生物信息学与系统生物学

张世华

中国科学院数学与系统科学研究院

课程信息

- http://www.aporc.org/doc/wiki/Course001

- Contains all course-related materials (lecture slides & further readings), regularly updated.

课程信息

- 答疑&讨论: 课后或思源楼 1012/1003

- 对课程的意见和建议

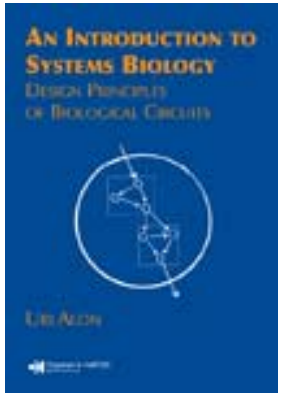
邮件：

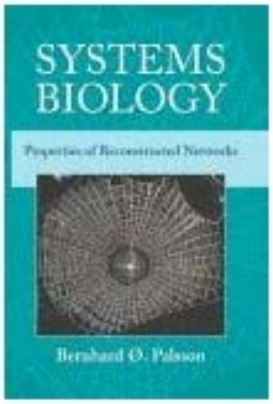
zsh@amss.ac.cn;

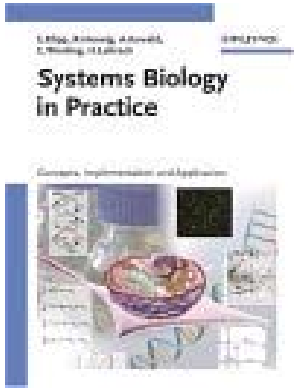
时间：2012.2.22---4.27，每周三、五下午13:30-16:10
地点: 中科院研究生院中关村教学楼N215教室

推荐书目

- An introduction to Systems Biology: Design Principles of Biological Circuits
  by Uri Alon.
  June 2006, Chapman&Hall/CRC, Taylor and Francis Group
- Systems Biology : Properties of Reconstructed Networks
  by Bernard Palsson.
  January 2006, published by Cambridge Univ. Press
- Systems Biology in Practice: Concepts, Implementation And Application
  Klipp, E et al. John Wiley & Sons Inc. 2005
- Systems Biology: A Textbook Edda Klipp, et al. 2009







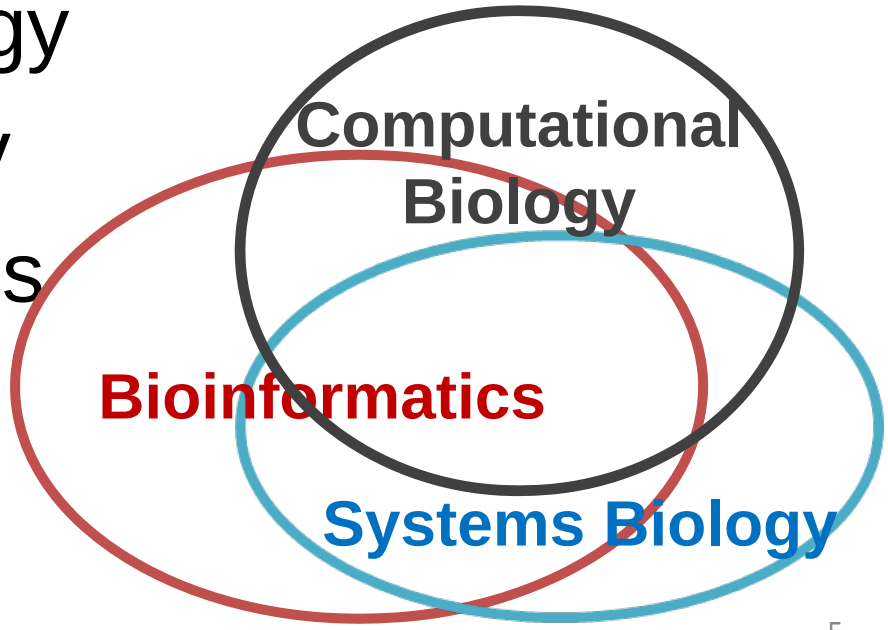
http://www.systems-biology.org

State-of-Arts

- Science, Nature, Cell, PNAS
- Molecular Systems Biology

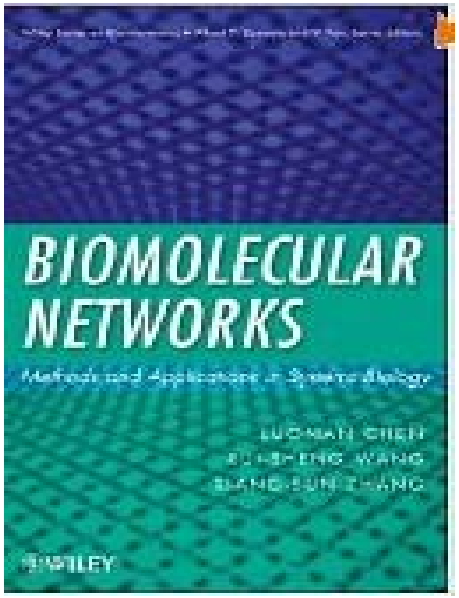
- BMC Systems Biology
- IET Systems Biology
- Other related journals

- Google, Wiki

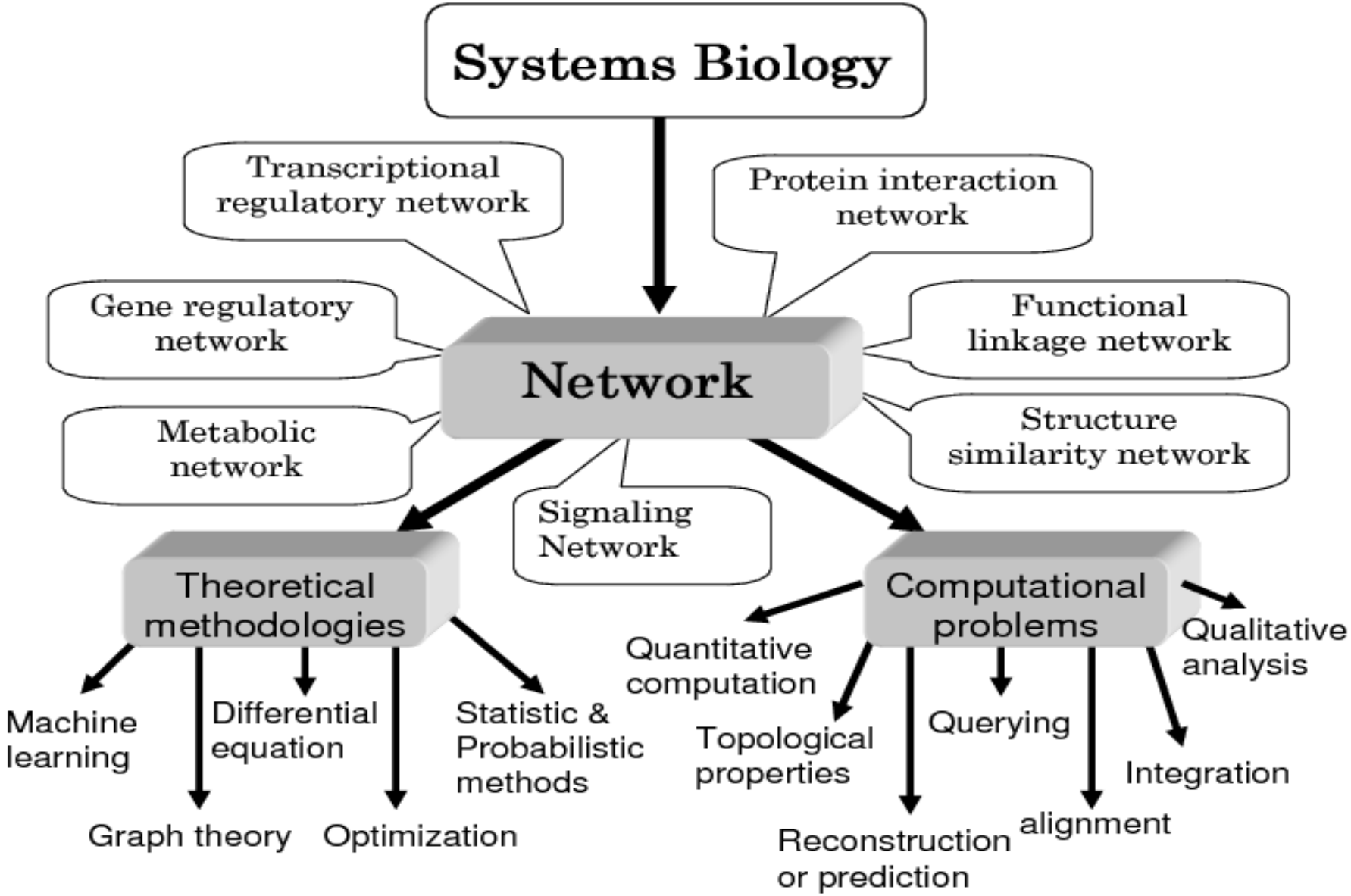


We focus on biomolecular networks

as well as highly related topics



Luonan Chen, Rui-Sheng Wang, Xiang-Sun Zhang.
Biomolecular Networks: Methods and Applications in Systems Biology. John Wiley & Sons, Hoboken, New Jersey. July, 2009.



Network Systems Biology


系统生物学

大纲

如何分析网络？（张世华）

1. 生物分子网络分析
2. 生物分子网络motif，　模块分析
3. 生物分子网络比对
4. 生物活性通路与网络标记物识别

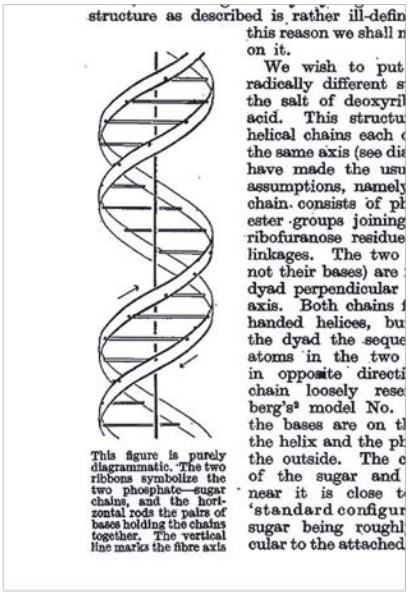
如何构建网络？（王勇）

1. 基因调控网络重建
2. 转录调控网络重建
3. 转录因子合作网络预测
4. 蛋白质相互作用网络预测


系统生物学

系统生物学

《Nature》1953



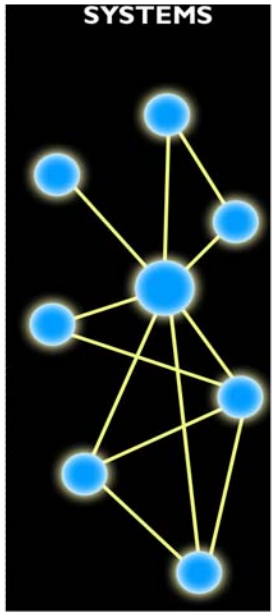
structure as described is rather ill-defin
this reason we shall n
on it.
We wish to put
radically different s
the salt of deoxyril
acid. This structu
helical chains each
the same axis (see di
have made the usu
assumptions, namely
chain consists of p
ester groups joining
ribofuranose residue
linkages. The two
not their bases) are
dyad perpendicular
axis. Both chains
handed helices, bu
the dyad the seque
atoms in the two
in opposite directi
chain loosely rese
berg's[3] model No.
the bases are on t
the helix and the p
the outside. The
of the sugar and
near it is close t
'standard configur
sugar being roughl
cular to the attached

This figure is purely diagrammatic. The two ribbons symbolize the two phosphate—sugar chains, and the horizontal rods the pairs of bases holding the chains together. The vertical line marks the fibre axis

