Student Online Workshop on

Application of Bioinformatics for Pedagogy of Plant Sciences

Organized by Kirori Mal College

(Under DBT Star Scheme)

23rd July 2021

Plant Cell Biology 101 meets Bioinformatics

By

Prof. Sudeshna Mazumdar-Leighton & Ph.D. Research Scholars of Plant-Biotic Interactions Lab,

Lab 15/18, Department of Botany, University of Delhi

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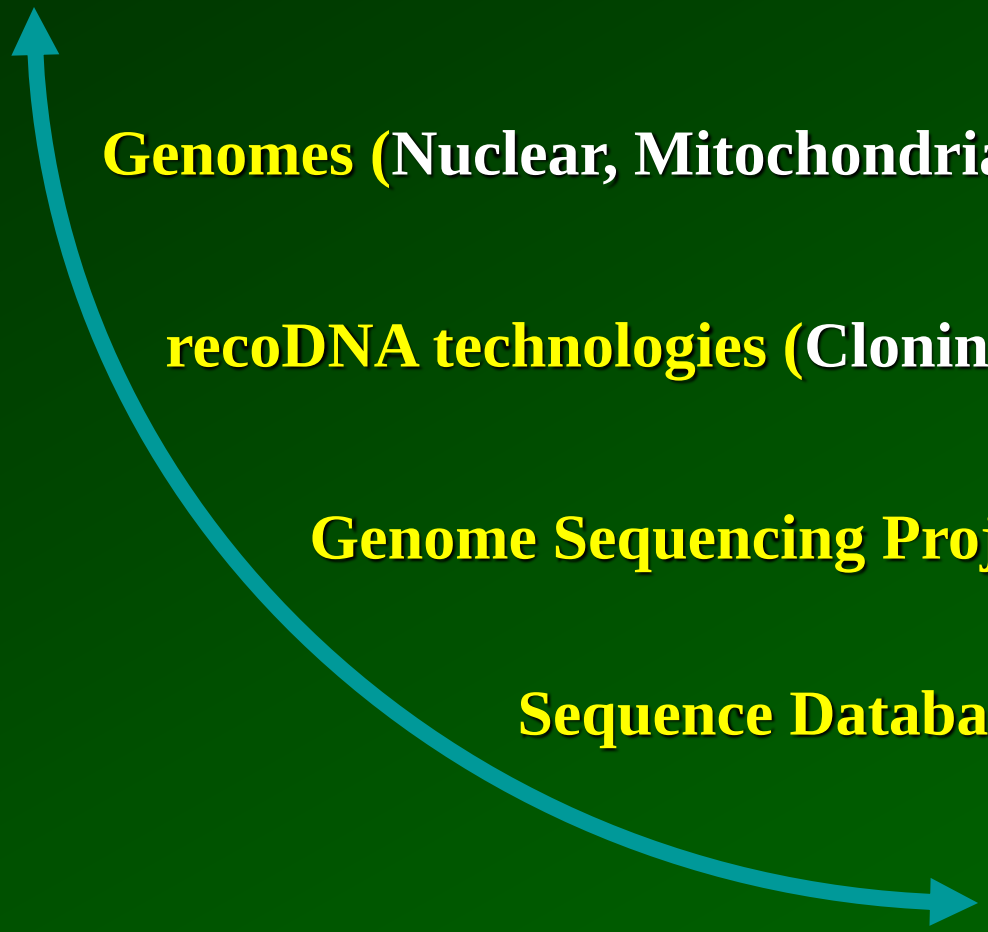
Online workshop contents

Sr. no.	Topics covered	Presenter	Duration
1.	Welcome address	Organizers	3.00 - 3.15 pm
2.	Bioinformatics and Actins in *Arabidopsis*	Prof. Sudeshna Mazumdar-Leighton	3.15 - 3.45 pm (35 min.)
3.	A brief overview of protein sorting; What is iPSORT and how does it work?	Aashima Mehra	3.45 - 4.00 pm (15 min)
4.	Retrieval of sequences from NCBI; Preparation of Fasta files; Prediction of localization sites of protein sequences	K. Tingneivah Mate	4.00 - 4.15 pm (15 min)
5.	Run amino acid index and Data analysis	Mansi Bansal	4.15 - 4.30 pm (15 min)
6.	Bayesian-based prediction software	Parul Bhardwaj	4.30 - 4.45 pm (15 min)
7.	Homework exercise and concluding session		4.45 – 5.00 pm

Overview



Cell (Animal, Plant, Bacteria, Virus + & -)

Genomes (Nuclear, Mitochondrial, Chloroplast)

recoDNA technologies (Cloning, PCR, DNA sequencing*)

Genome Sequencing Projects (HUGO, TAIR*)

Sequence Databases (NCBI, PDB)

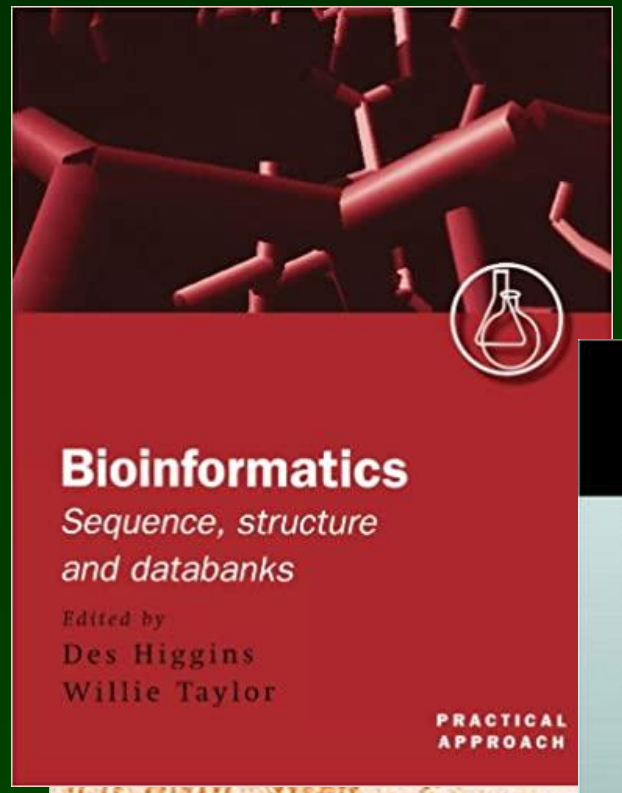
Computational Biology/
Bioinformatics

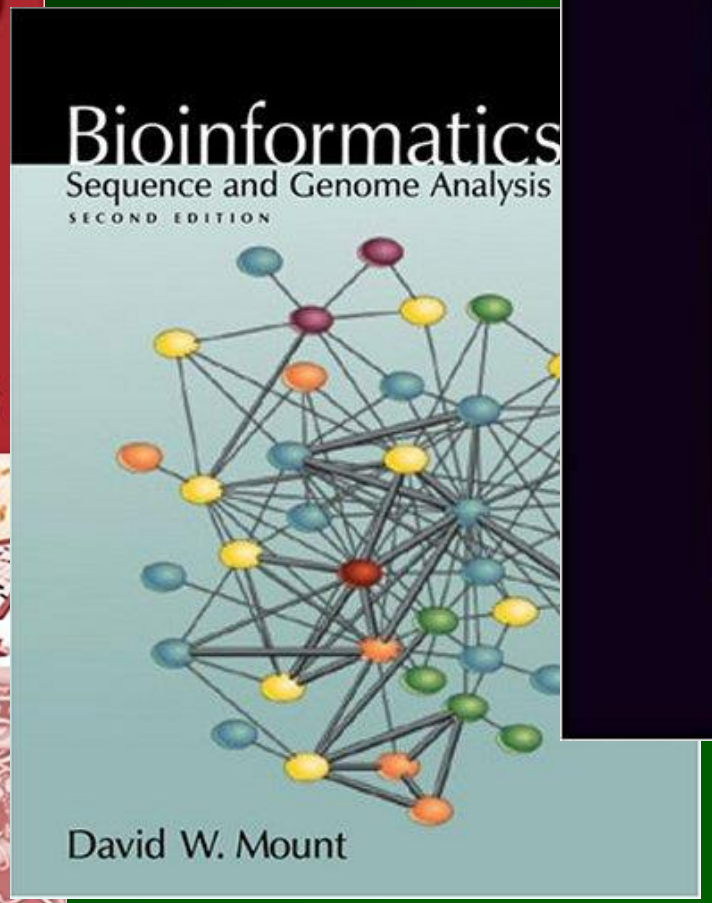
Sequence Databases

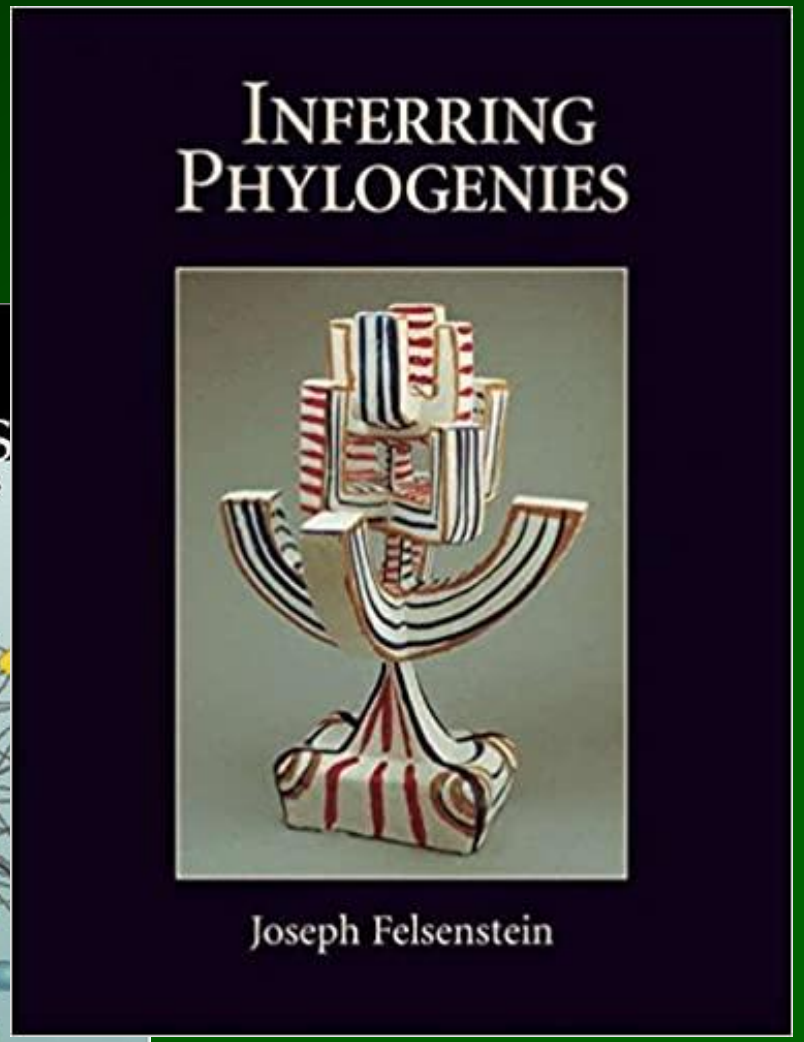
- ***History:*** **Margaret Dayhoff (1970s), Walter Goad (Los Alamos National Lab, NM,USA) (1980s)**
- **DDBJ, EMBL, NCBI (NA)**
- **PIR, Swiss-Prot, MIPS, JIPID (Proteins)**

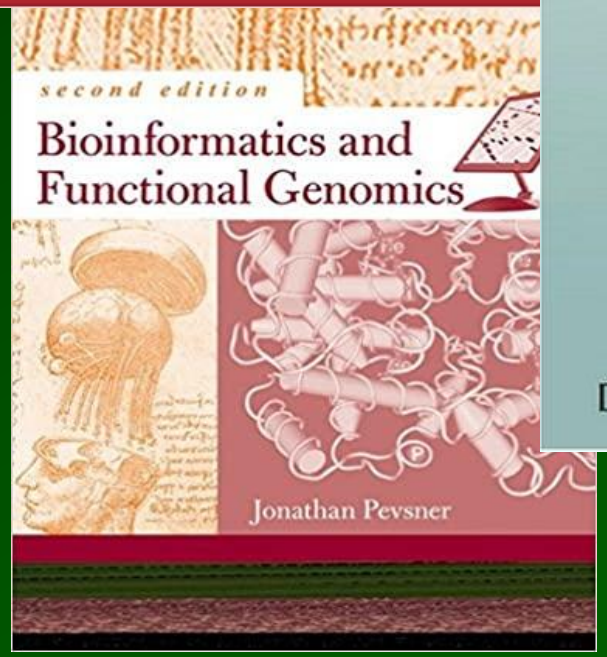
WE RECOMMEND USING FOR CLASS:

http://www.ncbi.nlm.nih.gov









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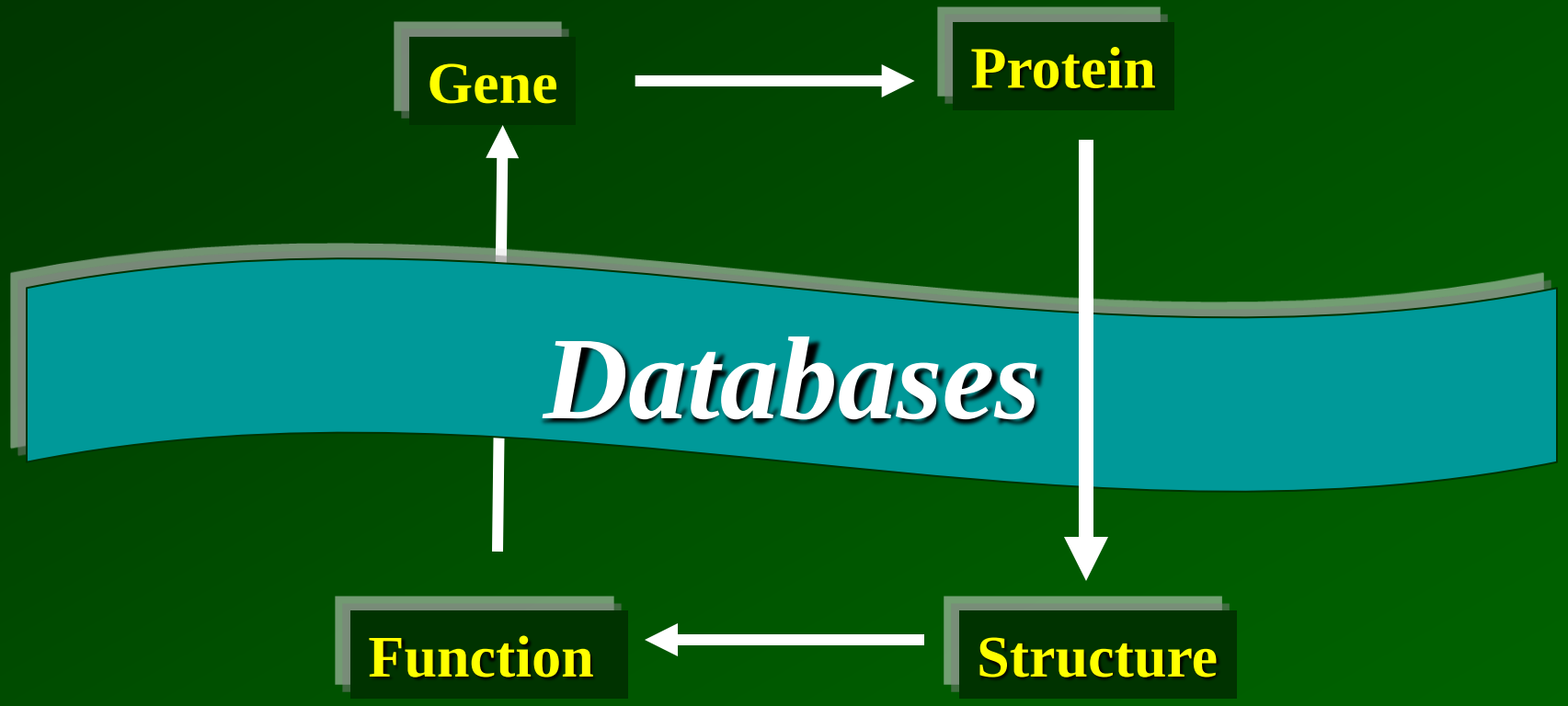
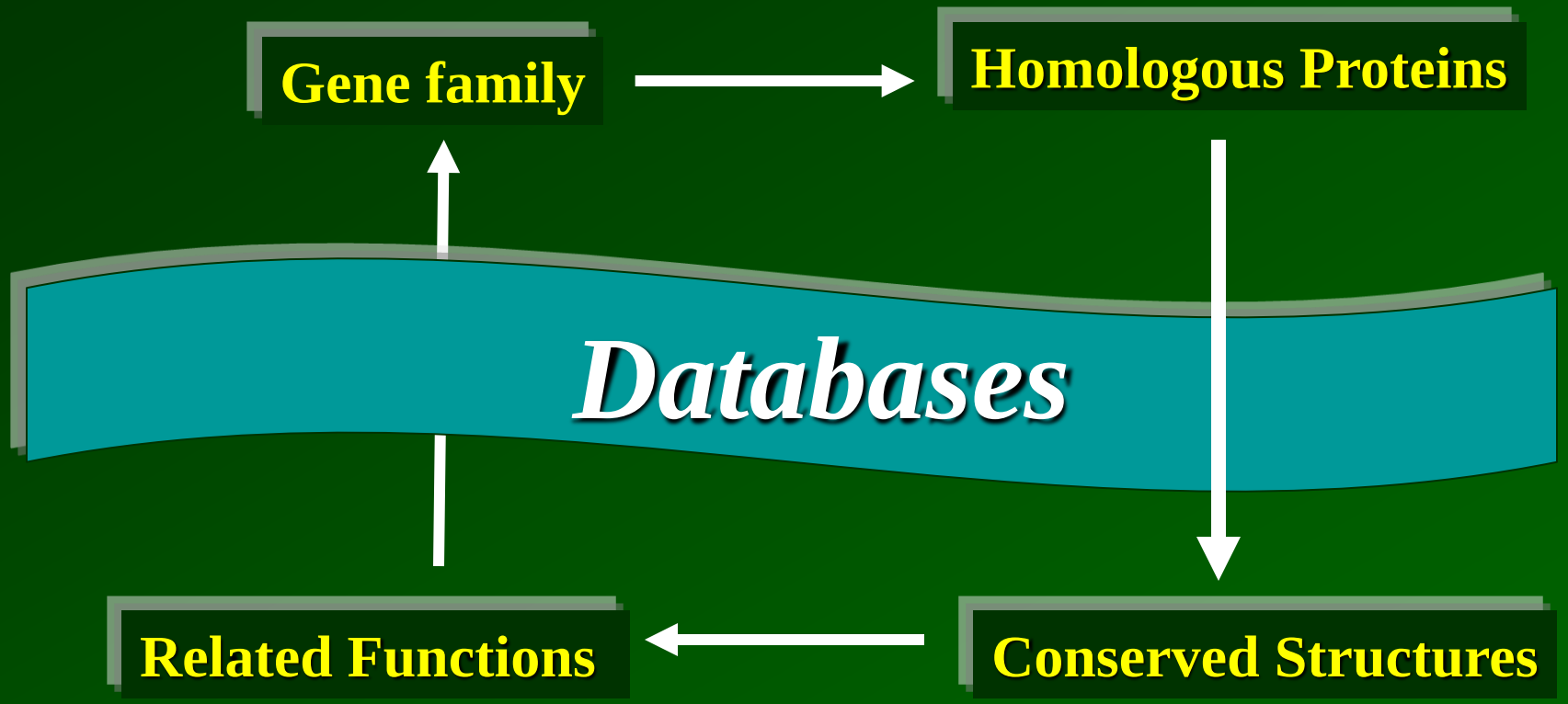
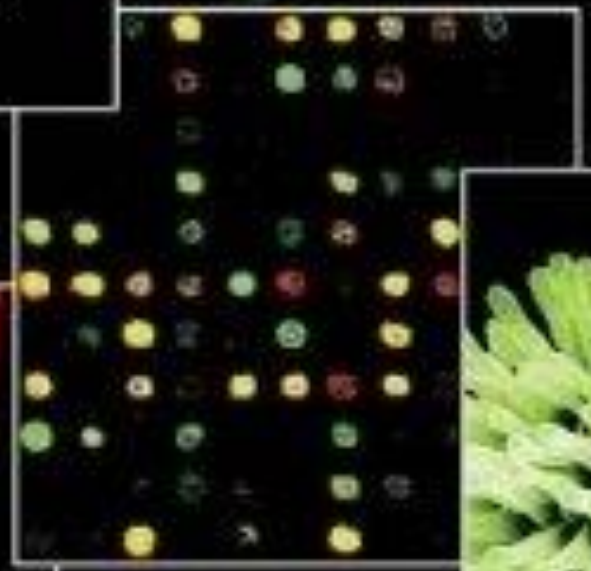
Bioinformatics/Computational Biology

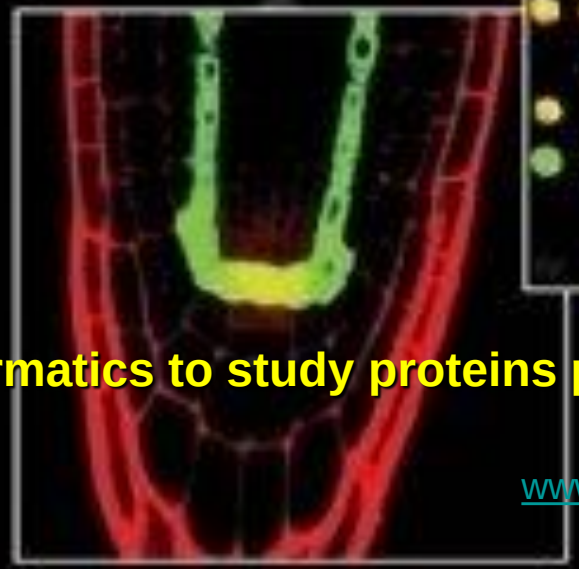


Bioinformatics/Computational Biology



Molecular Evolution of Actin genes in *Arabidopsis thaliana*





***Bioinformatics to study proteins participating in functional organization of cells**

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UNITE
A new NIH initiative to end structural racism and achieve racial equity in the biomedical research enterprise.

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Participating labs contribute over 70 tests for COVID-19 to the NIH Genetic Testing Registry
22 Jul 2021
During the COVID-19 pandemic, an

New RefSeq annotations for human, zebra finch, great white shark and more!
21 Jul 2021
In May and June, the NCBI Eukaryotic Genome Annotation Pipeline released

RefSeq release 207 is available!
16 Jul 2021
RefSeq release 207 is now available online, from the FTP site and through NCBI's Entrez programming utilities. E-

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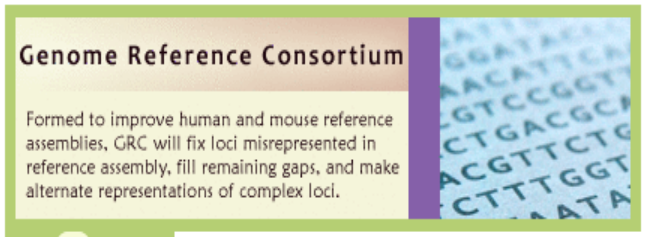
- Training & Tutorials
- Homology
- Small Molecules
- Variation



II 1 2 3

How To...

- Obtain the full text of an article
- Retrieve all sequences for an organism or taxon
- Find a homolog for a gene in another organism
- Find genes associated with a phenotype or disease
- Design PCR primers and check them for specificity
- Find the function of a gene or gene product
- Find syntenic regions between the genomes of two organisms

See all ...

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NLM/NCBI

- Newest H1N1 influenza sequences
- Submit flu sequences to GenBank
- Latest H1N1 citations in PubMed
- MedlinePlus (consumer health information)
- Enviro-Health links

Popular Resources

- PubMed

Done

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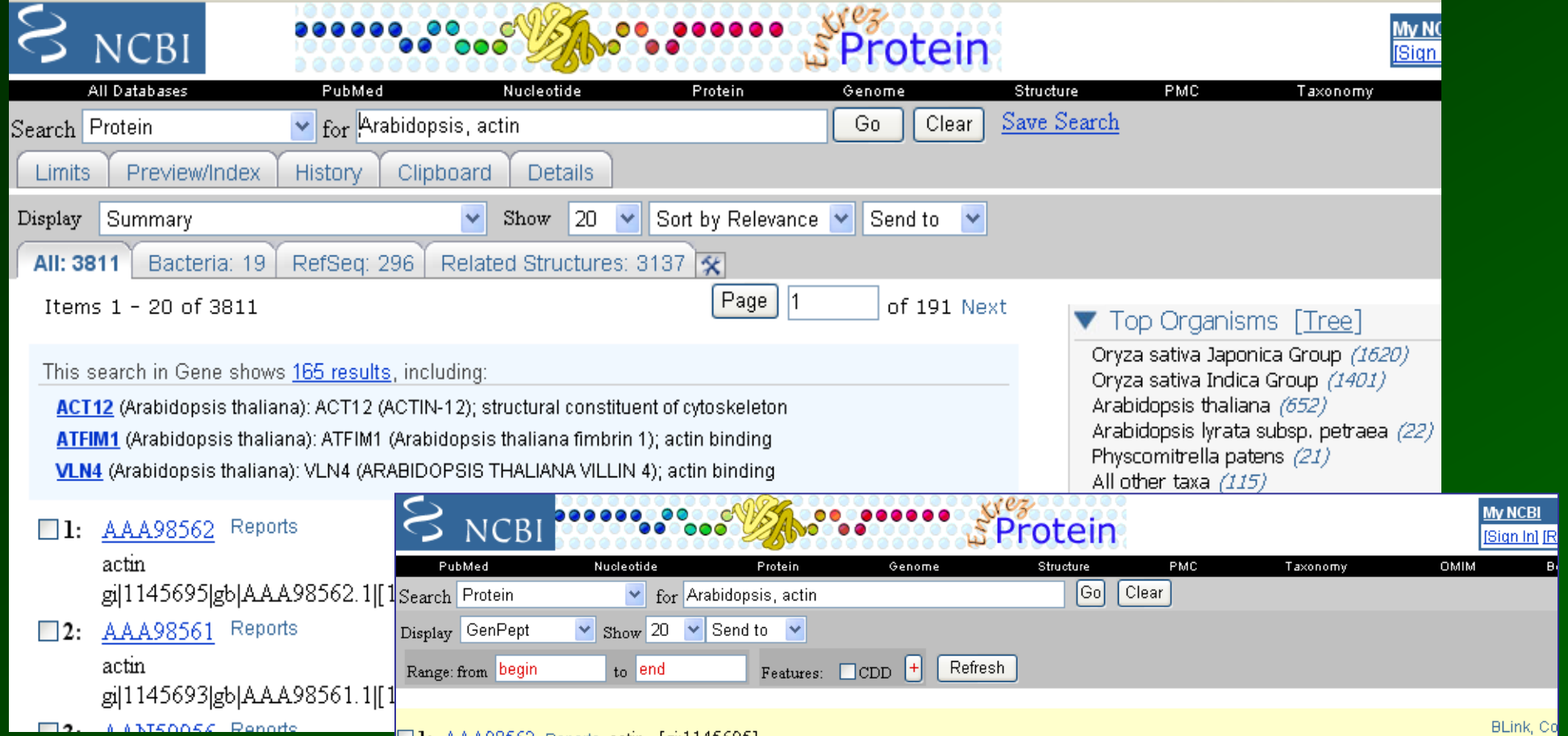

