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Úvod do bioinformatiky a bioinformatické databáze



EVROPSKÁ UNIE



MINISTERSTVO ŠKOLSTVÍ,
MLÁDEŽE A TĚLOVÝCHOVY



INVESTICE DO ROZVOJE VZDĚLÁVÁNÍ

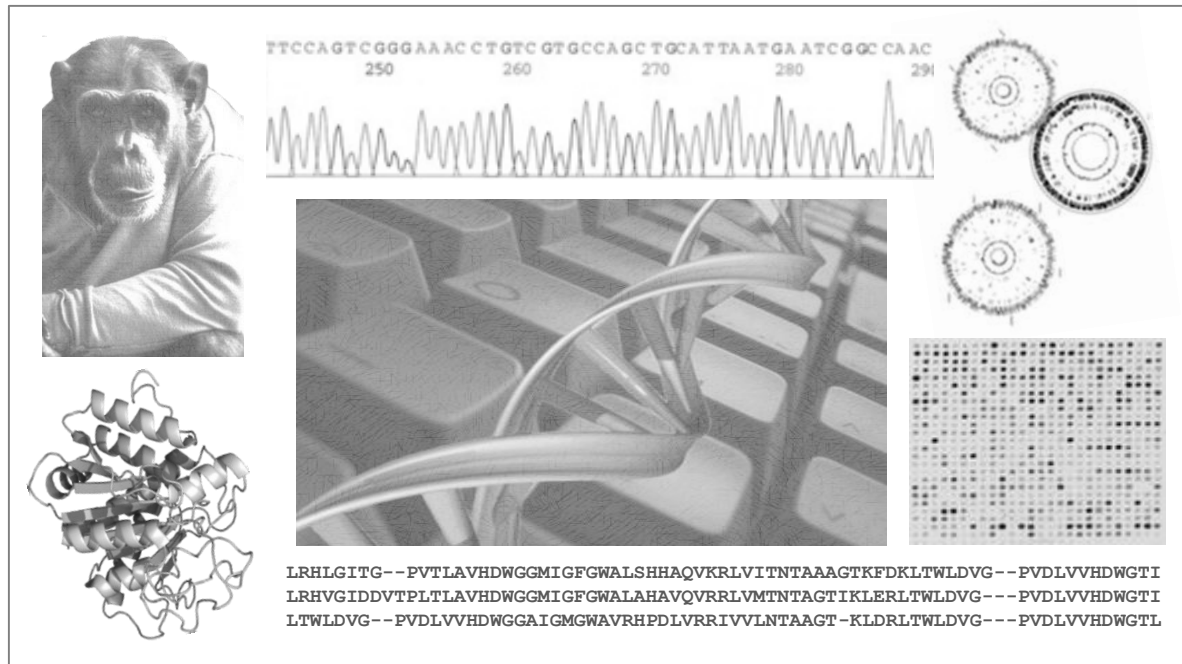
- ❑ Organizační informace
- ❑ Studijní literatura
- ❑ Historie bioinformatiky
- ❑ Bioinformatické instituce
- ❑ Bioinformatické databáze
- ❑ Prohledávání databází

- Kolokvium
 - Písemný test
 - Celkem 25 otázek s jednou i více správnými odpověďmi
 - Minimálně 17 správných odpovědí

- Bi5000 Bioinformatika I – nukleové kyseliny
- Bi9060 Bioinformatika II – proteiny
- Bi9061 Bioinformatika – cvičení

- ❑ Xiong, J. **Essential Bioinformatics**. Cambridge University Press, New York, 2006.
- ❑ Claverie, J., and Notredame, C. **Bioinformatics for Dummies** ^{2 ed.}. Wiley Publishing, Hoboken, 2006
- ❑ Cvrčková, F. **Úvod do praktické bioinformatiky**. Academia, Praha 2006.
- ❑ Misener, S., Krawetz S.A. **Bioinformatics: methods and protocols**. Humana Press, Totowa, New Jersey 2000.
- ❑ Attwood, T.K., Parry-Smith, D.J. **Introduction to bioinformatics**. Longman, Essex, 1999.
- ❑ Baxevanis, A.D., Ouellette, F.B.F. **Bioinformatics: a practical guide to the analysis of genes and proteins**. Wiley-Interscience, New York 1998.

