introduction to Network Science for Transcriptomics-guided Drug Discovery

박상민 _ 충남대학교

KSBI KOREAN SOCIETY FOR BIOINFORMATICS | 한국생명정보학회

본 강의 자료는 한국생명정보학회가 주관하는 BIML 2026 워크샵을 목적으로
제작된 것으로 해당 목적 이외의 다른 용도로 사용할 수 없음을 분명하게 알립니다.

이를 다른 사람과 공유하거나 복제, 배포, 전송할 수 없으며 만약 이러한 사항을 위반할 경우
발생하는 **모든 법적 책임은 행위자 본인에게 있음**을 알립니다.

KSBi-BIML 2026

Bioinformatics & Machine Learning (BIML) Workshop for Life Scientists

한국생명정보학회가 주최하는 BIML-2026 동계 Bioinformatics &Machine Learning 교육 워크숍에 여러분을 초대합니다.

BIML 워크숍은 생명정보학 연구자들이 최신 AI바이오 분야의 인공지능 기반 분석 기술과 바이오 데이터 분석 기법을 이론과 실습을 통해 체계적으로 배울 수 있는 전문 교육 프로그램입니다. 2015년에 시작된 BIML 워크숍은 올해로 12년 차를 맞이하며, 국내 생명정보학 분야의 최초이자 최고 수준의 교육 프로그램으로 자리 잡았습니다. 이번 워크숍은 크게 인공지능바이오(AI바이오) 분야와 디지털바이오 분야, 두 분야로 구성됩니다.

AI바이오 분야에서는 생명정보 분석에 폭넓게 응용되고 있는 다양한 인공지능 기반 자료 모델링 기법을 다룰 예정입니다. 특히, 인공지능 심층학습을 활용한 단백질 구조 예측, 유전체 분석, 신약 개발에 대한 이론 및 실습 강의가 진행됩니다.

또한 디지털바이오 분야에서는 단일세포오믹스, 공간오믹스, 멀티오믹스, 메타오믹스에 대한 강의도 마련되어 있어, 연구자들의 분석 역량 강화에 실질적인 도움을 줄 것으로 기대됩니다.

또한 2024년부터 추가된 의료정보 자료 분석을 다루는 강의를 올해도 지속해서 운영하고자 합니다. 이는 최근 의료정보 자료 분석에 관한 연구 수요 증가를 반영한 것으로, 관련 연구를 수행하는 의과학자 및 의료정보 연구자들에게 유용한 지침을 제공할 것입니다.

또한, 올해도 생명정보학 기술의 다양화에 발맞춰 온라인 강좌를 대폭 확대했습니다. 올해는 무료 강좌 10개를 포함한 총 40개 이상의 강좌가 개설되며, 연구 주제에 맞는 강좌 추천과 강연료 할인 혜택도 제공합니다.

BIML-2026는 국내 주요 연구 중심 대학의 전임 교수 및 각 분야 최고 전문가들의 강의로 구성되어 있으며, 기초 이론부터 최신 연구 동향까지 아우르는 심도 있는 교육의 장이 될 것으로 확신합니다.

여러분의 많은 관심과 참여를 기대합니다!

2026년 2월

한국생명정보학회장 류 성 호

강의개요

Introduction to Network Science for Transcriptomics-guided Drug Discovery

오믹스 데이터를 어떻게 신약 개발의 단서로 바꿀 수 있을까? 암, 만성질환, 퇴행성질환과 같은 복잡계 질환(complex disease)은 단일 유전자의 문제가 아니라, 분자 상호작용 네트워크의 재배선(rewiring)으로 나타나는 경우가 많다. 따라서 "어떤 표적을 선택할지", "어떤 약물이 효과를 낼지"를 예측하려면, one-drug&one-target 중심의 환원주의적 접근을 넘어 질병과 약물을 시스템 수준에서 해석하는 시각이 필요하다.

본 강의에서는 시스템 약리학(Systems Pharmacology)과 네트워크 과학(Network Science)을 바탕으로, 질병과 약물의 상호작용을 네트워크 관점에서 분석하는 방법을 제시한다. 수강생들은 네트워크를 이해하는 핵심 개념을 익히고, "약물–표적–경로–질병"으로 기전 축을 분석하는 과정을 학습한다. 또한 약물전사체(Pharmacotranscriptomics) 데이터를 활용하여 복합적인 약물의 작용 기전(MoA)을 추론하는 방법을 다룬다. 나아가 다양한 화합물/천연물 데이터베이스를 활용하여 네트워크를 제어할 수 있는 최적의 후보 물질을 발굴하고, 이를 약물 재창출(Drug Repositioning) 연구에 적용하는 실전 전략을 소개한다.

강의는 다음의 내용을 포함한다:

- 네트워크 과학(Network Science) 기본 개념
- 네트워크 약리학(Network pharmacology) 연구 방법
- 약물전사체학(Pharmacotranscriptomics) 연구 방법
- 약물재창출(Drug Repositioning) 및 효능 예측 사례

* 교육생준비물:
  R 및 Cytoscape 사용 가능 컴퓨터

* 강의 난이도: 초급

* 강의: 박상민 교수 (충남대학교 약학대학)

Curriculum Vitae

Speaker Name: Sang-Min Park, Ph.D.

▶ **Personal Info**

Name	Sang-Min Park
Title	Associate Professor
Affiliation	Chungnam National University (CNU)

▶ **Contact Information**

Address	99 Daehak-ro, Yuseong-gu, Daejeon 34134
Email	smpark@cnu.ac.kr

Research Interest

Pharmacotranscriptomics, Network medicine, Systems Biology, Virtual Cell

Educational Experience

2010	B.S. in Department of Bio and Brain Engineering, KAIST, Korea
2012	M.S. in Department of Bio and Brain Engineering, KAIST, Korea
2019	Ph.D. in Department of Bio and Brain Engineering, KAIST, Korea

Professional Experience

2019-2019	Postdoctoral Researcher, Institute of Information Electronics, KAIST, Korea
2019-2022	Senior researcher, KM data division, Korea Institute of Oriental Medicine (KIOM), Korea
2022-2025	Assistant professor, College of Pharmacy, Chungnam National University (CNU), Korea
2025-	Associate professor, College of Pharmacy, Chungnam National University (CNU), Korea

Selected Publications (3 maximum)

1. Yeo, Heerim, Sang-Yun Kim, and Sang-Min Park. "Harnessing transcriptomics for discovery of natural products to overcome acquired cancer resistance." *Archives of Pharmacal Research* (2025): 1-29.
2. Kim, Sang-Yun, et al. "Deciphering the immunomodulatory mechanisms of Bojungikki-tang via systematic transcriptomic and immune cell interaction network analysis." *Biomedicine & Pharmacotherapy* 188 (2025): 118129.
3. Park, Sang-Min, et al. "Integrative transcriptomic analysis identifies emetine as a promising candidate for overcoming acquired resistance to ALK inhibitors in lung cancer." *Molecular Oncology* 19.4 (2025): 1155-1169.

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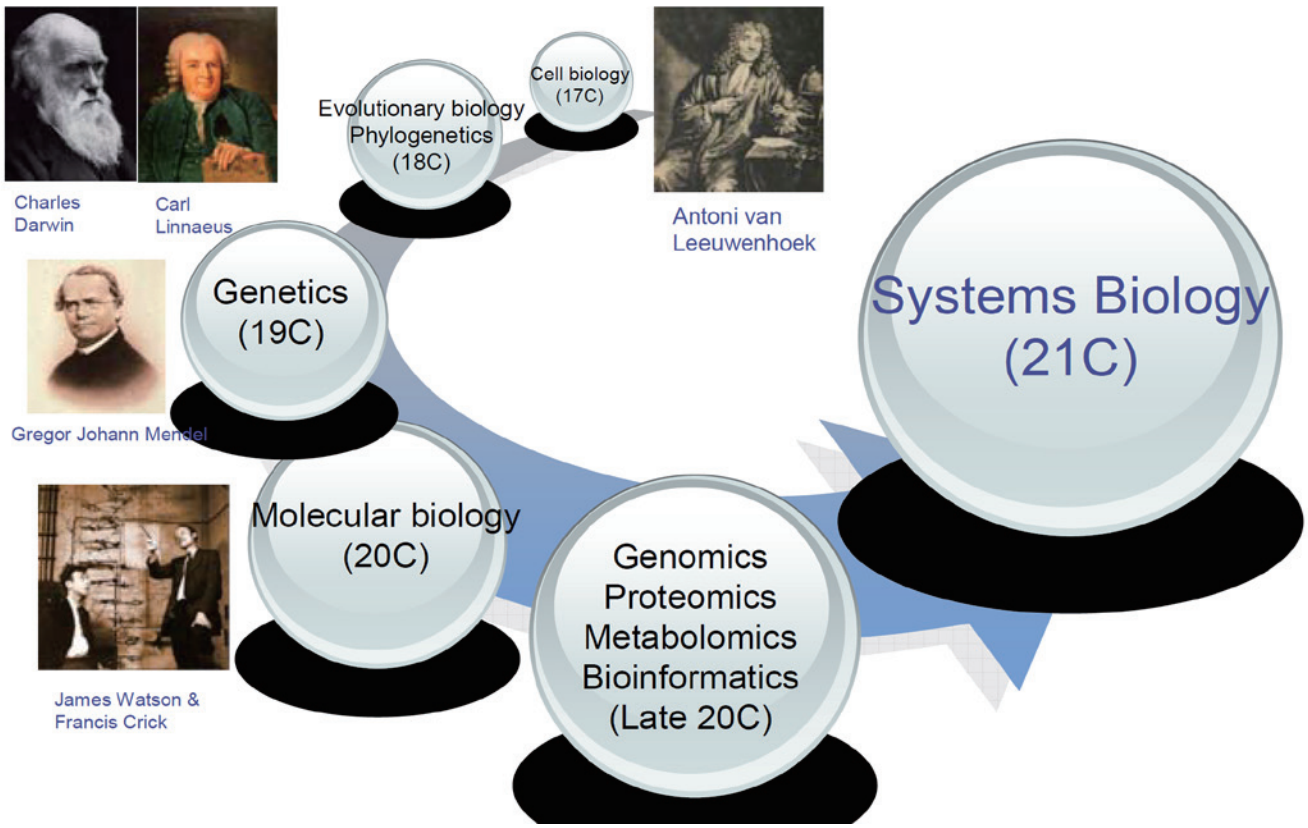
KSBi-BIML 2026

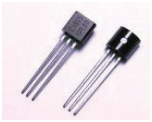
Introduction to Network Science for Transcriptomics-guided Drug Discovery

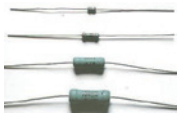
충남대학교 약학대학
박상민

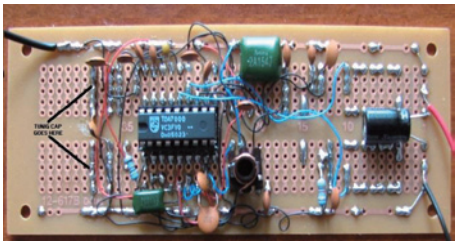
History of life science



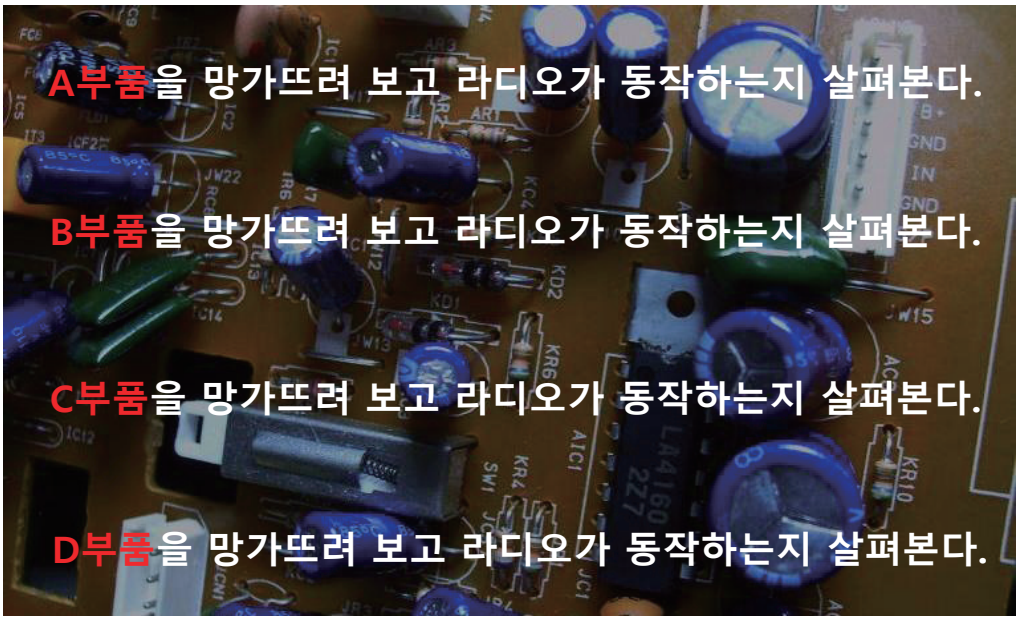
생물학자는 라디오를 고칠 수 있을까?



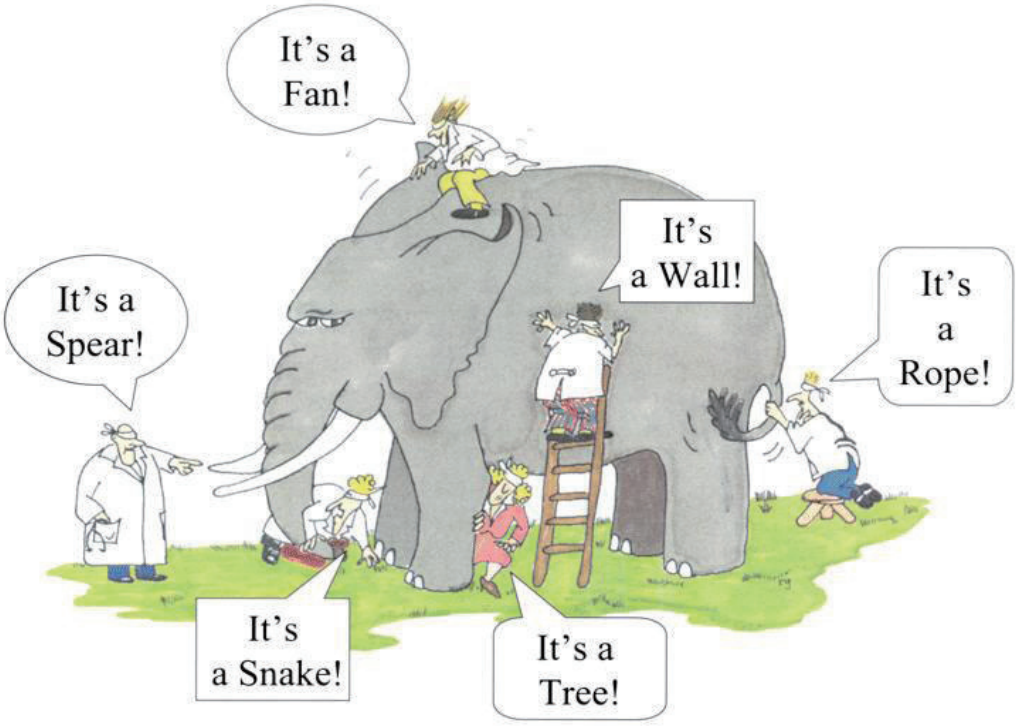




전통적인 생물학자의 접근 방식



전통 생물학: “장님 코끼리 만지기”



http://www.proprofs.com/quiz-school/story.php?title=blind-men--elephant

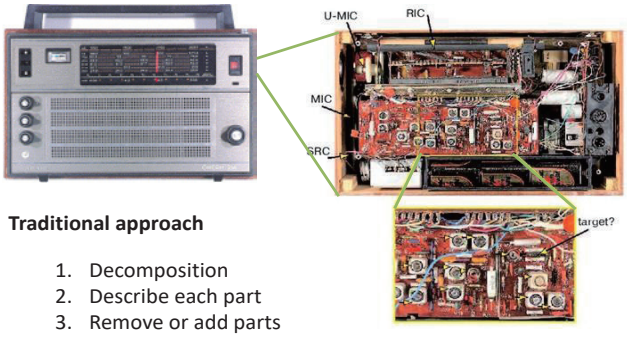
From the part to the whole – via the systems perspective

Cancer Cell

CORRESPONDENCE | VOLUME 2, ISSUE 3, P179-182, SEPTEMBER 01, 2002

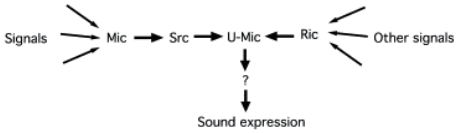
Can a biologist fix a radio?—Or, what I learned while studying apoptosis

Yuri Lazebnik

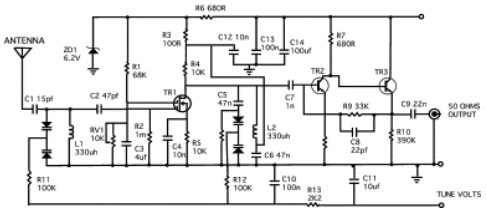


Traditional approach

1. Decomposition
2. Describe each part
3. Remove or add parts



Underlying systematic design principle

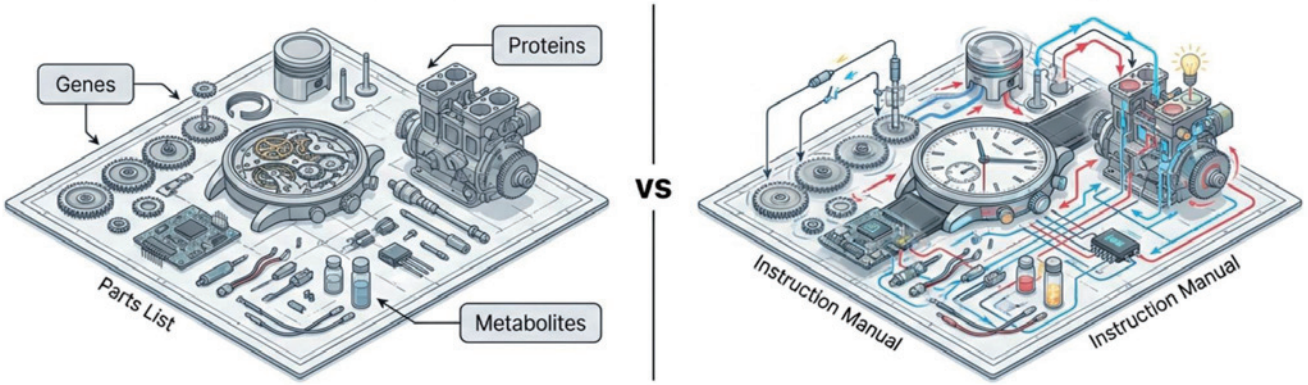


quantitative, testable, predictable

6

부품 목록(Parts List)만으로는 시스템을 이해할 수 없습니다

Human Genome (Static) — **VS** → **Functional Networks (Dynamic)**



게놈(Genome)의 한계

인간 게놈 프로젝트는 생명체의 '부품 목록'을 제공했지만, 부품 간의 상호작용인 '사용 설명서'는 제공하지 못했습니다.

환원주의의 실패

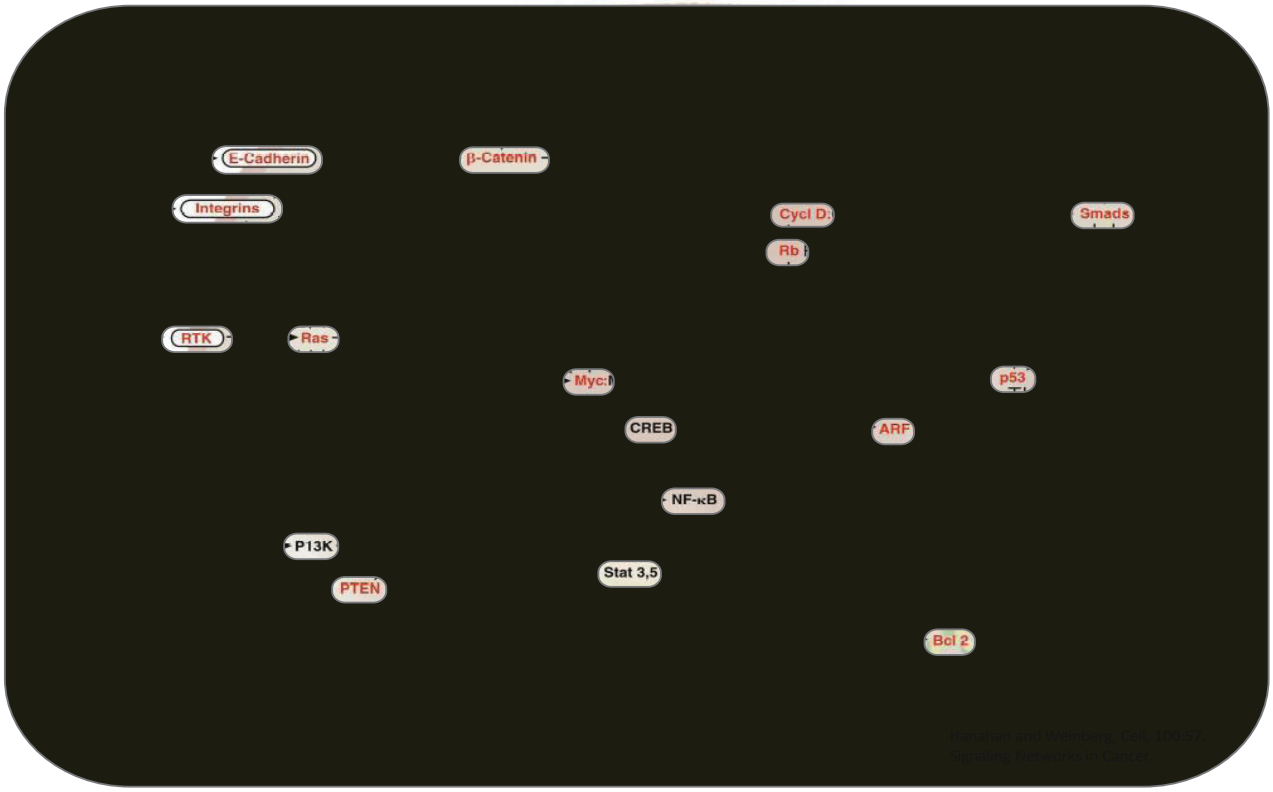
ALK 억제제와 같은 표적 치료제는 특정 변이(Mutation)를 공격하지만, 세포는 우회 경로를 통해 생존합니다.

연결성(Connectivity)의 부재

질병 유전자와 약물 간의 단순 연관성만으로는 인과관계나 회로 수준의 메커니즘을 규명할 수 없습니다. 시스템을 섭동(Perturbation)시키고 그 반응을 관찰해야 합니다.

From the part to the whole – via the systems perspective

Phenotype is an **emergent outcome of complicated interactions** of molecules that are orchestrated together.



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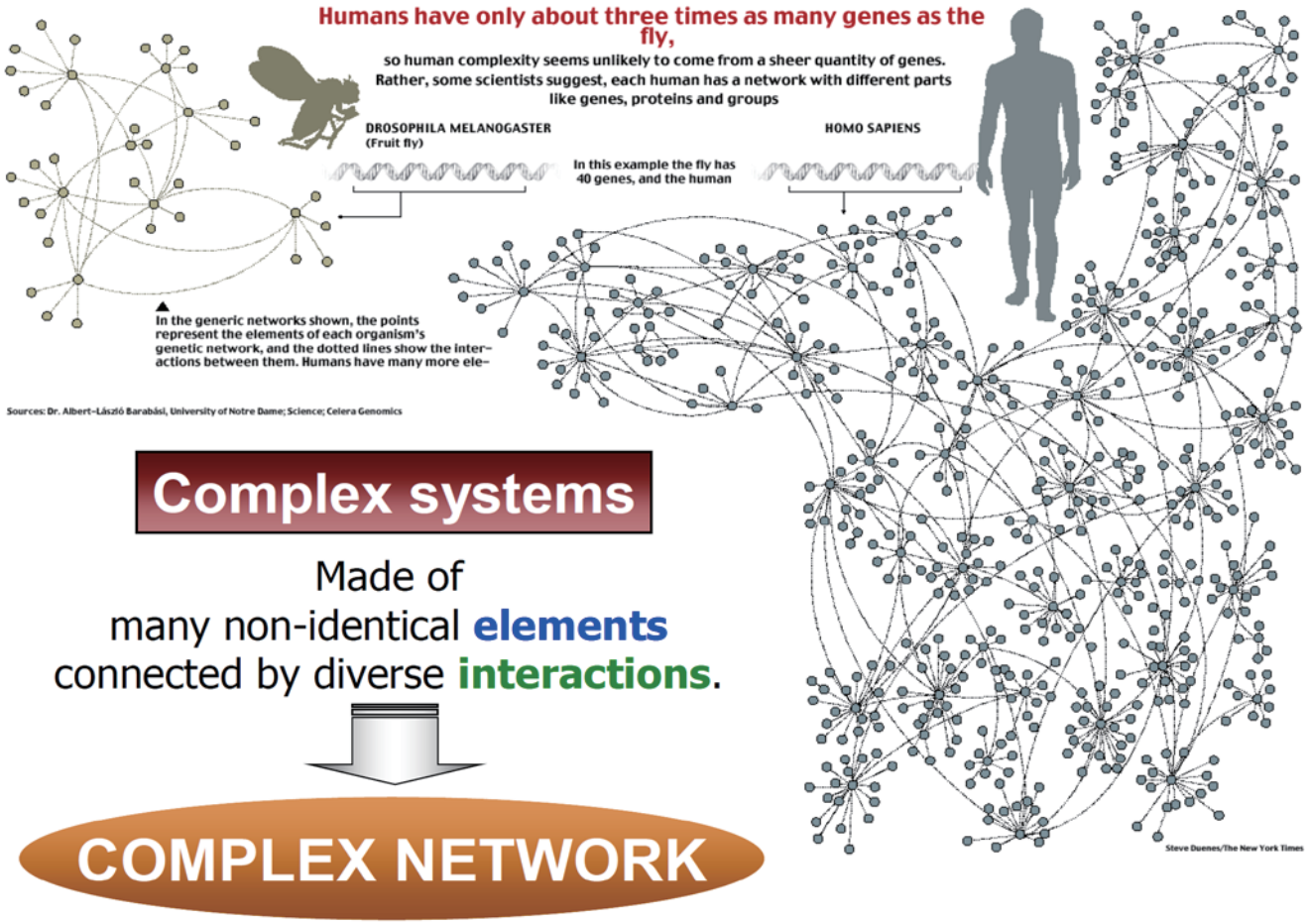
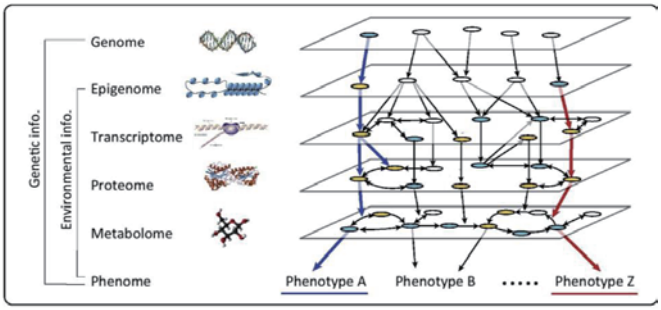


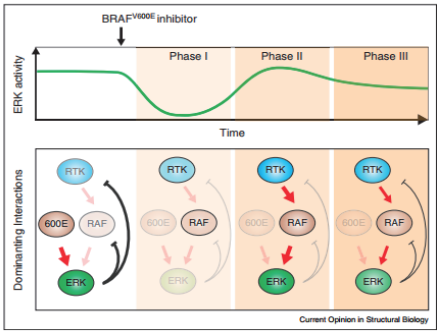
Understand and Control the network system

Disease as network perturbation

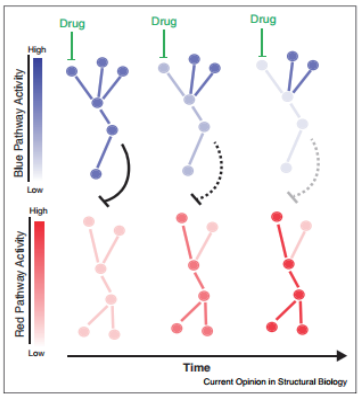


- **Complex diseases** (cancer, Parkinson's disease, and diabetes) are defined by dysregulated networks.
- We need to reconsider our strategies for drug design and selection of molecular targets for treatment.
- A network approach should provide the **framework for designing therapies.**

Drug as network control

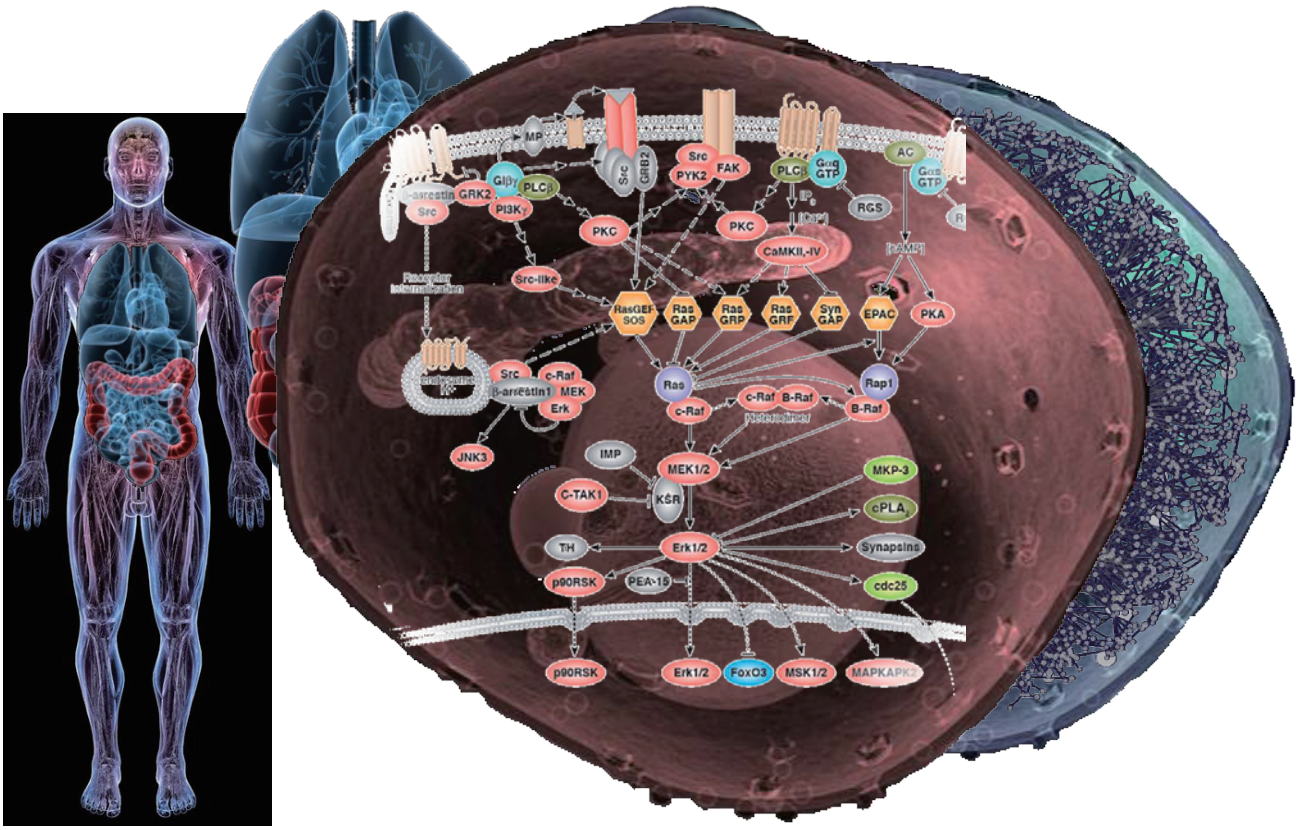


- Drug-induced rewiring in network feedback and crosstalk action can lead to **unexpected activation** of targeted or bypass pathways. => adapt to and counteract the drug effect.
- We need to develop **novel theoretical and experimental framework** to explore the dynamic complexity of cellular networks after multiple perturbations.



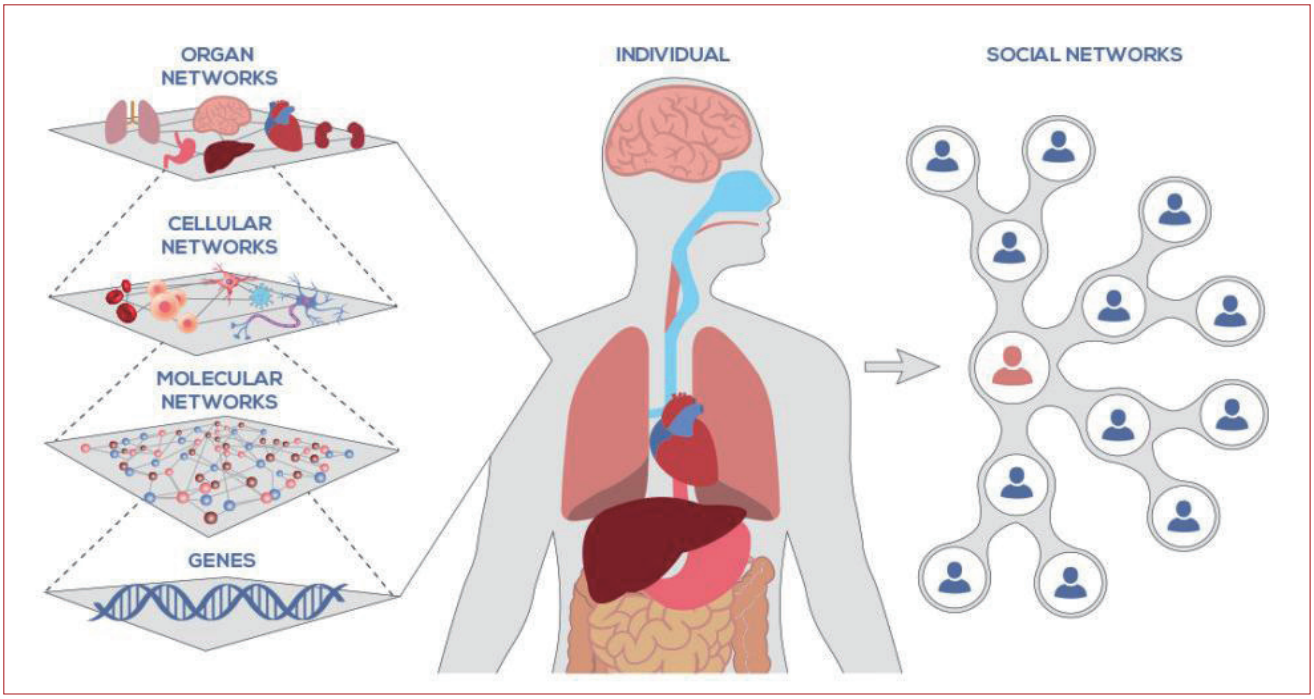
10

인체는 복잡한 네트워크가 계층적으로 구성되어 있다!



인체는 복잡한 네트워크가 계층적으로 구성되어 있다!

Network of Networks



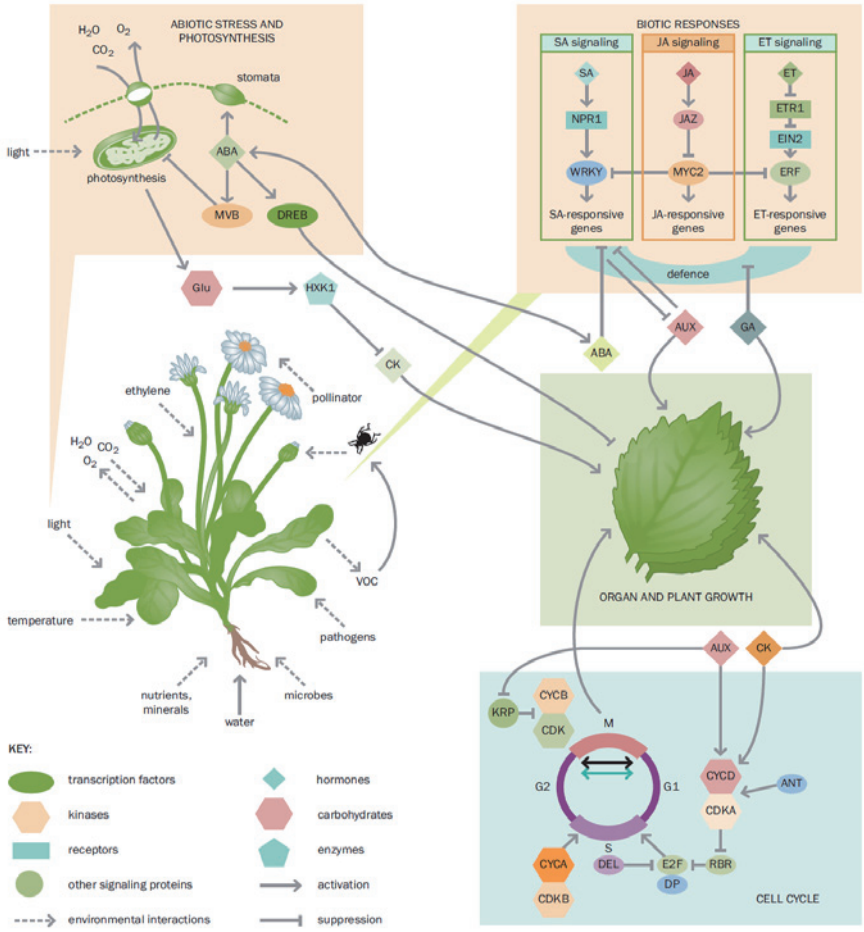
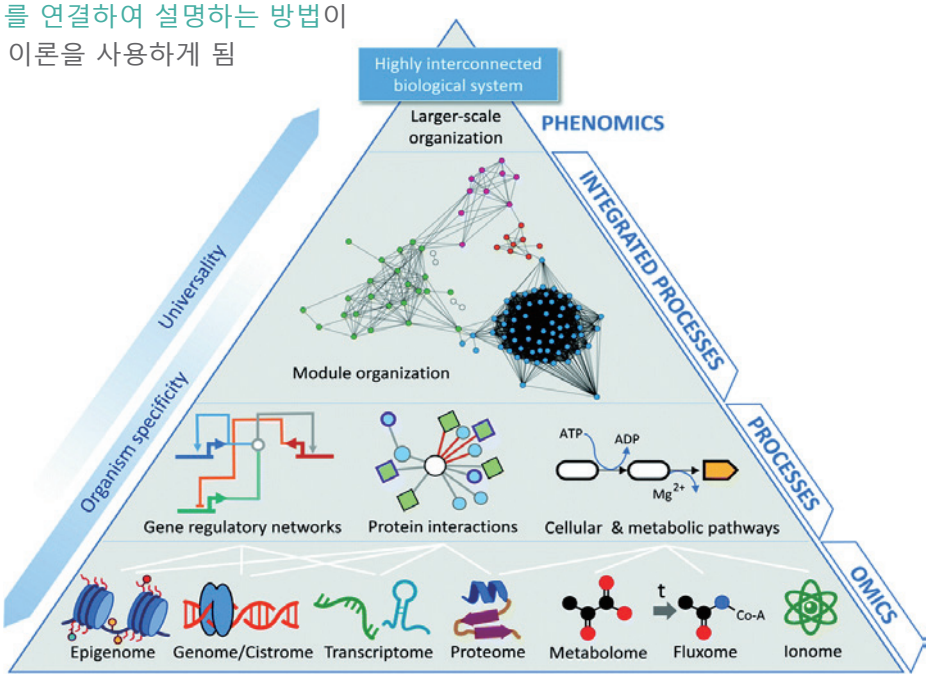


Figure 1.7 Stress responses are coordinated by systems at different levels of organization (cf. Figure 1.2). At the physiological level, the stress response system in plants includes changes at the cellular, organ, and whole-plant levels and also affects interactions of the plant with other species.

시스템 생물학의 대두

- 유전자, 분자, 세포 수준의 요소를 통해 그들 간의 관계를 찾고, 관계에 관한 정보들을 시스템 차원의 관점에서 통합하여 분석하는 학문
- 세포, 조직 수준에서 벗어나 유기체적 접근으로 인체를 이해해야 한다는 접근
- 유전체-전사체-단백체-대사체 : 유기체적 접근을 필요로 하는 omics 데이터

1)유기체 내에서의 상호작용을 설명하는 방법과
2)각각 다른 계층의 데이터를 연결하여 설명하는 방법이
필요했기 때문에 네트워크 이론을 사용하게 됨



What is complex networks?