DNA双螺旋结构发现，
开启分子生物学研究

《Science》2001

人类基因组计划完成



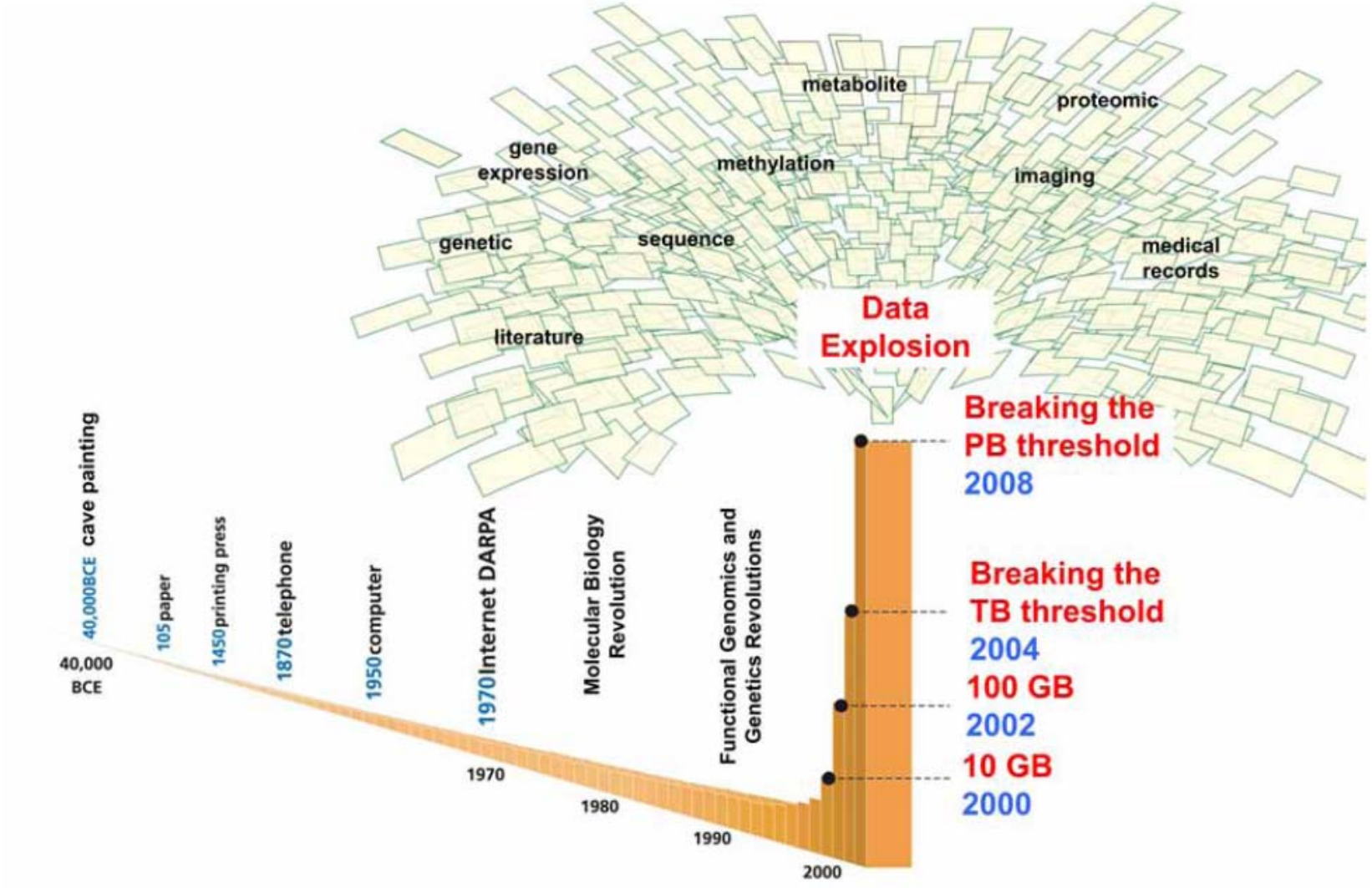
系统生物学

1950

1990

2002

生物信息学



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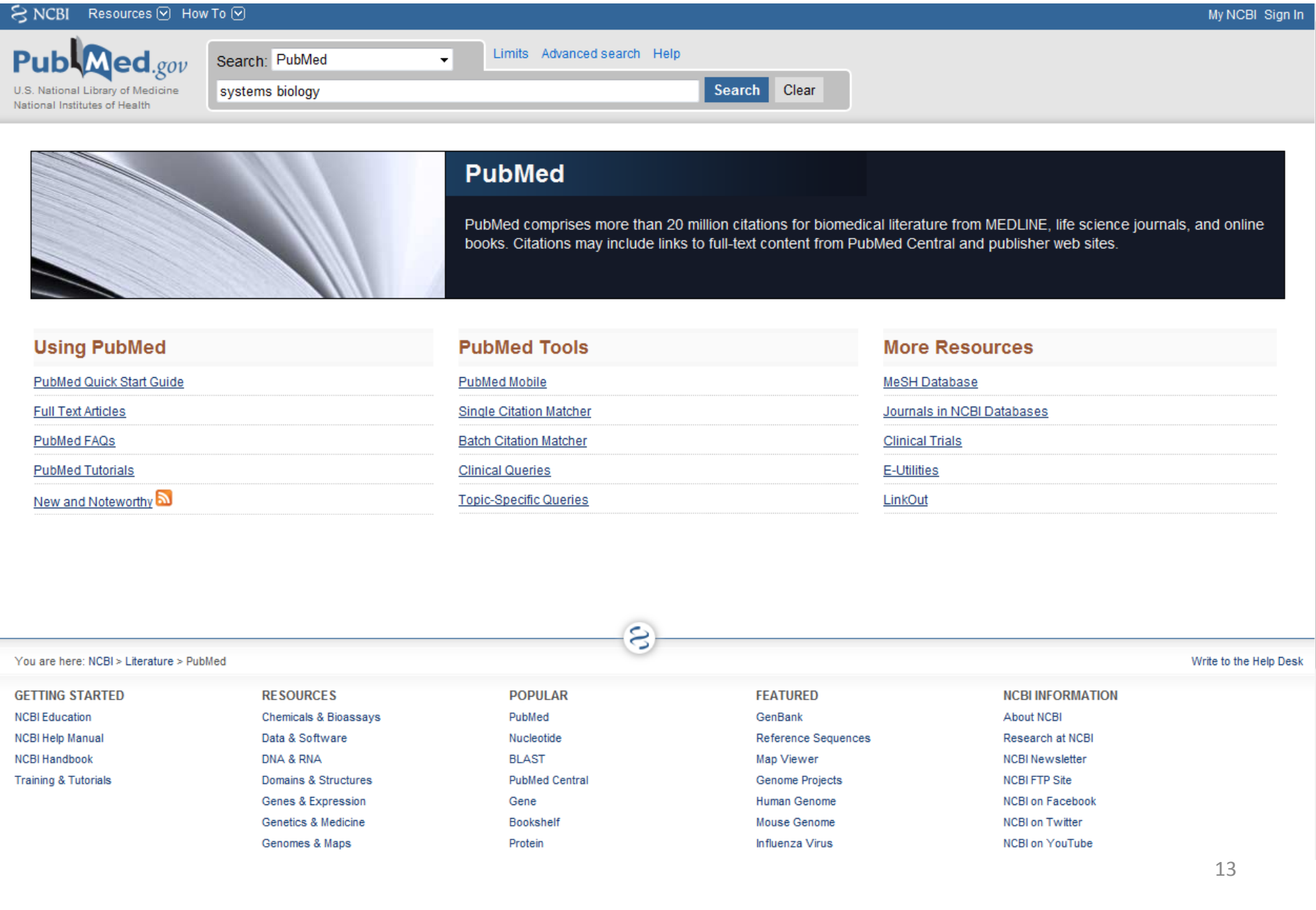
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Domains & Structures
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Genomes & Maps
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Bookshelf
Protein
FEATURED
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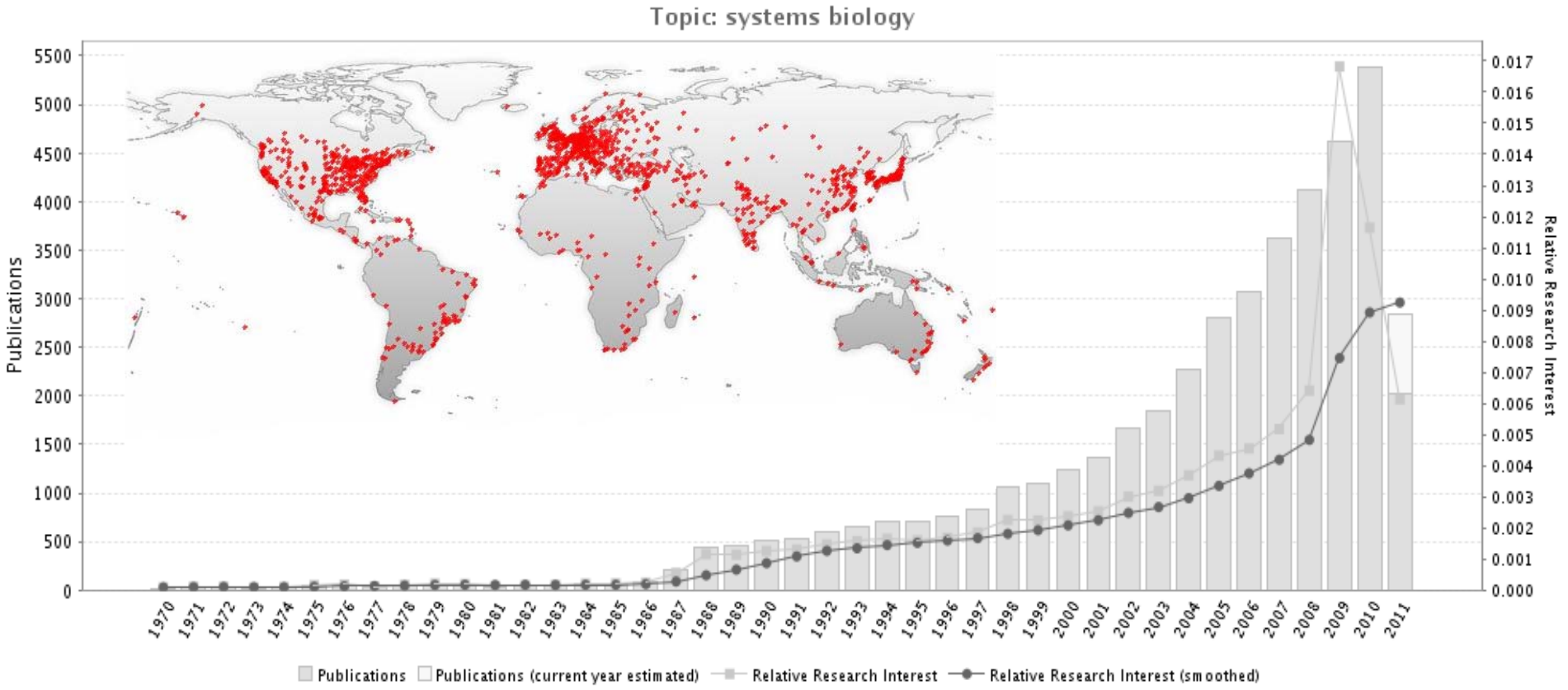
Topic: systems biology
Publications
Relative Research Interest
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
0.017
0.016
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1970 1971 1972 1973 1974 1975 1976 1977 1978 1979 1980 1981 1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997 1998 1999 2000 2001 2002 2003 2004 2005 2006 2007 2008 2009 2010 2011
Publications
Publications (current year estimated)
Relative Research Interest
Relative Research Interest (smoothed)

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小提示：只搜索中文(简体)结果，可在 学术搜索设置. 指定搜索语言

Systems biology: a brief overview — uu.nl 中的 [PDF]
H Kitano - Science, 2002 - sciencemag.org
Abstract To understand biology at the system level, we must examine the structure and dynamics of cellular and organismal function, rather than the characteristics of isolated parts of a cell or organism. Properties of systems, such as robustness, emerge as central issues, ...
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The systems biology markup language (SBML): a medium for representation and exchange of biochemical network models — oxfordjournals.org 中的 [PDF]
M Hucka, A Finney, HM Sauro, H Bolouri... - ..., 2003 - Oxford Univ Press
Abstract Motivation: Molecular biotechnology now makes it possible to build elaborate systems models, but the systems biology community needs information standards if models are to be shared, evaluated and developed cooperatively. Results: We summarize the ...
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H Kitano - Nature, 2002 - people.mbi.ohio-state.edu
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Evolving a lingua franca and associated software infrastructure for computational systems biology: the Systems Biology Markup Language (SBML) project — caltech.edu 中的 [PDF]
M Hucka, A Finney, BJ Bornstein... - Systems ..., 2004 - authors.library.caltech.edu
Biologists are increasingly recognising that computational modelling is crucial for making sense of the vast quantities of complex experimental data that are now being collected. The systems biology field needs agreed-upon informationstandards if models are to be shared ...
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A new approach to decoding life: systems biology — buscario.com.br 中的 [PDF]
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▪ Abstract Systems biology studies biological systems by systematically perturbing them (biologically, genetically, or chemically); monitoring the gene, protein, and informational pathway responses; integrating these data; and ultimately, formulating mathematical ...
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The protein data bank HM Berman, J Westbrook, Z Feng, G Gilliland, TN Bhat, H Weissig, IN ... Nucleic acids research 28 (1), 235-242	13295	2000
Protein structure alignment by incremental combinatorial extension (CE) of the optimal path. IN Shindyalov, PE Bourne Protein engineering 11 (9), 739-747	1516	1998
The protein data bank HM Berman, T Battistuz, TN Bhat, WF Bluhm, PE Bourne, K Burkhardt, Z Feng ... Acta Crystallographica Section D: Biological Crystallography 58 (6), 899-907	686	2002
The RCSB Protein Data Bank: a redesigned query system and relational database based on the mmCIF schema		

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Title / Author	Cited by	Year
Identification of overlapping community structure in complex networks using fuzzy c-means clustering S Zhang, RS Wang, XS Zhang Physica A: Statistical Mechanics and its Applications 374 (1), 483-490	141	2007
Quantitative function for community detection Z Li, S Zhang, RS Wang, XS Zhang, L Chen Physical Review E 77 (3), 036109	67	2008
Discovering functions and revealing mechanisms at molecular level from biological networks S Zhang, G Jin, XS Zhang, L Chen Proteomics 7 (16), 2856-2869	57	2007
Alignment of molecular networks by integer quadratic programming Z Li, S Zhang, Y Wang, XS Zhang, L Chen Bioinformatics 23 (13), 1631-1639	55	2007
Uncovering fuzzy community structure in complex networks S Zhang, RS Wang, XS Zhang	41	2007

h-index

h-index，又称为h指数或h因子（h-factor），是一种评价学术成就的新方法。h代表“高引用次数”（high citations），一名科研人员的h指数是指他至多有h篇论文分别被引用了至少h次。h指数能够比较准确地反映一个人的学术成就。一个人的h指数越高，则表明他的论文影响力越大

什么是系统生物学？

- 内涵？
- 外延？
- 问题？

Systems Biology

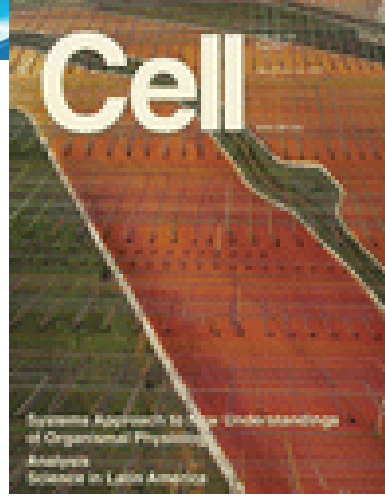
- Networking the whole biological system, rather than studying its isolated parts.