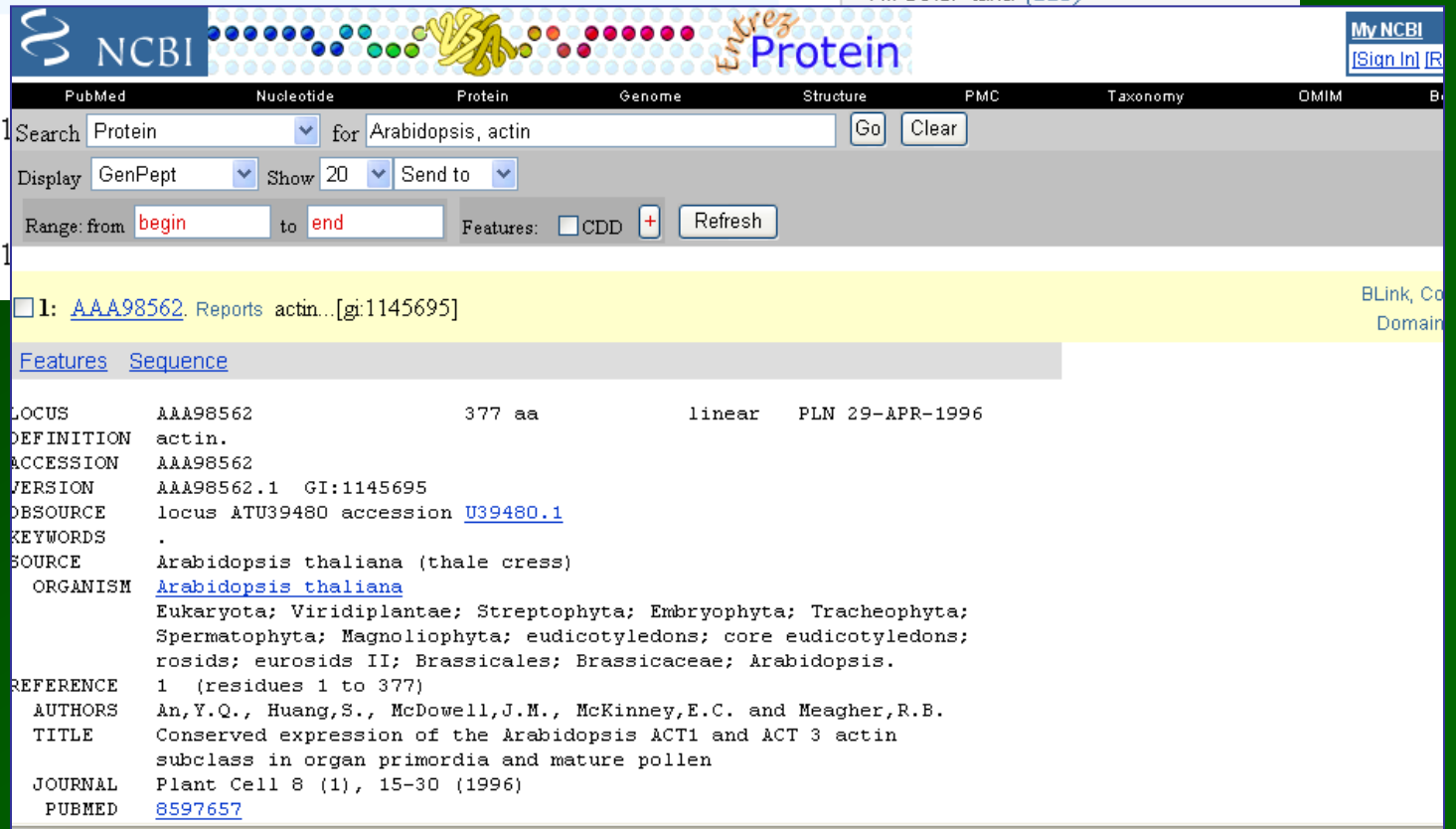

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REFERENCE   1  (residues 1 to 377)
  AUTHORS   An,Y.Q., Huang,S., McDowell,J.M., McKinney,E.C. and Meagher,R.B.
  TITLE     Conserved expression of the Arabidopsis ACT1 and ACT 3 actin
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  JOURNAL   Plant Cell 8 (1), 15-30 (1996)
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      121 mtqimfetfn apamyvaiqa vlslyasgrt tgivldsgdg vshtvpiyeg yalphailrl
      181 dlaqrdltda lmkiltergy sfttaaerei vrdikeklcy ialdyegele taktsssvek
```

A FASTA FILE

- >ACT1
  MADGEDIQPLVCDNGTGMVKAGFAGDDAPRAVFPSIVGRPRHTGVMVGMGQKDAYVGDEA
  QSKRGILTLKYPIEHGIVNNWDDMEKIWHHTFYNELRVAPEEHPILLTEAPLNPKANREKMTQI
  MFETFNAPAMYVAIQAVLSLYASGRTTGIVLDSGDGVSHTVPIYEGYALPHAILRLDLAGRDLT
  DALMKILTERGYSFTTTAEREIVRDIKEKLCYIALDYEQELETAKTSSSVEKNYELPDGQVITIGS
  ERFRCPEVLYQPSMIGMENAGIHETTYNSIMKCDVDIRKDLYGNIVLSGGTTMFPGIADRMSKE
  ITALAPSSMKIKVVAPPERKYSVWIGGSILASLSTFQQMWIAKAEYDESGPSIVHRKCF
- >ACT2
  MAEADDIQPIVCDNGTGMVKAGFAGDDAPRAVFPSVVGRPRHHGVMVGMNQKDAYVGDEA
  QSKRGILTLKYPIEHGVVSNWDDMEKIWHHTFYNELRIAPEEHPVLLTEAPLNPKANREKMTQI
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- >ACT3
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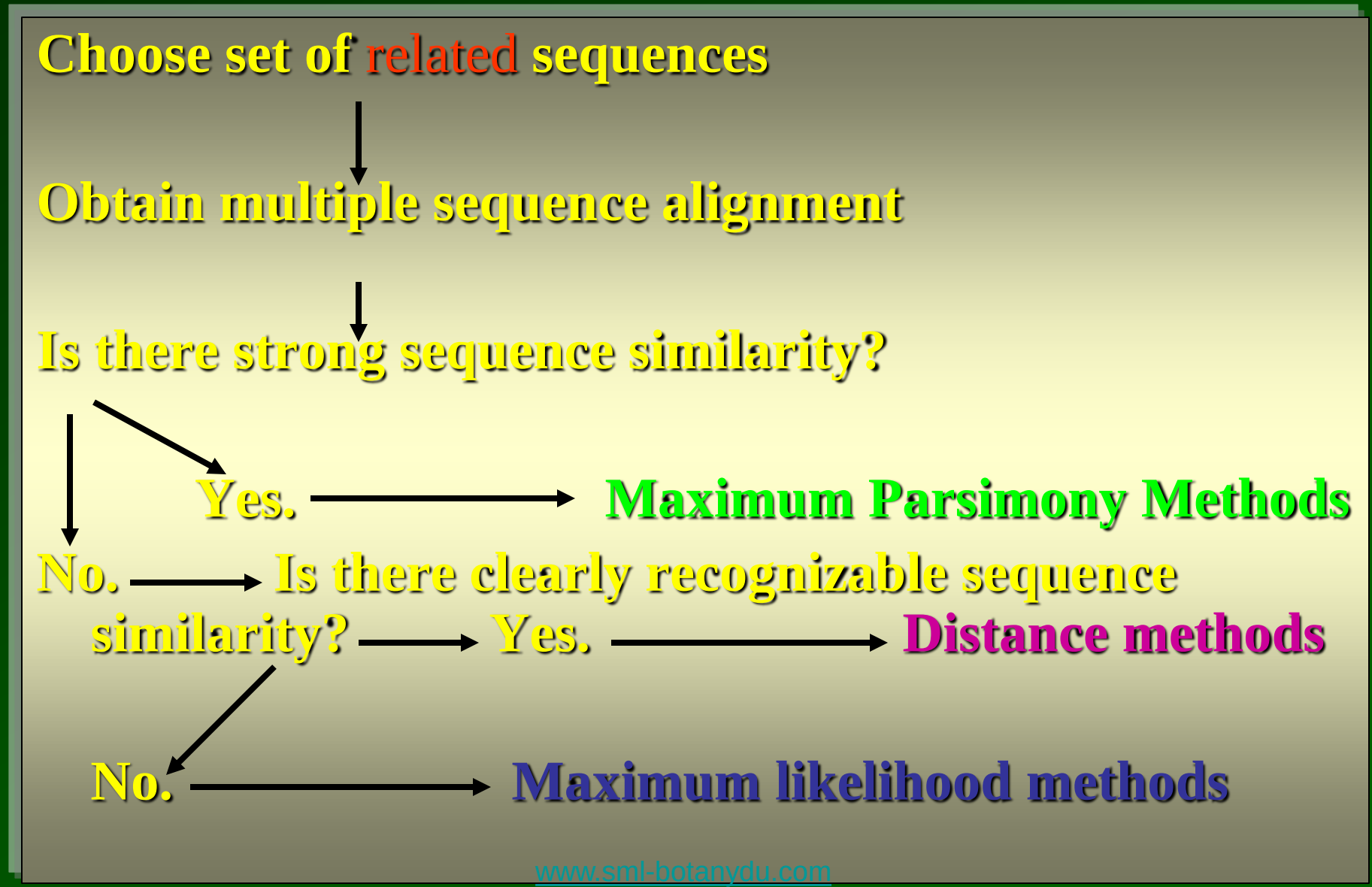
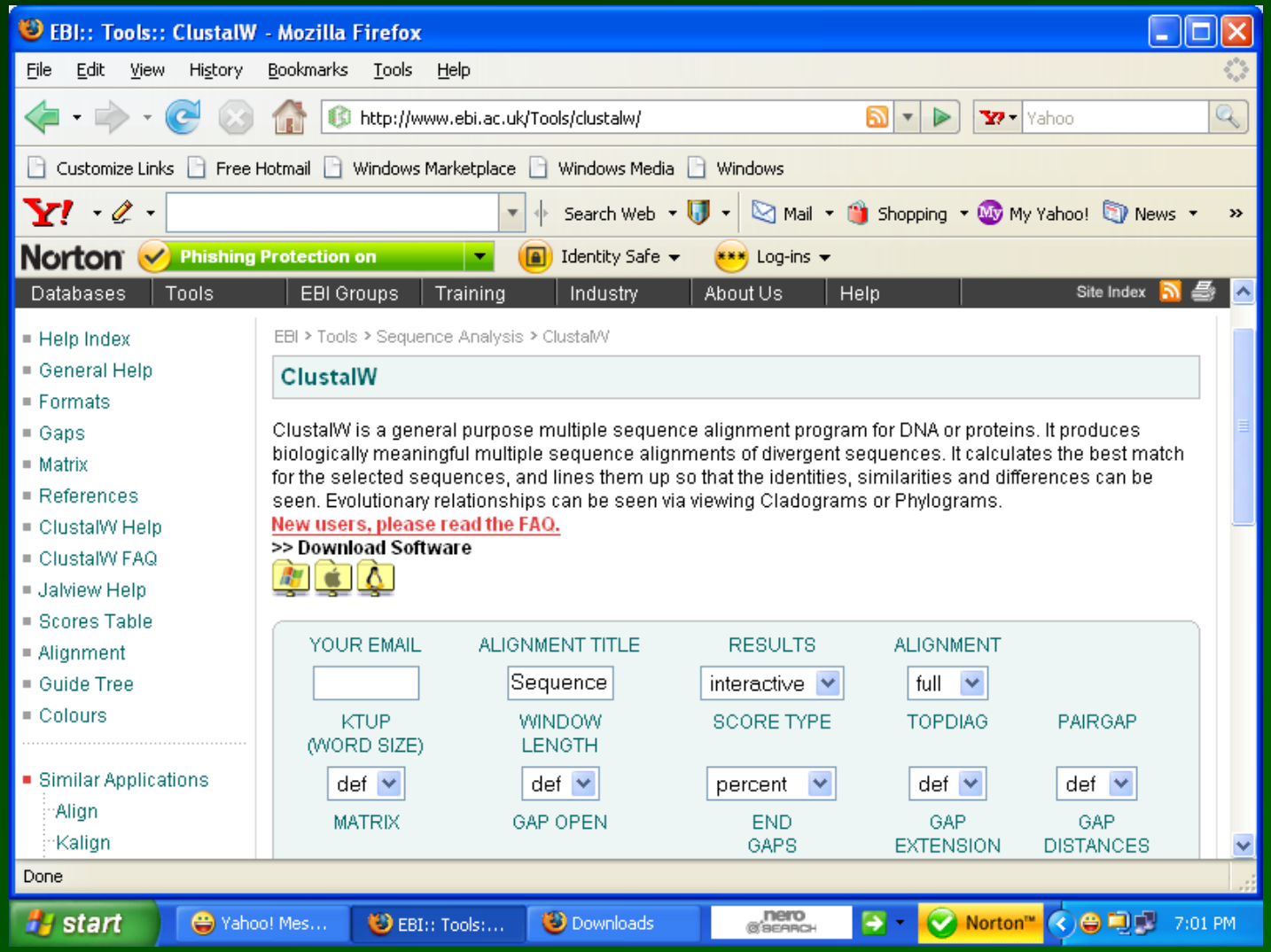
Methods



CLUSTAL W (http://www.ebi.ac.uk)



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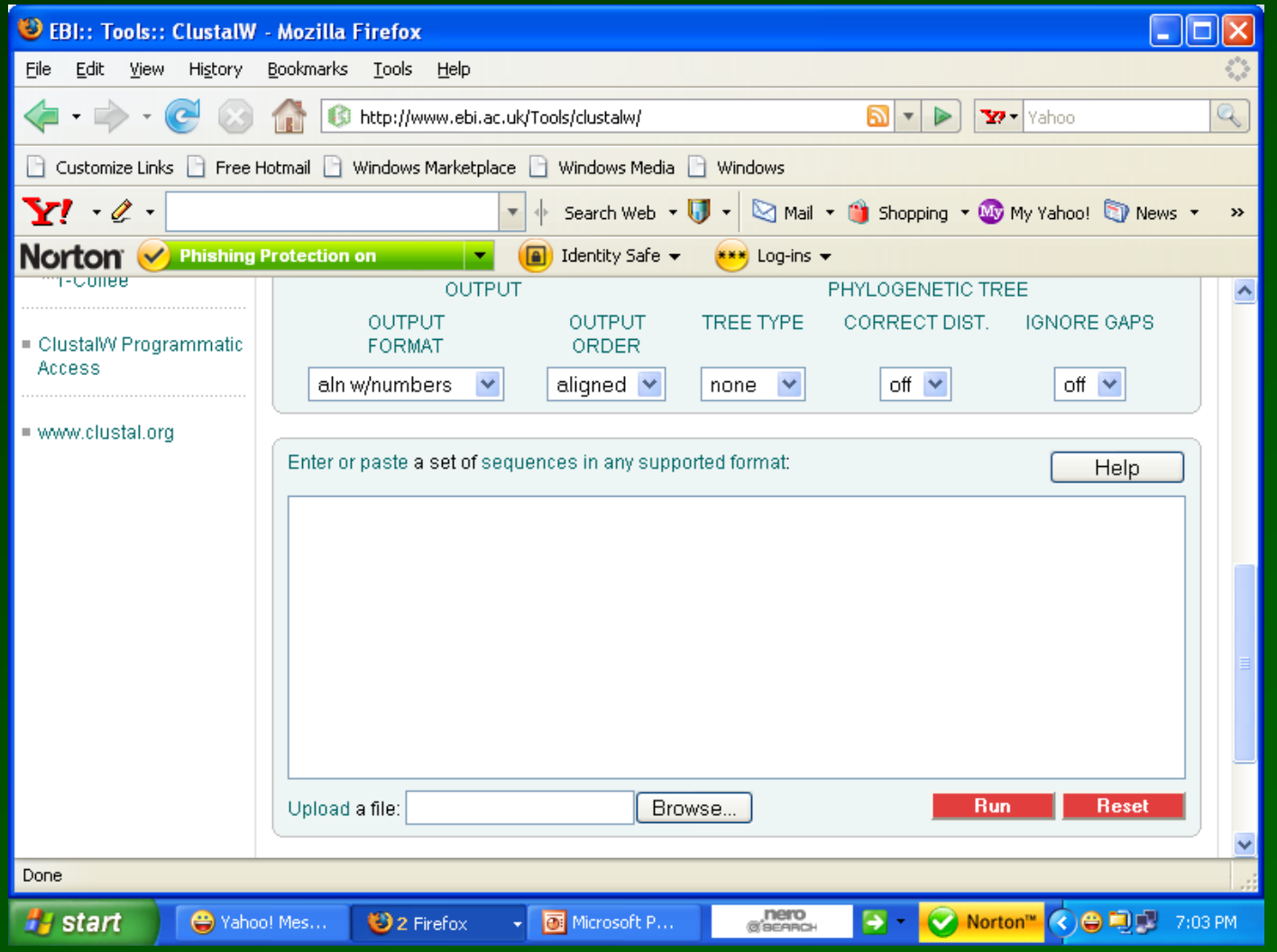


Sequence Alignments

- Pair-wise comparison….

LGPSSKQTGKGS--SRIWDN

LN--ITKSAGKGAIMRLGDA

GLOBAL ALIGNMENT

LOCAL ALIGNMENT

Sequence Alignment

- 2 sequences (protein and nucleotide)

Needleman & Wunsch, 1970 alignments

GATCTA
GATCΔA

		G	A	T	C	T	A
	G	1					
	A		2				1
	T			3		1	
	C				4		
Δ →	A		1				5 minus gap penalty

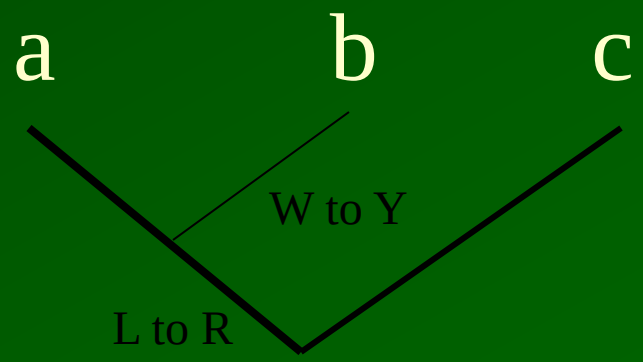
Aligning gene & protein sequences

- Margaret Dayhoff, 1972, 1978 (PIR) Matrices based PAM tables (percent amino acid substitutions)

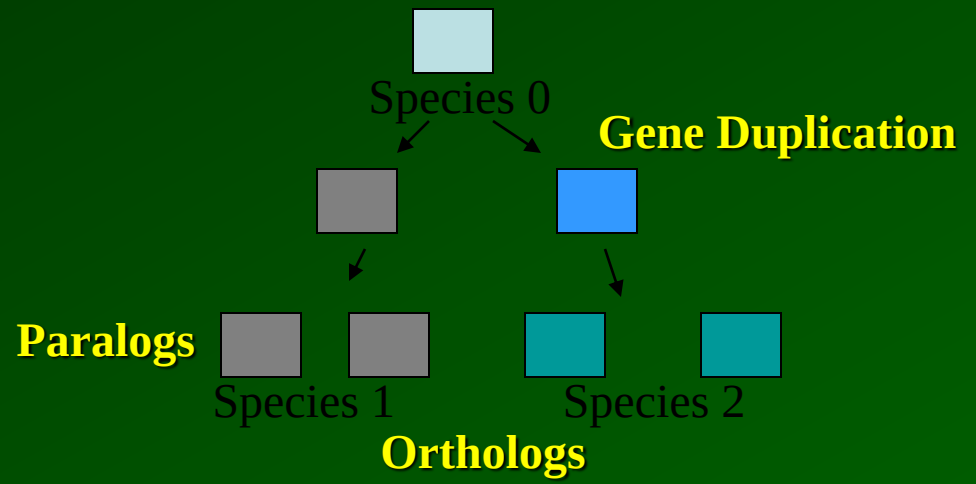
Organism a AWTVASAVRLSI

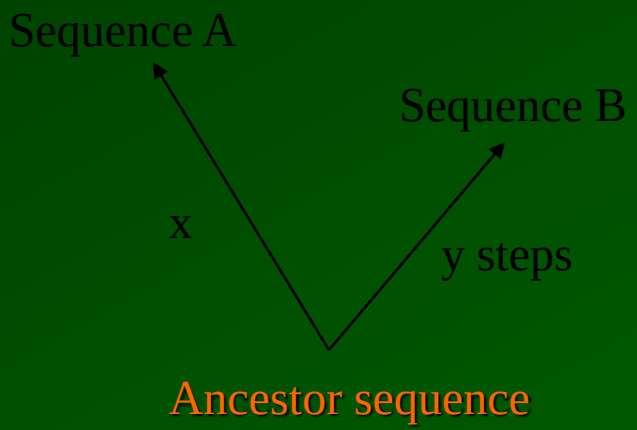
Organism b AYTVAAAVRLSI

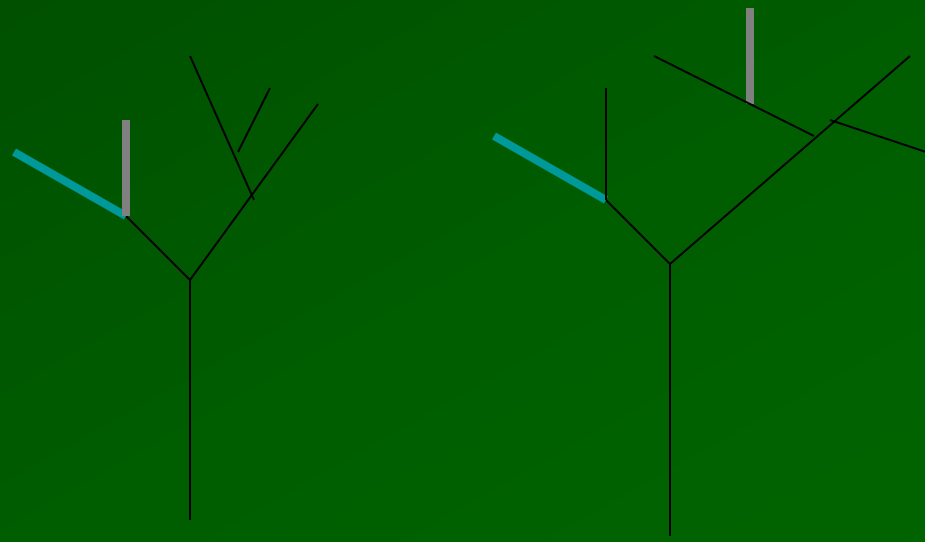
Organism c AWTVAAAVLTSI



Significance of Sequence Alignments

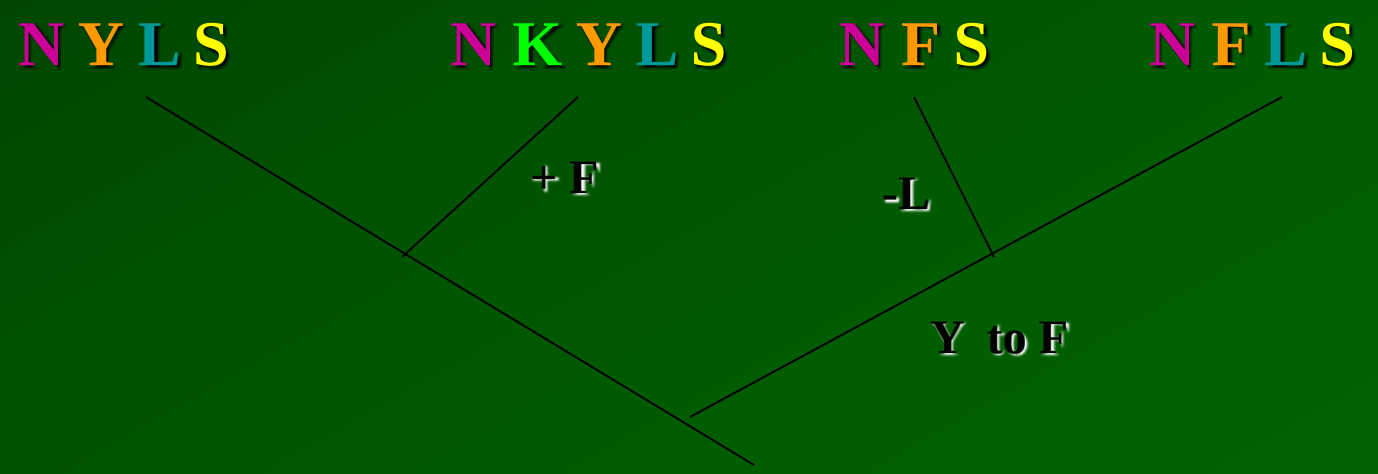






Multiple Sequence Alignment, MSA

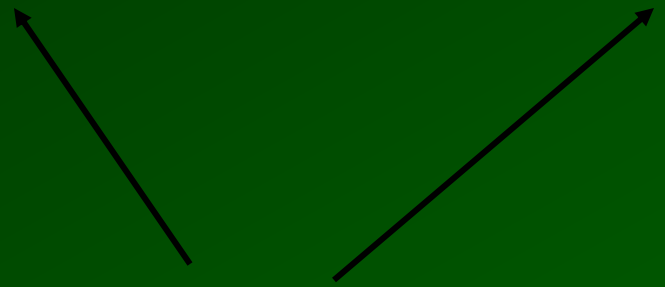
seqA N * F L S
seqB N * F - S
seqC N K Y L S
seqD N * Y L S



Multiple Sequence Alignment & Trees

- MSA is a foundation step in the determination of evolutionary relationships among multiple sequences. They can be of proteins or nucleotides.

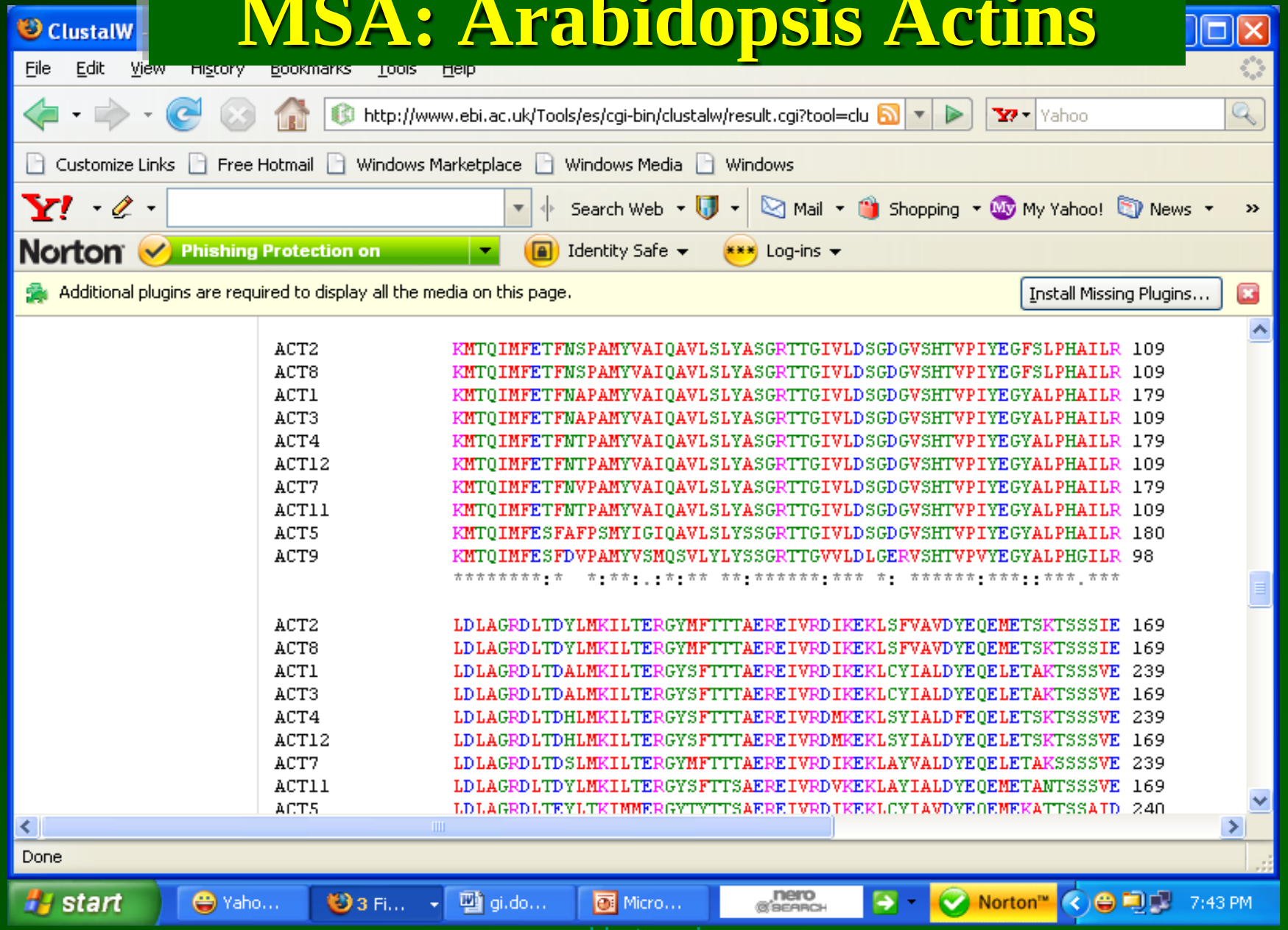
GAGTT **GAATC**



Ancestor: GA (G/A)T(C/T)

***Softwares convert MSA data into a tree using algorithms. Trees can be Rooted/Unrooted.**

MSA: Arabidopsis Actins



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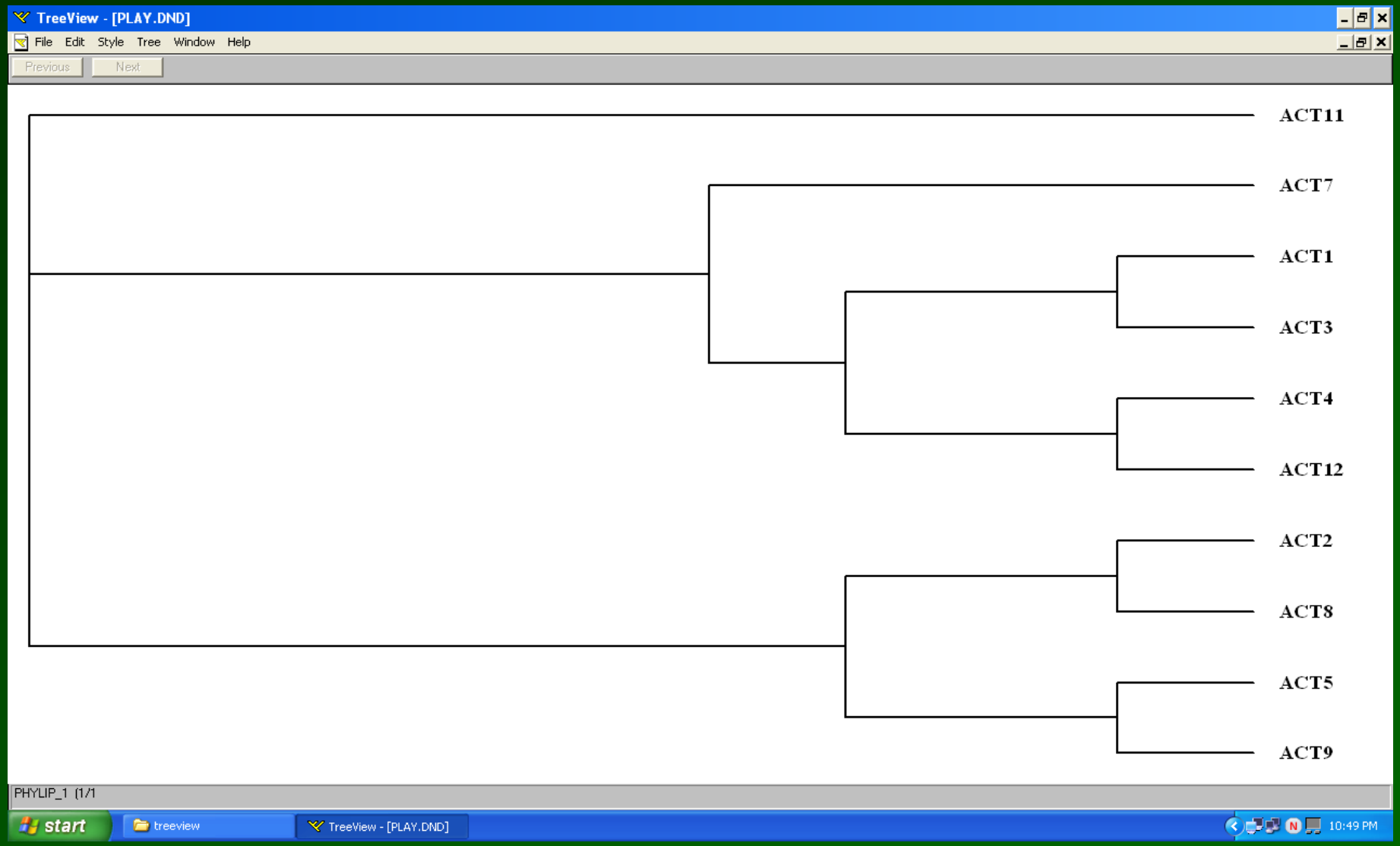
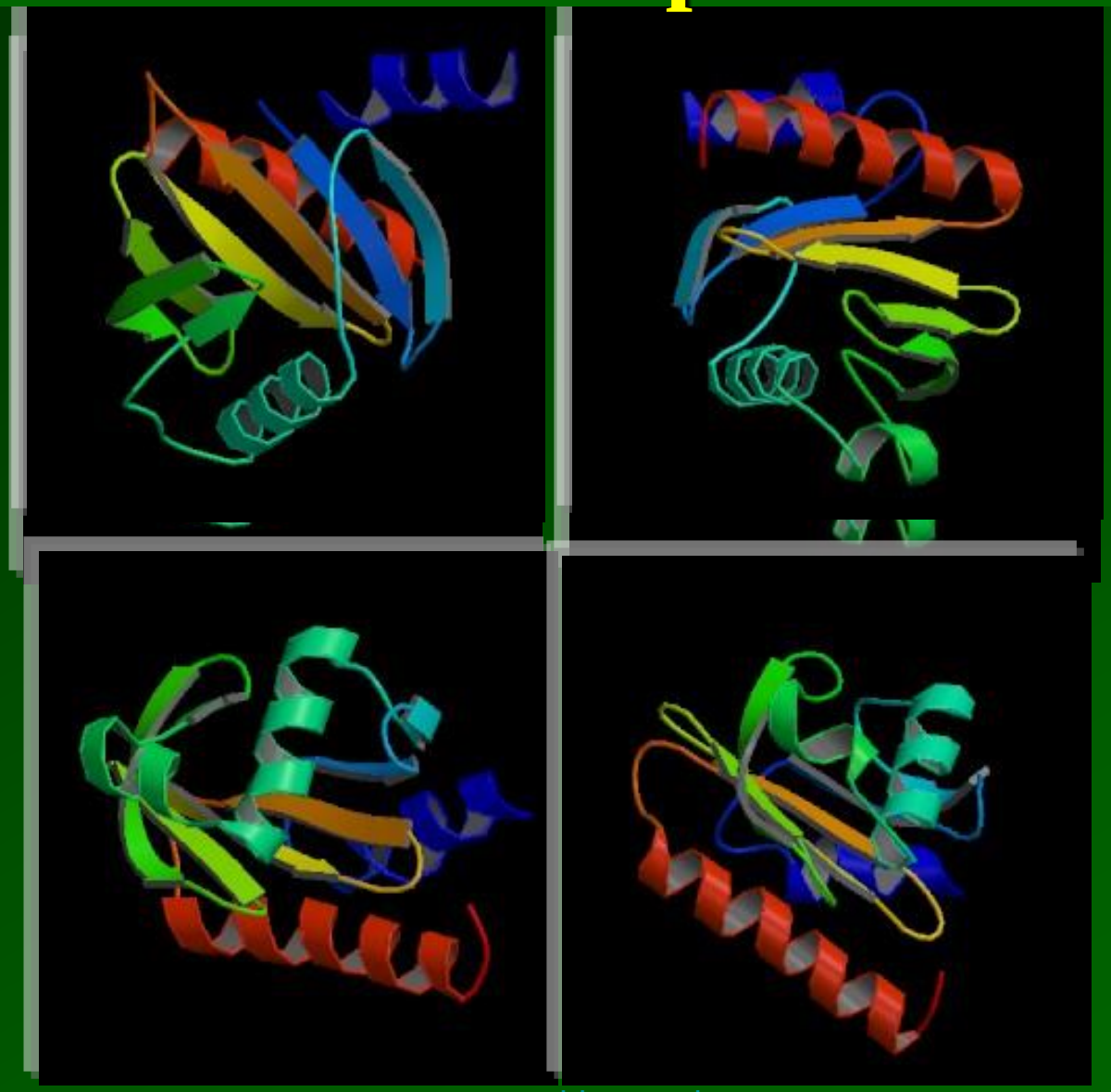
Tree of Arabidopsis actins



MSAs also describe protein structures



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REFERENCE   1  (residues 1 to 377)
  AUTHORS   An,Y.Q., Huang,S., McDowell,J.M., McKinney,E.C. and Meagher,R.B.
  TITLE     Conserved expression of the Arabidopsis ACT1 and ACT 3 actin
            subclass in organ primordia and mature pollen
  JOURNAL   Plant Cell 8 (1), 15-30 (1996)
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  JOURNAL   Submitted (25-OCT-1995) Yong-Qiang An, Deptartment of Genetics,
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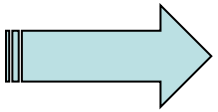
**Arabidopsis, Actin, Meagher



Identify Conserved Domains

Highlight Sequence Features

Find in this Sequence

Related information

Nucleotide

PubMed

Taxonomy

CDD Search Results

Conserved Domains (Concise)

Conserved Domains (Full)

Full text in PMC

Related Structures (List)

Related Structures (Summary)

Recent activity

Turn Off Clear

actin 1 [Arabidopsis thaliana]
Protein

Actin, Arabidopsis, meagher (56)
Protein

actin 4 [Arabidopsis thaliana]
Protein

actin-12 [Arabidopsis thaliana]
Protein

actin [Oryza sativa Japonica Group]
Protein

See more...

NCBI Genome Data Viewer

ncbi.nlm.nih.gov/genome/gdv/

Genome Data Viewer

GDV supports the exploration and analysis of *NCBI-annotated* and selected non-NCBI annotated eukaryotic genome assemblies. Currently, over 1250 assemblies are available.

Switch view

Search organisms: Homo sapiens (human)

To view more organisms in the tree, click on nodes that have '+' signs. Press and hold the '+' to expand and reveal all the subgroups. Or, search for an organism using the search box above.

New! Click on Switch view at the top to see another way of navigating genomes.

Homo sapiens (human)

Search in genome

Location, gene or phenotype

Examples: TXLNA, chr1:32178000-32200000, DNA repair

Assembly: GRCh38.p13

Browse genome | BLAST genome

Download via NC

Explore this genome in Genome Data Viewer

Assembly details

Name	GRCh38.p13
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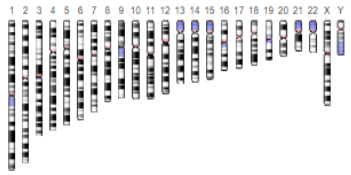
GenBank accession	GCA_000001405.28
Submitter	Genome Reference Consortium
Level	Chromosome
Category	Reference genome
Replaced by	GCF_000001405.25

Annotation details

Annotation Release	109
Release date	May 16, 2021



https://www.ncbi.nlm.nih.gov/genome/gdv/browser/genome/?id=GCF_000001405.39#gdvl=...

Type here to search

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“Seeking more...”

Arabidopsis (Arabidopsis thaliana

ncbi.nlm.nih.gov/genome/gdv/?org=arabidopsis-thaliana&group=brassicaceae

Genome Data Viewer

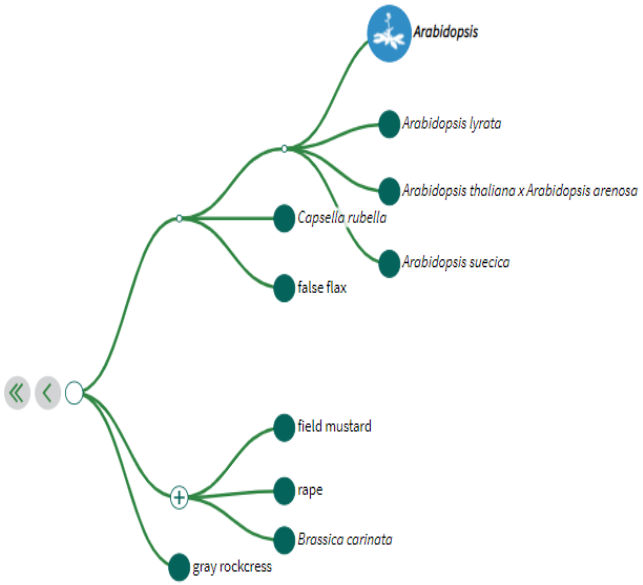
GDV supports the exploration and analysis of NCBI-annotated and selected non-NCBI annotated eukaryotic genome assemblies. Currently, over 1250 assemblies are available.

Switch view

Search organisms: Arabidopsis thaliana (thale cress)

To view more organisms in the tree, click on nodes that have '+' signs. Press and hold the '+' to expand and reveal all the subgroups. Or, search for an organism using the search box above.

New! Click on Switch view at the top to see another way of navigating genomes.



Arabidopsis thaliana (thale cress)

Search in genome: Actin

Genes | Other

Name	Location
ACT12	Chr3: 17,128,211 - 17,131,466
ACT12	Chr3: 17,128,211 - 17,131,466
ARP2	Chr3: 9,952,479 - 9,955,982
ARP2	Chr3: 9,952,479 - 9,955,982
DIS1	Chr1: 4,494,924 - 4,498,469
DIS1	Chr1: 4,494,924 - 4,498,469
ADF1	Chr3: 16,909,217 - 16,910,845
ADF1	Chr3: 16,909,217 - 16,910,845

Examples: VHA-A1, chr2:12208000-12218000, DNA repair

Assembly: TAIR10.1

Browse genome | BLAST genome

Download via NCBI Datasets

Assembly details

Name	TAIR10.1
RefSeq accession	GCF_000001735.4
GenBank accession	GCA_000001735.2
Submitter	The Arabidopsis Information Resource (TAIR)
Level	Chromosome
Category	Reference genome
Replaced by	GCF_000001735.2

Annotation details

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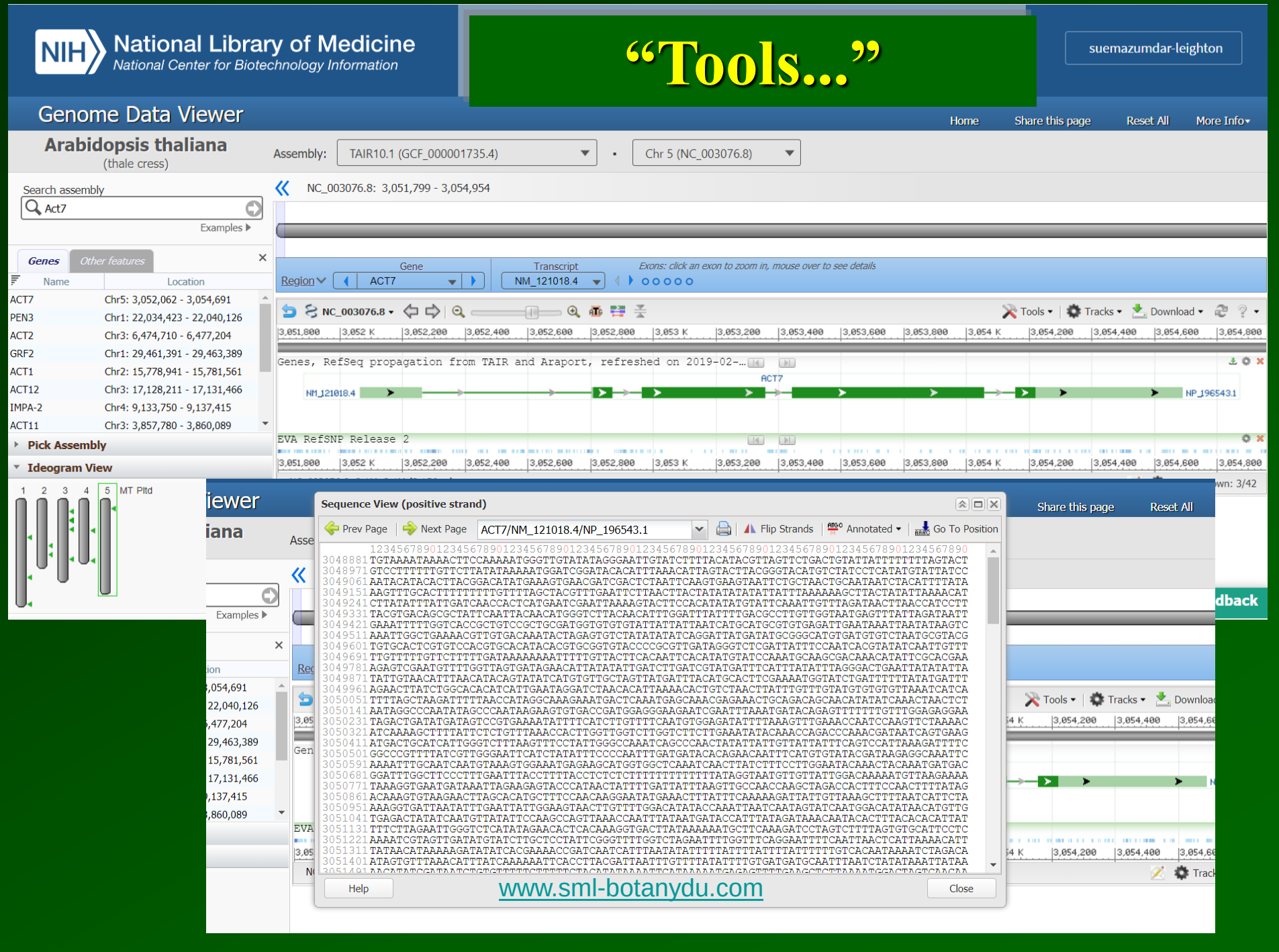
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National Center for Biotechnology Information
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More Info
Arabidopsis thaliana
(thale cress)
Assembly:
TAIR10.1 (GCF_000001735.4)
Chr 5 (NC_003076.8)
Search assembly
Act7
Examples
Genes
Other features
Name
Location
ACT7 Chr5: 3,052,062 - 3,054,691
PEN3 Chr1: 22,034,423 - 22,040,126
ACT2 Chr3: 6,474,710 - 6,477,204
GRF2 Chr1: 29,461,391 - 29,463,389
ACT1 Chr2: 15,778,941 - 15,781,561
ACT12 Chr3: 17,128,211 - 17,131,466
IMPA-2 Chr4: 9,133,750 - 9,137,415
ACT11 Chr3: 3,857,780 - 3,860,089
Pick Assembly
Ideogram View
NC_003076.8: 3,051,799 - 3,054,954
Region
Gene
ACT7
Transcript
NM_121018.4
Exons: click an exon to zoom in, mouse over to see details
Tools
Tracks
Download
Genes, RefSeq propagation from TAIR and Araport, refreshed on 2019-02-...
NM_121018.4
NP_196543.1
EVA RefSNP Release 2
Sequence View (positive strand)
Prev Page
Next Page
ACT7/NM_121018.4/NP_196543.1
Flip Strands
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Go To Position
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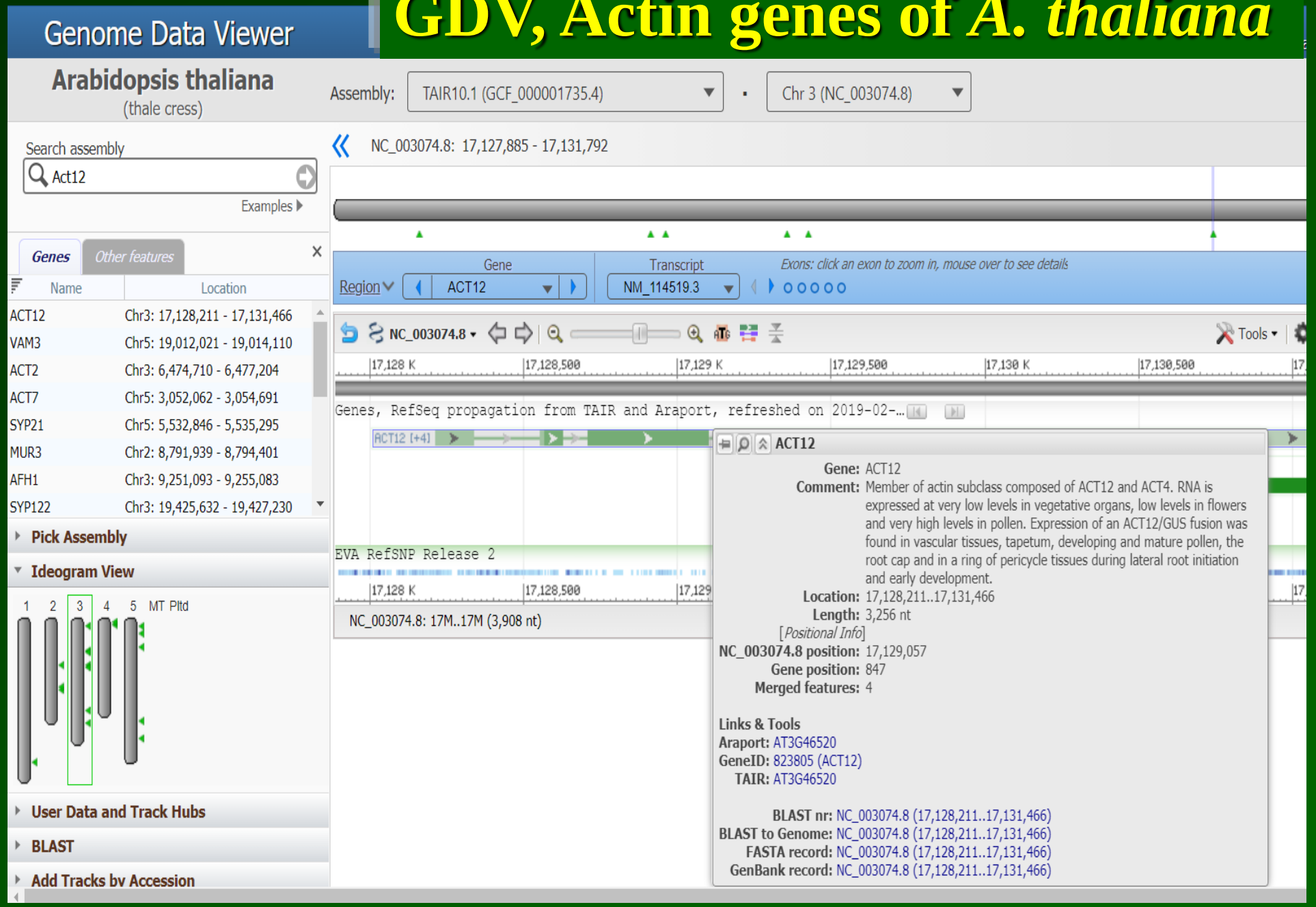
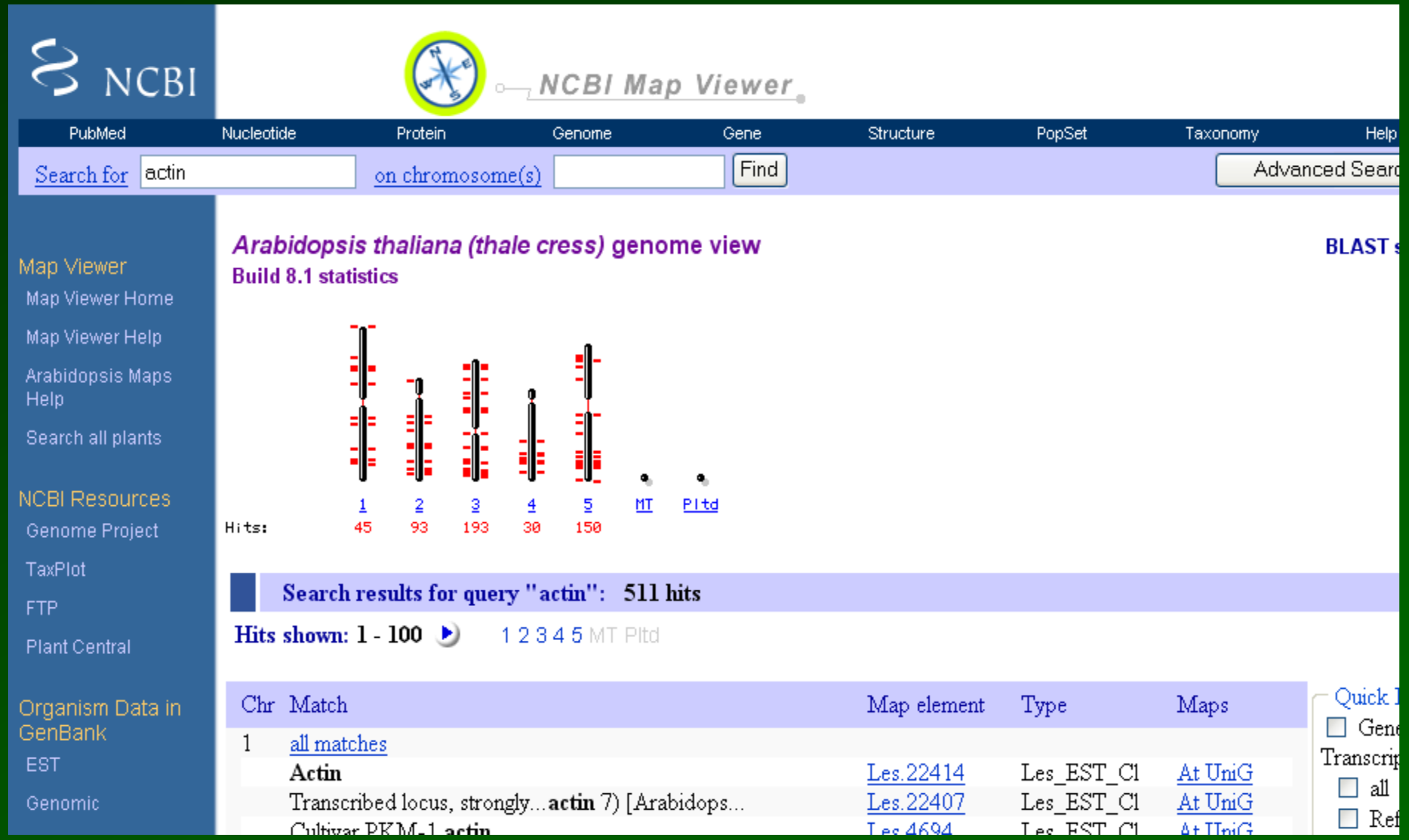
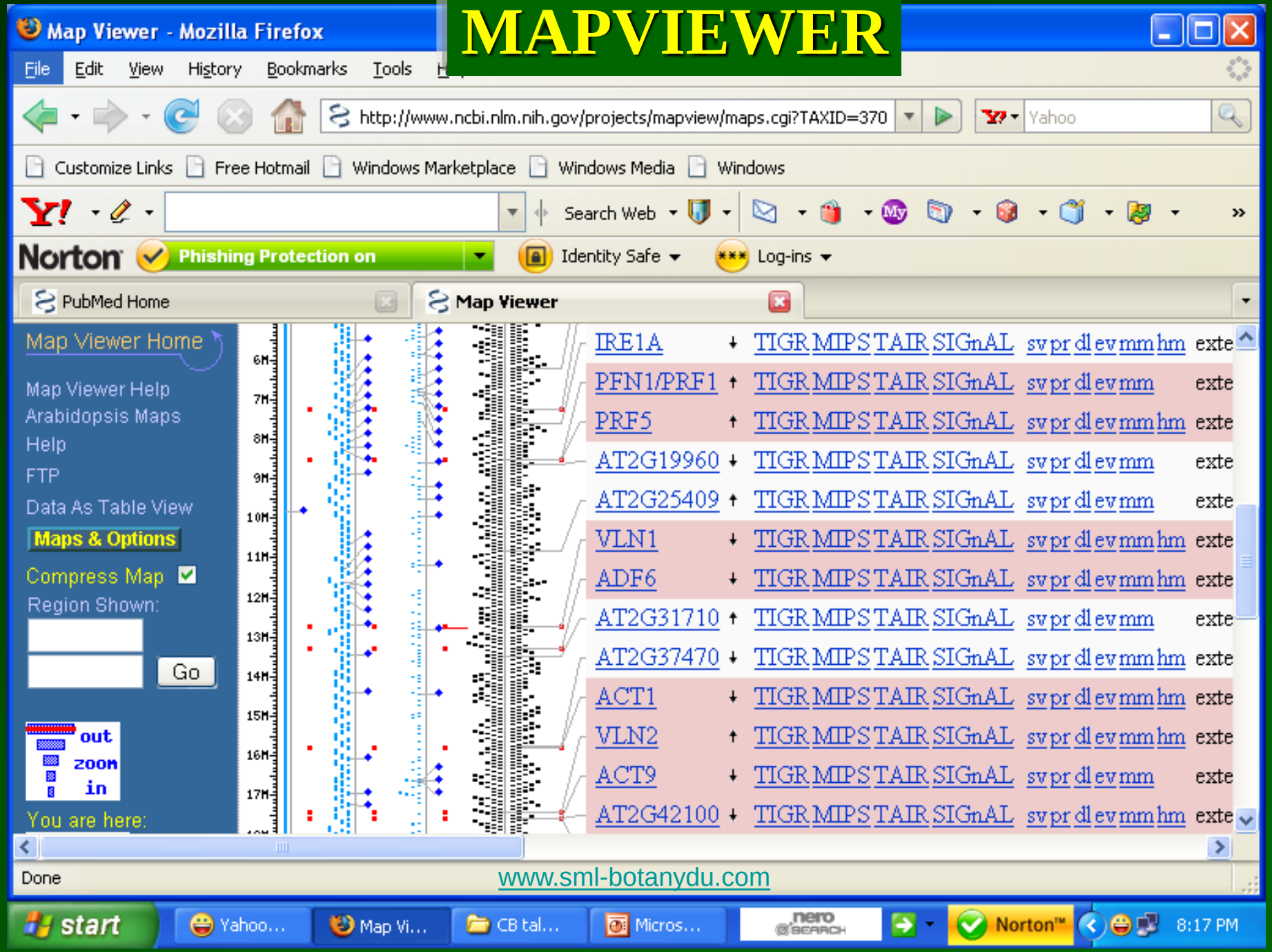
GDV, Actin genes of *A. thaliana*



MAPVIEWER: *A. thaliana* ACTIN



MAPVIEWER



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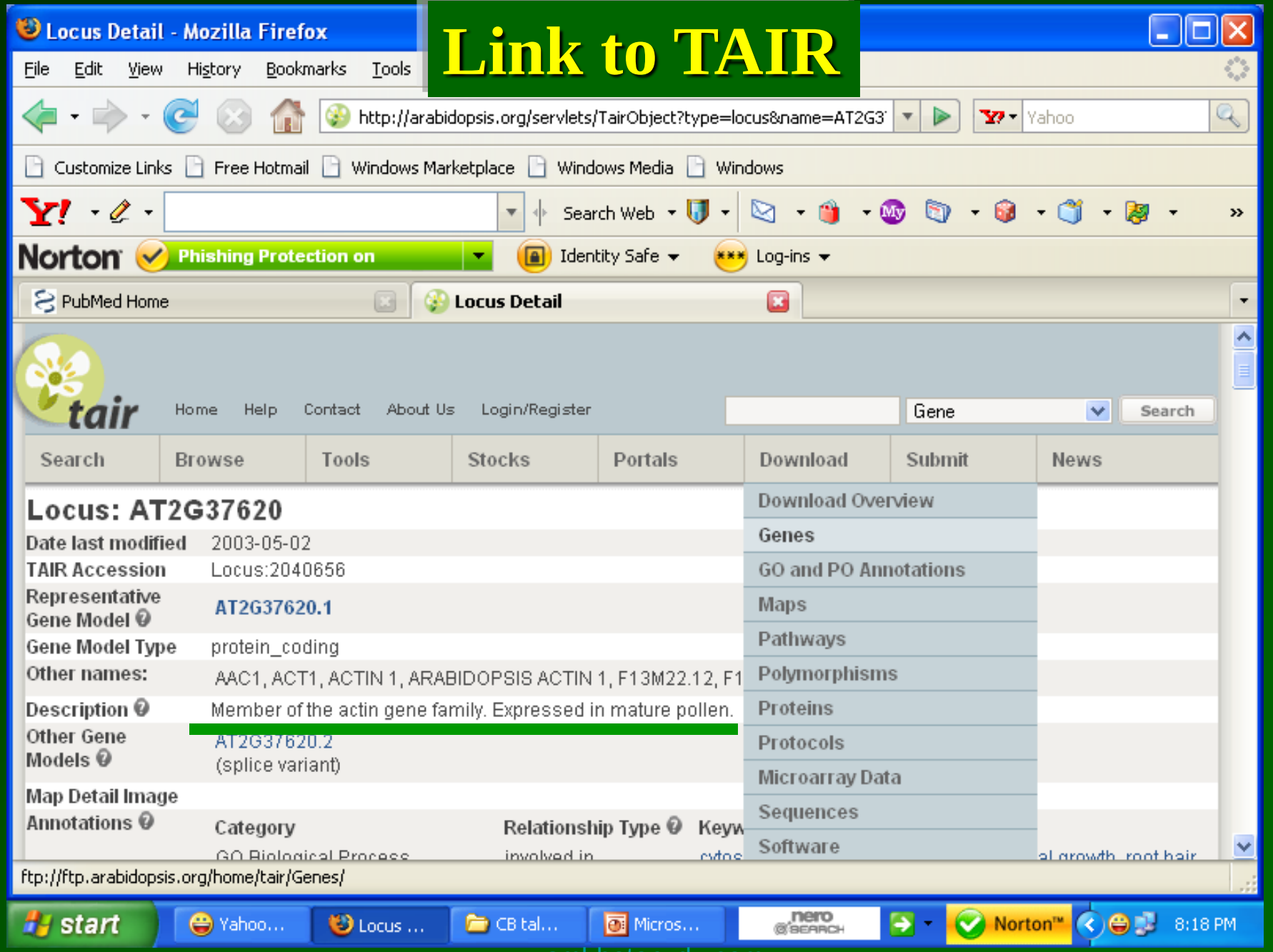
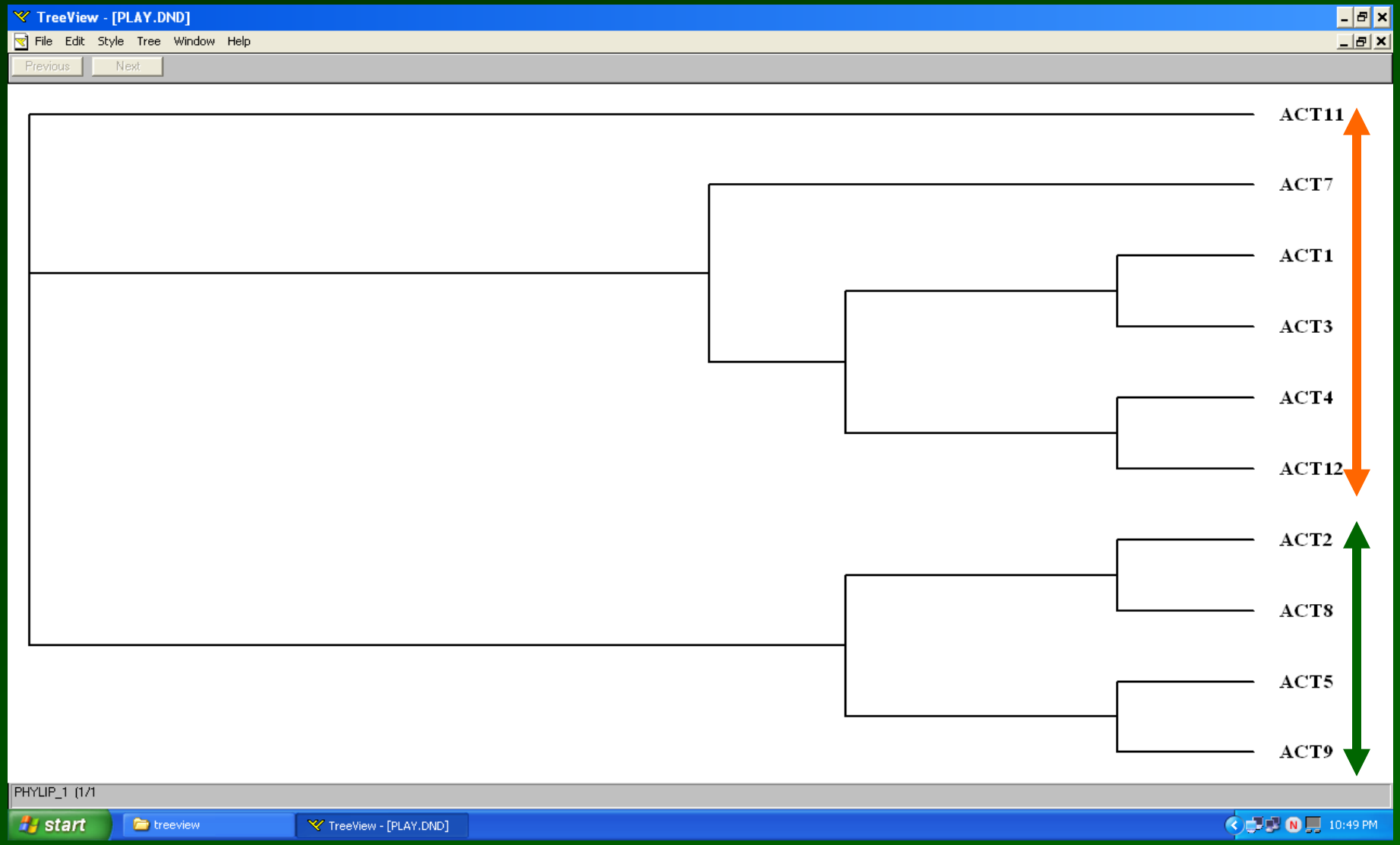
Link to TAIR



A FASTA FILE

- >ACT1 **(POLLEN)**
- MADGEDIQPLVCDNGTGMVKAGFAGDDAPRAVFPSIVGRPRHTGVMVGMGQKDAYVGDEA
  QSKRGILTLKYPIEHGIVNNWDDMEKIWHHTFYNELRVAPEEHPILLTEAPLNPKANREKMTQI
  MFETFNAPAMYVAIQAVLSLYASGRTTGIVLDSGDGVSHTVPIYEGYALPHAILRLDLAGRDLT
  DALMKILTERGYSFTTTAEREIVRDIKEKLCYIALDYEQELETAKTSSSVEKNYELPDGQVITIGS
  ERFRCPEVLYQPSMIGMENAGIHETTYNSIMKCDVDIRKDLYGNIVLSGGTTMFPGIADRMSKE
  ITALAPSSMKIKVVAPPERKYSVWIGGSILASLSTFQQMWIAKAEYDESGPSIVHRKCF
- >ACT2 **(ROOT, STEM, LEAVES of mature plants)**
- MAEADDIQPIVCDNGTGMVKAGFAGDDAPRAVFPSVVGRPRHHGVMVGMNQKDAYVGDEA
  QSKRGILTLKYPIEHGVVSNWDDMEKIWHHTFYNELRIAPEEHPVLLTEAPLNPKANREKMTQI
  MFETFNSPAMYVAIQAVLSLYASGRTTGIVLDSGDGVSHTVPIYEGFSLPHAILRLDLAGRDLT
  DYLMKILTERGYMFTTTAEREIVRDIKEKLSFVAVDYEQEMETSKTSSSIEKNYELPDGQVITIG
  AERFRCPEVLFQPSFVGMEAAGIHETTYNSIMKCDVDIRKDLYGNIVLSGGTTMFSGIADRMSK
  EITALAPSSMKIKVVAPPERKYSVWIGGSILASLSTFQQVKIDQILFRILLHAN
- >ACT3 **(POLLEN, OVULES)**
  MADGEDIQPLVCDNGTGMVKAGFAGDDAPRAVFPSIVGRPRHTGVMVGMGQKDAYVGDEA
  QSKRGILTLKYPIEHGIVNNWDDMEKIWHHTFYNELRVAPEEHPILLTEAPLNPKANREKMTQI
  MFETFNAPAMYVAIQAVLSLYASGRTTGIVLDSGDGVSHTVPIYEGYALPHAILRLDLAGRDLT
  DALMKILTERGYSFTTTAEREIVRDIKEKLCYIALDYEQELETAKTSSSVEKNYELPDGQVITIGS
  ERFRCPEVLYQPSMIGMENAGIHETTYNSIMKCDVDIRKDLYGNIVLSGGTTMFPGIADRMSKE
  ITALAPSSMKIKVVAPPERKYSVWIGGSILASLSTFQQMWIAKAEYDESGPSIVHRKCF
- >ACT4 **(SEEDS)**

Tree of Arabidopsis actins



Structure and Evolution of the Actin Gene Family in *Arabidopsis thaliana*