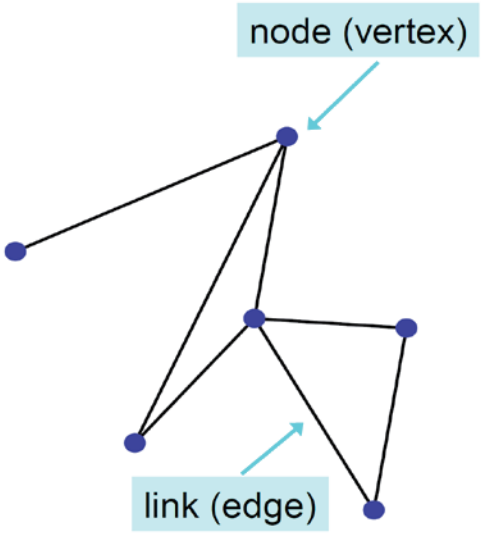
- Network

  = Graph in math

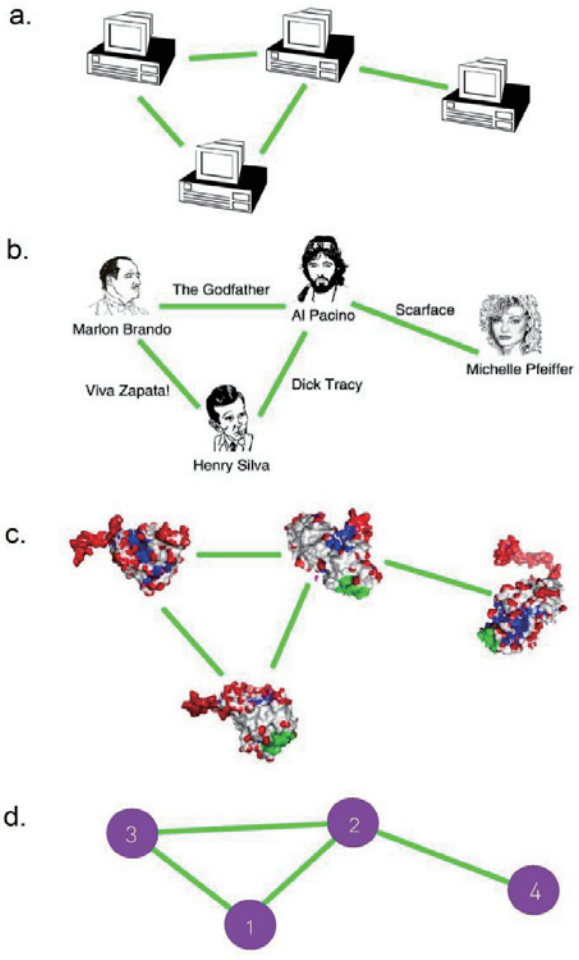
  = (Points + Lines)

  = (Nodes + Links)

  = (Vertices + Edges)



Different Networks, Same Graph



RESEARCH ARTICLE | APPLIED PHYSICAL SCIENCES

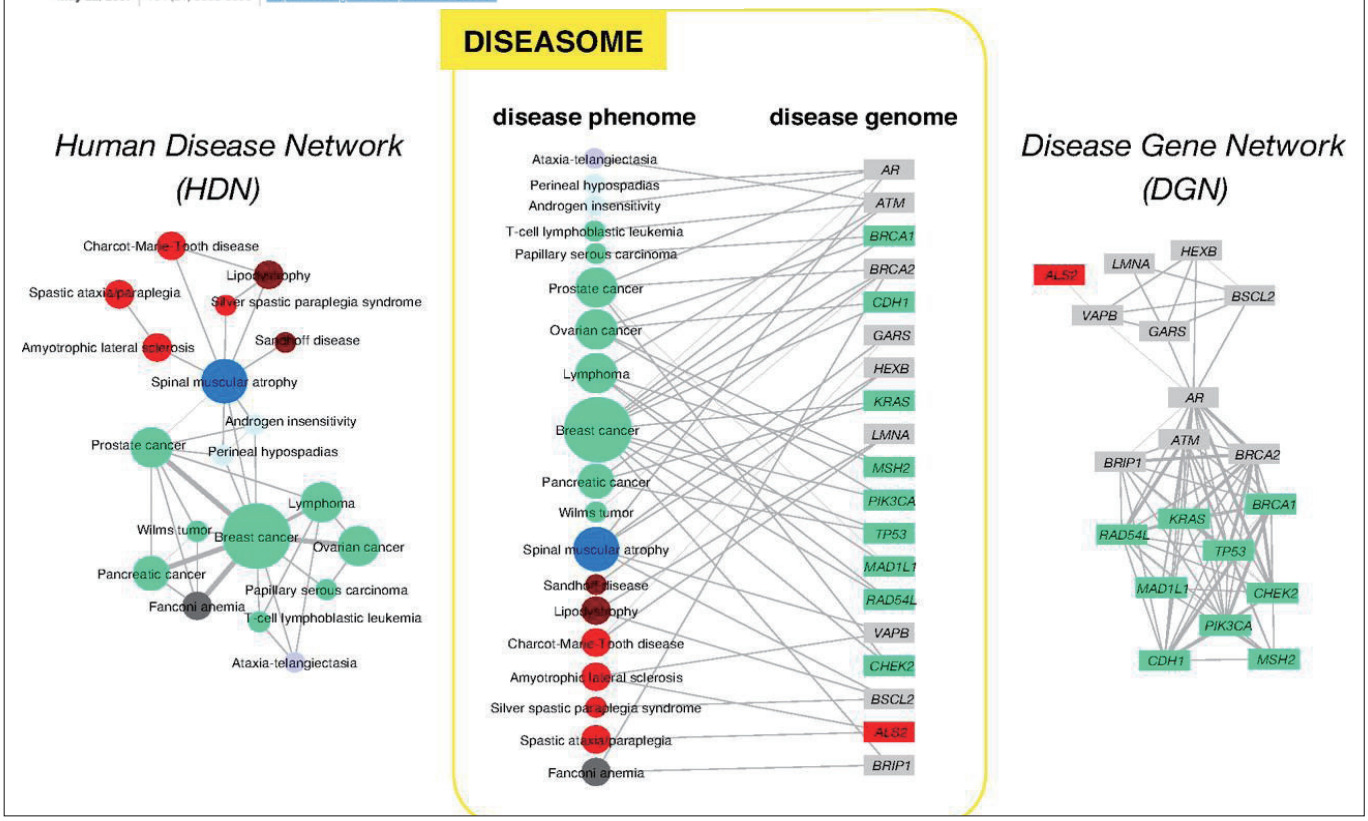
PNAS

The human disease network

Kwang-Il Goh, Michael E. Cusick, David Valle, +2, and Albert-László Barabási Authors Info & Affiliations

Edited by H. Eugene Stanley, Boston University, Boston, MA, and approved April 3, 2007

May 22, 2007 | 104 (21) 8685-8690 | https://doi.org/10.1073/pnas.0701361104



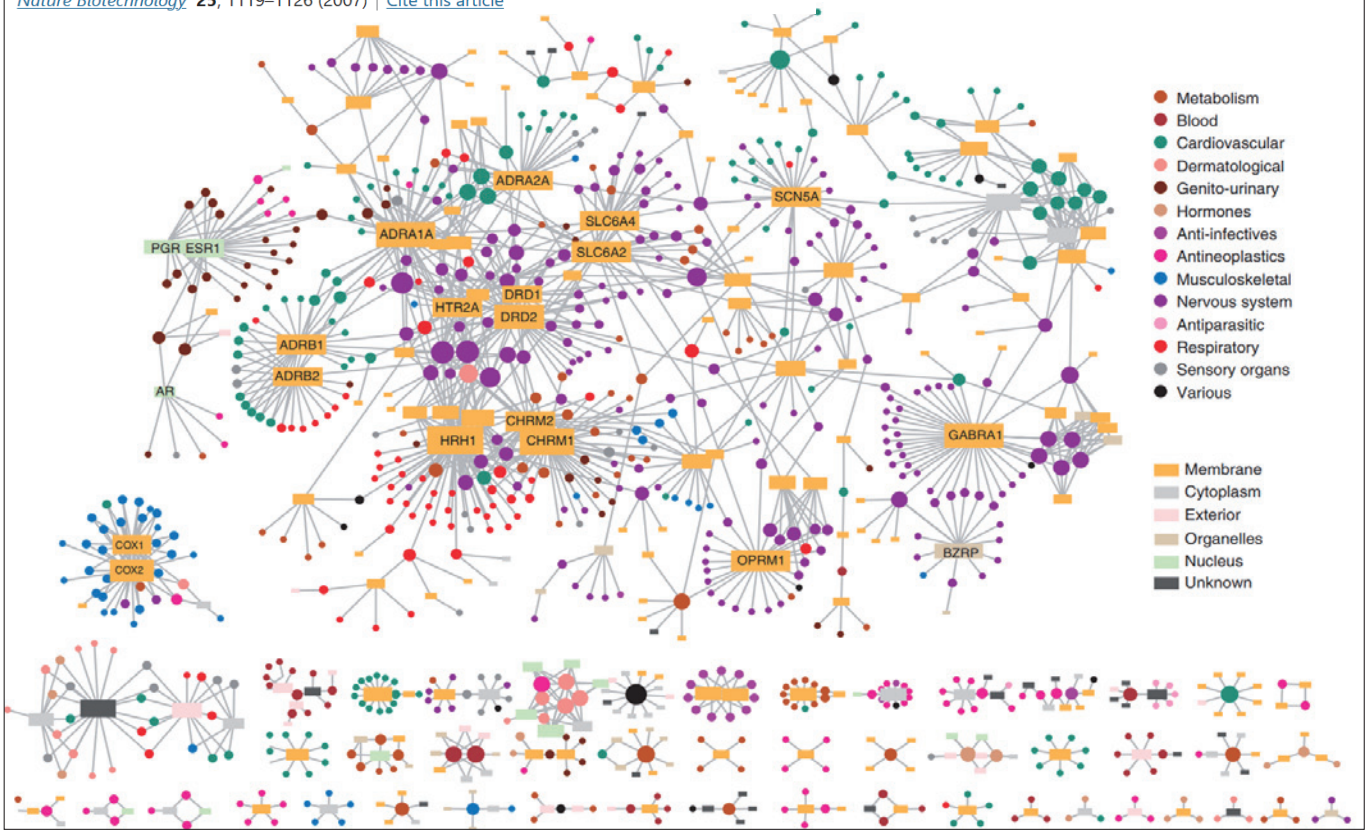
Analysis | Published: 05 October 2007

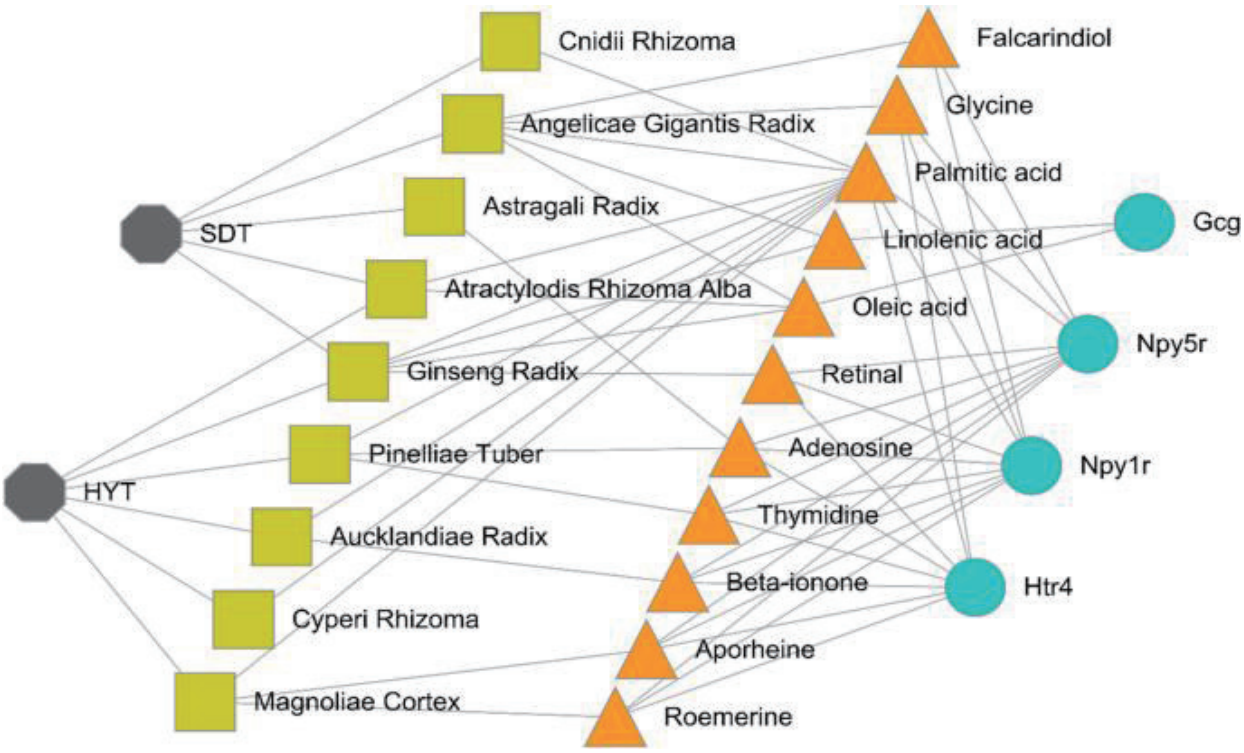
Drug–target network

nature biotechnology

Muhammed A Yıldırım, Kwang-Il Goh, Michael E Cusick, Albert-László Barabási & Marc Vidal

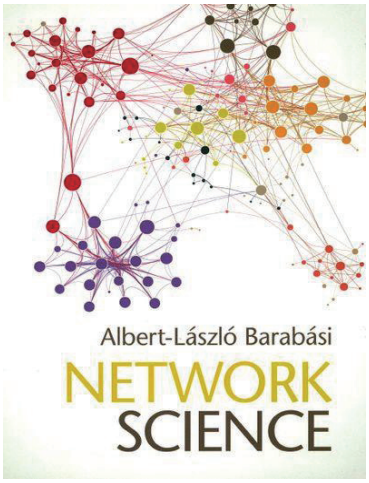
Nature Biotechnology **25**, 1119–1126 (2007) | Cite this article

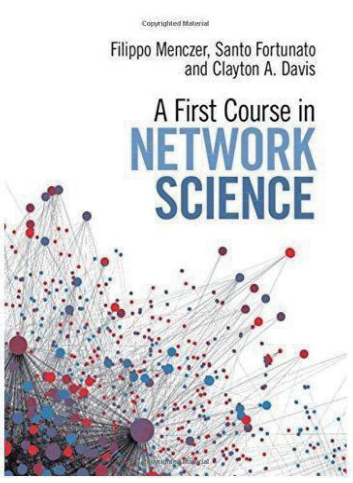


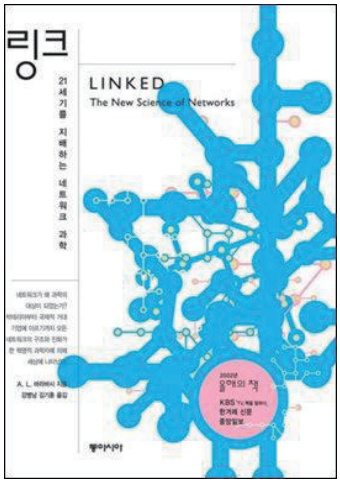


prescription-herb-compound-target network

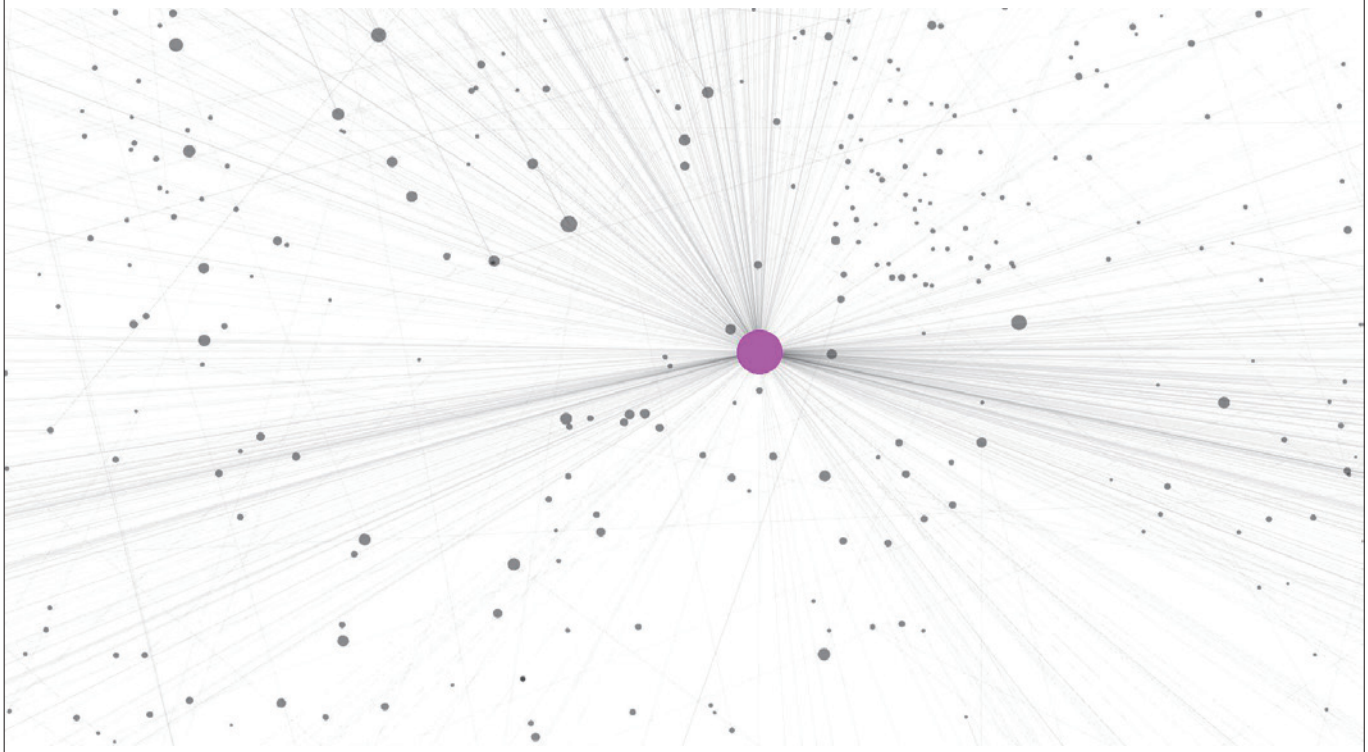
Reference







Zooming into the World Wide Web

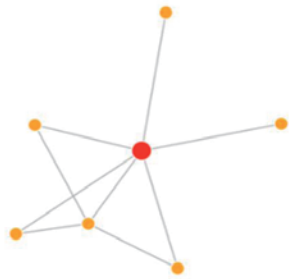
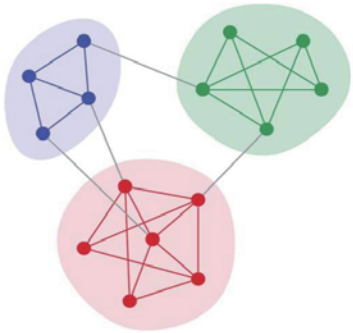
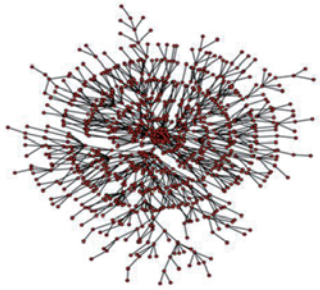


점(Node)와 선(Edge)를 이용하여
네트워크를 정의하고 만들어진 네트워크의
구조(Topology)와 변화(Dynamics)를
이용하여 현상을 설명, 예측하는 방법

Collective dynamics of **'small-world'networks**
DJ Watts, SH Strogatz - nature, 1998 - nature.com
… The neural **network** of the worm Caenorhabditis elegans, the power grid of the western …
to be **small-world networks**. Models of **dynamical** systems with **small-world** coupling display …
☆ 저장 99 인용 56543회 인용 관련 학술자료 전체 136개의 버전 Web of Science: 29365

Emergence of scaling in random networks
AL Barabási, R Albert - science, 1999 - science.org
Systems as diverse as genetic networks or the World Wide Web are best described as networks with complex topology. A common property of many large networks is that the vertex connectivities follow a scale-free power-law distribution. This feature was found to be a consequence of two generic mechanisms:(i) networks expand continuously by the addition of new vertices, and (ii) new vertices attach preferentially to sites that are already well connected. A model based on these two ingredients reproduces the observed stationary …
☆ 저장 99 인용 47950회 인용 관련 학술자료 전체 62개의 버전 Web of Science: 24977 »

Analysis of network structure (topology)

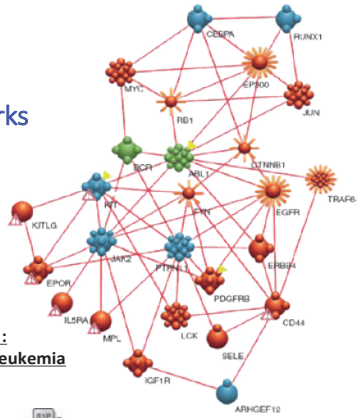
Micro-level (local structure of individual nodes)	Meso-level (structure at the intermediate level of network)	Macro-level (structure of entire network)
		

Macroscale properties of various networks

Social Network

Twitter follow network

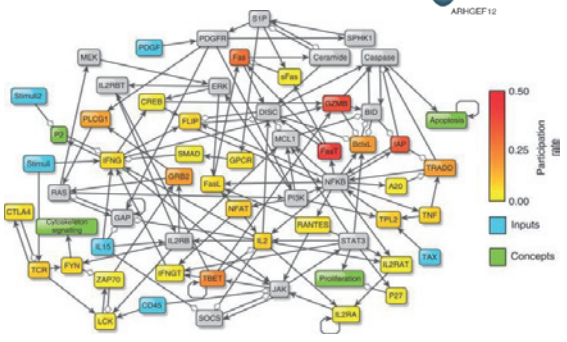
Biological Networks



Protein interaction network :
Related to chronic myeloid leukemia

Transport Network

Delta airline domestic routes network



T cell survival signaling network

- What are network measures that characterize the topology of these networks?
- How are these measures related to macroscopic properties of the networks?

Fig. 0.8 Three biological networks. Left: Protein interaction network of yeast. Node size is proportional to the number of interacting proteins. Center: Neural network of the roundworm *Caenorhabditis elegans*. Large and red nodes represent neurons with more outgoing and incoming synapses, respectively. Right: Food web of species in the Florida Everglades. A directed link goes from a prey to a predator species. The weight (width) of a link represents the energy flux between the two species. Node size and color represent incoming and outgoing links, respectively, so that large blue nodes are the species at the top of the food chain, while small red nodes are the species at the bottom.

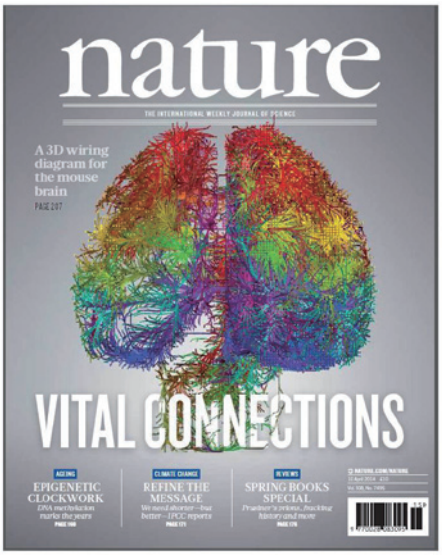
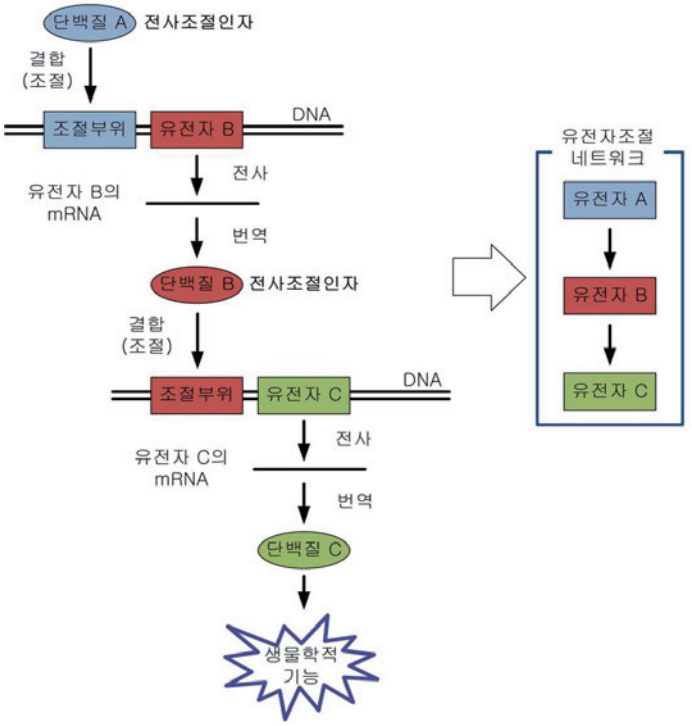


Figure 1.4
Mapping the Brain

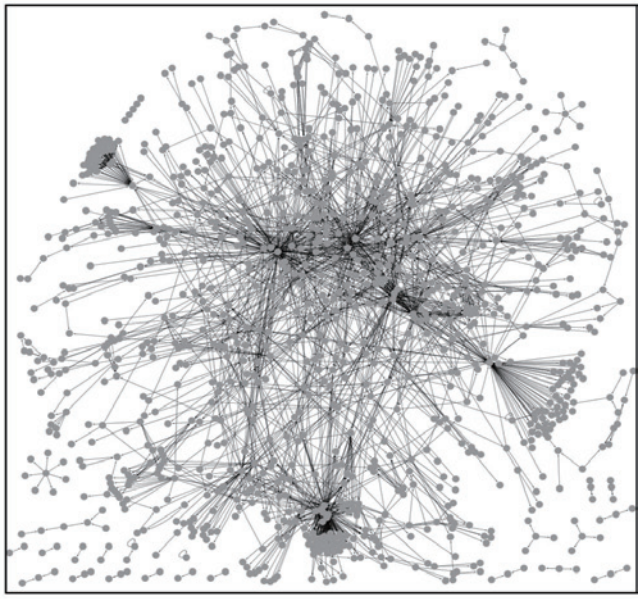
An exploding application area for network science is brain research. The wiring diagram of a complete nervous system has long been available for C. elegans, a small roundworm, but neuronal connectivity data for larger animals has been missing until recently. That is changing thanks to major efforts by the scientific community to develop technologies that can map out the brain's wiring diagram. The image shows the cover of the April 10, 2014 issue of *Nature*, reporting an extensive map of the laboratory mouse [4] generated by researchers at the Allen Institute in Seattle.

Figure 1.5
Network Biology and Medicine

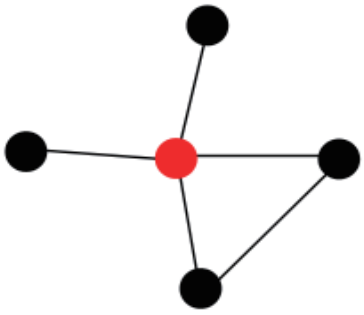
The cover of two issues of *Nature Reviews Genetics*, the leading review journal in genetics. The journal has devoted exceptional attention to the impact of networks: the 2004 cover focuses on *network biology* [8] (top), the 2011 cover discusses *network medicine* [9] (bottom).



인간의 유전자조절네트워크



Degree



Degree: The degree k_i of node i is equal to the number of edges attached to node i.
The red node has degree $k = 4$.

NETWORK	NODES	LINKS	DIRECTED UNDIRECTED	N	L	⟨k⟩
Internet	Routers	Internet connections	Undirected	192,244	609,066	6.34
WWW	Webpages	Links	Directed	325,729	1,497,134	4.60
Power Grid	Power plants, transformers	Cables	Undirected	4,941	6,594	2.67
Mobile Phone Calls	Subscribers	Calls	Directed	36,595	91,826	2.51
Email	Email addresses	Emails	Directed	57,194	103,731	1.81
Science Collaboration	Scientists	Co-authorship	Undirected	23,133	93,439	8.08
Actor Network	Actors	Co-acting	Undirected	702,388	29,397,908	83.71
Citation Network	Paper	Citations	Directed	449,673	4,689,479	10.43
E. Coli Metabolism	Metabolites	Chemical reactions	Directed	1,039	5,802	5.58
Protein Interactions	Proteins	Binding interactions	Undirected	2,018	2,930	2.90

Table 2.1
Canonical Network Maps

The basic characteristics of ten networks used throughout this book to illustrate the tools of network science. The table lists the nature of their nodes and links, indicating if links are directed or undirected, the number of nodes (N) and links (L), and the average degree for each network. For directed networks the average degree shown is the average in- or out-degrees $\langle k \rangle = \langle k_{in} \rangle = \langle k_{out} \rangle$ (see Equation (2.5)).

Characteristic of networks – degree distribution

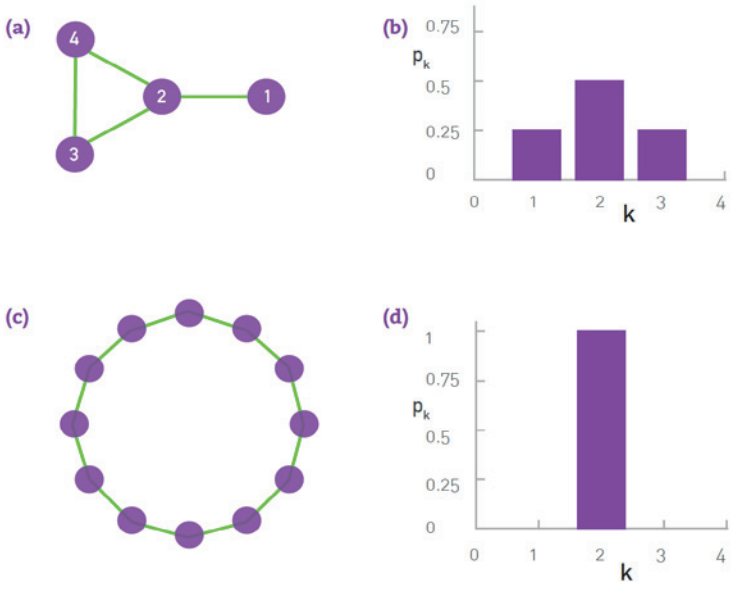


Figure 2.3
Degree Distribution

The degree distribution of a network is provided by the ratio (2.7).

(a) For the network in (a) with $N = 4$ the degree distribution is shown in (b).

(b) We have $p_1 = 1/4$ (one of the four nodes has degree $k_1 = 1$), $p_2 = 1/2$ (two nodes have $k_3 = k_4 = 2$), and $p_3 = 1/4$ (as $k_2 = 3$). As we lack nodes with degree $k > 3$, $p_k = 0$ for any $k > 3$.

(c) A one dimensional lattice for which each node has the same degree $k = 2$.

(d) The degree distribution of (c) is a Kronecker's delta function, $p_k = \delta(k - 2)$.

Graphical and matrix representation of networks

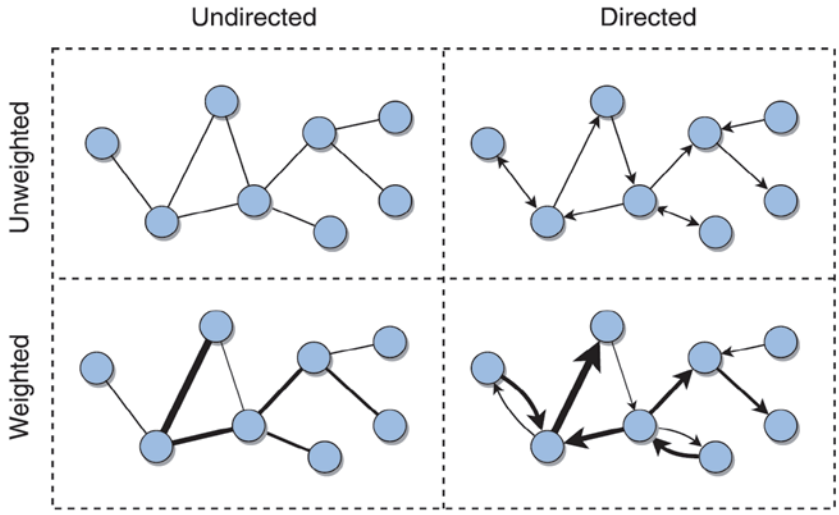


Fig. 1.1 Graphical representations of undirected, directed, and weighted networks. The circles represent the nodes. Pairs of adjacent nodes are connected by a line (link) or arrow (directed link). Arrows indicate the direction of the links. The thickness of a link represents its weight in weighted networks.

Graphical and matrix representation of networks

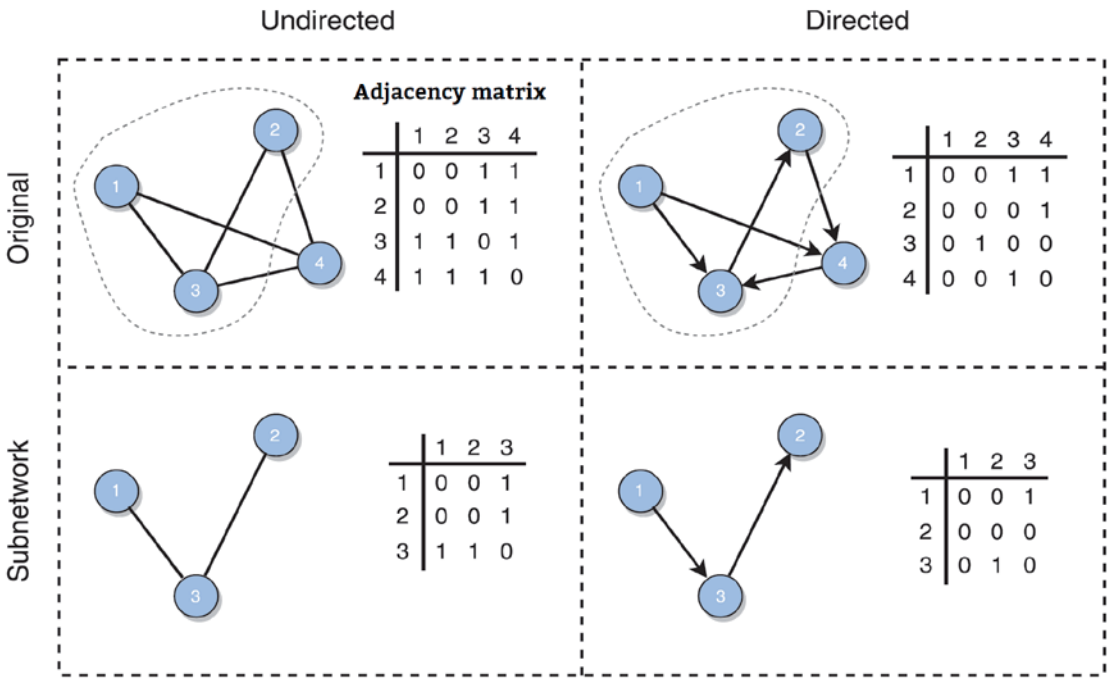
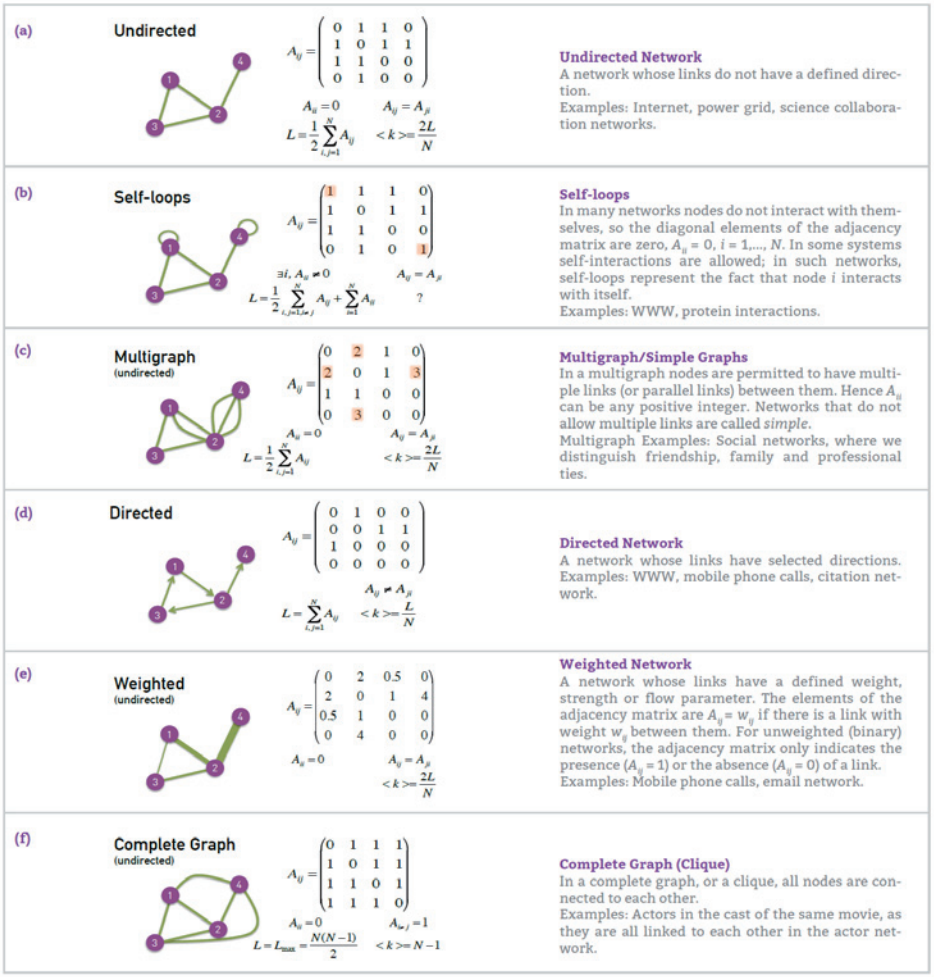


Fig. 1.3 Network and subnetwork examples. We also show the adjacency matrix representation of each network (see Section 1.9).



Graphical and matrix representation of networks

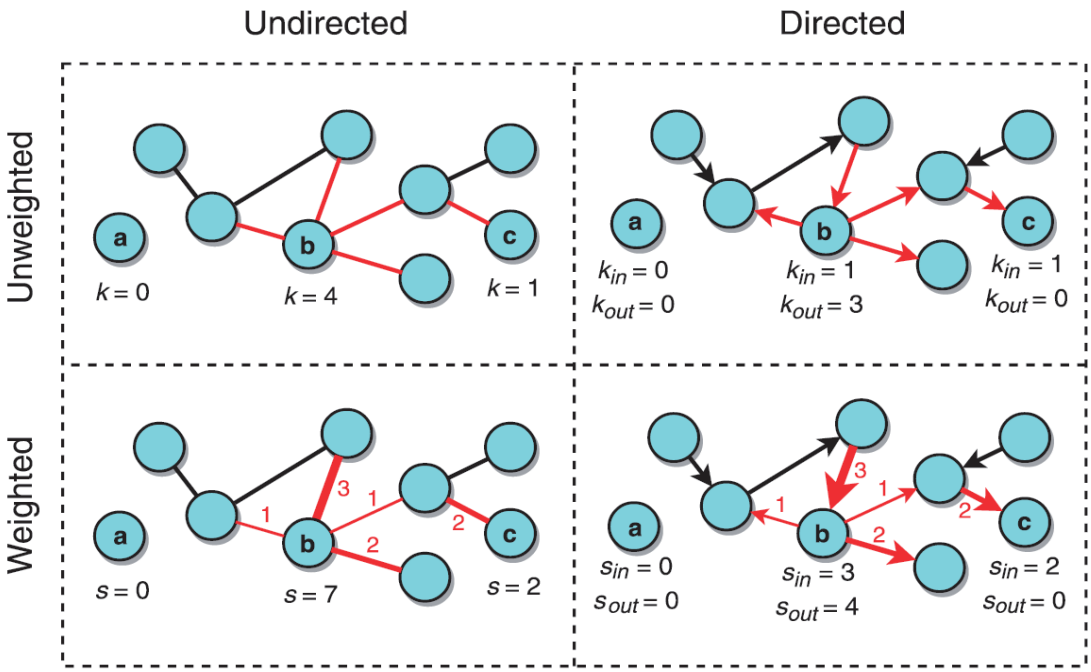


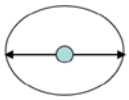
Fig. 1.4 Illustrations of degree and strength in directed, undirected, weighted, and unweighted networks. The links of nodes **a**, **b**, and **c** along with their weights are highlighted in red, and their degrees or strengths are shown.

Important measures…
(How to find important node?)

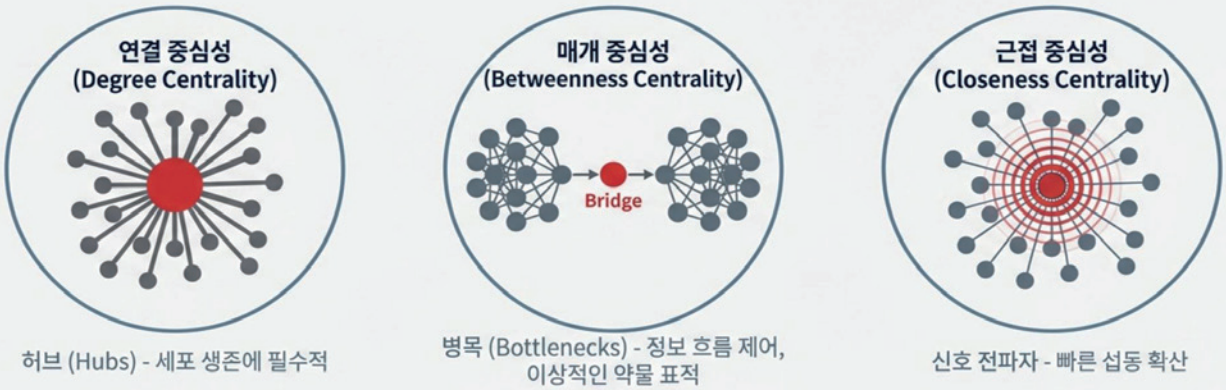
- Degree centrality (Hub:마당발)
  – Node with lots of connections

- Betweeness centrality (Linker:매개자)
  – Node with lots of traffic

- Closeness centrality (Center:중심자)
  – Node in the middle of the network



토폴로지 지표와 약물 표적 선정



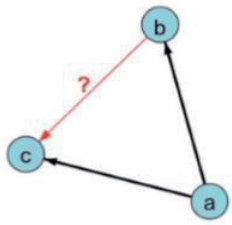
허브 (Hubs) - 세포 생존에 필수적

병목 (Bottlenecks) - 정보 흐름 제어, 이상적인 약물 표적

신호 전파자 - 빠른 섭동 확산

지표 (Metric)	정의 (Definition)	생물학적 의미 (Biological Implication)
Degree Centrality	연결된 엣지의 수	필수 단백질(Hub). 독성 문제로 직접 공략이 어려울 수 있음.
Betweenness Centrality	최단 경로에 위치하는 빈도	기능적 모듈 간의 연결 고리. 효과적인 약물 표적(VIP).
Closeness Centrality	모든 노드까지의 거리의 역수	네트워크 전체로 신호를 빠르게 전달하는 능력.

