

生物情報工学II

11月29日

生物情報工学(Bioinfomatics)ってなに?

> 生物が持っている物質(DNA、タンパク質、その他代謝産物など) の情報を分析する学問分野。



>情報をもとにその物質の機能や構造を推定。

>ただし、解析には様々な物質に関する情報の蓄積が必要。

Bioinfomaticsの台頭 - DNA配列解析の場合 -

ABI社DNA analyzerで、配列取得に10年、データ 解析に3年の歳月と3000億円の費用をかけて解析。

1990年-2003年 ヒトゲノム計画

Illumina社HiseqXで、5名分のゲノ ム情報を10日70万円で解析完了。

https://jp.illumina.com/content/dam/illuminamarketing/apac/japan/documents/pdf/primer _illumina_sequencing_introduction-j.pdf



https://upload.wikimedia.org/wikipedi a/commons/c/cb/Sequencing.jpg 1977年 Dideoxy法(サンガー法)



https://upload.wikimedia.org/wikipedia/commons/th umb/7/78/370A_automated_DNA_sequencer.jpg/7 38px-370A_automated_DNA_sequencer.jpg

1987年 ABI社370 DNA sequencer発売



http://www.biochemsoctrans.org/con tent/ppbiost/43/1/1/F4.medium.gif

2006年 Solexa社(現Illumina社) Genome Analyzer発売



http://www.biotechniques.com/multimedia/archive/00190/2013-04-03-read-len_190429a.png

2011年 Pacific bioscience社 Pacbio RS発売



古典的な分子生物学



現在の分子生物学



ゲノム、転写産物、たんぱく質、表現型の各階層内・階層間での複雑な相互作用

一つ一つの要素だけに注目していても、生命現象の本質的な理解には至らない? 木を見て森を見ず?





複雑な相互作用ネットワークから成る生命システムを、分解せず複雑なネットワークとして理解する。

システムバイオロジー

オミクスデータをもとに、統計学やグラフ理論を駆使して、それぞれの要素の 間にある相互関係を解き明かし、ネットワーク動態で生命現象を説明する。

けど、今のところ生命システムが複雑すぎて無理ゲー。

ひたすらオミクスで情報を蓄積させている。



システムバイオロジーの申し子「KEGG」

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	ウェブ 画像 動画 ニュース 地	□図 もっと見る マ 検索ツール
	約 4,690,000 件 (0.34 秒)	
	KEGG: Kyoto Encyclopedia of Gen www.genome.jp/kegg/ マこのページを訳す KEGG is a database resource for understanding biological system, such as the cell, the organism level information, especially large-scale molecula	es and Genomes high-level functions ar and the ecosystem, for ar datasets generated
	KEGG Pathway	KEGG GENES D Googleで"KEGG"を検索
	KEGG2 - Gene - Brite - Module	prokaryotic genomes was
	Kyoto Encyclopedia of Gene KEGG は分子レベルの情報から細 胞、個体、エコシステムといった高 次	KEGG Database KEGG Database. KEGG (Kyoto Encyclopedia of Genes and
	KEGG2	KEGG Mapper
	Category, Entry Point, Search & Compute, DBGET Search	Search&Color Pathway - Search Pathway - Reconstruct Pathway
	genome.jp からの検索結果 »	

システムバイオロジーの申し子「KEGG」

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🗀 RNAseq 🦳 news 🗋 Journals 🦳 R & programing 🗋 統計学 🗋 Web tools 🦳 Rice DB 🦳 Data base 🦳 植物工場 🧰 Others (🗎 Hobbies



KEGG Home

Release notes Current statistics Plea from KEGG

KEGG Database

KEGG overview Searching KEGG **KEGG** mapping Color codes

KEGG Objects

Pathway maps Brite hierarchies

KEGG Software

KegTools **KEGG API** KGMI

KEGG FTP Subscription

GenomeNet

DBGET/LinkDB

Feedback

Kanehisa Labs

KEGG: Kyoto Encyclopedia of Genes and Genomes

KEGG is a database resource for understanding high-level functions and utilities of the biological system, such as the cell, the organism and the ecosystem, from molecular-level information, especially large-scale molecular datasets generated by genome sequencing and other high-throughput experimental technologies (See Release notes for new and updated features).