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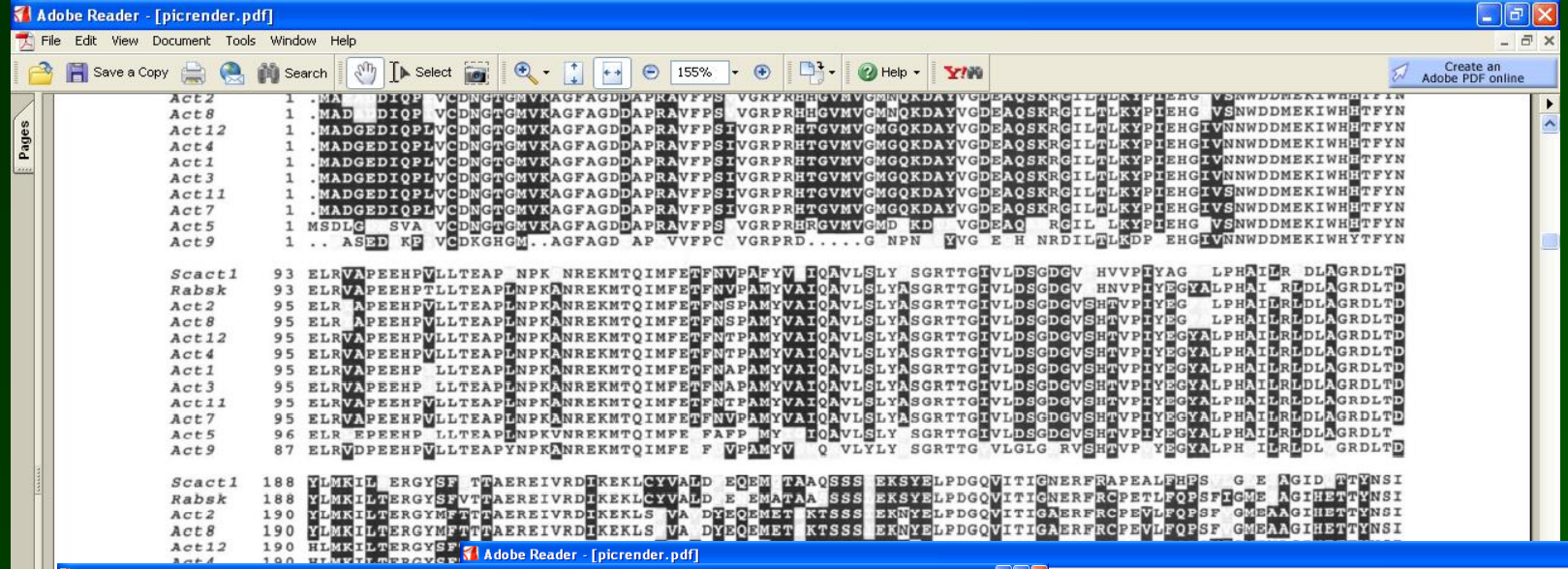
Accepted for publication October 27, 1995

ABSTRACT

Higher plants contain families of actin-encoding genes that are divergent and differentially expressed. Progress in understanding the functions and evolution of plant actins has been hindered by the large size of the actin gene families. In this study, we characterized the structure and evolution of the actin gene family in *Arabidopsis thaliana*. DNA blot analyses with gene-specific probes suggested that all 10 of the Arabidopsis actin gene family members have been isolated and established that Arabidopsis has a much simpler actin gene family than other plants that have been examined. Phylogenetic analyses suggested that the Arabidopsis gene family contains at least two ancient classes of genes that diverged early in land plant evolution and may have separated vegetative from reproductive actins. Subsequent divergence produced a total of six distinct subclasses of actin, and five showed a distinct pattern of tissue specific expression. The concordance of expression patterns with the phylogenetic structure is discussed. These subclasses appear to be evolving independently, as no evidence of gene conversion was found. The Arabidopsis actin proteins have an unusually large number of nonconservative amino acid substitutions, which mapped to the surface of the actin molecule, and should effect protein-protein interactions.



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Act2      1  .MA  DIQP VCDNGTGMVKAGFAGDDAPRAVFPS VGRPRHHGVMVGMNQKDAYVGDEAQSKRGILTLKYPIEHG VSNWDDMEKIWHHTFYN
Act8      1  .MAD DIQP VCDNGTGMVKAGFAGDDAPRAVFPS VGRPRHHGVMVGMNQKDAYVGDEAQSKRGILTLKYPIEHG VSNWDDMEKIWHHTFYN
Act12     1  .MADGEDIQPLVCDNGTGMVKAGFAGDDAPRAVFPSIVGRPRHTGVMVGMGQKDAYVGDEAQSKRGILTLKYPIEHGIVNNWDDMEKIWHHTFYN
Act4      1  .MADGEDIQPLVCDNGTGMVKAGFAGDDAPRAVFPSIVGRPRHTGVMVGMGQKDAYVGDEAQSKRGILTLKYPIEHGIVNNWDDMEKIWHHTFYN
Act1      1  .MADGEDIQPLVCDNGTGMVKAGFAGDDAPRAVFPSIVGRPRHTGVMVGMGQKDAYVGDEAQSKRGILTLKYPIEHGIVNNWDDMEKIWHHTFYN
Act3      1  .MADGEDIQPLVCDNGTGMVKAGFAGDDAPRAVFPSIVGRPRHTGVMVGMGQKDAYVGDEAQSKRGILTLKYPIEHGIVNNWDDMEKIWHHTFYN
Act11     1  .MADGEDIQPLVCDNGTGMVKAGFAGDDAPRAVFPSIVGRPRHTGVMVGMGQKDAYVGDEAQSKRGILTLKYPIEHGIVSNWDDMEKIWHHTFYN
Act7      1  .MADGEDIQPLVCDNGTGMVKAGFAGDDAPRAVFPSIVGRPRHTGVMVGMGQKDAYVGDEAQSKRGILTLKYPIEHGIVSNWDDMEKIWHHTFYN
Act5      1 MSDLG  SVA VCDNGTGMVKAGFAGDDAPRAVFPS VGRPRHRGVMVGMD KD  VGDEAQ  RGIL LKYPIEHG VSNWDDMEKIWHHTFYN
Act9      1  .. ASED KP VCDKGHGM..AGFAGD AP VVFPC VGRPRD.....G NPN  YVG E H NRDILTLKDP EHGIVNNWDDMEKIWHYTFYN

Scact1   93 ELRVAPEEHPVLLTEAP NPK NREKMTQIMFETFNVPAFYV IQAVLSLY SGRTTGIVLDSGDGV HVVPIYAG  LPHAIIR DLAGRDLTD
Rabsk    93 ELRVAPEEHPTLLTEAPLNPKANREKMTQIMFETFNVPAMYVAIQAVLSLYASGRTTGIVLDSGDGV HNVPIYEGYALPHAI RLDLAGRDLTD
Act2     95 ELR APEEHPVLLTEAPLNPKANREKMTQIMFETFNSPAMYVAIQAVLSLYASGRTTGIVLDSGDGVSHTVPIYEG  LPHAIIRLDLAGRDLTD
Act8     95 ELR APEEHPVLLTEAPLNPKANREKMTQIMFETFNSPAMYVAIQAVLSLYASGRTTGIVLDSGDGVSHTVPIYEG  LPHAIIRLDLAGRDLTD
Act12    95 ELRVAPEEHPVLLTEAPLNPKANREKMTQIMFETFNTPAMYVAIQAVLSLYASGRTTGIVLDSGDGVSHTVPIYEGYALPHAIIRLDLAGRDLTD
Act4     95 ELRVAPEEHPVLLTEAPLNPKANREKMTQIMFETFNTPAMYVAIQAVLSLYASGRTTGIVLDSGDGVSHTVPIYEGYALPHAIIRLDLAGRDLTD
Act1     95 ELRVAPEEHP LLTEAPLNPKANREKMTQIMFETFNAPAMYVAIQAVLSLYASGRTTGIVLDSGDGVSHTVPIYEGYALPHAIIRLDLAGRDLTD
Act3     95 ELRVAPEEHP LLTEAPLNPKANREKMTQIMFETFNAPAMYVAIQAVLSLYASGRTTGIVLDSGDGVSHTVPIYEGYALPHAIIRLDLAGRDLTD
Act11    95 ELRVAPEEHPVLLTEAPLNPKANREKMTQIMFETFNTPAMYVAIQAVLSLYASGRTTGIVLDSGDGVSHTVPIYEGYALPHAIIRLDLAGRDLTD
Act7     95 ELRVAPEEHPVLLTEAPLNPKANREKMTQIMFETFNVPAMYVAIQAVLSLYASGRTTGIVLDSGDGVSHTVPIYEGYALPHAIIRLDLAGRDLTD
Act5     96 ELR EPEEHP LLTEAPLNPKVNREKMTQIMFE FAPP MY  IQAVLSLY SGRTTGIVLDSGDGVSHTVPIYEGYALPHAIIRLDLAGRDLT
Act9     87 ELRVDPEEHPVLLTEAPYNPKANREKMTQIMFE F VPAMYV  Q VLYLY SGRTTG VLGLG RVSHTVP YEGYALPH IIRLDL GRDLTD

Scact1  188 YLMKIL ERGYSF TTAEREIVRDIKEKLCYVALD FEQEM TAAQSSS EKSYELPDGQVITIGNERFRAPEALFHPS  G E AGID TTYNSI
Rabsk   188 YLMKILTERGYSFVTTAEREIVRDIKEKLCYVALD E EMATAA SSS EKSYELPDGQVITIGNERFRCPETLFQPSFIGME AGIHETTYNSI
Act2    190 YLMKILTERGYMFTTTAEREIVRDIKEKLS VA DYEQEMET KTSSS EKNYELPDGQVITIGAERFRCPEVLFQPSF GMEAAGIHETTYNSI
Act8    190 YLMKILTERGYMFTTTAEREIVRDIKEKLS VA DYEQEMET KTSSS EKNYELPDGQVITIGAERFRCPEVLFQPSF GMEAAGIHETTYNSI
Act12   190 HLMKILTERGYSFTTTAEREIVRDIKEKLCYVALD FEQEM TAAQSSS EKSYELPDGQVITIGNERFRAPEALFHPS  G E AGID TTYNSI
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changes. Neighbor joining and maximum likelihood trees were reconstructed in the PHYLIP package (version 3.5) (FELSENSTEIN 1993). Third codon positions were assigned a weight of zero in every case. The inputs for the neighbor joining program were distance matrices constructed by KIMURA's two parameter method. Other methods of calculating genetic distance were also employed and yielded trees with very similar branching orders.

Construction of space-filling models for plant and human actins: Sequences for human Act-b, Act-g, Act-c, Act-s, Act-a, and Act-h were obtained from GenBank and aligned to identify variable residues. Structural coordinates for the model of rabbit skeletal actin-DNaseI complex (KABSCH *et al.* 1990) were retrieved from the Bookhaven Database. Rabbit skeletal actin is identical in sequence and presumably in structure to human Act-s and was used as the basis for building a model plant actin. The DNaseI molecule was deleted from this model using Nitro (Tripos Assoc. Inc.). Building plant *ACT2* model structure required making 52 amino acid substitutions within the above skeletal muscle actin. Changing residue 7 from ala7 in Act-s to pro7 in *ACT2* could not be done without making a minor change in conformation of the peptide backbone. Residues which varied within the plant or animal families were located within the Act-s and *ACT2* structures, respectively, and displayed in a spacefilling model.

	ACT1	*ACT2*	*ACT3*	*ACT4*	*ACT5*	*ACT7*	*ACT8*	*ACT9*	*ACT11*	*ACT12*	*SCER*
ACT1	0	0.0666	0.0023	0.0251	0.0994	0.0420	0.0647	0.1787	0.0317	0.0257	0.1550
ACT2	1.297	0	0.0660	0.0635	0.1018	0.0426	0.0046	0.1814	0.0518	0.0648	0.1619
ACT3	0.6055	1.133	0	0.0269	0.0994	0.0420	0.0641	0.1800	0.0347	0.0251	0.1561
ACT4	1.242	1.677	1.432	0	0.1026	0.0494	0.0604	0.1789	0.0293	0.0046	0.1570
ACT5	1.452	1.969	1.366	1.444	0	0.1068	0.0973	0.1608	0.0935	0.1059	0.1887
ACT7	0.9957	1.176	1.192	1.483	1.776	0	0.0408	0.1806	0.0403	0.0469	0.1616
ACT8	1.067	0.5571	1.228	1.351	1.603	1.045	0	0.1769	0.0493	0.0598	0.1634
ACT9	1.552	1.562	1.458	1.434	0.3960	1.676	1.292	0	0.1729	0.1759	0.2499
ACT11	1.100	1.097	1.289	1.438	1.342	1.250	1.218	1.170	0	0.0293	0.1571
ACT12	1.447	1.722	1.331	0.8351	1.535	1.569	1.764	1.667	1.426	0	0.1641
SCER	NAN	NAN	NAN	NAN	NAN	NAN	NAN	NAN	NAN	NAN	0

FIGURE 2.—Nonsynonymous and synonymous nucleotide substitutions among Arabidopsis actin genes. Nonsynonymous (RNS) and synonymous (SNS) substitutions (above and below the diagonal, respectively) were calculated for all pairwise comparisons of the Arabidopsis actin protein coding sequences (see MATERIALS AND METHODS). The numbers shown were corrected for multiple hit kinetics and are given as a fraction of the total number possible substitutions (*i.e.*, in the RNS comparison of *ACT1 vs. ACT2* the value of 0.0666 means that 6.66% of the total possible changes occured). Values which corrected to numbers >2.0 (200%) are listed as NAN.

RESULTS

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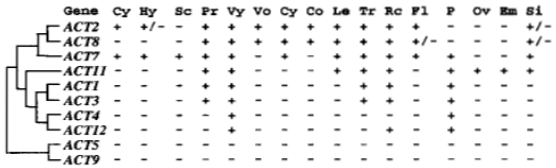

FIGURE 8.—Summary of the expression patterns of the Arabidopsis gene actin genes. The phylogenetic relationships of the 10 Arabidopsis actin genes, based on protein coding sequence, is presented on the left. To the right is a table that outlines the expression of the genes in the following tissues and organs: Cy, tissues of cotyledons excluding young vascular tissue; Hy, hypocotyl; Sc, seed coat; Pr, organ primordia and meristems; Vy, young vascular tissue; Vo, old vascular tissue; Cy, young cortical tissue; Co, old cortical tissue, Le, leaf epidermis; Rc, root cap; P, pollen; Ov, developing ovules; Em, embryo; Fl, flower (*i.e.*, sepals, petals, stigma, style) but excluding pollen, pollen sack, developing ovules; and Si, siliques. The + and − score expression and no expression, respectively, and a +/− score implies very weak expression or that expression is limited to a small subset of the cells present in this organ or tissue. These data are summarized from several recent manuscripts from this laboratory (Y.-Q.AN, S. HUANG, J. M. MCDOWELL, E. C. MCKINNEY and R. B. MEAGHER; Y.-Q. AN, J. M. MCDOWELL, S. HUANG, E. C. MCKINNEY, S. CHAM-

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Hypothesis

"The macro-evolution of vegetative and reproductive plant structures is linked to the molecular evolution of two, differentially regulated classes of cytoskeletal genes that physically direct development."

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            http://www.genoscope.cns.fr
COMMENT     Information on performance of analysis and a more detailed
            annotation of this entry and other sequences of chromosomes 3, 4
            and 5 can be viewed at: http://www.mips.biochem.mpg.de/proj/thal/
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                     /db_xref="InterPro:IPR004001"
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                     /db_xref="UniProtKB/Swiss-Prot:P53497"
ORIGIN
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       61 qskrgiltlk ypiehgivnn wddmekiwhh tfynelrvap eehpvlltea plnpkanrek
      121 mtqimfetfn tpamyvaiqa vlslyasgrt tgivldsgdg vshtvpiyeg yalphailrl
      181 dlagrdltdh lmkiltergy sftttaerei vrdmkeklsy ialdyeqele tsktsssvek
```