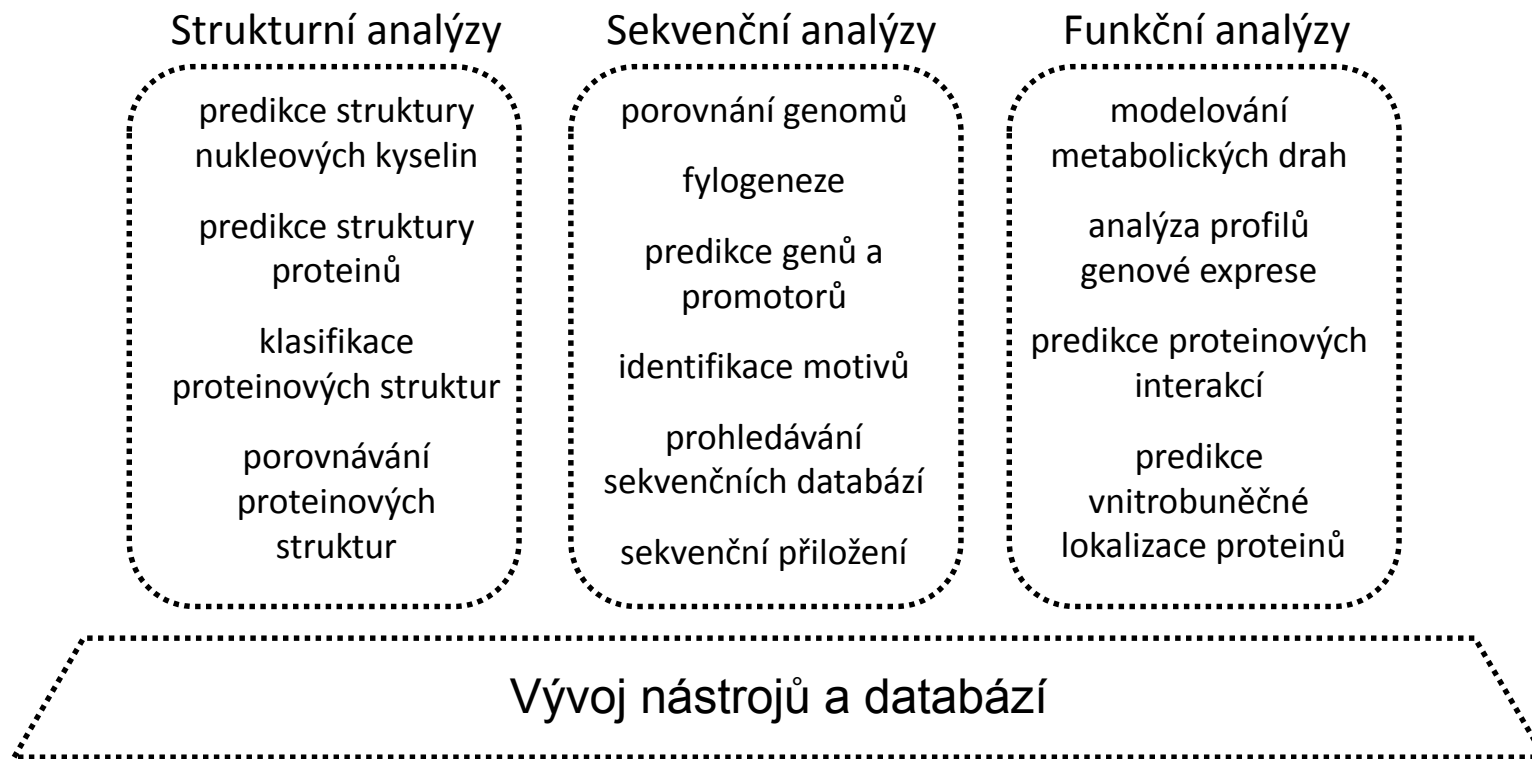
- Informační technologie sloužící k **získávání, uchování, analýze a distribuci informací** týkajících se biomakromolekul