- Integrating large amounts of data in the context of biological network (Sequence, structure, function, gene expression, protein expression, protein interaction, protein-DNA interaction, and literature data).

Systems Biology——Procedure

- System Perturbation
- Generating of comprehensive global data
- Identification of key molecules
- Network modelling
- Generation of hypotheses
- Validation of hypotheses

- Journal club



A Predictive Model for Transcriptional Control of Physiology in a Free Living Cell

Richard Bonneau et. al. Cell, Vol 131, 1354-1365, 28 Dec. 2007

Institute for Systems Biology, Seattle, WA 98103, USA
Center for Genomics & Systems Biology, New York University, New York, NY 10003, USA

On the cover:

Brightly colored blooms of halophlic (喜盐的) organisms in the salt flats of the South San Francisco Bay (photograph by Michael Melford, courtesy Getty Images) serve as a vibrant backdrop(背景) for a segment of a predictive environmental and gene regulatory circuit determined for one of this ecosystem's principal inhabitants, the archaeon(古代生物) Halobacterium salinarium NRC-1(一种嗜盐的古生菌，一般只生存在盐水池塘或是盐湖中).

This organism possesses **a number of fascinating adaptations** for life in hypersaline (高盐) environments including the **production of membrane pigments** (细胞膜上产生色素) that mediate light-driven energy production and **flotation devices** called gas vesicles for vertical mobility in search of favorable oxic regimes (氧载体). While the availability of unique adaptations is important, the integrated regulation of these and many other core physiological processes (生理学过程) is vital for survival in this dynamic environment.

In this issue,

Bonneau et al. report a systems level regulatory circuit for the transcriptional control of **80% of all genes** in this organism. This regulatory model accurately predicts the transcriptional changes that occur when Halobacterium is challenged with **new environmental** and **genetic perturbations**.

Significantly, this study supports the claim that fundamental properties of biological systems and their environments should enable the rapid construction of highly accurate, predictive models of global gene regulation for both traditional model systems and for many more currently uncharacterized organisms.

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- Physiology
- Plant Biology
- Psychiatry
- Public Health & Epidemiology
- Renal Biology

Other comments

- **Research Highlight by *Nature Reviews Microbiology* 6, 92 (February 2008)**

- **Bio-IT World's Systems Biology newsletter.**(In the closing days to 2007, a really nice piece of systems biology work was published in the journal *Cell*)

Why this paper

- **Cell** publish computational biology work
- From Institute for Systems Biology, Seattle
- The ISB founder, also the founder of systems biology Lee Hood is one of the co-authors.
- To taste the flavor of systems biology **(network+perturbation+data integration)**

What did they study?

- A largely uncharacterized organisms
- Easy to be cultured
- The environment significantly influences the dynamic expression

Methodology

- Experiments:

1. Microarray data: Total 413 experiments (Time-course and steady state, 8 environment effects perturbation, combinatorial perturbation. 33 gene deletion and GTF overexpression)

   266 experiments in training set

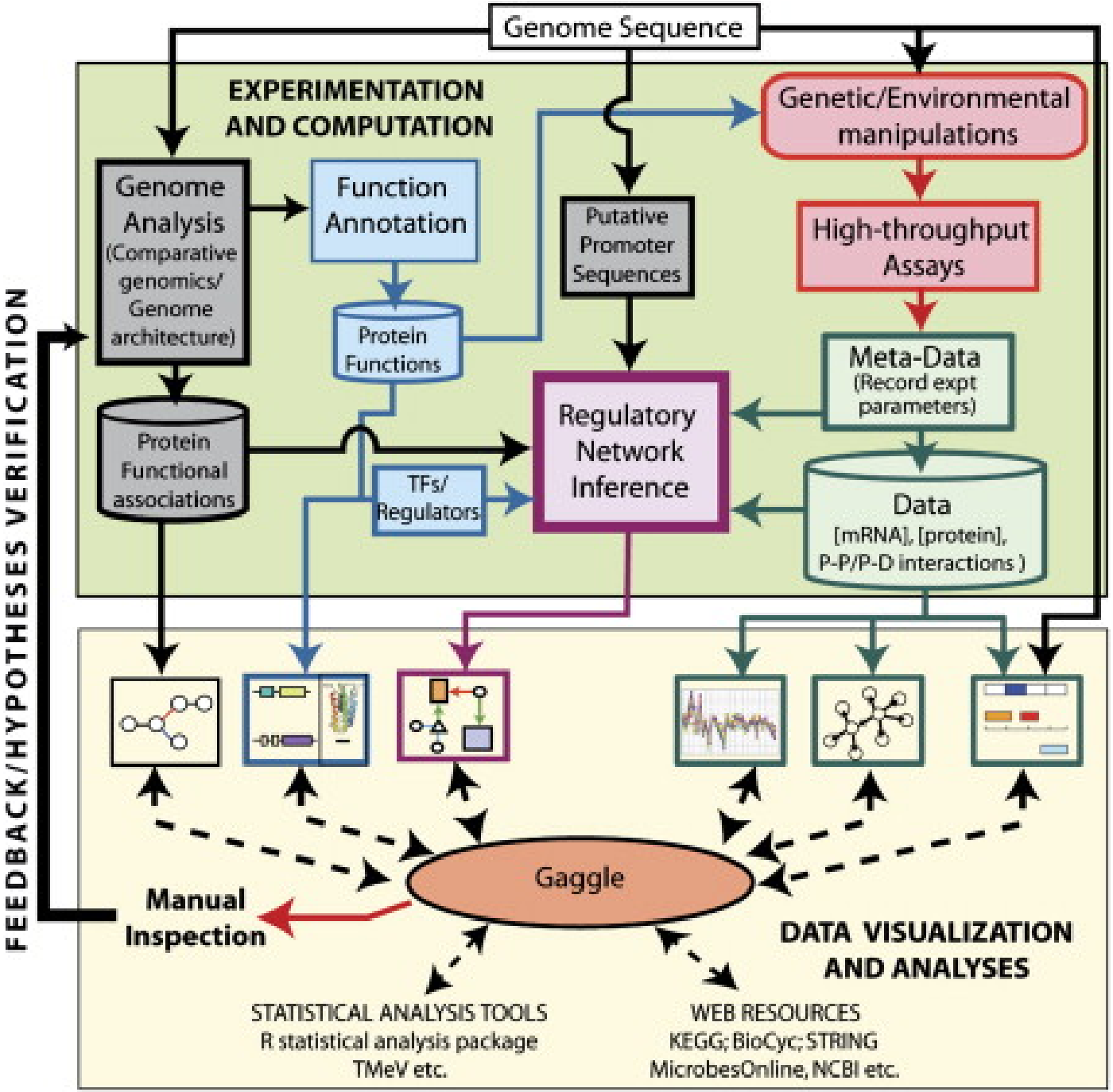
   147 new experiments

2. ChIP-chip data

http://baliga.systemsbiology.net/egrin.php

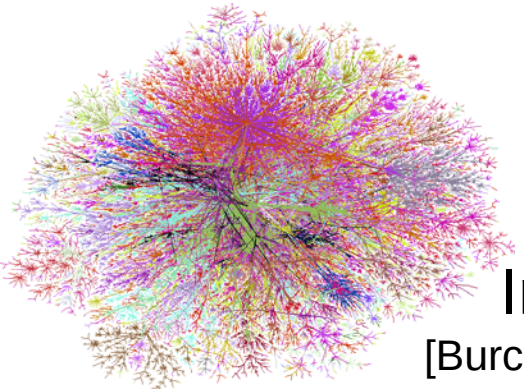
- Computational prediction

1. Protein structure prediction
2. Function annotation algorithm
3. Biclustering algorithm (Data integration and dimensionality reduction)
4. Transcriptional regulatory network inference

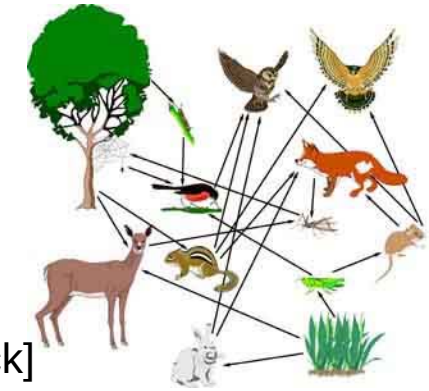

Genome Sequence
EXPERIMENTATION AND COMPUTATION
Genetic/Environmental manipulations
Genome Analysis (Comparative genomics/ Genome architecture)
Function Annotation
Putative Promoter Sequences
High-throughput Assays
Protein Functions
Meta-Data (Record expt parameters)
Protein Functional associations
Regulatory Network Inference
TFs/ Regulators
Data [mRNA], [protein], P-P/P-D interactions)
FEEDBACK/HYPOTHESES VERIFICATION
Gaggle
Manual Inspection
DATA VISUALIZATION AND ANALYSES
STATISTICAL ANALYSIS TOOLS
R statistical analysis package
TMeV etc.
WEB RESOURCES
KEGG; BioCyc; STRING
MicrobesOnline, NCBI etc.

网络生物学

Networks as a universal language

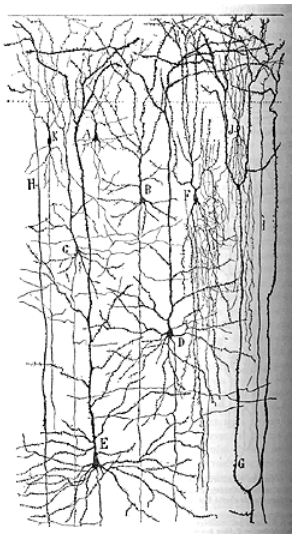


Internet
[Burch & Cheswick]

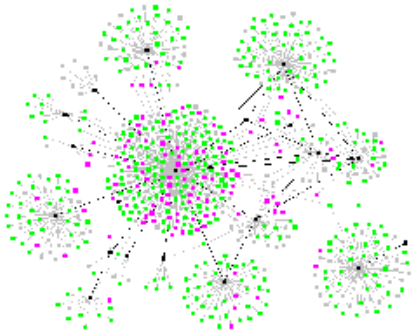


Food Web

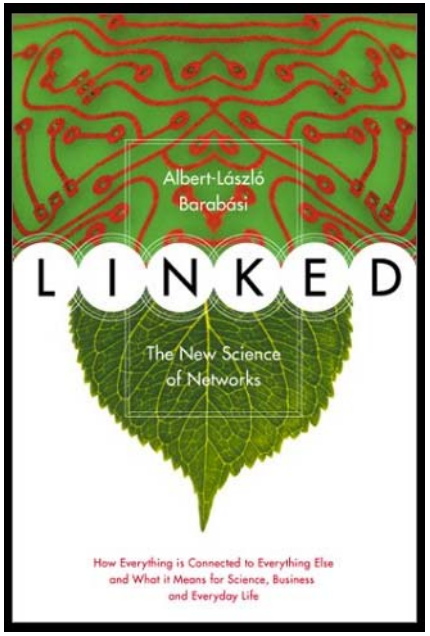
Electronic Circuit



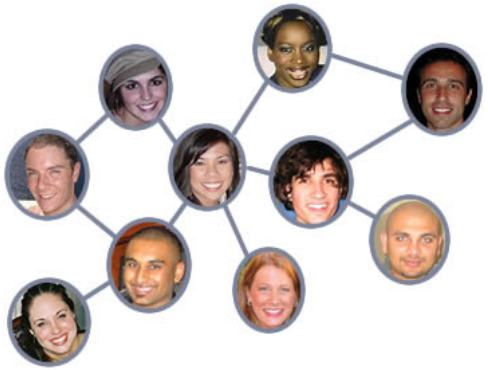
Neural Network
[Cajal]