Local clustering coefficient



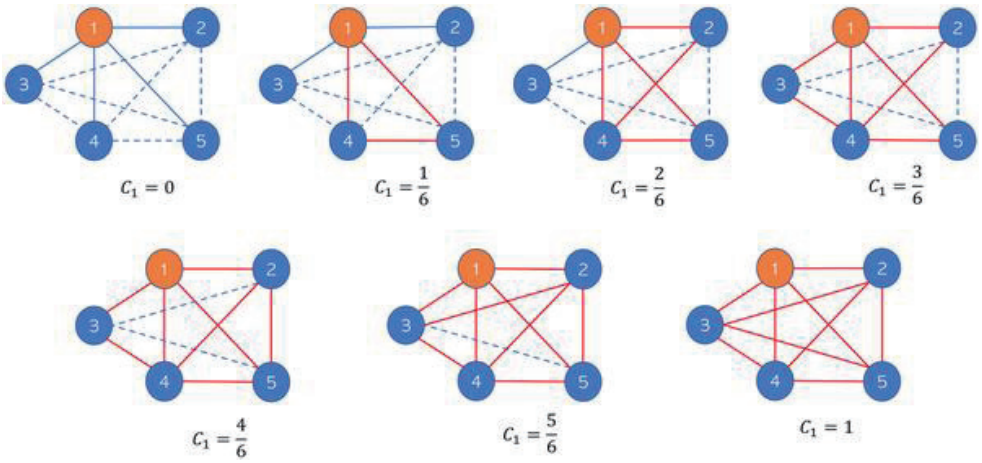
- for a node i, the **local clustering coefficient** captures the fraction of its neighbours that are directly connected
- **undirected networks**

$$C_i := \frac{2 \cdot k(i)}{d_i(d_i - 1)} = \frac{k(i)}{\binom{d_i}{2}}$$

- **directed networks**

$$C_i := \frac{k(i)}{d_{out}(i)(d_{out}(i) - 1)}$$

for $k(i) := |\{(j,k) \in E : (i,j) \in E \wedge (i,k) \in E\}|$



Network measures

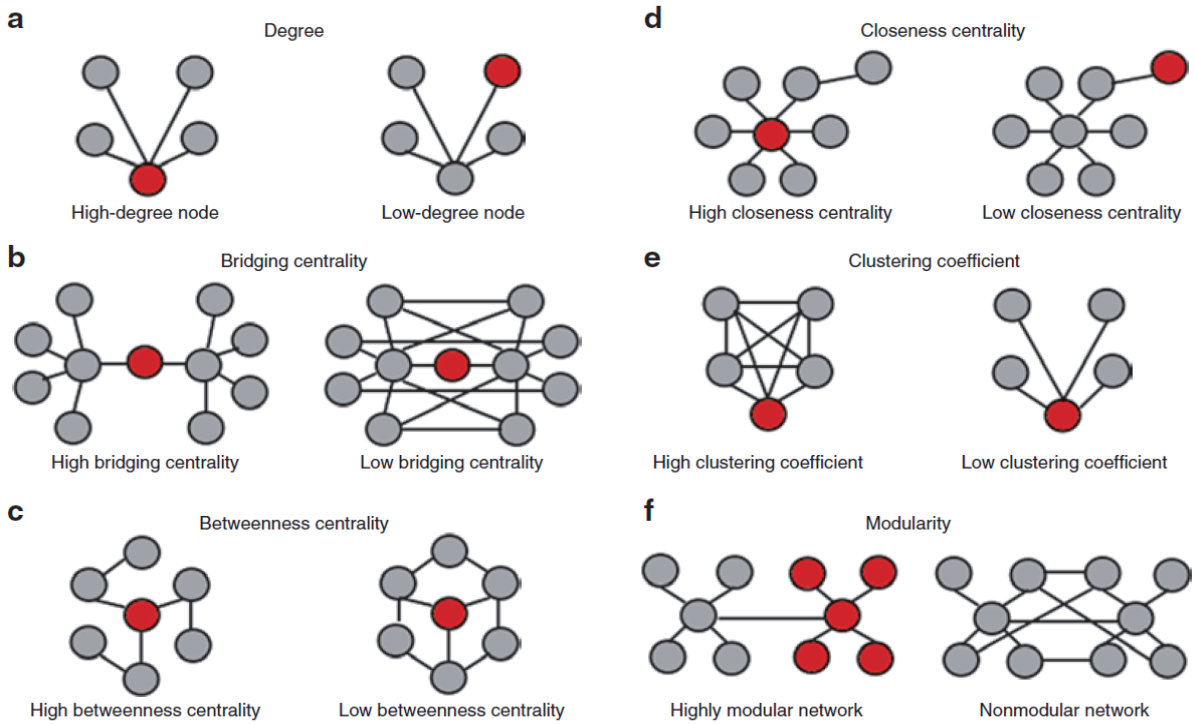
Clinical Pharmacology & Therapeutics

State of the Art

Connecting the Dots: Applications of Network Medicine in Pharmacology and Disease

A Jacunski, N P Tatonetti

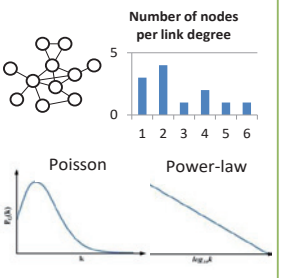
First published: 29 August 2013 | https://doi.org/10.1038/clpt.2013.168 | Citations: 11



Networks can be characterized by many network properties.

Network Properties

Degree distribution



Network heterogeneity

$$H = \frac{\sqrt{\mathrm{Var}(k)}}{\mathrm{mean}(k)}$$

Node accessibility

Characteristic path length

$\bar{l} = \mathrm{avg}(l(i,j))$

$\bar{l}(i) = \mathrm{avg}(l(i,j))$

Graph Diameter

$D = \max(l(i,j))$

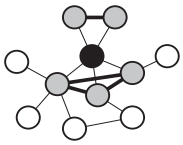
Closeness centrality

$$C_c(i) = \frac{1}{\bar{l}(i)}$$

Betweenness centrality

$$B(m) = \sum_{i \neq j} \frac{B(i,m,j)}{B(i,j)}$$

Clustering coefficient



Clustering coefficient of Black node

$$C_x = \frac{4}{\binom{5}{2}} = 0.4$$

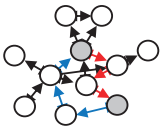
Clustering coefficient of Whole graph

$\bar{C} = \mathrm{avg}(C_i)$

Small worldness

High $\bar{C}$, low $\bar{l}$

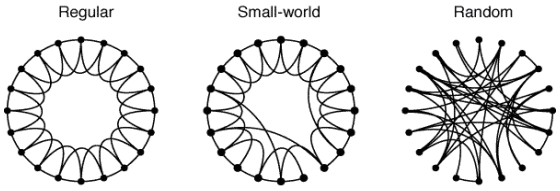
Directionality

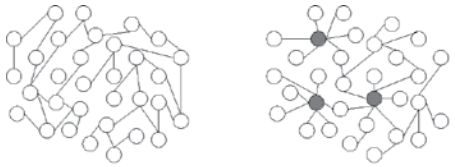


Directed graphs have separate '**directed**' and '**undirected**' properties.

e.g. In-degree and out-degree distribution
Direction-considered characteristic path length

Network Types





(a) Random network (b) Scale-free network

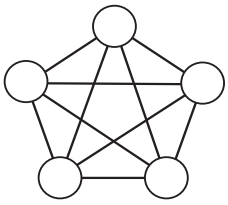
The hidden networks of everything

https://youtu.be/RfgjHoVCZwU

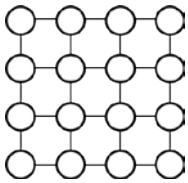
Regular networks and random networks

Regular networks

Generating methods

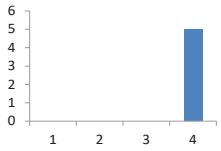


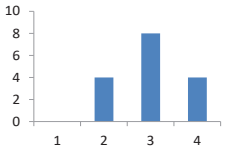
All nodes have same number of links



Similar number of links

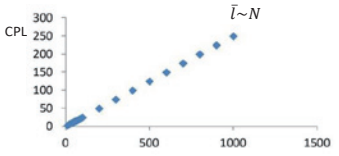
Degree distribution





Regular networks

Characteristic path length



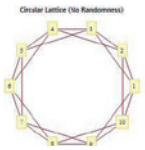
Number of nodes

Clustering coefficient

Ring lattice with degree k:

$$C = \frac{3(k-2)}{4(k-1)} \gg p$$

(Different for general regular networks)

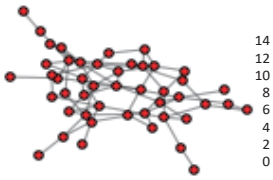


Ring lattice with degree 4

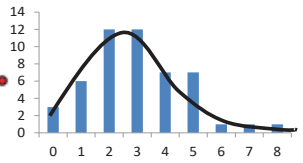
Random networks

$G(n,p)$ All node-pairs have same probability of connection p

$G(n,M)$ A graph is chosen random-uniformly from all possible graphs with M edges

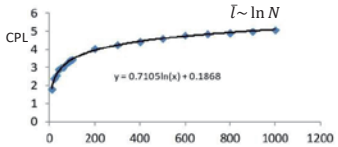


Random network with n=50, M=75



Poisson Distribution

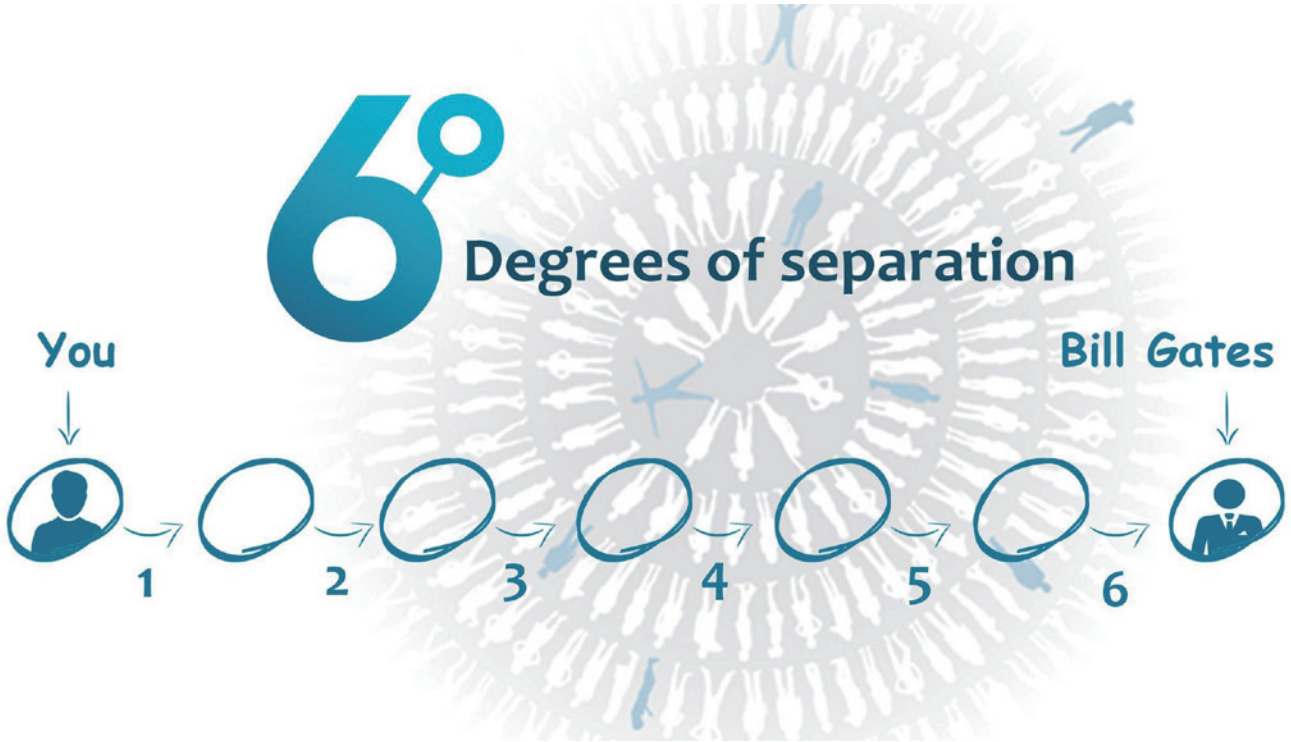
Random networks



Number of nodes

Expectation value of clustering coefficient: p

It's a Small World



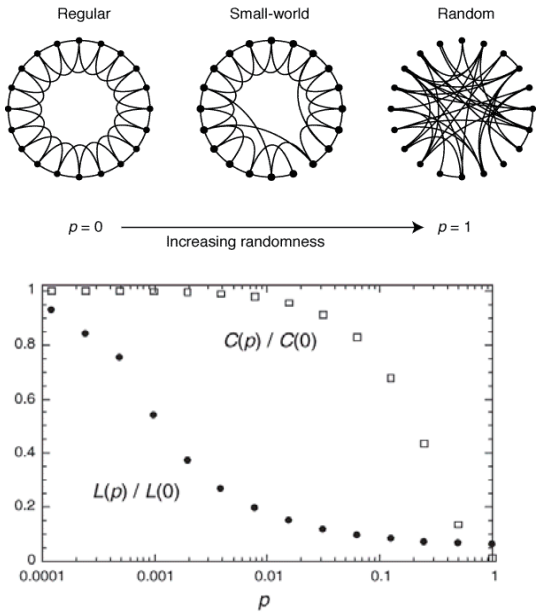
Small-world networks

https://mathinsight.org/applet/small_world_network

Watts-Strogatz small-world model

Generation: Start with ring lattice, rewire each edge randomly by probability p

Characteristics

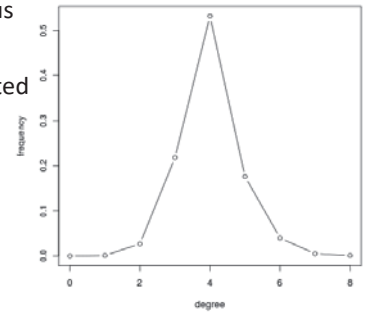


Network	Lattice, Ordered	Small World	Random, Disordered
Clustering Coefficient	High	High	Low
Mean Path Length	Long	Short	Short

- Generation of Watts-Strogatz small-world network. $p = 0$ and $p = 1$ obtains regular lattice and random network respectively.

- **General Small-worldness**
  - Highly clustered than random networks
  - Small characteristic path length like random networks (**at least** $\bar{l} \sim \log n$)
  - High 'small world coefficient' $\sigma = \frac{C/C_{rand}}{L/L_{rand}}$

- Generally homogeneous degree distribution
  - Many less-concentrated hubs



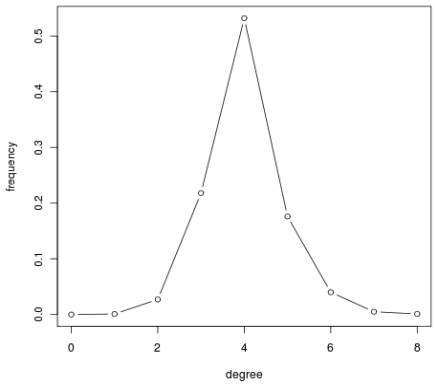
- Real-world advantages: Efficient information flow, robust to perturbations via high clustering

Small-world networks

Watts-Strogatz small-world model

Limitations of Watts-Strogatz model

- Unrealistic degree distribution:
  Real world networks follow power law, which cannot be explained by Watts-Strogatz model



- Degree distribution of Watts-Strogatz model (1000 nodes and 2000 edges, p=0.1) Homogeneous distribution: peak on average

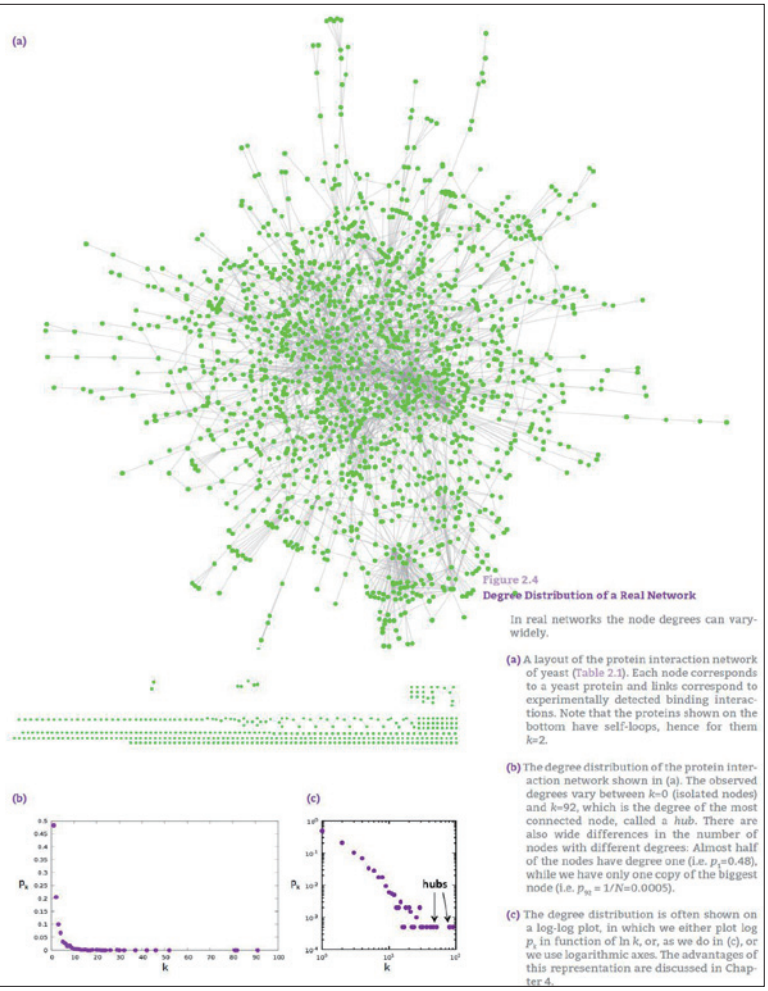


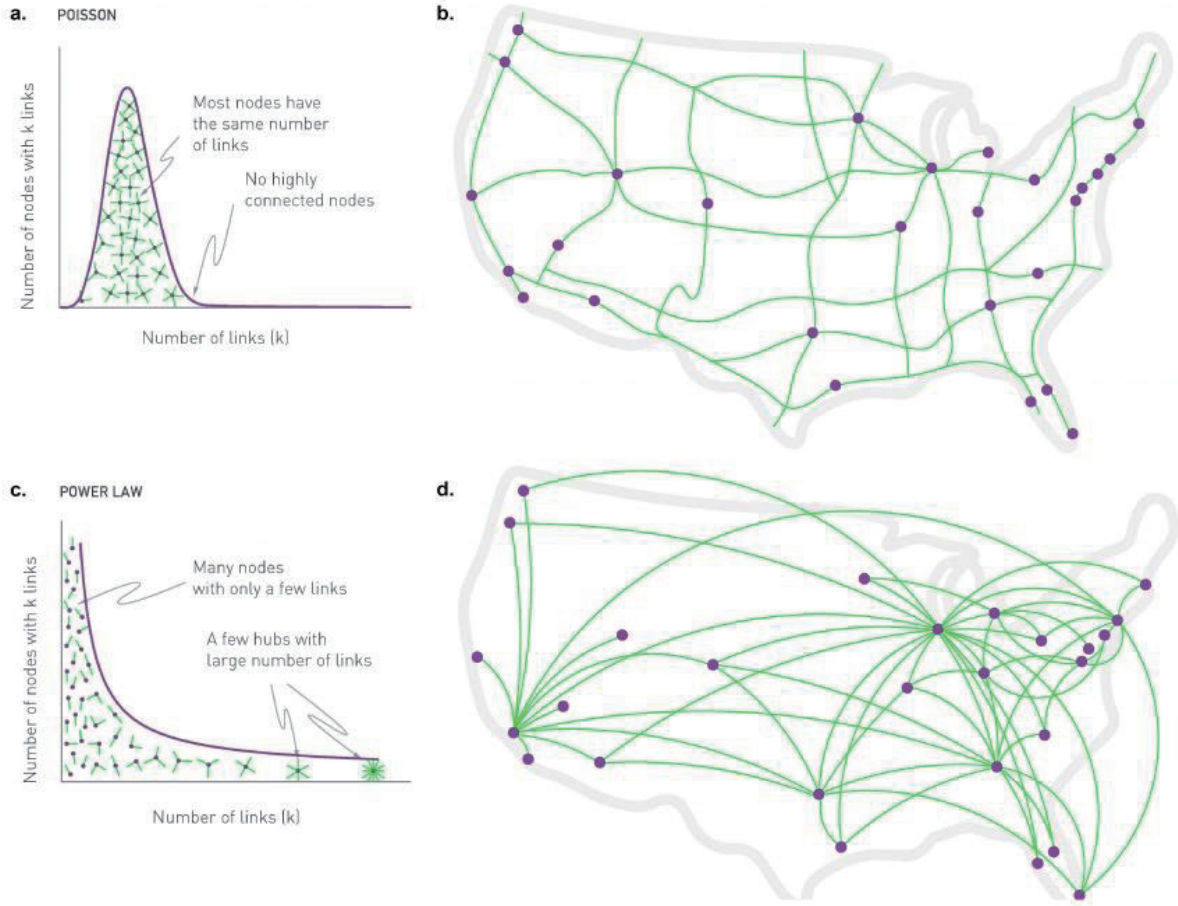
Figure 2.4
Degree Distribution of a Real Network

In real networks the node degrees can vary widely.

(a) A layout of the protein interaction network of yeast (Table 2.1). Each node corresponds to a yeast protein and links correspond to experimentally detected binding interactions. Note that the proteins shown on the bottom have self-loops, hence for them $k=2$.

(b) The degree distribution of the protein interaction network shown in (a). The observed degrees vary between $k=0$ (isolated nodes) and $k=92$, which is the degree of the most connected node, called a *hub*. There are also wide differences in the number of nodes with different degrees: Almost half of the nodes have degree one (i.e. $p_k=0.48$), while we have only one copy of the biggest node (i.e. $p_{92} = 1/N=0.0005$).

(c) The degree distribution is often shown on a log-log plot, in which we either plot log p_k in function of ln k, or, as we do in (c), or we use logarithmic axes. The advantages of this representation are discussed in Chapter 4.

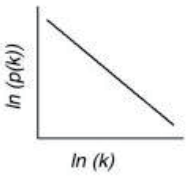


Scale-free networks

- **Definition: Power-law degree distribution**

$$P(k) \sim k^{-\gamma}$$

  - Graph steeper as larger γ
  - Scale-free: no characteristic value k on the graph



- **Characteristics**

(1) Extremely small characteristic path length:

$$\bar{l} \sim \log(\log(N))$$

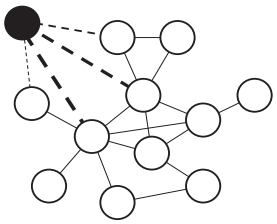
(2) Relatively many super-hubs (long tail)
(3) More robust to random error.
(4) More fragile to hub-targeted attacks.

- **Generation: Preferential attachment**

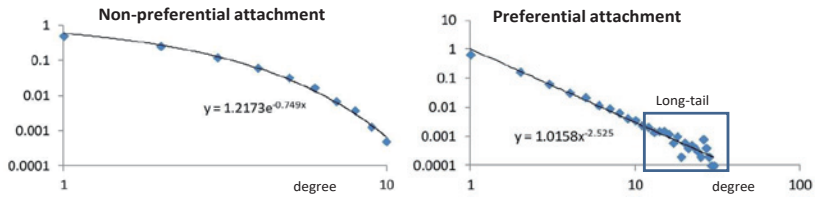
$$P(i) \sim \frac{(k_i + A)}{\sum_i (k_i + A)}$$

  - Higher probability of link addition for hubs
  - Larger $A \rightarrow$ larger γ

$$A = 0\text{: } \gamma \sim 3$$

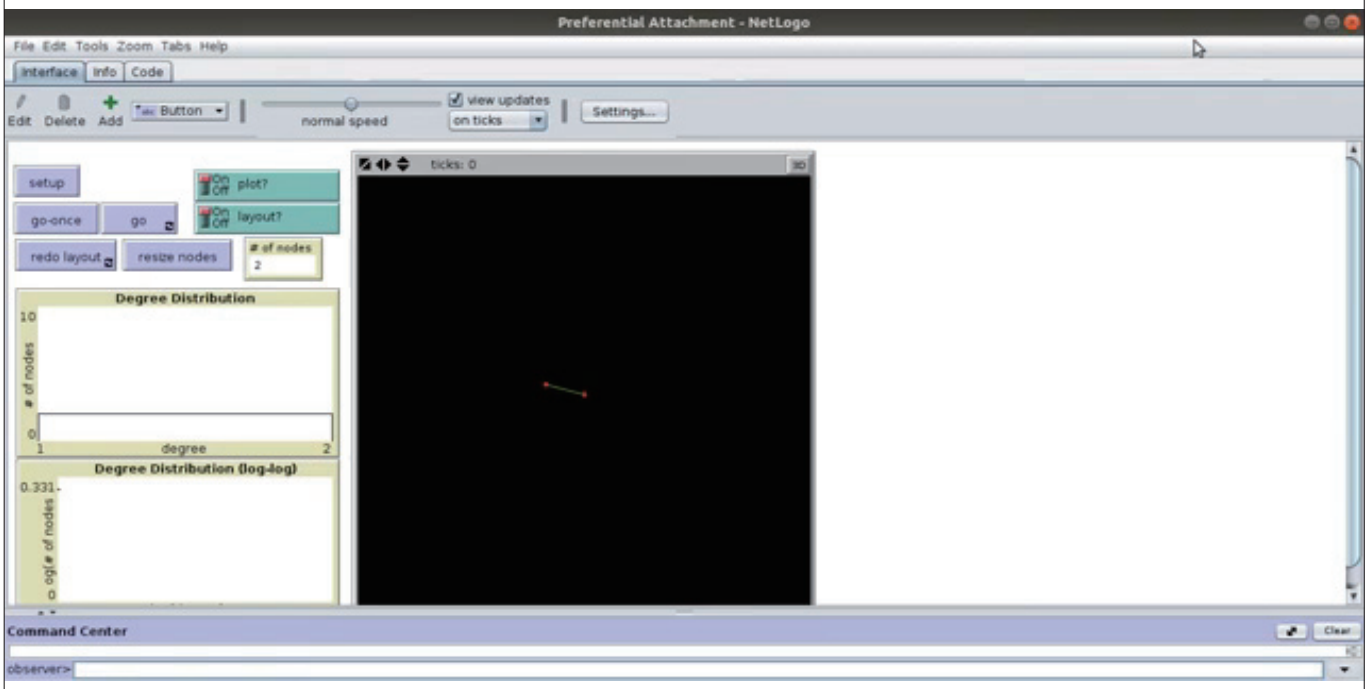


Degree distribution



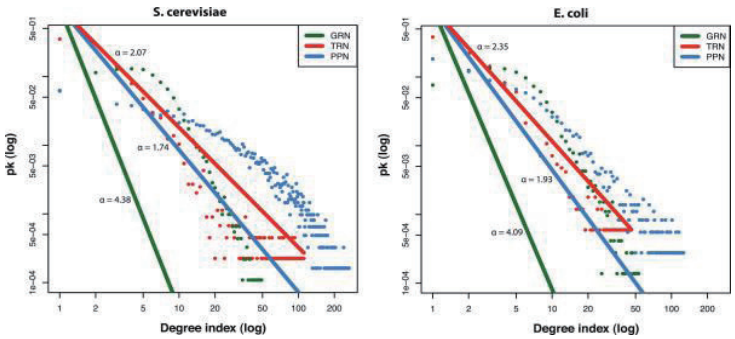
  - Preferential attachment can generate network with power law degree distribution.

Scale-free networks



Scale-free properties of biological networks

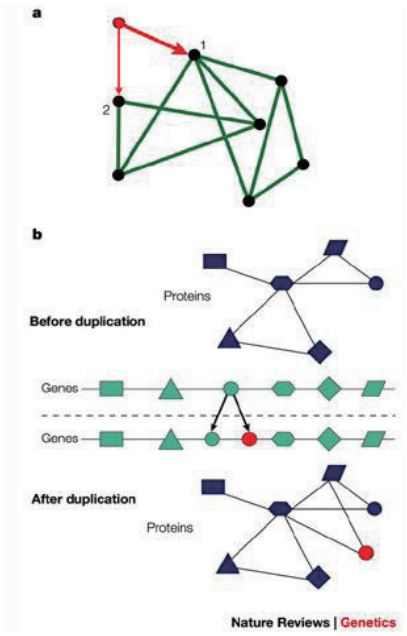
- Scale-free networks are more 'fit-to-survive' than random networks, because biological errors occur mainly by random events, not targeted attacks.
- Signaling, gene regulation, metabolic, protein-protein inter-action networks all have scale-free properties.
- In particular, metabolic and PPI networks also have high clustering coefficient (thus small-worldness), which provides advantages on information flow and local robustness.



Fitted power-law distribution for the gene regulatory network (GRN), transcriptional regulatory network (TRN), and protein-protein interaction network (PPI) of *S. cerevisiae* and *E. coli* .

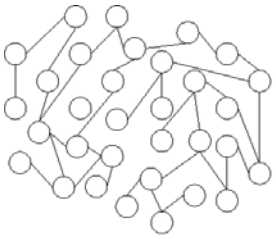
Biological origin

Duplication-Divergence model



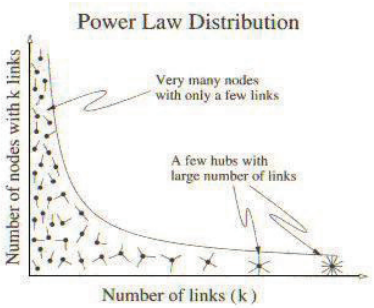
Scale-freeness of biological networks may be result of preferential attach-ment by gene duplication.

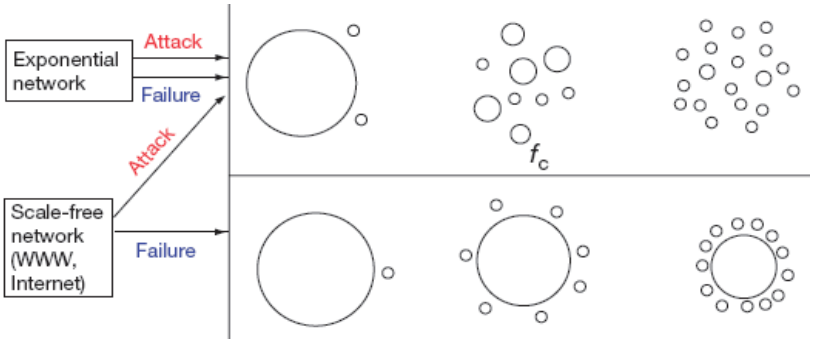
Structure-function relationship



Exponential
(a) Random network

Scale-free
(b) Scale-free network





Error and attack tolerance of complex networks

Réka Albert, Hawoong Jeong & Albert-László Barabási

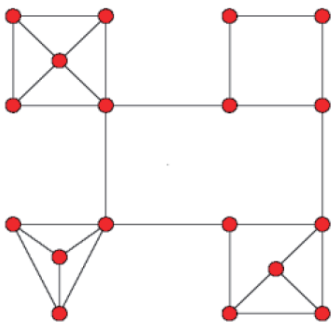
Department of Physics, 225 Nieuwland Science Hall, University of Notre Dame, Notre Dame, Indiana 46556, USA

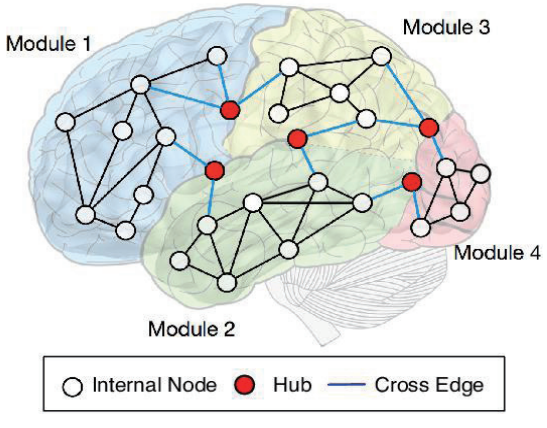
- Failure : selection and removal of random nodes
- Attack : selection and removal of a few nodes that play a vital role in maintaining the network's connectivity

BUT THERE IS Modularity!!!

- High C → real networks are fragmented into group or modules
  - Internet: Vasquez, Pastor-Satorras, Vespignani (2001).
  - Society: Granovetter, M. S. (1973) ; Girvan, M., & Newman, M.E.J. (2001); Watts, D. J., Dodds, P. S., & Newman, M. E. J. (2002).
  - WWW: Flake, G. W., Lawrence, S., & Giles. C. L. (2000).
  - Biology: Hartwell, L.-H., Hopfield, J. J., Leibler, S., & Murray, A. W. (1999).

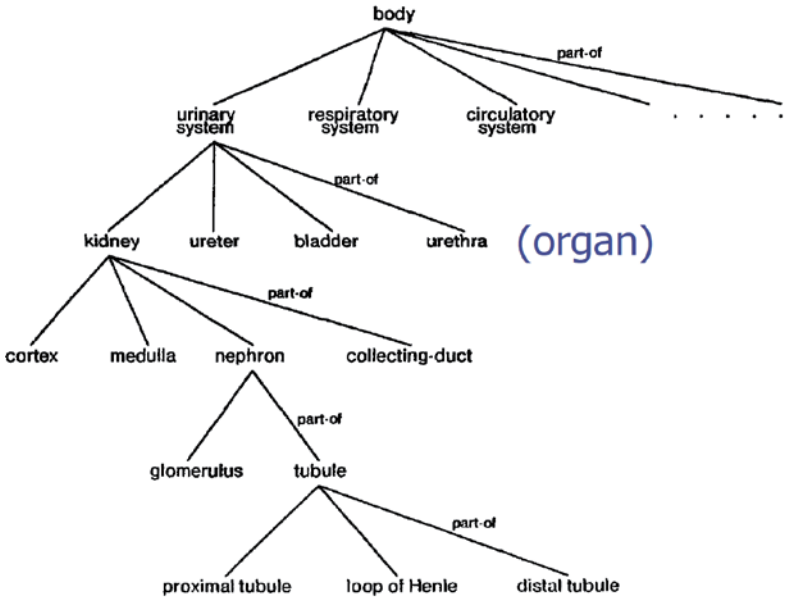
- Traditional view of modularity:

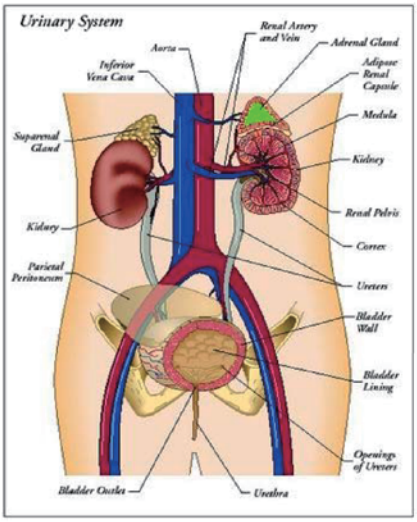




Meso-level property

Modules in biology





Patil, Ramesh S. *Causal Representation of Patient Illness for Electrolyte and Acid-Base Diagnosis.* MIT Lab for Comp. Sci. TR-267 (1981).

www.faqs.org

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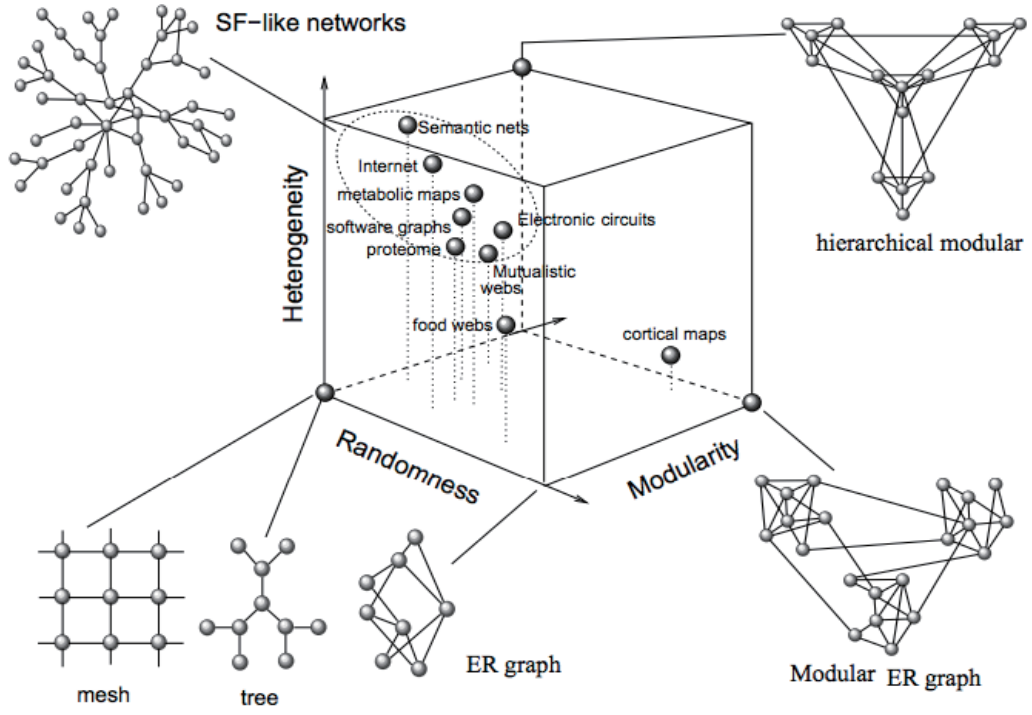
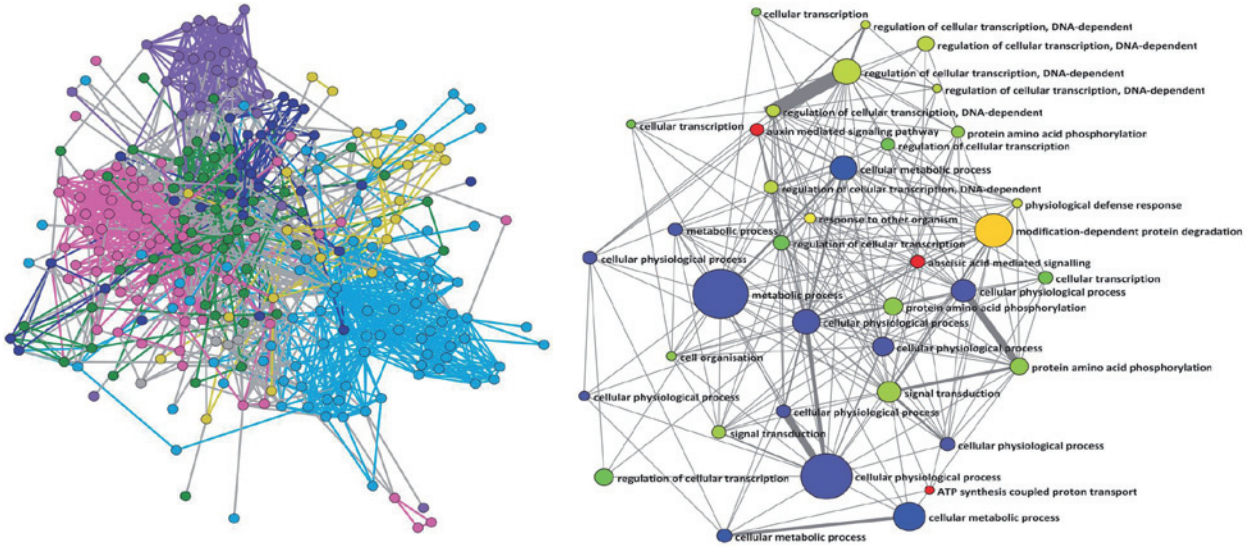


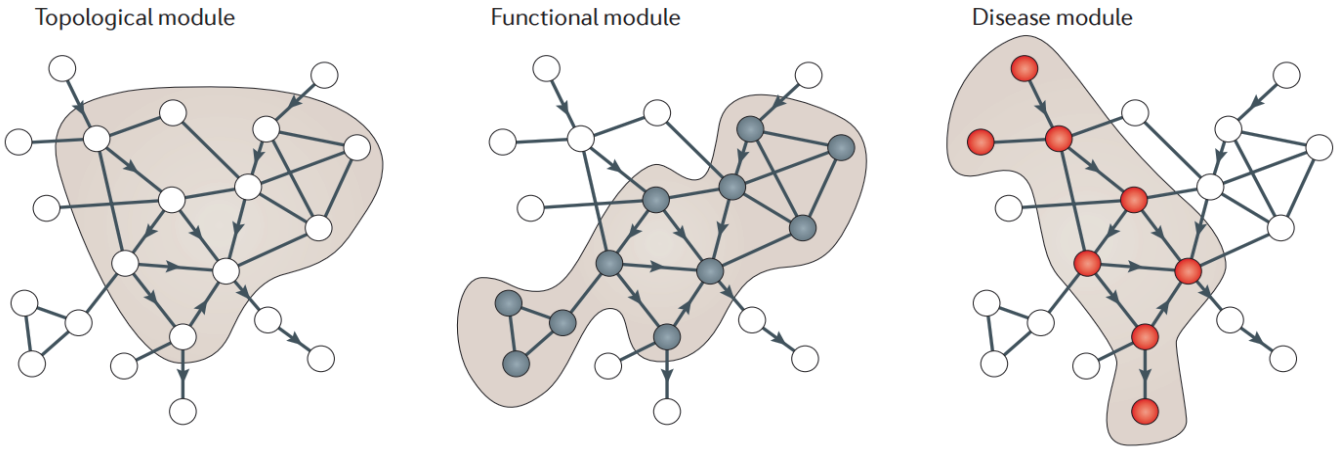
FIG. 3 A zoo of complex networks. In this qualitative space, three relevant characteristics are included: randomness, heterogeneity and modularity. The first introduces the amount of randomness involved in the process of network's building. The second measures how diverse is the link distribution and the third would measure how modular is the architecture. The position of different examples are only a visual guide. The domain of highly heterogeneous, random hierarchical networks appears much more occupied than others. Scale-free like networks belong to this domain.

