ちょっと整理しておきたいのですが…

▶ 生物情報工学(バイオインフォマティクス)ってなに?

分子生物学研究の結果、大量のDNA配列データが蓄積されてきた。 Gene A: ATGAAGTTTAGACCGATCAGTACT.... Gene B: ATGCAGTACGAAGTACGATAGACAAGT...

新奇遺伝子が見つかった。さて、これは既知のものと同じ機能か否か?

Novel Gene: ATGCAGTACTAAGTTTAGACCGAT....

さらに、ゲノムプロジェクトの進展で大量のDNA配列データが手に入った。 さて、配列が分かってもどこが遺伝子か分からない…。

> じゃあ、過去の知見をもとに遺伝子領域を予測しよう! BLAST、ORF finder、Softberry/FGENESH

DNAシーケンサーの発達により、ゲノム配列情報がさらに充実。 ゲノムを種間比較して、進化学的な研究をしよう⇒比較ゲノミクス



▶ 生物情報工学(バイオインフォマティクス)ってなに?

古典的な分子生物学



ちょっと整理しておきたいのですが...

▶ 生物情報工学(バイオインフォマティクス)ってなに?

分子生物学の発展



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 ーつー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?

ちょっと整理しておきたいのですが…

▶ 生物情報工学(バイオインフォマティクス)ってなに?

分子生物学の発展



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

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のまま理解する。

オミクス(Omics)

- Genomics (ゲノム)
- Transcriptomics (転写産物)
- Proteomics (タンパク質)
- Metabolomics (代謝産物)
- Glycomics (糖鎖付加)
- Epigenomics (ゲノム修飾)
- Phenomics (表現型)

データを数理モデルやネット ワークモデルに落とし込んで、 生命システムを理解したい。 ⇒ システムバイオロジー

システムバイオロジーの申し子「KEGG」

🛞 KEGG: Kyoto Er	ncyclope 🗙 🚺 生物情報工学(第1部) 🗙 🖌 G	KEGG - Google 検索 X 📃		
⊢ → C' <u> </u> h	https://www.google.co.jp/webhp?sou	rceid=chrome-instant&ion	=1&espv=2&ie=UT	
🖹 RNAseq 🗎 nev	vs 🛅 Journals 📋 R & programing 🧰 統計学	🗀 Web tools 📋 Rice DB 📋 [Data base 📋 植物工場 (
G <mark>g</mark> gle	KEGG		. С то	
	ウェブ 画像 動画 ニュース 地	図 もっと見る ▼ 検索ツー	ル	
	約 4,690,000 件(0.34 秒)			
	KEGG: Kyoto Encyclopedia of Gene 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	ihe	
	KEGG Pathway Map01100 - Search Pathway - KEGG2 - Gene - Brite - Module	KEGG GENES D GOO The KEGG GENES database for prokaryotic genomes was	gleで"KEGG"を検索	索
	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 Category, Entry Point, Search & Compute, DBGET Search	KEGG Mapper 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」

🎊 KEGG: Kyoto Encyclope 🗴 📣 https://www.agr.nagoy 🗙 🎊 KEGG: Kyoto Encyclope 🗴 📃	
← → C 🗋 www.genome.jp/kegg/) 🖬 👷
🗀 RNAseq 🦳 news 🗀 Journals 🦳 R & programing 🦳 統計学 🦳 Web tools 🦳 Rice DB 🦳 Data base 🦳 植物工場 🛄 Ot	ners 🧰 Hobbies

- 000				
	KEGG	•	Search	Help
				» Japanese

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

KegTools KEGG API KGML

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 Update notes				
🥔 Data-oriented e	ntry points				
KEGG PATHWA	KEGG pathway maps [Pathway list]				
KEGG BRITE	TE functional hierarchies [Brite list]				
KEGG MODULE	modules [Module list Statistics]				
KEGG ORTHOL	groups [KO system Annotation]				
KEGG GENOME	G [KEGG organisms]				
KEGG GENES	(V = C = C = C = C = C = C = C = C = C =				
KEGG COMPOU	KEGG PATHWAY 27997				
KEGG REACTIO	N Biochemical reactions [Reaction modules]				
KEGG DISEASE	Human diseases [Cancer Pathogen]				
KEGG DRUG	Drugs [ATC drug classification]				
KEGG MEDICUS	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.nagoy × G システムズバイオロジー 🛛 × 🕒 www.fbs.osaka-u.ac.jp/ × 🛄
$\leftarrow \rightarrow \mathbb{C}$ www.genome.jp/kegg/pathway.html $\bigcirc \mathbb{Q} \cong \mathbb{C}$
🗀 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
KEGG2 PATHWAY BRITE MODULE KO GENOME GENES LIGAND DISEASE DRUG DBGET
Select prefix Enter keywords
map Organism plant hormone G Upp [New pathway Odate history]
Pathway Maps
KEGG PATHWAY is a collection of manually drawn pathway "Plant hormone"をキーワード検索 molecular interaction and reaction networks for:
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