Disease Spread
[Krebs]



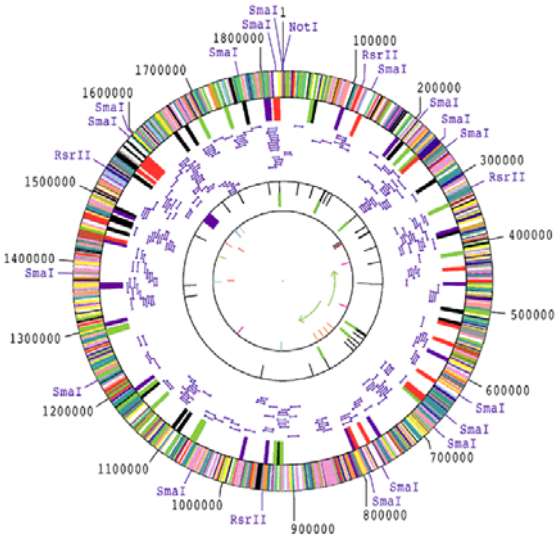
Protein Interactions
[Barabasi]



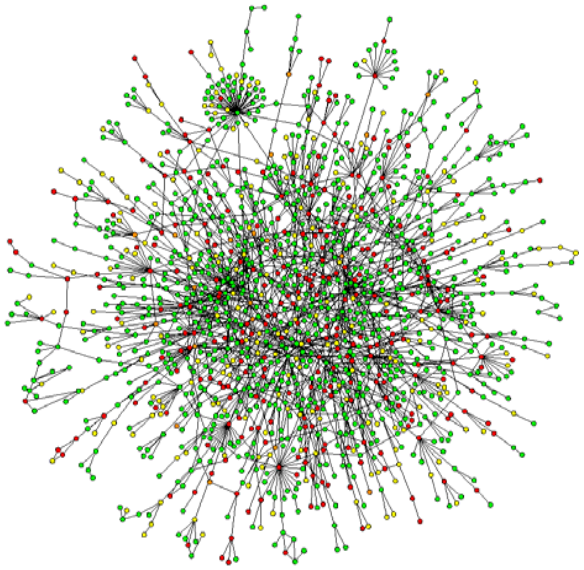
Social Network

生物分子网络

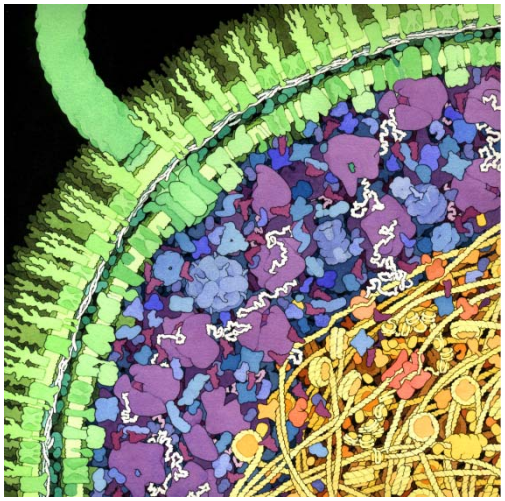
- 图作为基本工具用来强调相互作用并直观表示复杂的生物系统
- 节点代表生物分子，边代表他们之间在生命过程中的某种关系



1D: Complete Genetic Partslist



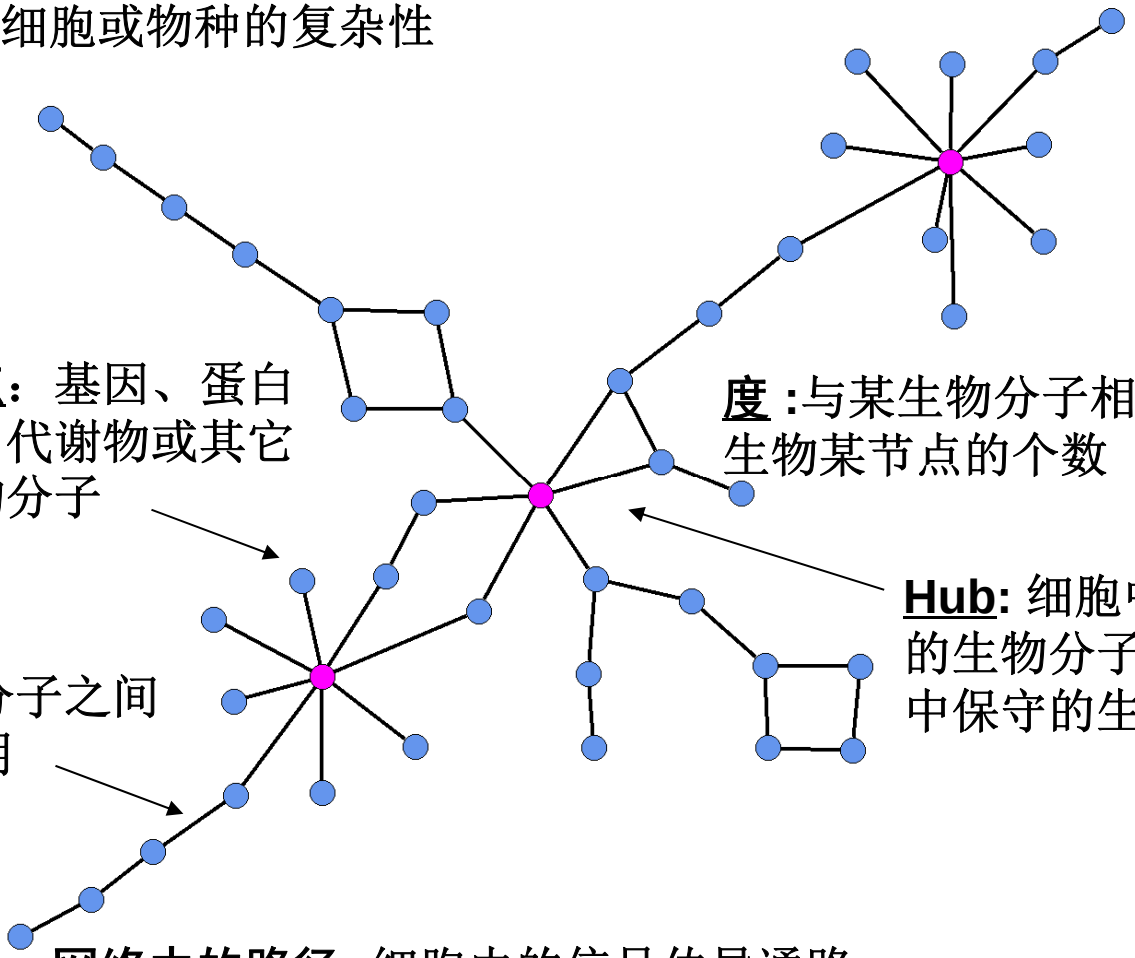
~2D: Bio-molecular Network



3D: Detailed structural understanding of cellular machinery

生物学语言下的网络

网络规模:细胞或物种的复杂性



节点：基因、蛋白质、代谢物或其它生物分子

度 :与某生物分子相互作用的其它生物某节点的个数

Hub: 细胞中具有重要功能的生物分子，或者是进化中保守的生物分子

边：生物分子之间的相互作用

网络中的路径: 细胞内的信号传导通路

At molecular level

Emerging area

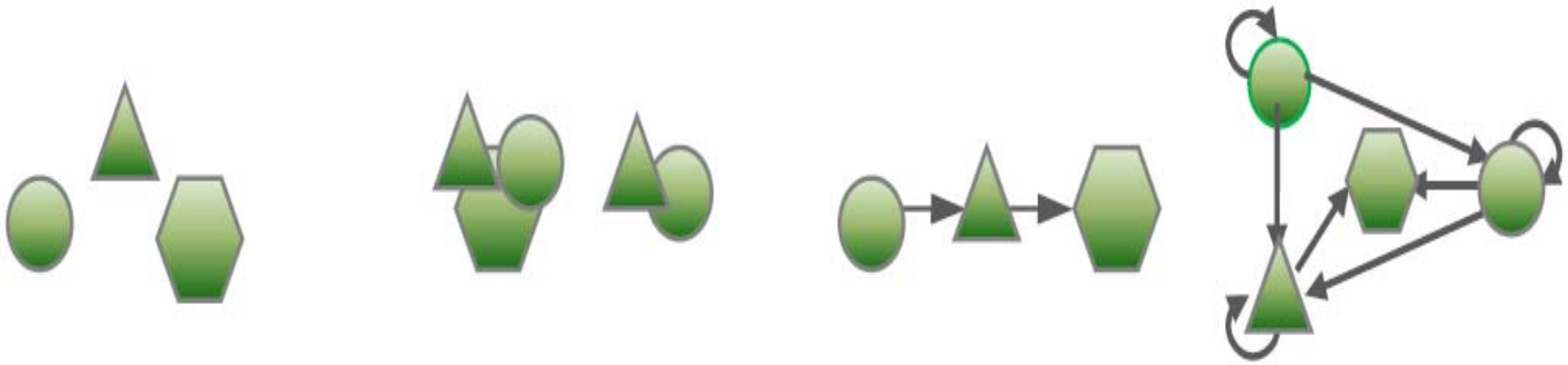
Network Systems Biology?

Instead of analyzing individual components or aspects of an organism,

We study how an organism, viewed as a **dynamical network** of biomolecules and biochemical reactions, eventually gives rise to a complex life.

Main ingredients?

Molecules **Interactions** **Pathways** **Networks**



Individual molecules ⇨ Pairwise interactions ⇨ Local structures ⇨ Global networks

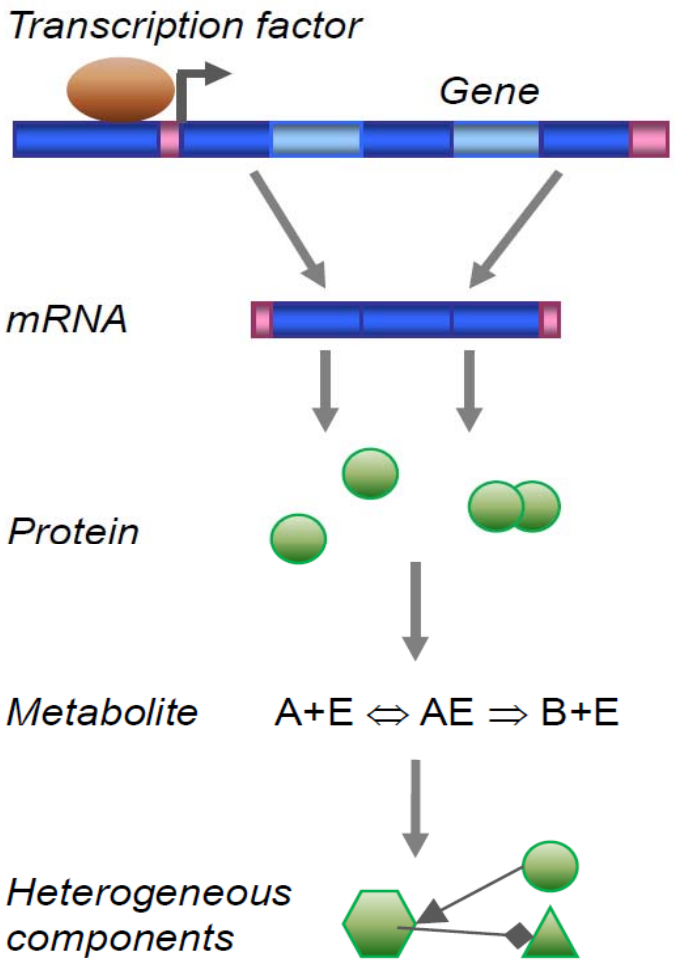
Local → Global

Hierarchical Relations

Biological networks

- Elements: gene, proteins, etc. Node
- Interactions: Regulation, physical interaction, genetic interaction, metabolic reaction, modification, etc. Edges
- Local structures: Motif, community, functional module, complex, etc.
- Global structures: Scale-free, small world, etc.

Biological networks



Transcription regulatory network
(DNA-TF interactions)

Gene regulatory network
(gene-gene interactions)

Protein interaction network
(protein-protein interactions)

Metabolic network
(enzyme-substrate interactions)

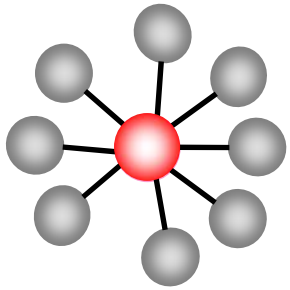
Signaling network
(molecule-molecule interactions)

Central Dogma of Biology

Molecules vs. **Networks**

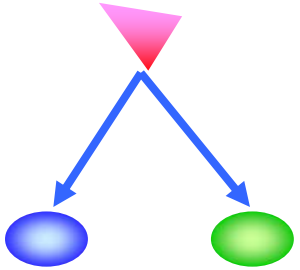
Types of Biological networks

Genetic network: Interactions between genes, gene products, small molecules
Transcriptional regulatory network: Network of control decisions to turn genes on / off, Subset of genetic network
Signal transduction network: Network of the movement of signals from outside the cell to inside.