New articles

- KEGG as a reference resource for gene and protein annotation
- BlastKOALA and GhostKOALA: KEGG tools for functional characterization of genome and metagenome sequences

Main entry point to the KEGG web service

KEGG2 **KEGG** Table of Contents Data-oriented entry points **KEGG PATHWAY** KEGG BRITE **KEGG MODULE** KEGG ORTHOLO **KEGG GENOME KEGG GENES** KEGG COMPOUNI **KEGG REACTION** KEGG DISEASE KEGG DRUG KEGG MEDICUS

KEGG pathway maps [Pathway list] functional hierarchies [Brite list] nodules [Module list | Statistics] roups [KO system | Annotation] [KEGG organisms]

"KEGG PATHWAY"をクリック

Update notes

Biochemical reactions [Reaction modules] Human diseases [Cancer | Pathogen] Drugs [ATC drug classification] Health information resource [Drug labels search]

KEGG

京都大学バイオインフォマ ティクスセンターが管理し ているバイオインフォマテ ィクス研究用データベース。 システムバイオジー的なコ ンセプトを基にしており、 遺伝子間、分子間の相互作 用ネットワークに関する情 報をデータベース化してあ る。

KEGGのコアデータベースKEGG PATHWAY

🎊 KEGG PATHWAY Databa 🗴 🕻 https://www.agr.nago/ 🗙 🕻 G システムズバイオロジー 🔹 🌔 www.fbs.osaka-u.ac.jp 🗴 🛄
← → C www.genome.jp/kegg/pathway.html ⊕
🗀 RNAseq 📋 news 📋 Journals 🗀 R & programing 🗋 統計学 🗋 Web tools 🗋 Rice DB 🦳 Data base 🛅 植物工場 🦲 Others 🗋 Hobbies 👒
KEGG PATHWAY Database
Wiring diagrams of molecular interactions, reactions, and relations
Select prefix Enter keywords plant hormone Genes LIGAND DISEASE DROG DBGET
[New pathway Maps
KEGG PATHWAY is a collection of manually drawn pathway "Plant hormone"をキーワード検索
1. Metabolism

KEGGで植物ホルモンシグナル伝達系を俯瞰する



イネにおける植物ホルモンシグナル伝達系遺伝子

 C www.kegg.jp/kegg-bin/highlight_pathway?scale=1 RNAseq news Journals R & programing 第計学 Web tools Note Plant hormone signal transduction - Reference pathway Pathway menu Organism menu Pathway entry User data mapping] Reference pathway Go 100% V Cucumis sativus (cucumber) Cucumis quercas Populus trichocarpa (black cottonwood) Vity vinifera (wing grape) Solanum tuberosum (potato) Bola vulgaris (sugar beet) Oryza sativa japonica (Japanese rice) (RefSeq) Oryza sativa japonica (Japanese rice) (RefSeq) Oryza sativa japonica (Japanese rice) (RefSeq) Oryza sativa japonica (Japanese rice) (RAPDDB) Oryza sativa japonica (Japanese rice) (RAPDDB) Populus trichocarpa (black cottonwood) Vity a acuminata (wing right) West a cutination Catina biosy Catina	Pathway Search Result × 🔀 KEGG PATHWAY: Plant × 🔀 KEGG PATHWAY:
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イネのジベレリン受容



