Grundpraktikum Bioinfo - Week 2

Biological sequence analysis

Carl Herrmann
IPMB - Universität Heidelberg

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Institut für Pharmazie und Molekulare Biotechnologie

UNIVERSITÄT HEIDELBERG
ZUKUNFT SEIT 1386

Themen des Grundkurses

IPMB Institut für Pharmazie und Molekulare Biotechnologie

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- **Statistische Datenanalyse** - Woche 1
  - Beschreibende Statistik, graphische Darstellung von Daten
  - Inferenzstatistik
  - Datenanalyse
  - Umsetzung der Konzepte mit R

Carl Herrmann
Maiwen Caudron-Herger

- **Sequenzanalyse** - Woche 2
  - Untersuchung von unbekannten Sequenzen
  - Sequenzalignments
  - Phylogenetische Rekonstruktion
  - Genomische Daten - Pre-Prozessierung von RNA-seq Daten

Carl Herrmann
Benedikt Brors

- **Analyse von RNA-seq Daten** - Woche 3
  - Normalisierung
  - Differentielle Analysen

Simon Anders

Woche 2 - Sequenzanalyse

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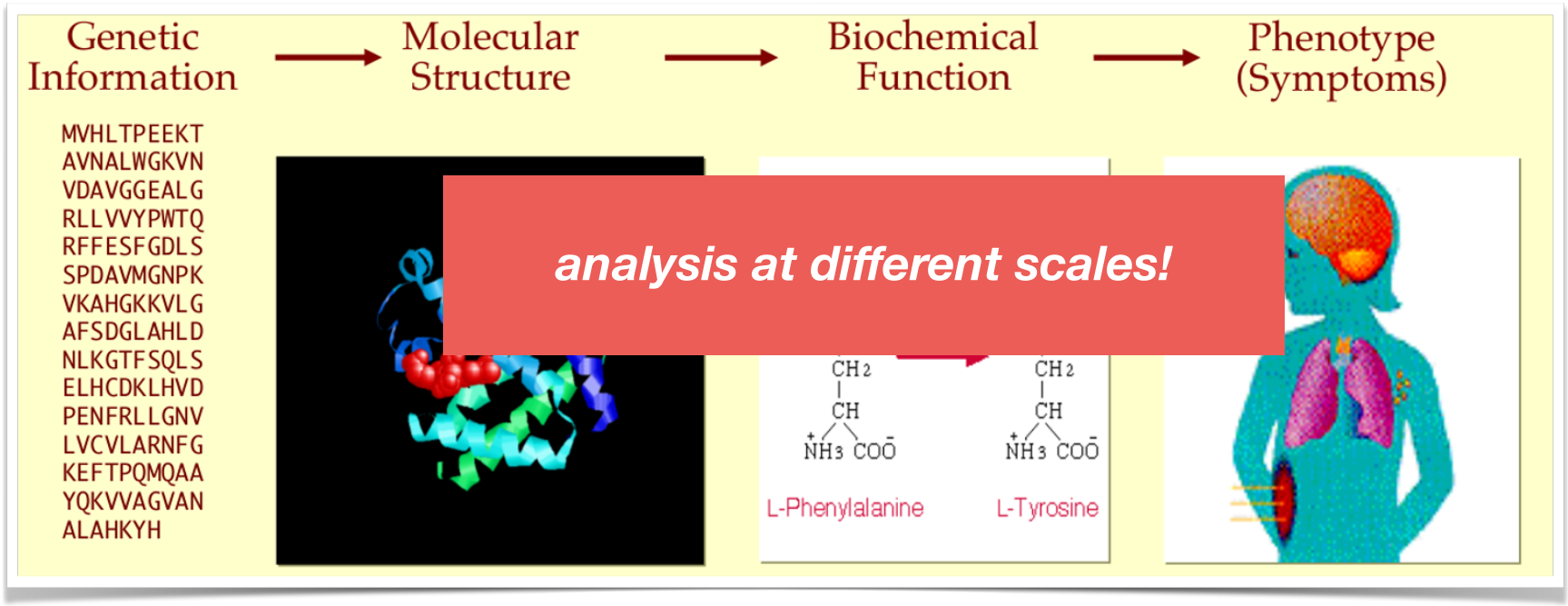
	Vormittags	Nachmittags (Albert Li, Robin Droit)
Montag	Einführung in Sequenzanalyse	**Annotathon!** Annotation metagenomischer Sequenzen
Dienstag	Alignments; BLAST	
Mittwoch	Multiples Sequenzalignment; phylogenetische Rekonstruktion	
Donnerstag	Hochdurchsatzsequenzierung (Benedikt Brors)	Untersuchung von HTS-Daten mit Genome Browser (IGV)
Freitag		pre-prozessierung von RNA-seq Daten

What is Bioinformatics??

Bioinformatics: The science of **information** and **information flow** in biological systems, especially of the use of **computational methods** in genetics and **genomics**. (Oxford English Dictionnary)



Why is bioinformatics necessary?

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Genome annotation

Find german
words for animals

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F	J	B	H	U	N	D	J	M	C	R	J	A	N	P
R	K	Z	P	U	O	Y	H	W	X	T	R	U	J	Z
H	A	R	M	B	S	R	W	O	G	A	N	S	F	G
I	F	G	C	P	F	P	R	L	I	H	F	O	J	B
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A	G	R	N	J	I	C	H	M	Z	S	G	G	K	X

Genome annotation

Find klingon
words for whatever...

Without bioinformatics...

Genome wide association studies

EDITORIALS

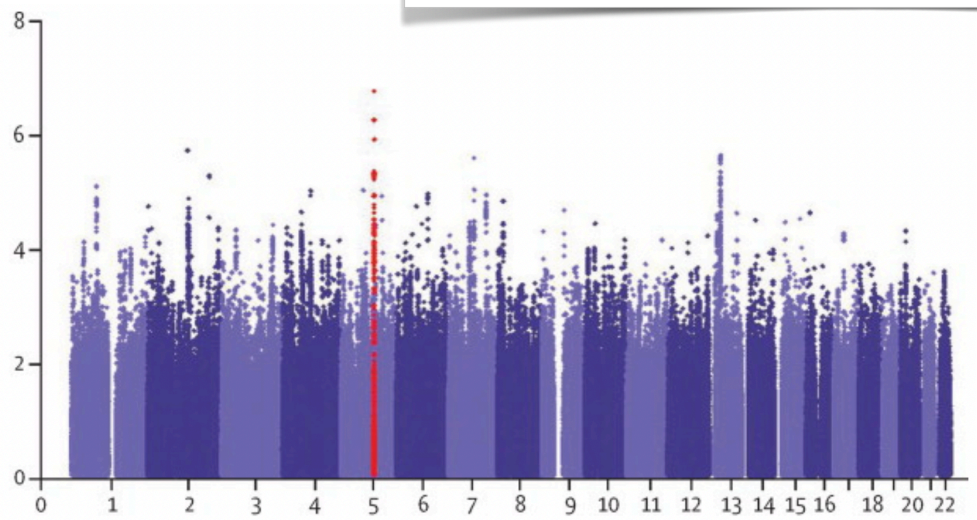
Finding a Needle in the Haystack

Leveraging Bioinformatics to Identify a Functional Genetic Risk Factor for Sepsis Death*

Meyer, Nuala J. MD, MS

Author Information

Critical Care Medicine 43(1):p 242-243, January 2015. | *DOI:* 10.1097/CCM.0000000000000664



[Rautanen et al., Lancet Resp. Med (2015)]

- Single-nucleotide variants (SNPs)
- ~ 4-5 milllion per genome
- 600 million different SNPs identified so far...
- **Which ones are associated to disease phenotype?**

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Biological databases

Bioinformatics

Sequence alignments

Genome annotation

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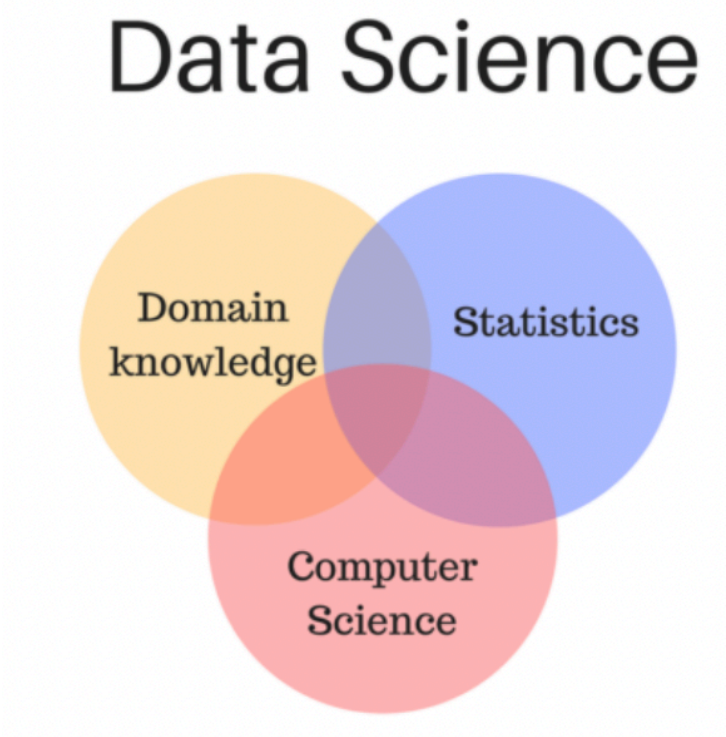
ML & Artificial Intelligence