More about the gene ACT12

Member of actin subclass composed of ACT12 and ACT4. RNA is expressed at very low levels in vegetative organs, low levels in flowers and ver...
Also Known As: AT3G46520, ACTIN, actin...

Homologs of the ACT12 gene

The ACT12 gene is conserved in human, chimpanzee, Rhesus monkey, dog, cow, mouse, rat, chicken, zebrafish, fruit fly, rice, and frog.

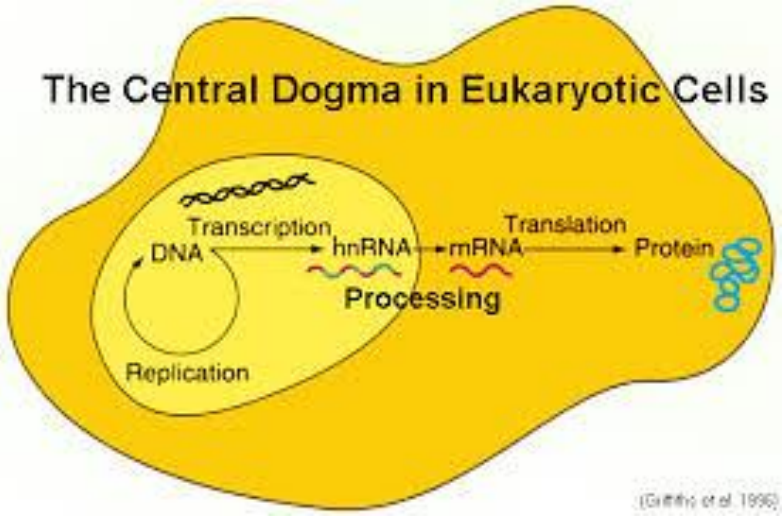
Related information

- BioProject
- Nucleotide
- Taxonomy
- BioSystems
- CDD Search Results
- Conserved Domains (Concise)
- Conserved Domains (Full)
- Gene
- Genome
- PubMed (Weighted)
- Related Structures (List)
- Related Structures (Summary)

Suggested Readings

- RB Meagher, EC McKinney and AV Vitale, 1999 “The evolution of new structures: clues from plant cyto-skeletal genes” TIG 15:7, 278-284.
- Bioinformatics: A Practical Approach, Higgins & Taylor, OUP (Indian ed.) Rs. 295
- Biological Sequence Analysis : Probabilistic Models of Proteins and Nucleic Acids, Durbin et al., CUP (Indian ed.) Rs. 395.
- *Surf the web!!*

Protein sorting in plant cells

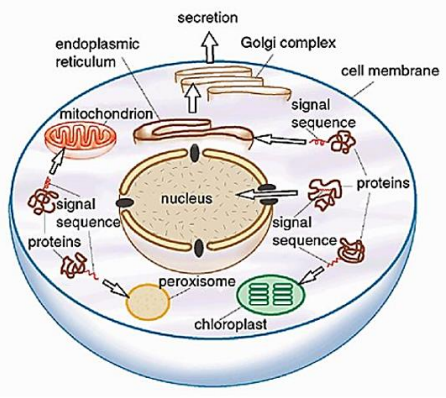


1974 Nobel Prize in Physiology/Medicine
– George Palade
• *"for discoveries concerning the structural and functional organization of the cell"*

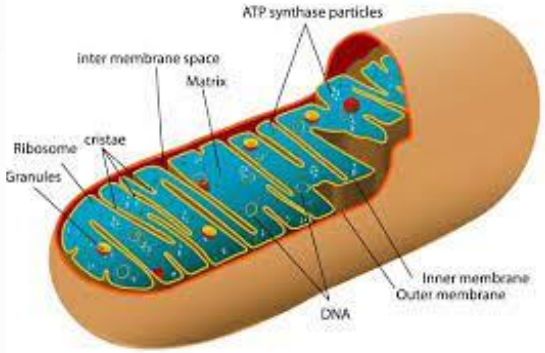
1999 Nobel Prize in Physiology/Medicine
– Günter Blobel
• *"for the discovery that proteins have intrinsic signals that govern their transport and localization in the cell"*

- **Protein sorting** is the mechanism by which a cell transports proteins to the appropriate positions in the cell or outside of it.
- Valuable annotations for novel proteins
- Proteins can move between compartments in different ways –
  - Gated transport (Nucleus)
  - Transmembrane transport (Mitochondria, Peroxisomes)
  - Vesicular transport (ER)

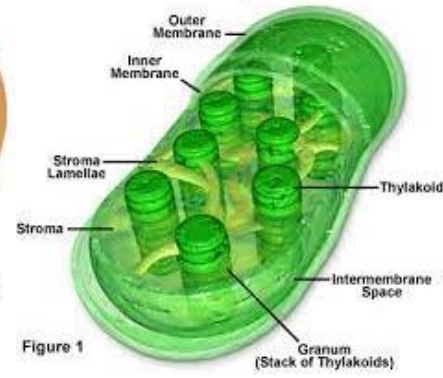
Compartmentalization in cellular organelles



Eukaryotic cell



Mitochondria



Chloroplast

Protein subcellular localization

Some signals are easily recognizable while others are difficult to understand

Proteins must have **intrinsic signals for their localization – a cellular address (eg. N-terminal signal sequences)**

➢The pre-sequences of the targeting peptides are often found at the **N-terminal** extension.

➢It is composed of between 6 to 136 basic and hydrophobic amino acids.

➢Signal sequences are removed from the finished protein by specialized signal peptidases once the sorting process has been completed.

Enough experimental data exists to build highly accurate computational predictors of localization.