Modular representation can reduce the complexity of network structure



- Abstraction of intracellular biomolecular interactions into networks is useful for data integration and graph analysis.
- Network analysis tools facilitate predictions of novel functions for proteins, prediction of functional interactions and identification of intracellular modules.
- These efforts are linked with drug and phenotype data to accelerate drug-target and biomarker discovery.

Module identification methods for different purposes



- Topological modules correspond to locally dense neighbourhoods of the interactome, and represent a pure network property.
- Functional modules correspond to network neighbourhoods in which there is a statistically significant segregation of nodes of related function.
- A disease module represents a group of nodes whose perturbation (mutations, deletions, copy number variations or expression changes) can be linked to a particular disease phenotype.

Modularity in graph theory

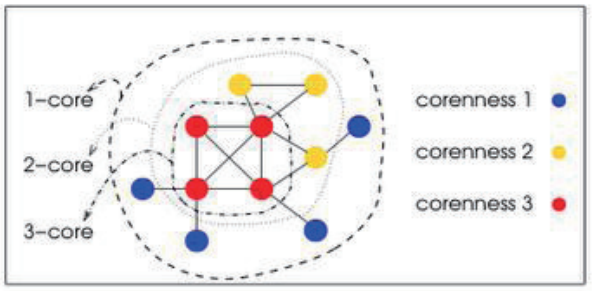
- Network modularity is the degree to which it can be separated into nearly independent subnetworks.
- Briefly, the Newman and Girvan algorithm finds the division of the nodes into modules that maximize a measure Q.

$$Q = \sum_{s=1}^{K} \left[\frac{l_s}{L} - \left(\frac{d_s}{2L} \right)^2 \right]$$

Where K is the number of modules, L is the number of edges in the network, l_s is the number of edges between nodes in module s, and d_s is the sum of the degrees of the nodes in module s.

- The rationale for this modularity measure is as follows:
  A good partition of a network into modules must comprise many within-module edges and as few as possible between-module edges.

Module identification using K-Core decomposition



- In the first round, all nodes with one or less edges are removed from the graph, and all their edges are deleted.
- In the second round, all nodes with two edges or less are removed from the graph and their edges deleted.
- Similarly, at the i-th iteration all nodes with less than i neighbors are removed from the graph.

Pseudocode

Stage 1: Vertex Weighting
procedure MCODE-VERTEX-WEIGHTING
  input: **graph**: G = (V,E)
  for all *v* in G **do**
    N = find neighbors of *v* to depth 1
    K = Get highest *k*-core graph from N
    k = Get highest *k*-core number from N
    d = Get density of K
    Set weight of *v* = *k* × *d*
  end for
end procedure

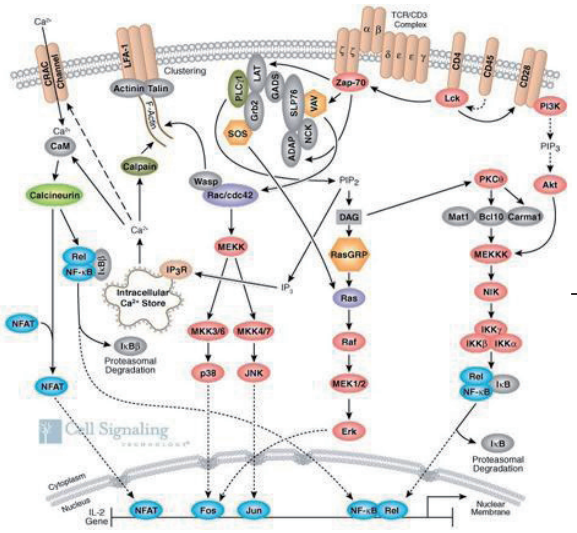
Stage 2: Molecular Complex Prediction
procedure MCODE-FIND-COMPLEX
  input: **graph**: G = (V,E); **vertex weights**: W;
    vertex weight percentage: *d*; **seed vertex**: *s*
  if *s* already seen **then return**
  for all *v* neighbors of *s* **do**
    if weight of *v* > (weight of *s*)(1 - *d*) **then** add *v* to complex C
    call: MCODE-FIND-COMPLEX (G, W, *d*, *v*)
  end for
end procedure
procedure MCODE-FIND-COMPLEXES
  input: **graph**: G = (V,E); **vertex weights**: W;
    vertex weight percentage: *d*
  for all *v* in G **do**
    if not already seen v **then call**: MCODE-FIND-COMPLEX(G, W, *d*, *v*)
  end for
end procedure

Stage 3: Post-Processing (optional)
procedure MCODE-FLUFF-COMPLEX
  input: **graph**: G = (V,E); **vertex weights**: W;
    fluff density threshold: *d*; **complex graph**: C = (U,F)
  for all *u* in C **do**
    if weight of *u* >*d* **then** add *u* to complex C
  end for
end procedure
procedure MCODE-POST-PROCESS
  input: **graph**: G = (V,E); **vertex weights**: W; **haircut flag**: *h*; **fluff flag**: *f*;
    fluff density threshold: *t*; **set of predicted complex graphs**: C
  for all *c* in C **do**
    if *c* not 2-core **then** filter
    if *h* is TRUE **then** 2-core complex
    if *f* is TRUE **then call**: MCODE-FLUFF-COMPLEX(G, W, *t*, *c*)
  end for
end procedure

Overall Process
procedure MCODE
  input: **graph**: G = (V,E); **vertex weight percentage**: *d*;
    haircut flag: *h*; **fluff flag**: *f*; **fluff density threshold**: *t*;
    set of predicted complex graphs: C
  call: W = MCODE-VERTEX-WEIGHTING (G)
  call: C = MCODE-FIND-COMPLEXES (G, W, *d*)

Meso-level property

- **What can be identified as a module in the signal transduction network?**



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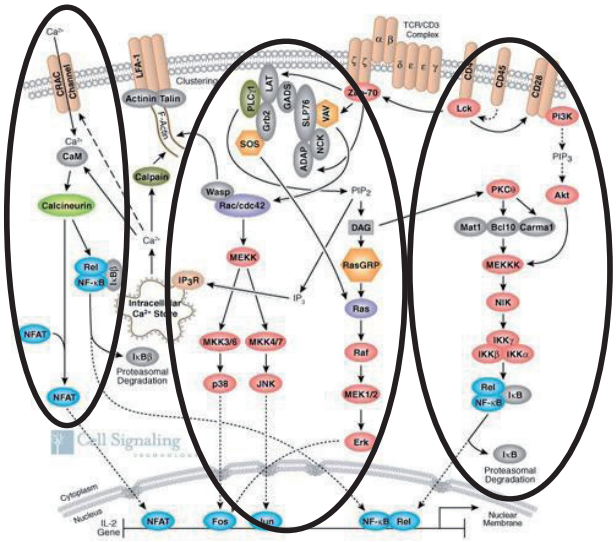
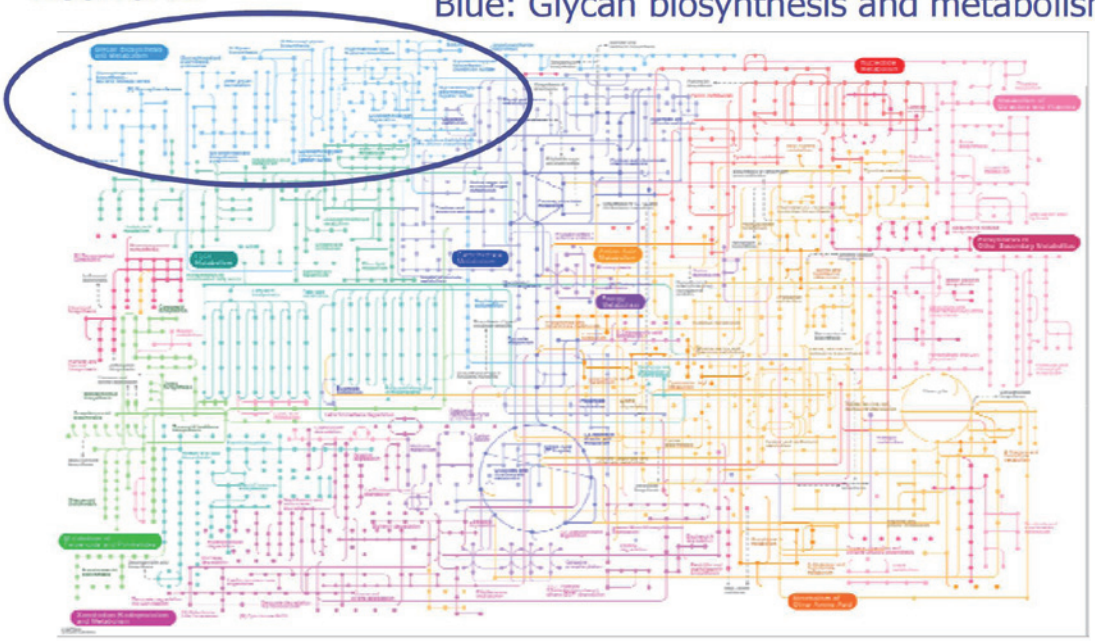


Signaling pathways can be candidates of modules.

Meso-level property

- Each color represents the functional role of metabolic network.

Blue: Glycan biosynthesis and metabolism



http://www.genome.jp/kegg/pathway/map/map01100.html

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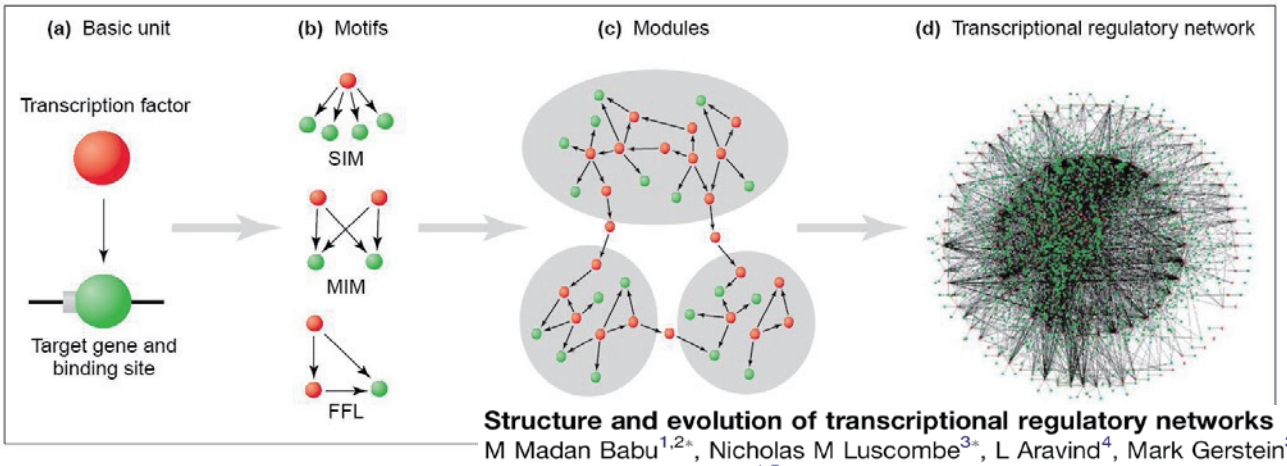
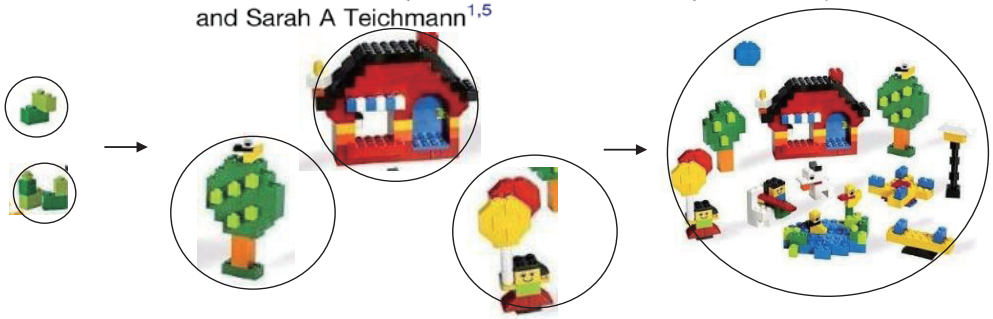
Different ways of study of biological networks

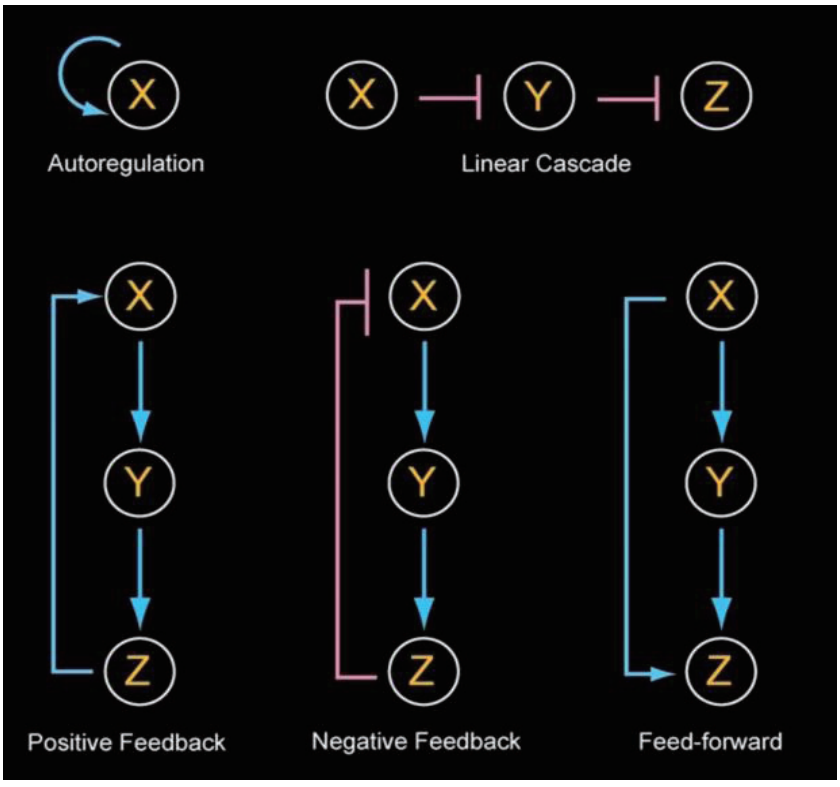


Structure and evolution of transcriptional regulatory networks
M Madan Babu[1,2*], Nicholas M Luscombe[3*], L Aravind[4], Mark Gerstein[3] and Sarah A Teichmann[1,5]



Structure-function relationship!

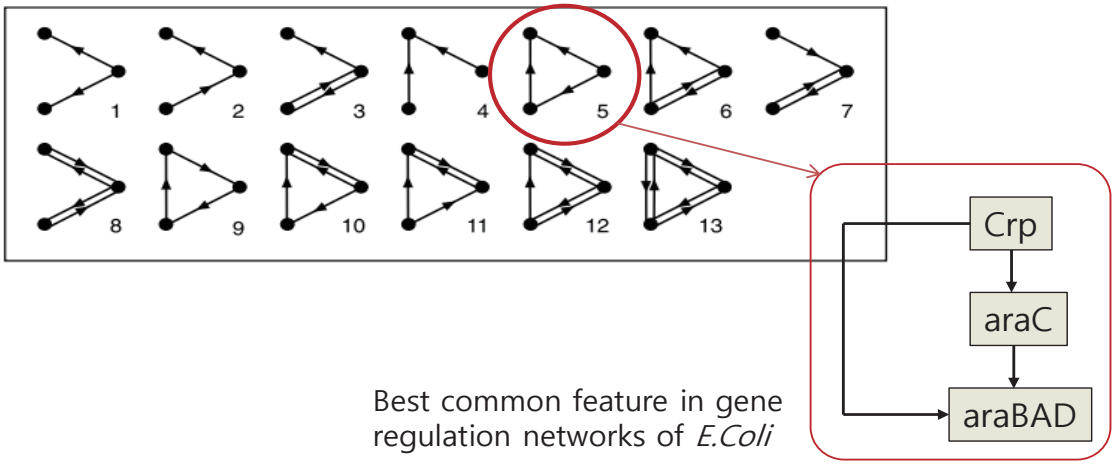
Micro-level property: Motifs



Building block

Network Motif
basic interaction patterns that recur throughout biological networks, much more often than in random networks.

n=1 Self-loops and isolated nodes
n=2 An edge, or a loop of two nodes
n=3 13 types of connected directed graphs



Best common feature in gene regulation networks of *E.Coli*

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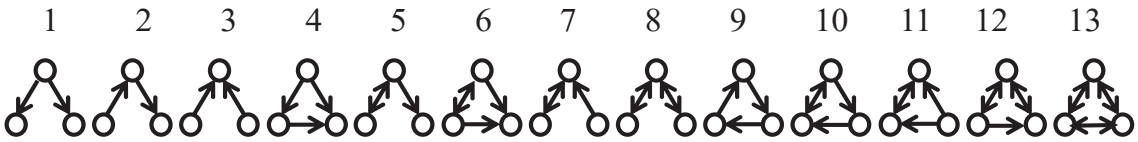
Micro-level property

- Sub-graphs



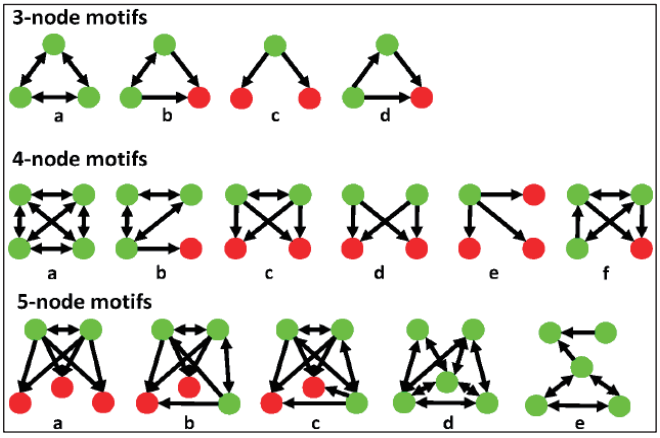
- Network Motifs are defined as patterns of interconnections that recur in many different parts of a network at frequencies much higher than those found in randomized networks.
- Network motif = basic functional unit= Basic building block

Why do we study network motifs?

- In order to explore the connection with various functions by dividing the network into the smallest unit.
- Forecasting of operation and response in the network under given situations.

Micro-level property

- **How to find?**
  - Comparison with random network to find statistically significant motifs.
  - By generating several random networks (R) with the same number of nodes and links as the target network (N), the significance of network motifs is determined by considering the average number of motifs and their standard deviation.



$$Z = \frac{< S >_N - < S >_R}{\sigma_R}$$

- $<S>_N$: Number of structures found in the target network
- $<S>_R$: Average of the number of structures found in a random network
- σ_R : Standard deviation of the number of structures found in a random network

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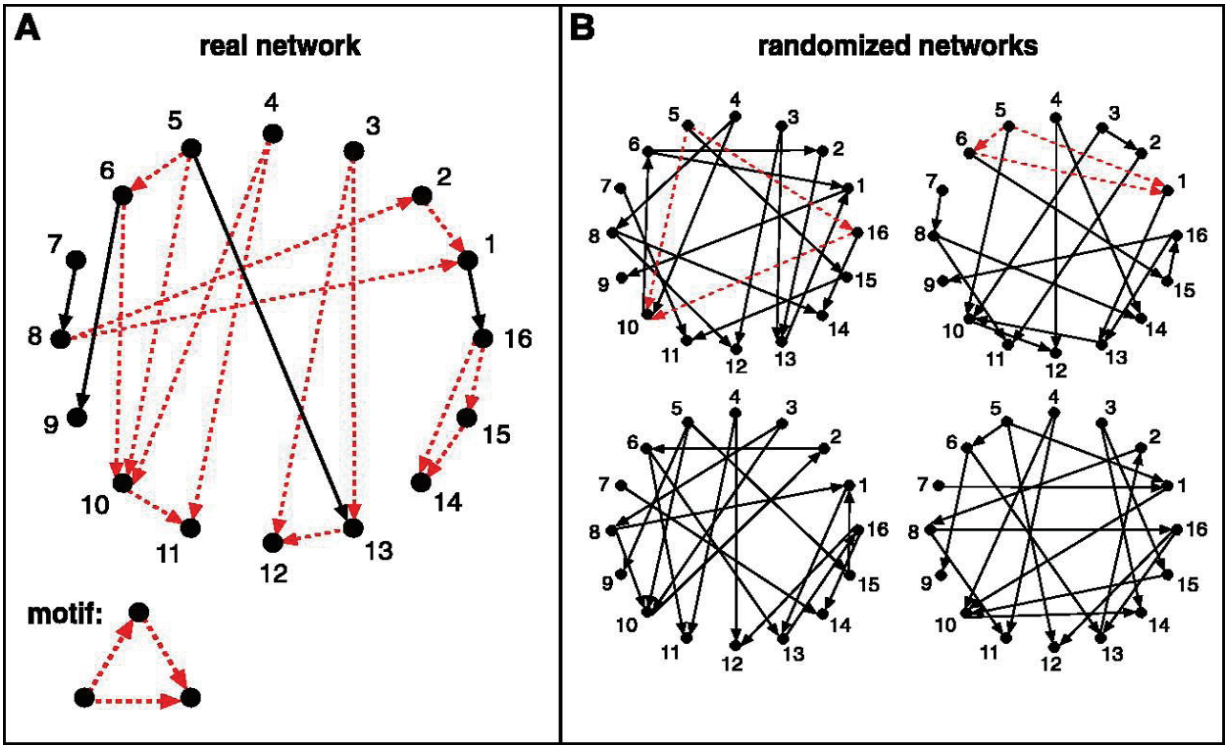
Micro-level property

Milo, Ron, et al. "Network motifs: simple building blocks of complex networks." *Science* 298.5594 (2002): 824-827.

- **Network motifs: simple building blocks of complex networks**



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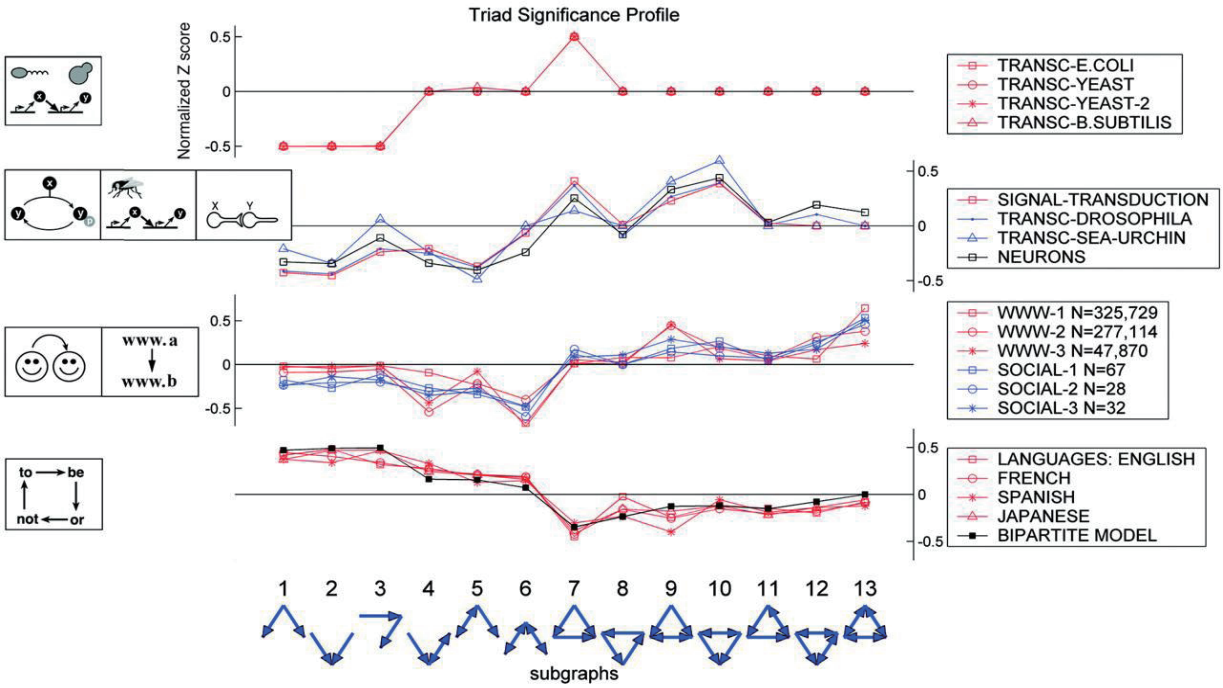
Micro-level property

Milo, Ron, et al. "Superfamilies of evolved and designed networks." *Science* 303.5663 (2004): 1538-1542.

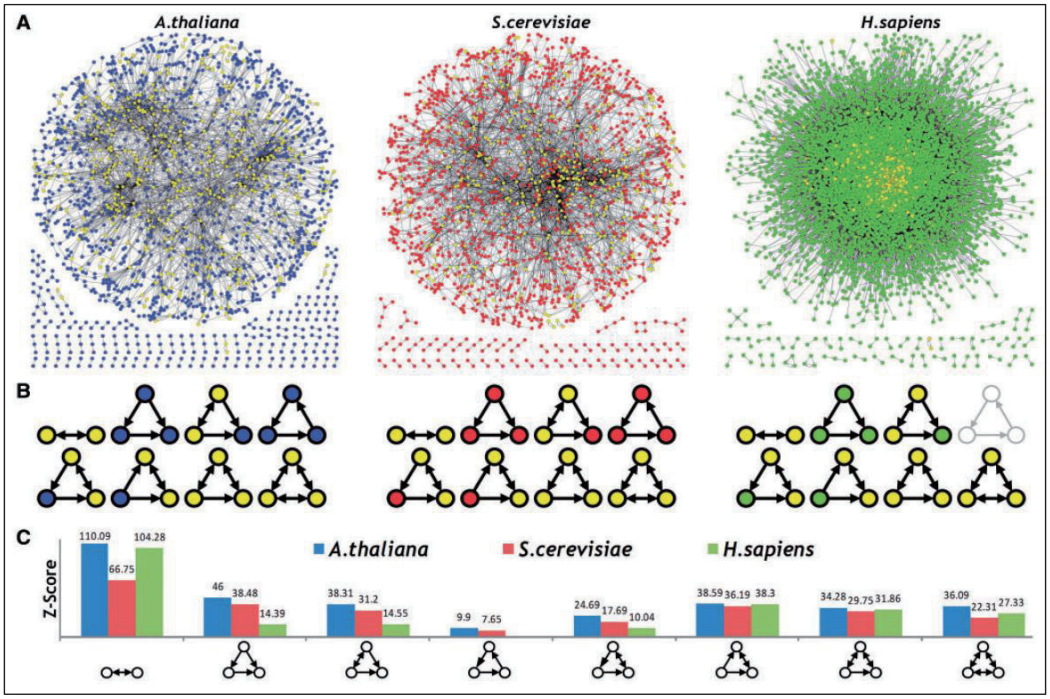
- **Superfamilies of evolved and designed networks**



Micro-level property

Kim, Tae-Hwan, et al. "Evolutionary design principles and functional characteristics based on kingdom-specific network motifs." *Bioinformatics* 27.2 (2011): 245-251.

- **Evolutionary design principles and functional characteristics based on kingdom-specific network motifs**



KSBI | 한국생명정보학회

Introduction to Network Science for Transcriptomics-guided Drug Discovery

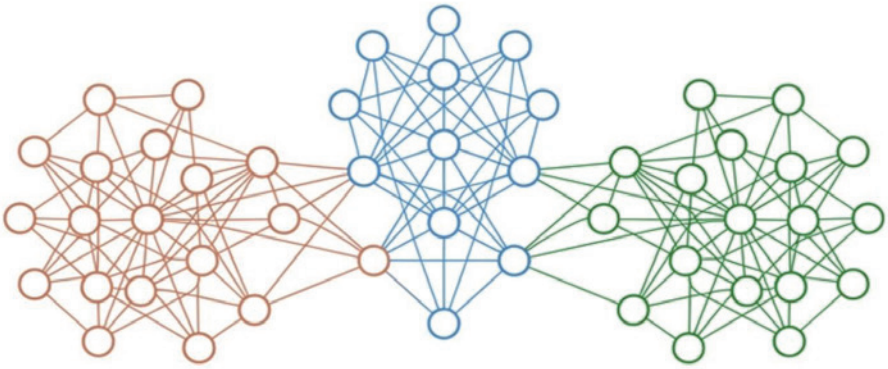
SMPARKLAB

KSBI | 한국생명정보학회

KSBi-BIML 2026

Introduction to Network Science for Transcriptomics-guided Drug Discovery PART II

충남대학교 약학대학
박상민



Network Analysis & Visualization

Choosing the Right Tool for Your Data Journey

모든 도구가 모든 상황에 적합한 것은 아닙니다. 현재 데이터의 특성과 분석 목적에 따라 최적의 도구를 선택하십시오.

Cytoscape

- **Best For:** 생물학/복잡계 네트워크의 직관적 탐색
- **Key Strength:** GUI 기반, 강력한 플러그인 생태계
- **User Profile:** 코딩보다 마우스 조작을 선호하는 연구자

R (igraph/ggraph)

- **Best For:** 통계적 분석 및 출판용 고품질 정적 시각화
- **Key Strength:** 강력한 통계 패키지 연동, 아름다운 그래픽 문법
- **User Profile:** 통계적 엄밀함과 시각적 커스터마이징을 중시하는 분석가

Python (NetworkX)

- **Best For:** 대규모 데이터 파이프라인 구축 및 머신러닝 연동
- **Key Strength:** 확장성, 알고리즘 구현 용이성
- **User Profile:** 엔지니어링 배경이 있거나 자동화가 필요한 데이터 과학자

Cytoscape: Interactive Exploration Without Code

WORKFLOW GUIDE

01. Data Import

Menu: File → Import → Network from File...

Detail: 엑셀(.xlsx) 또는 CSV 파일을 로드합니다. Source Node와 Target Node 컬럼을 지정하여 관계를 정의하고, 속성(Attribute) 데이터를 매핑합니다.

02. Analysis

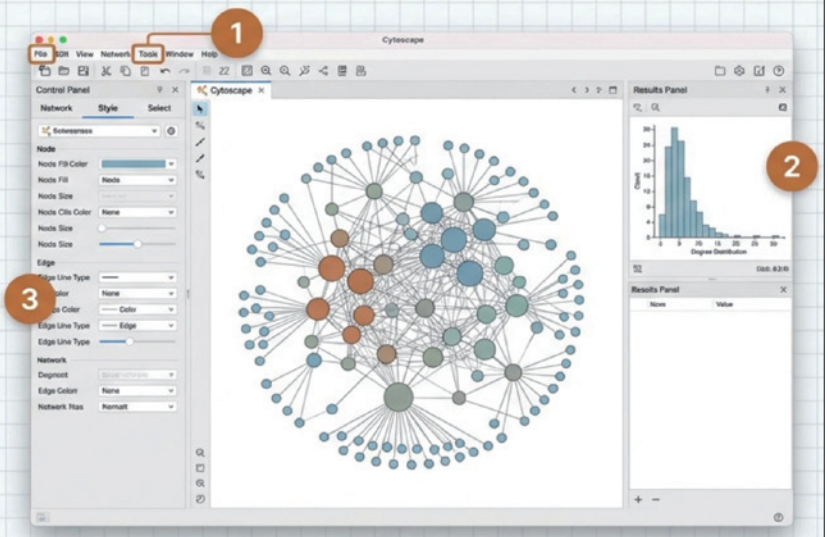
Menu: Tools → Network Analyzer → Network Analysis → Analyze Network

Detail: 클릭 한 번으로 Degree, Betweenness Centrality, Clustering Coefficient 등의 주요 지표를 자동 계산합니다.

03. Visualization

Menu: Style Tab & Layout Menu

Detail: Layout은 'Prefuse Force Directed'를 선택. Mapping은 Node Size를 Degree에, Node Color를 Betweenness에 연결하여 시각화합니다.



R: Statistical Rigor Meets Publication-Quality Graphics

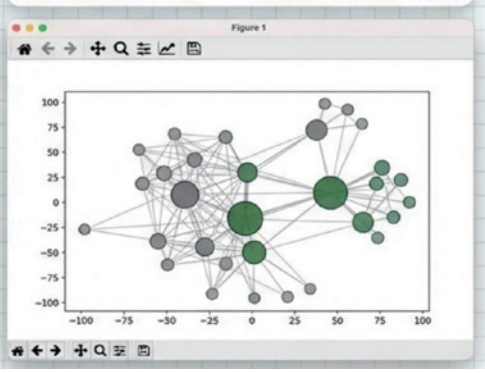
```r
# 01. Setup & Load
library(tidyverse); library(tidygraph); library(ggraph)
nodes <- read_csv("nodes.csv")
edges <- read_csv("edges.csv")
# 데이터 프레임을 그래프 객체로 변환
graph_obj <- tbl_graph(nodes = nodes, edges = edges, directed = TRUE)

# 02. Analysis (Centrality Calculation)
graph_obj <- graph_obj %>%
  activate(nodes) %>%
  mutate(degree = centrality_degree(),
         betweenness = centrality_betweenness())

# 03. Visualization (Grammar of Graphics)
ggraph(graph_obj, layout = 'fr') +
  geom_edge_link(aes(width = weight), alpha = 0.8) +
  geom_node_point(aes(size = degree, color = betweenness)) +
  theme_graph()
```

Python: Scalable Pipelines & Algorithmic Power

```python
# 01. Data Preparation
import networkx as nx
import pandas as pd
import matplotlib.pyplot as plt

df = pd.read_csv('network_data.csv')
# Pandas DataFrame에서 그래프 객체 생성
G = nx.from_pandas_edgelist(df, source='source', target='target')

# 02. Algorithmic Analysis
# 중심성 계산 (Dictionary 형태 반환)
degree_dict = nx.degree_centrality(G)
nx.set_node_attributes(G, degree_dict, 'degree')

# 03. Visualization
pos = nx.spring_layout(G)
nx.draw_networkx_nodes(G, pos, node_size=[v * 1000 for v in degree_dict.values()])
nx.draw_networkx_edges(G, pos, alpha=0.5)
plt.show()
```

	source	target	weight
1	A	1	5
2	A	2	3
3	1	3	3
4	2	4	5
5	3	4	8
6	4	6	1

DataFrame (Pandas) → Network Graph (NetworkX)



The Analyst's Cheat Sheet: Feature Comparison

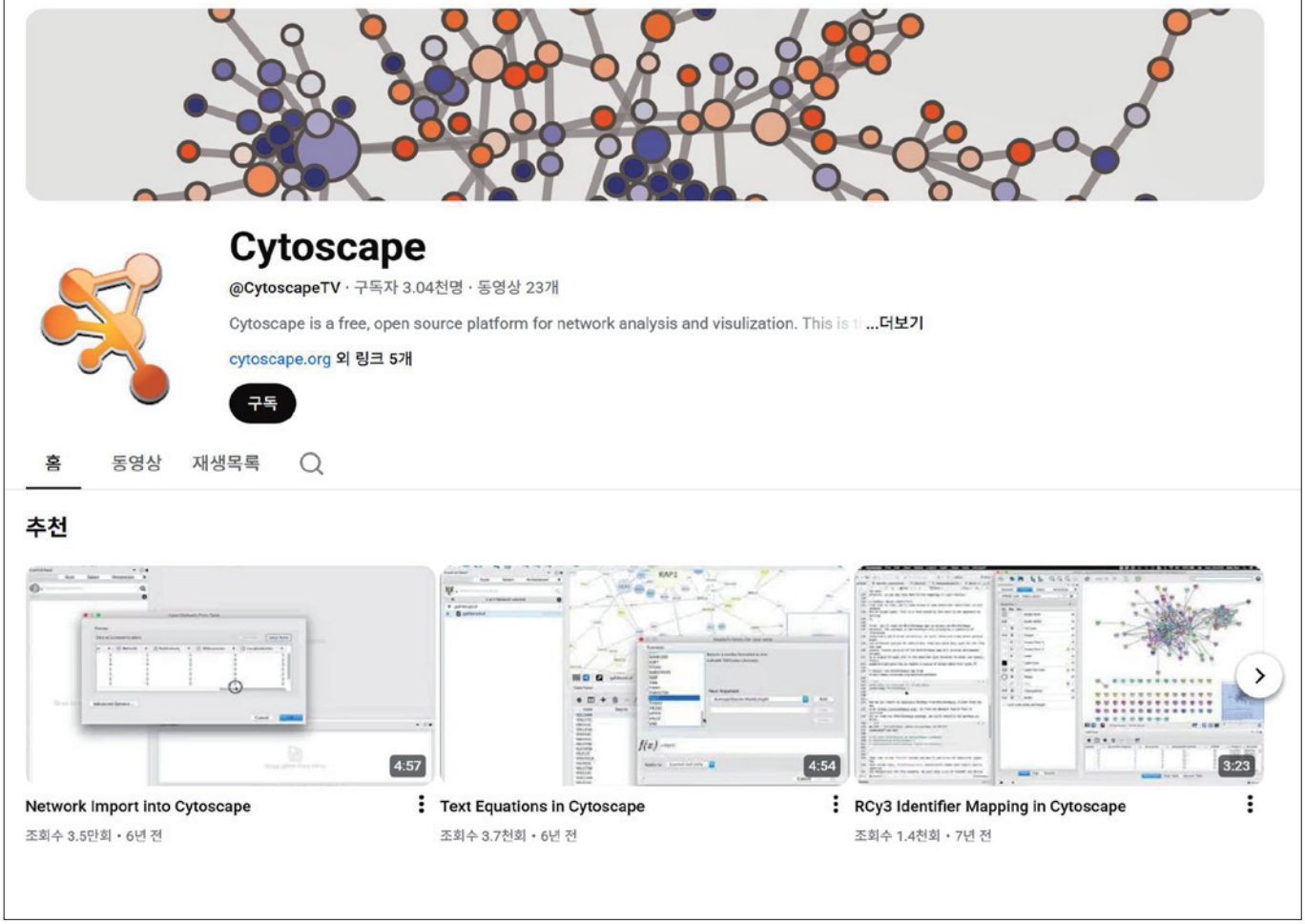
Feature	Cytoscape	R	Python
데이터 로드 (Data Load)	Excel/CSV Import (GUI Menu)	read_csv() + tbl_graph()	Pandas DataFrame Integration
분석 방식 (Analysis)	Click-based "Network Analyzer"	tidygraph (Pipe Operator %>%)	networkx methods & scipy
시각화 철학 (Visualization)	WYSIWYG Style Mapping Panel	Layered Grammar (ggraph + ggplot2)	Object-oriented Plotting (matplotlib)
확장성 (Scalability)	Plugin Dependent / Memory Intensive	In-memory (Medium scale)	High (Integration with Big Data tools)

💡 **Key Takeaway:** 데이터 탐색과 가설 설정 단계에서는 **Cytoscape**, 논문용 고품질 차트 제작은 **R**, 대규모 시스템 및 파이프라인 구현은 **Python**이 가장 효율적입니다.

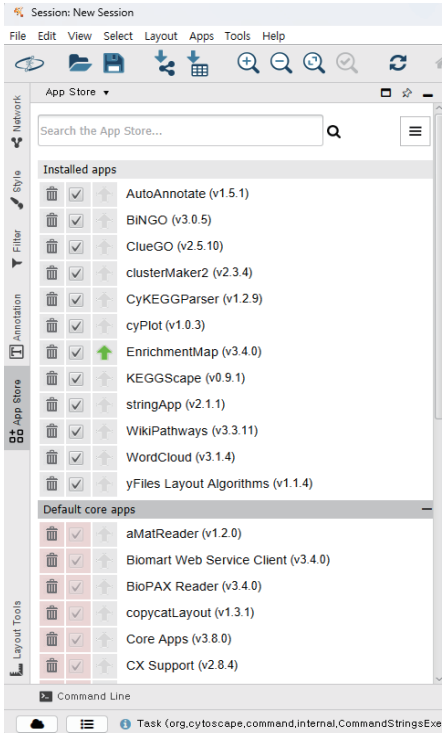
Cytoscape is an open source software platform for visualizing complex networks and integrating these with any type of attribute data. A lot of *Apps* are available for various kinds of problem domains, including bioinformatics, social network analysis, and semantic web.
Learn more...