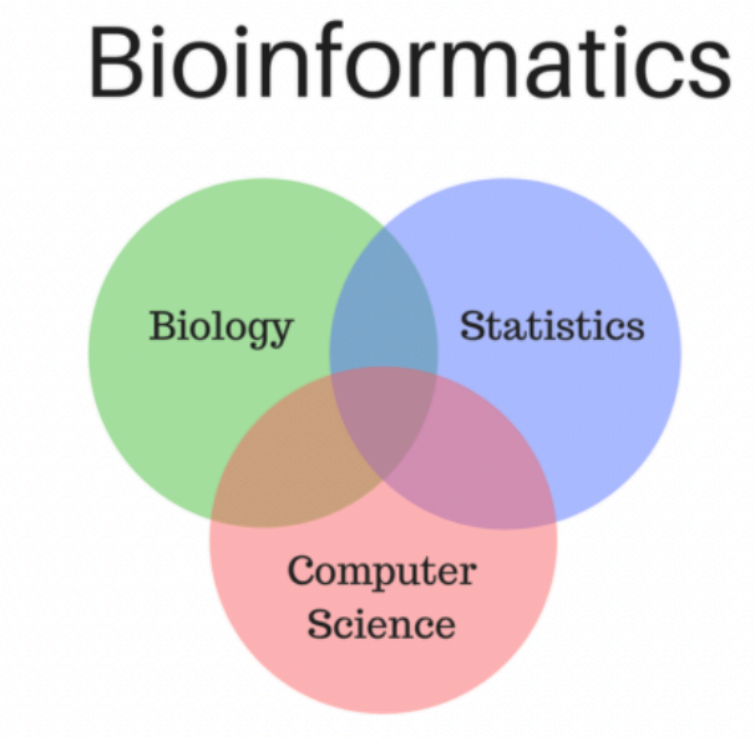
Computational Biology

Data Science

Systems Biology

Bioinformatics = data analysis?





[OMGenomics]

Aspects of bioinformatics/computational biology

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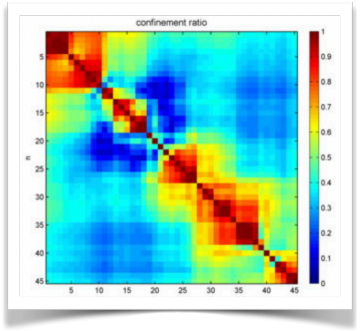
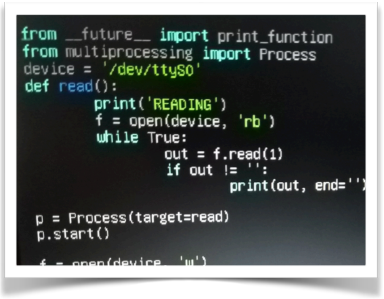
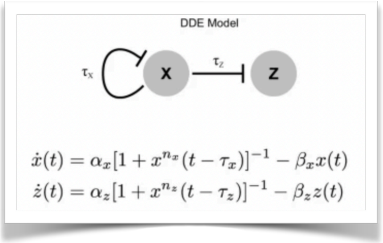
1. **Data analysis**: Going from raw data, to clean data, to statistical and visual interpretations of the results



2. **Bioinformatics software development**: Developing software to do bioinformatics analysis, big enough software products to publish as independent methods papers and to be used by other scientists.



3. **Modeling**: Performing simulations and writing equations to represent biological systems ("systems biology")



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1. **Data analysis**: Going from raw data, to clean data, to statistical and visual interpretations of the results

2. **Bioinformatics software development**: Developing software to do bioinformatics analysis, big enough software products to publish as independent methods papers and to be used by other scientists.

3. **Modeling**: Performing simulations and writing equations to represent biological systems.

what we are doing in these 3 weeks !

data =

- ***numerical data***
- ***sequence data***
- ***genomics data***

[OMGenomics]

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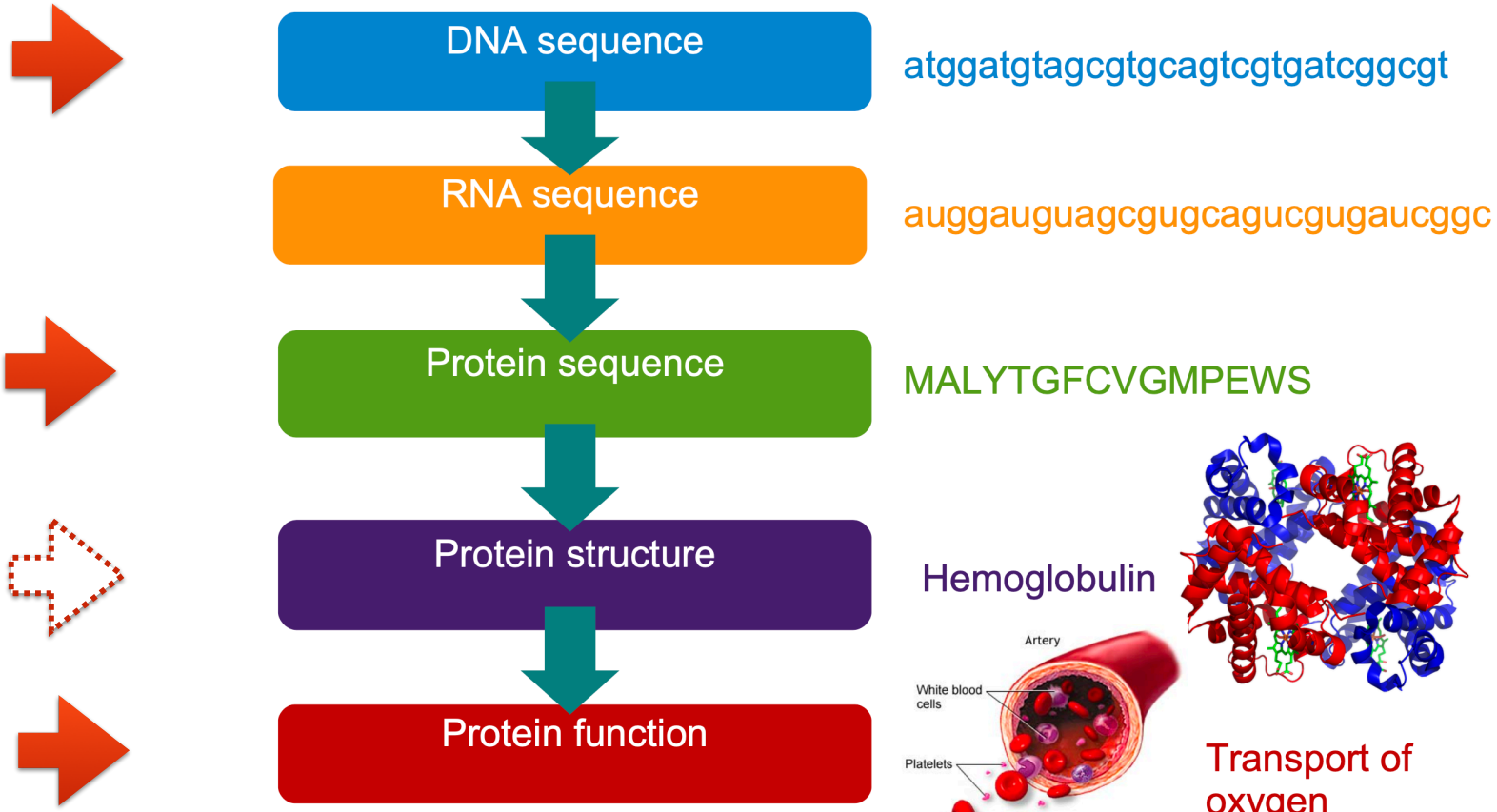
Sequence analysis

Carl Herrmann

What sequences?



What sequences?

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DNA / RNA sequences
4 bases

```
5' A G T A C G 3'
3' T C A T G C 5'
```

FASTA formated sequence:

```
>free text annotation
AGTACGGGTAATGCGTAGCATG
TACGTATGCTATCTGTACGA
```

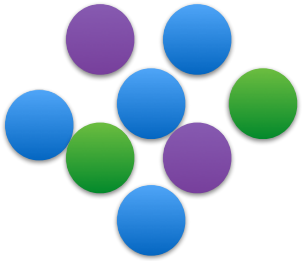
Protein sequences
20 amino acids

N_{term} **M H P G C V** C_{term}

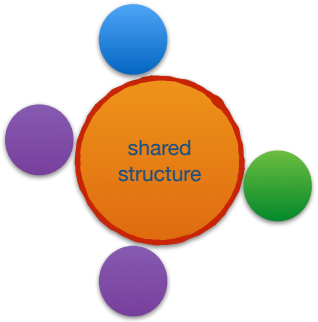
FASTA formated sequence:

```
>free text annotation
MHPGCVGTRFSPMNWVAFGRDS
```

Initial protein models...