Common structure of N-terminal signal peptide

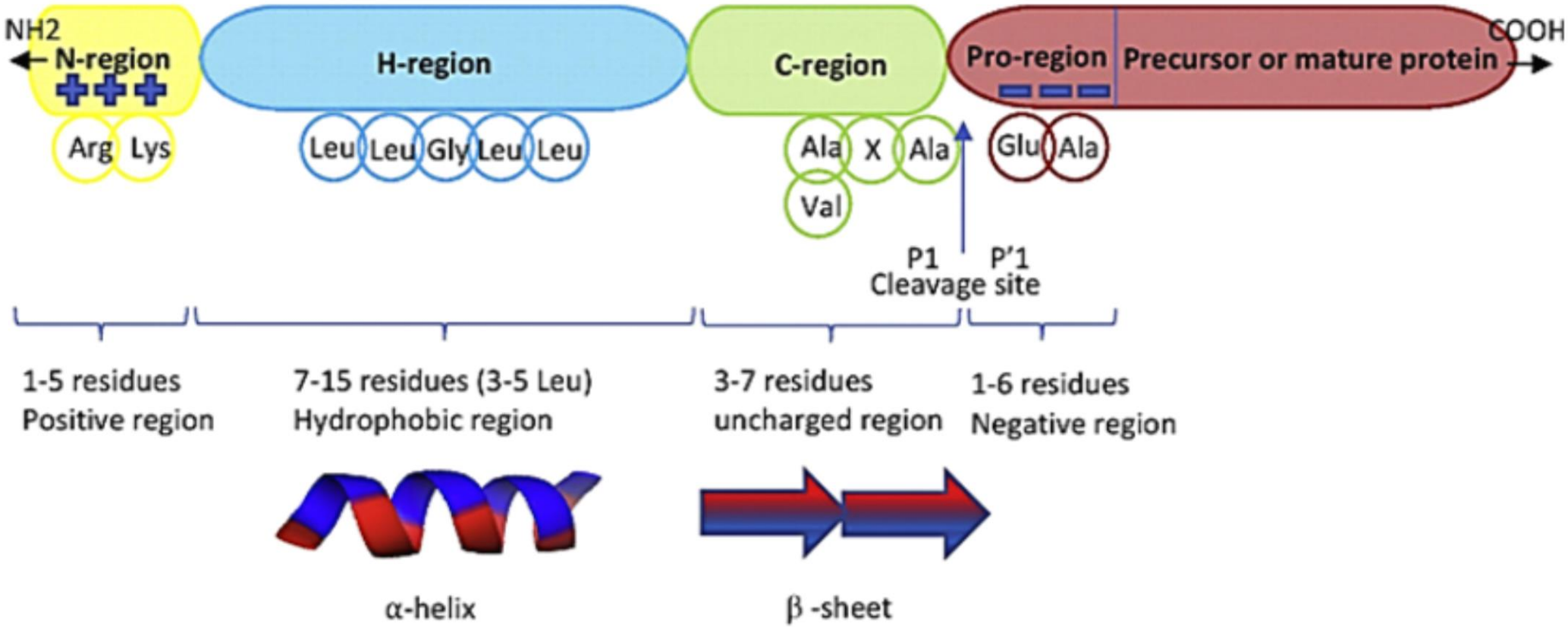
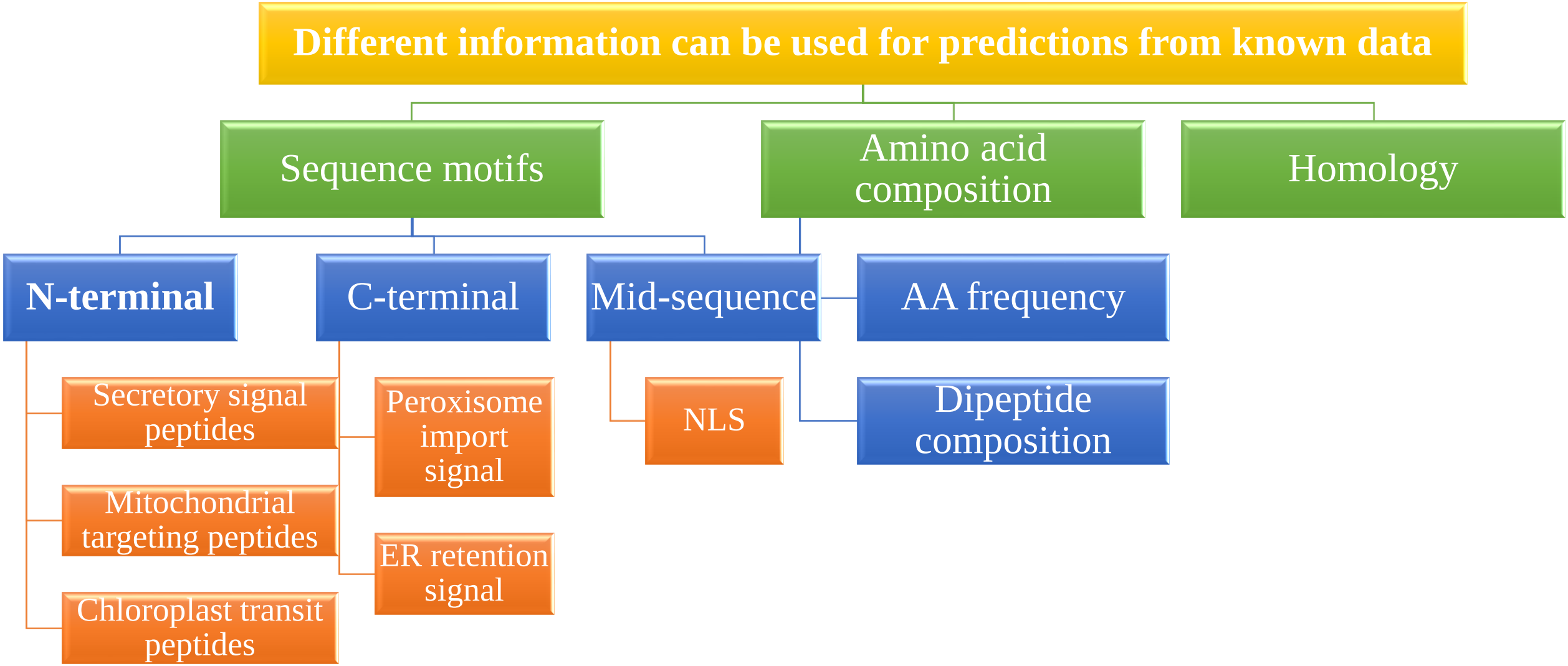


Fig. 2. The general structure of an SP. It is composed of three main parts: 1) N-region- the positive-charged domain 2) H-region- the hydrophobic core, forming α-helix 3) C-region- the cleavage site, forming β-sheet. The initial part of protein, important to protein secretion, is called Pro-region. Residues before the cleavage site are called as P1 and after the cleavage site are called as P'1. Cleavage occurs at AXA or VXA motif.

Predictions from known data



The PSORT family

The PSORT family server (http://psort.nibb.ac.jp/; http://psort.org/) contains several variant tools for the prediction of protein localization sites in cells.

It receives the information of an amino acid sequence and its source origin, e.g., Gram-negative bacteria, as inputs.

Then, it analyzes the input sequence by applying the stored rules for various sequence features of known protein sorting signals.

Finally, it reports the possibility for the input protein to be localized at each candidate site with additional information.

Variant tools of the PSORT family

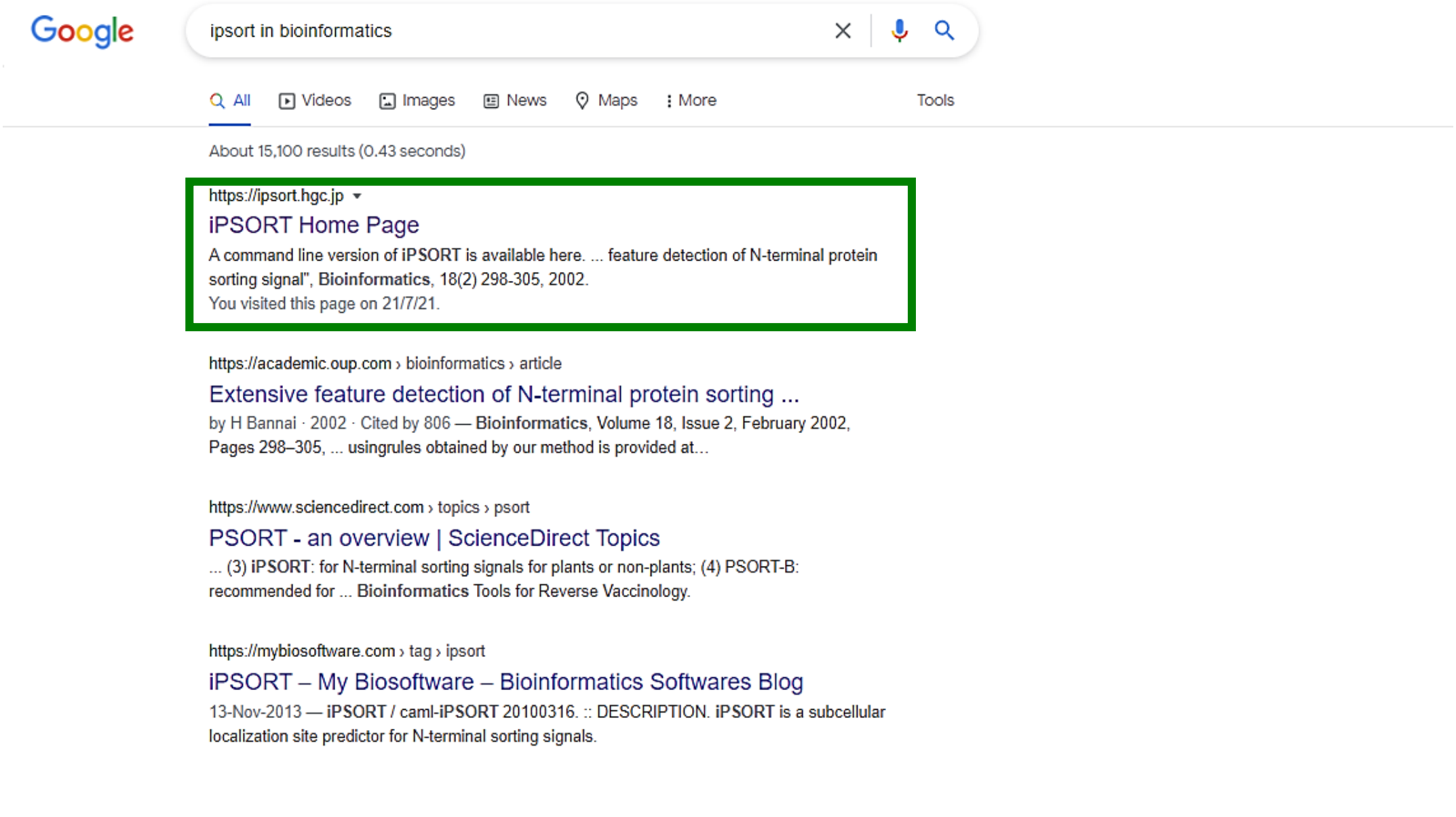
- **PSORT**: an old version for plants and bacteria
- **PSORT II**: recommended for yeast and animal
- **iPSORT**: for N-terminal sorting signals for plants or non-plants
- **PSORT-B**: recommended for Gram-negative bacteria
- **WoLF PSORT**: recommended for animal, plant and fungi

What is iPSORT – Overview

iPSORT is a subcellular localization site predictor for **N-terminal** sorting signals.

Given a protein sequence, it will predict whether it contains a (Signal Peptide **SP**), Mitochondrial Targeting Peptide (**mTP**), or Chloroplast Transit Peptide (**cTP**).

Getting started with iPSORT



iPSORT homepage opens

ipsort.hgc.jp

Welcome to the iPSORT WWW Service

This page is currently maintained by Yoshinori Tamada at Hirosaki University and Division of Health Medical Intelligence, Human Genome Center, Institute of Medical Science, University of Tokyo.
Questions, comments, bug reports, etc. should be directed to: Hideo Bannai <hdbn.dsc@tmd.ac.jp> and Yoshinori Tamada.
Best viewed with a style sheet capable browser.

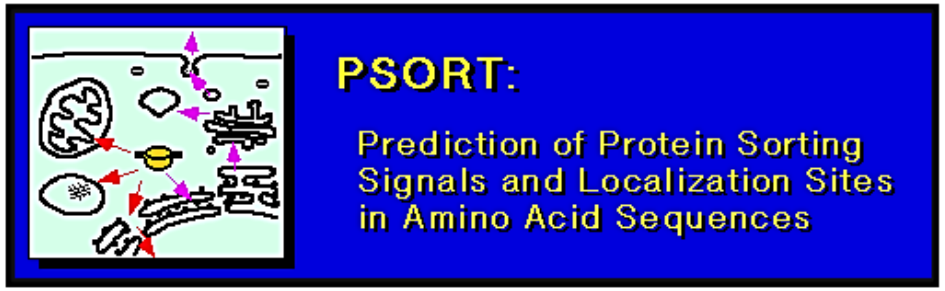
A command line version of iPSORT is available here. The program has been rewritten in the OCaml language, and is different from the one used for this web predictor (but should give the same predictions).

Contents

iPSORT Prediction

Paste your amino acid sequence below:
*** Characters except the standard 20 codes will be removed off
*** Only the first 30 residues are used for prediction

Link to PSORT www service (PSORT, PSORT II):
The original PSORT and PSORT II



PSORT WWW Server

PSORT is a computer program for the prediction of protein localization sites in cells. It receives the information of an amino acid sequence and its source orgin, *e.g.*, Gram-negative bacteria, as inputs. Then, it analyzes the input sequence by applying the stored rules for various sequence features of known protein sorting signals. Finally, it reports the possiblity for the input protein to be localized at each candidate site with additional information.

PSORT is mirrored at Tokyo, Okazaki, and Peking

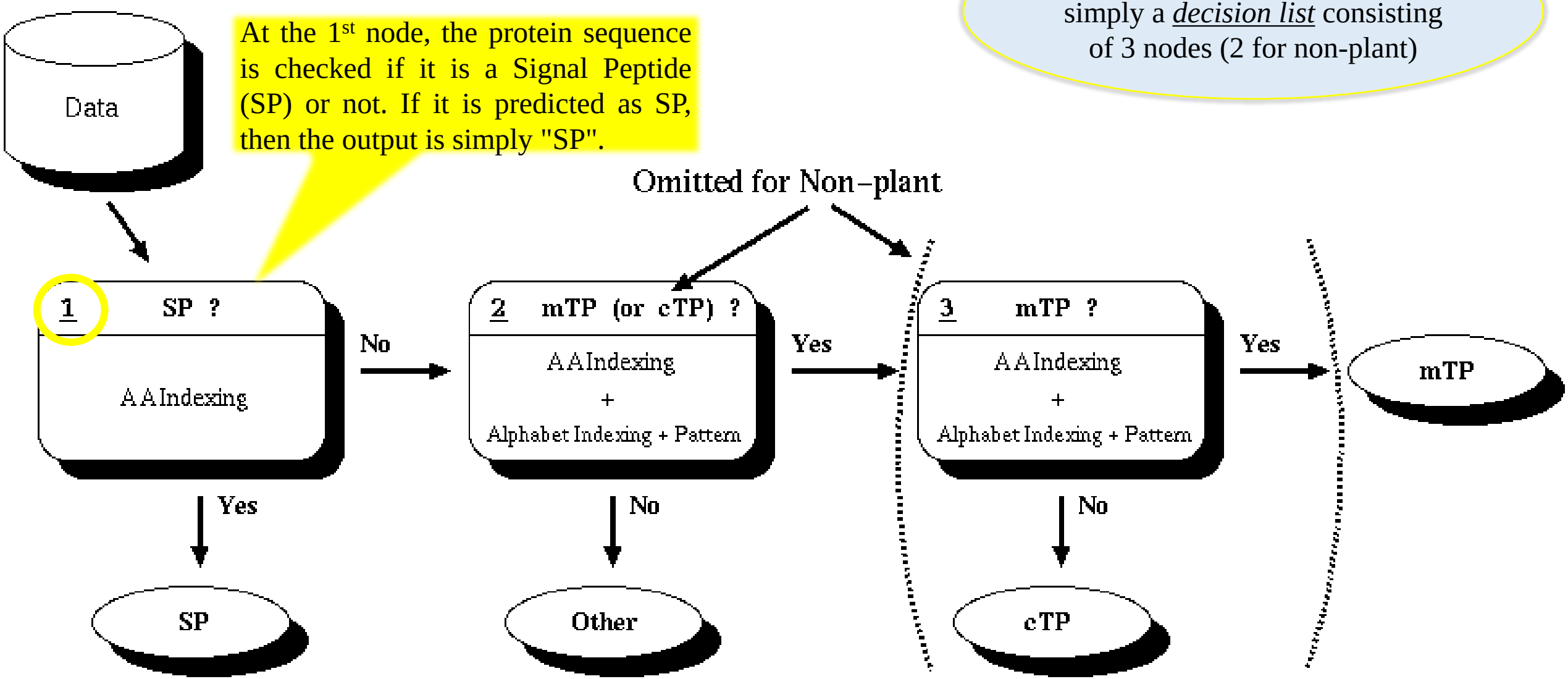
- December 1, 1998, Official release of the PSORT II package
- June 1, 1999, K. Nakai moved to Univ. Tokyo
- October 13, 1999, The Web server has been moved from Osaka to Tokyo
- March 11, 2001, Introduction of iPSORT
- September 23, 2001, New mirror site at Peking University
- December 22, 2001, Distribution of caml-iPSORT
- January 18, 2003, Replacing the training data for PSORT II at Peking
- February 22, 2003, Rebuilding the PSORT II server at Tokyo
- April 16, 2003, Minor update of the top page
- November 9, 2003, Minor updates of several pages
- May 27, 2005, Link to WoLF PSORT; update some links
- January 5, 2007, Modification of the link to WolfPSORT

---

iPSORT – Structure

The structure of iPSORT is simply a *decision list* consisting of 3 nodes (2 for non-plant)

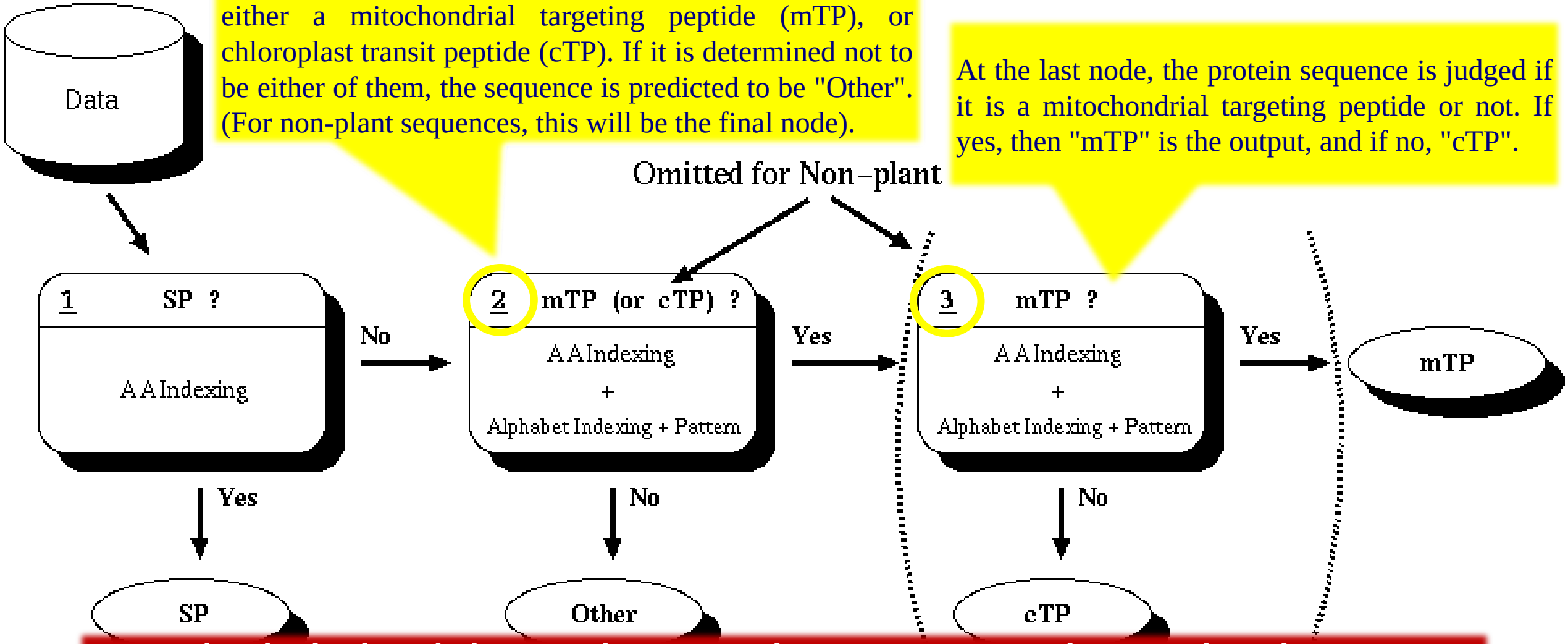
At the 1st node, the protein sequence is checked if it is a Signal Peptide (SP) or not. If it is predicted as SP, then the output is simply "SP".



iPSORT – Structure

At the 2nd node, the protein sequence is judged if it is either a mitochondrial targeting peptide (mTP), or chloroplast transit peptide (cTP). If it is determined not to be either of them, the sequence is predicted to be "Other". (For non-plant sequences, this will be the final node).

At the last node, the protein sequence is judged if it is a mitochondrial targeting peptide or not. If yes, then "mTP" is the output, and if no, "cTP".



The rules deciding whether or not the given signals contain a certain signal consists of two elements:
an *amino acid index rule*, and an *alphabet indexing+pattern rule*. (except for SP with only an amino acid index rule).
To be judged "yes" at each node, *the input amino acid sequence must satisfy both of the two rules* (except SP).

Suggested readings for iPSORT

- Bannai, H., Tamada, Y., Maruyama, O., Nakai, K., and Miyano, S., "*Extensive feature detection of N-terminal protein sorting signal*", Bioinformatics, 18(2) 298-305, 2002.
- Bannai, H., Tamada, Y., Maruyama, O., Nakai, K., Miyano, S., *Views: Fundamental Building Blocks in the Process of Knowledge Discovery*, In Proceedings of the 14th International FLAIRS Conference, 233-238, AAAI Press, 2001.
- Gardy, J. L., Spencer, C., Wang, K., Ester, M., Tusnady, G. E., Simon, I., ... & Brinkman, F. S. (2003). *PSORT-B: Improving protein subcellular localization prediction for Gram-negative bacteria*. Nucleic acids research, 31(13), 3613-3617.
- Horton, P., Park, K. J., Obayashi, T., Fujita, N., Harada, H., Adams-Collier, C. J., & Nakai, K. (2007). *WoLF PSORT: protein localization predictor*. Nucleic acids research, 35(suppl_2), W585-W587.
- Hiller, K., Grote, A., Scheer, M., Münch, R., & Jahn, D. (2004). *PrediSi: prediction of signal peptides and their cleavage positions*. Nucleic acids research, 32(suppl_2), W375-W379.
- Zheng, Z., Chen, Y., Chen, L., Guo, G., Fan, Y., & Kong, X. (2012). *Signal-BNF: a Bayesian network fusing approach to predict signal peptides*. Journal of Biomedicine and Biotechnology, 2012.

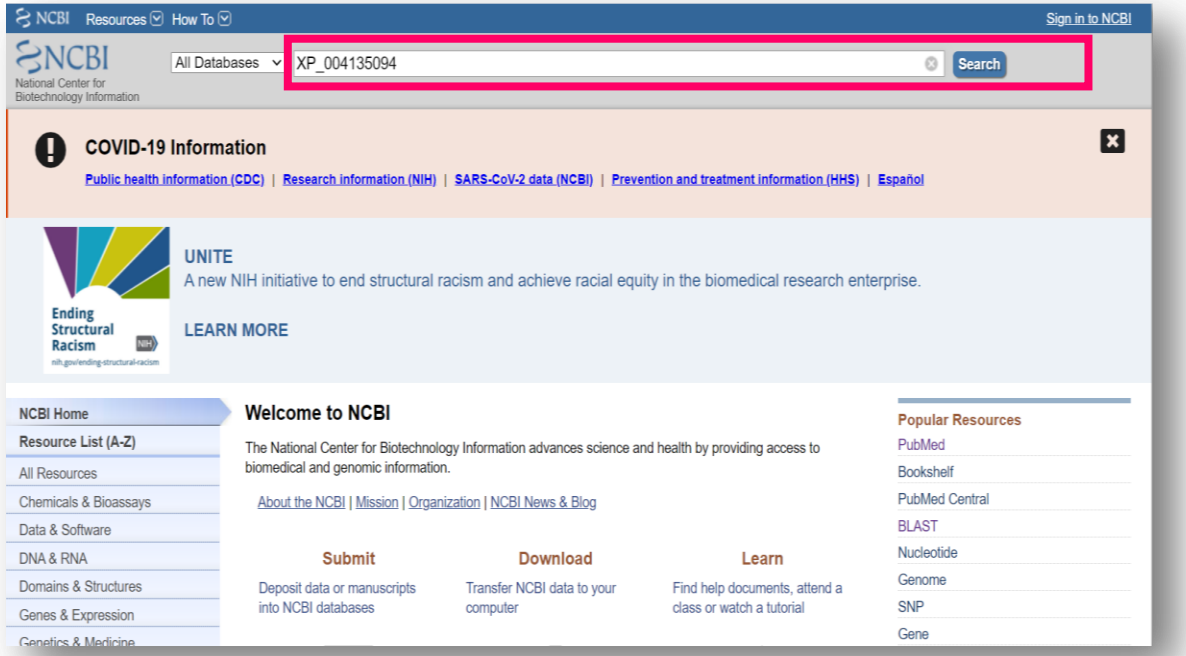
Sequence retrieval from database

- Search the Gene database with the desired gene name, species, or accession number.
- Nucleotide/ Protein sequence: Basic Local Alignment Search Tool (BLAST) tool.

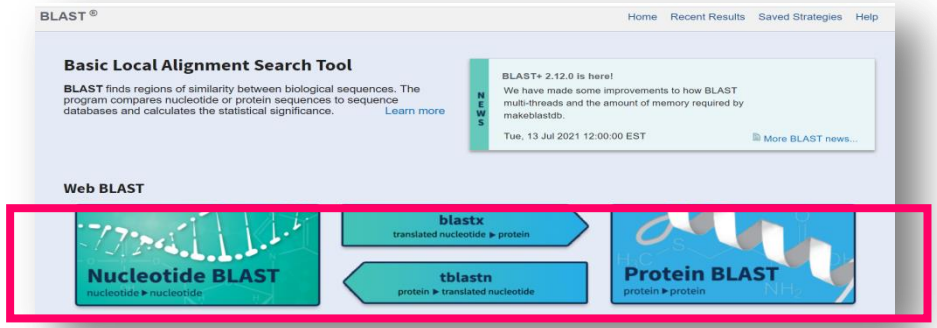
1

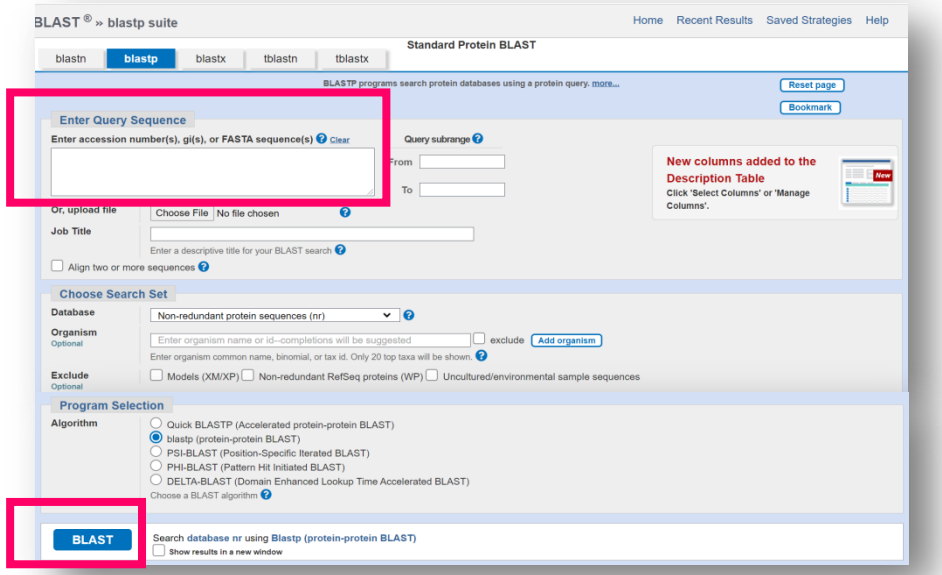
NCBI database website:
https://www.ncbi.nlm.nih.gov/

2



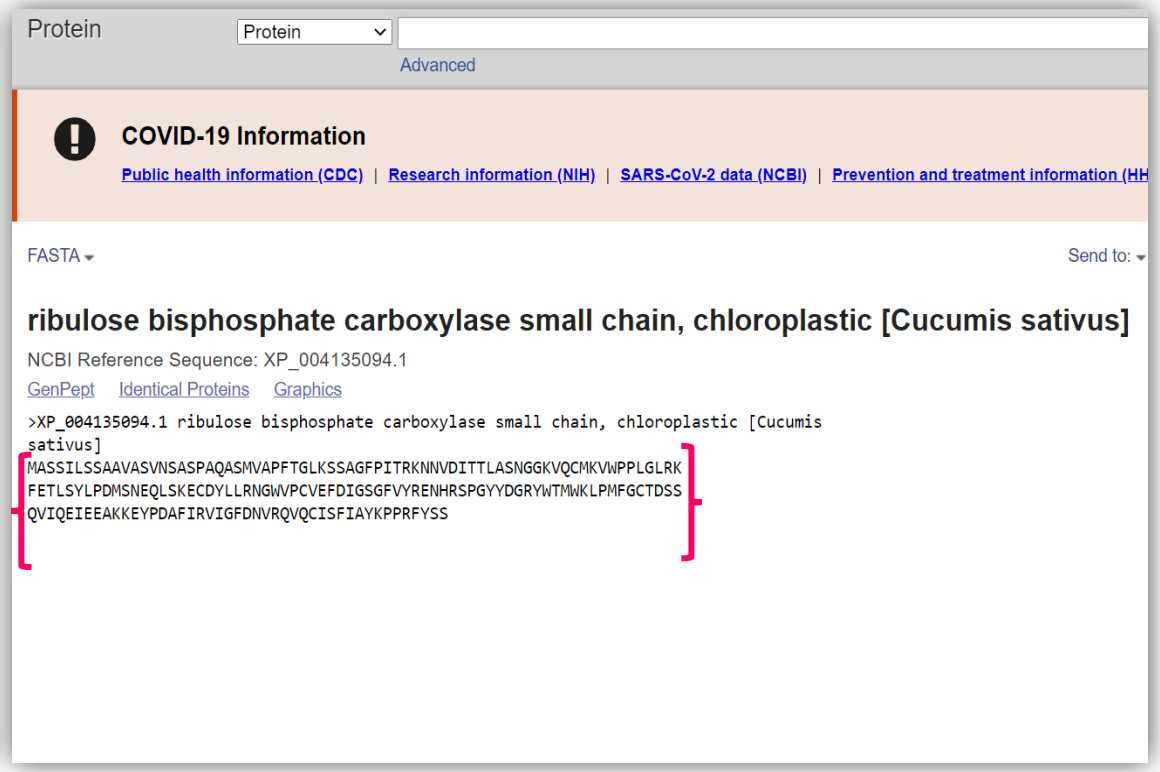
3





Preparation of FASTA files

1



2

Preparation of FASTA files

>XP_004135094

MASSILSSAAVASVNSASPAQASMVAPFTGLKSSAGFPITRKNNVDITTLASN
GGKVQCMKVWPPLGLRKFETLSYLPDMSNEQLSKECDYLLRNGWVPCVEF
DIGSGFVYRENHRSPGYYDGRYWTMWKLPMFGCTDSSQVIQEIEEAKKEYP
DAFIRVIGFDNVRQVQCISFIAYKPPRFYSS