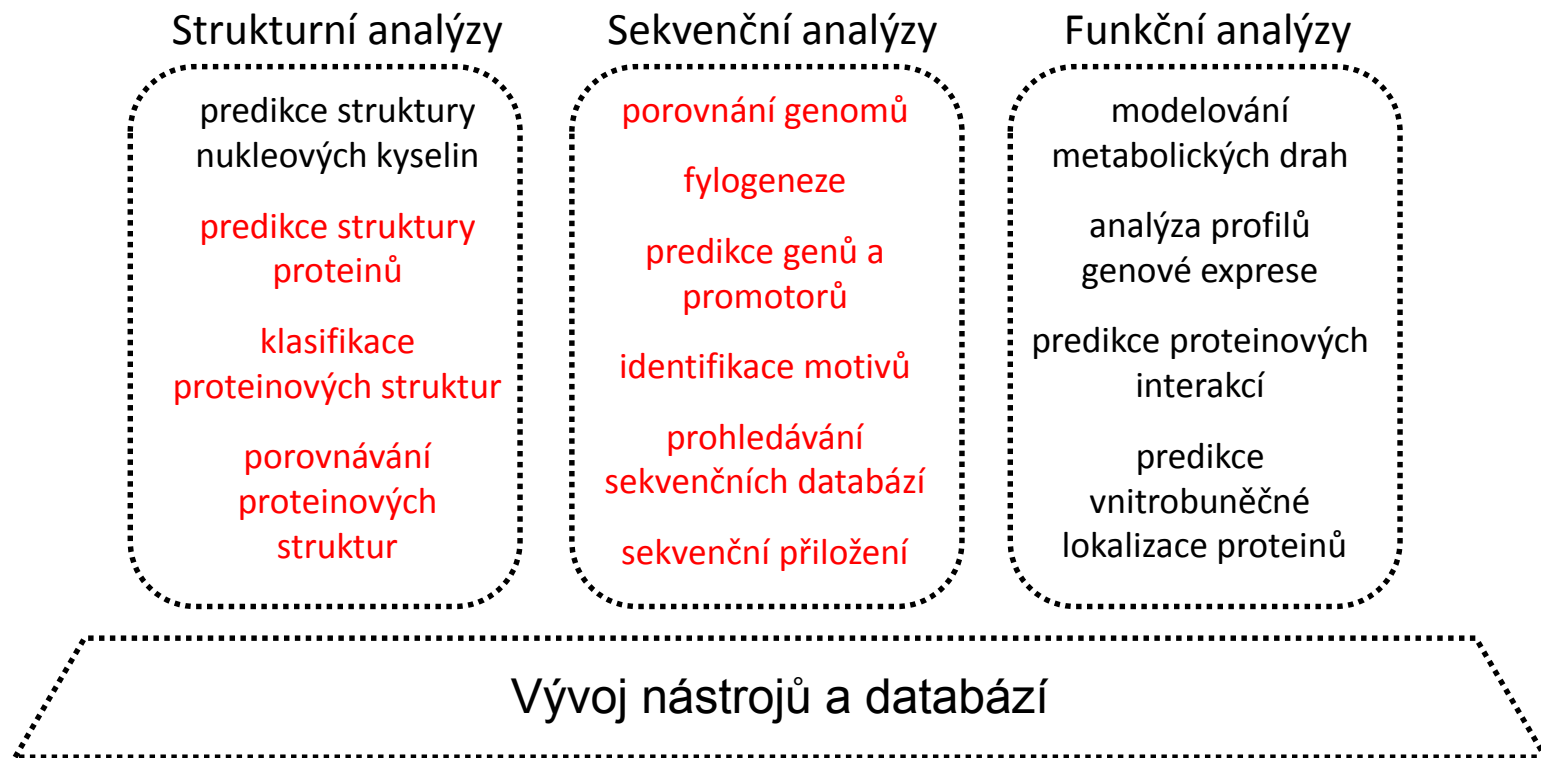
- Informační technologie sloužící k **získávání, uchovávání, analýze a distribuci informací** týkajících se biomakromolekul

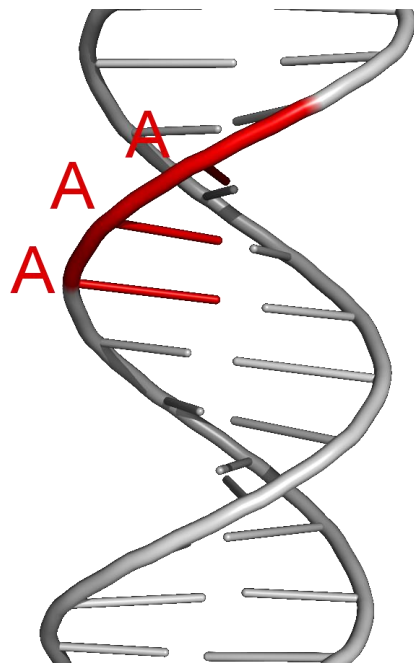
Vývoj nástrojů a databází

- Informační technologie sloužící k **získávání, uchovávání, analýze a distribuci informací** týkajících se biomakromolekul