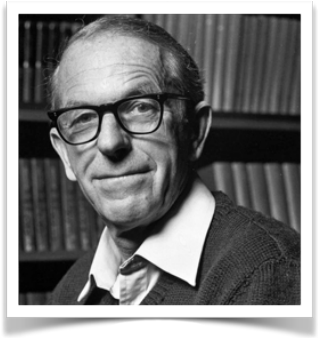


"soup" of amino-acids?



Shared structure + micro-heterogeneity?

Fred Sanger,
sequencing of
insulin protein
1951/1952

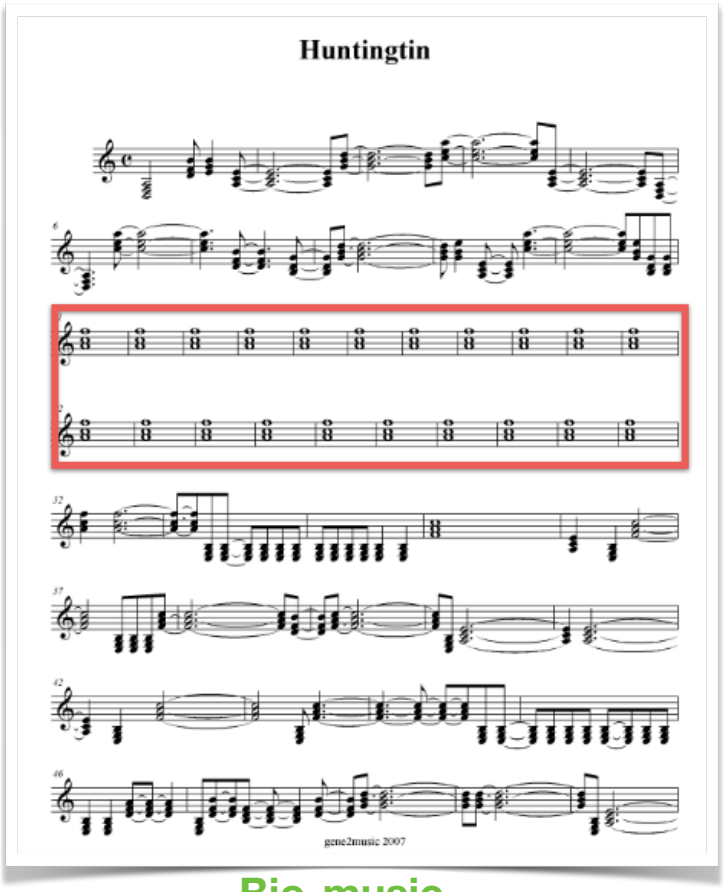


"Proteins have a unique linear sequence"

Nonetheless, the correctness of the concept that all molecules of a very carefully prepared protein have the same unique structure and configuration is still controversial, as shown by the divergent conclusions in two recent reviews (124,

[Colvin, Smith, Cook (1954)]

Initial protein models...



Bio-music

[Takahashi & Miller (2007)

```
>sp|P42858|HD_HUMAN Huntingtin
MATLEKLMKAFESLKSFQQQQQQQQQQQQQQQQQQQQPPPPPPPPPPQLPQPPPQAQP
LLPQPQPPPPPPPPPPGPAVAEEPLHRPKKELSATKKDRVNHCLTICENIVAQSVRNSPE
FQKLLGIAMELFLLCSDDAESDVRMVADECLNKVIKALMDSNLPRLQLELYKEIKKNGAP
RSLRAALWRFAELAHLVRPQKCRPYLVNLLPCLTRTSKRPEESVQETLAAAVPKIMASFG
NFANDNEIKVLLKAFIANLKSSSPTIRRTAAGSAVSICQHSRRTQYFYSWLLNVLLGLLV
PVEDEHSTLLILGVLLTLRYLVPLLQQQVKDTSLKGSFGVTRKEMEVSPSAEQLVQVYEL
TLHHTQHQDHNVVTGALELLQQLFRTPPPELLQTLTAVGGIGQLTAAKEESGGRSRSGSI
VELIAGGGSSCSPVLSRKQKGKVLLGEEEALEDDSESRSDVSSSALTASVKDEISGELAA
SSGVSTPGSAGHDIITEQPRSQHTLQADSVDLASCDLTSSATDGDEEDILSHSSSQVSAV
PSDPAMDLNDGTQASSPISDSSQTTTEGPDSAVTPSDSSEIVLDGTDNQYLGLQIGQPQD
EDEEATGILPDEASEAFRNSSMALQQAHLLKNMSHCRQPSDSSVDKFVLRDEATEPGDQE
NKPCRIKGDIGQSTDDDSAPLVHCVRLLSASFLLTGGKNVLVPDRDVRVSVKALALSCVG
AAVALHPESFFSKLYKVPLDTTEYPEEQYVSDILNYIDHGDPQVRGATAILCGTLICSIL
```

Bio-literature

Decode biological sequences...

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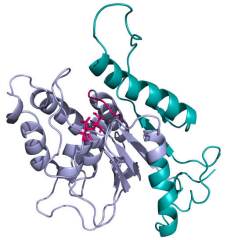
```
VNNBM SSDII XZOWR TIEHI FQKNN
WKCSS DGLHG GXEMJ IWKBA YZGWJ
QTAHK AUSVR SCJTR OQ
```

Mignonne allons voir si la rose
Qui ce matin avait éclose
Sa robe pourpre au soleil

```
MTQFDKQYNSIIKDIxINNGISDEEFDVRTKWDSDGTPAHTLSVISKQMRFDNSEVPILTT
KKVAWKTAIKELLWIWQLKSNDVNDLNMMGVHIWDQWKQEDGTIGHAYGFQLGKKNRSLN
GEKVDQVDYLLHQLKNNPSSRRHITMLWNPDELDAMALTPCVYETQWYVKHGKLHLEVRA
RSNDMALGNPFNVFQYNVLQRMIAQVTGYELGEYIFNIGDCHVYTRHIDNLKIQMEREQF
EAPELWINPEVKDFYDFTIDDFKLINYKHGDKLLFEVAV
```

Tyrosine kinase /
response to osmotic stress



Which questions can we answer?