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RNAseq 🛄] news 🦲 Journals 🔝 R & programing 🦲 統計字 🦲 Web tools 🦲 Rice DB 🚺 Data base	
KEGG	Oryza sativa japonica (Japanese rice) (RAPDB): Os05t0407500- 01	
Entry	0s05t0407500-01 CDS T02163	
Gene name	OsO5g0407500, GIBBERELLIN_INSENSITIVE_DWARF1, GID1	
Definition KO	(RAP-DB) Alpha/beta hydrolase fold-3 domain containing protein. K14493 gibberellin receptor GID1 [EC:3]	
Or gan i sm	dosa Oryza sativa japonica (Japanese rice) (RAPDB)	
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Motif	Pfam: Abhydrolase_3 Abhydrolase_5 COesterase Hydrolase_4 PAF-AH_p_II Motif	
Other DBs	RAP-DB: 0s05t0407500-01 Oryzabase: 7353	
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Position	chr05:join(1986890719868945,1986958919870614)	
AA seq	354 aa AA seq DB search MAGSDEVNRNECKTVVPLHTWVLISNFKLSYNILRRADGTFERDLGEYLDRRVPANARPL EGVSSFDHIIDGSVGLEVRIYRAAAEGDAEEGAAAVTRPLLEFLIDAPAAEPFPVIIFFH GGSFVHSSASTIYDSLCRRFVKLSKGVVVSVNYRRAPEHRYPCAYDDGHTALKWYMSOP FMMSGGDAGARVFLSGDSSGGNIAHHWAVRAADEGVKVCGNILLNAMFGGTENTESERR DGKYFVTLODRDWYWKAYLPEDADRDHPACNPFGPNGRRLGGLPFAKSLIIVSGLDLTCI RCLAYADALREDGHHVKVVOCNATVGFYLLPNTVHYHEVMEEISDFLNANLYY	
NT seq	1065 nt NT seq al georgeoage sacgaggt caacegeaageagt get geoget caacege t ggst get catet ceaact te ageet get acaacat te geoge gead geoget get geoget geoget t te sacge geoget acet george geoget get geoget geoget geoget agesgest get get geoget george geoget geoget geoget geoget t aces geoget geoget geoget geoget geoget geoget geoget t aces geoget geoget geoget geoget geoget geoget geoget t aces geoget geoget geoget geoget geoget geoget geoget t te satter te geoget geoget geoget geoget geoget geoget t te satter te geoget geoget geoget geoget geoget geoget geoget t te satter te geoget ge	
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🗋 RNAseq 🗋 news 🎦 Journals 🗋 R & programing 🗋 統計学 🎦 Web tools 🛄 Rice DB 🎦 Data base 📋 植物工場 📋 Othe

"MOTIF"をクリック

出席と宿題の提出 提出方法

リンク集

データベース検索:

- 1. PubMed: 論文検索
- 2. <u>Entrez</u>:総合データベース
- 3. Google:何でも検索
- 4. Google Scholar: 科学に関する検索
- 5. <u>特許データベース</u>

ホモロジー検索:

- 1. BLAST [GenomeNET]
- 2. FASTA [GenomeNET]

配列解析:

- 1. DNA → AA : DNA配列をアミノ酸配列に変換
- 2. <u>Spidey</u>: DNAとcDNAのマッチング
- 3. <u>BLAST(NCBI)</u>:遺伝子のホモロジー検索
- 4. <u>BLAST(DDBJ)</u>:遺伝子のホモロジー検索
- 5. <u>Softberry/FGENESH</u>:遺伝子の予測
- 6. <u>GeneMark</u>:遺伝子の予測
- 7. <u>GENESCAN</u>:遺伝子の予測
- 8. <u>clustalW</u>: アライメント
- 9. InterProScan:ドメイン解析
- 10. <u>PSORT</u>:細胞内局在性予測
- 11. GEO: 遺伝子発現解析
- 12. Gene Ontology:用語を用いた検索
- 13. <u>SSPN</u>: スプライシングの予測
- 14. ORF Finder: ORFの予測
- 15. TFSEARCH : 転写因子結合部位の予測
- 16. <u>MOTIF</u>: タンパク質モチーフ検索
- 17. <u>pI/Mw</u>: 等電点、分子量の予測
- 18. <u>RAP-DB</u>: イネのゲノムデータベース