Undirected

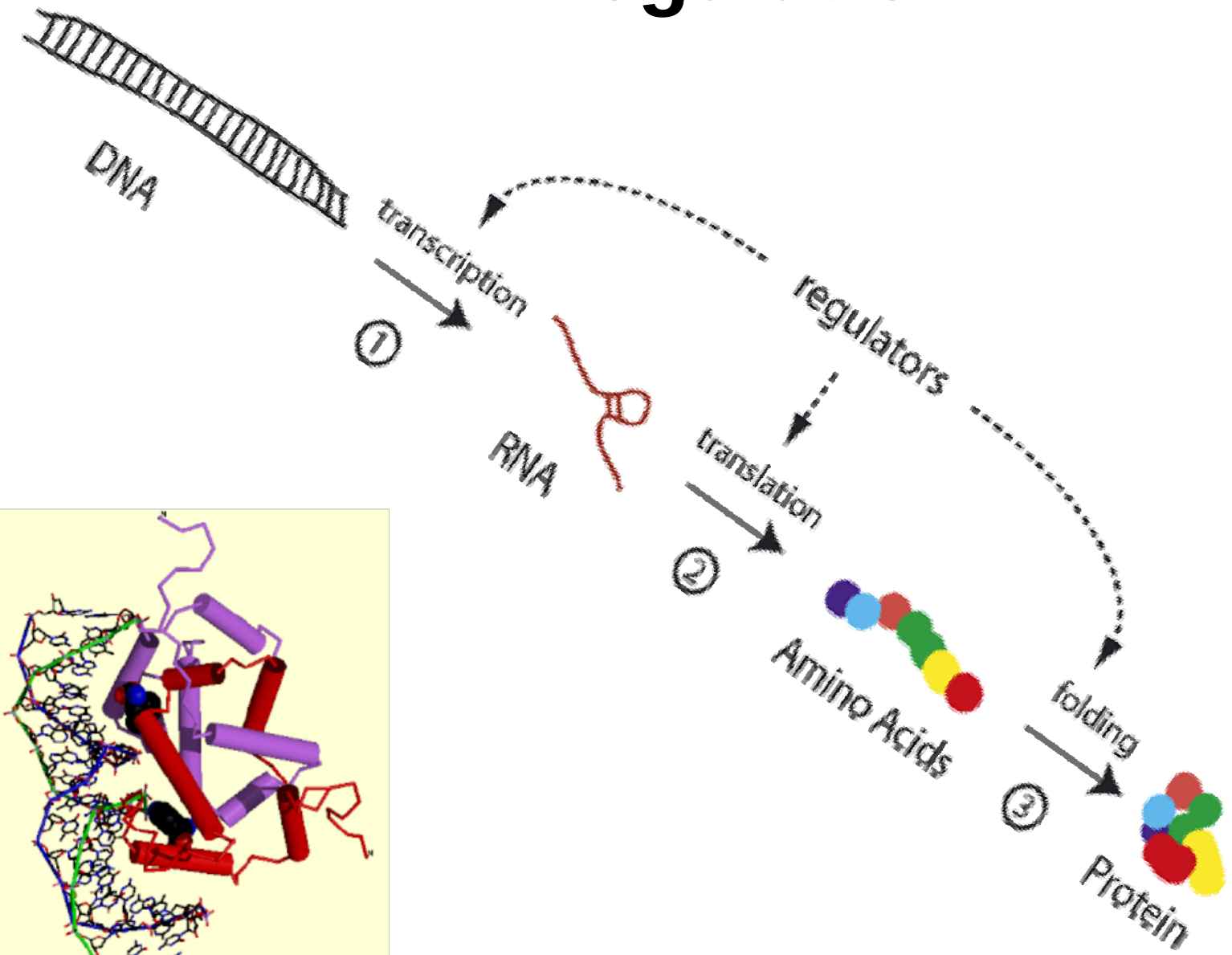
Protein-protein interaction network: Physical or genetic network
Metabolic network: Network of interactions between proteins, Synthesize / break down molecules (enzymes, cofactors)



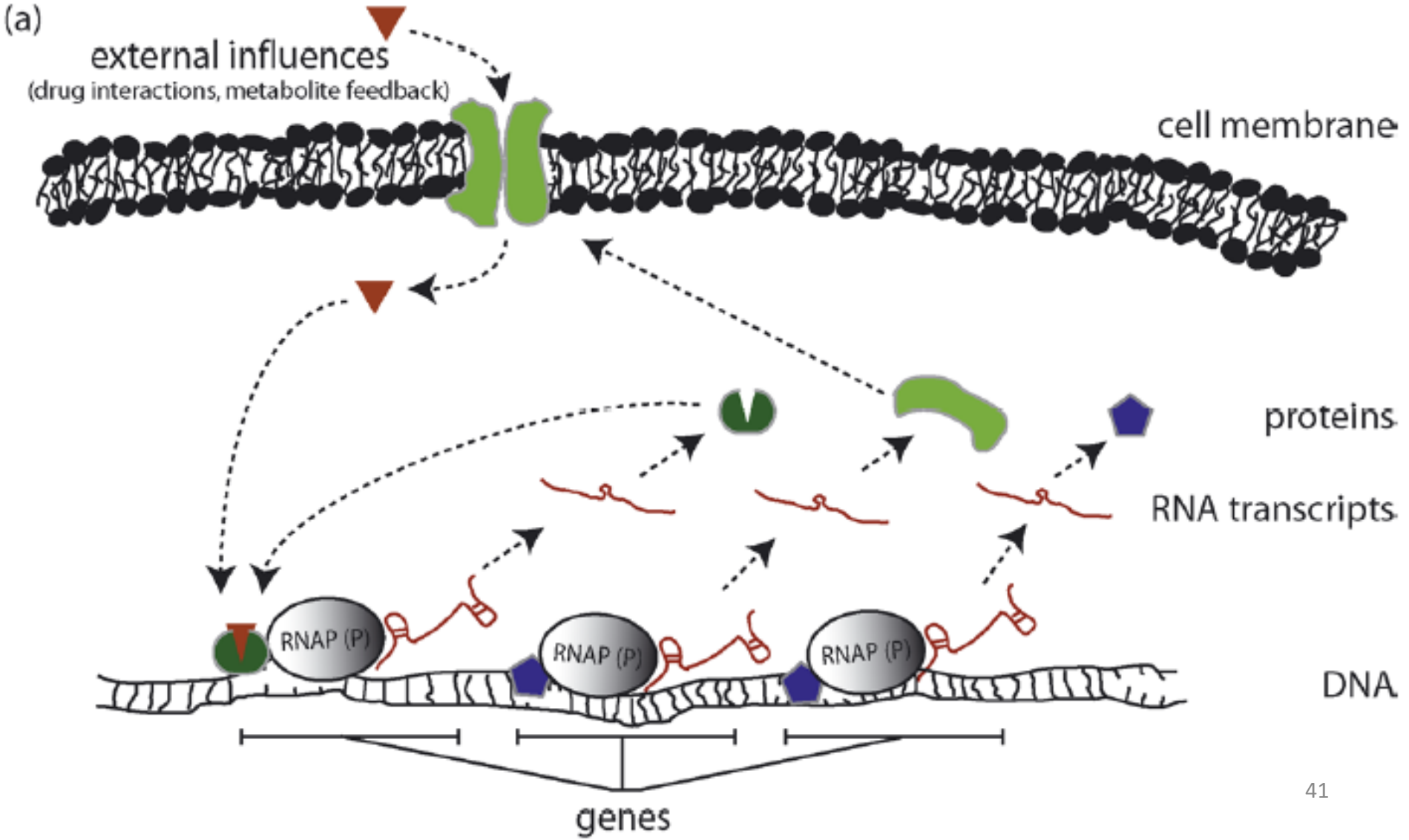
Directed

Others: Gene co-expression network, Functional linkage network, protein structure network, protein folding network, neural network, Domain interaction network

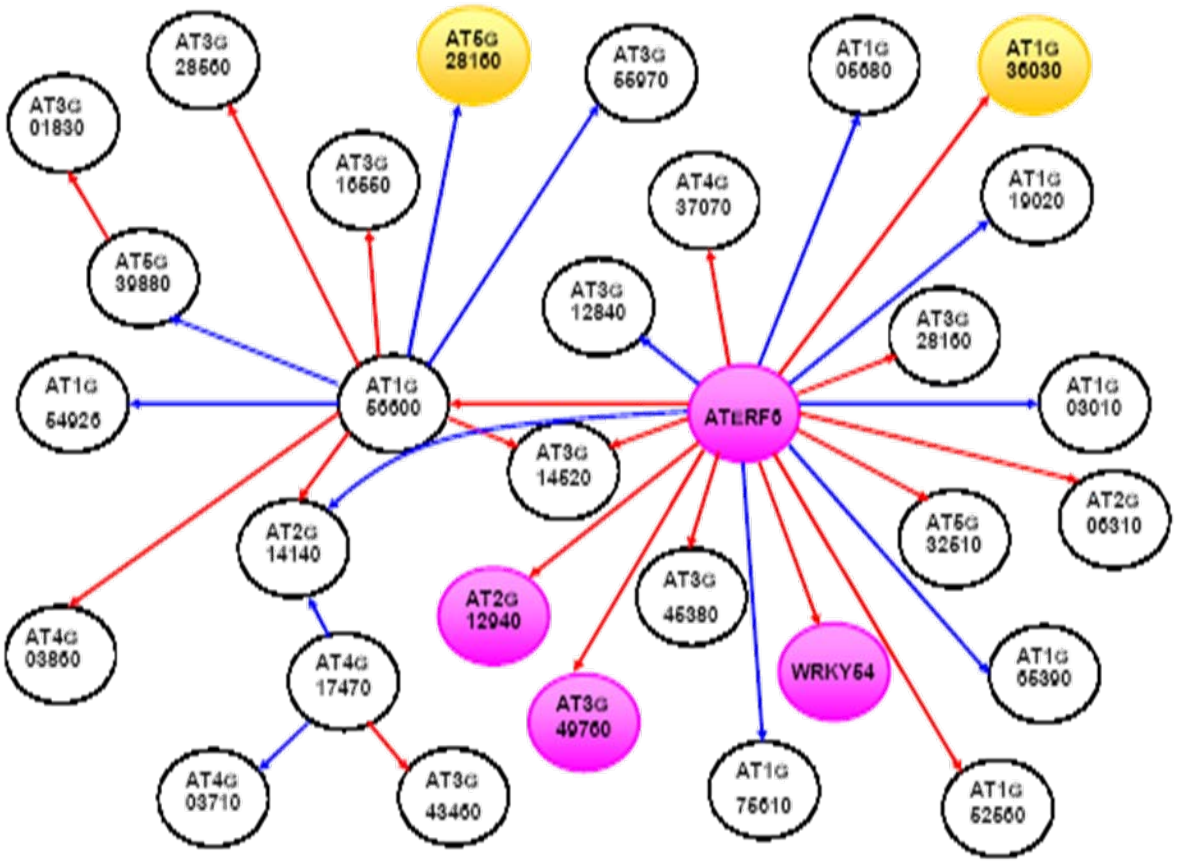
Regulation


DNA
transcription
regulators
RNA
translation
Amino Acids
folding
Protein

Direct and indirect regulation



Genetic network



Node: gene

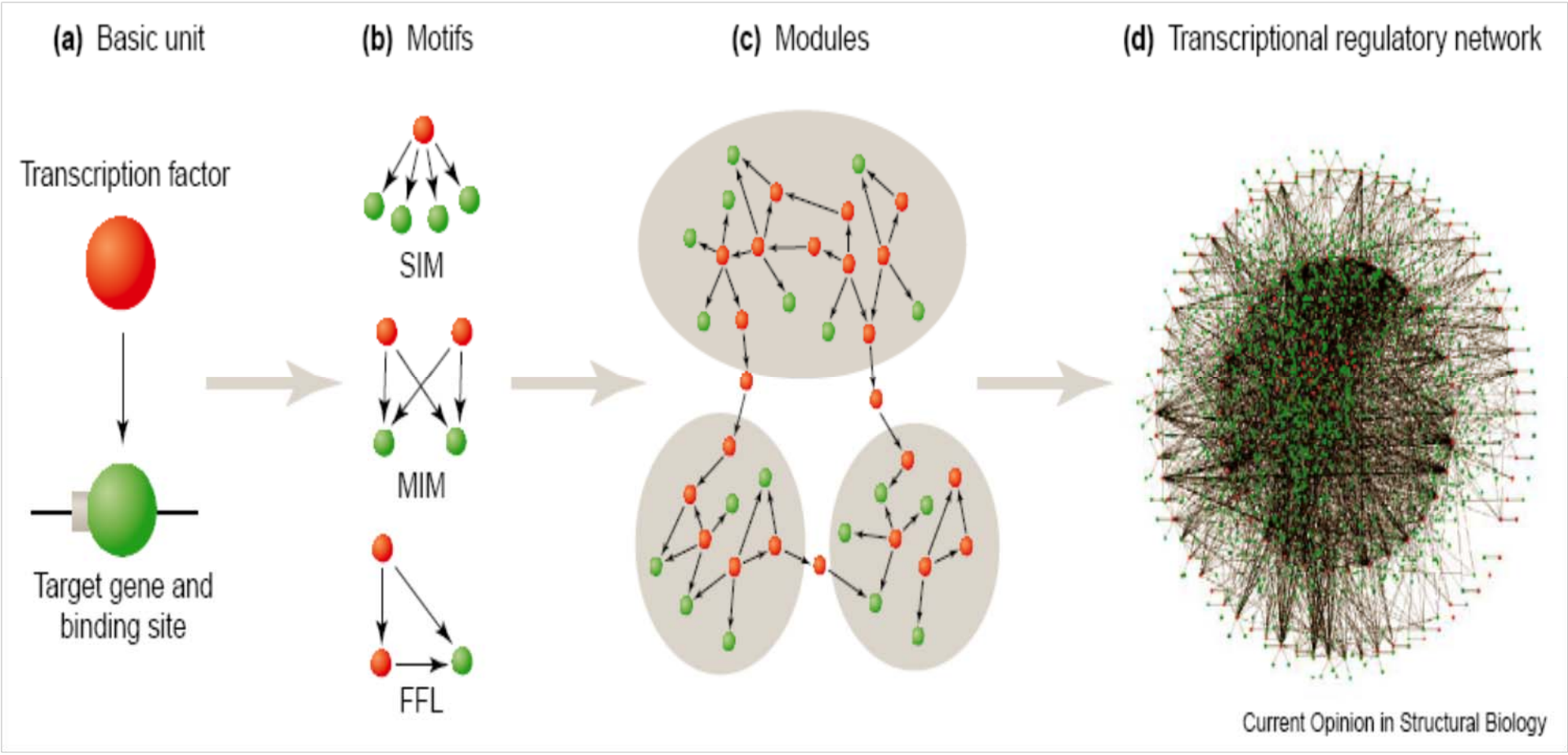
Edge: causality regulatory relationships