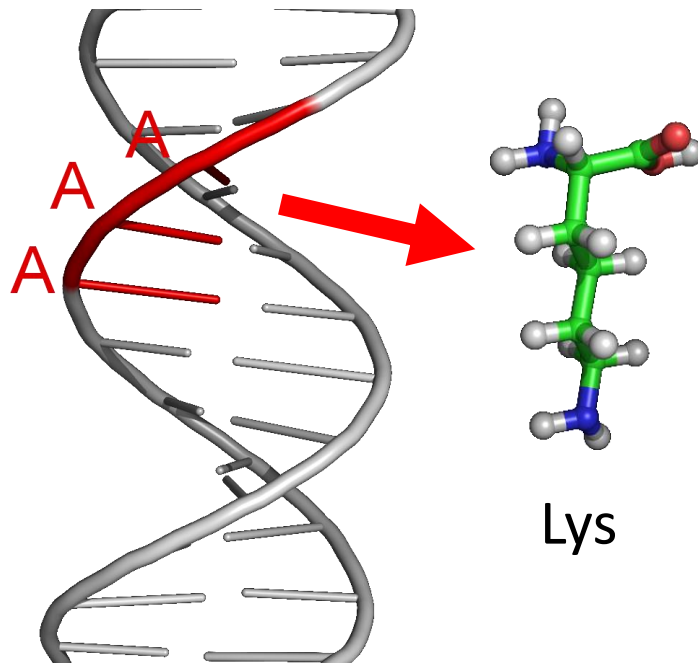


- Informační technologie sloužící k získávání, uchovávání, analýze a distribuci informací týkajících se biomakromolekul