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```
GGAACACTCGCGCTCGTTGAGGTAGACGGCGTTGCTGTGCGAGTCGGCCAGCACCTGGATCTCGATGTGGCGCGGCTCCTCCACGAACTTCTCCACCAGC
ATGGCGTCGTCGCCAAAGGAGGCGCGCGCCTCCTGGATGGAGAGGTGGTAGCCCTCGCGCGCCTCGGTGTCGTTGTAGGCCACGCGCATGCCCTTGCCGC
CGCCGCCGGCCGAGGCCTTGATCATGACCGGGTAGCCGATCTCGCGCGCGATCTCGAGCATGTGCGCCTCGTCGCGCACCTCGCCCACAAAGCCGGGCAC
CACGTTGATGCCCGCCTCGGTGGCGATGCGCTTGCTGGCGATCTTGGCGCCCATCACCTCGAGCGCGTGCTGCTTGGGCCCCACGAAGGTGACGCCGTGC
TTCTCGAGCAGGTCGCAGAACTTGGTGTTCTCCGAGAGGAACCCGTAGCCGGGGTGGACCGCGTCGGCGCCCGTCTCGACGCACGCCTCGAGGATGCGGT
CCATGGCCAGGTAGGACTCGGAGGACGCGGCCGGCCCCACGTGCCTCGACTCGTCCGCCATCTGAACGTGCTTGGACGACGCGCGGGCGACGAGTACACC
GCCACCGTCGGGATCCCCATCCTGCGCGCGGTCGCAAACACGCGGCACGCGATCTCGCCCCGGTTGGCCACCAGGAGCTTGGTCACTCCGGTGGAGGCTG
CTGCTGCGGCTGCGGCGGAGAGCCTGCGCGAGGGCCTCCTCCTCACCACCGCCACGTTCTTGGACCGTGCTGCGCGGATCA
```

Does this sequence contain a coding gene?

Find ORFs; Alignment with known sequences (BLAST,...)

What could be the function of this gene?

Identification of protein domains (InterPro,...)

What is the origin of this sequence?

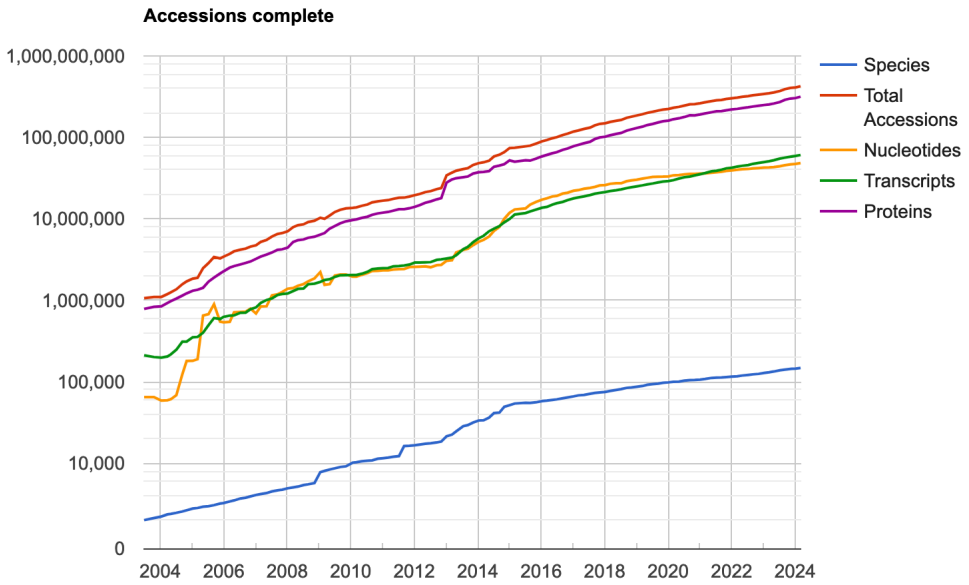
Multiple sequence alignments; phylogenetic tree reconstruction

What is the 3D structure of the protein?

Structural prediction methods (MD, AlphaFold,...)

Sequence databases

NCBI GeneBank / RefSeq
comprehensive, integrated, non-redundant, well-annotated set
of sequences, including genomic DNA, transcripts, and proteins



Homo sapiens oligodendrocyte transcription factor 2 (OLIG2), RefSeqGene on chromosome 21

NCBI Reference Sequence: NG_011834.1

FASTA Graphics

Go to:

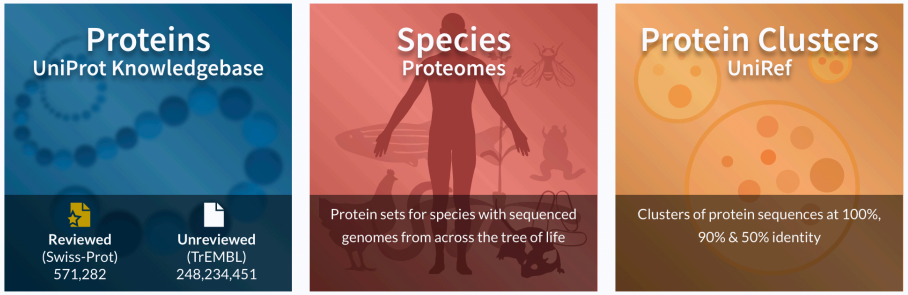
```
LOCUS       NG_011834              10262 bp    DNA     linear   PRI 15-JUN-2020
DEFINITION  Homo sapiens oligodendrocyte transcription factor 2 (OLIG2),
            RefSeqGene on chromosome 21.
ACCESSION   NG_011834
VERSION     NG_011834.1
KEYWORDS    RefSeq; RefSeqGene.
SOURCE      Homo sapiens (human)
  ORGANISM  Homo sapiens
            Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi;
            Mammalia; Eutheria; Euarchontoglires; Primates; Haplorrhini;
            Catarrhini; Hominidae; Homo.
COMMENT     REVIEWED REFSEQ: This record has been curated by NCBI staff. The
            reference sequence was derived from AP000286.1 and AP000287.1.
            This sequence is a reference standard in the RefSeqGene project.