>WP_140970218

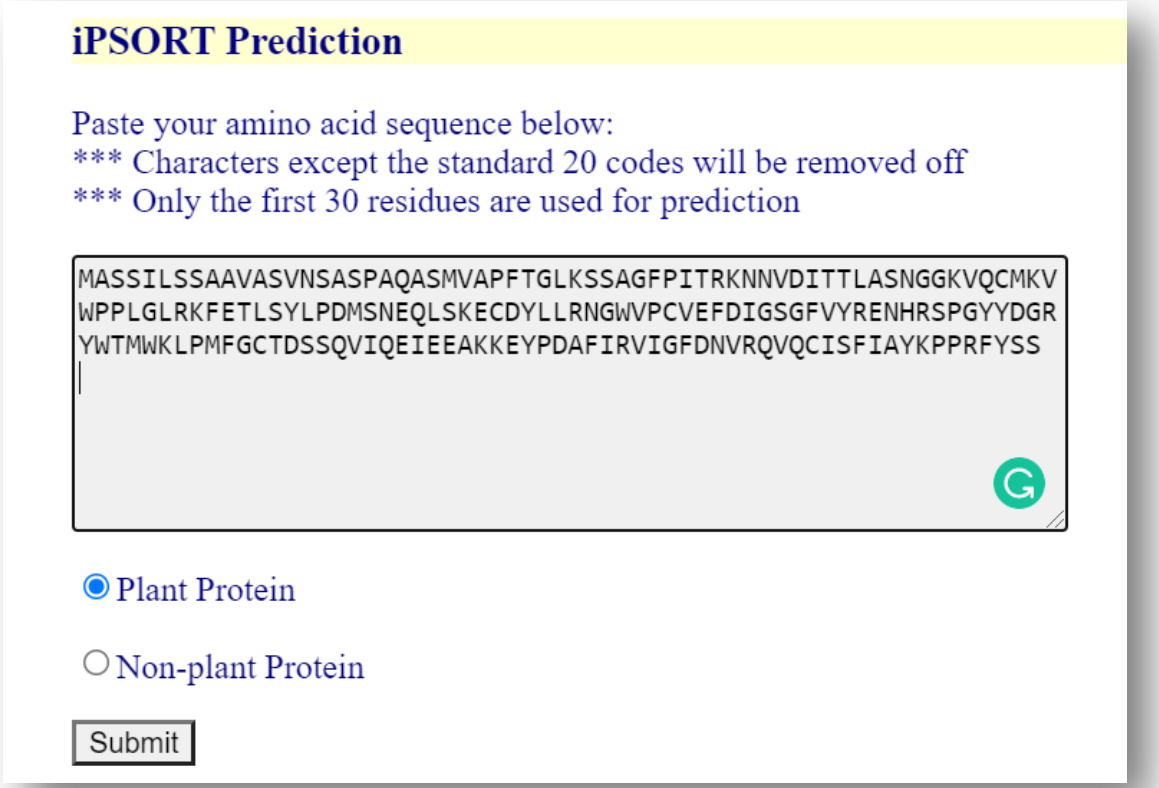
MLKKAIAEFIGTFVLVLFGTGVAVLGGGIEGIGTLGIAMAFGLSIVAMAYSIG
TISGCHINPAVSVAMFINKRMNAMELCYYVLAQILGGLLGTATLVTILKSAK
APLDNLGQNGFGTLGLSGAFLVEFILTFVFVLVIVAVTGKKGSSSLAGLVIGFT
LVLIHLLGIPLTGTSVNPARSIAPALFAGGEALSQLWVFIVAPILGGIVAAIVGK
FILNTEK

Localization sites of protein sequences

- Protein Sorting Signals:
  - Signal Peptides (SP)
  - Chloroplast transit peptides (cTP)
  - Mitochondrial targeting peptides (mTP)

- SP has conserved three-region structure: a positively charged n-region, a hydrophobic h-region, and a polar c-region.
- cTP are known to be rare in acidic residues.
- mTP are rich in arginine (R), alanine (A), and serine (S), while negatively charged amino acid residues (aspartic acid (D) and glutamic acid (E)) are rare.

iPSORT domain address:
https://ipsort.hgc.jp/



Bannai *et al.*, 2002

Localization sites of protein sequences

1. XP_004135094 (*Cucumis sativus* - Rubisco)

Predicted as: *having a chloroplast transit peptide*

Sequence (Type: plant)

```
  1 PMASS ILSSA AVASV NSASP AQASM VAPFT GLKSS AGFPI TRKNN VDITT
 51 LASNG GKVQC MKVWP PLGLR KFETL SYLPD MSNEQ LSKEC DYLLR NGWVP
101 CVEFD IGSGF VYREN HRSPG YYDGR YWTMW KLPMF GCTDS SQVIQ EIEEA
151 KKEYP DAFIR VIGFD NVRQV QCISF IAYKP PRFYS S
```

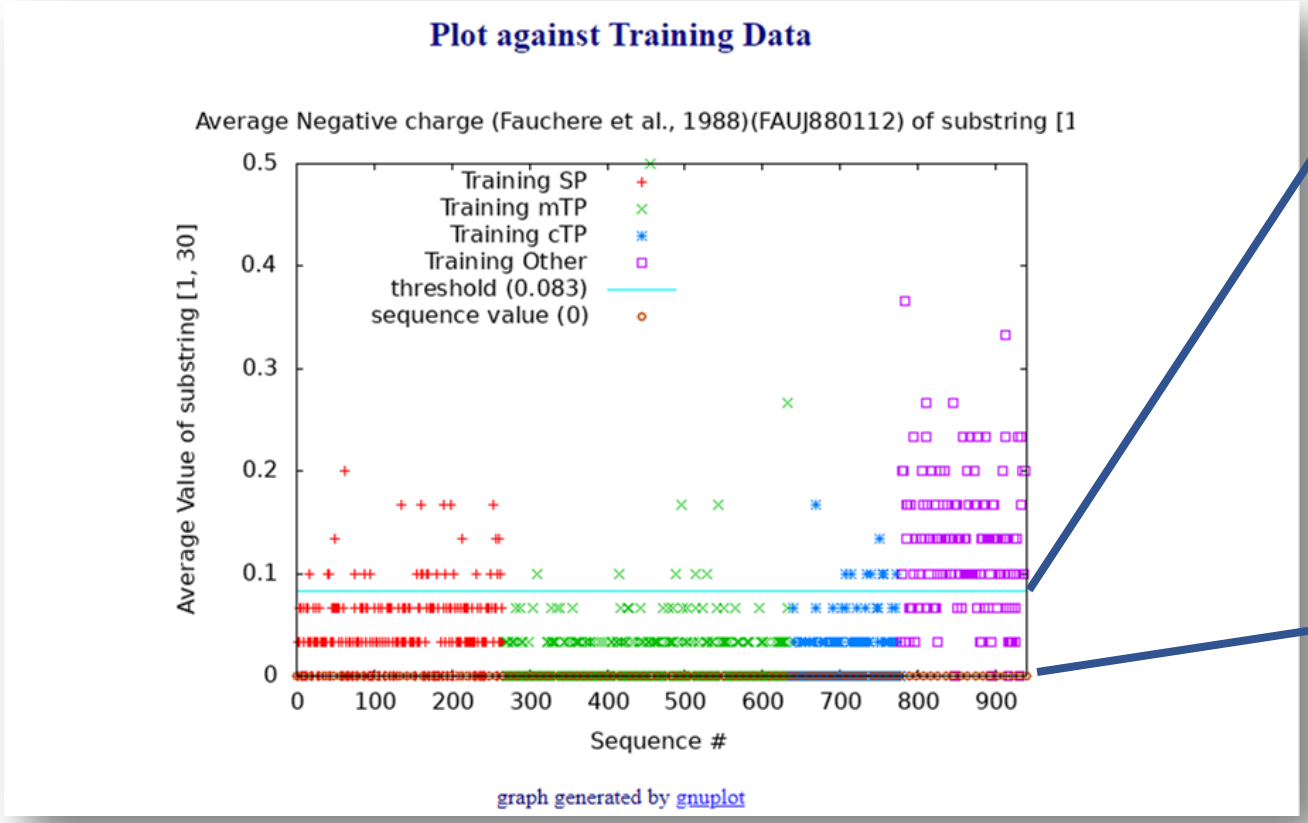
Values used for reasoning

Node	Answer	View	Substring	Value(s)	Plot
1. Signal peptide?	**No**	Average Hydropathy (KYTJ820101)	[6,25]	0.8 (>= 0.9225? No)	show
2. Mitochondrial or chloroplast ?	**Yes**	Average Negative Charge (FAUJ880112)	[1,30]	0 (< 0.083? Yes)	show
		Indexing: AI1 Pattern: 22121222 (ins/del <= 2)	[1,30]	PMAS-SILSSAAVASVNSASPAQASMVAPFT 2222-2122222222202222222222222222 22121222	--
3. Mitochondrial?	**No**	Average Isoelectric Point (ZIMJ680104)	[1,15]	5.89067 (>= 6.21? No)	show
		Indexing: AI2 Pattern: 100100110 (ins/del <= 3)	[1,15]	PMASSILSSAAVASV 200002000000000 NOMATCH	--

* This color means "not used".

Localization sites of protein sequences

1. XP_004135094 (*Cucumis sativus*- Rubisco)



Threshold = 0.083

Sequence Value = 0

Localization sites of protein sequences

2. WP_140970218 (*Bacillus*- Aquaporin)

Predicted as: *having a signal peptide*

Sequence (Type: nonplant)

```
  1 MLKKA IAEFI GTFVL VLFGT GVAVL GGGIE GIGTL GIAMA FGLSI VAMAY
 51 SIGTI SGCHI NPAVS VAMFI NKRMN AMELC YYVLA QILGG LLGTA TLVTI
101 LKSAK APLDN LGQNG FGTLG LSGAF LVEFI LTFVF VLVIV AVTGK KGSSS
151 LAGLV IGFTL VLIHL LGIPL TGTSV NPARS IAPAL FAGGE ALSQL WVFIV
201 APILG GIVAA IVGKF ILNTE K
```

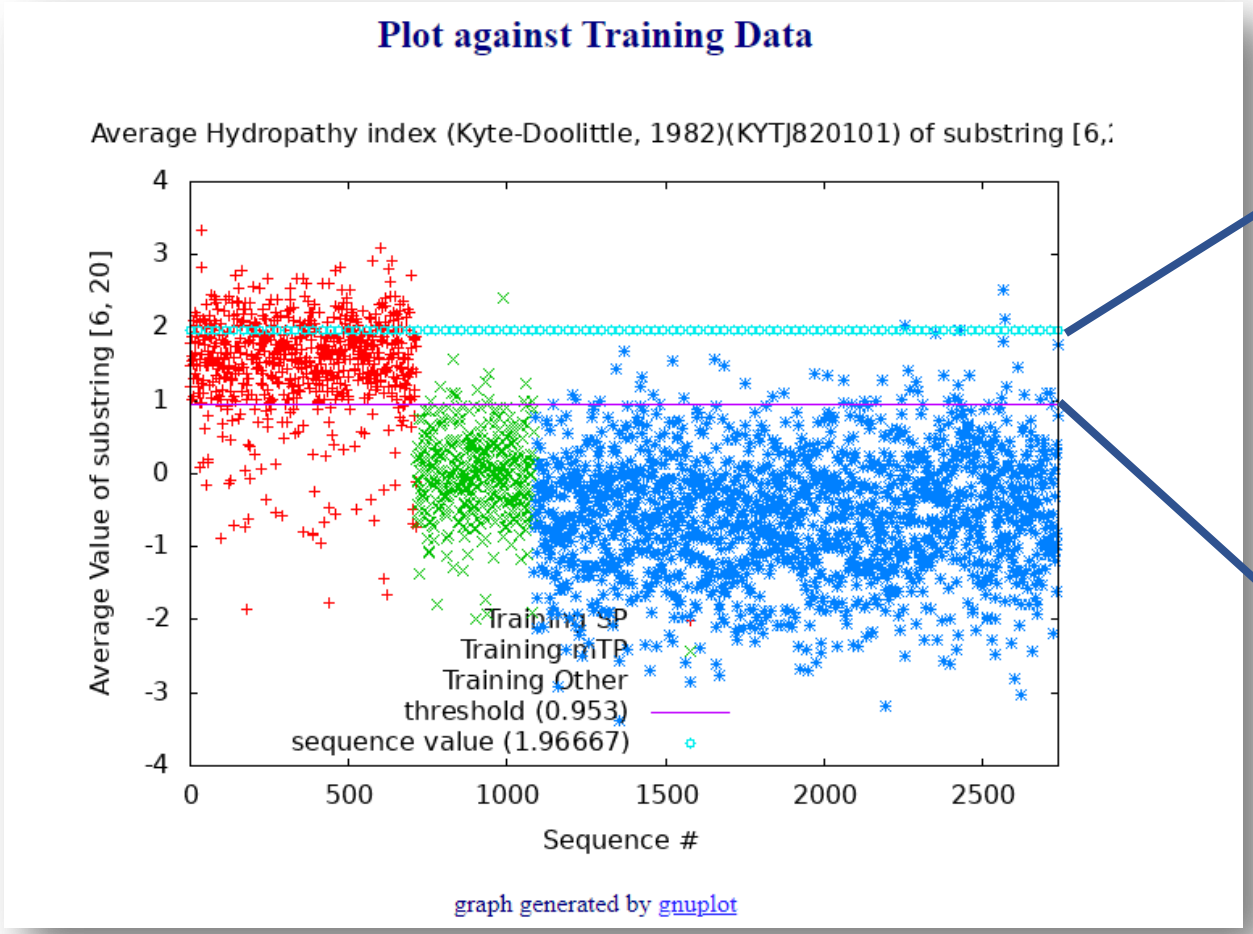
Values used for reasoning

Node	Answer	View	Substring	Value(s)	Plot
1. Signal peptide?	Yes	Average Hydropathy (KYTJ820101)	[6,20]	1.96667 (>= 0.953? Yes)	show
2. Mitochondrial ?	No	Average Net Charge (KLEP840101)	[1,30]	0 (>= 0.083? No)	show
		Indexing: AI1 Pattern: 221121122 (ins/del <= 3)	[1,30]	MLKKAIAEFIGTFVLVLFGTGVAVLGGGIE 220021202102222222020222200010 NOMATCH	--

* This color means "not used".

Localization sites of protein sequences

2. WP_140970218 (*Bacillus*- Aquaporin)



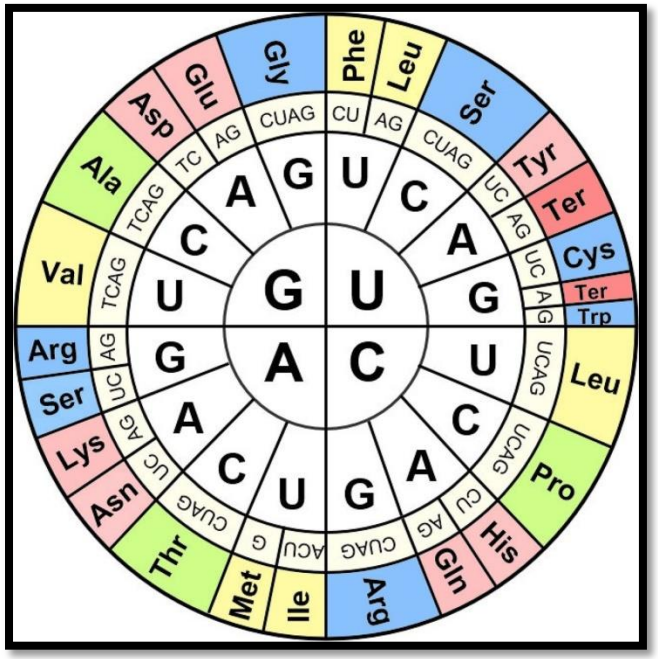
Sequence Value = 1.96667

Threshold = 0.953

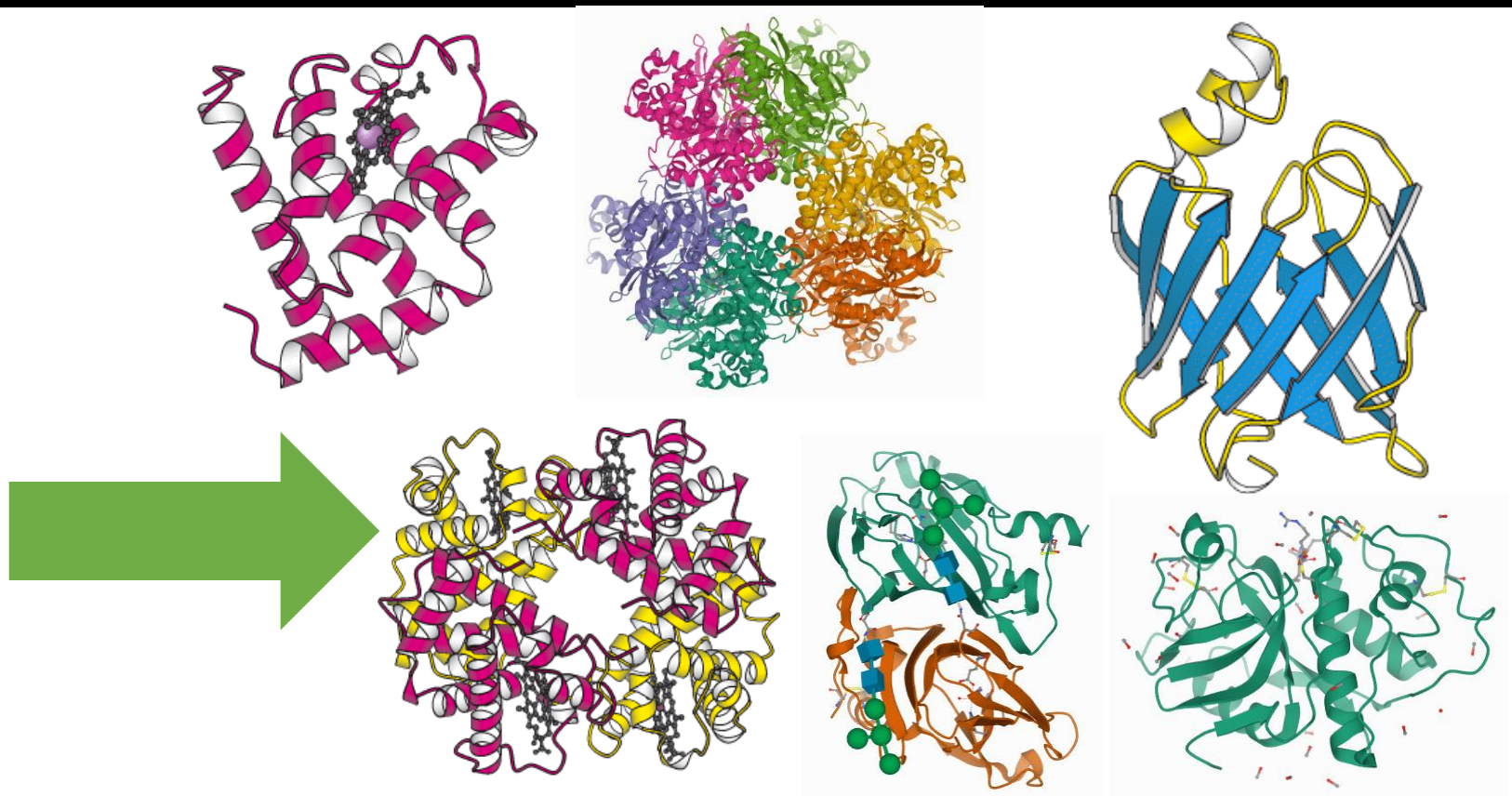
Amino acid index analysis

- **Amino Acid indices**
- **Amino Acid Index analysis tool at iPSORT WWW service**

Proteins are built from a repertoire of 20 Amino Acids



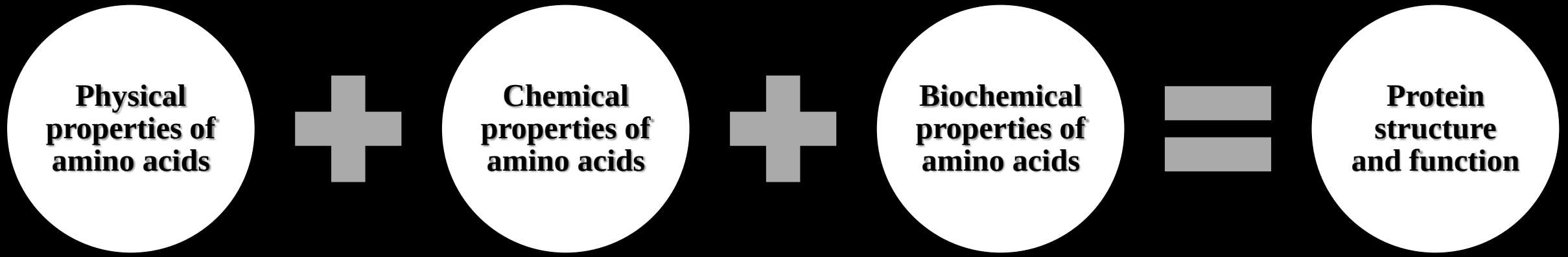
Genetic code encodes 20 basic amino acids which are the building blocks of all proteins



Three dimensional structure of Mygolobin, RuBiSCo, Fatty acid binding protein , Haemoglobin tetramer, Auxin binding protein, Papain.

Source : Berg et al., 2002, www.rcsb.org

Properties of Amino Acids determine Protein structure



- **The amino acid composition determines the primary structure of the protein.**
- **The spatial arrangement of the amino acid sequence in three-dimensional space determine the secondary and tertiary structure of the protein.**
- **The constituent amino acid has multifaceted properties that are responsible for the specificity and diversity of protein structure and function.**

Source: Berg et al., 2002; Kawashima & Kanehisa. 2000

AminoAcid Index or AA Index

Examples: Isoelectric point, Hydrophobicity, Hydropathy index, Alpha helix propensity

AA INDEX

AA index is a database of amino acid indices and amino acid mutation matrices

AA INDEX I

An amino acid index is a set of 20 numerical values representing various physico-chemical and biochemical properties of amino acids.

AA INDEX II

An amino acid mutation matrix is generally 20 × 20 numerical values representing similarity of amino acids

Source: Kawashima & Kanehisa. 2000

Running Amino Acid Index analysis tool at iPSORT WWW Service

Welcome to the iPSORT WWW Service

This page is currently maintained by Yoshinori Tamada at Hirosaki University and Division of Health Medical Intelligence, Human Genome Center, Institute of Medical Science, University of Tokyo.
Questions, comments, bug reports, etc. should be directed to: Hideo Bannai <hdbn.dsc@tmd.ac.jp> and Yoshinori Tamada.
Best viewed with a style sheet capable browser.

A command line version of iPSORT is available here. The program has been rewritten in the OCaml language, and is different from the one used for this web predictor (but should give the same predictions).

Contents

- What is iPSORT and how does it work?
- Predict localization sites of protein sequences
- Run amino acid index analysis
- Reference

iPSORT Prediction

Paste your amino acid sequence below:
*** Characters except the standard 20 codes will be removed off
*** Only the first 30 residues are used for prediction

(•) Plant Protein

( ) Non-plant Protein

Submit

AAindex Analysis

Choose amino acid index:

QIAN880131 - Weights for coil at the window position of -2 (Qian-Sejnowski, 1988)
QIAN880132 - Weights for coil at the window position of -1 (Qian-Sejnowski, 1988)
QIAN880133 - Weights for coil at the window position of 0 (Qian-Sejnowski, 1988)
QIAN880134 - Weights for coil at the window position of 1 (Qian-Sejnowski, 1988)
QIAN880135 - Weights for coil at the window position of 2 (Qian-Sejnowski, 1988)
QIAN880136 - Weights for coil at the window position of 3 (Qian-Sejnowski, 1988)
QIAN880137 - Weights for coil at the window position of 4 (Qian-Sejnowski, 1988)

Paste your sequences here:

Step 1 : Visit iPSORT WWW Service home page through your web browser

Welcome to the iPSORT WWW Service

iPSORT homepage URL : https://ipsort.hgc.jp

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---

iPSORT Prediction

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*** Only the first 30 residues are used for prediction

Step 2 : Click on the ‘Run amino acid index analysis’ option in ‘Contents’

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iPSORT Prediction

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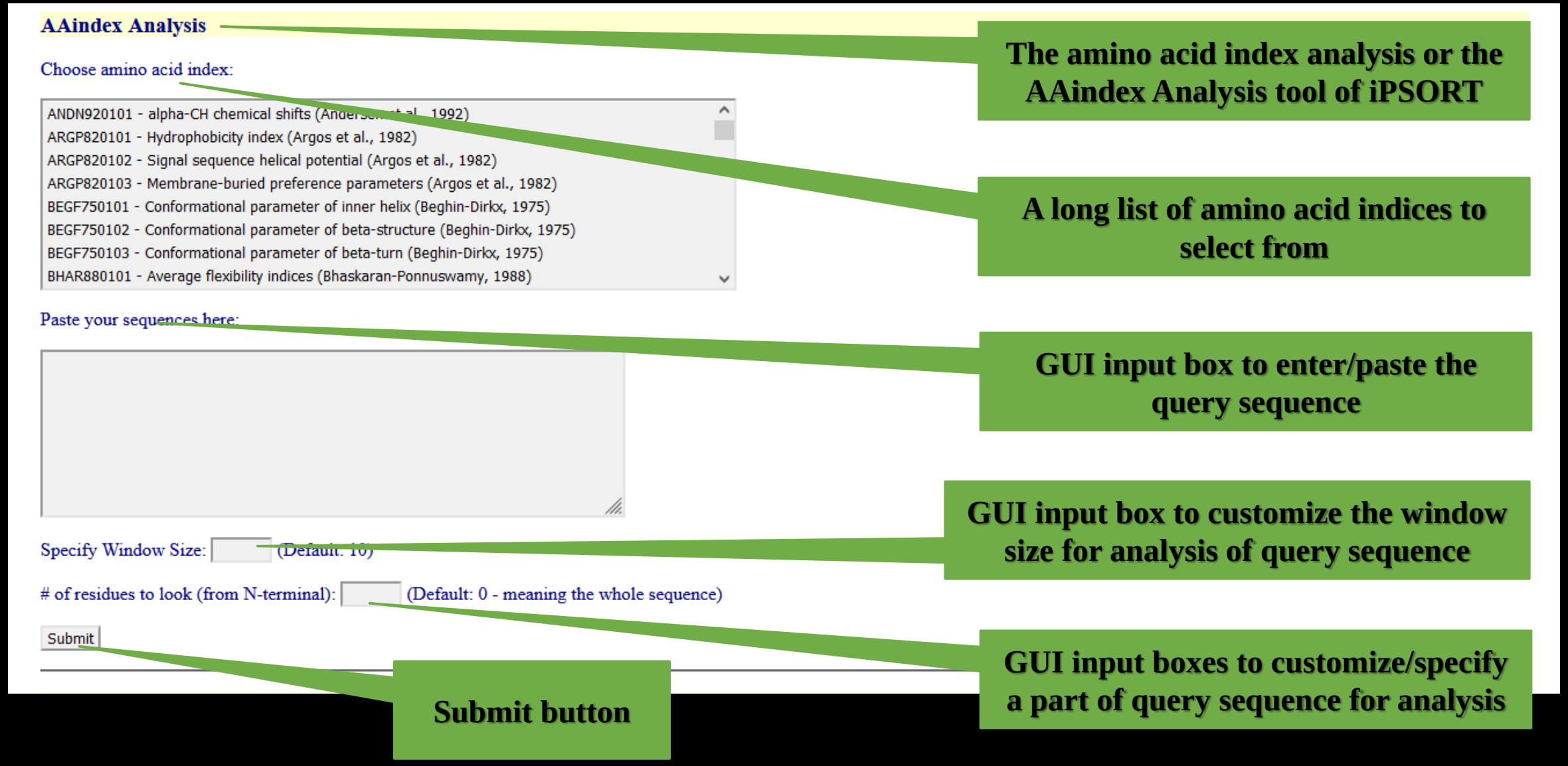
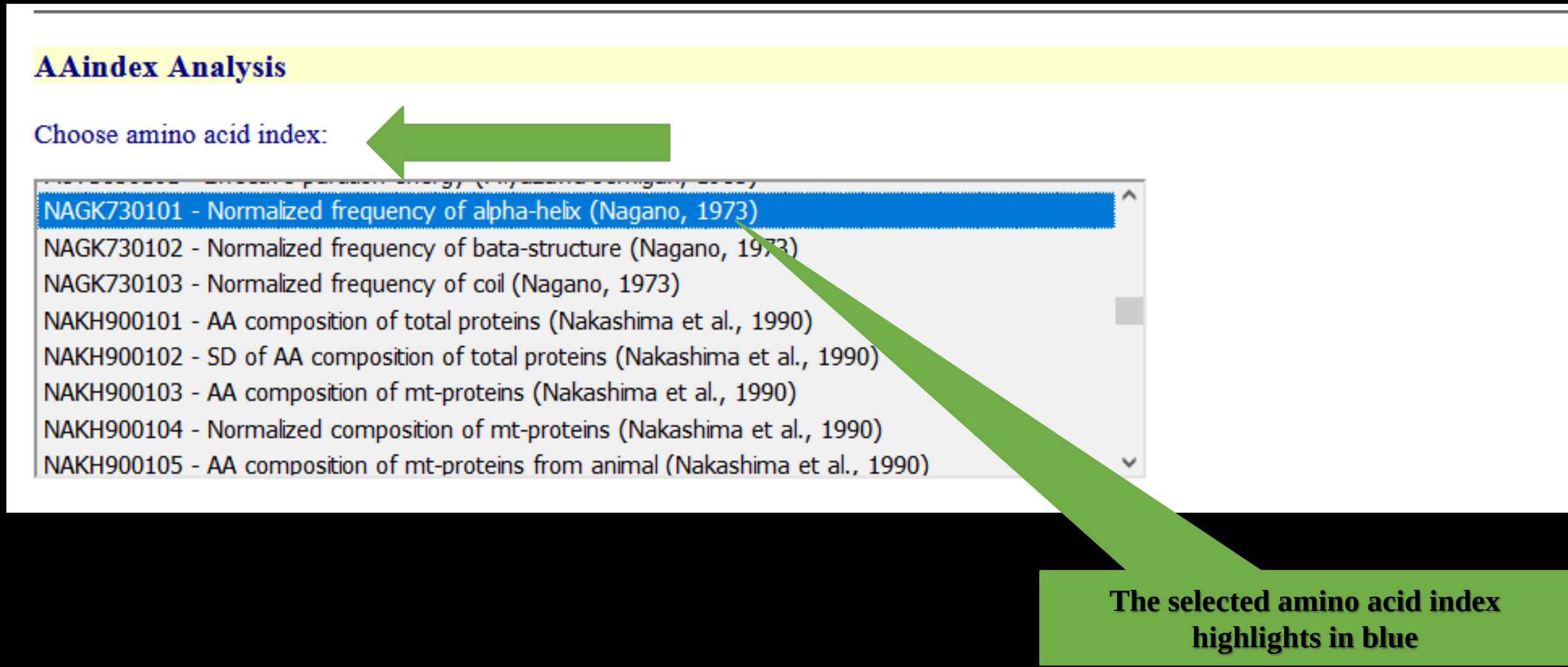
*** Only the first 30 residues are used for prediction