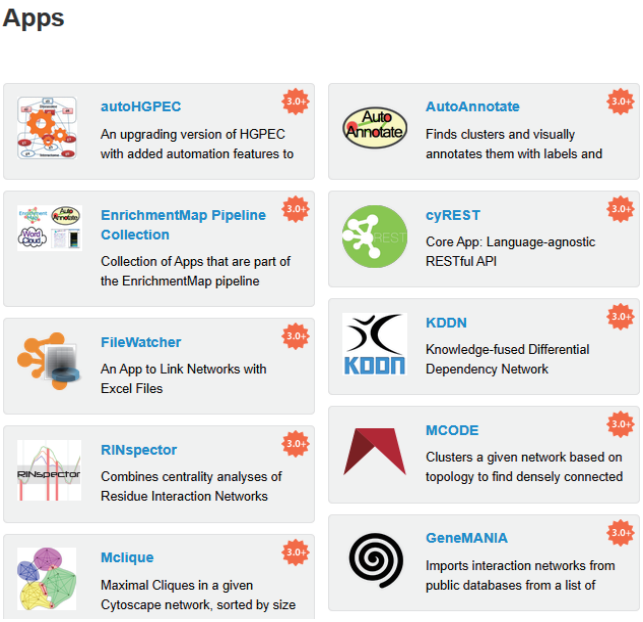
Release Notes

Sample Visualizations



Cytoscape를 활용해봅시다

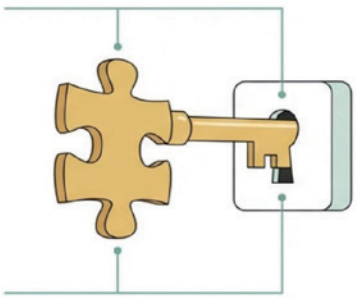




[Cytoscape App Store]

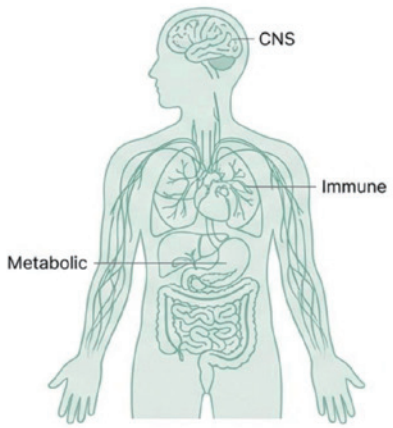
기존 약물 연구의 한계: 'Magic Bullet'의 종말

The Reductionist View



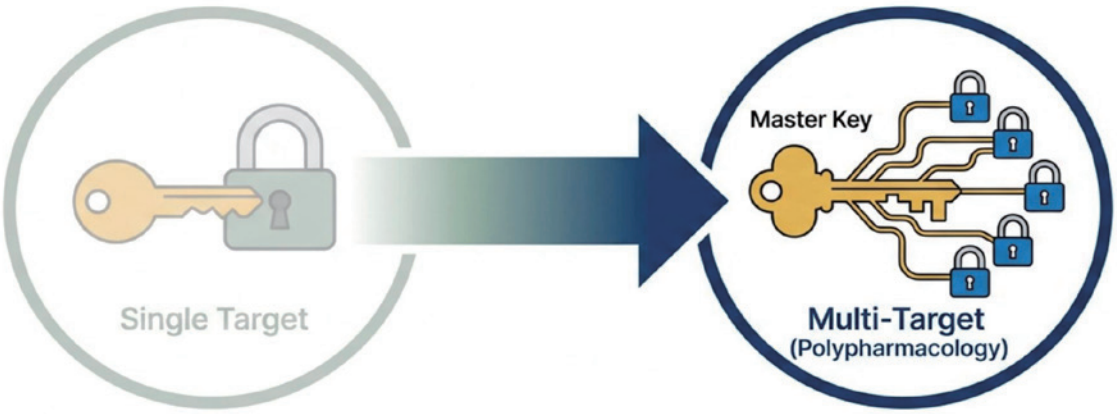
1 Drug = 1 Target (Lock & Key)
질환을 일으키는 단일 인자만 제거하는 이상적인 표적 치료제.

The Reality: Multifactorial Disorders



Complex Diseases (Diabetes, Cancer, Alzheimer's)
단일 약물로는 복잡한 다인자성 질환 제어 불가능.

네트워크 약리학: 증상 치료를 넘어 원인 메커니즘의 치유로



Old Paradigm

부작용 발생 가능성 높음
복합 질환에 낮은 효능

Network Medicine

Drug-Multi-Target-Disease 관계 탐색
질병 네트워크 자체를 조절하여 근본적 치료
(Curing Causal Mechanisms)

Review Article | Published: 17 December 2010

Network medicine: a network-based approach to human disease

Albert-László Barabási, Natali Gulbahce & Joseph Loscalzo

Nature Reviews Genetics **12**, 56–68 (2011) | Cite this article

51k Accesses | **4404** Citations | **105** Altmetric | Metrics

Article | Open access | Published: 13 March 2019

Network-based prediction of drug combinations

Feixiong Cheng, István A. Kovács & Albert-László Barabási

Nature Communications **10**, Article number: 1197 (2019) | Cite this article

79k Accesses | **757** Citations | **66** Altmetric | Metrics

RESEARCH ARTICLE | SYSTEMS BIOLOGY

Network medicine framework for identifying drug-repurposing opportunities for COVID-19

Deisy Morselli Gysi, Ítalo do Valle, Marinka Zitnik, +7, and Albert-László Barabási | Authors Info & Affiliations

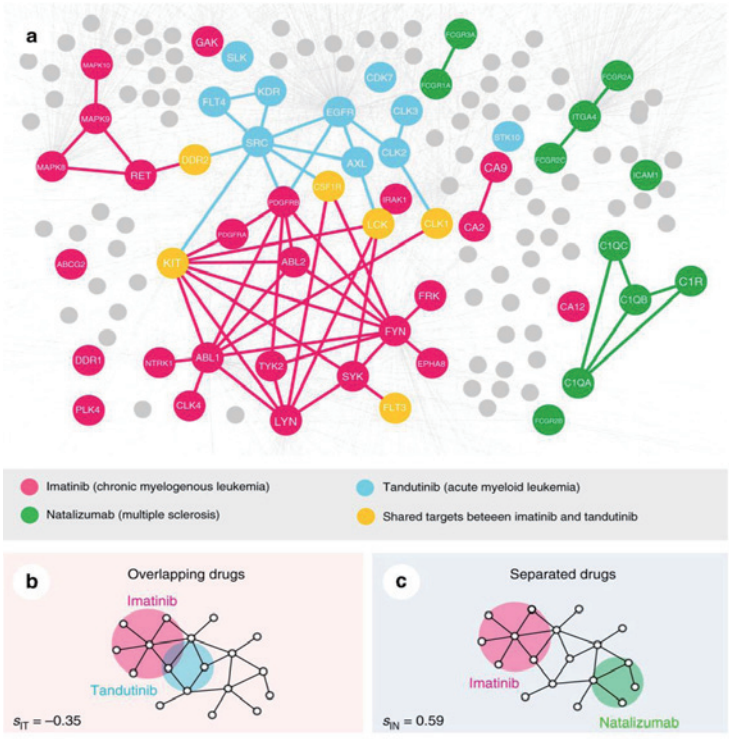
Edited by Eugene V. Koonin, NIH, Bethesda, MD, and approved March 30, 2021 (received for review December 12, 2020)

April 27, 2021 | 118 (19) e2025581118 | https://doi.org/10.1073/pnas.2025581118

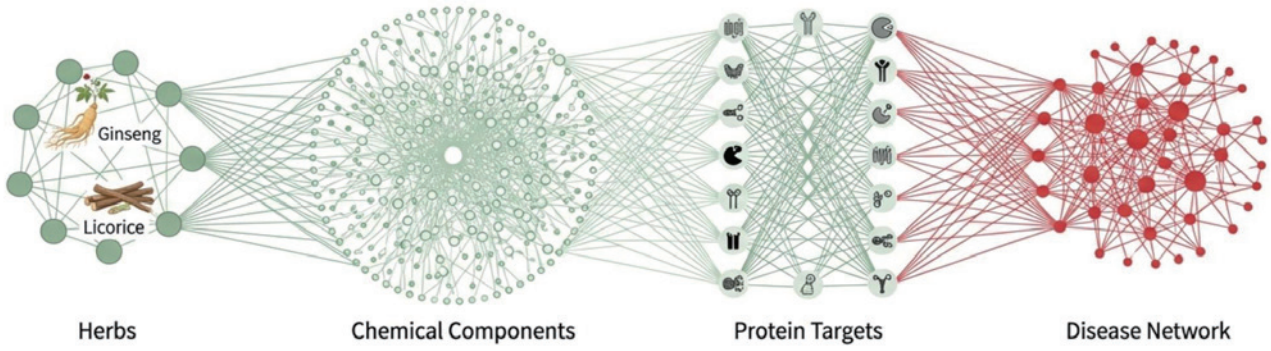
REVIEW · Volume 43, Issue 2, P136-150, February 2022 · *Open Access* | Download Full Issue

Network pharmacology: curing causal mechanisms instead of treating symptoms

Cristian Nogales[1,6] · Zeinab M. Mamdouh[1,2,6] · Markus List[3] · Christina Kiel[4] · Ana I. Casas[1,5] · Harald H.H.W. Schmidt[1]



전통 의학의 재해석: 다성분, 다표적(Multi-component, Multi-target) 전략

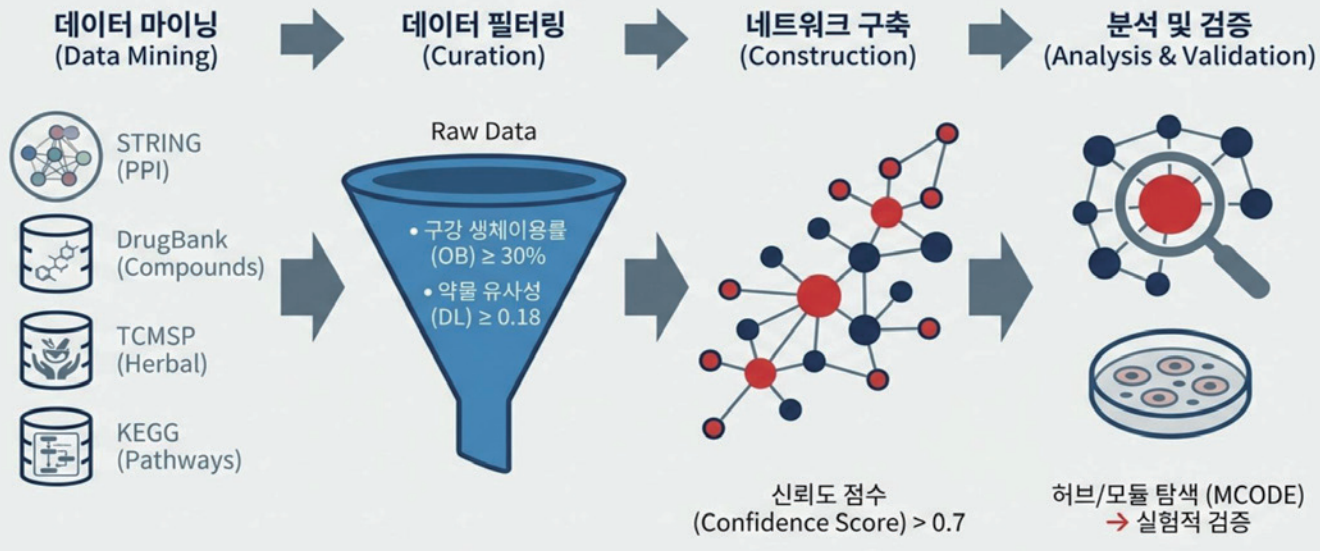


네트워크 약리학(Network Pharmacology):
한약(Herbal Medicine)이 단일 성분이 아니라 수십 가지 성분의 상호작용을 통해 효과를 낸다는 것을 증명합니다.

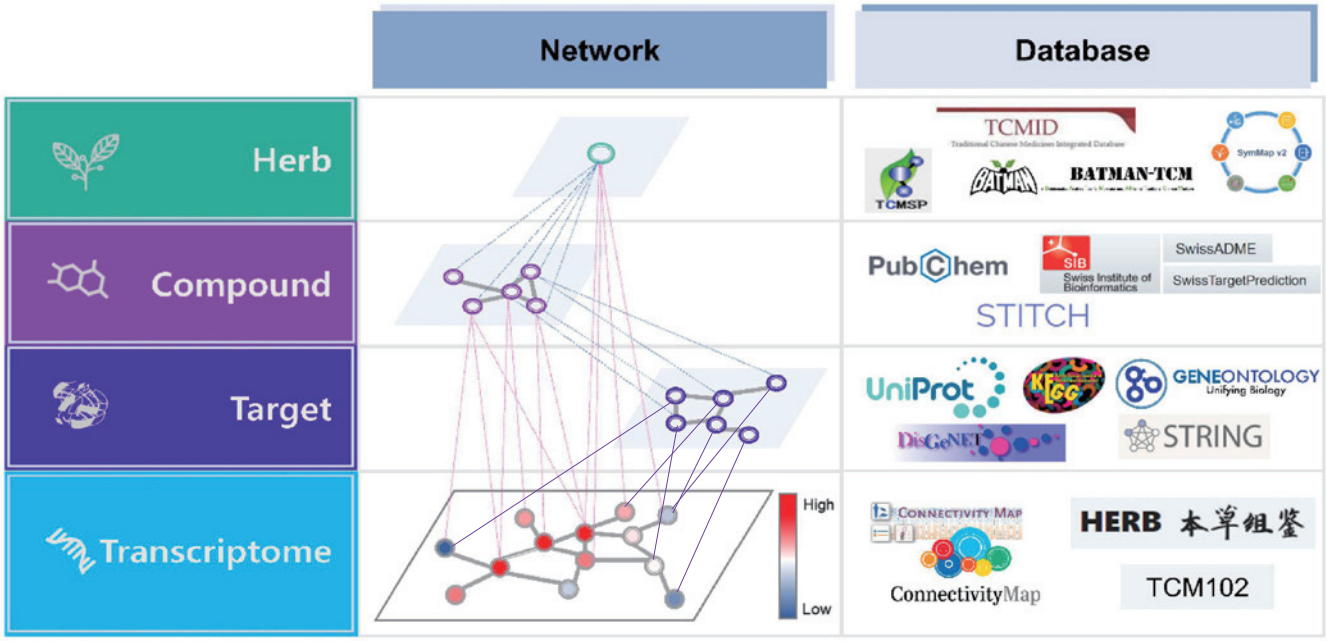
시너지 효과:
다중 성분이 질병 네트워크의 여러 허브(Hub)를 동시에 타격하여, 단일 표적 약물의 한계를 극복하고 부작용을 최소화합니다.

분석 프로세스:
1. 성분 및 표적 식별 (TCMSP, UniProt)
2. PPI (Protein-Protein Interaction) 네트워크 구축
3. 분자 도킹(Molecular Docking) 및 동역학 시뮬레이션 검증

네트워크 약리학 모델링 워크플로우



Data-Driven Drug Discovery in Herbal Medicine

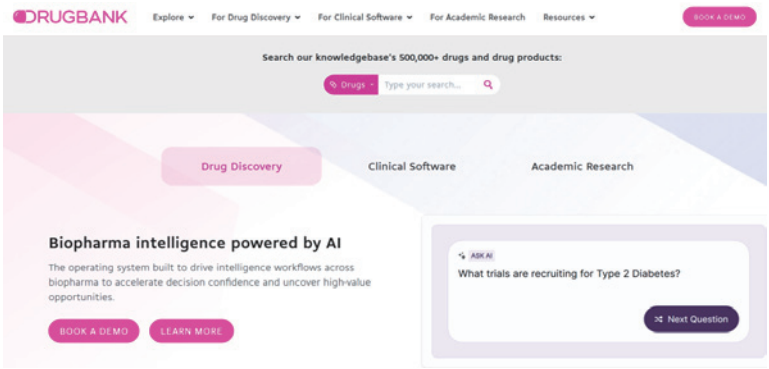


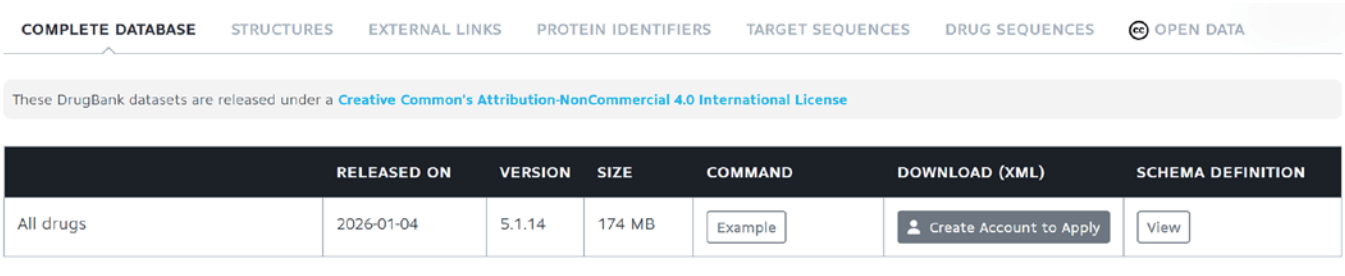
"Systems pharmacology approaches in herbal medicine research: a brief review." *BMB reports* 55.9 (2022): 417.

01. 타겟 데이터베이스

0. DrugBank

- ✓ FDA 승인 약물을 포함하여 수천 개 이상의 의약품에 대한 화학적, 약리학적, 제약적 데이터를 통합해 제공하는 포괄적인 온라인 데이터베이스
- ✓ 분자 구조, 약물 표적, 상호작용, 대사 등 상세한 정보를 통해 신약 개발 및 임상 연구에 활용

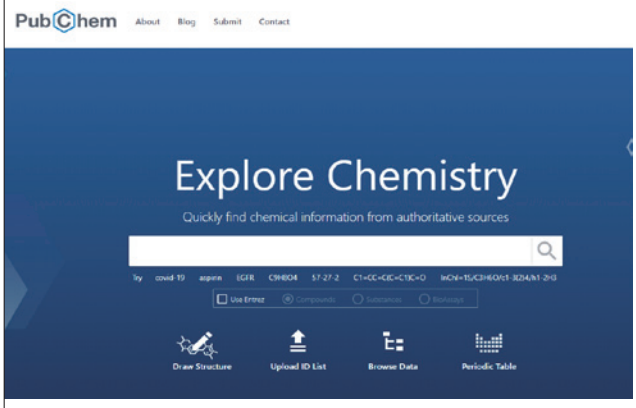


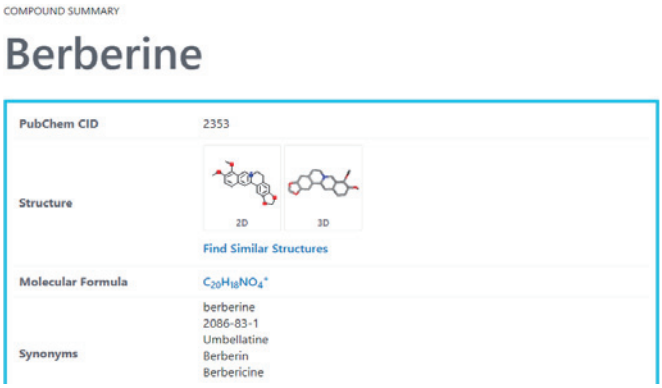


01. 타겟 데이터베이스

1. Pubchem

- ✓ Compound database
- ✓ Compound 정보 검색 (약동학적 성질, 관련 질환, 관련 타겟, 관련 논문 등)

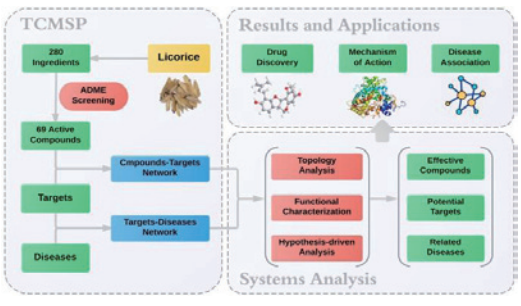


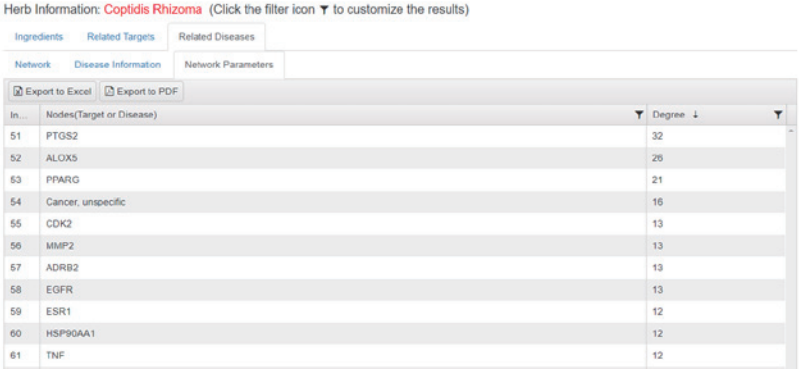


01. 타겟 데이터베이스

2. TCMSP

- ✓ 현재 가장 잘 알려지고 유명한 플랫폼
- ✓ Compound 선정 시 OB, DL, Lipinski rule of five, BBB 등의 약동학적 성질 이용
- ✓ Drug-Target interaction 예측 시 인공지능 사용(RF, SVM)
- ✓ 식물성 약재가 대부분이기 때문에, 동물성 약재, 광물성 약재가 거의 없으며 많이 사용하는 한약재가 없는 것이 단점 (예 : 녹용, 원지)
- ✓ 미리 계산해 놓은 값을 데이터베이스 형태로 제공





01. 타겟 데이터베이스

http://www.tcmip.cn/ETCM/
http://www.tcmip.cn/ETCM2/

3. ETCM

JOURNAL ARTICLE

ETCM: an encyclopaedia of traditional Chinese medicine

Hai-Yu Xu ✉, Yan-Qiong Zhang, Zhen-Ming Liu, Tong Chen, Chuan-Yu Lv, Shi-Huan Tang, Xiao-Bo Zhang, Wei Zhang, Zhi-Yong Li, Rong-Rong Zhou ... Show more

Author Notes

Nucleic Acids Research, Volume 47, Issue D1, 08 January 2019, Pages D976–D982, https://doi.org/10.1093/nar/gky987

Published: 26 October 2018 **Article history**

Acta Pharmaceutica Sinica B

Volume 13, Issue 6, June 2023, Pages 2559-2571

TOOLS

ETCM v2.0: An update with comprehensive resource and rich annotations for traditional Chinese medicine

01. 타겟 데이터베이스

JOURNAL ARTICLE

SymMap: an integrative database of traditional Chinese medicine enhanced by symptom mapping

Yang Wu, Feilong Zhang, Kuo Yang, Shuangsang Fang, Dechao Bu, Hui Li, Liang Sun, Hairuo Hu, Kuo Gao, Wei Wang ... Show more

Author Notes

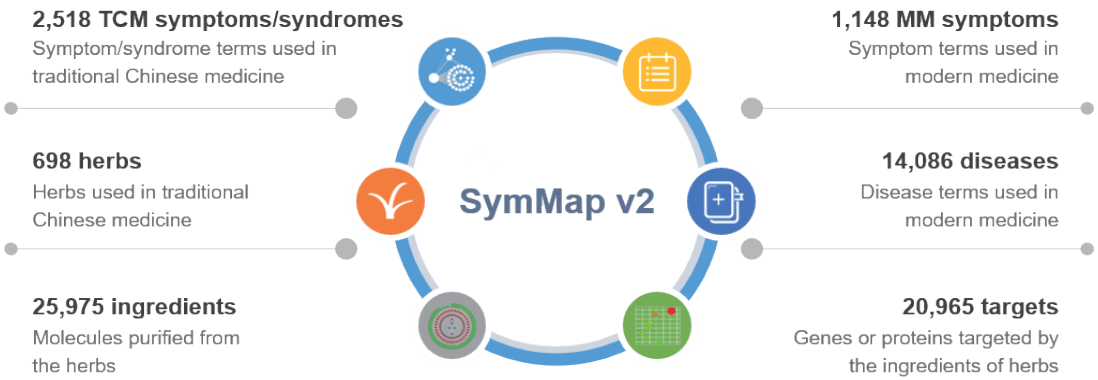
Nucleic Acids Research, Volume 47, Issue D1, 08 January 2019, Pages D1110–D1117, https://doi.org/10.1093/nar/gky1021

Published: 31 October 2018 **Article history**

4. SymMap

http://www.symmap.org/

SymMap integrates traditional Chinese medicine (TCM) with modern medicine (MM) through both **internal molecular mechanism** and **external symptom mapping**, thus provides massive information on herbs/ingredients, targets, as well as the clinical symptoms and diseases they are used to treat for drug screening efforts.

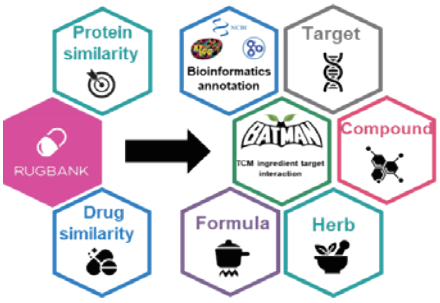


01. 타겟 데이터베이스

http://bionet.ncpsb.org.cn/batman-tcm/#/home

5. BATMAN-TCM

- ✓ Drug-Target interaction 예측 시 이미 알려져 있는 정보를 이용하여 scoring하여 제공
- ✓ 본초 이름 혹은 SMILES string만 있으면 서버에서 계산하기 때문에 DB에 수록되지 않은 성분도 **예측 가능**하다는 장점이 있음
- ✓ DTI 상호작용 예측 시 상호작용 근거를 찾기 어려움 (효과 있음/부작용을 분리할 수 없음)



Article | Open access | Published: 16 February 2016

BATMAN-TCM: a Bioinformatics Analysis Tool for Molecular mechANism of Traditional Chinese Medicine

Zhongyang Liu, Feifei Guo, Yong Wang, Chun Li, Xinlei Zhang, Honglei Li, Lihong Diao, Jiangyong Gu, Wei Wang, Dong Li & Fuchu He

Scientific Reports 6, Article number: 21146 (2016) | Cite this article

JOURNAL ARTICLE

BATMAN-TCM 2.0: an enhanced integrative database for known and predicted interactions between traditional Chinese medicine ingredients and target proteins

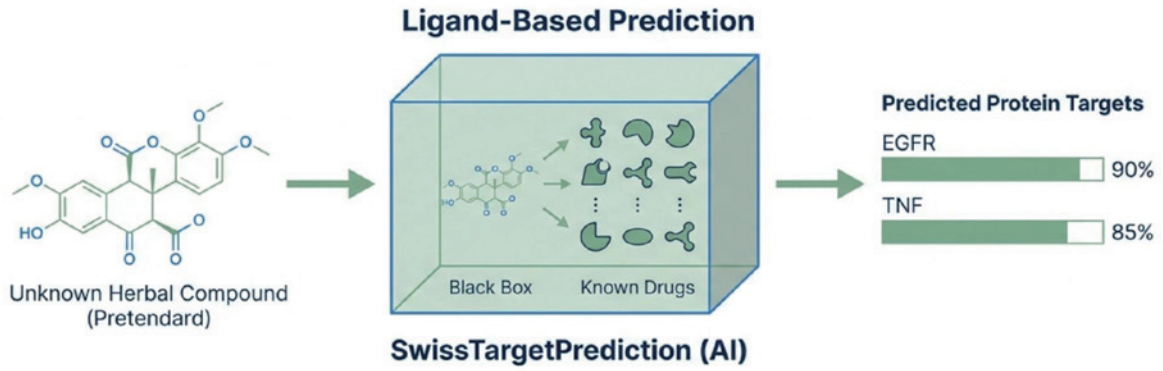
Xiangren Kong, Chao Liu, Zuzhen Zhang, Meiqi Cheng, Zhijun Mei, Xiangdong Li, Peng Liu, Lihong Diao, Yajie Ma, Peng Jiang ... Show more

Author Notes

Nucleic Acids Research, Volume 52, Issue D1, 5 January 2024, Pages D1110–D1120, https://doi.org/10.1093/nar/gkad926

Published: 30 October 2023 **Article history**

타겟 예측: 인공지능의 활용

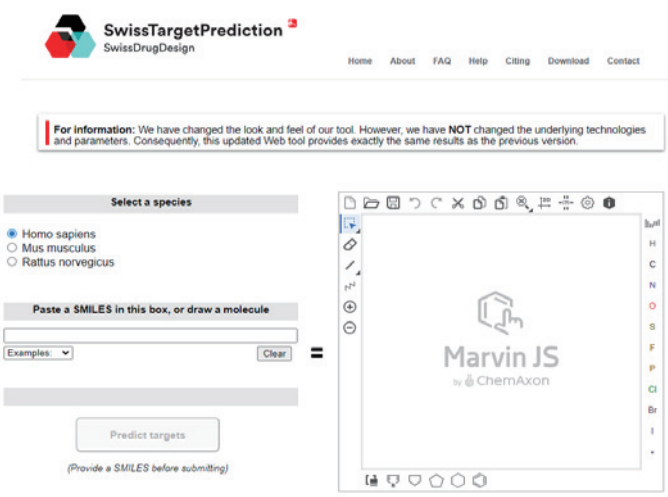


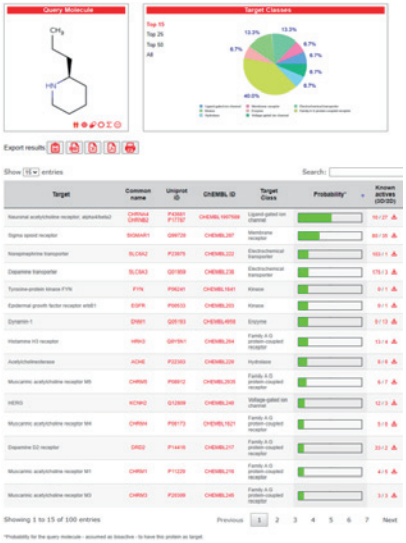
실험 데이터가 없는 성분의 타겟을 어떻게 찾을까?
SwissTargetPrediction: 화합물의 화학적 구조 유사성(Structural Similarity)을 분석하여 결합 가능한 단백질을 예측.

02. 타겟 예측

1. SwissTargetPrediction

화합물의 화학적 구조를 기반으로 그 화합물이 표적할 수 있는 단백질을 예측하는 온라인 도구 기존에 알려진 약물-표적 상호작용 데이터와 유사성 검색 알고리즘을 사용하여, 사용자가 입력한 화합물이 어느 단백질과 상호작용할 가능성이 높은지를 예측

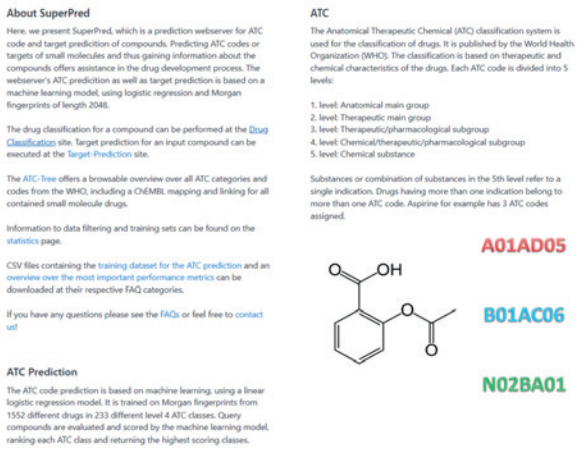


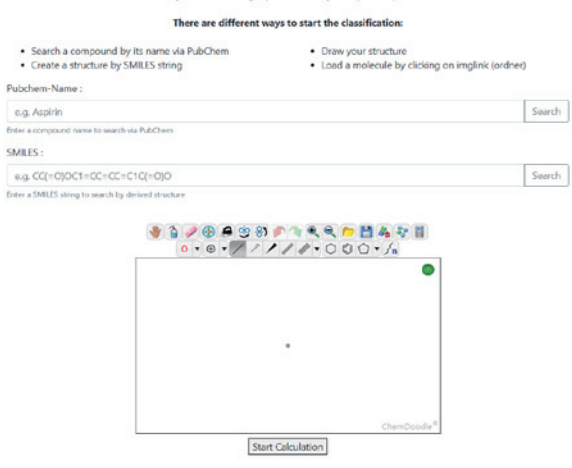


02. 타겟 예측

2. SuperPred

화합물의 화학적 구조를 기반으로 약물이 결합할 수 있는 표적 단백질을 예측하고, 약물 재창출 또는 부작용 예측을 돕는 웹 기반 도구. 화합물의 구조적 유사성을 활용해 기존 약물의 표적과 비교하여, 새로운 약물의 표적이나 상호작용을 예측

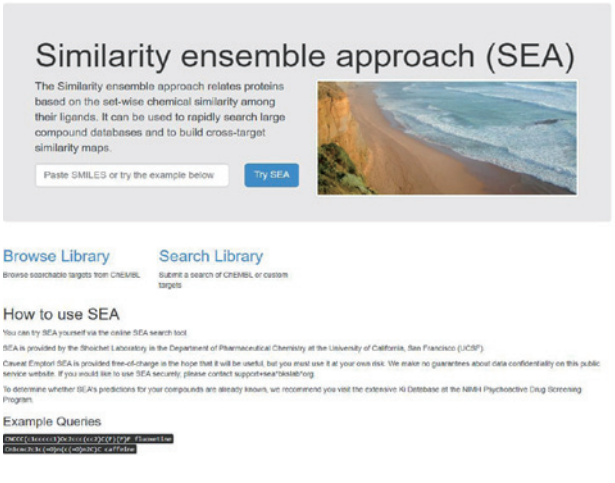


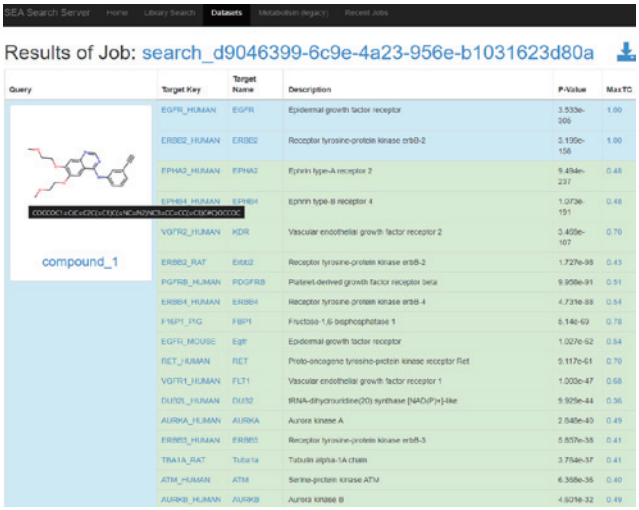


02. 타겟 예측

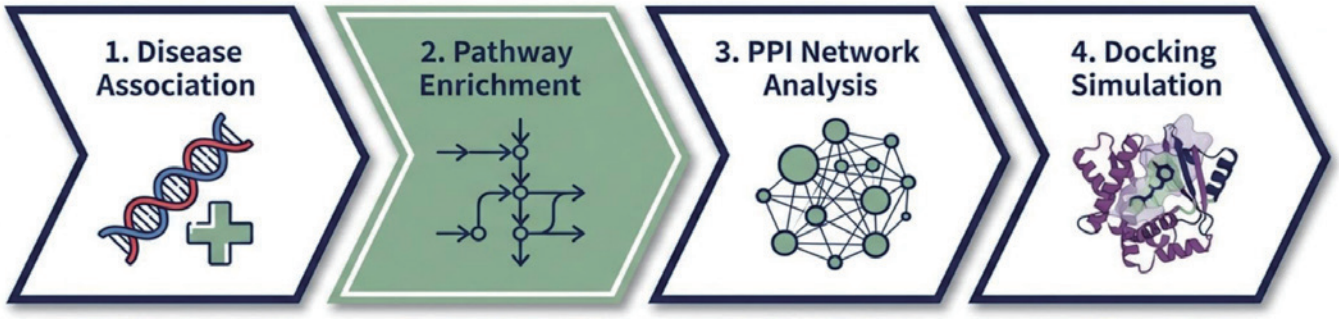
3. Similarity Ensemble Approach

화합물의 화학적 구조 유사성을 기반으로 약물 표적을 예측하는 웹 기반 도구. 기존에 알려진 약물-표적 상호작용 데이터를 바탕으로, 입력된 화합물이 기존 약물과 얼마나 유사한지 분석하여, 해당 화합물이 결합할 가능성이 높은 표적 단백질을 예측





네트워크 약리학 구축 이후의 분석 전략



유전자-질병 연관성 분석 (DisGeNET, OMIM)

생물학적 기전 도출 (KEGG, Reactome)

단백질 상호작용 및 허브 유전자 탐색 (STRING)

성분-타겟 결합 친화도 예측 (AutoDock)

Disease Association Analysis: 유전자와 질병의 연결 고리

Widely used databases for gene–disease association

DisGeNET

Integrates data from UniProt, CTD, and literature. Best for broad association mining.

CTD

Comparative Toxicogenomics Database. Focuses on chemical–gene–disease relationships.

OMIM

Online Mendelian Inheritance in Man. Specializes in genetic disorders and phenotypes.

GeneCards

Integrates functional information and disease links from multiple sources.

MalaCards

A comprehensive disease-centric database.

Pathway Enrichment Analysis의 원리

Over-Representation Analysis (ORA) Methodology

LIST OF DEGs

HAO1
STAT5
NFKB
AKR1C4
IL2R
BAAT
SLC2A2
FCER1G
ABL1
AGPAT2
ACY5
EE2F
CTF1
FOS
…

+

PATHWAY DATABASE

Pathway Name	Gene Set
Insulin pathway	INS, INSR, IRS1, IRS2, …
Fatty acid biosynthesis	FASN, FASB, MECR, …
Th1 differentiation	NOTCH3, NFKB, IL2R, STAT5, IL4…
Breast cancer	ER, RAF, RAS, HER2…
Cell cycle	RB, ARF, MDM2, P21, CDC24…
…	…

=

ENRICHED PATHWAYS

Fibrosis	P-value
Phagocytosis	
STAT3 signaling pathway	
Th1 differentiation	
Glycolysis	
Protein degradation	
Apoptosis	

Hypergeometric Test / Fisher's Exact Test를 통해
우연보다 더 자주 등장하는 경로를 통계적으로 산출.

주요 경로 데이터베이스 가이드 (Pathway Databases)

Metabolism & Signaling

KEGG
The standard for metabolic and signaling pathways. Curated maps.

Reactome
Detailed molecular events and reactions. High-resolution biological processes.

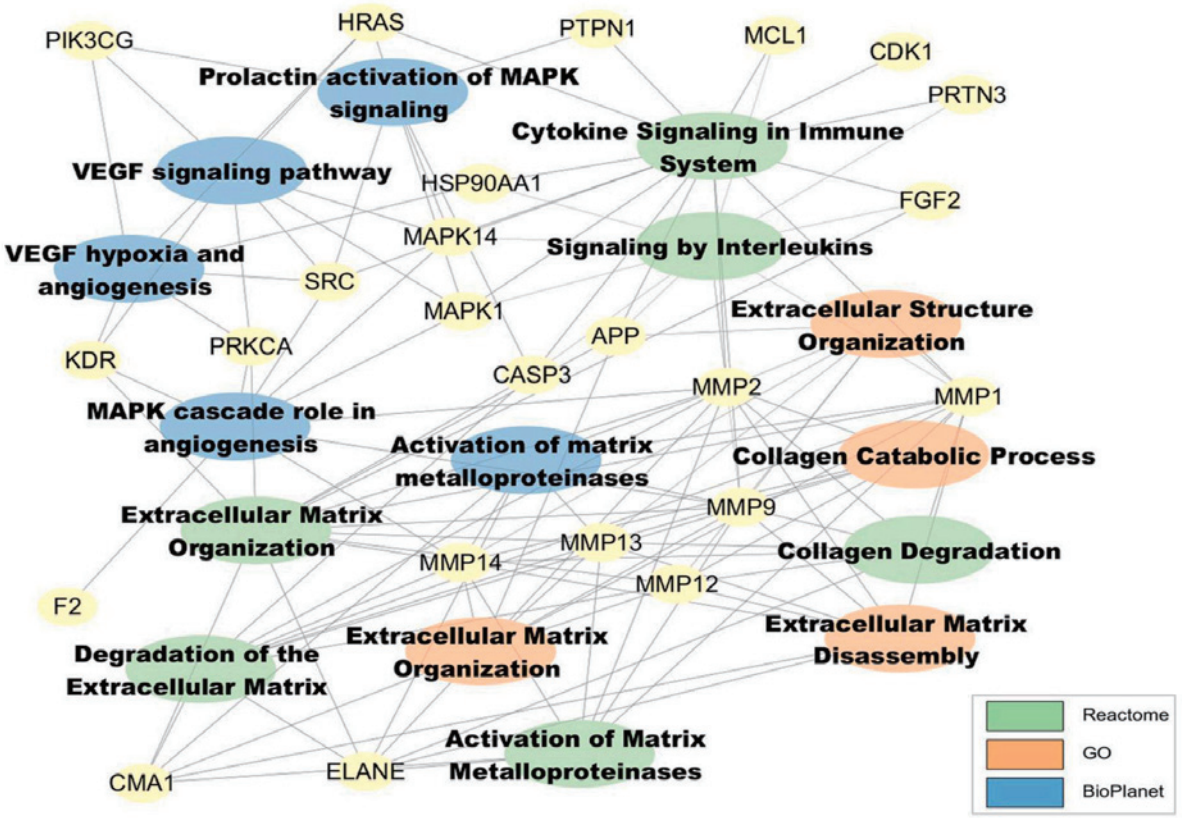
WikiPathways
Community-curated, open source, and frequently updated.

Function & Signatures

Gene Ontology (GO)
Classifies genes into BP (Process), MF (Function), and CC (Component).

MSigDB
Molecular Signatures Database. Used for GSEA (Hallmarks, Oncogenic signatures).

Life Sciences (2025): 123951.

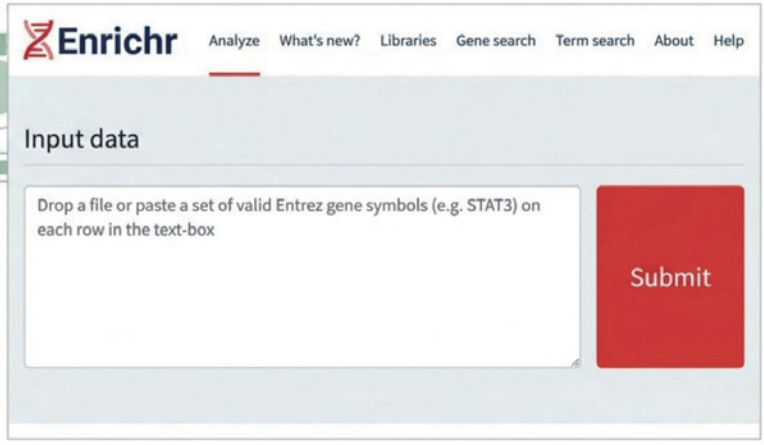


Tool Spotlight: Enrichr

Web-Based Analysis
No installation required.

Comprehensive Libraries
Access to KEGG, GO, Reactome, and 180+ others.

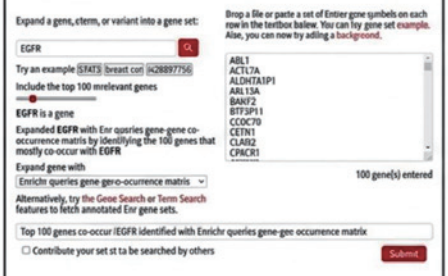
Multi-Dimensional
Analyzes Pathways, Diseases, Transcription Factors, and Drug Targets.



Interactive interface for instant gene list enrichment.