Pathway S	earch Result 🔹 🔀 KEGG T02163: Os05t0- 🗙 🕼 https://www.agr.nagoy 🗙 💶	
⇒ C'	www.kegg.jp/dbget-bin/www_bget?dosa:0s05t0407500-01	
RNAseq 📋] news 🦳 Journals 🧰 R & programing 🧰 統計学 🧰 Web tools 🧰 Rice DB 🧰 Data ba	se
K	Oryza sativa japonica (Japanese rice) (RAPDB): Os05t0407500- 01 Help	
ntry	0s05t0407500-01 CDS T02163	
iene name	OSU5gU4U/5UU, GIBBERELLIN_INSENSIIIYE_DWARFI, GIDI	
KO	K14493 gibberellin receptor GID1 [FC:3]	
Organism	dosa Oryza sativa japonica (Japanese rice) (RAPDB)	
Pathway	dosa04075 Plant hormone signal transduction	
ir ite	KEds Orthology (KO) EB:365300001] Environmental Information Processing Signal transduction 04075 Plant hormone signal transduction 0505t0407500-01 (0s05g0407500) Enzymes [BR:dosa01000] 3. Hydrolases 3 3 0.055t0407500-01 (0s05g0407500) EBITE hierarchy	
SSDB	Ortholog Paralog GFIT	
lotif	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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'osition	chrU5:join(1986890719868945,1986958919870614)	
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← → C 🔒 https://www.agr.nagoya-u.ac.jp/~bioinfo/Ashikari/index.html

📄 RNAseq 🦳 news 🗀 Journals 🗀 R & programing 🦳 統計学 🦳 Web tools 📋 Rice DB 🦳 Data base 📋 植物工場 🦳 Othei

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. <u>PubMed</u>: 論文検索

2. <u>Entrez</u>:総合データベース

3. <u>Google</u> : 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. <u>DNA → AA</u> : 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. GENESCAN : 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

"MOTIF"をクリック

解析用配列

<u>1. ある遺伝子AのgenomeDNA配列</u>

Pathway Search Result ×	(M KEGG 102163: Os05t04 ×	MOTIF: Searching P	rote ×		
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NAseq 🧰 news 🛅 Jou	rnals 📋 R & programing 🧰 🖁	統計学 🦲 Web tools 🧎	Rice DB Data base 🤅	📄 植物工場 🦲 Others 🧰 Hobbie	es 🖸 Ir
	MOTIF Se	arch			
Search Motif Li	brary Search Seq	uence Database	Generate Profil	e KEGG2	
Enter que ry see	quence: (in one of the th	ree forms)		Compute Clear	
Sequence ID		(Example) mja:MJ	_1041		
Local file name	ファイルを選択 選択されてい	ません			
Sequence data	MAGSDEVNRNECKTVVPLHTWVL	ISNFKLSYNILRRADGTFE	RDLGEYLDRRVPANA 🔄		
ſ	RPL EGVSSEDHTIDQSVGLEVRIYRA	A AEGDAEEGA AAV TRP II E			
Select motif lib	raries : (Help)				
Databases		Cut-off score (Click each datab	ase to get help for	アミノ酸配列をペ て "Compute"を	ース
Pfam		1.0 * E-	value	C, Compute 2	111