Step 2 : Click on the ‘Run amino acid index analysis’ option in ‘Contents’



Step 3 : Choose amino acid index of your interest



Step 4 : Enter/Paste query sequence

Paste your sequences here:

```
MASSILSSAAVASVNSASPAQASMVAPFTGLKSSAGFPITRKNNVDITTLASNGGKVQCMKV
WPPLGLRK
FETLSYLPDMSNEQLSKECDYLLRNGWVPCVEFDIGSGFVYRENHRSPGYYDGRYWTMWKLP
MFGCTDSS
QVIQEIEEAKKEYPDAFIRVIGFDNVRQVQCISFIAYKPPRFYSS
```

Specify Window Size: (Default: 10)

# of residues to look (from N-terminal): (Default: 0 - meaning the whole sequence)

Submit

The query protein sequence is pasted in the GUI box provided

The search can be customized for window size or a part of protein

If not stated, the default window size of 10 is selected and entire sequence is analysed

Step 5 : Click on ‘Submit’ Button

Paste your sequences here:

```
MASSILSSAAVASVNSASPAQASMVAPFTGLKSSAGFPITRKNNVDITTLASNGGKVQCMKV
WPPLGLRK
FETLSYLPDMSNEQLSKECDYLLRNGWVPCVEFDIGSGFVYRENHRSPGYYDGRYWTMWKLP
MFGCTDSS
QVIQEIEEAKKEYPDAFIRVIGFDNVRQVQCISFIAYKPPRFYSS
```

Specify Window Size: (Default: 10)

# of residues to look (from N-terminal): (Default: 0 - meaning the whole sequence)

Submit

Example 1

AAindex Analysis

Choose amino acid index:

NAGK730101 - Normalized frequency of alpha-helix (Nagano, 1973)
NAGK730102 - Normalized frequency of bata-structure (Nagano, 1973)
NAGK730103 - Normalized frequency of coil (Nagano, 1973)
NAKH900101 - AA composition of total proteins (Nakashima et al., 1990)
NAKH900102 - SD of AA composition of total proteins (Nakashima et al., 1990)
NAKH900103 - AA composition of mt-proteins (Nakashima et al., 1990)
NAKH900104 - Normalized composition of mt-proteins (Nakashima et al., 1990)
NAKH900105 - AA composition of mt-proteins from animal (Nakashima et al., 1990)

Paste your sequences here:

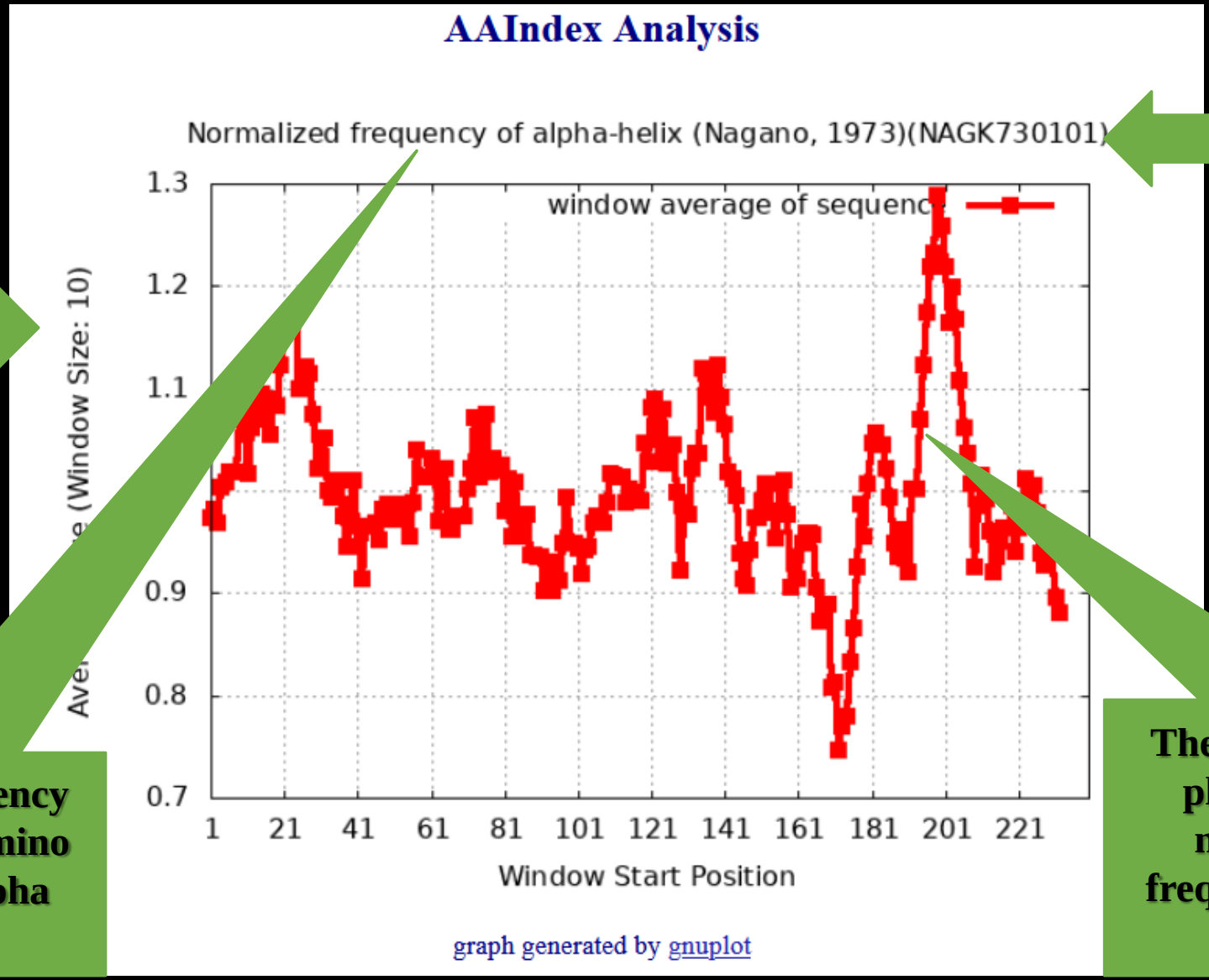
```
>XP_004135094.1 ribulose bisphosphate carboxylase small chain,
chloroplastic [Cucumis sativus]
MASSILSSAAVASVNSASPAQASMVAPFTGLKSSAGFPITRKNNVDITTLASNGGKVQCMKV
WPPLGLRK
FETLSYLPDMSNEQLSKECDYLLRNGWVPCVEFDIGSGFVYRENHRSPGYYDGRYWTMWKLP
MFGCTDSS
QVIQEIEEAKKEYPDAFIRVIGFDNVRQVQCISFIAYKPPRFYSS
```

Specify Window Size: (Default: 10)

# of residues to look (from N-terminal): (Default: 0 - meaning the whole sequence)

Submit

Example 1



It is the overall frequency calculated for each amino acid to occur in a alpha helix

The output graph shows the plot of average values of normalized alpha helix frequency for amino acids in selected window size

Example 2

AAindex Analysis

Choose amino acid index:

ZASB820101 - Dependence of partition coefficient on ionic strength (Zaslavsky et al., 1982)
ZIMJ680101 - Hydrophobicity (Zimmerman et al., 1968)
ZIMJ680102 - Bulkiness (Zimmerman et al., 1968)
ZIMJ680103 - Polarity (Zimmerman et al., 1968)
ZIMJ680104 - Isoelectric point (Zimmerman et al., 1968)
ZIMJ680105 - RF rank (Zimmerman et al., 1968)
AURR980101 - Normalized positional residue frequency at helix termini N4'(Aurora and Rose, 1998)
AURR980102 - Normalized positional residue frequency at helix termini N''' (Aurora and Rose, 1998)

Paste your sequences here:

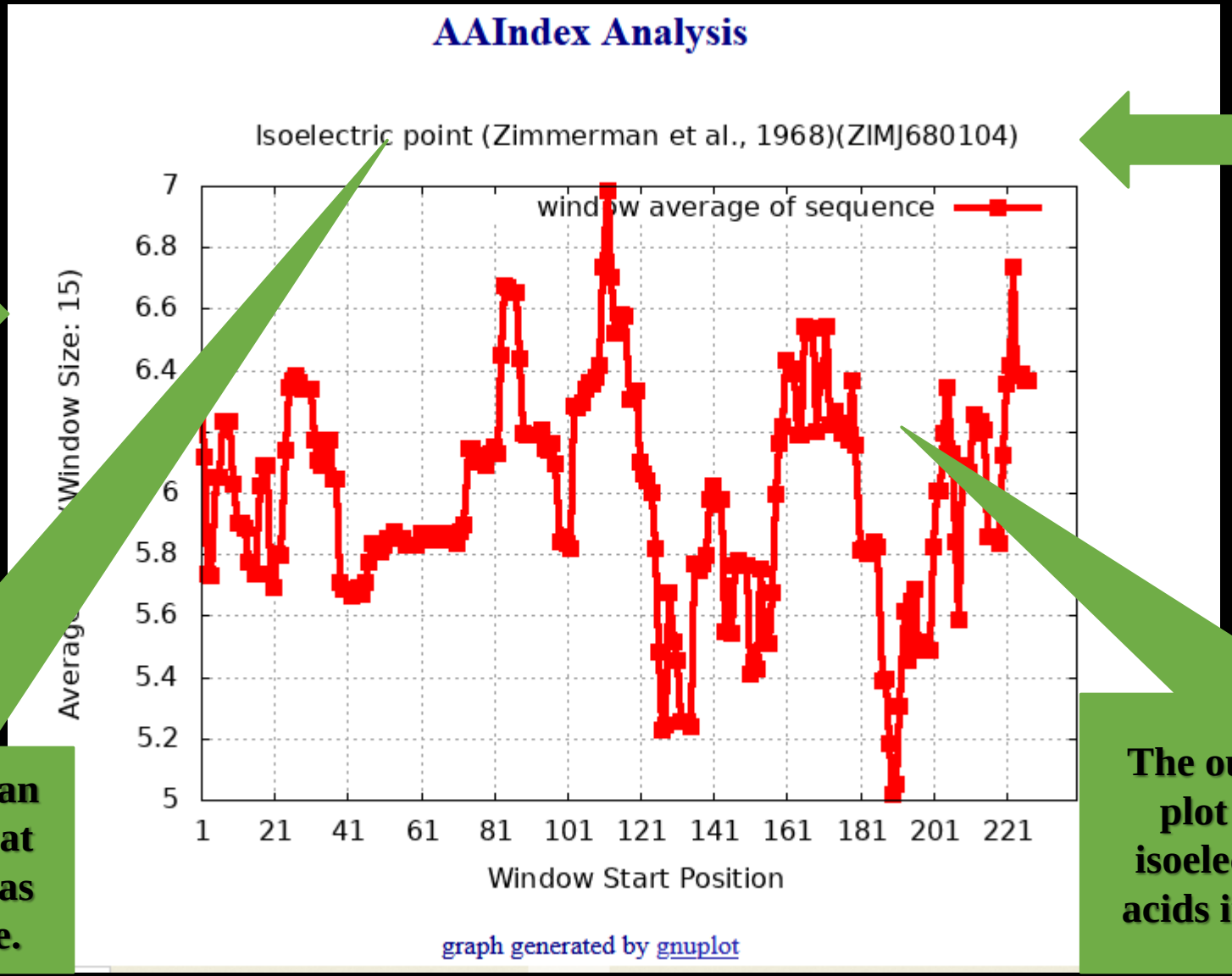
```
>XP_004135094.1 ribulose bisphosphate carboxylase small chain,
chloroplastic [Cucumis sativus]
MASSILSSAAVASVNSASPAQASMVAPFTGLKSSAGFPITRKNNVDITTLASNGGKVQCMKV
WPPLGLRK
FETLSYLPDMSNEQLSKECDYLLRNGWVPCVEFDIGSGFVYRENHRSPGYYDGRYWTMWKLP
MFGCTDSS
QVIQEIEEAKKEYPDAFIRVIGFDNVRQVQCISFIAYKPPRFYSS
```

Specify Window Size: 15 (Default: 10)

# of residues to look (from N-terminal): (Default: 0 - meaning the whole sequence)

Submit

Example 2



The isoelectric point of an amino acid is the point at which the amino acid has no net electrical charge.

The output graph shows the plot of average values of isoelectric points for amino acids in selected window size

Exploring AAindex database further

Paste your sequences here:

```
>XP_004135094.1 ribulose bisphosphate carboxylase small chain,
chloroplastic [Cucumis sativus]
MASSILSSAAVASVNSASPAQASMVAPFTGLKSSAGFPITRKNNVDITTLASNGGKVQCMKV
WPPLGLRK
FETLSYLPDMSNEQLSKECDYLLRNGWVPCVEFDIGSGFVYRENHRSPGYYDGRYWTMWKLP
MFGCTDSS
QVIQEIEEAKKEYPDAFIRVIGFDNVRQVQCISFIAYKPPRFYSS
```

Specify Window Size: 15 (Default: 10)

# of residues to look (from N-terminal): (Default: 0 - meaning the whole sequence)

Submit

Reference

- Bannai, H., Tamada, Y., Maruyama, O., Nakai, K., and Miyano, S., *"Extensive feature detection of N-terminal protein sorting signal"*, Bioinformatics, 18(2) 298-305, 2002. (My version that I'm allowed to post, is here. The copyright has been transferred to Oxford University Press.) [Pubmed]
- Bannai, H., Tamada, Y., Maruyama, O., Nakai, K., Miyano, S., *Views: Fundamental Building Blocks in the Process of Knowledge Discovery*, In Proceedings of the 14th International FLAIRS Conference, 233-238, AAAI Press, 2001. (postscript, gzipped postscript, PDF) (C) AAAI

Links

- PSORT www service (PSORT, PSORT II): The original PSORT and PSORT II.
- AAindex Database: A database of amino acid indices.

Exploring AAindex database further

AAindex

Amino acid indices, substitution matrices and pair-wise contact potentials

AAindex is a database of numerical indices representing various physicochemical and biochemical properties of amino acids and pairs of amino acids. AAindex consists of three sections now: AAindex1 for the amino acid index of 20 numerical values, AAindex2 for the amino acid mutation matrix and AAindex3 for the statistical protein contact potentials. All data are derived from published literature.

Search or Download

Search AAindex **by DBGET bfind for** Go Clear

(e.g. Hydrophobicity, MIRL960101)

- AAindex Help
- Search AAindex by DBGET/LinkDB [DBGET Help]
- Download by anonymous FTP
- Download by HTTPS

Figures and Lists

- Lists of the current database entries

Exploring AAindex database further

AAindex: Amino Acid Index Database

Release 9.2, Feb 2017

Introduction

An amino acid index is a set of 20 numerical values representing any of the different physicochemical and biological properties of amino acids. The AAindex1 section of the Amino Acid Index Database is a collection of published indices together with the result of cluster analysis using the correlation coefficient as the distance between two indices. This section currently contains 566 indices.

Another important feature of amino acids that can be represented numerically is the similarity between amino acids. Thus, a similarity matrix, also called a mutation matrix, is a set of 210 numerical values, 20 diagonal and 20x19/2 off-diagonal elements, used for sequence alignments and similarity searches. The AAindex2 section of the Amino Acid Index Database is a collection of published amino acid mutation matrices together with the result of cluster analysis. This section currently contains 94 matrices.

In the release 9.0, we added a collection of published protein pairwise contact potentials to AAindex as AAindex3. This section currently contains 47 contact potential matrices.

How to search AAindex

AAindex entries can be retrieved by keyword search against the description lines of AAindex (D line in each entry) using DBGET. For example, the user can retrieve a list of entries to input keywors such as 'alpha-helix' or 'hydrophobicity' on the text-box of AAindx home page or the DBGET search page. In the DBGET system, the "bfind" mode is used to get the list of entries including the specified keywords and the "bget" mode is used to get an database entry by specifing an entry ID.

AAindex Home https://www.genome.jp/aaindex/
AAindex search by DBGET https://www.genome.jp/dbget-bin/www_bfind?aaindex

Exploring AAindex database further

```
List of 566 Amino Acid Indices in AAindex ver.9.2

The columns correspond to the AAindex accession number and the description of
each index.

ANDN920101 alpha-CH chemical shifts (Andersen et al., 1992)
ARGP820101 Hydrophobicity index (Argos et al., 1982)
ARGP820102 Signal sequence helical potential (Argos et al., 1982)
BEGF750101 Conformational parameter of inner helix (Beghin-Dirkx, 1975)
BEGF750102 Conformational parameter of beta-structure (Beghin-Dirkx, 1975)
BEGF750103 Conformational parameter of beta-turn (Beghin-Dirkx, 1975)
BHAR880101 Average flexibility indices (Bhaskaran-Ponnuswamy, 1988)
BIGC670101 Residue volume (Bigelow, 1967)
BIOV880101 Information value for accessibility; average fraction 35% (Biou et al., 1988)
BIOV880102 Information value for accessibility; average fraction 23% (Biou et al., 1988)
BROC820101 Retention coefficient in TFA (Browne et al., 1982)
BROC820102 Retention coefficient in HFBA (Browne et al., 1982)
BULH740101 Transfer free energy to surface (Bull-Breese, 1974)
BULH740102 Apparent partial specific volume (Bull-Breese, 1974)
BUNA790101 alpha-NH chemical shifts (Bundi-Wuthrich, 1979)
BUNA790102 alpha-CH chemical shifts (Bundi-Wuthrich, 1979)
BUNA790103 Spin-spin coupling constants 3JHalpha-NH (Bundi-Wuthrich, 1979)
BURA740101 Normalized frequency of alpha-helix (Burgess et al., 1974)
BURA740102 Normalized frequency of extended structure (Burgess et al., 1974)
CHAM810101 Steric parameter (Charton, 1981)
CHAM820101 Polarizability parameter (Charton-Charton, 1982)
CHAM820102 Free energy of solution in water, kcal/mole (Charton-Charton, 1982)
CHAM830101 The Chou-Fasman parameter of the coil conformation (Charton-Charton, 1983)
CHAM830102 A parameter defined from the residuals obtained from the best correlation of  the Chou-Fasman parameter of beta-sheet (Charton-Charton, 1983)
CHAM830103 The number of atoms in the side chain labelled 1+1 (Charton-Charton, 1983)
CHAM830104 The number of atoms in the side chain labelled 2+1 (Charton-Charton, 1983)
CHAM830105 The number of atoms in the side chain labelled 3+1 (Charton-Charton, 1983)
CHAM830106 The number of bonds in the longest chain (Charton-Charton, 1983)
CHAM830107 A parameter of charge transfer capability (Charton-Charton, 1983)
CHAM830108 A parameter of charge transfer donor capability (Charton-Charton, 1983)
CHOC750101 Average volume of buried residue (Chothia, 1975)
CHOC760101 Residue accessible surface area in tripeptide (Chothia, 1976)
CHOC760102 Residue accessible surface area in folded protein (Chothia, 1976)
CHOC760103 Proportion of residues 95% buried (Chothia, 1976)
```

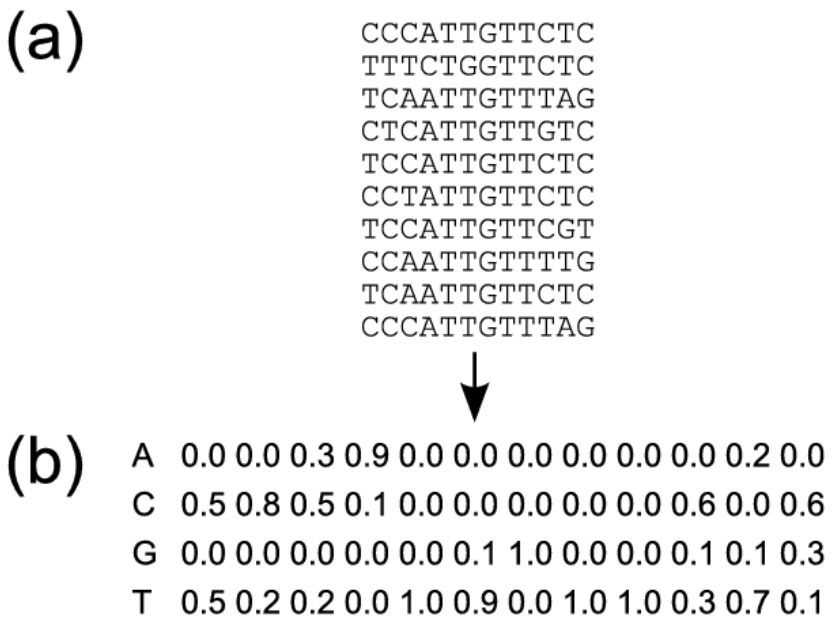
PrediSi

PREDIction of SIgnal peptides

PrediSi

PREDIction of SIgnal peptides

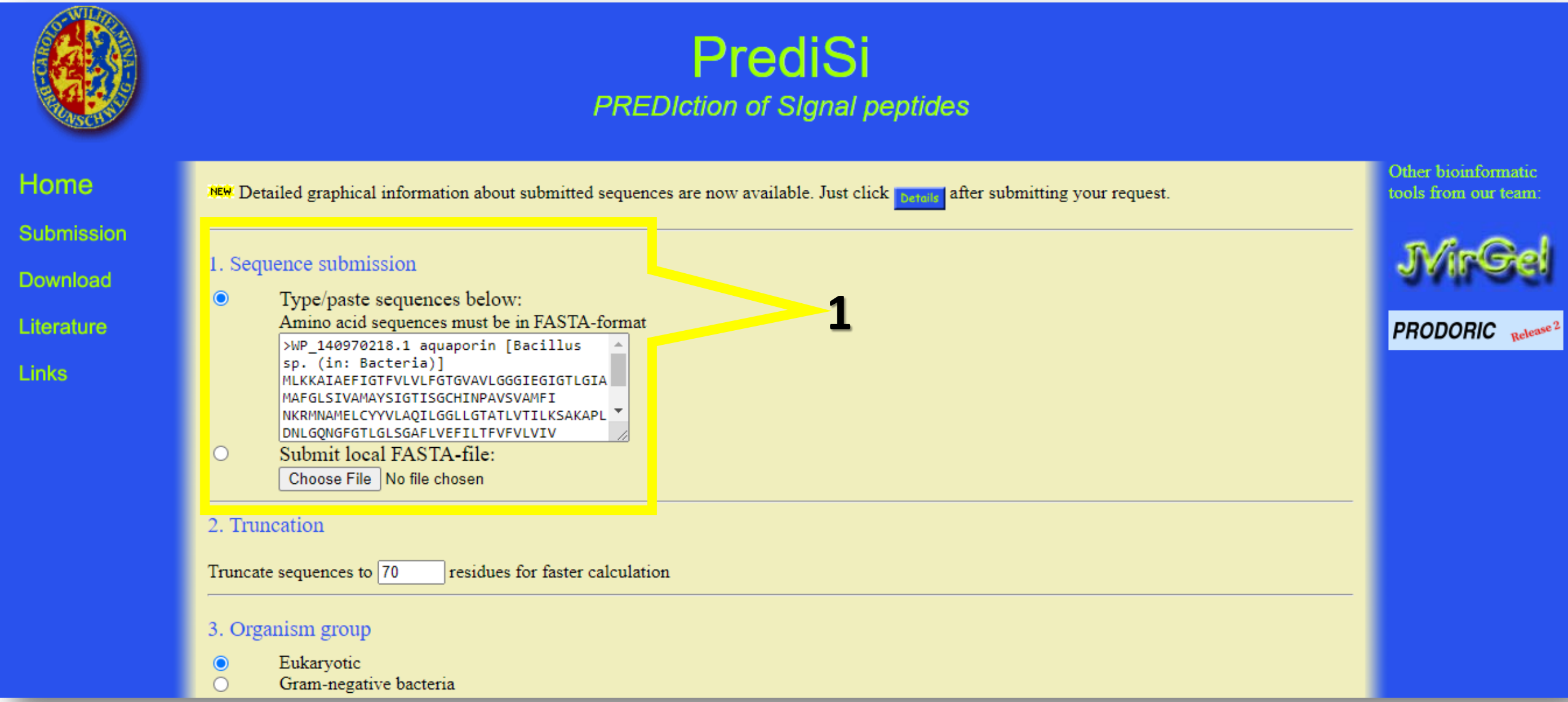
- **PrediSi** allows the evaluation of whole proteome datasets i.e. analysis of large datasets in real time with high accuracy.
- The method employed is based on a **position weight matrix** approach.
- A **freely available**, user-friendly web interface tool (http://www.predisi.de)
- Presentation of the **results** in **user-** as well as **computer-friendly** formats such as HTML, XML and CSV.
- Free availability as a **Java package** for integration into other software projects.