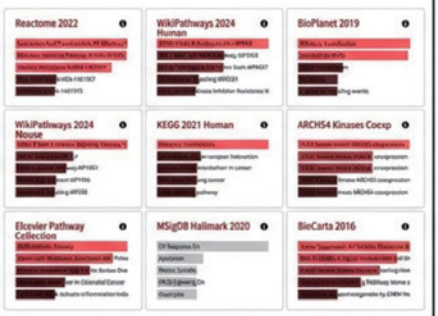
Enrichr 사용 가이드 (User Guide)

Step 1: Input Data



Paste Gene List / Upload File.

Step 2: Select Library

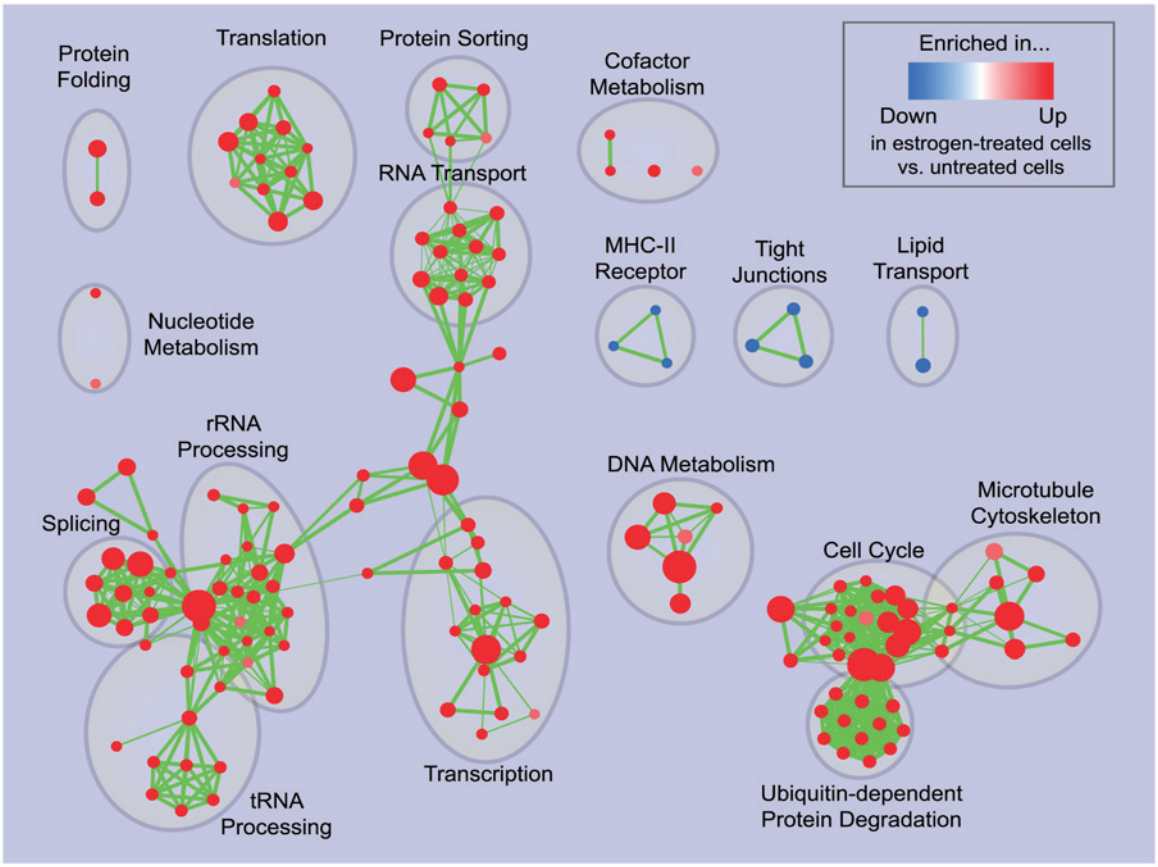


Choose database (e.g., Reactome, KEGG).

Step 3: Result & Export

Check P-value, visualize, and export (.txt).

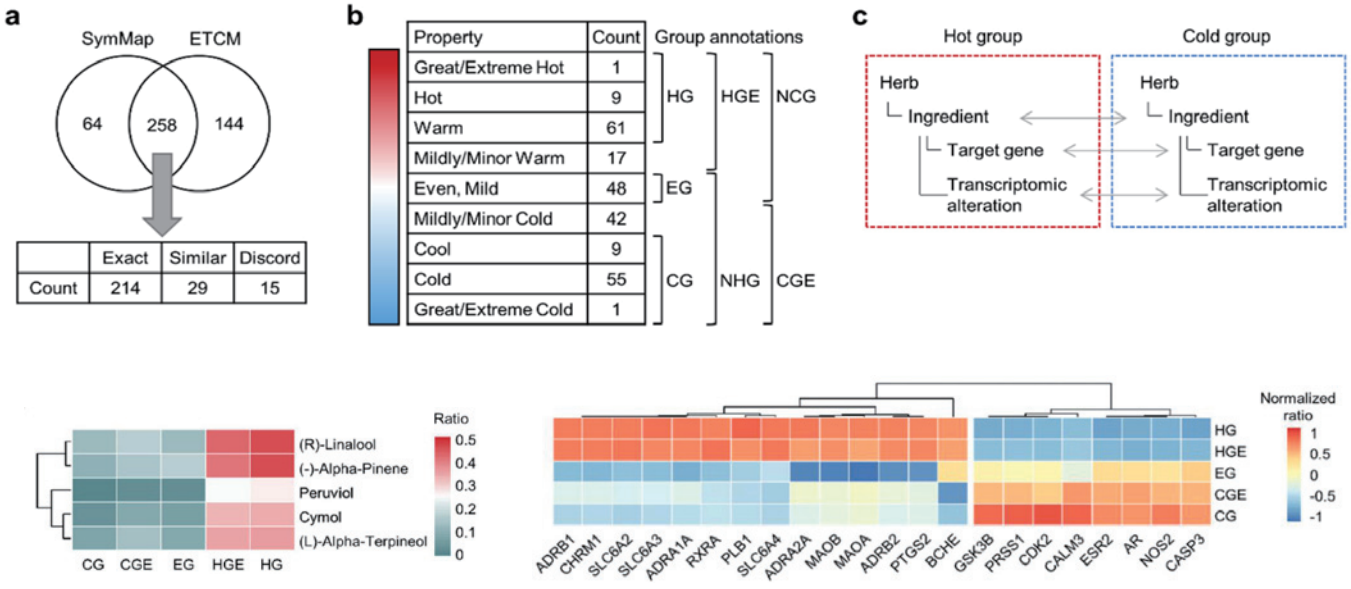
Reimand, Jüri, et al. "Pathway enrichment analysis and visualization of omics data using g: Profiler, GSEA, Cytoscape and **EnrichmentMap**." *Nature protocols* 14.2 (2019): 482-517.



Open Access | Editor's Choice | Article

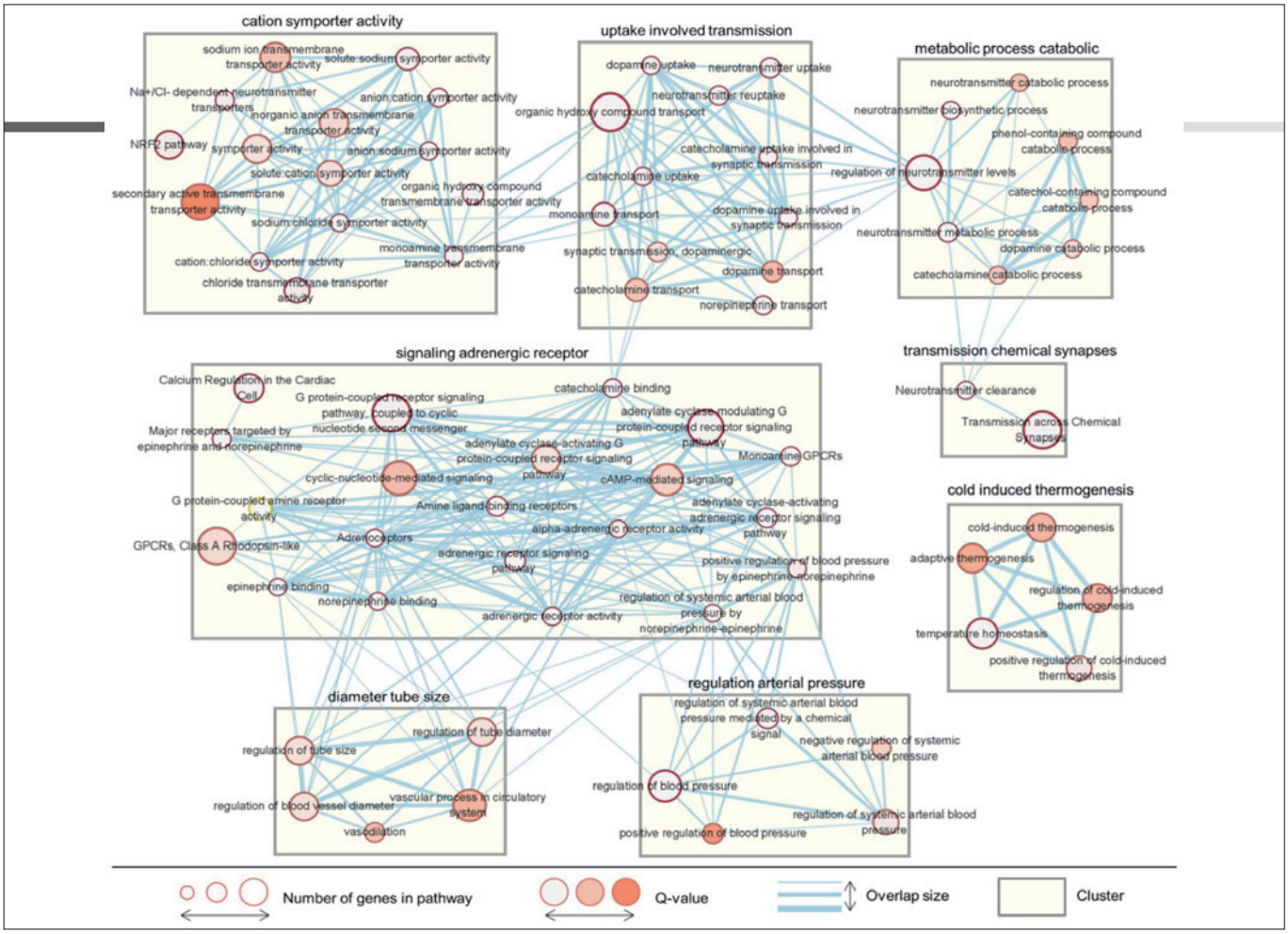
Systematic Analysis of the Molecular Mechanisms of Cold and Hot Properties of Herbal Medicines

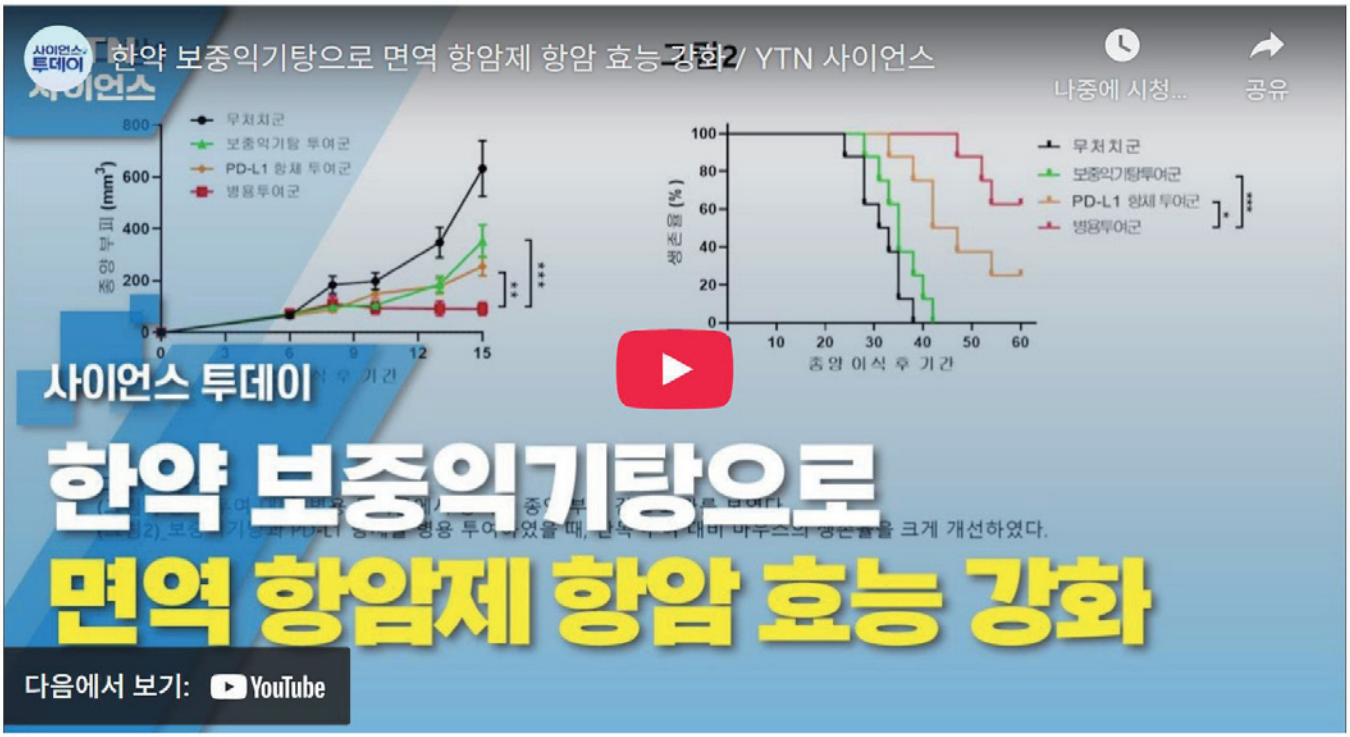
by Sang-Min Park [1,2], Su-Jin Baek [1], Hyo-Jeong Ban [1], Hee-Jeong Jin [1] and Seongwon Cha [1,*]



Group-specific Ingredient

Group-specific target gene



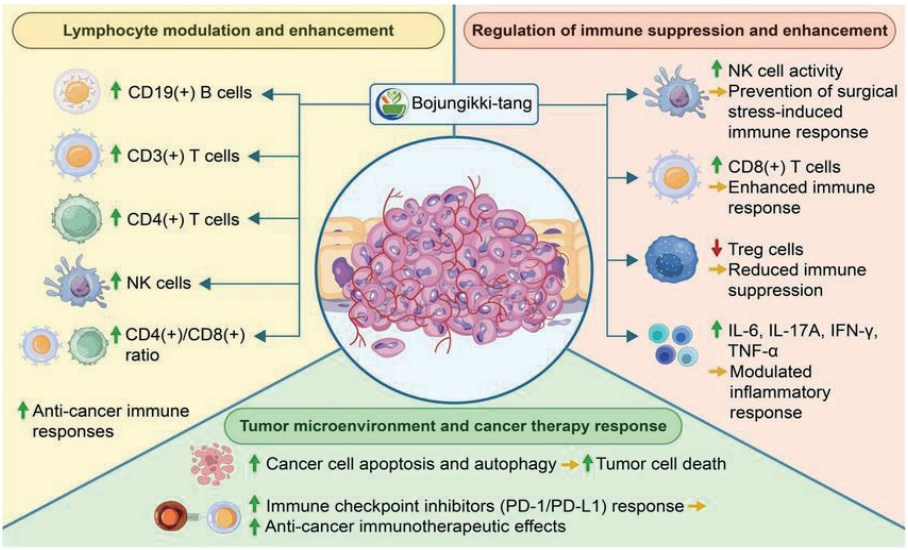


한약 보중익기탕으로 면역 항암제 항암 효능 강화

2022년 08월 11일 17시 32분

Case 1: BJIKT with Network Pharmacology

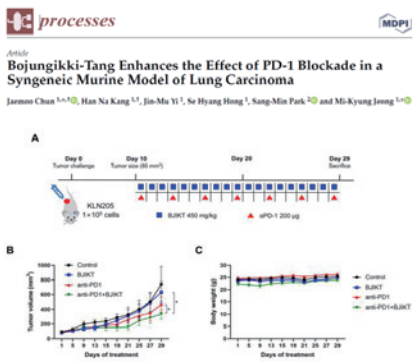
'Bojungikki-tang (BJIKT)' in South Korea
'Buzhongyiqi-Tang' in China
'Hochuekkito' in Japan

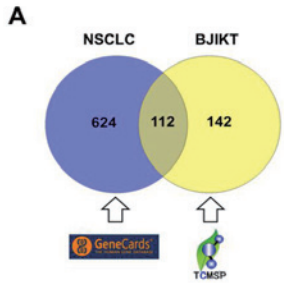


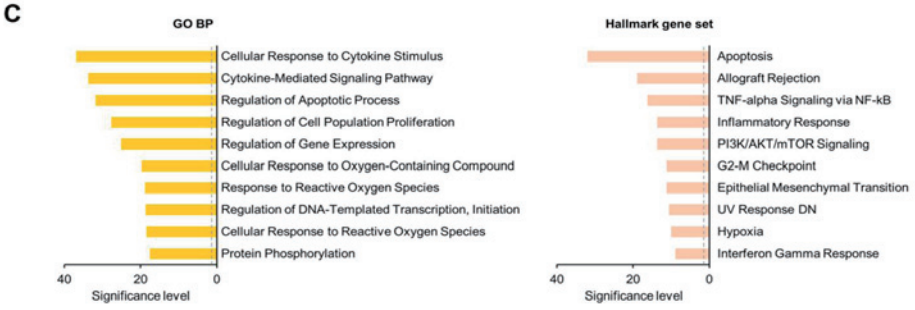
BMC cancer 24.1 (2024): 1169.

Dr. Mi-Kyung Jeong
KM Data Division, Korea Institute of Oriental Medicine

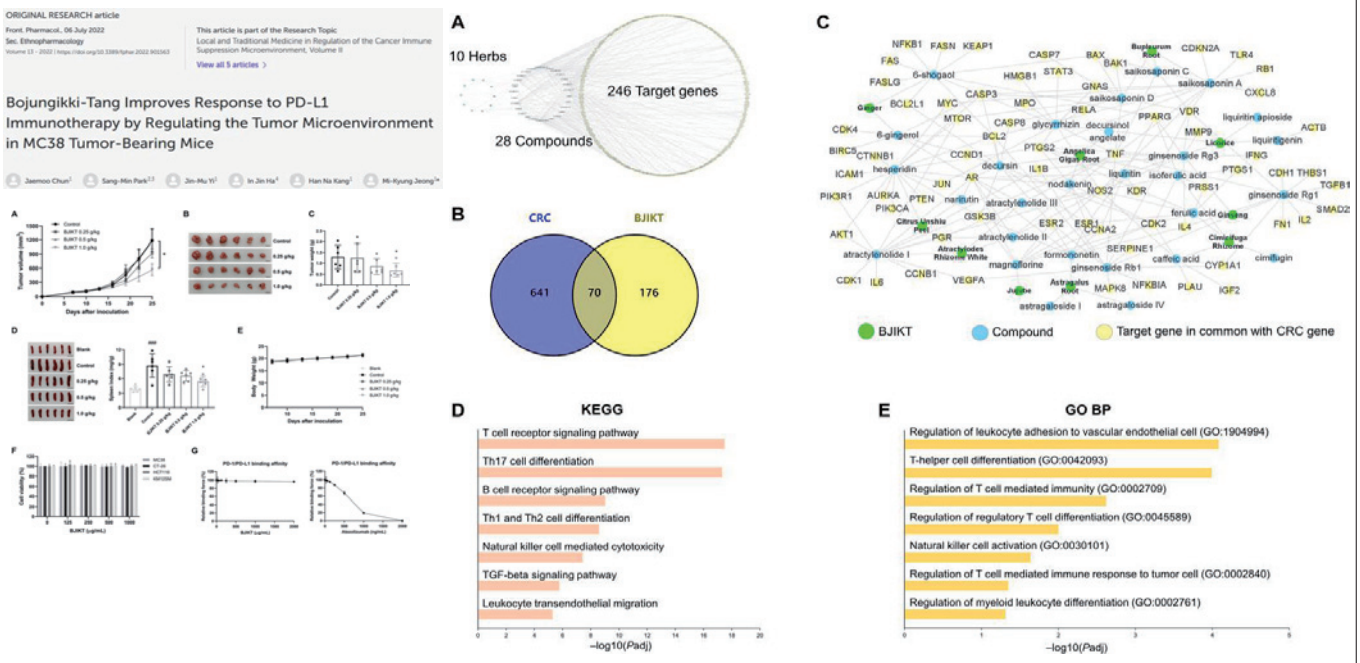
Case 1: BJIKT with Network Pharmacology







Case 1: BJIKT with Network Pharmacology



Limitations

1. 연구 편향(Study bias)으로 인한 중심성 과대평가

- 잘 알려진 질환 유전자(예: 대표적 oncogene)나 유명 화합물은 문헌과 실험 데이터가 풍부해 DB에 많이 기록됨
  → 이들이 실제 생물학적 중요도보다 과도하게 중심 노드로 나타날 수 있음
- 반대로 덜 연구된 타깃은 과소평가되어 **새로운 기전 후보가 사라지는** 위험이 있음

2. 타깃 예측의 간접성

- 네트워크 약리학에서 사용되는 타깃 정보는 DB 기반 예측에 의존
  → **실제 결합 여부나 결합 친화도는 반영되지 않음**

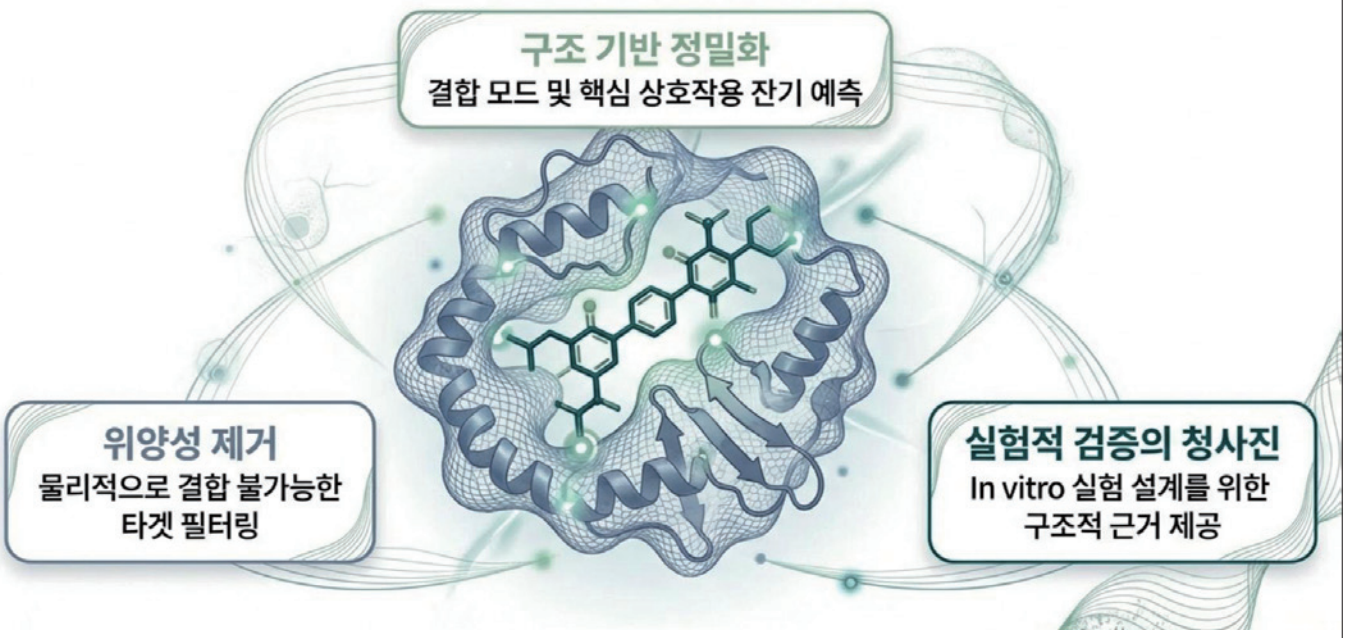
➔ **도킹의 역할:** 예측된 타깃–리간드 쌍 중 **구조적으로 결합 가능성이 있는 상호작용만 선별**하여 네트워크의 신뢰도를 보완

3. 기능적 효과 방향성 부족 및 정적 네트워크의 한계

- 네트워크 약리학은 "연결됨"은 보여주지만 **활성화인지 억제인지**, 병리적 효과인지 보호 효과인지는 구분하지 못함
- 또한 "화합물–타깃–경로"를 **고정된 연결 구조**로 표현하여 질환 상태, 시간, 세포 환경에 따른 **동적 변화 반영 불가**

➔ **전사체 분석의 역할:** 실제 질환 조건에서 어떤 유전자와 경로가 **활성화/억제되는지**를 보여줌

해결책: 분자 도킹 시뮬레이션의 통합



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Molecular docking, network pharmacology and experimental verification to explore the mechanism of Wulongzhiyangwan in the treatment of pruritus

Lyu Anqi & Shan Shijun

Scientific Reports 13, Article number: 361 (2023) | Cite this article

https://www.nature.com/articles/s41598-023-27593-5


Research | Open access | Published: 28 August 2020

Application of network pharmacology and molecular docking to elucidate the potential mechanism of *Eucommia ulmoides-Radix Achyranthis Bidentatae* against osteoarthritis

Gong-hui Jian, Bing-zhu Su, Wen-jia Zhou & Hui Xiong

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Molecular docking, network pharmacology and experimental verification to explore the mechanism of Wulongzhiyangwan in the treatment of pruritus

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https://www.nature.com/articles/s41598-023-27593-5


Research article | Open access | Published: 02 March 2020

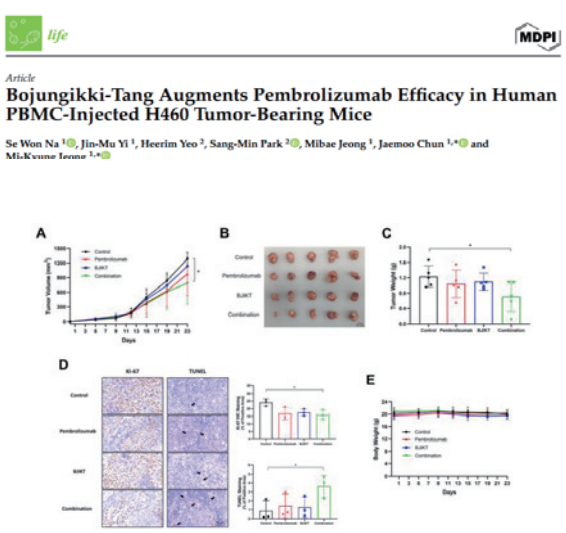
Investigating the multi-target pharmacological mechanism of danhong injection acting on unstable angina by combined network pharmacology and molecular docking

Siyu Guo, Jiarui Wu, Wei Zhou, Xinkui Liu, Jingyuan Zhang, Shanshan Jia, Ziqi Meng, Shuyu Liu, Mengwei Ni & Yingying Liu

BMC Complementary Medicine and Therapies 20, Article number: 66 (2020) | Cite this article

https://bmccomplementmedtherapies.biomedcentral.com/articles/10.1186/s12906-020-2853-5

Case 2: BJIKT with Transcriptomics

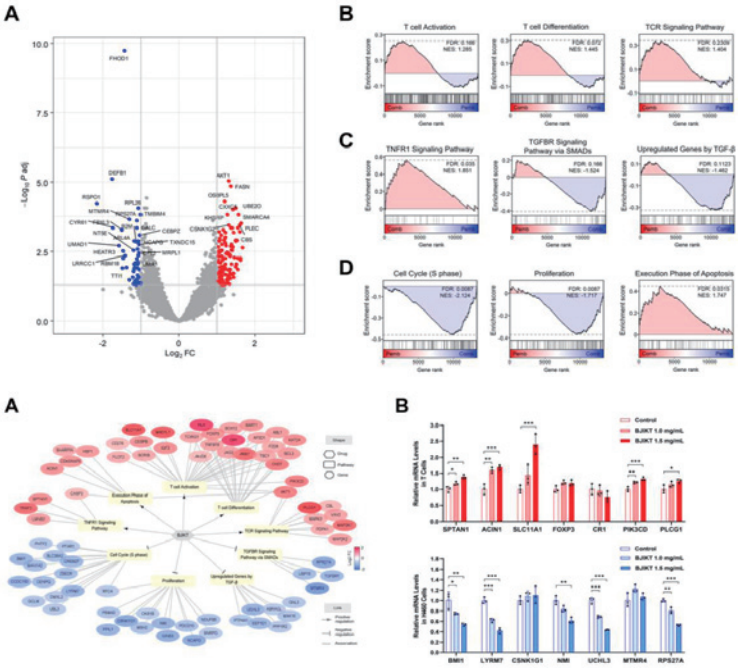

life

MDPI

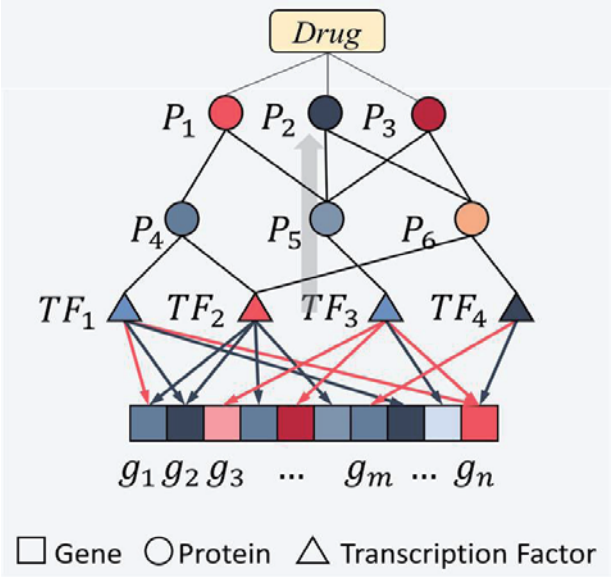
Article

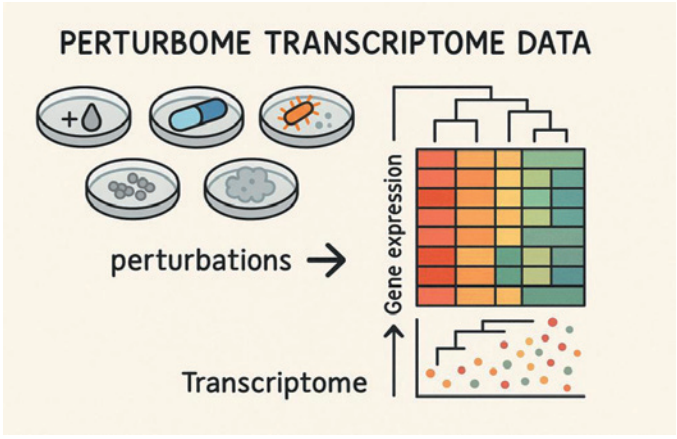
Bojungikki-Tang Augments Pembrolizumab Efficacy in Human PBMC-Injected H460 Tumor-Bearing Mice

Se Won Na [1], Jin-Mu Yi [1], Heerim Yeo [2], Sang-Min Park [2], Mibae Jeong [1], Jaemoo Chun [1,*] and Mi-Kyung Jeong [1,*]



"Perturbome" data analysis – via transcriptomics





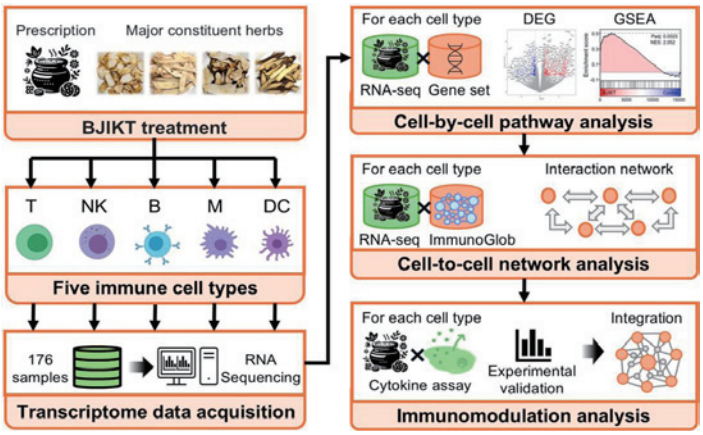
Case 2: BJIKT with Transcriptomics

Biomedicine & Pharmacotherapy
Volume 188, July 2025, 118129

Deciphering the immunomodulatory mechanisms of Bojungikki-tang via systematic transcriptomic and immune cell interaction network analysis

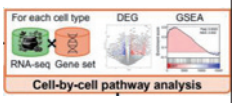
Sang-Yun Kim [a 1], Jin-Mu Yi [b 1], Jaemoo Chun [b], Musun Park [c], Heerim Yeo [a], Sang-Min Park [a], Mi-Kyung Jeong [b]

Systematic transcriptome analysis reveal how herbal medicine modulates immunity.

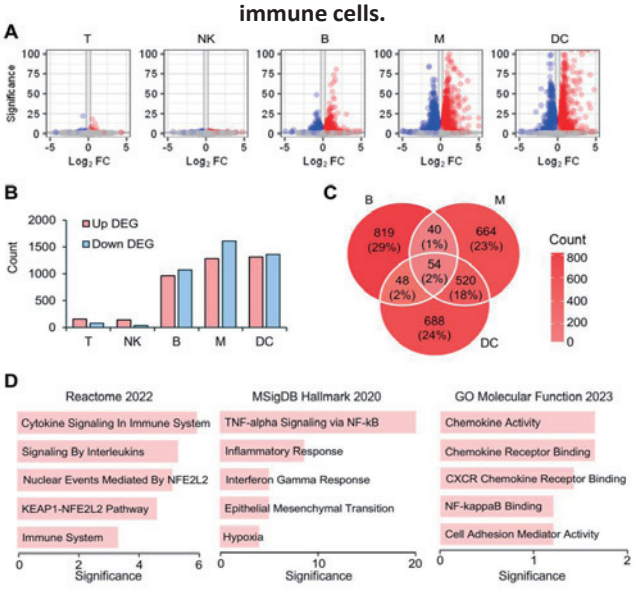


Large-scale RNA-seq data from five immune cell types were analyzed within a network.

Case 2: BJIKT with Transcriptomics



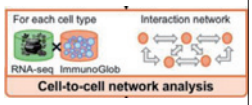
Gene expression analysis in BJIKT-treated immune cells.



Gene set enrichment analysis (GSEA) of immune cell responses to BJIKT treatment.

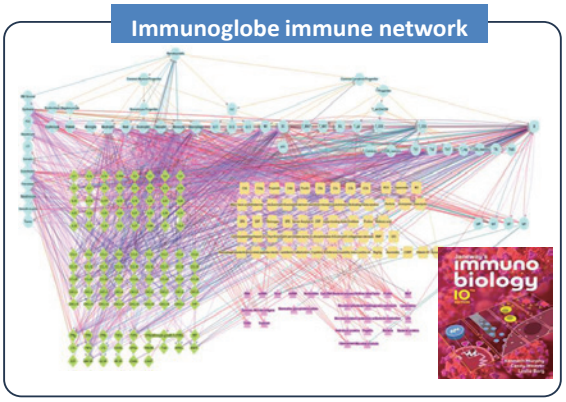
BJIKT upregulates IFN-γ, TNF-α, and inflammatory pathways in B cells, Macrophages, and DCs.

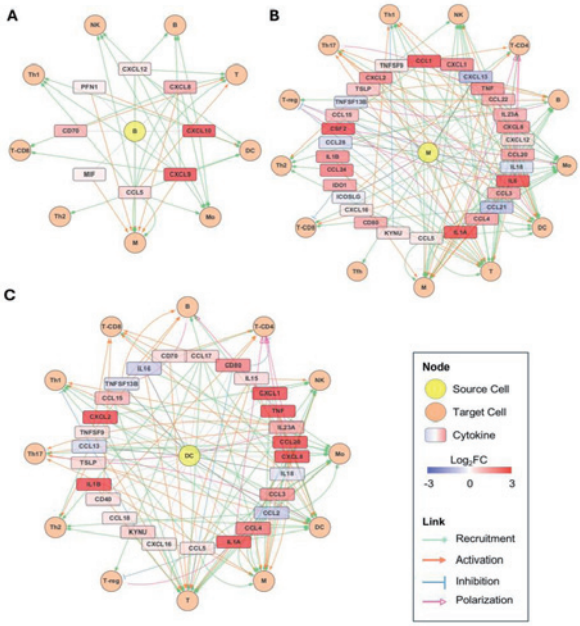
Case 2: BJIKT with Transcriptomics



Cell-to-cell interaction networks for BJIKT-treated immune cells.

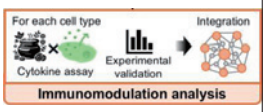
Immunoglobe immune network



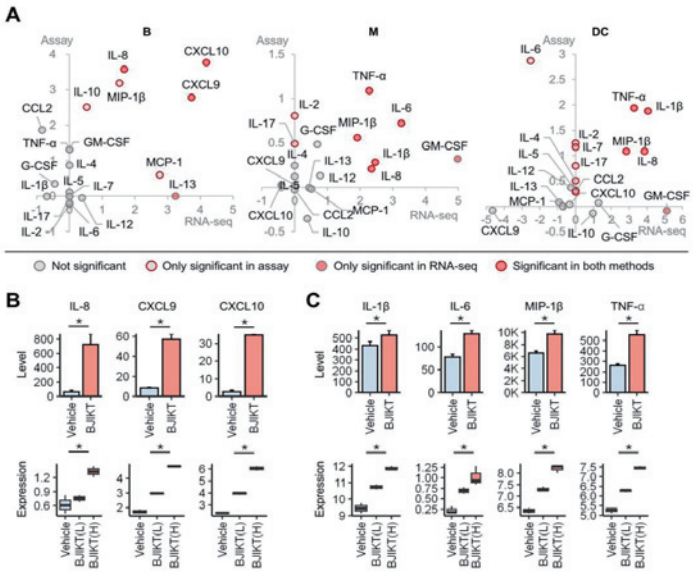


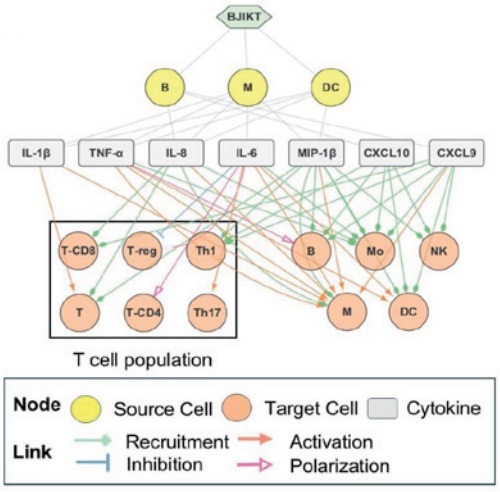
BJIKT influences T cells via cytokines, activating and recruiting immune cells.

Case 2: BJIKT with Transcriptomics



Cytokine level changes in immune cells following BJIKT treatment.

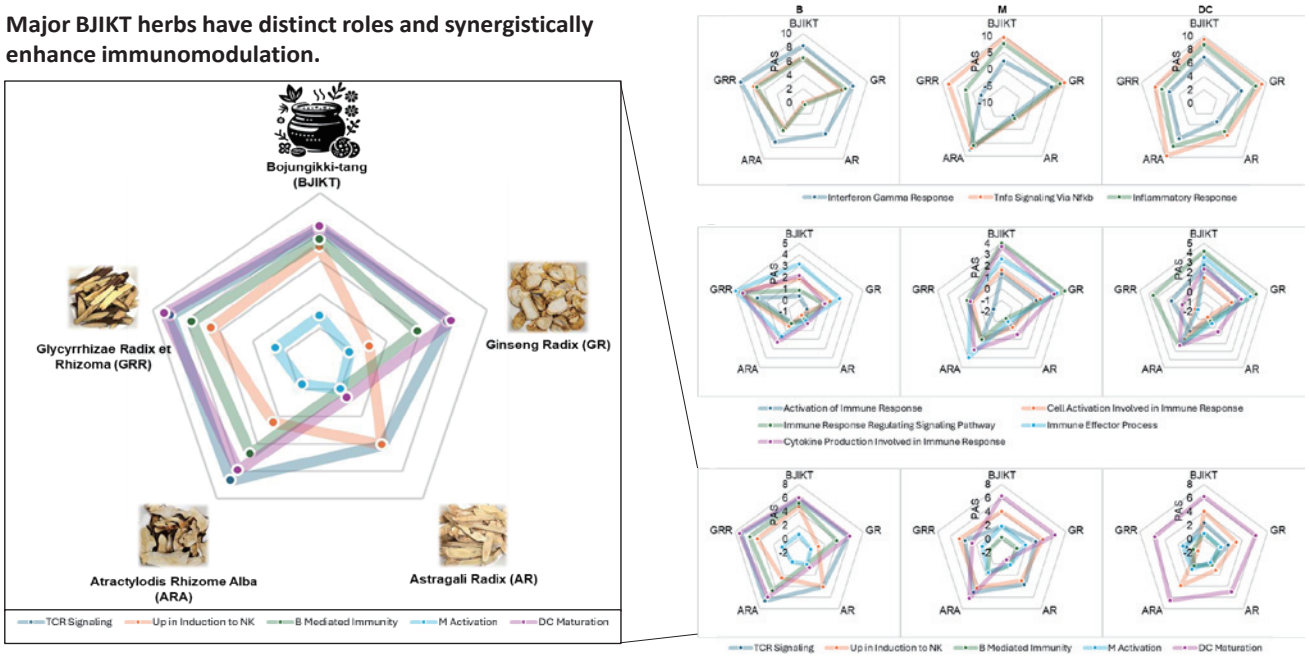




Integrated network for key cytokines induced by BJIKT treatment and their effects on immune cells

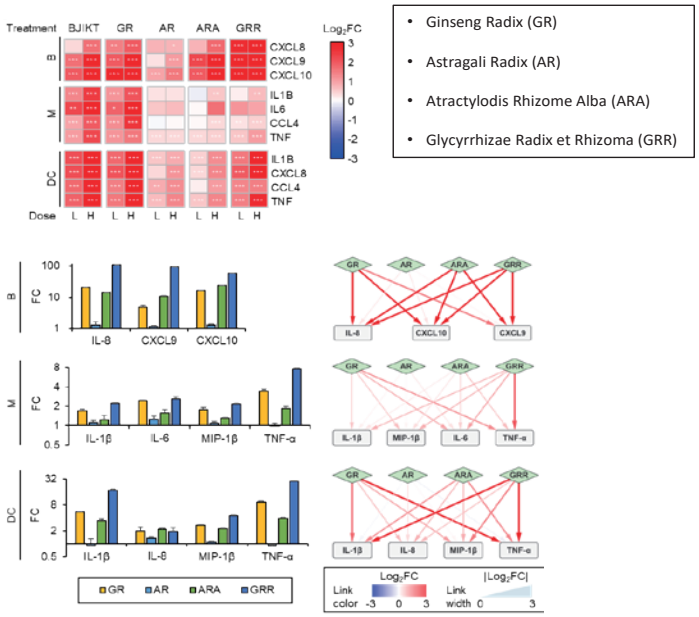
Case 2: BJIKT with Transcriptomics

Major BJIKT herbs have distinct roles and synergistically enhance immunomodulation.