            Summary: This gene encodes a basic helix-loop-helix transcription
            factor which is expressed in oligodendroglial tumors of the brain.
            The protein is an essential regulator of ventral neuroectodermal
            progenitor cell fate. The gene is involved in a chromosomal
            translocation t(14;21)(q11.2;q22) associated with T-cell acute
            lymphoblastic leukemia. Its chromosomal location is within a region
            of chromosome 21 which has been suggested to play a role in
            learning deficits associated with Down syndrome. [provided by
            RefSeq, Jul 2008].
PRIMARY     REFSEQ_SPAN         PRIMARY_IDENTIFIER PRIMARY_SPAN        COMP
            1-4501              AP000286.1         18016-22516
            4502-10262          AP000287.1         1-5761
FEATURES             Location/Qualifiers
     source          1..10262
                     /organism="Homo sapiens"
                     /mol_type="genomic DNA"
                     /db_xref="taxon:9606"
                     /chromosome="21"
                     /map="21q22.11"
     gene            5005..8255
```

[Link to the sequence]

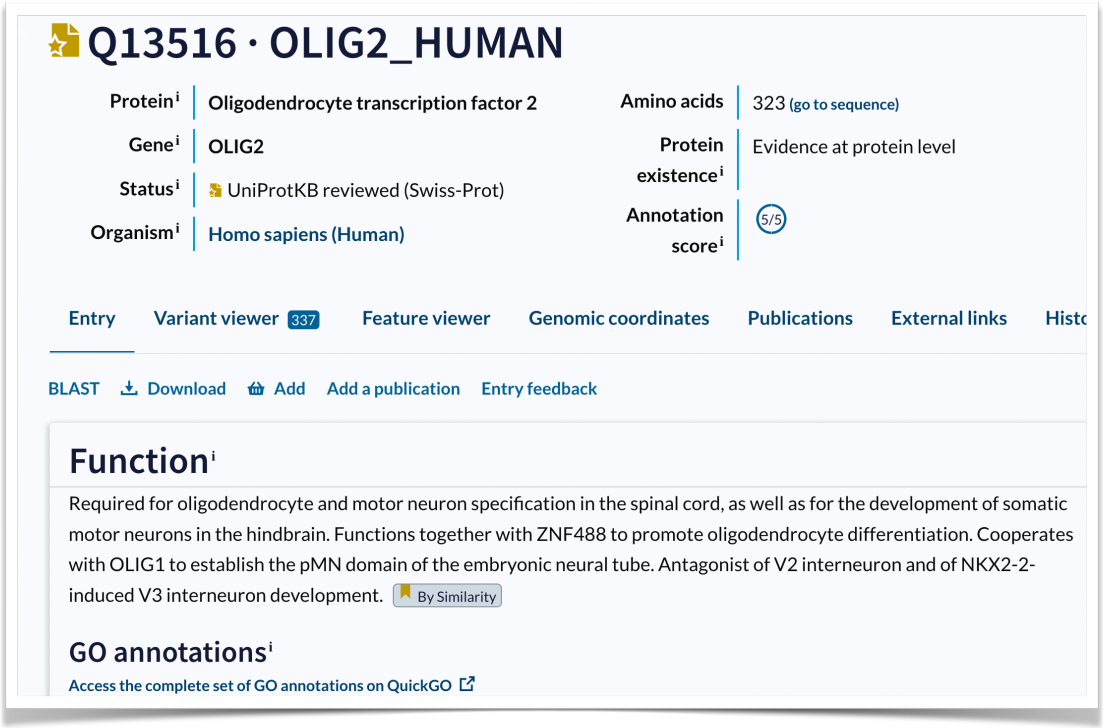
Sequence databases

UniProt/Swissprot
reference protein databases containing manually curated entries and automatic translations



Total number of entries in this release of UniProtKB

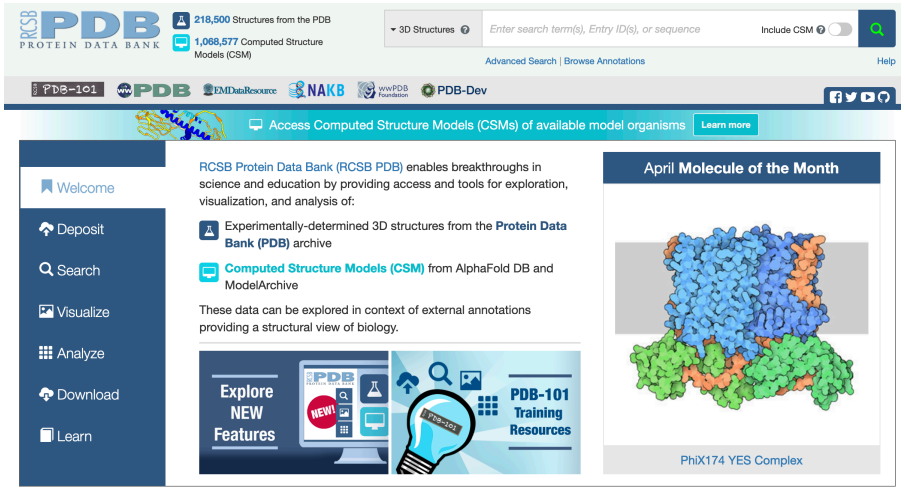
Section	Number of entries in total	Number of entries with an annotation update
UniProtKB	248,805,733	117,146,151
Reviewed (Swiss-Prot)	571,282	436,850
Unreviewed (TrEMBL)	248,234,451	116,709,301

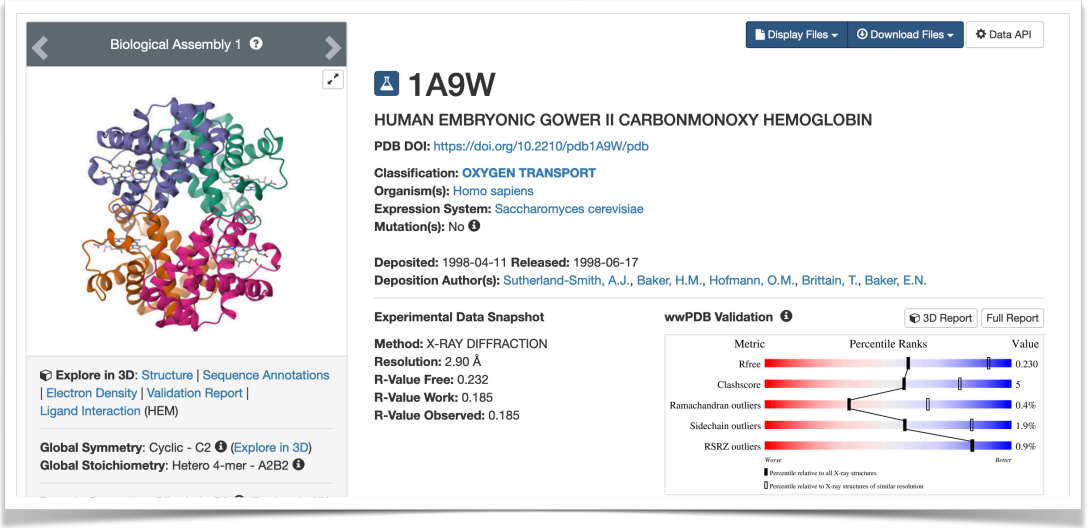


[Link to the sequence]

Sequence databases

Protein Databank (PDB)
database of protein sequences including structural 3D conformation

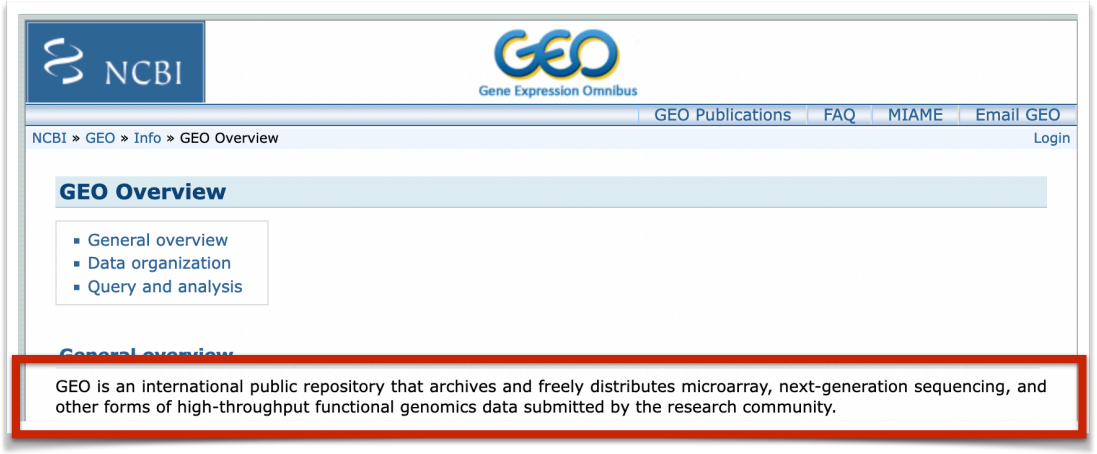




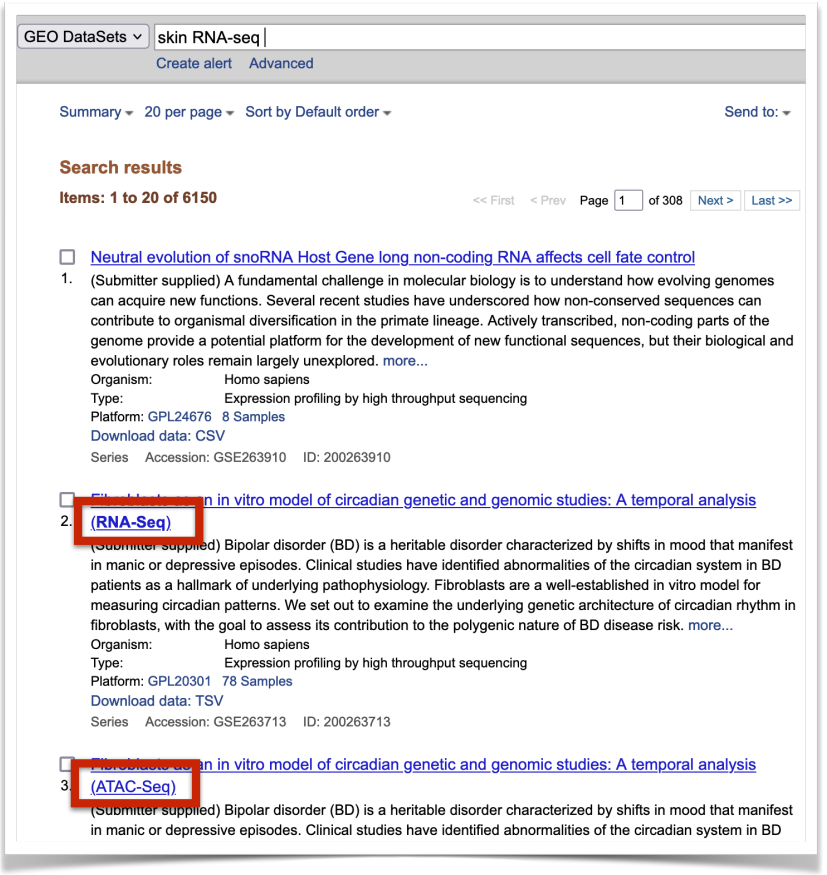
[link to entry]

Genomic databases

Gene Expression Omnibus (GEO)
database of gene expression / high-throughput sequencing data (RNA-seq / ChIP-seq / ATAC-seq / ...)

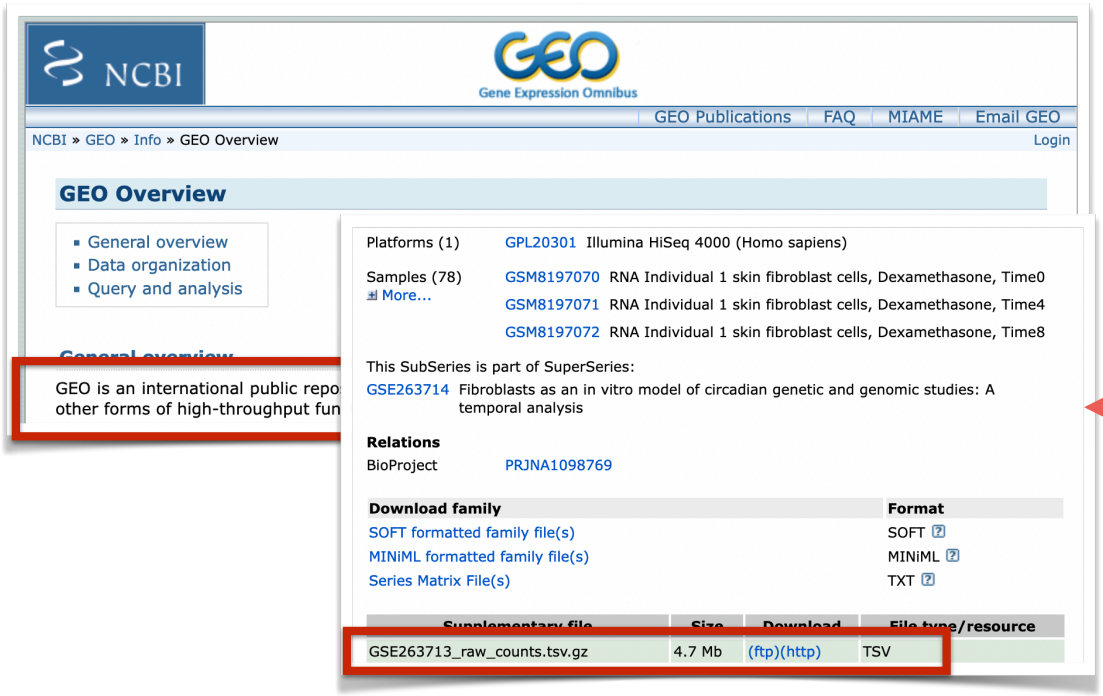


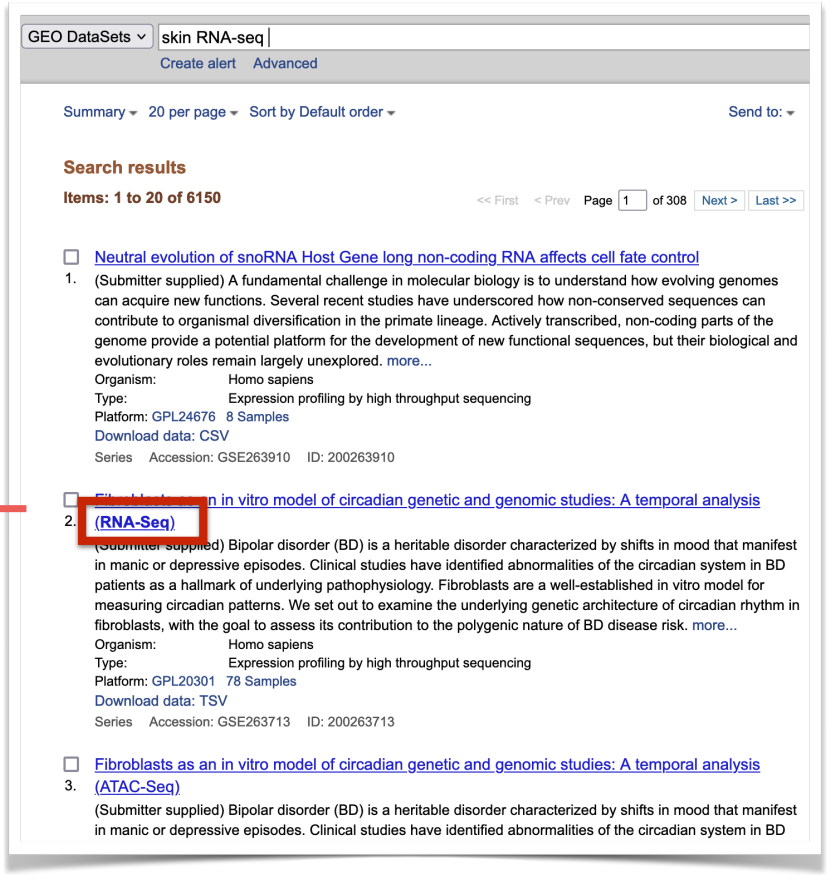
(→ Thursday lab!)



Genomic databases

Gene Expression Omnibus (GEO)
database of gene expression / high-throughput sequencing data (RNA-seq / ChIP-seq / ATAC-seq / ...)





Functional database

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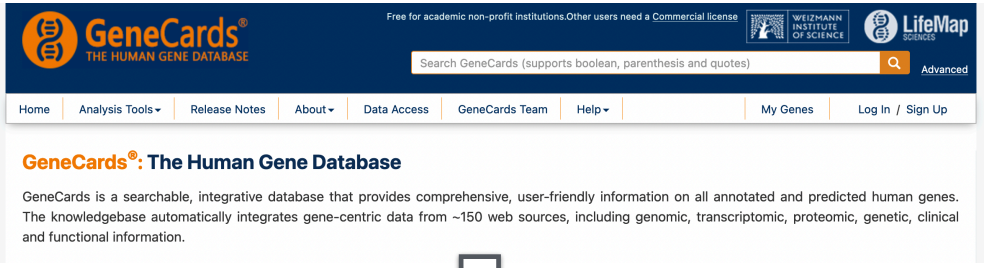
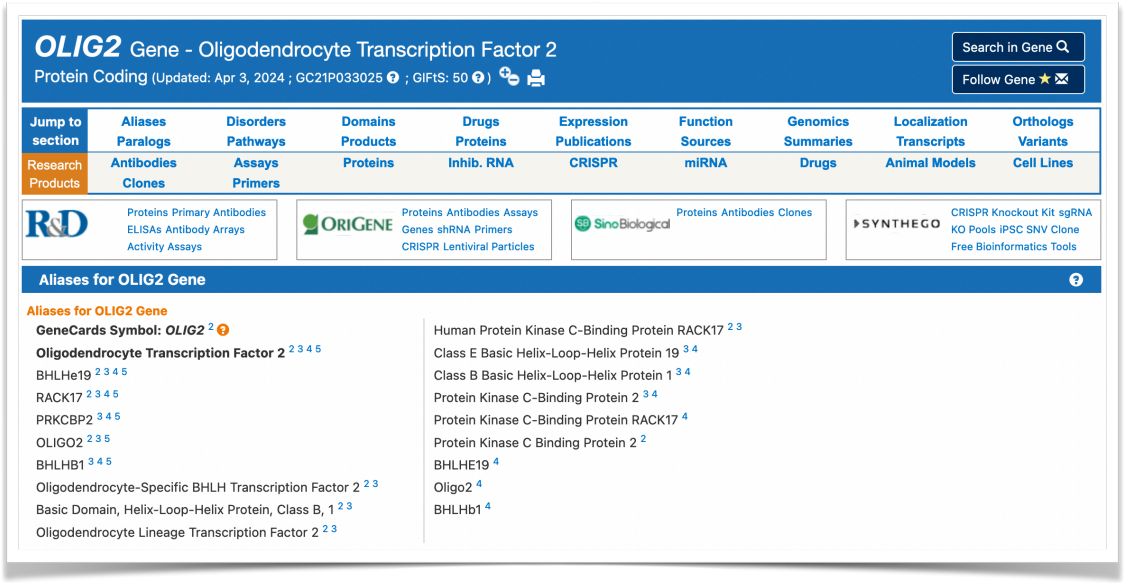
GeneCards

Gene centric database summarizing all information about human genes (diseases, functions, proteins, tissues, ...)





Version 5.20: 10 April 2024