Directed

Edge weighted

Genetic network consists of set of genes, proteins, small molecules, and their mutual regulatory interactions。

Transcriptional regulatory network

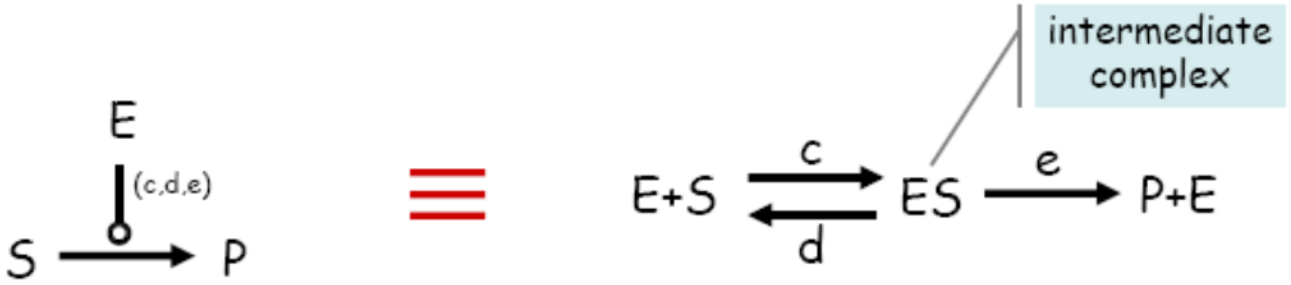


Subset of genetic network

Node: TF and genes, Edge: regulation relationships
Directed, Edge weighted

Enzymatic Reactions

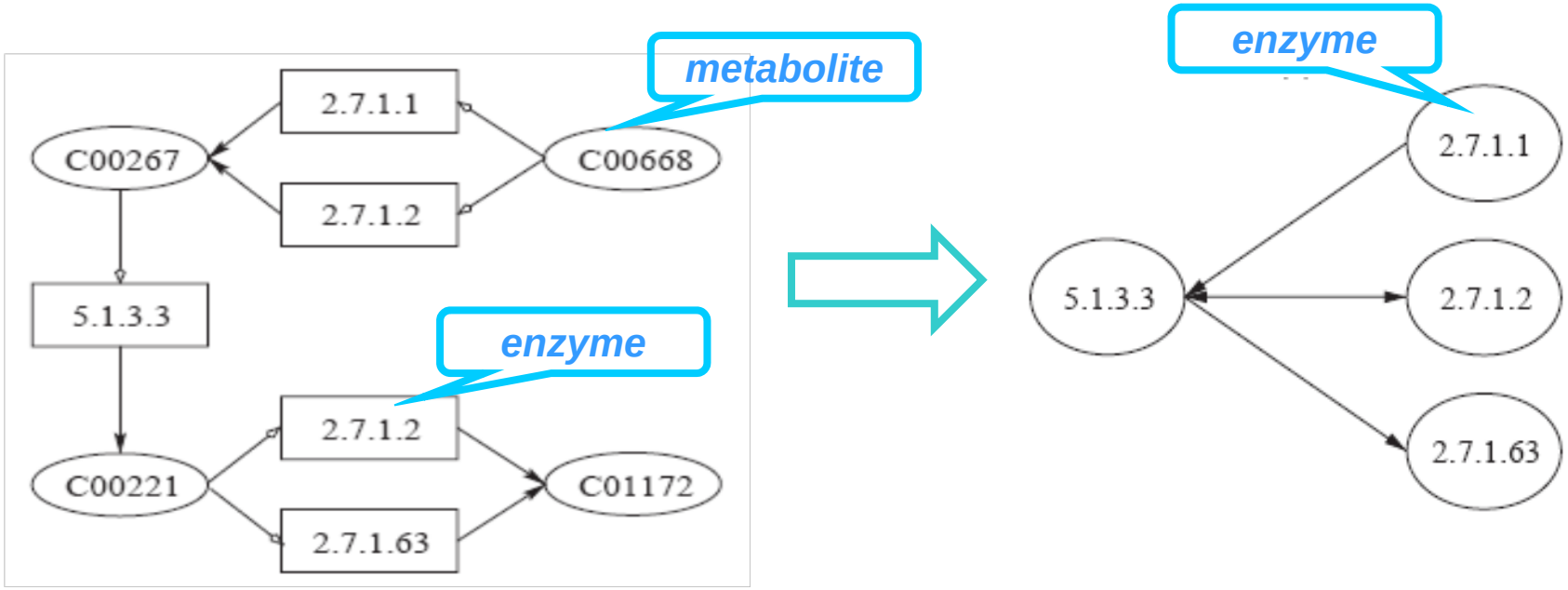
Reaction View

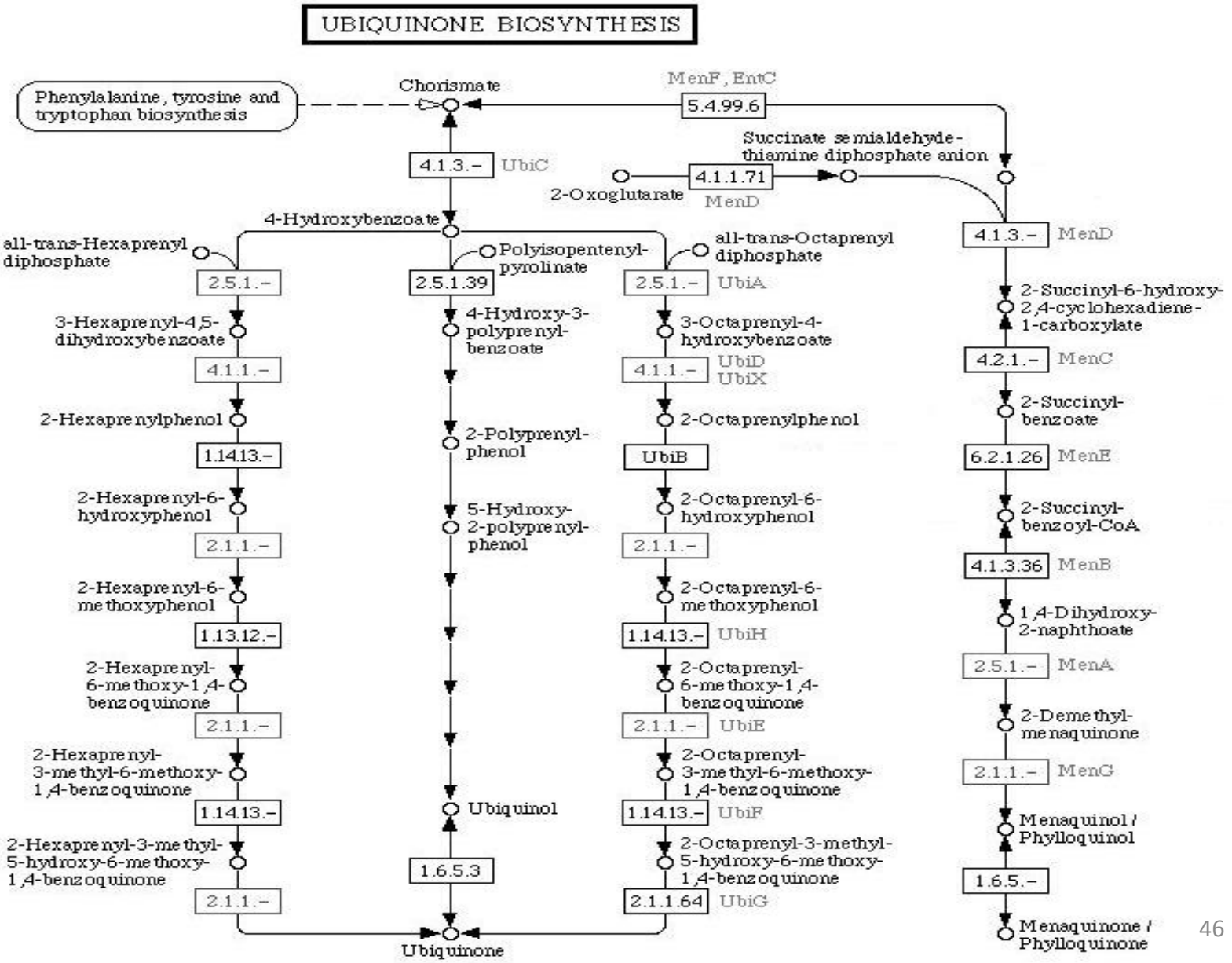


- **Definition of Metabolic network G*(V,E)* :**
  - **For every enzyme z_i in Z - a node v_i exists**
  - **(v_i,v_j) in E iff z_j consumes the product of z_i**