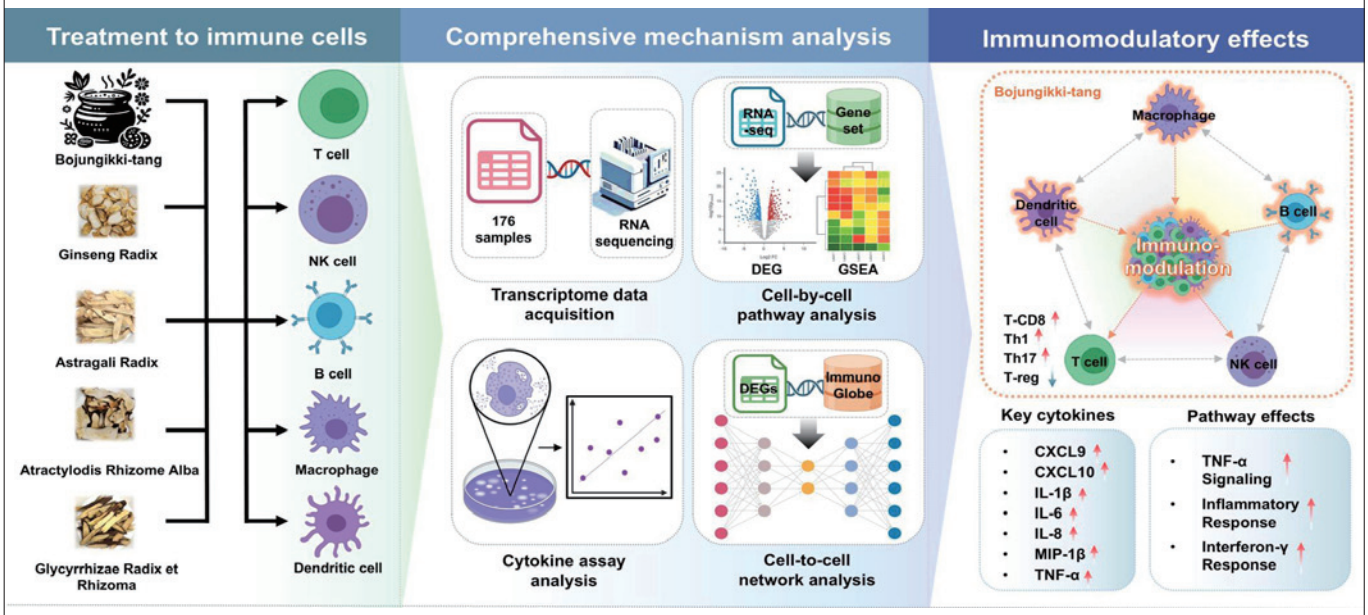
Case 2: BJIKT with Transcriptomics

Major BJIKT herbs have distinct roles and synergistically enhance immunomodulation.



- Ginseng Radix (GR)
- Astragali Radix (AR)
- Atractylodis Rhizome Alba (ARA)
- Glycyrrhizae Radix et Rhizoma (GRR)

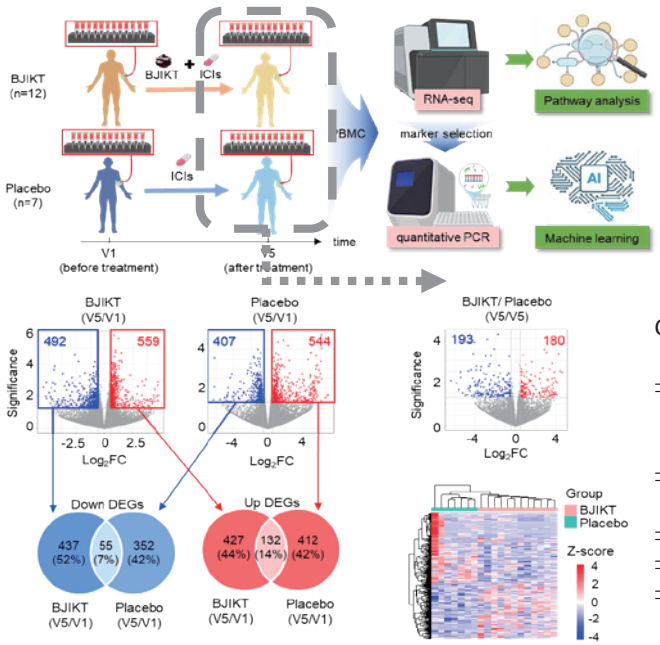
Case 2: BJIKT with Transcriptomics



Biomedicine & Pharmacotherapy (2025) 188, 118129

Case 2: BJIKT with Transcriptomics

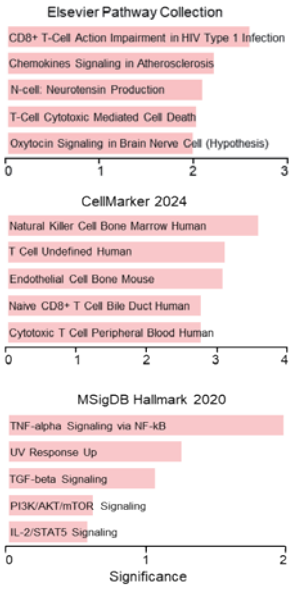
Unpublished



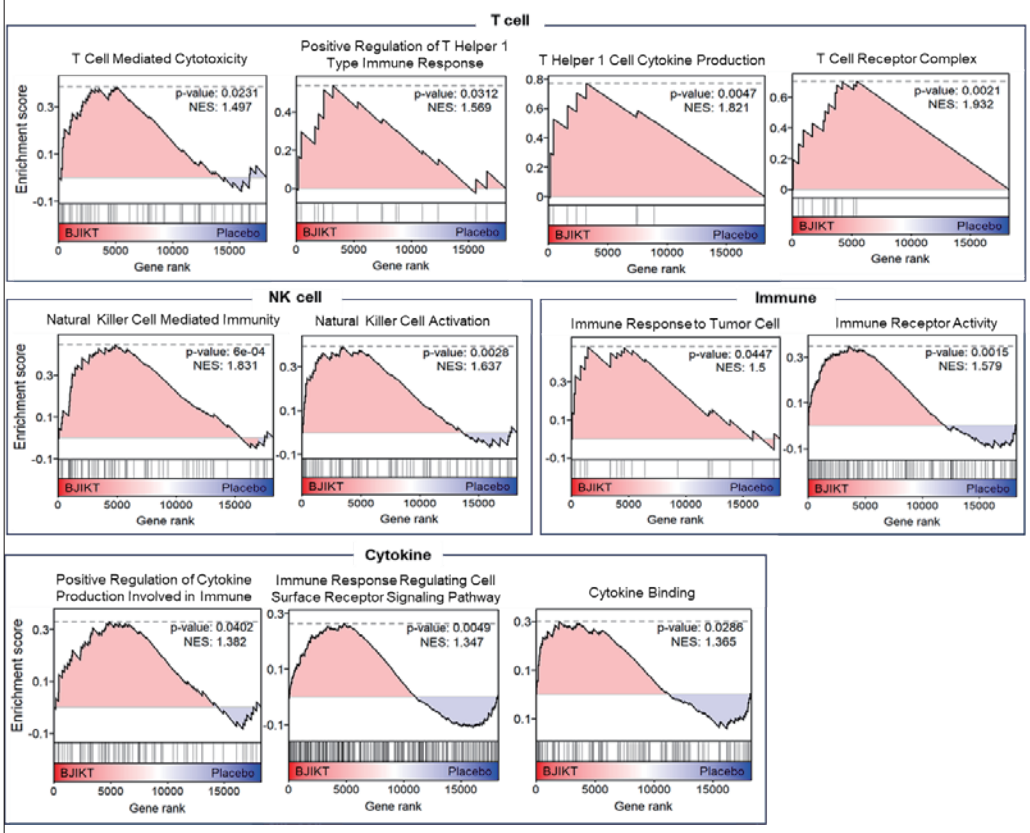
Patients with NSCLC
receiving atezolizumab (anti–PD-L1)

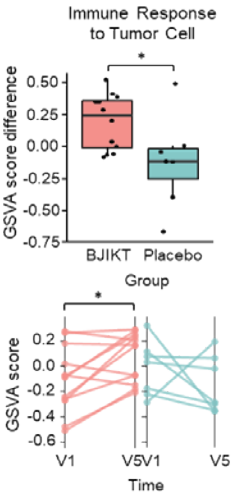
Cross-sectional comparison

⇒ BJIKT-upregulated genes highlighted immune-effector programs
⇒ *TNF-α signaling via NF-κB pathway*
⇒ *IL–2/STAT5 signaling*
⇒ *NK cell markers*
⇒ *cytotoxic T-cell mediated cell death*

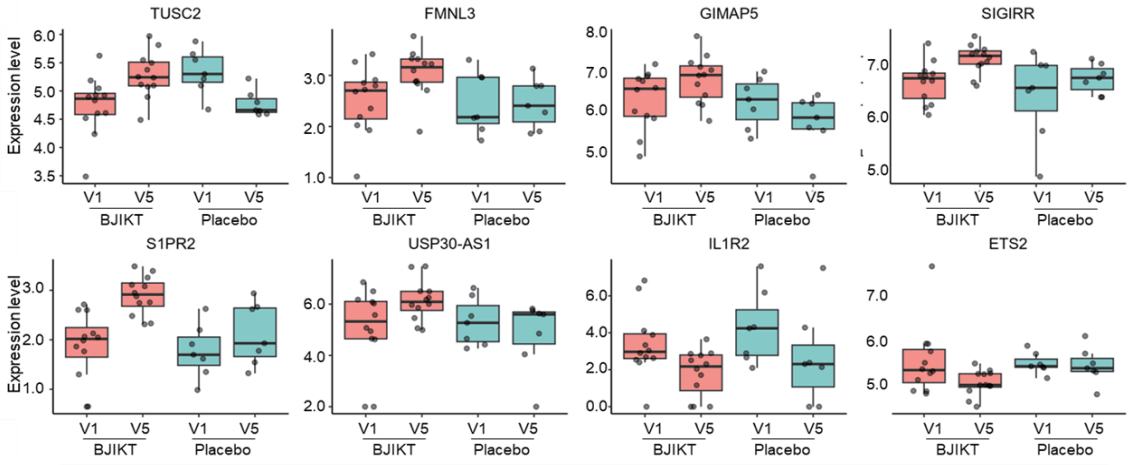


Case 2: BJIKT with Transcriptomics





Case 2: BJIKT with Transcriptomics

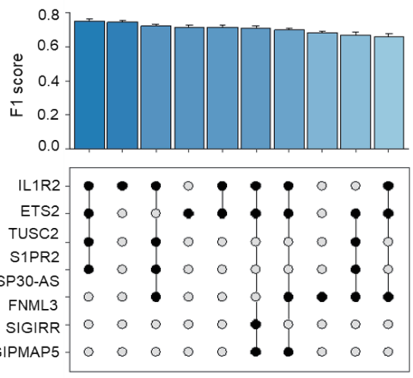


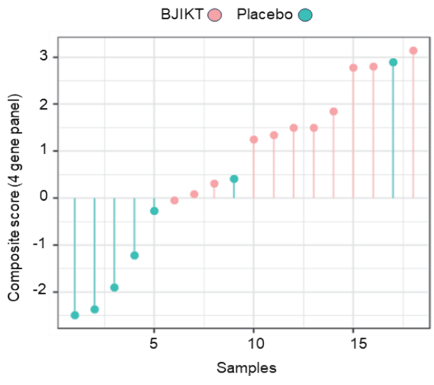
Machine learning

qPCR (V5/V1 fold change)

5-fold cross validation, repeated 1000 times

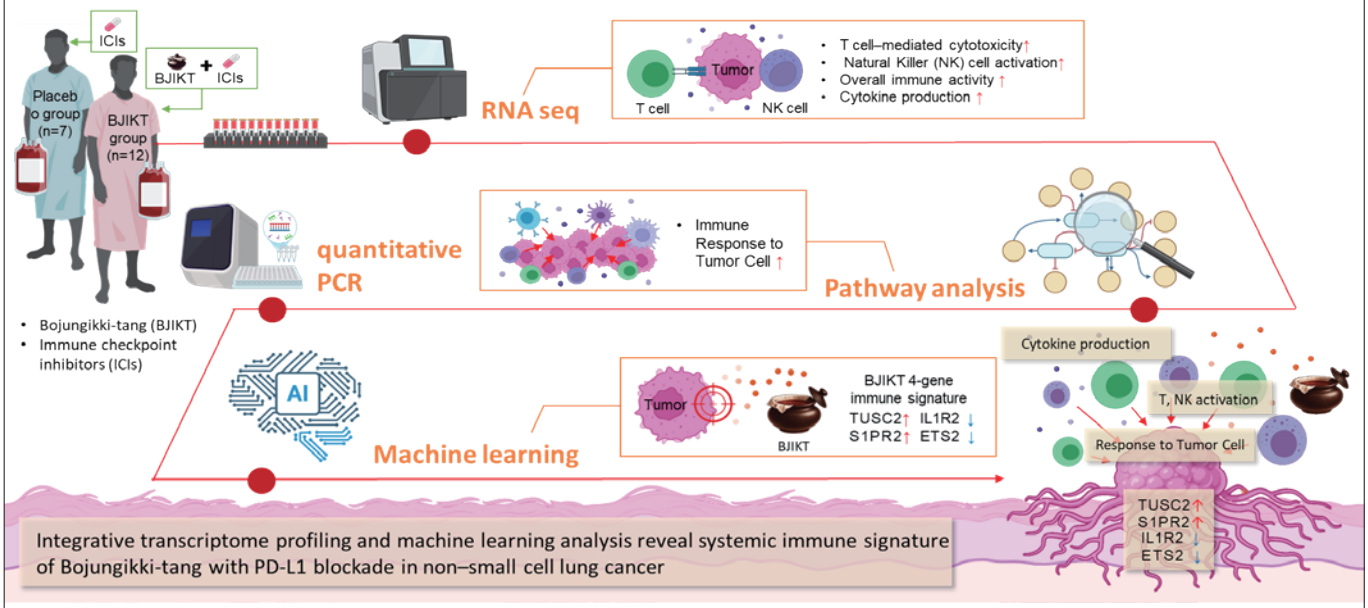
Logistic regression





Case 2: BJIKT with Transcriptomics

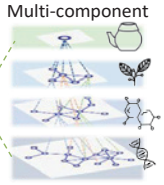
Unpublished



Integrative transcriptome profiling and machine learning analysis reveal systemic immune signature of Bojungikki-tang with PD-L1 blockade in non–small cell lung cancer

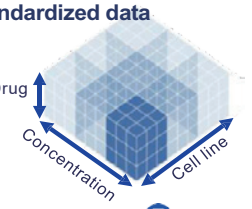
Digital transformation of herbal medicine

Multi-component



Multi-target

• **Standardized data**



- **Preparations: 24 mixed, 57 herbs**
- **3 treatment concentrations** (based on IC20)
- **Number of repetitions: 3**
- **4 human tissue-derived cell lines**

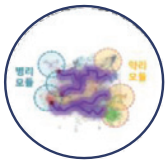
HepG2 A549 HT29 SW1783

13,000 herbal medicine-responsive signature genes

KORE-Map: analysis service platform development (Web & analysis tools)

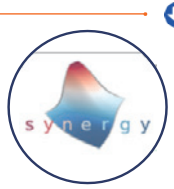
Disease pathology module

Cardiovascular and metabolic diseases, chronic diseases



Pathology-pharmacology network

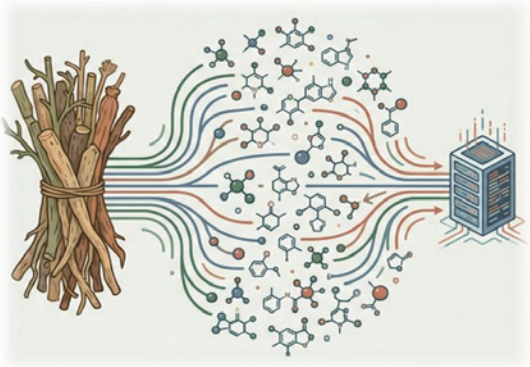
Pathology-pharmacology module network



Drug combination prediction

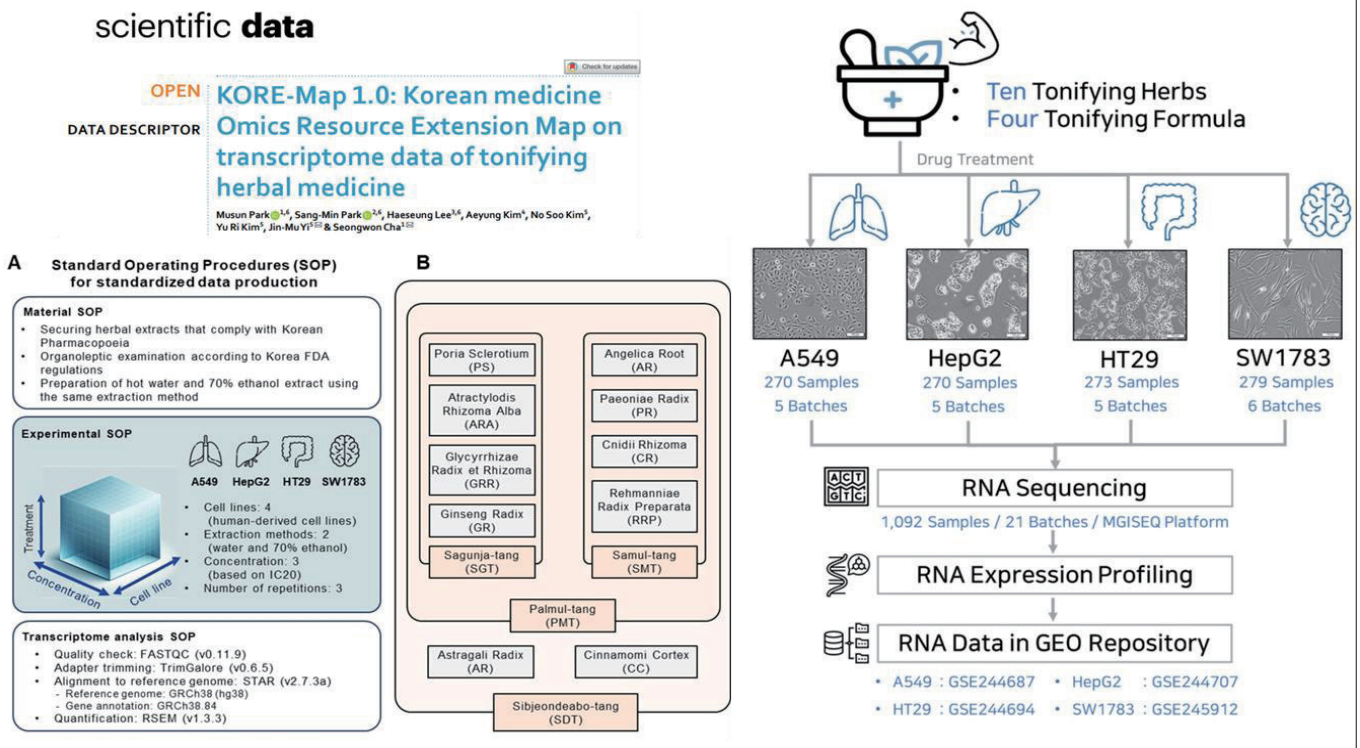
Herbal-herbal medicine
Herbal-western medicine

Verification: in vitro/in vivo experiments



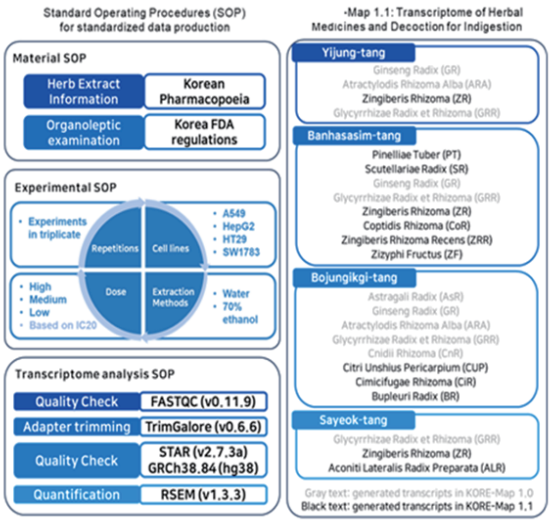
Dr. Seongwon Cha
KM Data Division, Korea Institute of Oriental Medicine

Digital transformation of herbal medicine

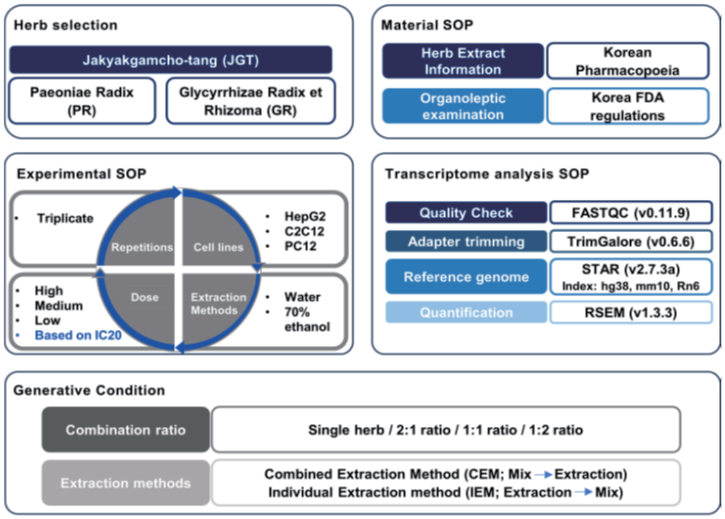


Digital transformation of herbal medicine

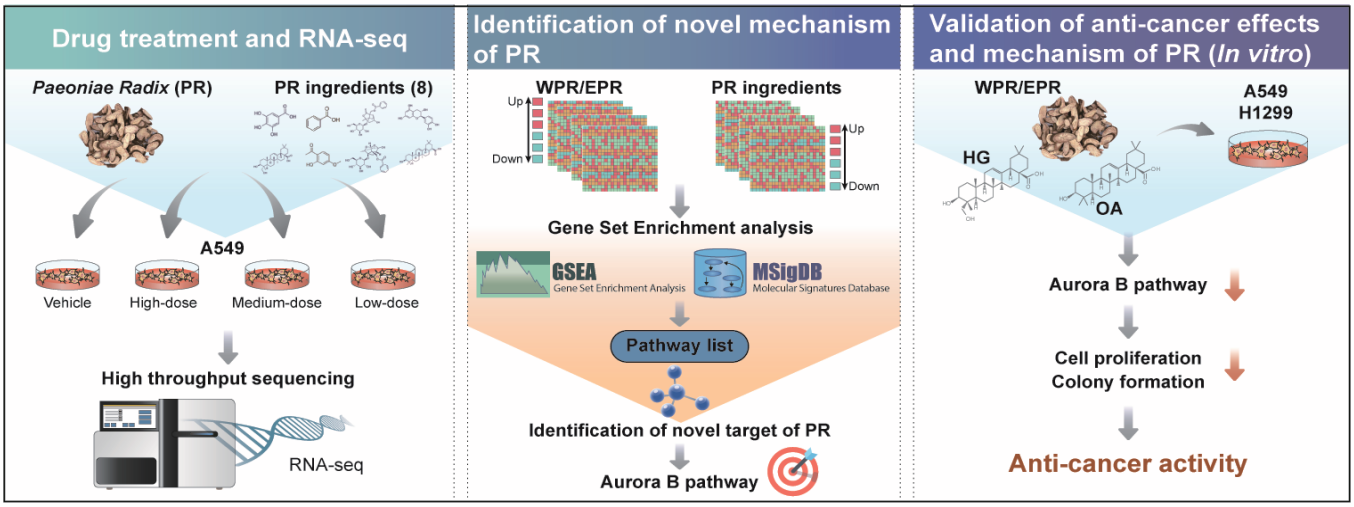
KORE-Map 1.1: Korean Medicine Omics Resource Extension Map on Transcriptome Data of Dyspepsia Herbal Medicine



Multidimensional transcriptome dataset for systematic evaluation of Jakyakgamcho-tang-induced cell signatures



Case 3: Systems analysis for medicinal herbs #1

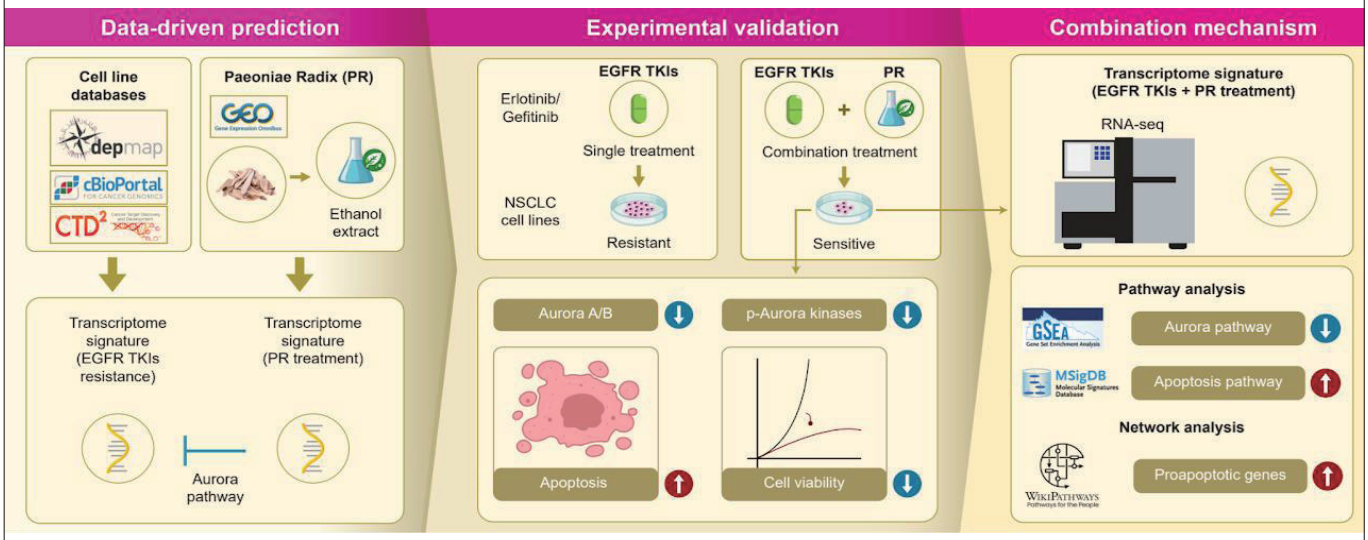


Baek SJ et al., *Biomedicine & Pharmacotheapy* (2022)

Identification of a novel anticancer mechanism of Paeoniae Radix extracts
based on **systematic transcriptome analysis**

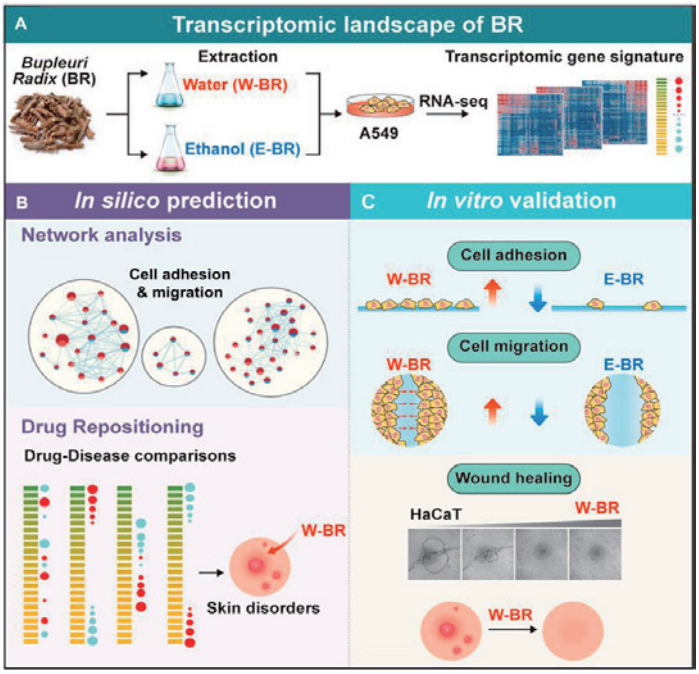
Case 3: Systems analysis for medicinal herbs #2

Life Sciences (2024): 123097.

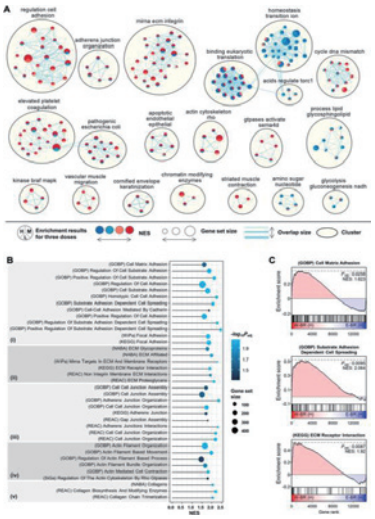


Identification of a novel anticancer mechanism of Paeoniae Radix extracts
based on **systematic transcriptome analysis**

Case 3: Systems analysis for medicinal herbs #3

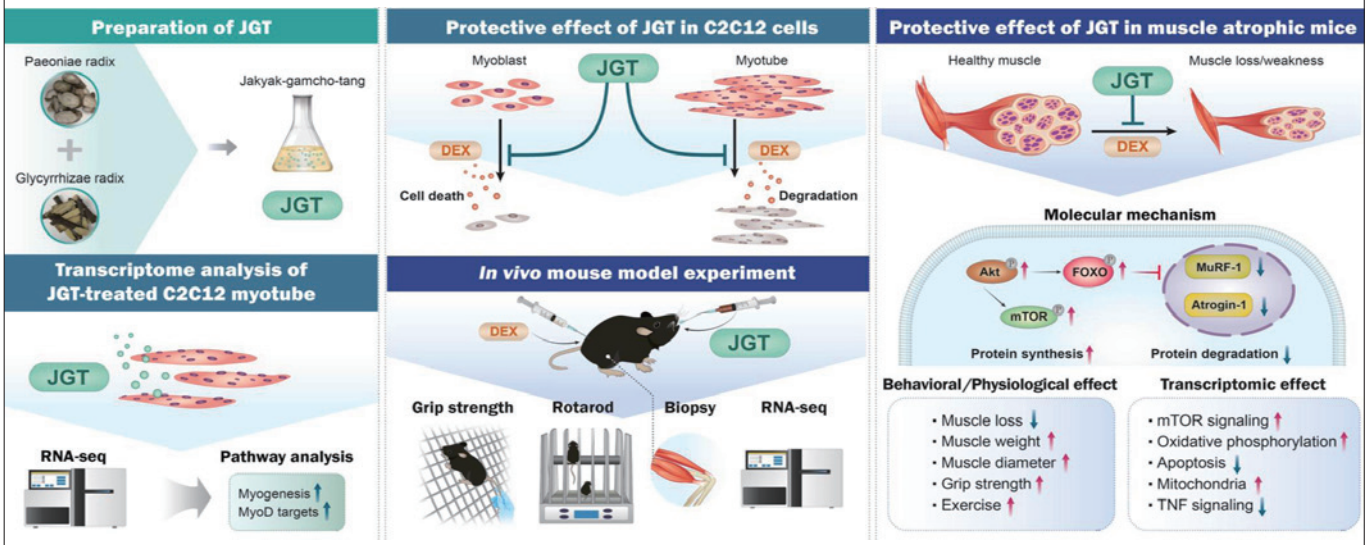


Frontiers in Pharmacology (2022)



Systematic transcriptome analysis reveals molecular mechanisms and indications of Bupleuri Radix

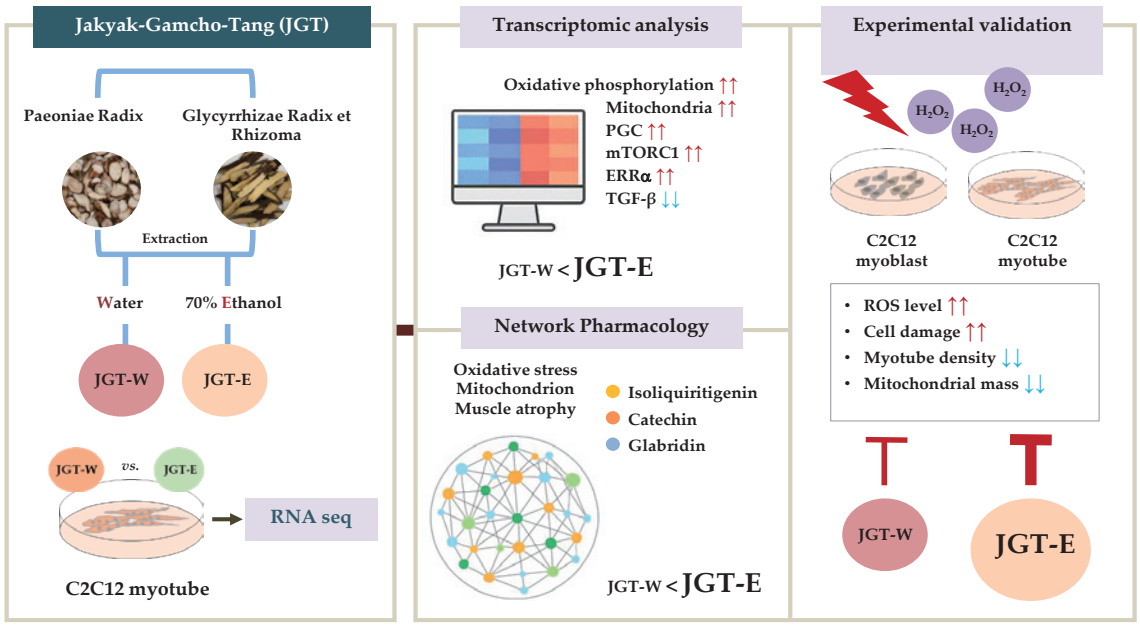
Case 3: Systems analysis for medicinal herbs #4 (combination)



Jakyak-gamcho-tang, a decoction of Paeoniae Radix and Glycyrrhizae Radix et Rhizoma, ameliorates dexamethasone-induced muscle atrophy and muscle dysfunction

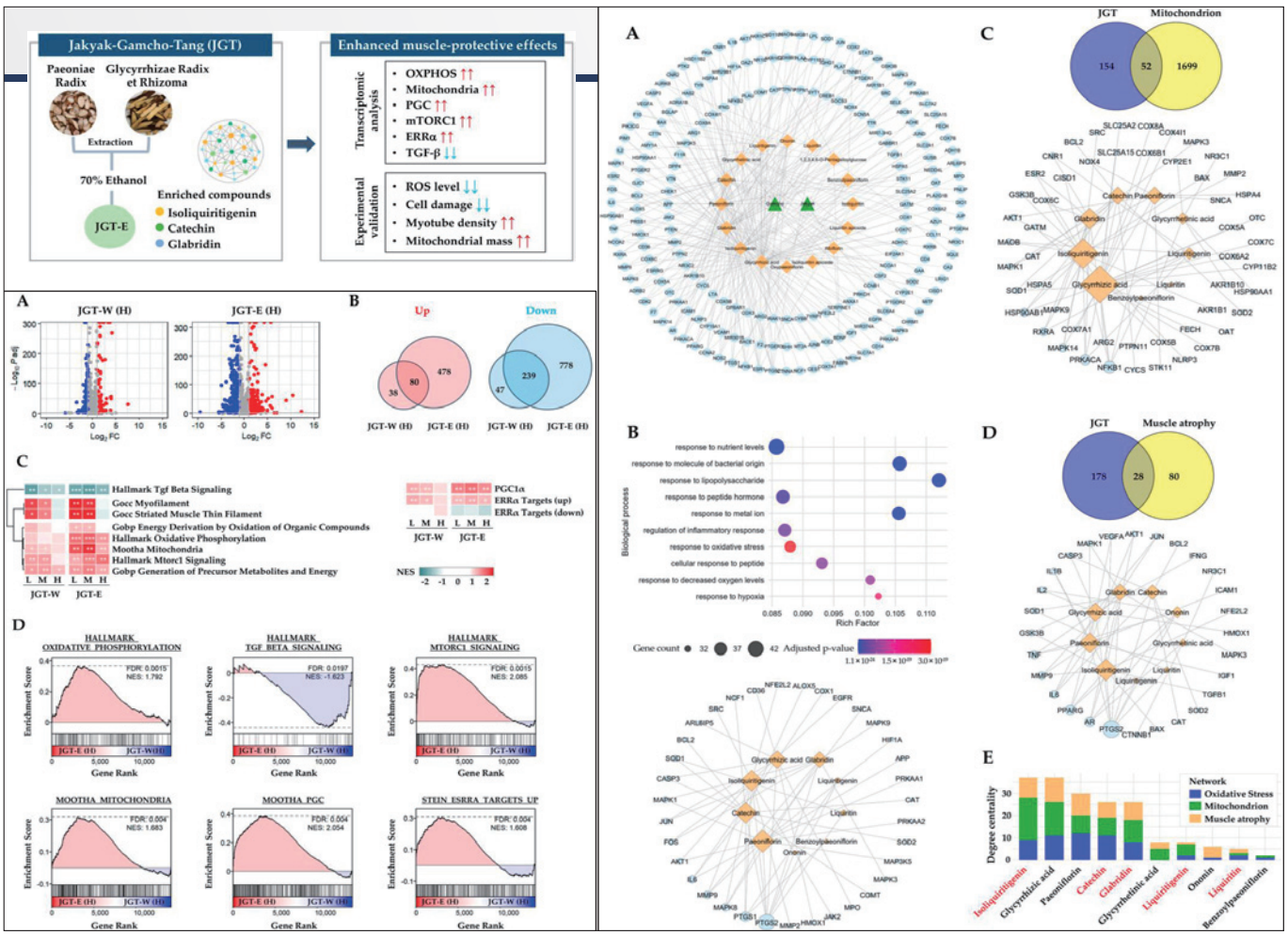
Phytomedicine 123 (2024): 155057.

Case 3: Systems analysis for medicinal herbs #5 (phytochemical)

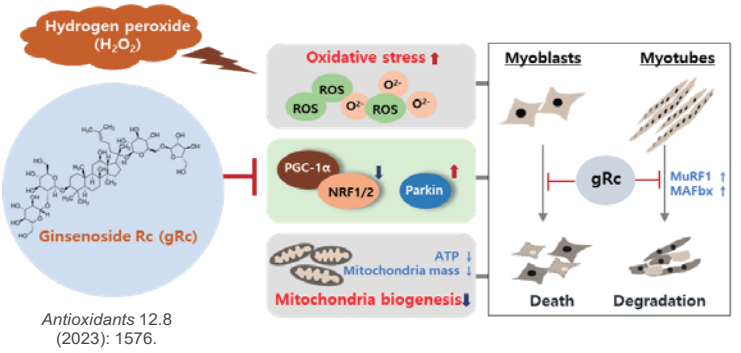


Integration of Transcriptomic Analysis, Network Pharmacology, and Experimental Validation Demonstrates Enhanced Muscle-Protective Effects of Ethanol Extract of Jakyak-Gamcho-Tang

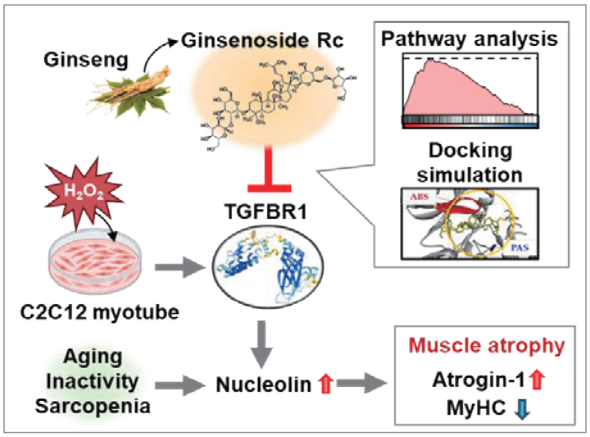
Antioxidants 14.7 (2025): 795



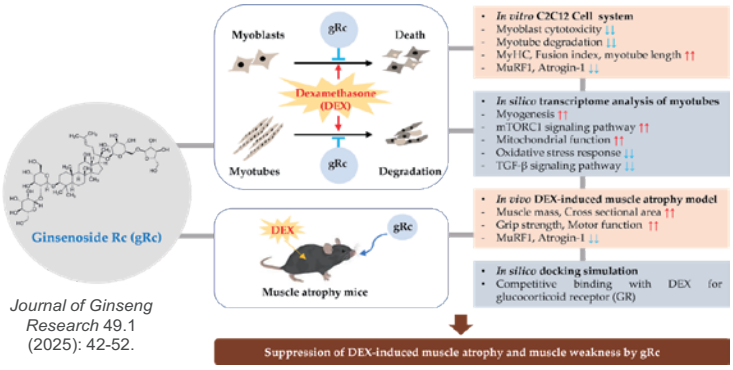
Case 4: Systems analysis for phytochemicals – example 1



Antioxidants 12.8 (2023): 1576.