解析用配列

1. ある遺伝子AのgenomeDNA配列

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Aseq 📋 news 📋 Jo	urnals 🦳 R & programing 🦳 統計学 🦳 Web tools 🦳 Rice DB 🦳 Data base 🦳 植物工場 🦳 Others 🦳 Hobbies 💶 Ir
	MOTIF Search
Search Motif L	ibrary Search Sequence Database Generate Profile KEGG2
Enter query se	Equence: (in one of the three forms)
Local file name	(Example) mja:MJ_1041
Sequence data	
	RPL EGVSSFDHIIDQSVGLEVRIYRAAAEGDAEEGAAAVTRPILEFLTDAPAAEPFPVII FFH GGSFVHSSASSTIYDSLCRRFVKLSKGVVVSVNYRRAPEHRYPCAYDDGWTALKW
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Result of Mod Number of found m	tifFinder otifs: 5				
Query 0	100		200	300	354
	Abhy	ydrolase_3			
	Abhy COest PAF-A	ydrolase_5 erase WH_p_II H	ydrolase_4		

Pfam (5 motifs)

Pfam	Position(Independent E-value) Description
Abhydrolase_3	116329(1.3e-56) Deta	PF07859, alpha/beta hydrolase fold
Abhydrolase_5	115256(5.3e-05) Deta	PF12695, Alpha/beta hydrolase family
COesterase	110208(0.00015) Deta	PF00135, Carboxylesterase family
Hydrolase_4	189234(0.042) Deta	PF12146, Serine aminopeptidase, S33
PAF-AH_p_II	111161(0.08) Deta	PF03403, Platelet-activating factor acetylhydrolase, isoform II

KEGG からモチーフサーチ結果への直接リンク

→ G	www.kegg.jp/dbget-bin/www_bget?dosa:0s05t040/500-01
RNAseq) news 🦳 Journals 🦳 R & programing 🦳 統計学 🦳 Web tools 🦳 Rice DB 🦳 Data base
KEGG	Oryza sativa japonica (Japanese rice) (RAPDB): Os05t0407500- 01 Help
Entry	Os05t0407500-01 CDS T02163
Gene name	OsO5g0407500, GIBBERELLIN_INSENSITIVE_DWARF1, GID1
Definition	(RAP-DB) Alpha/beta hydrolase fold-3 domain containing protein.
KU On man 1 am	K14493 gibberellin receptor GIVI [EU:3]
Organism Dothmou	dosa Uryza sativa japonica (Japanese rice) (NAPUD)
Brite	KEGG Orthology (KD) [BR:dose00001]
	Environmental Information Processing Signal transduction 04075 Plant hormone signal transduction 050510407500-01 (0605g0407500) Enzymes [BR:dosa01000] 3. Hydrolases 3 3 9 0.050510407500-01 (0s05g0407500) BRITE hierarchy
SSDB	Ortholog Paralog GFIT
Motif	Pfam: Abhydrolase_3 Abhydrolase_5 COesterase Hydrolase_4 PAF-AH_p_II Motif
Other DBs	RAP-DB: 000000000000000000000000000000000000
Li nkDB	All DBs
St ruct ure	[™] ・ 「Motif"ボタンをクリッ
	Jmol
Position	chrU5:join(1986890719868945,1986958919870614)
AA seq	1304 aa AA seq DB search MAGSDEVNRNECKTVYPLHTWYLISNFLRAARDGTFERDLGEYLDRRVPANARPL EGYSSFDHIJDOSVGLEVFLYRAAREGDAEEGAAVTRPILEFLTDAPAAEPFPVIIFFH GGSFVHSSASSTIYDSLCRRFVKLSKGVVSSNYRRAPEHRYPCAYDDGWTALKWVMSOP FMRSGGDAGARVFLSGDSSGONIAHHVAVRAADEGVVCCNILLNAMFGGTERTESERRL DGXYFVTLODRUWWKAYLPEDADRDHPACNPFGPNGRRLGCIPFAKSLITVSGLDLTCD ROLAYADALREDGHHVKVVQCENATVGFYLLPNTVHYHEVMEEISDFLNANLYY
NT seq	1065 nt NT seq
	al ggor ggo ag sag gag to acc graac gat g caag ac g t g g c g ot caaca t ggst got act to caact to ag ot g c g a caag act to t g c g c g g c g g c g g c g c g c g g a g g g a c t c g a g g g g g g g g g g g g g g g g g