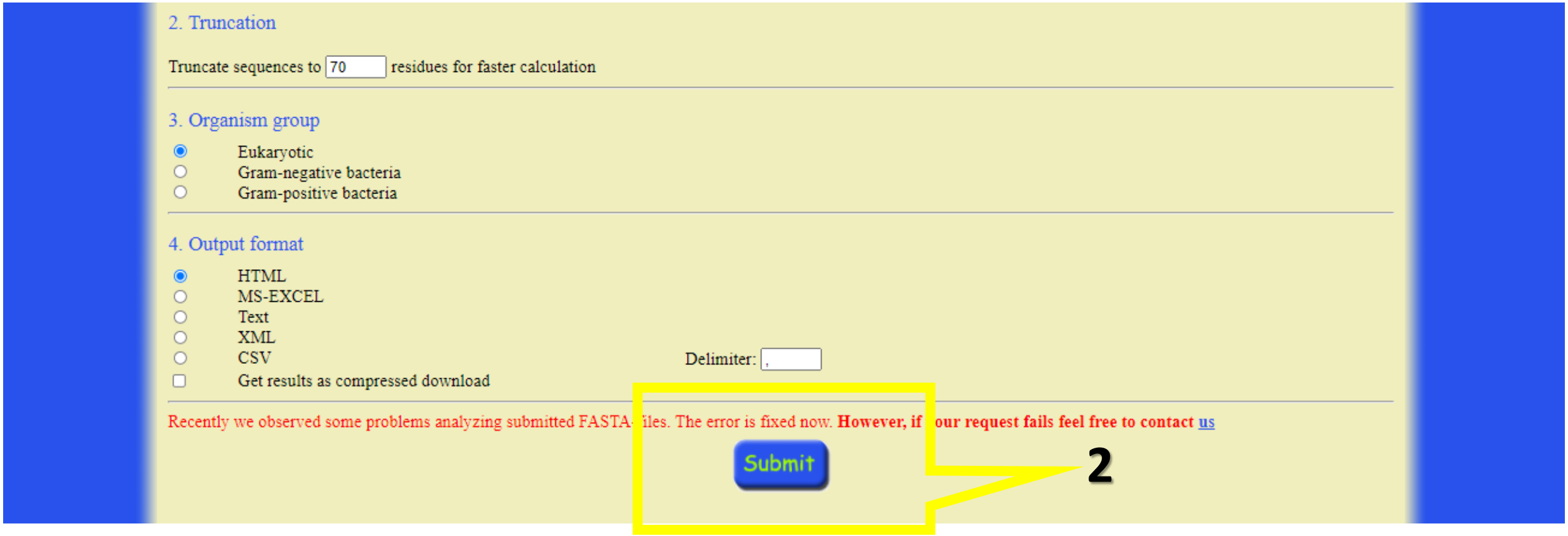
Hiller et al., 2004; Kilpatrick, 2015

Steps to follow

http://www.predisi.de/



Steps to follow



Settings:

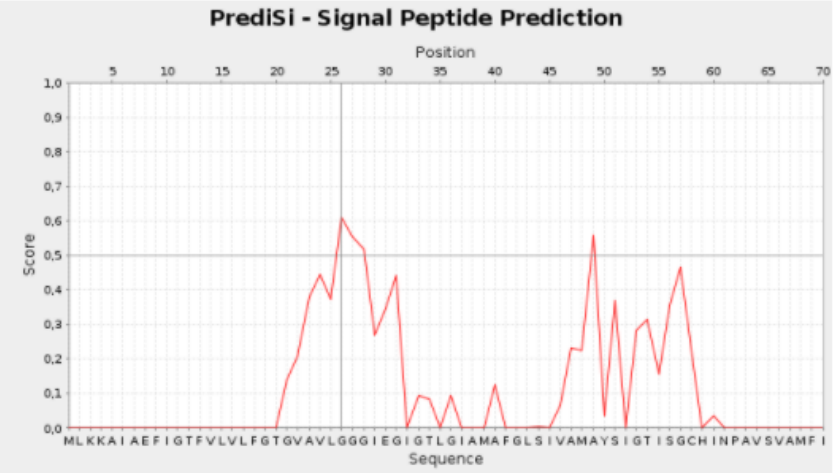
Matrix:	null
Truncation:	70 residues
Output:	null

Result

FASTA-ID	Score	Cleavage Position	Signal Peptide ?	Chart
WP_140970218.1 aquaporin [Bacillus sp. (in: Bacteria)]	0.6092	26	Y	Details

Details:

Matrix:	Eukarya
Truncation:	70 residues
Cleavage position:	26
Score:	0.6092
Secreted protein:	predicted for secretion



WP_140970218.1 aquaporin [Bacillus sp. (in: Bacteria)]:

```
MLKKAIAEFIGTFVLVLFGTGVAVLGGGIEGIGTLGIAMAFGLSIVAMAYSIGTISGCHINPAVSVAMFI
|    |    |    |    |    |    |    |    |    |    |    |    |    |    |
1        10        20        30        40        50        60        70
```

Detailed Results

Bibliography

PrediSi

PREDIction of SIgnal peptides

Home

Submission

Download

Literature

Links

Literature:

- von Heijne, G. (1985) **Signal sequences. The limits of variation.** *Journal of molecular biology* **184** , 99-105 [PUBMED]
- Rapoport, TA., Jungnickel, B. & Kutay, U. (1996) **Protein transport across the eukaryotic endoplasmic reticulum and bacterial inner membranes.** *Annu. Rev. Biochem.* **61**, 271-303 [PUBMED]
- Nielsen, H., Engelbrecht, J., Brunak, S. & von Heijne, G. (1997) **Identification of prokaryotic and eukaryotic signal peptides and prediction of their cleavage sites.** *Protein Eng.* **10**, 1-6 [PUBMED]
- Zheng, N. and Gierasch, L..M. (1996) **Signal sequences: the same yet different.** *Cell* **86**, 849-852 [PUBMED]
- Rapoport T.A., Jungnickel B. and Kutay U. (1996) **Protein transport across the eukaryotic endoplasmic reticulum and bacterial inner membranes.** *Annual review of biochemistry* **65**, 271-303 [PUBMED]
- Nielsen, H., Engelbrecht, J., von Heijne, G. and Brunak, S. (1996) **Defining a Similarity Threshold for a Functional Protein Sequence Pattern: The Signal Peptide Cleavage Site.** *Proteins* **24** , 165-177 [PUBMED]
- Menne, K. M. L., Hermjakob, H. and Apweiler, R. (2000) **A comparison of signal sequence prediction methods using a test set of signal peptides.** *Bioinformatics* **16**, 741-742 [PUBMED]
- Schreiber M. and Brown C. (2002) **Compensation for nucleotide bias in a genome by representation as a discrete channel with noise.** *Bioinformatics* **18** , 507-512 [PUBMED]
- Boeckmann B., Bairoch A., Apweiler R., Blatter M.-C., Estreicher A., Gasteiger E., Martin M.J., Michoud K., O'Donovan C., Phan I., Pilbout S. and Schneider M. (2003) **The SWISS-PROT protein knowledgebase and its supplement TrEMBL in 2003.** Nucleic Acids Research. **31**, 365- 370 [PUBMED]
- Hiller, K., Schobert, M., Hundertmark, C., Jahn, D. & Münch, R. (2003) **JVirGel: calculation of virtual two-dimensional protein gels.** *Nucleic Acids Res.* **31**, 3862-3865 [PUBMED]

Other bioinformatic tools from our team:

JVirGel

PRODORIC Release 2

Algorithms for Prediction Softwares

- Signal peptides serve as “address tags”. It is highly desirable to develop the fast and accurate algorithms to identify the signal sequences and predict their cleavage sites. Based on different kinds of characteristics, several algorithms such as neural networks, and **Hidden Markov Models** have been used.
- **Bayesian network** is a method of statistical inference in which some kind of evidence or observations are used to calculate the probability if a hypothesis may be true.

Hidden Markov Model & Bayes Theorem

Life of a Science student

Experiment worked!!

Experiment failed!!

Exceptions

Experiment worked!!

0.8

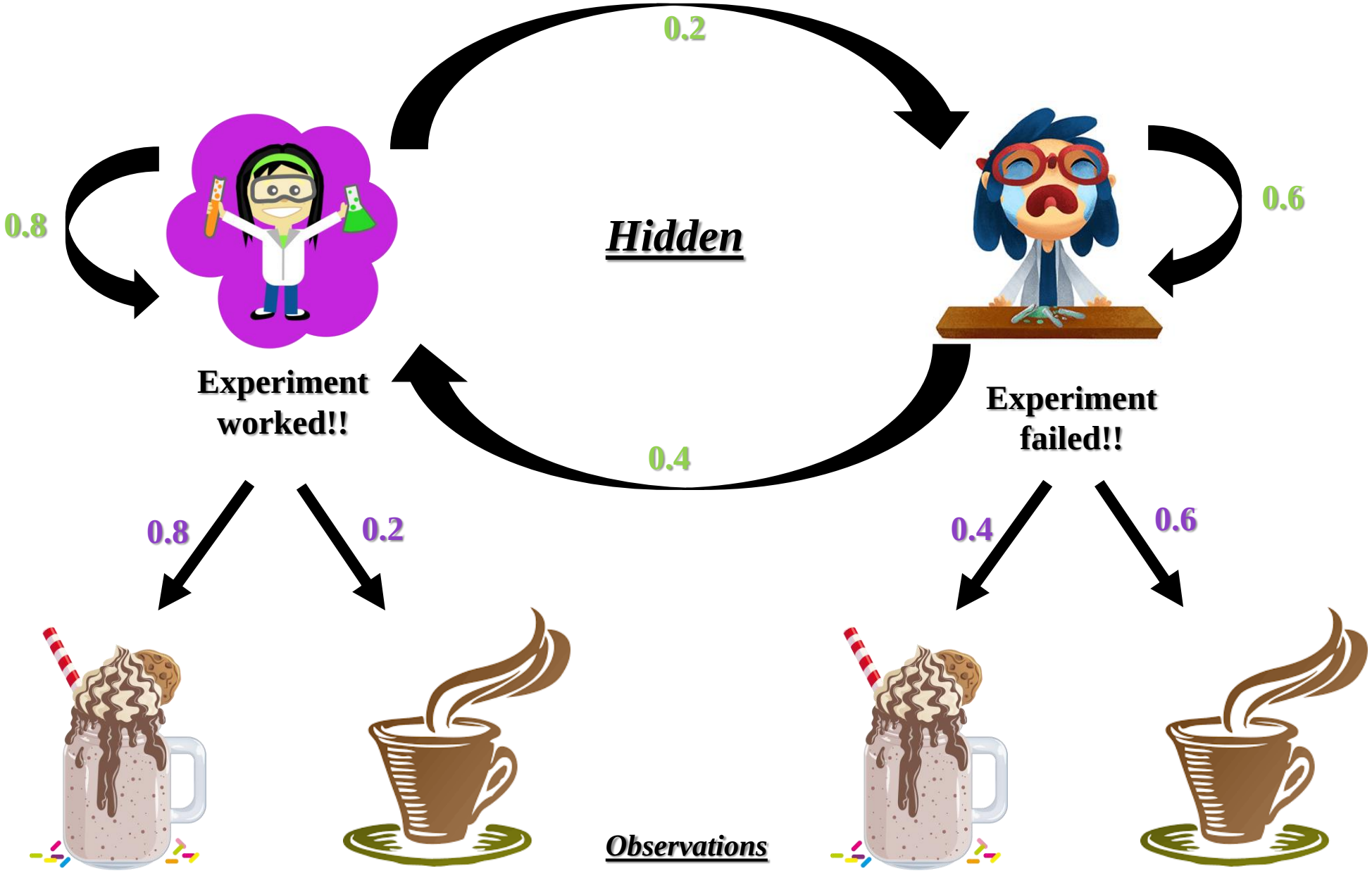
0.2

Experiment failed!!

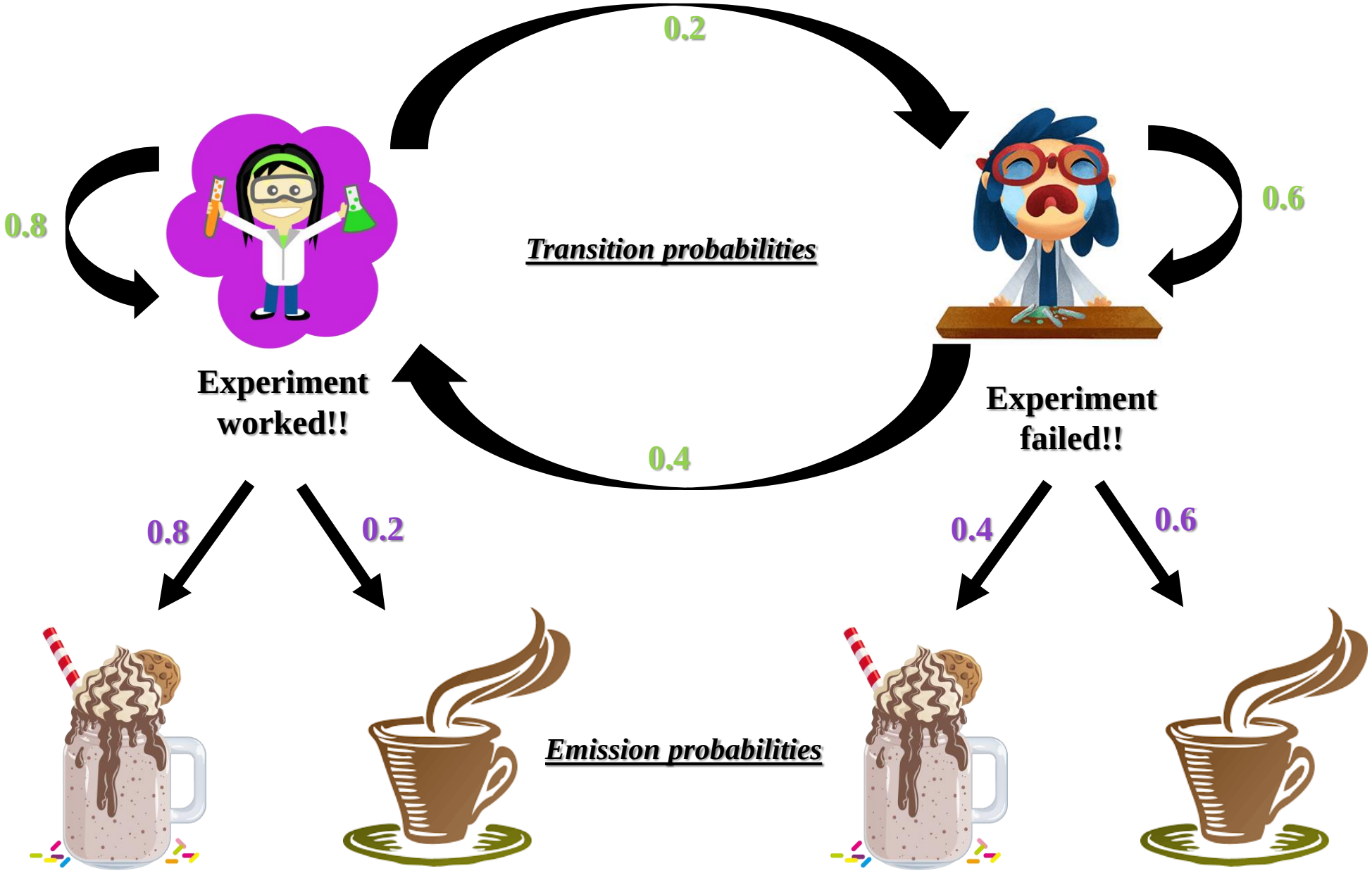
0.4

0.6

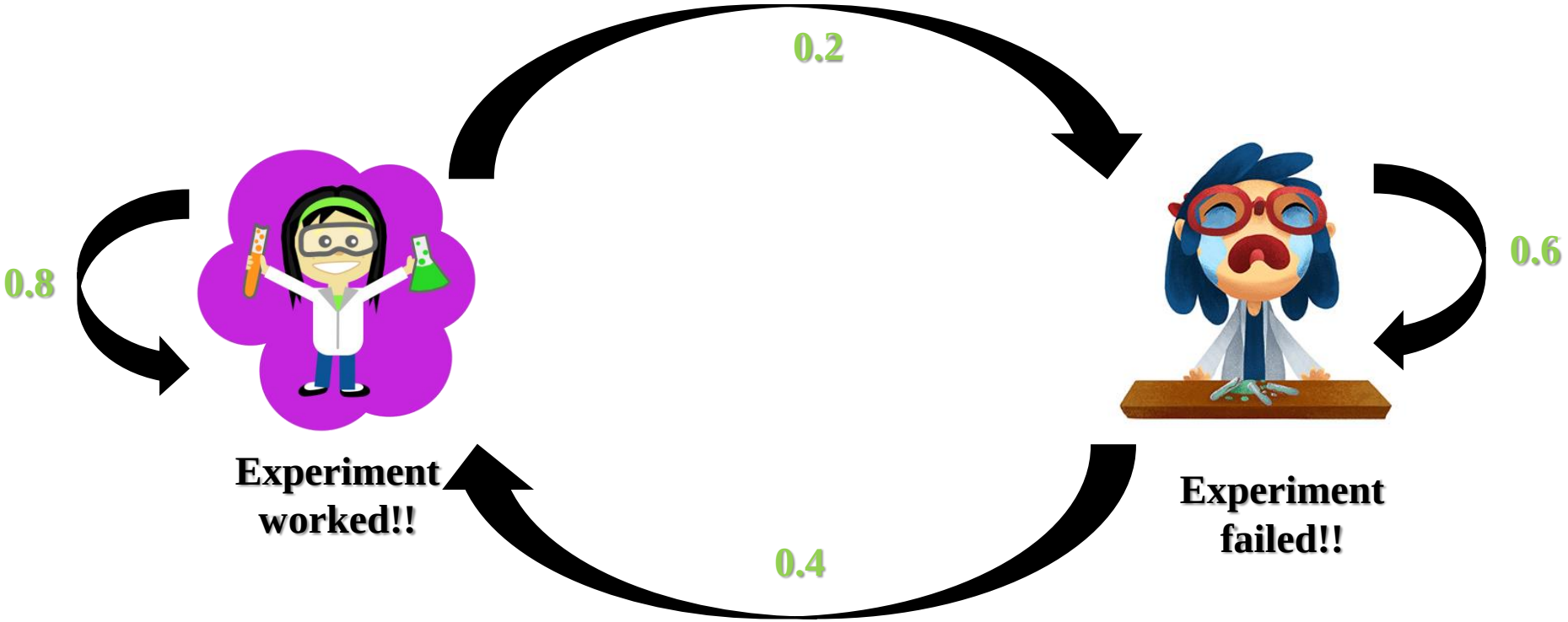
Hidden Markov Model



Hidden Markov Model



Probability of an experiment working or failing on a Random day?

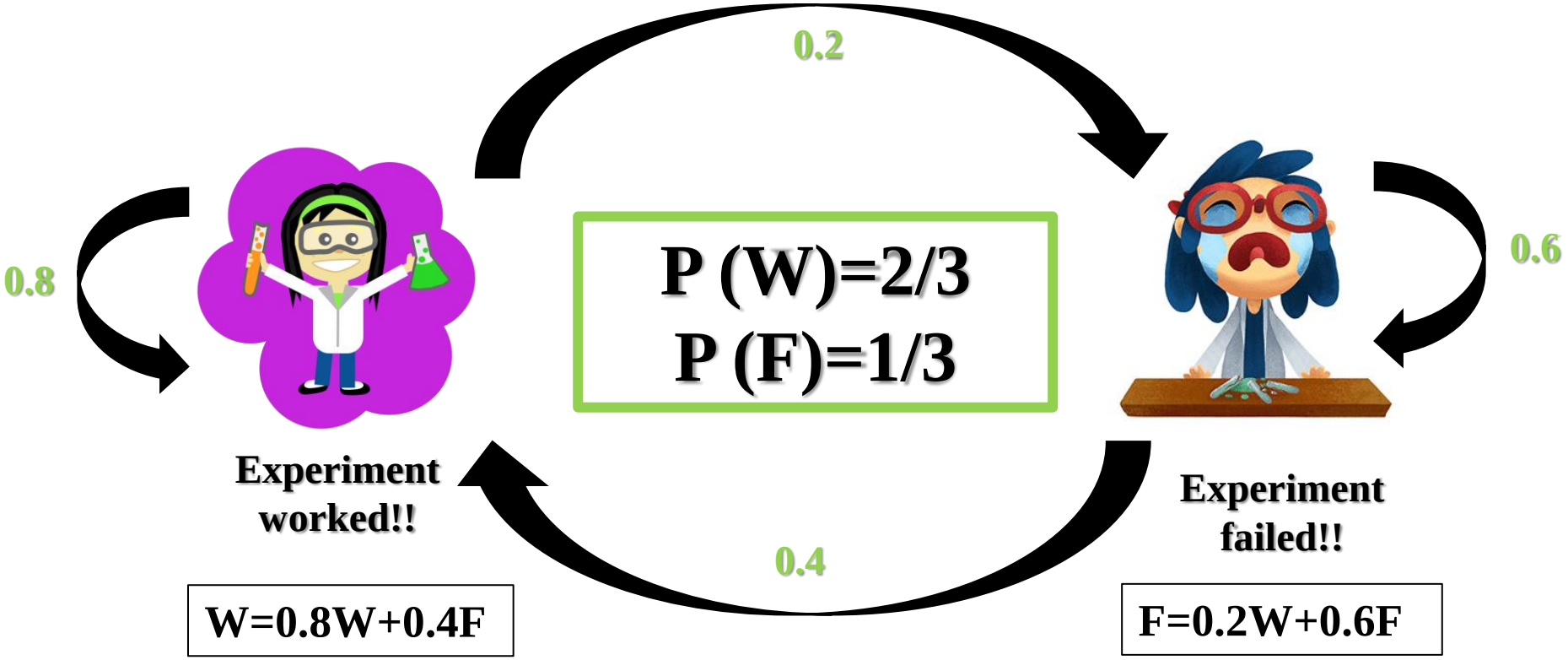


$$W=0.8W+0.4F$$

$$F=0.2W+0.6F$$

$$W+F=1$$

Probability of an experiment failing or working on a Random day?



W+F=1

Probability of an experiment failing or working if I ordered Oreo shake?

Experiment worked!!

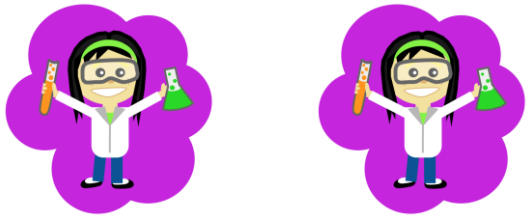
Experiment failed!!

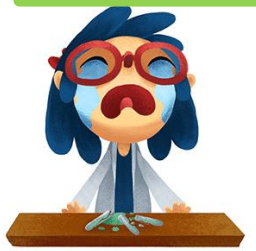
P (W)=2/3
P (F)=1/3

Prior Probability

Bayes Theorem

P(W)=2/3 ← **Prior Probability** → **P(F)=1/3**



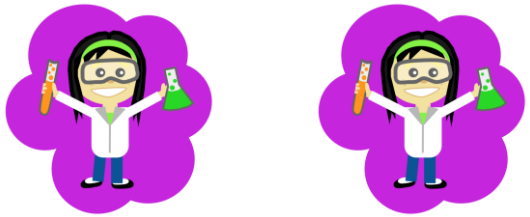


0.8

0.2

Bayes Theorem

P(W)=2/3 ← **Prior Probability** → **P(F)=1/3**



0.8

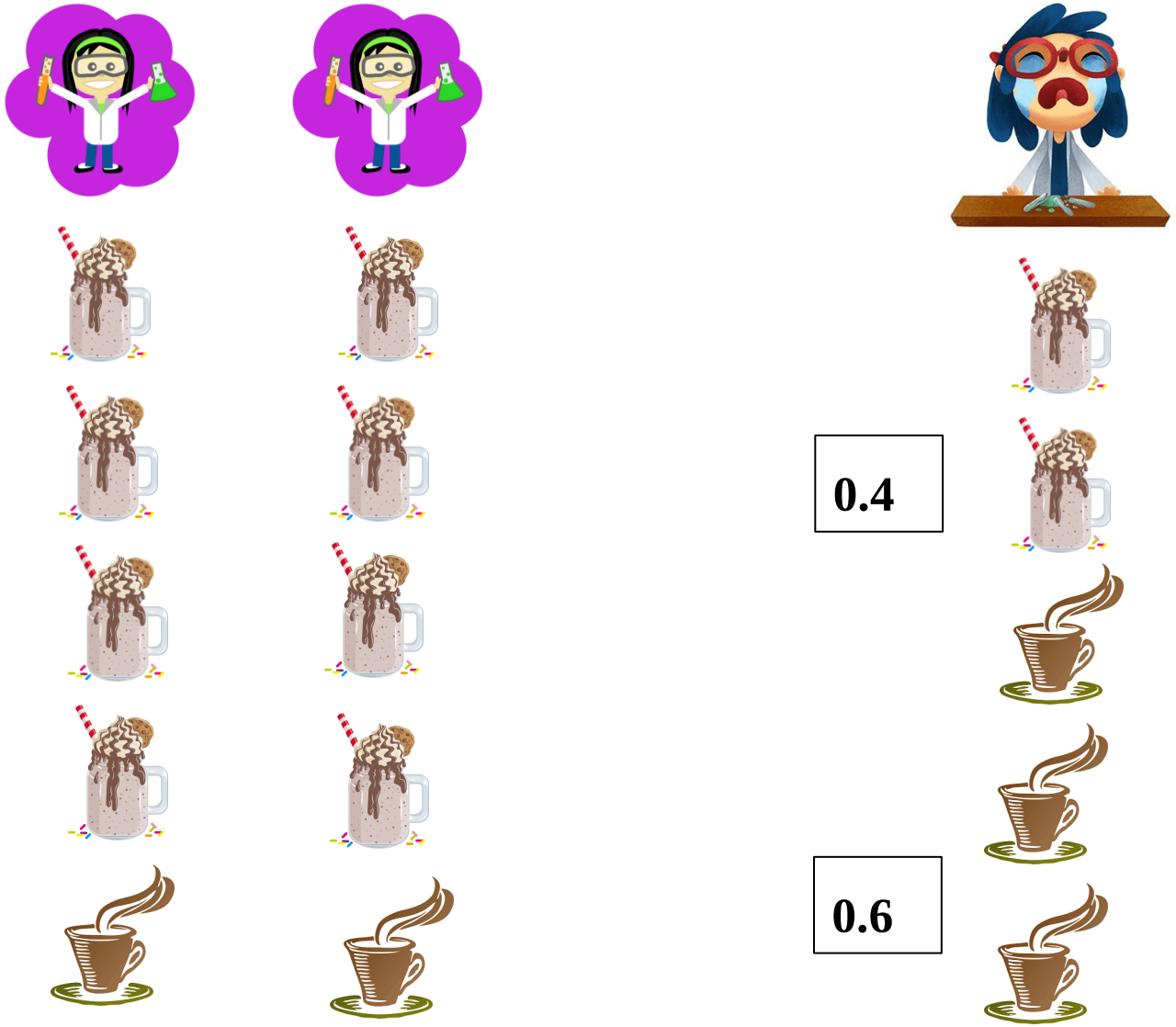
0.4

0.2

0.6

Bayes Theorem

P(W)=2/3 ← Prior Probability → P(F)=1/3



0.8

0.2

0.4

0.6

If OS,

P (W|OS)= 8/10

P (F|OS)=2/10

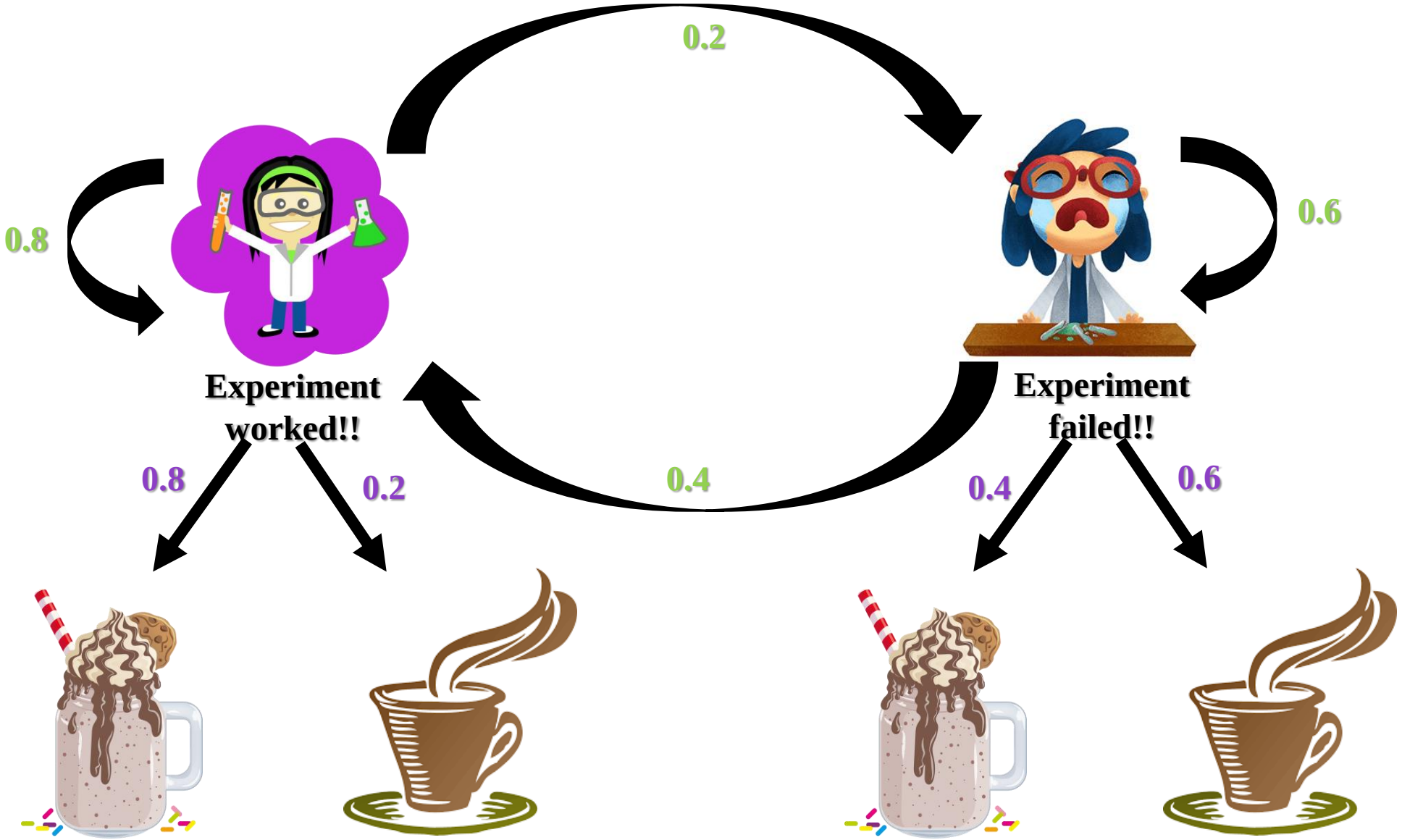
Posterior Probabilities

If C,

P (W|C)= 2/5

P (F|C)=3/5

Maximum Likelihood- Home Exercise



If for 2 consecutive days I ordered Oreo shake, what was the status of my experiments?

Hint

No. of possibilities= 2^n where n=2 in this case

I

Experiment worked!!

Experiment worked!!

II

Experiment failed!!

Experiment failed!!

III

Experiment worked!!

Experiment failed!!

IV

Experiment failed!!

Experiment worked!!

Acknowledgements

Students of B. Sc (H) Botany, KMC, University of Delhi

Student Online Workshop on

Application of Bioinformatics for Pedagogy of Plant Sciences

Organized by Kirori Mal College

(Under DBT Star Scheme)

23rd July 2021

Plant Cell Biology 101 meets Bioinformatics