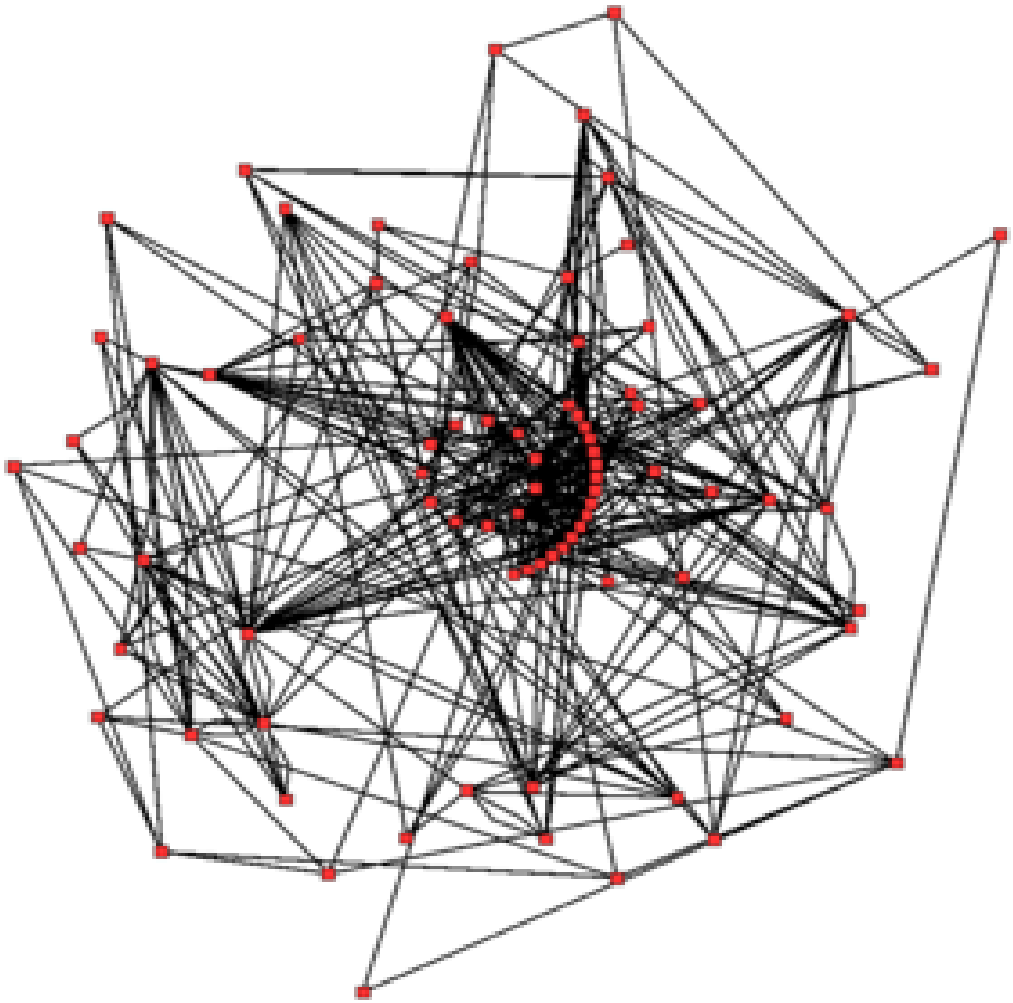
  酶A的一个产物是酶B 的一个底物

- **Example:**




UBIQUINONE BIOSYNTHESIS
Phenylalanine, tyrosine and tryptophan biosynthesis
Chorismate
MenF, EntC
5.4.99.6
4.1.3.– UbiC
Succinate semialdehyde-thiamine diphosphate anion
2-Oxoglutarate
4.1.1.71 MenD
4-Hydroxybenzoate
all-trans-Hexaprenyl diphosphate
Polyisopentenyl-pyrolinate
all-trans-Octaprenyl diphosphate
2.5.1.–
2.5.1.39
2.5.1.– UbiA
4.1.3.– MenD
3-Hexaprenyl-4,5-dihydroxybenzoate
4-Hydroxy-3-polyprenyl-benzoate
3-Octaprenyl-4-hydroxybenzoate
2-Succinyl-6-hydroxy-2,4-cyclohexadiene-1-carboxylate
4.1.1.–
4.1.1.– UbiD UbiX
4.2.1.– MenC
2-Hexaprenylphenol
2-Polyprenyl-phenol
2-Octaprenylphenol
2-Succinyl-benzoate
1.14.13.–
UbiB
6.2.1.26 MenE
2-Hexaprenyl-6-hydroxyphenol
5-Hydroxy-2-polyprenyl-phenol
2-Octaprenyl-6-hydroxyphenol
2-Succinyl-benzoyl-CoA
2.1.1.–
2.1.1.–
4.1.3.36 MenB
2-Hexaprenyl-6-methoxyphenol
2-Octaprenyl-6-methoxyphenol
1,4-Dihydroxy-2-naphthoate
1.13.12.–
1.14.13.– UbiH
2.5.1.– MenA
2-Hexaprenyl-6-methoxy-1,4-benzoquinone
2-Octaprenyl-6-methoxy-1,4-benzoquinone
2-Demethyl-menaquinone
2.1.1.–
2.1.1.– UbiE
2.1.1.– MenG
2-Hexaprenyl-3-methyl-6-methoxy-1,4-benzoquinone
2-Octaprenyl-3-methyl-6-methoxy-1,4-benzoquinone
Menaquinol / Phylloquinol
1.14.13.–
Ubiquinol
1.14.13.– UbiF
1.6.5.–
2-Hexaprenyl-3-methyl-5-hydroxy-6-methoxy-1,4-benzoquinone
1.6.5.3
2-Octaprenyl-3-methyl-5-hydroxy-6-methoxy-1,4-benzoquinone
2.1.1.–
2.1.1.64 UbiG
Menaquinone / Phylloquinone
Ubiquinone

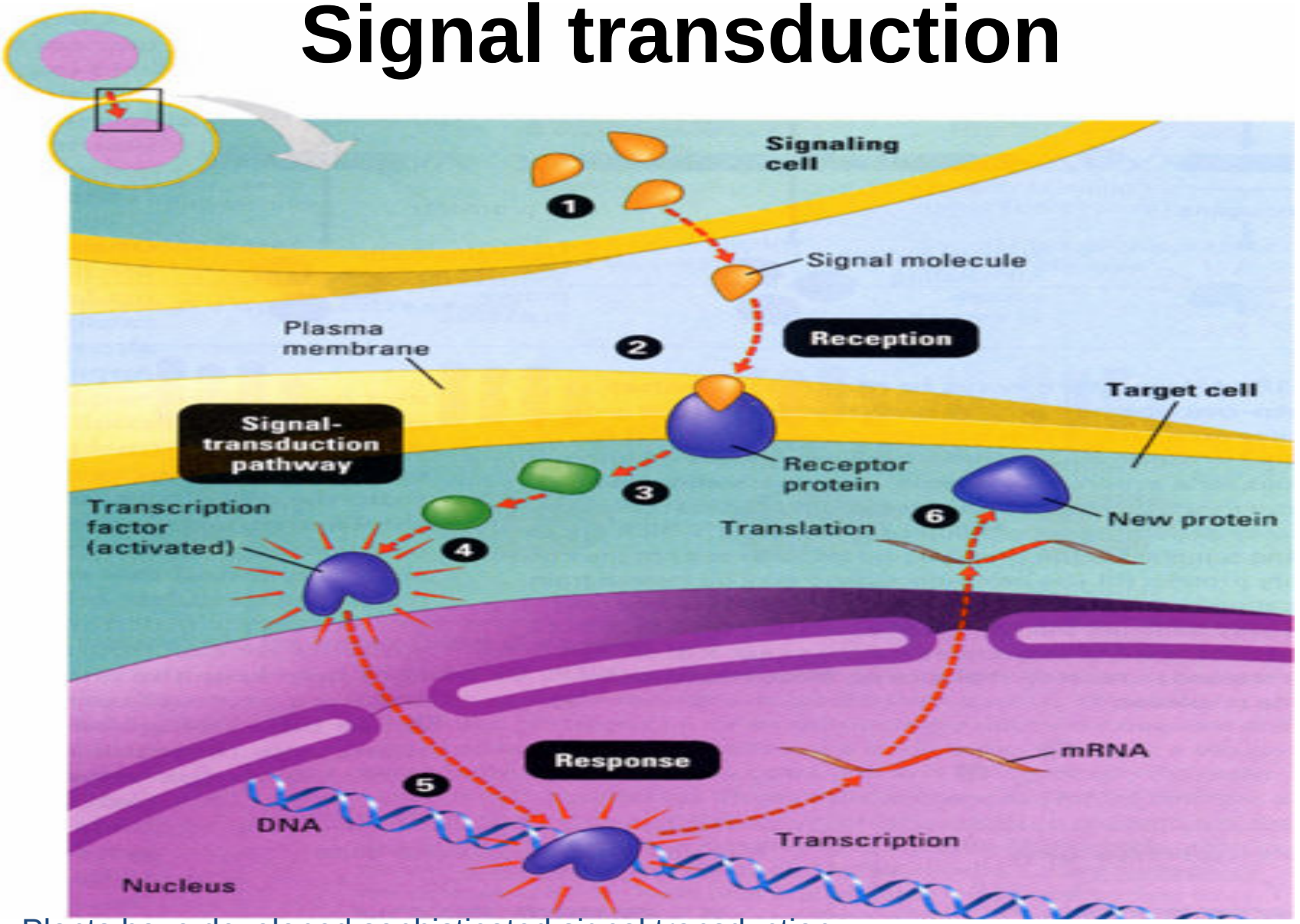
Metabolic network



Representation 1:
Node: metabolites
Edge: enzymatic steps
Directed
Unweighted

Representation 2:
Node: Enzymes
Edge: Enzymes working on adjacent steps
Undirected
Unweighted

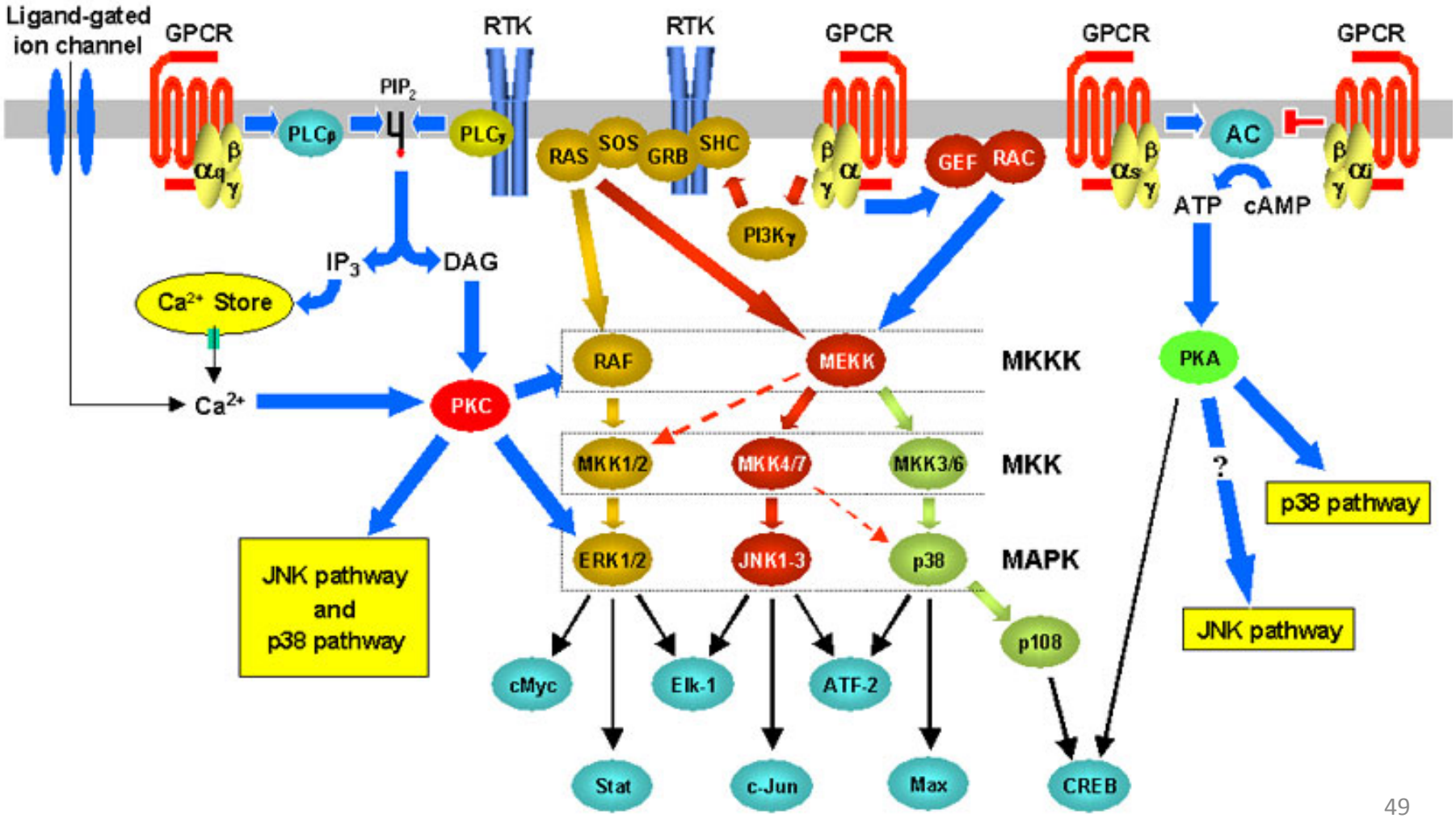
Signal transduction



Plants have developed sophisticated signal transduction mechanisms to be able to respond to changing environmental conditions.