KEGG からモチーフサーチ結果への直接リンク

🙆 Pathway Search Result 🗙 👩 SSDB Motif Search Resux	-
← → C 🗋 www.kegg.jp/ssdb-bin/ssdb_motif?kid=dosa:Os05t0407500-01	
🗀 RNAseq 🦳 news 🗀 Journals 🦳 R & programing 🗀 統計学 🦳 Web tools 🦳 Rice DB 🦳 Data base 🦳 植物工場 🦳 Others 🦳 Hobbies 💶 Ir	troduction to P… 🛛 🙏 http
SSDB Motif Search Result	
Organism: Oryza sativa japonica (Japanese rice) (RAPDB) Gene: Os05t0407500. GIBBERELLIN_INSENSITIVE_DWARF1, GID1; Alpha/beta hydrolase fold-3 domain containing protein.; K14493 gibberellin receptor Motif id From To Definition E value Score pf:/Ocesterase 110 208 (Carboxylesterase family 0.00015 - pf:Abhydrolase_3 206 (Alpha/beta hydrolase fold 1.3e-56 - pf:Abhydrolase_3 116 329 alpha/beta hydrolase fold 1.3e-56 - pf:Hydrolase_4 189 234 Putative lysophospholipase 0.042 - Search GENES with the same motifs dosa:0s050t0407500-01 50 100 150 200 250 300 350 (354) pf:RbHydrolase_5 pf:RbHydrolase_13 pf:RbHydrolase_6 pf:Hydrolase_4	иr GID1 [EC:3,]

ジベレリン受容体GID1は、加水分解酵素!?

ジベレリン受容体GID1は、加水分解酵素!?



図1 リボンモデルで表示したジベレリン受容体とリパーゼの立体構造の比較 a ジベレリン受容体、b リパーゼ。両者の基本構造は非常によく似ている。a、bにおいてそれぞれ薄紫色、金色で示したの がa/β水解酵素型構造。a、bにおいてそれぞれ濃緑色、濃紫色で示したのがN末端のリッド(ふた)。



N-末端の スウィッチ領域 (腕と手) GID1 ジベレリン受容体

DELLAタンパク質

ジベレリンを分解することなく、 結合による構造変化でシグナルを伝達。

図2 ジベレリン受容体のジベレリン(GA) 結合ポケットの拡大図 活性型ジベレリン(GA4)は炭素原子をオレンジ、酸素原子を赤で表示した。リパーゼ触媒アミノ酸トリオに相当する Ser198とAsp296は、炭素原子を黄色、酸素原子を赤で表示した。オキシアニオン結合部位は紫色、ジベレリン結合ポケッ トの「ふた」は水色で表示した。