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Result of	MotifFinder								
Number of fou	ınd motifs: 5								
Pfam								054	
Query I . 0	100	· ·	· ·	200		300	<u>, </u>	304	
		Abhydrolas	e_3						
	F	Abhydrolas	e_5						
	CO	esterase	_	ulualaca d					
	Ph	нг-нп_р_11	n <u>y</u>	jaroiase_4					
Pfam (5 motifs	;)								
Pfam	Position(Independent	E-value)			Descripti	ion			
Abhydrolase_3	116329(1.3e-56)	Detail	PF07859, alı	oha/beta h	ydrolase fold				
Abhydrolase_5	115256(5.3e-05)	Detail	PF12695, Al	pha/beta h	ydrolase fam	nily			
COesterase	110208(0.00015)	Detail	PF00135, Ca	rboxyleste	erase family				
Hydrolase_4	189234(0.042)	Detail	PF12146, Se	rine amino	opeptidase, S	33			

KEGG からモチーフサーチ結果への直接リンク

🙆 Pathway S	earch Result 🗙 👩 KEGG T02163: Os05t0: 🗙 🕼 https://www.agr.nago) 🗴 🦲
- → C	www.kegg.jp/dbget-bin/www_bget?dosa:0s05t0407500-01
RNAsea	
J raw beq _	
KEGG	Oryza sativa japonica (Japanese rice) (RAPDB): Os05t0407500- 01
Entry	Os05t0407500-01 CDS T02163
Gene name	OsO5g0407500, GIBBERELLIN_INSENSITIVE_DWARF1, GID1
Definition	(RAP-DB) Alpha/beta hydrolase fold-3 domain containing protein.
КО	K14493 gibberellin receptor GID1 [EC:3]
Organism	dosa Oryza sativa japonica (Japanese rice) (KAPDB)
Pathway	dosaU4U/5 Plant hormone signal transduction
	Environmental Information Processing Signal transduction 04075 Plant hormone signal transduction 0s05t0407500-01 (0s05g0407500) Enzymes [Br:dosa01000] 3. Hydrolases 3 3 3 0s05t0407500-01 (0s05g0407500) BRITE hierarchy
SSDB	Ortholog Paralog GEIT
Motif	Pfam: Abhydrolase_3 Abhydrolase_5 COesterase Hydrolase_4 PAF-AH_p_II
Other DBs	RAP-DB: Oryzabas
LinkDB	All DBs
St ruct ure	『Motif"ボタンをクリッ
	Jmol
Position	chr05:join(1986890719868945,1986958919870614)
AA seq	354 aa AA seg DB search MAGSDEFWRHECKTYVPLHTWVLISDRFKLSYNILRRADGTFERDLGEYLDRYVPANARPL EGYSSFDHIIDGSYGLEVRIYRAAAEGDAEGAAAYTRPILEFLTDAPAAEPFPVIIFFH GGSFVHSSASSTIYDSLCRFFVKLSKGVVVSYNYRRAPEHRYPCAYDDGWTALKWVMSOP FMRSGGDAGARVFLSGDSSGGNIAHHVAVRAADEGVKVCGNILLNAMFGGTERTESERRL DGKYFVTLODRDWYWKAYLPEDADRDHPACNPFGPNGRRLGGLPFAKSLIVSGLDLTCD RGLAYADALREDGHHVKVVGCENATVGFYLLPNTVHYHEVMEEISDFLNAMLYY
NT seq	1065 nt NT seq atggccggcaggaggaggtcaaccgcaacgagtgcaagacggtggtgccgctccacaca tgggtgccacctccacacttcaagctgtcgtacaacattctgcggcgggggggg

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 💶 Introduction to P… 🔺 H						
SSDB Motif Search Result						
Organism : Oryza sativa japonica (Japanese rice) (RAPDB) Gene : Os05t0407500-01 Definition : Os05g0407500, GIBBERELLIN INSENSITIVE_DWARF1, GID1; Alpha/beta hydrolase fold-3 domain containing protein.; K14493 gibberellin receptor GID1 [EC:3]						
Motif id From To Definition E value Score						
pf:COesterase 110 208 Carboxylesterase family 0.00015 -						
pf:PAF-AH_p_II 111 161 isoform II 0.08 -						
pf:Abhydrolase_5 115 256 Alpha/beta hydrolase family 5.3e-05 -						
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:0s05t0407500-01 50 100 200 250 300 350 (354) pf:C0esterase pf:PAF-AH_p_II pf:Abhydrolase_5 pf:Abhydrolase_3 pf:Hydrolase_4						
GENES KEGG GenomeNet]						

ジベレリン受容体GID1は、加水分解酵素!? 16

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o/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)。