- **466,349 Entries**, 43,839 HGNC approved, 21,601 Protein coding, 291,492 RNA genes including 130,365 lncRNAs, 111,811 piRNAs, and 49,316 other ncRNAs.
- **MalaCards:** Revamped user interface, with AI-generated summaries in a new Overview section, a new navigation pane, searchable and downloadable tables, and more. Visit www.malacards.org - we welcome your feedback.

[link to entry]

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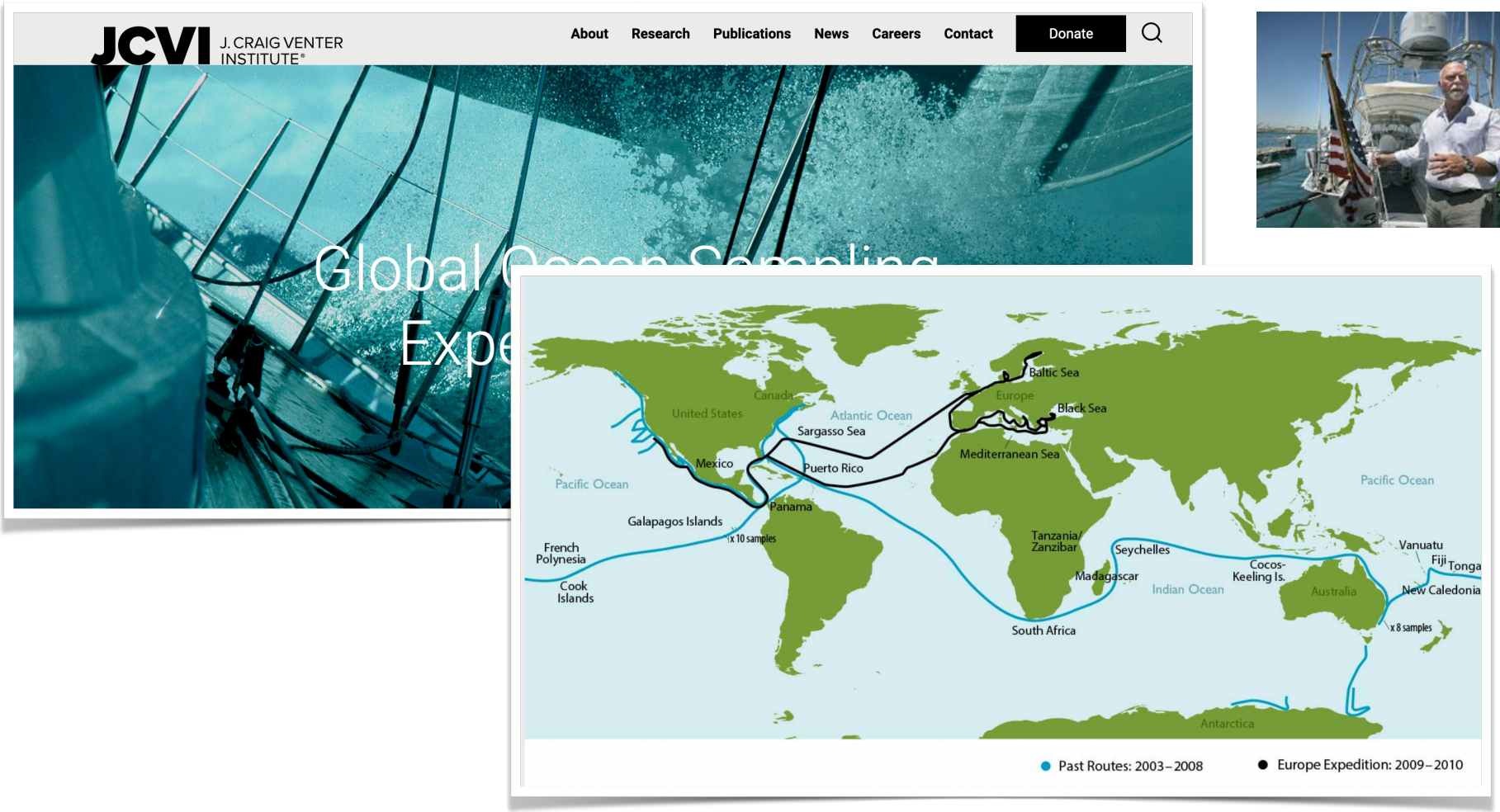
ZUKUNFT SEIT 1386

Analysis of metagenomic sequences

Carl Herrmann

Institut für Pharmazie und Molekulare Biotechnologie | Abt. Bioinformatik

Ocean metagenomics



ID	Sample Location	Country	Date, mm/dd/yy	Time	Location	Sample Depth, m	Water Depth, m	T (°C)[a]	S[b] (ppt)	Size Fraction (μm)	Habitat Type	Chl *a* Sample Month (Annual ± SE) mg/m^{-3}	Good Sequences
GS00a	Sargasso Stations 13 and 11	Bermuda (UK)	02/26/03	3:00	31°32′6″n; 63°35′42″w	5.0	>4,200	20.0 20.5	36.6	0.1–0.8	Open ocean	0.17 (0.0.9 ± 0.02)	644,551
				10:10	31°10′50″n; 64°19′27″w				36.7				
GS00b	Sargasso Stations 13 and 11	Bermuda (UK)	02/26/03	3:35	31°32′10″n; 63°35′70″w	5.0	>4,200	20.0 20.5	36.6	0.22–0.8	Open ocean	0.17 (0.0.9 ± 0.02)	317,180
				10:43	31°10′50n; 64°19′27″w				36.7				
GS00c	Sargasso Stations 3	Bermuda (UK)	02/25/03	13:00	32°09′30″n; 64°00′36″w	5.0	>4,200	19.8	36.7	0.22–0.8	Open ocean	0.17 (0.0.9 ± 0.02)	368,835
GS00d	Sargasso Stations 13	Bermuda (UK)	02/25/03	17:00	31°32′6″n; 63°35′42″w	5.0	>4,200	20.0	36.6	0.22–0.8	Open ocean	0.17 (0.0.9 ± 0.02)	332,240
GS01a	Hydrostation S	Bermuda (UK)	05/15/03	11:40	32°10′00″n 64°30′00″w	5.0	>4,200	22.9	36.7	3.0–20.0	Open ocean	0.10 (0.10 ± 0.01)	142,352
GS01b	Hydrostation S	Bermuda (UK)	05/15/03	11:40	32°10′00″n; 64°30′00″w	5.0	>4,201	22.9	36.7	0.8–3.0	Open ocean	0.10 (0.10 ± 0.01)	90,905
GS01c	Hydrostation S	Bermuda (UK)	05/15/03	11:40	32°10′00″n; 64°30′00″w	5.0	>4,202	22.9	36.7	0.1–0.8	Open ocean	0.1 (0.1 ± 0.01)	92,351
GS02	Gulf of Maine	USA	08/21/03	6:32	42°30′11″n; 67°14′24″w	1.0	106	18.2	29.2	0.1–0.8	Coastal	1.4 (1.12 ± 0.19)	121,590
GS03	Browns Bank, Gulf of Maine	Canada	08/21/03	11:50	42°51′10″n; 66°13′2″w	1.0	119	11.7	29.9	0.1–0.8	Coastal	1.4 (1.12 ± 0.19)	61,605
GS04	Outside Halifax, Nova Scotia	Canada	08/22/03	5:25	44°8′14″n; 63°38′40″w	2.0	142	17.3	28.3	0.1–0.8	Coastal	0.4 (0.78 ± 0.17)	52,959
GS05	Bedford Basin, Nova Scotia	Canada	08/22/03	16:21	44°41′25″n; 63°38′14″w	1.0	64	15.0	30.2	0.1–0.8	Embayment	6 (6.76 ± 0.98)	61,131
GS06	Bay of Fundy, Nova Scotia	Canada	08/23/03	10:47	45°6′42″n; 64°56′48″w	1.0	11	11.2		0.1–0.8	Estuary	2.8 (1.87 ± 0.18)	59,679
GS07	Northern Gulf of Maine	Canada	08/25/03	8:25	43°37′56″n; 66°50′50″w	1.0	139	17.9	31.7[c]	0.1–0.8	Coastal	1.4 (1.12 ± 0.19)	50,980