http://www.kyoto-

u.ac.jp/static/ja/news_data/h/h1/news6/2008/081127_1.htm

脂質加水分解酵素リパーゼの基質結合部位に変異 が起こり、ジベレリンと結合できるようになった。

バイオインフォマティクスの真骨頂:比較ゲノミクス



Phytozome

数十の植物種のゲノム情報を統合 し、そのゲノム情報を比較する目 的に特化したデータベース。

植物種間横断的にBLAST解析を行ったり、とある遺伝子のホモログやパラログを容易に検索できる。

通常のNCBIのBLASTなどに比べて、 検索される情報が整理されている ので扱いが容易。

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BLAT JBrowse PhytoMine BioMart Flagships All genomes and families Early Release Genomes All released species Amaranthus hypochondriacus Amborella trichopoda v1.0 Image: Comparison of the provided set of the prov		Documentation • View a tree representation of the species in Phytozome v12.1 • View a Quick Start Guide to using Phytozome • Check out the FAQs
About Phytozome 12.1.4	News (details)	System Status (2017-11-20 02:05)
Phytozome, the Plant Comparative Genomics portal of the Department of Energy's Joint Genome Institute, provides JGI users and the broader plant science community a hub for accessing, visualizing and analyzing JGI-sequenced plant genomes, as well as selected genomes and datasets that have been sequenced elsewhere. As of release v12.1, Phytozome hosts 77 assembled and annotation genomes, from 74 viridiplantae species. Forty-three of these genomes have been sequenced assembled and annotated with JGI Plant Science program resources By integrating this large collection of plant genomes into a single resource and performing comprehensive and uniform annotation and analyzes, Phytozome facilitates accurate and insightful comparative genomics studies. All gene sets in Phytozome have been annotated with KIG, KEGG, ENZYME, Pathway and the interPro family of protein analysis tools. Inparanoid pairwise orthology and paralogy groups have been calculated across all Phytozome proteomes. Families of related genes representing the modern descendants of putative ancestral genes are constructed at key phylogenetic nodes. These families provide additional insight into clade-specific orthology/paralogy relationships as well as clade-specific novelties and expansions. Search and visualization tools let users quickly find and analyze genes or genomic regions of interest. Query-based data access is provided by Phytozome's InterMine and BioMart instances, while bulk data sets can be accessed via the JGI's Genome Portal. JBrowse genome browsers are available for all genomes.	(2017-10-11) Olive genome released (2017-09-28) 2 <i>P.</i> hallii genomes + sunflower (2017-09-07) Chickpea and Bsylaticum added	 ✓ Search ★ BLAST ✓ Database ★ BLAT ✓ PhytoMine
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Ath(シロイヌナズナ)のGID1周辺の遺伝子をクリックすると Bra(ブラシカラパ)のGID1周辺遺伝子もハイライトされる。 ただし、ATGID1BとATGID1AまたはATGID1C周辺では、 ハイライトされる遺伝子が異なる。

Ge	nes i	n Family	Function	nal Annotation	MSA raminy misu	ory			
1	M	Views	Org	ID	Alias/Symbol	Defline		Domains Synteny Exons	
	F	GB	Bdi	Bradi2g25600 1	Readi2a25600 v2		(Blast2GO)		
E	F	GB	Osa	LOC_Os Auto: (E=	25590.1.p is a membe 1e-257) PF01535//PF	r of Family 93519195: 🖄 13041 - PPR repeat (PPR)	putative, expre	-	Zapa
	F	GB	Ath	AT3G63 // PPR re	peat family (PPR_2)		erfamily protein		
E	F	GB	Ath	AT3G05120.1	ATGID1A	alpha/beta-Hydrolases su	perfamily protein		
100	F	GB	Ath	AT5G27320.1	ATGID1C	alpha/beta-Hydrolases su	perfamily protein		
	F	GB	Bra	Brara.D00038.1		(1 of 4) K14493 - gibberell	in receptor GID1 (
	F	GB	Bra	Brara.E03404.1		(1 of 2) PTHR23024:SF222	7 - GIBBERELLIN		
	F	GB	Bra	Brara.F02873.1		(1 of 2) PTHR23024:SF222	7 - GIBBERELLIN	00000	
100	F	GB	Bra	Brara.G01992.1		(1 of 4) K14493 - gibberell	in recept <mark>or GID1 (</mark>		



一番トのBra(フラシカラバ)のGID1周辺遺伝子は、 ATGID1B周辺と近いが、どちらかといえばBra(ブラ シカラパ)の一番上のエントリーと似ている。

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CLUSTALW Result

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