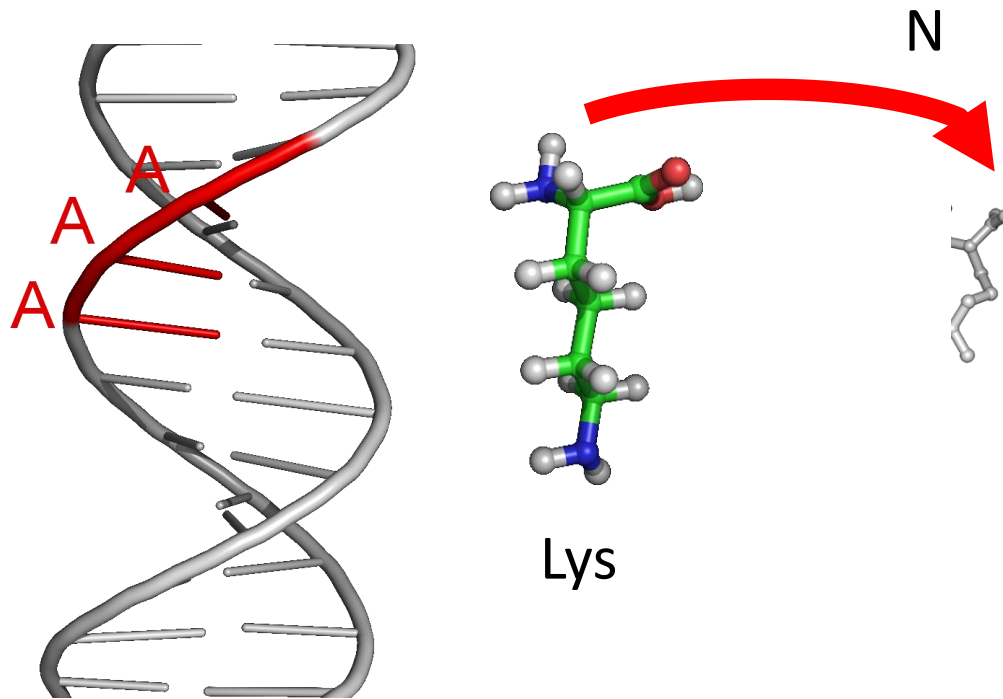




Nukleové kyseliny



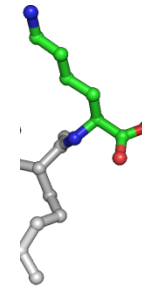
Nukleové kyseliny



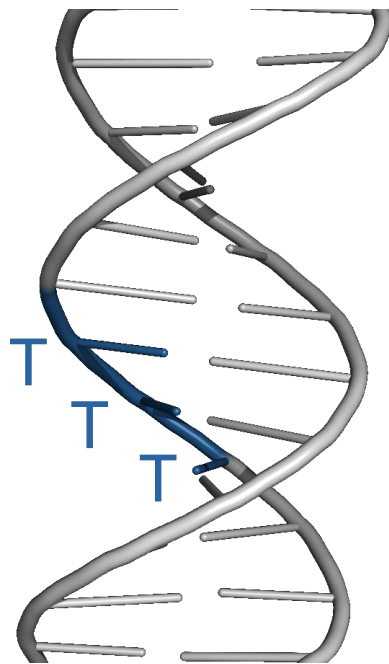
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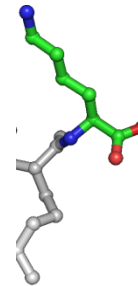
N-Lys



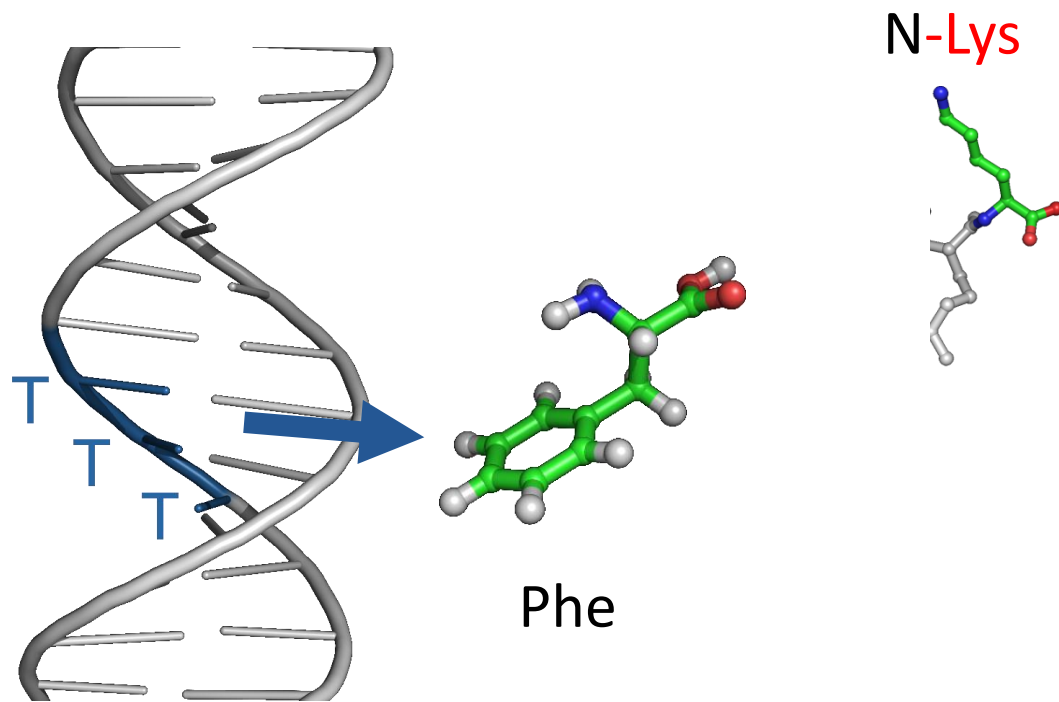