GS08	Newport Harbor, RI	USA	11/16/03	16:45	41°29′9″n; 71°21′4″w	1.0	12	9.4	26.5[c]	0.1–0.8	Coastal	2.2 (1.59 ± 0.17)	129,655
GS09	Block Island, NY	USA	11/17/03	10:30	41°5′28″n; 71°36′8″w	1.0	32	11.0	31.0[c]	0.1–0.8	Coastal	4.0 (2.72 ± 0.24)	79,303
GS10	Cape May, NJ	USA	11/18/03	4:30	38°56′24″n; 74°41′6″w	1.0	10	12.0	31.0[c]	0.1–0.8	Coastal	2.0 (2.75 ± 0.33)	78,304
GS11	Delaware Bay, NJ	USA	11/18/03	11:30	39°25′4″n; 75°30′15″w	1.0	8	11.0		0.1–0.8	Estuary	4.8 (9.23 ± 1.02)	124,435
GS12	Chesapeake Bay, MD	USA	12/18/03	11:32	38°56′49″n; 76°25′2″w	1.0	25	3.2	3.47[c]	0.1–0.8	Estuary	21.0 (15.0 ± 1.01)	126,162
GS13	Off Nags Head, NC	USA	12/19/03	6:28	36°0′14″n; 75°23′41″w	1.0	20	9.3		0.1–0.8	Coastal	3.0 (2.24 ± 0.25)	138,033
GS14	South of Charleston, SC	USA	12/20/03	17:12	32°30′25″n; 79°15′50″w	1.0	31	18.6		0.1–0.8	Coastal	1.70 (1.92 ± 0.25)	128,885
GS15	Off Key West, FL	USA	01/08/04	6:25	24°29′18″n; 83°4′12″w	2.0	47	25.3	36.0	0.1–0.8	Coastal	0.2 (0.27 ± 0.09)	127,362
GS16	Gulf of Mexico	USA	01/08/04	14:15	24°10′29″n; 84°20′40″w	2.0	3,333	26.4	35.8	0.1–0.8	Coastal sea	0.16 (0.11 ± 0.01)	127,122
GS17	Yucatan Channel	Mexico	01/09/04	13:47	20°31′21″n; 85°24′49″w	2.0	4,513	27.0	35.8	0.1–0.8	Open ocean	0.13 (0.09 ± 0.01)	257,581
GS18	Rosario Bank	Honduras	01/10/04	8:12	18°2′12″n; 83°47′5″w	2.0	4,470	27.4	35.4	0.1–0.8	Open ocean	0.14 (0.09 ± 0.01)	142,743
GS19	Northeast of Colón	Panama	01/12/04	9:03	10°42′59″n; 80°15′16″w	2.0	3,336	27.7	35.4	0.1–0.8	Coastal	0.23 (0.15 ± 0.02)	135,325
GS20	Lake Gatun	Panama	01/15/04	10:24	9°9′52″n; 79°50′10″w	2.0	4	28.5	0.06	0.1–0.8	Fresh water		296,355
GS21	Gulf of Panama	Panama	01/19/04	16:48	8°7′45″n; 79°41′28″w	2.0	76	27.6	30.7	0.1–0.8	Coastal	0.50 (0.73 ± 0.22)	131,798
GS22	250 miles from Panama City	Panama	01/20/04	16:39	6°29′34″n; 82°54′14″w	2.0	2,431	29.3	32.3	0.1–0.8	Open ocean	0.33 (0.28 ± 0.02)	121,662
GS23	30 miles from Cocos Island	Costa Rica	01/21/04	15:00	5°38′24″n; 86°33′55″w	2.0	1,139	28.7	32.6	0.1–0.8	Open ocean	0.07 (0.19 ± 0.02)	133,051
GS25	Dirty Rock, Cocos Island	Costa Rica	01/28/04	10:51	5°33′10″n; 87°5′16″w	1.1	30	28.3	31.4	0.8–3.0	Fringing reef	0.11 (0.19 ± 0.01)	120,671
GS26	134 miles NE of Galapagos	Ecuador	02/01/04	16:16	1°15′51″n; 90°17′42″w	2.0	2,376	27.8	32.6	0.1–0.8	Open ocean	0.22 (0.28 ± 0.02)	102,708
GS27	Devil's Crown, Floreana	Ecuador	02/04/04	11:41	1°12′58″s; 90°25′22″w	2.0	2.3	25.5	34.9	0.1–0.8	Coastal	0.40 (0.38 ± 0.03)	222,080
GS28	Coastal Floreana	Ecuador	02/04/04	15:47	1°13′1″s; 90°19′11″w	2.0	156	25.0[c]		0.1–0.8	Coastal	0.35 (0.35 ± 0.02)	189,052
GS29	North James Bay, Santigo	Ecuador	02/08/04	18:03	0°12′0″s; 90°50′7″w	2.0	12	26.2	34.5	0.1–0.8	Coastal	0.40 (0.39 ± 0.03)	131,529