Life Sciences (2025): 124011.



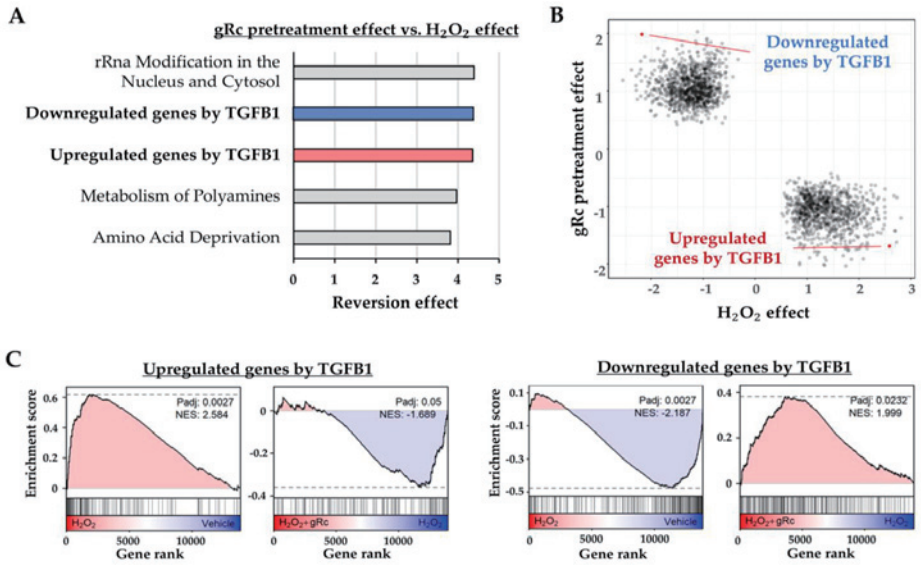
Journal of Ginseng Research 49.1 (2025): 42-52.

Dr. Aeyung Kim

Korean Medicine (KM) Application Center,
Korea Institute of Oriental Medicine

Molecular targets for the muscle protective effects of gRc

Life sciences (2025)

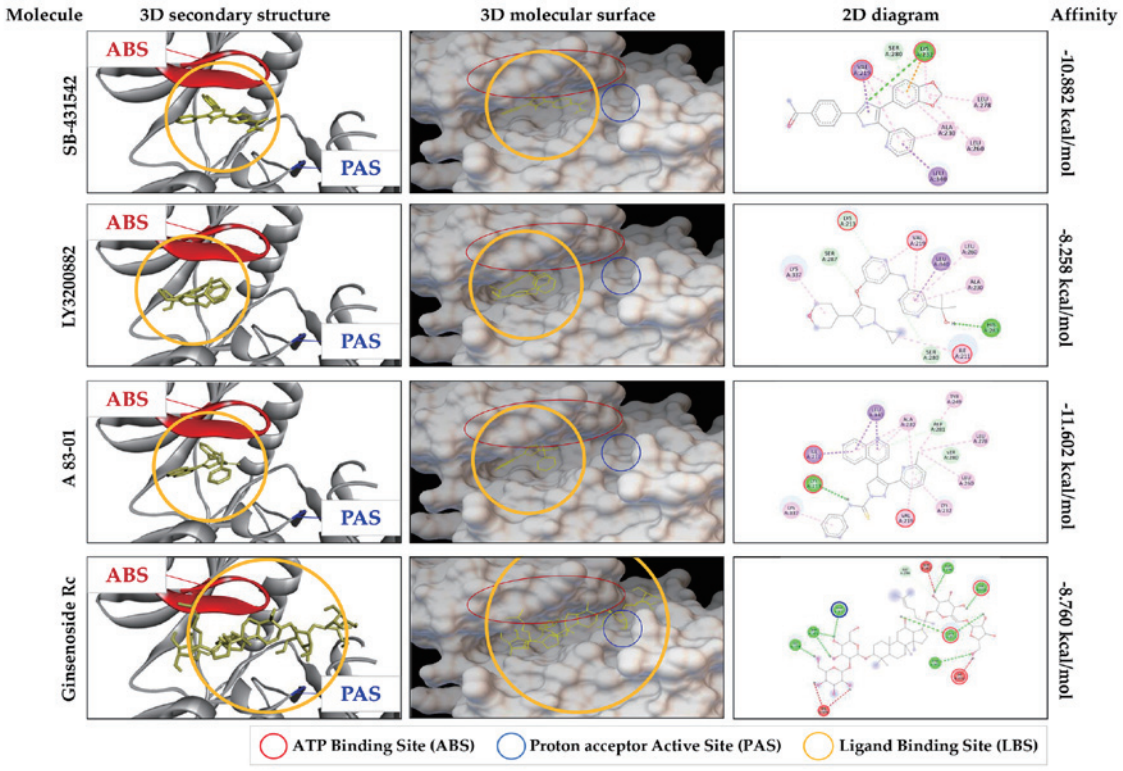


gRc protects myotubes from oxidative stress-induced degradation via TGF-β inhibition.

Molecular targets for the muscle protective effects of gRc

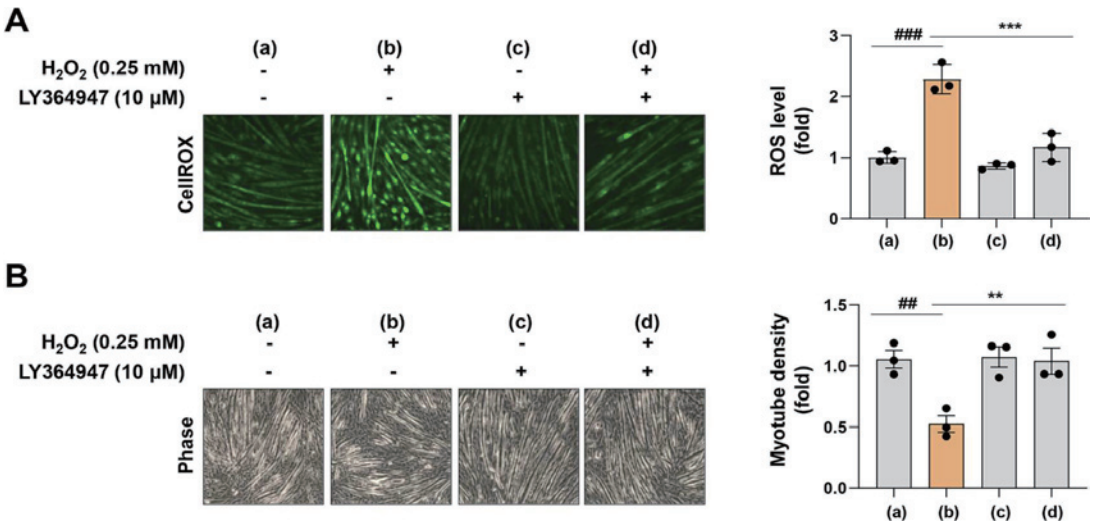
Molecular docking suggests gRc directly binds and inhibits TGF-β receptor 1 (TGFBR1)

Life sciences (2025)



Molecular targets for the muscle protective effects of gRc

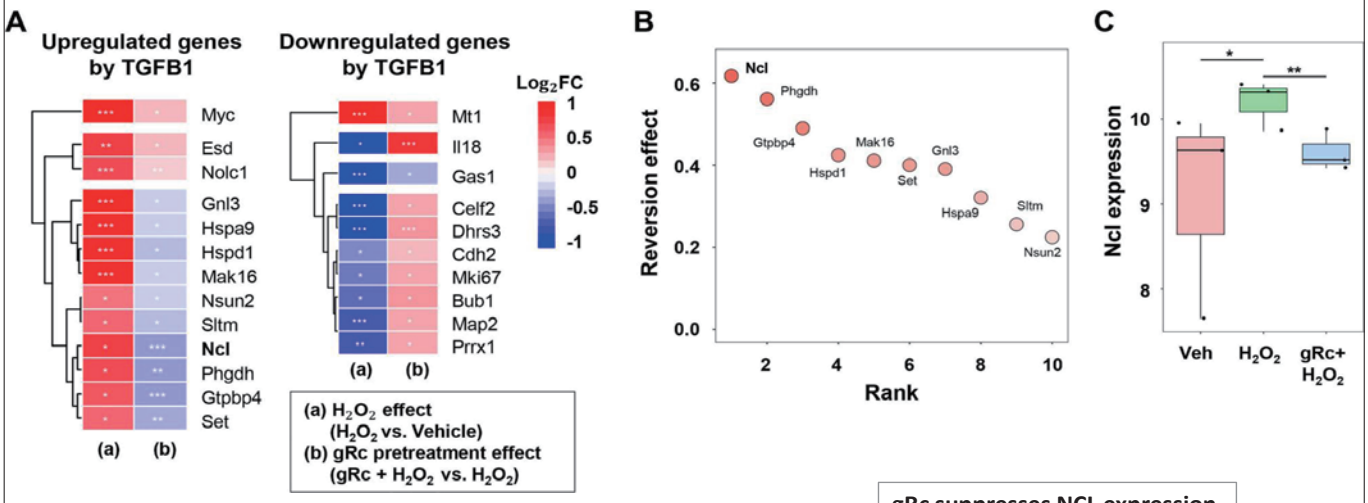
Life sciences (2025)



Effects of a TGF-β inhibitor on H_2O_2-induced ROS generation and cellular damage in C2C12 myotubes

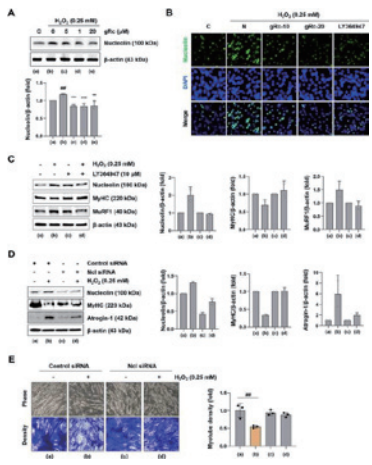
Molecular targets for the muscle protective effects of gRc

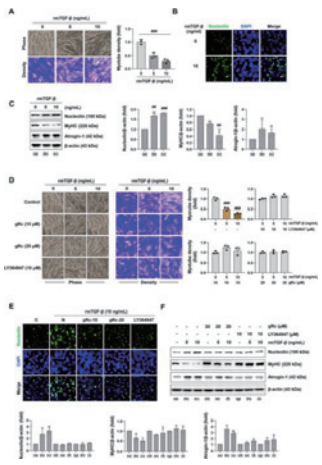
Life sciences (2025)

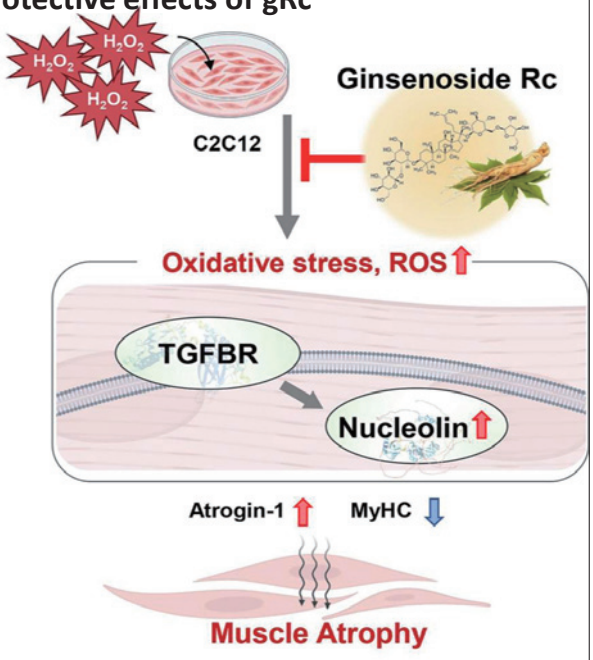


gRc suppresses NCL expression, a key downstream target of TGF-β signaling in muscle

Molecular targets for the muscle protective effects of gRc



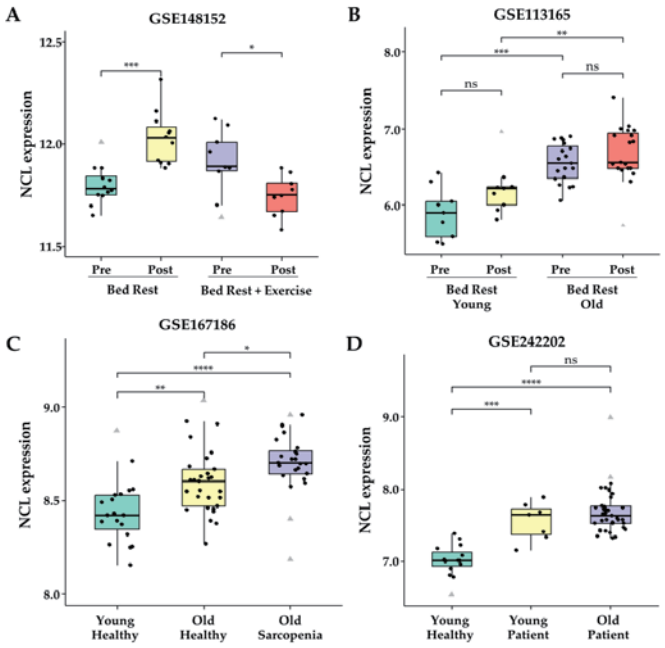




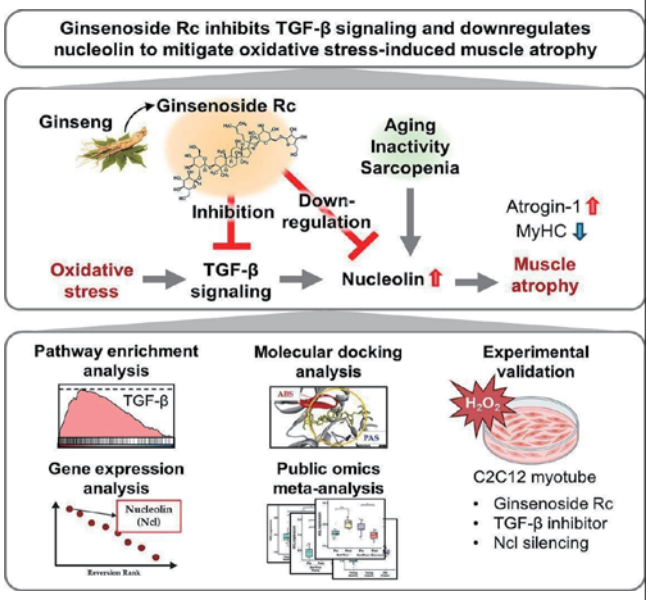
gRc attenuates TGF-β-induced
- Smad activation
- Ncl upregulation
- myotube degradation ← Ncl silencing prevents

Molecular targets for the muscle protective effects of gRc

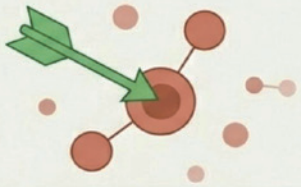
Life sciences (2025)



Human transcriptome data confirm NCL elevation in aging, inactivity, and sarcopenia



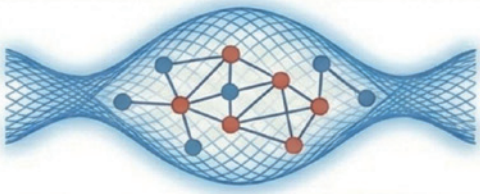
패러다임의 전환: 타겟 중심에서 시스템 기반 접근으로



Target-based Approach

특정 유전자 변이(Mutation) 하나만 공격
(예: HER2, EGFR).

나무만 보는 접근



Systems-based Approach

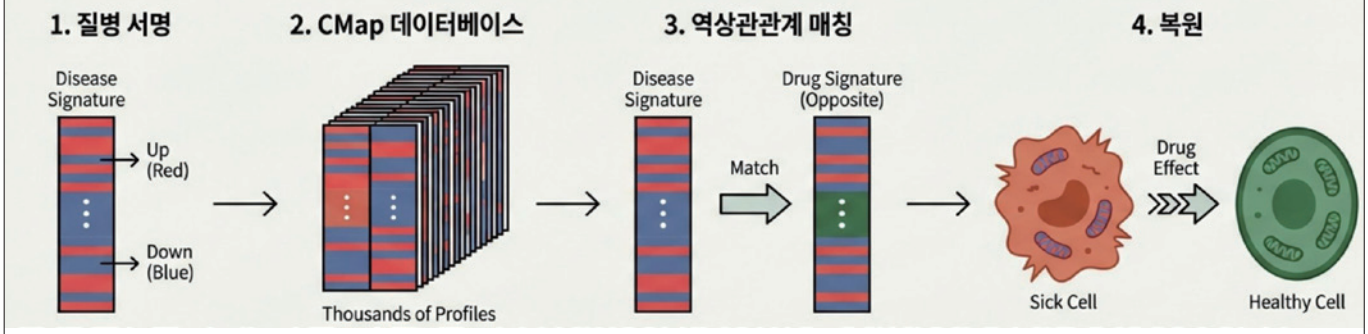
질병으로 인해 변형된 분자적 상태(Signature)를 총체적으로 분석.

숲을 보고 생태계를 복원하는 접근

"단일 변이 타겟팅만으로는 복잡한 시스템을 제어하기 어렵습니다.
변형된 분자 상태를 총체적으로 되돌리는 약물을 찾아야 합니다."
– Chen B. et al., Nat Rev Gastroenterol Hepatol (2020)

방법론: 전사체 기반 약물 탐색 (Transcriptome-Guided Drug Discovery)

Connectivity Map (CMap) 활용



OXFORD

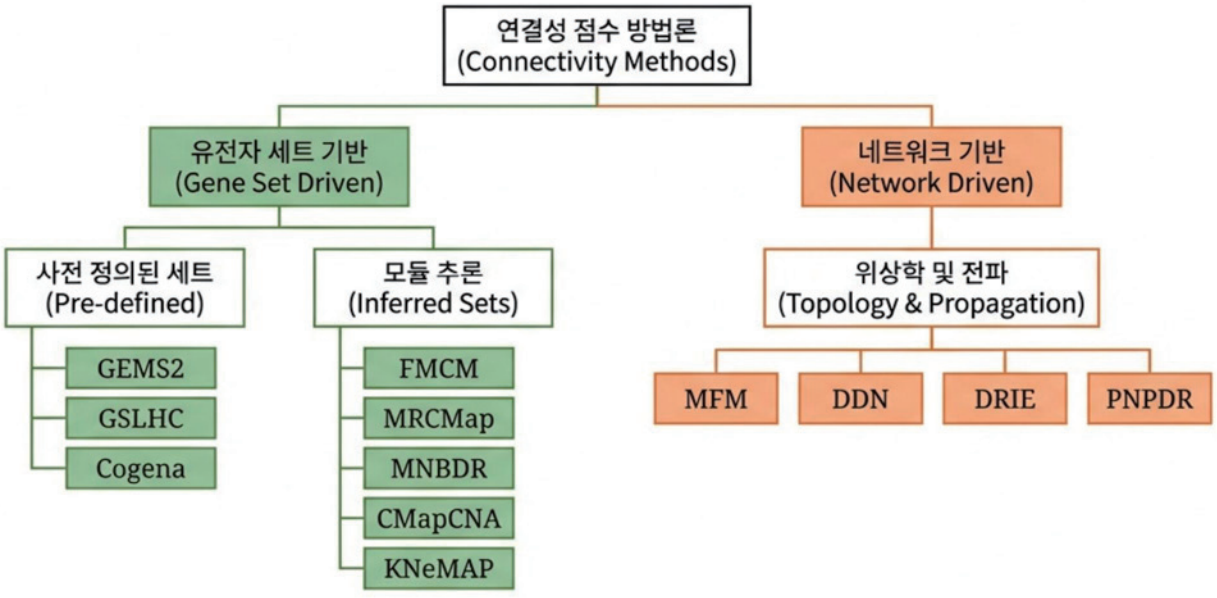
Briefings in Bioinformatics, 2025, **26(4)**, bbaf387

https://doi.org/10.1093/bib/bbaf387

Review

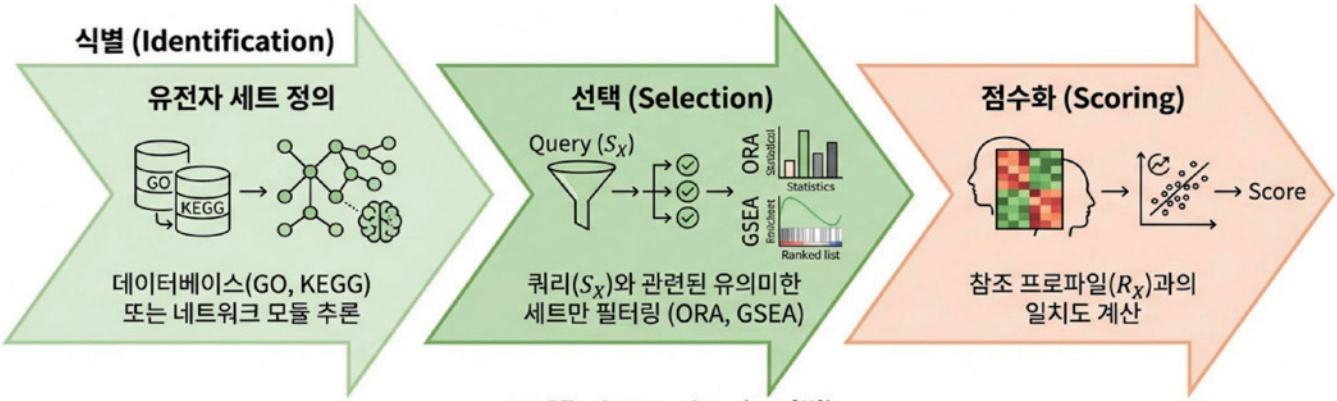
Reconciling multiple connectivity-based systems biology methods for drug repurposing

12가지 연결성 방법론의 분류 체계



모든 방법론은 '지식 통합 방식'에 따라 크게 두 가지로 분류됩니다.

유전자 세트 기반 방법론의 공통 워크플로우



Unified Notation (표기법)

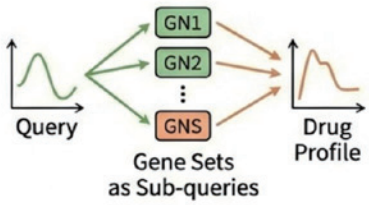
- S_X: : 쿼리(질병)와 관련된 유전자 세트
- R_X: : 참조(약물)와 관련된 유전자 세트
- $v_{ref}()$, $v_{qry}()$: 유전자 발현 점수 벡터

사전 정의된 유전자 세트 활용 (Pre-defined Gene Sets)
GEMS2, GSLHC, Cogena

핵심 메커니즘:
외부 지식 베이스(KEGG, GO, MSigDB) 직접 활용

GEMS2

Sub-query Strategy

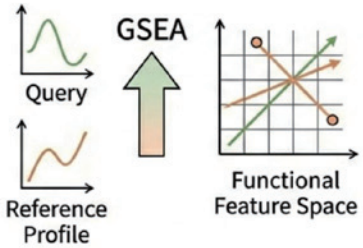


유전자 세트를 'Sub-query'로 사용하여 각 약물 프로파일과 비교.

ES_{up} 및 ES_{down} 점수 계산

GSLHC

Functional Feature Space

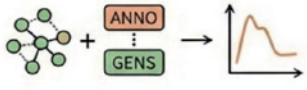


GSEA를 사용하여 쿼리와 참조 프로파일을 '기능적 특징 공간'으로 투영.

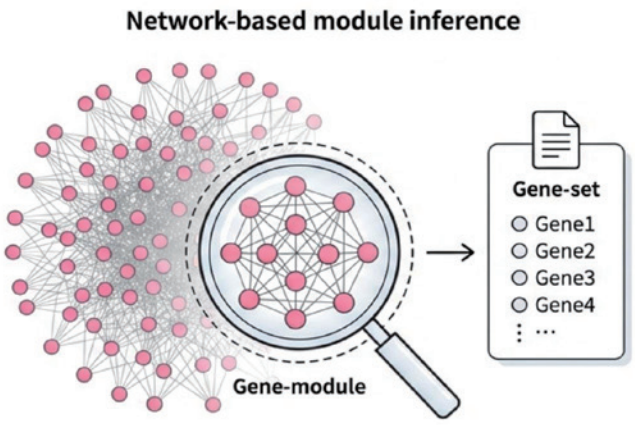
Cogena

Co-expression & Annotation

1. 공동 발현 유전자 클러스터링
2. 기능적 데이터베이스로 주석 처리
3. 약물 서명과 비교



네트워크 추론 기반 유전자 모듈 (Network-Inferred Gene Modules)
FMCM, MRCMap, MNBDR, KNeMAP



핵심 메커니즘:
실험 데이터와 네트워크 위상(Topology)을 결합하여 '조건 특이적' 유전자 모듈 생성.

주요 방법론:
- **FMCM:** PPI 네트워크 + 유전자 공발현 네트워크(GGIN) 통합. 기능적 모듈 식별.
- **MRCMap:** 전사 인자(TF) 중심의 조절 네트워크(Regulon) 구축. 질병의 핵심 조절 인자 타겟팅.
- **MNBDR:** 모듈 네트워크 구축 후 PageRank 알고리즘 적용.

스코어링 전략: 모듈형 vs 전역형

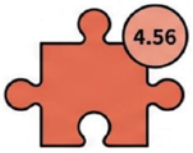
모듈형 점수 (Modular Scores)

Methods:
FMCM, GEMS2, MRCMap, Cogena

Definition:
각 유전자 세트(또는 모듈)별로 개별 점수 산출 ($gems_{r,i}$, $fmcm_{r,i}$)

Use Case:
특정 생물학적 경로(Pathway)나 기전(Mechanism)을 타겟하는 약물 발굴

전역형 점수 (Global Scores)



Methods:
MNBDR, GSLHC, KNeMAP

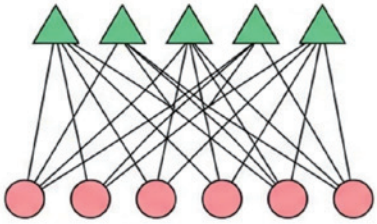
Definition:
전체 프로파일의 유사도를 하나의 숫자로 요약

Use Case:
가장 유망한 약물 후보의 빠른 순위 매기기(Ranking)

Note: FMCM과 MRCMap은 모듈 점수 기반의 '전역 선택 프로세스'도 제공함.

네트워크 기반 접근법의 핵심 개념

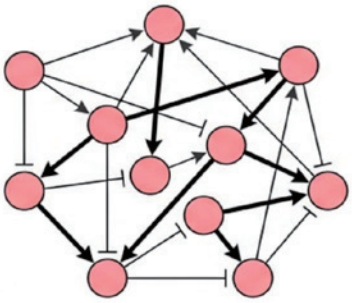
1. 이분 그래프 (Bipartite Network)



Used in PNPDR

약물-경로 등 두 가지 다른 유형의 노드 연결

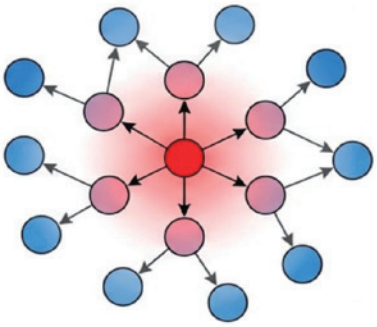
2. 방향성 가중치 네트워크 (Weighted Directed Network)



Used in DDN, DRIE

유전자 간의 활성/억제 흐름 파악

3. 네트워크 전파 (Network Propagation)



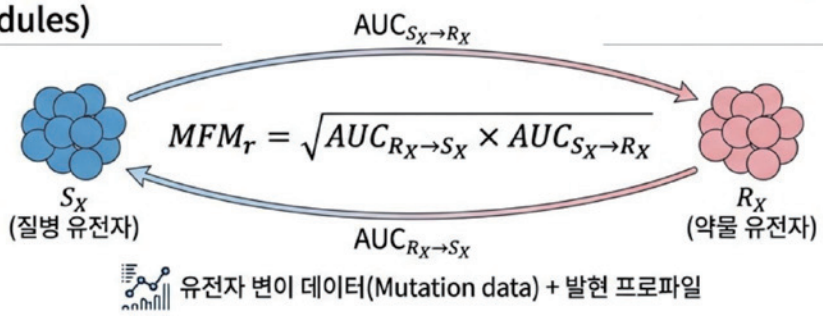
Used in PNPDR, MNBDR

'유죄 연좌제(Guilt-by-association)' 원리: 정보 확산

상호 예측성과 네트워크 전파 (Mutual Predictability & Propagation)

MFM (Method of Functional Modules)

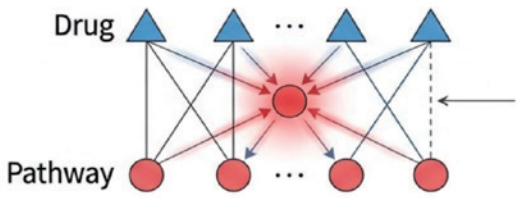
기능적 연관 네트워크 상에서 질병 유전자(S_X)와 약물 유전자(R_X) 간의 상호 예측성 측정.



유전자 변이 데이터(Mutation data) + 발현 프로파일

PNPDR (Pathway-based Network Propagation)

약물(Drug)과 경로(Pathway) 노드로 구성된 이분 그래프 (Bipartite Graph) 활용.



반지도 학습(Semi-supervised learning) 기반의 라벨 전파(Label Propagation).

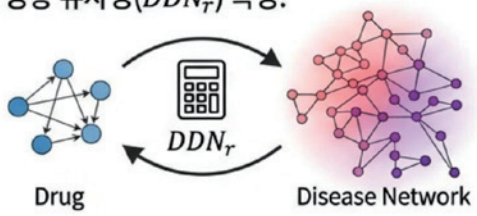
알려지지 않은 약물-질병 경로 간의 숨겨진 링크 예측.

경로 위상학적 분석: 활성 및 억제 모델링

DDN & DRIE

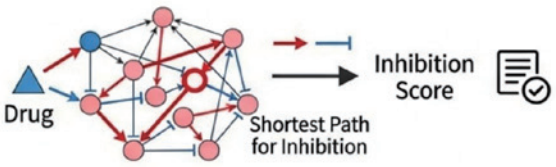
DDN (DrugDiseaseNet)

섭동 인자(Perturbation Factor)를 계산하여
시스템 영향 유사성(DDN_r) 측정.



DRIE

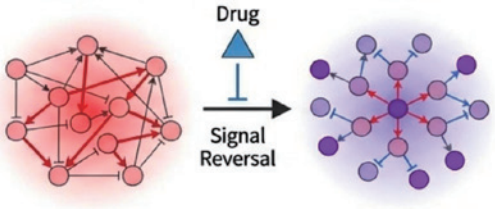
최단 경로(Shortest Path) 분석을 통한
억제 점수(Inhibition Score) 산출.



핵심 논리 및 목표 (Core Logic & Goal)

KEGG 신호전달 경로의 흐름과 상호작용 유형(Type of Interaction) 고려.
$\lambda_{gh} = 1$ (Activation) vs. $\lambda_{gh} = -1$ (Inhibition).

목표: 질병 신호를 역전(Reverse)시키는 약물 식별.



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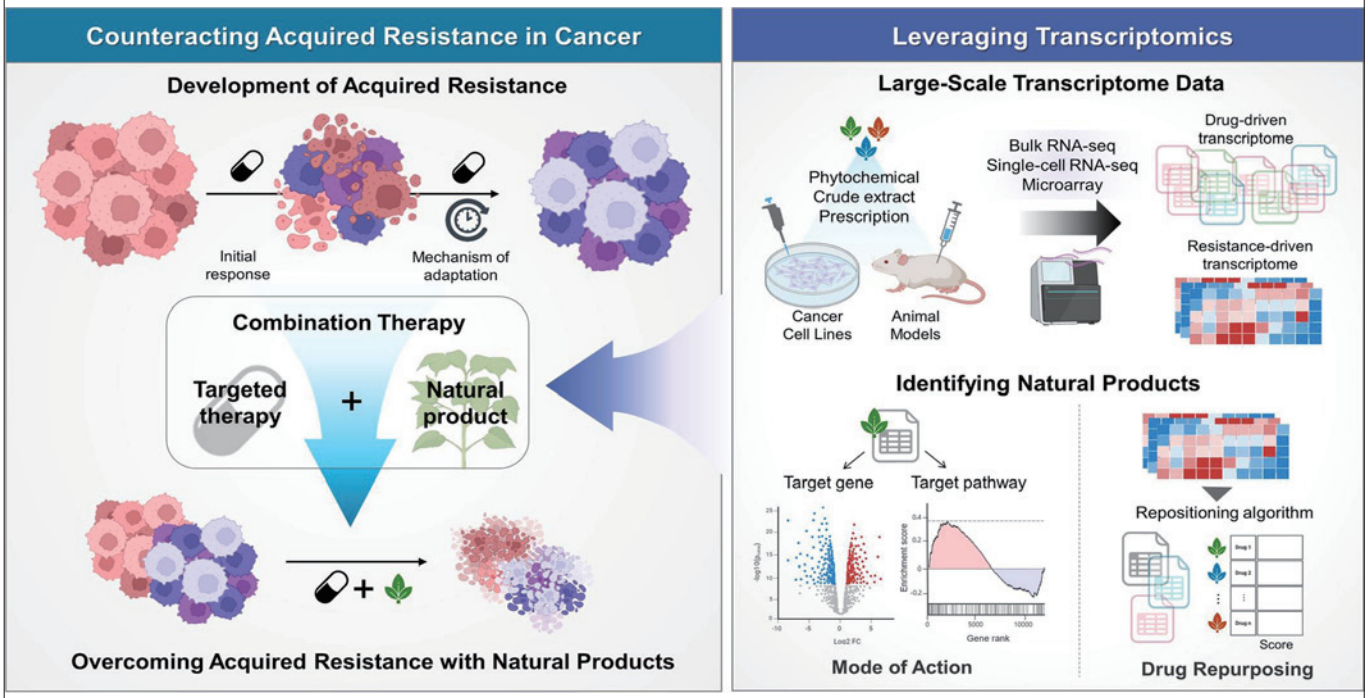
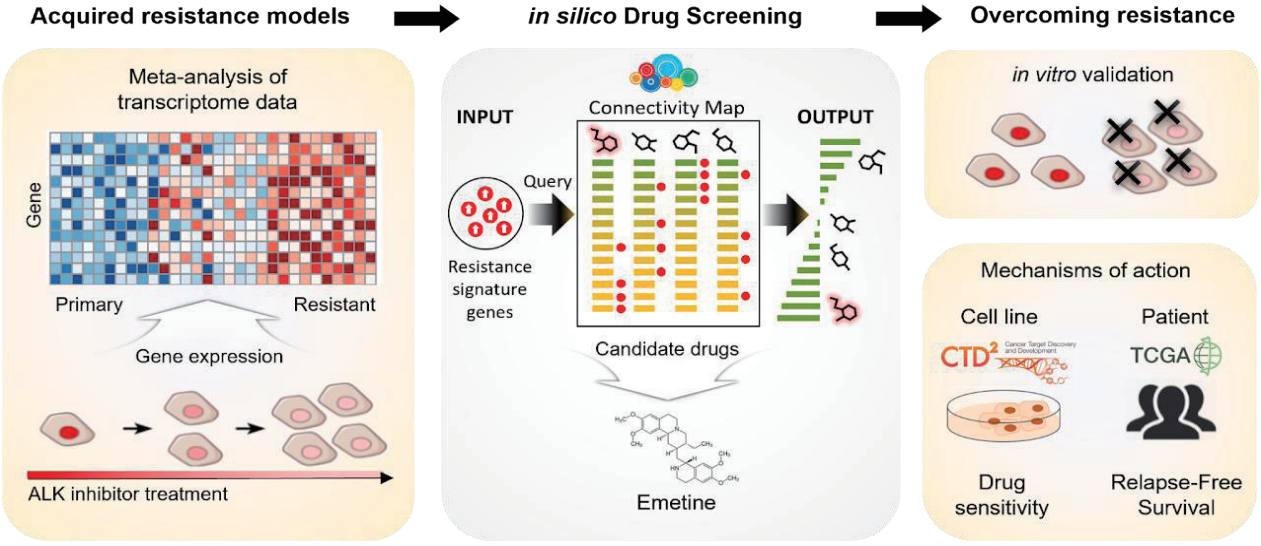
Harnessing transcriptomics for discovery of natural products to overcome acquired cancer resistance

Review | Published: 08 December 2025



Case 4: **Drug repositioning for acquired cancer resistance**



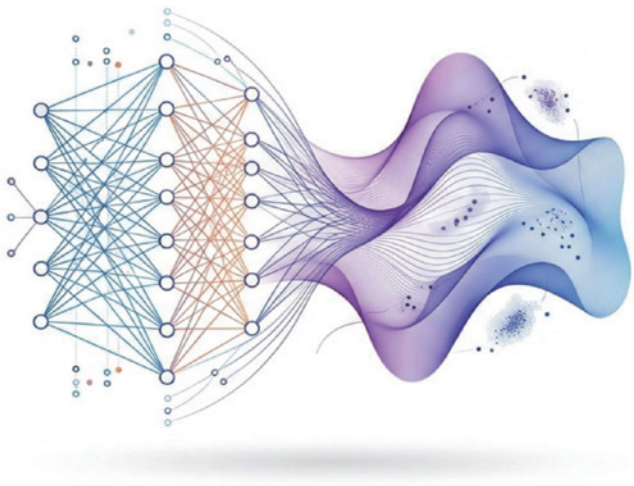
Molecular oncology (2024)

Integrative Transcriptomic Analysis Identifies Emetine as a Promising Candidate for Overcoming Acquired Resistance to ALK Inhibitors in Lung Cancer

Prof. Haeseung Lee

College of Pharmacy and
Research Institute for Drug Development,
Pusan National University

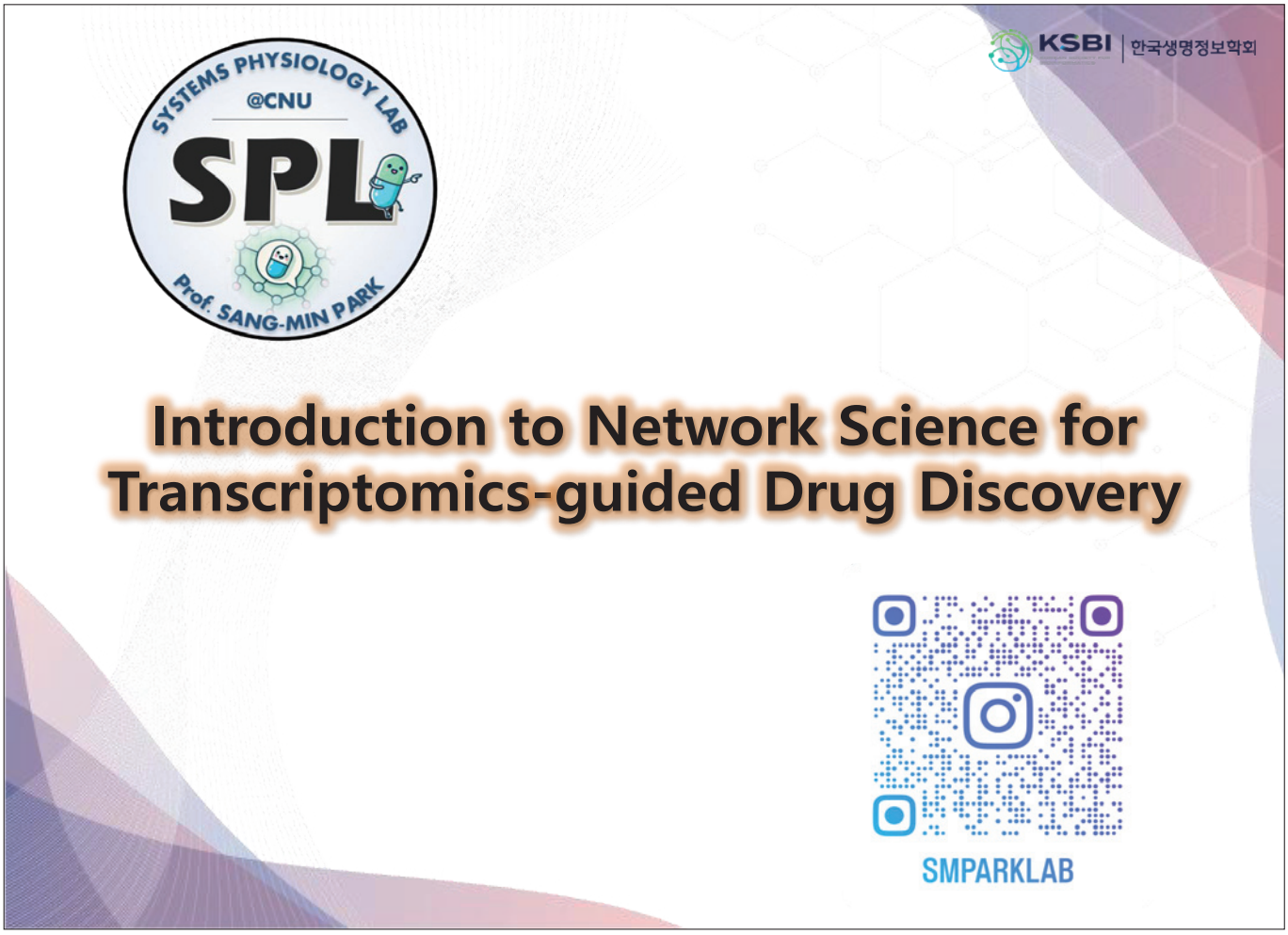
미래 전망: AI와 딥러닝의 통합



Latent Representations (잠재 표현):
수동 네트워크 기능 공학에서
'임베딩(Embeddings)' 학습으로 이동.

Deep Learning:
Graph Convolutional Networks
(GCNs)를 이용한 이질적인 데이터 융합.

LLMs & RAG:
거대 언어 모델(LLM)과 검색 증강 생성(RAG)을 활용하여 표현형(Phenotype)에 맞는 오믹스 데이터셋 자동 검색 및 가설 생성.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Introduction to Network Science for Transcriptomics-guided Drug Discovery
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