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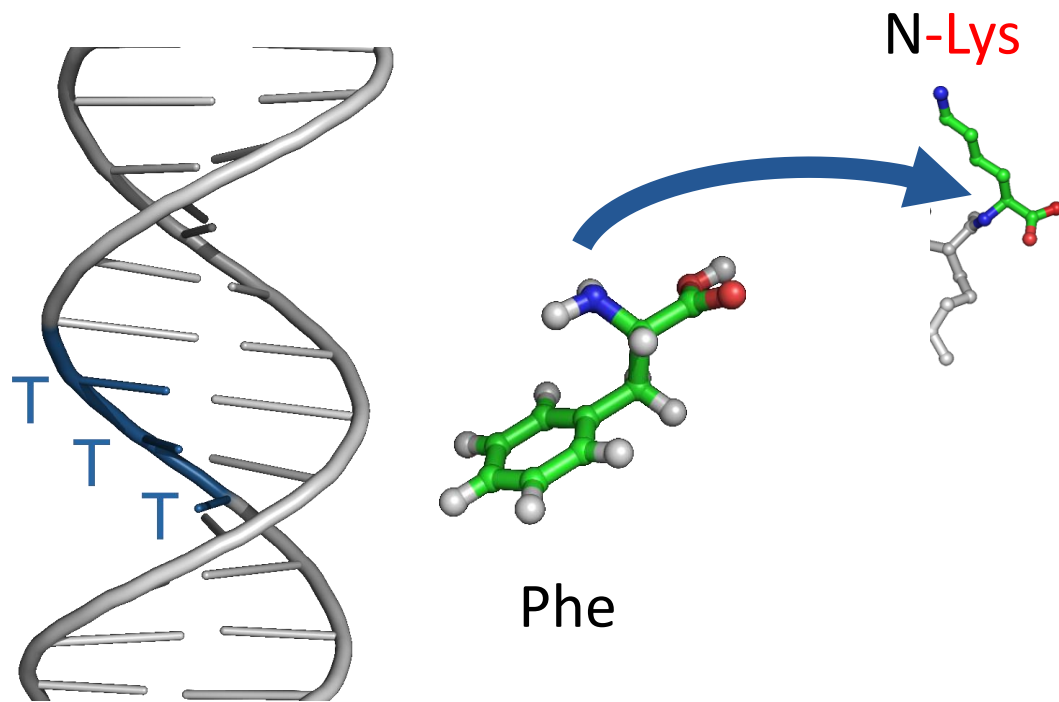
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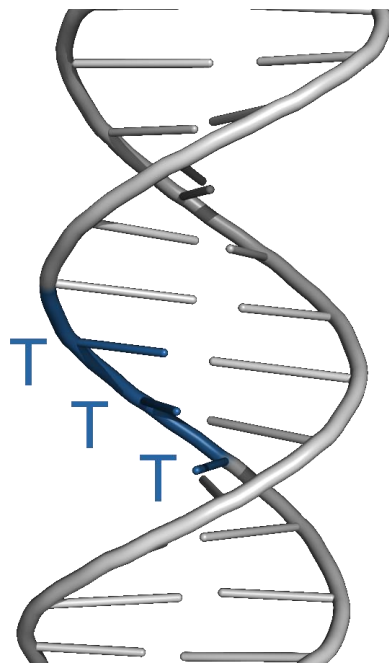
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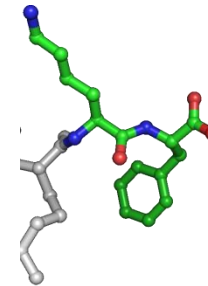
Nukleové kyseliny