GS30	Warm seep, Roca Redonda	Ecuador	02/09/04	11:42	0°16′20″n; 91°38′0″w	19.0	19	26.9		0.1–0.8	Warm seep		359,152
GS31	Upwelling, Fernandina	Ecuador	02/10/04	14:43	0°18′4″s; 91°39′6″w	12.0	19	18.6		0.1–0.8	Coastal upwelling	0.35 (0.39 ± 0.03)	436,401
GS32	Mangrove, Isabella	Ecuador	02/11/04	11:30	0°35′38″s; 91°4′10″w	0.3	0.67	25.4		0.1–0.8	Mangrove		148,018
GS33	Punta Cormorant Lagoon, Floreana	Ecuador	02/19/04	13:35	1°13′42″s; 90°25′45″w	0.2	0.33	37.6	46[c]	0.1–0.8	Hypersaline		692,255
GS34	North Seamore	Ecuador	02/19/04	17:06	0°22′59″s; 90°16′47″w	2.0	35	27.5		0.1–0.8	Coastal	0.36 (0.35 ± 0.02)	134,347
GS35	Wolf Island	Ecuador	03/01/04	16:44	1°23′21″n; 91°49′1″w	2.0	71	21.8	34.5	0.1–0.8	Coastal	0.28 (0.31 ± 0.02)	140,814
GS36	Cabo Marshall, Isabella	Ecuador	03/02/04	12:52	0°1′15″s; 91°11′52″w	2.0	67	25.8	34.6	0.1–0.8	Coastal	0.65 (0.45 ± 0.05)	77,538
GS37	Equatorial Pacific TAO Buoy	International	03/17/04	16:38	1°58′26″s; 95°0′53″w	2.0	3,334	28.8		0.1–0.8	Open ocean	0.21 (0.24 ± 0.02)	65,670
GS47	201 miles from French Polynesia	International	03/28/04	15:25	10°7′53″s; 135°26′58″w	30.0	2,400	28.6	37.3	0.1–0.8	Open ocean		66,023
GS51	Rangirora Atoll	French Polynesia	05/22/04	7:04	15°8′37″s; 147°26′6″w	1.0	10	27.3	34.2	0.1–0.8	Coral reef atoll		128,982
Total													7,697,926

[a]Temperature.
[b]Salinity.
[c]Measurements were acquired from nearby vessels and/or research stations.
doi:10.1371/journal.pbio.0050077.t001

[Rusch DB, Halpern AL, Sutton G, Heidelberg KB, Williamson S, Yooseph S, et al. (2007)]

Goals

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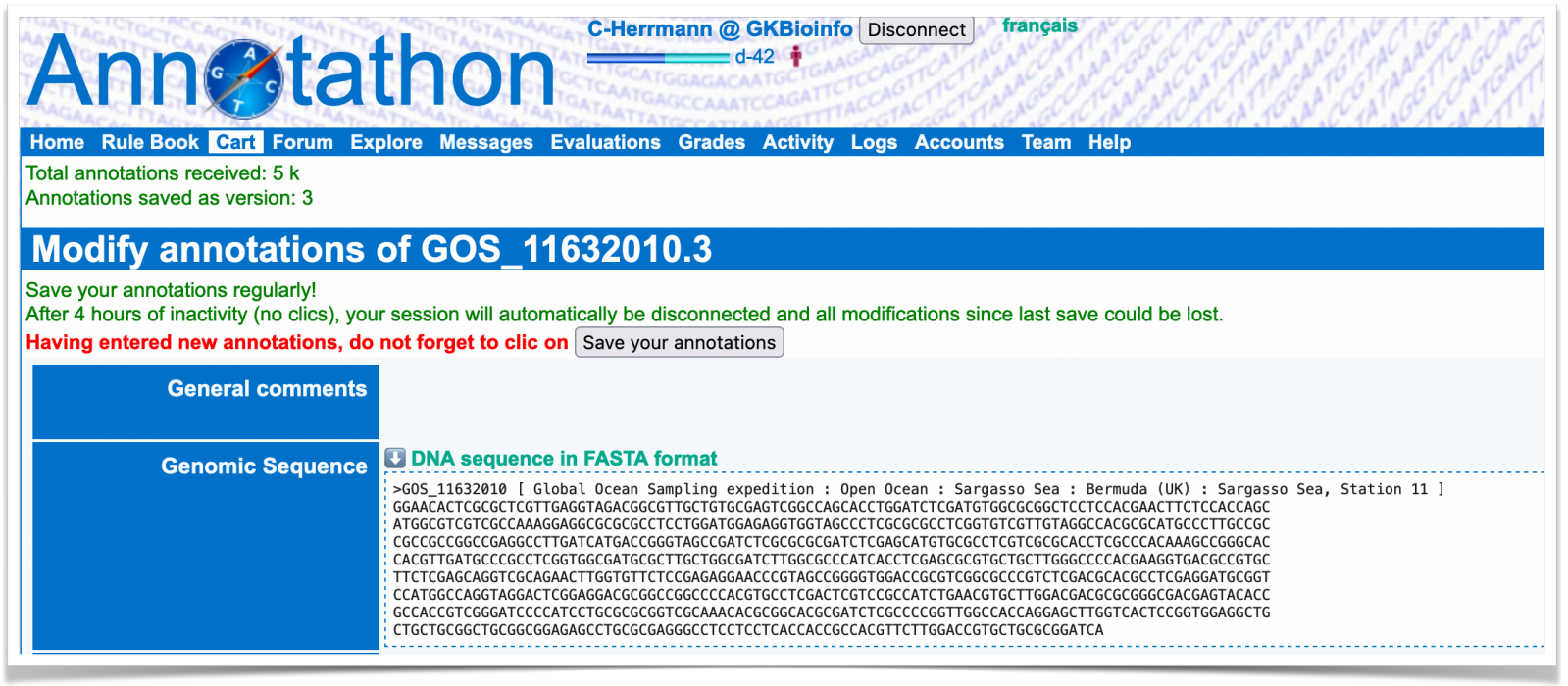
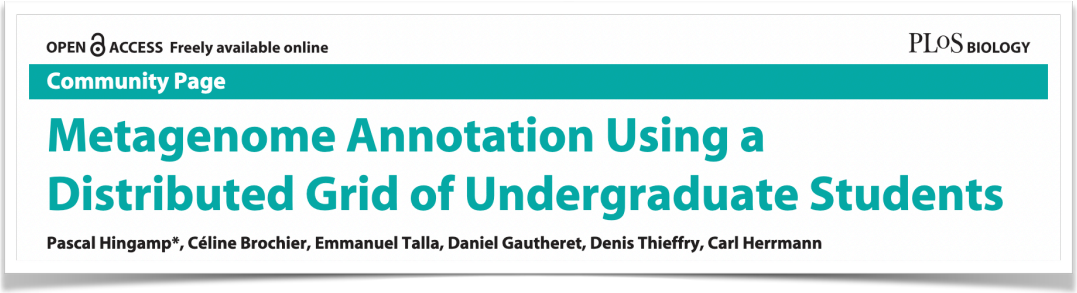
ZUKUNFT SEIT 1386

Perform a full bioinformatics annotation of an unknown metagenomic sequence

- Pick a random sequence from the GOS dataset Use bioinformatics online tools to ask:
  - does the DNA code for a **protein**?
  - does the DNA have **homologs** in GENBANK?
  - can we predict the protein's **function**?
  - can we predict from what **life form** the DNA came from?

Annotathon





[Hingamp, ... Herrmann, PLOS Biology (2008)]

Workflow

Sample random metagenomc sequence

Step 1
identify open reading frames

Step 2
identify protein domains / protein families

Step 3
identify homologous sequences using BLAST

Step 4
Perform multiple sequence alignment

Step 5
Reconstruction phylogenetic tree

Step 6
Summarize your findings

- Is the DNA fragment **coding**?
- What are the protein **domains**?
- What are **homologous** sequences?
- What could be the biological **function** of the gene?
- What is the **evolutionary origin** of this sequence?

Let's dive...