DELLAタンパク質 N-末端の スウィッチ領域 (腕と手) 本分子 GID1 デベレリン GID1 デベレリン受容体

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

8	Google	phytozome		५
		ウェブ ニュース 画像 ショッピン	グ 動画 もっと見る▼	検索ツール
v		約 149,000 件 (0.38 秒) 他のキーワード: ncbi phytozome使い方		
F		Phytozome v10.3: Home phytozome.jgi.doc 10.3.3. Phytozome Energy's Joint Geno descendants of ance rat	nomics portal of the Department of ted genes representing the modern at key phylogenetic nodes.	
		blast	Arabidopsis thaliana TA	IR10
		sequence Google C"Pl	nytozome"を	検索
		Search for genes, families a Search for genes, families and sequences. 1. Select a Target. 0	Release Notes Release Notes. What's new. The v10.3.1 release of Phytozome	
3		JGI The Soybean (Glycine max) genome project was initiated	Eucalyptus grandis v1.1 Eucalyptus grandis v1.1 (Eucalyp Eucalyptus	otus)
		doe.gov からの検索結果 »		
3 C		Phytozome: a comparative platform www.ncbi.nlm.nih.gov > > PubMed Central DM Goodstein 著 - 2012 - 引用元 705 - 間違記事 2011/11/22 - Phytozome ((http://www.phytozon a centralized hub that enables users with varying sophistication to access annotated plant gene fa	n for green plant genomics (PMC) ▼ このページを訳す ne.net), first released in 2008, provi g degrees of computational milies, to navigate the	des
t		Phytozome: a comparative platform www.ncbi.nlm.nih.gov/pubmed/22110026 ▼ DM Goodstein 著 - 2012 - 引用元 700 - 関連記事 Nucleic Acids Res. 2012 Jan:40(Database issue	f or green plant genomics このページを訳す):D1178-86. doi: 10.1093/nar/dkr94/	j. 4.

Nucleic Acids Res. 2012 Jan;40(Database issue):D1178-86. doi: 10.1093/nar/gkr944 Epub 2011 Nov 22. Phytozome: a comparative platform for green plant genomics. Goodstein DM(1), Shu S, Howson R, Neupane R, Hayes RD, Fazo J, ...

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。

🔀 Pathway Search Result 🗴 🛟 Phytozome v10.3: Hom 🗴 🗍 生物情報工学(第1部) 🗴 🎓 GenomeNet - Bioinform 🗴 😒 Domains & Structures - 🗴 🕝 比較ゲノミクス バイオイ	×
← → C D phytozome.jgi.doe.gov/pz/portal.html	☆ =
🗀 RNAseq 🗋 news 🗋 Journals 🧰 R & programing 🧰 統計学 🗋 Web tools 🦳 Rice DB 😭 Data base 🦳 植物工場 🦳 Others 🎦 Hobbies 📁 Introduction to P… 🔥 https://	www.agr
Image: Species + Tools + Info + Download + Help + Cart Subscribe	
Keyword search Phytozo BLAST (advanced)	Help with Phytozome
BLAT JBrowse PhytoMine BioMart All released species Unit vi.0 Search in Click an image or type species/node name BioKart Click an image or type species/node name Mall genomes and families Early Release Genomes Carly	 Documentation View a tree representation of the species in Phytozome v10 View a Quick Start Guide to using Phytozome Check out the FAQs
About Phytozome 10.3.3 News (details)	System Status (2015-11-30 05:04)
Phytozome is the Plant Comparative Genomics portal of the Department of Energy's Joint Genome Institute. Families of related genes representing the modern descendants of ancestral genes are constructed at key phylogenetic nodes. These families allow easy access to clade-specific orthology/paralogy relationships as well as insights into clade-specific novelties and expansions. As of release v10.3.1, Phytozome provides access to sixty-one sequenced and annotated green plant genomes, forty-seven of which have been clustered into gene families at 12 evolutionarily significant nodes. Each gene has been annotated with PFAM, KOG, KEGG, PANTHER and GO assignments, where possible. Query-based data access is provided by Phytozome's PhytoMine and BioMart instances, while bulk data sets can be accessed via the JGI's Genome Portal (registration required). JBrowse genome browsers are available for all genomes. (2015-10-02) Take our user survey here	 Search BLAST BLAT PhytoMine Database
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Brachypodium distachyon v2.1 Oryza sativa v7.0 **Brassicaceae** Arabidopsis thaliana TAIR10 Brassica rapa FPsc v1.3



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