Signal transduction network

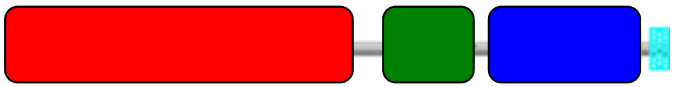
Node: proteins, signal molecules, Edge: interaction relationships, Undirected, Unweighted



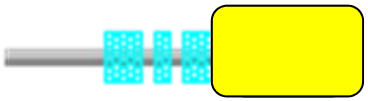
Protein Interaction

Proteins: **Domains:**

P02994



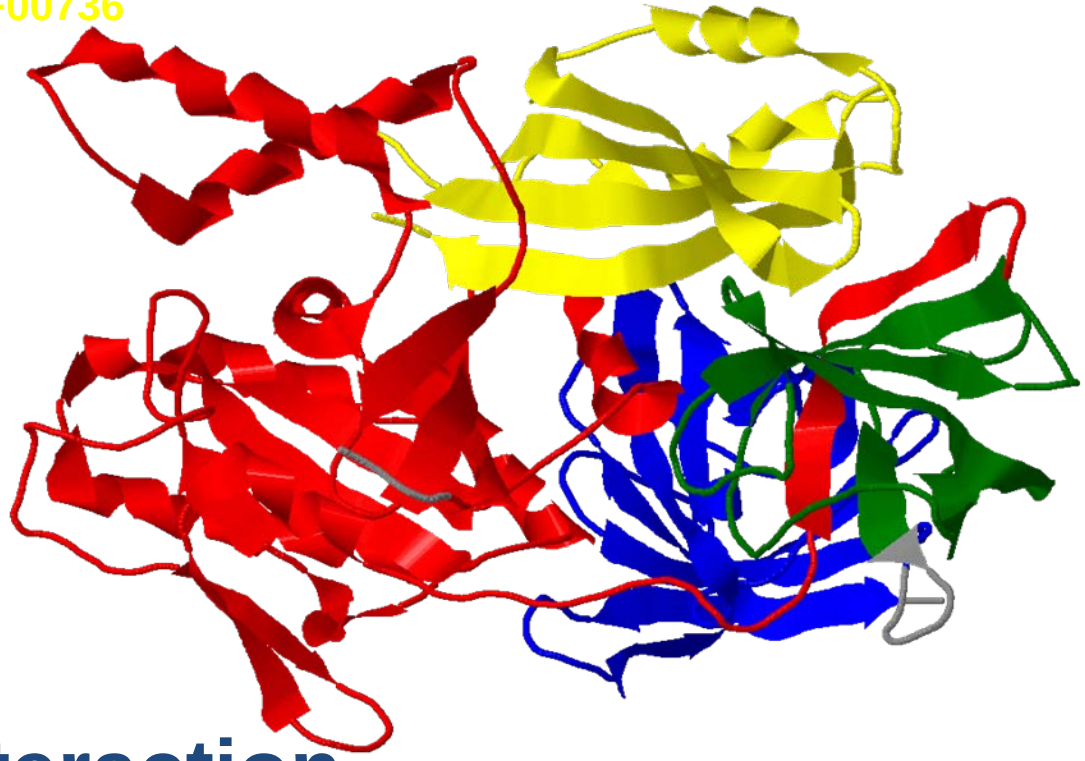
P32471



ORFs: **Interactions:**

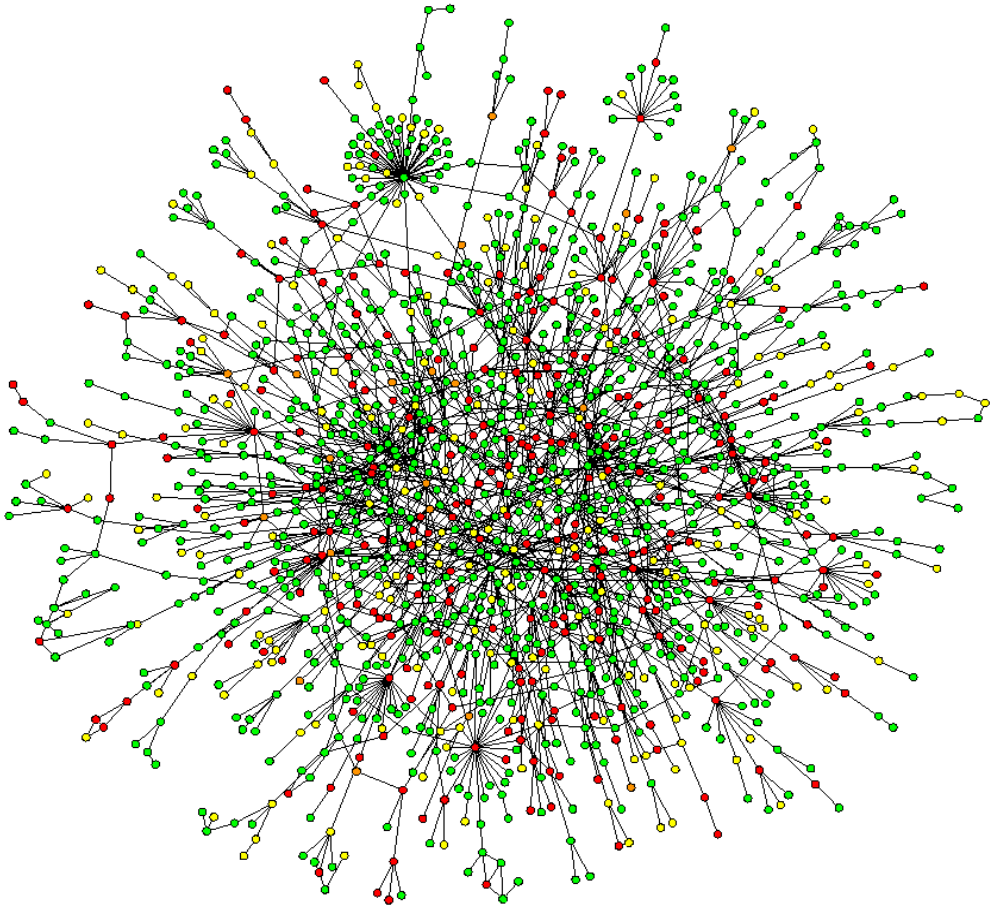
YBR118W←→YAL003W PF03144 PF00009 ← → PF00736
YBR118W←→YAL003W PF03143 PF00009 ← → PF00736
YBR118W←→YAL003W PF03143 PF03144 ← → PF00736

YPR080W←→YAL003W PF03144 PF00009 ← → PF00736
YPR080W←→YAL003W PF03143 PF00009 ← → PF00736
YPR080W←→YAL003W PF03143 PF03144 ← → PF00736



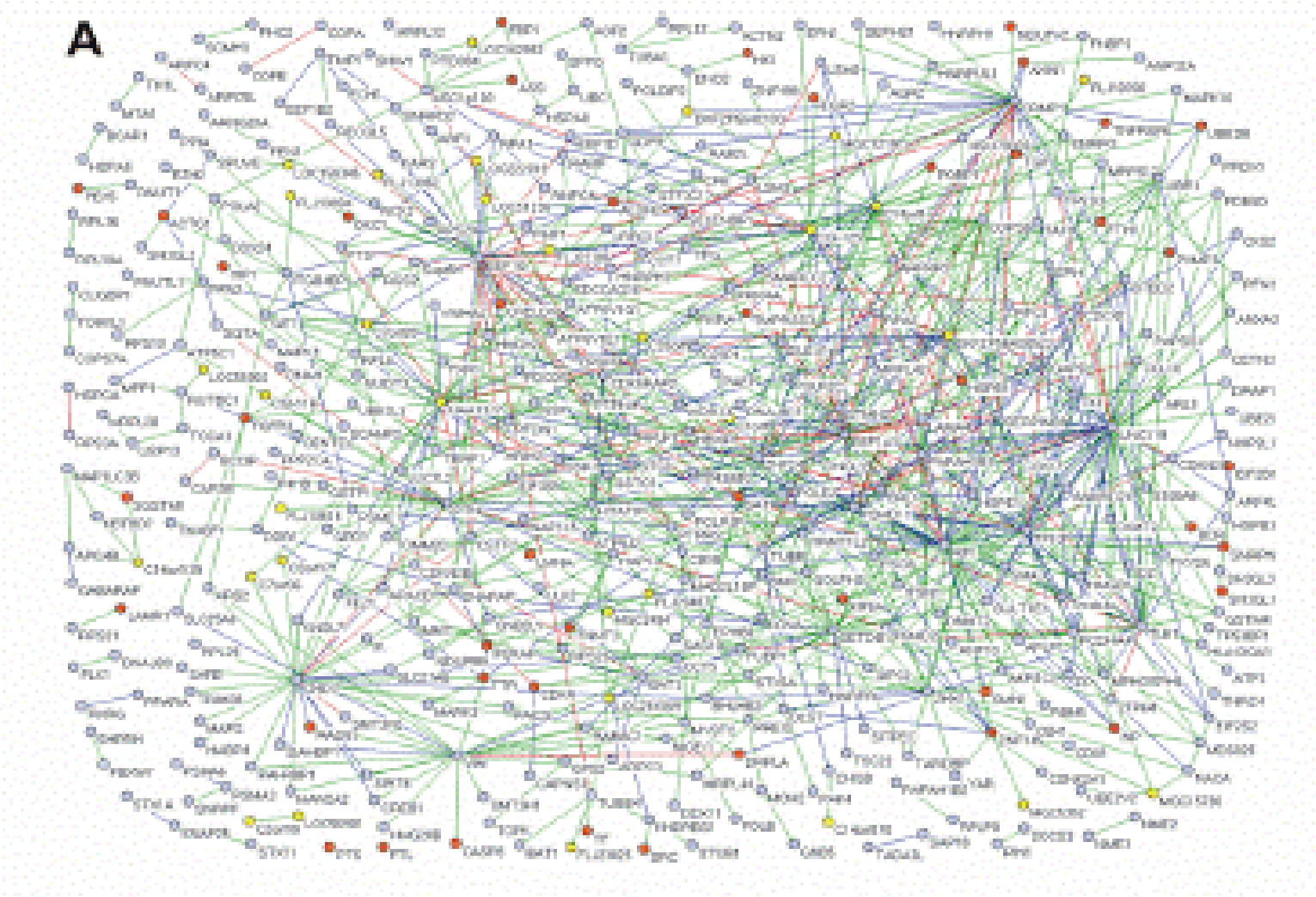
Protein interaction

Protein Interaction Network

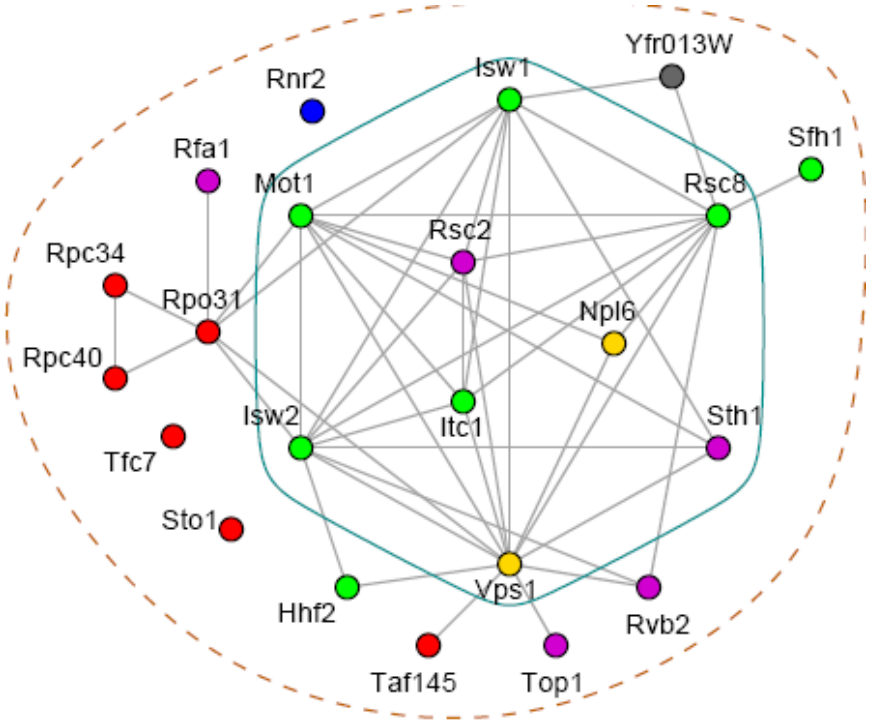


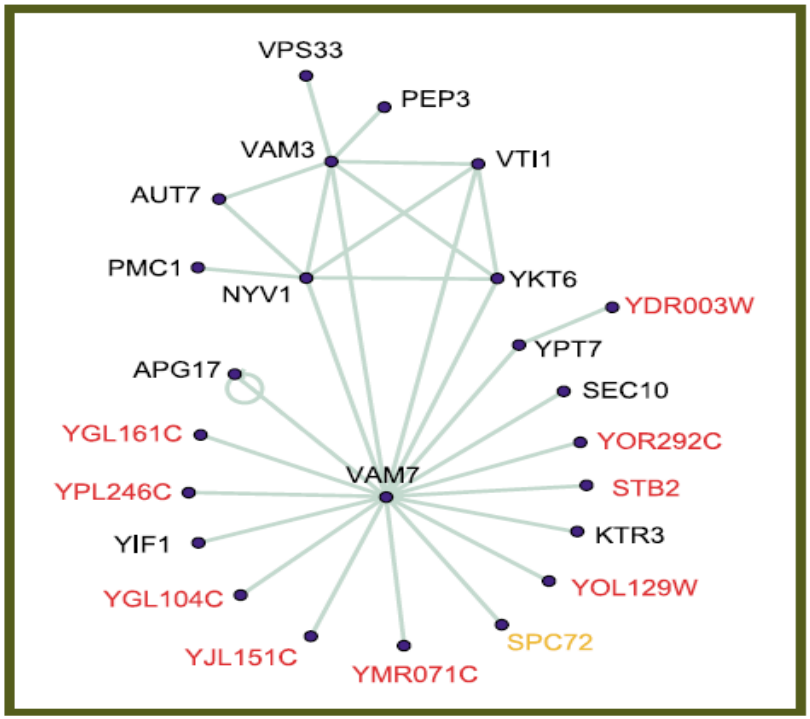
Yeast protein interaction network

Protein interaction network in Human by yeast two-hybrid method, 2006. Protein number: 1705, links： 3186



Representation of PPI network





Node: proteins, Edge: interaction relationships, Undirected, Weighted (Binary or Strengthed)

生物分子网络研究的科学问题

- 如何构建网络？ （王勇）

建模，数据处理、集成

- 如何分析网络？ （张世华）

静态：结构，功能等

动态：不同条件，进化

致谢！

该PPT课件的制作基于2010、2011版本，并有适当增删。

感谢章祥荪研究员、吴凌云和王勇博士以及整个课题组！

感谢许多工作的原始作者，限于时间和篇幅文献和作者未能及时标注。