Nukleové kyseliny



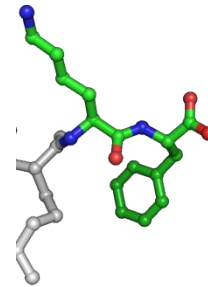
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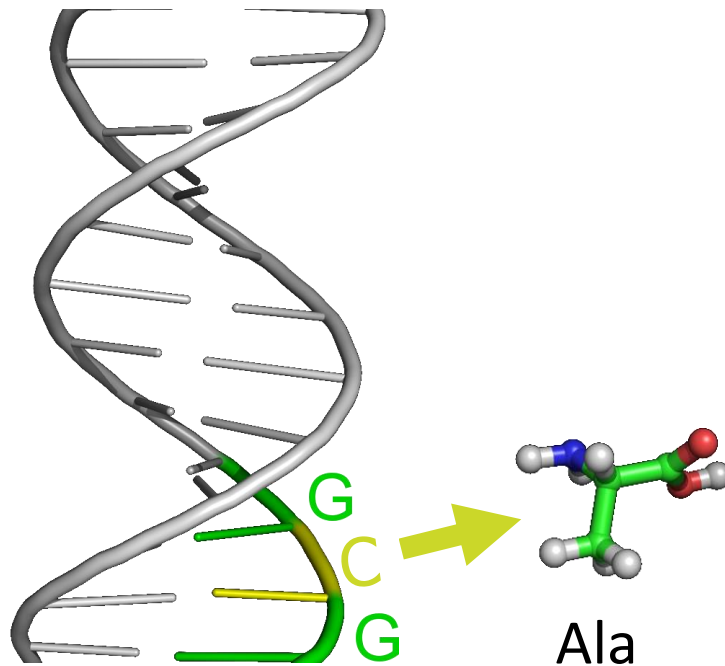
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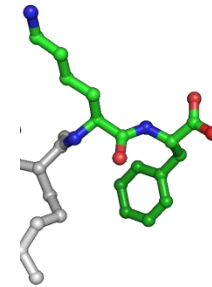
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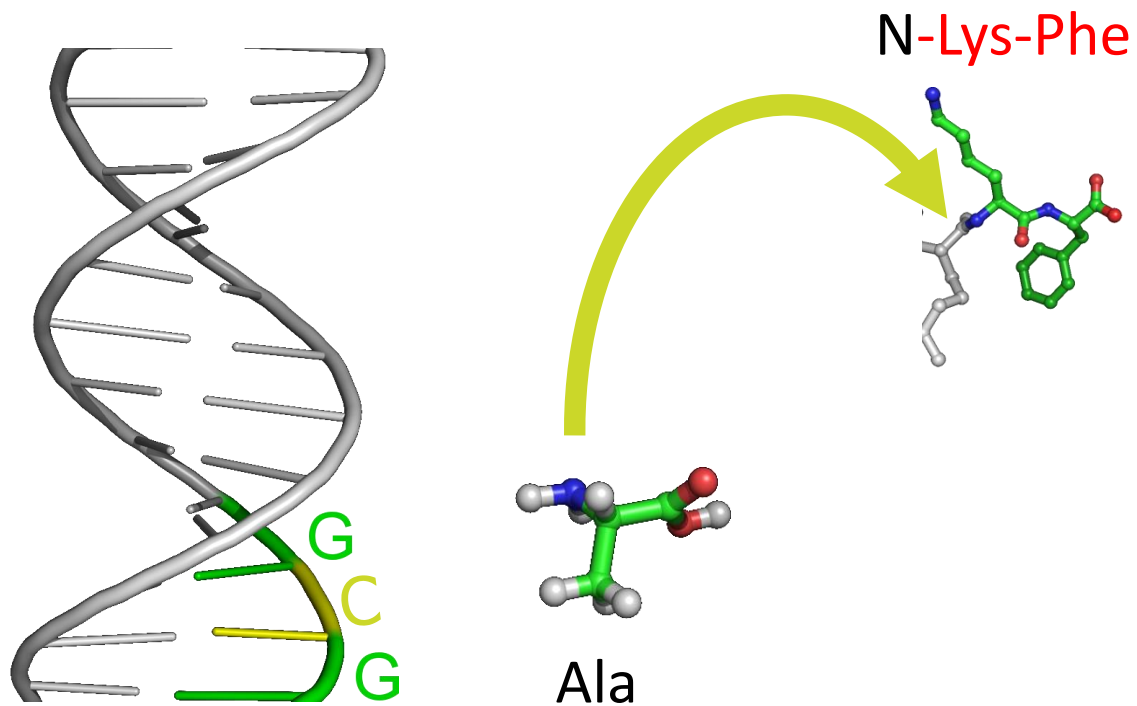
Nukleové kyseliny



N-Lys-Phe



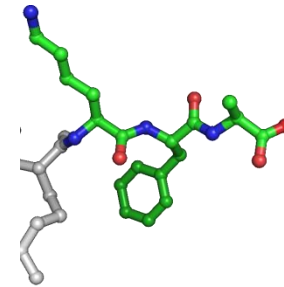
Nukleové kyseliny



Nukleové kyseliny

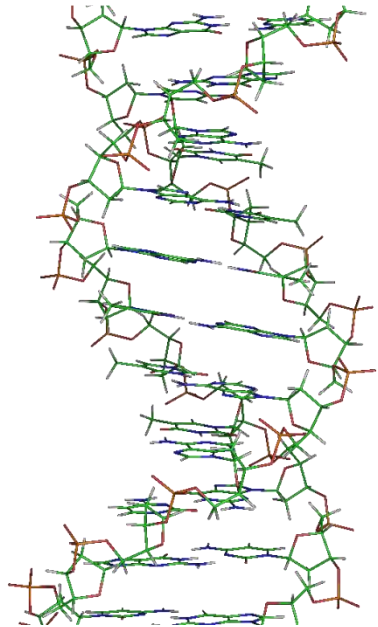


N-Lys-Phe-Ala

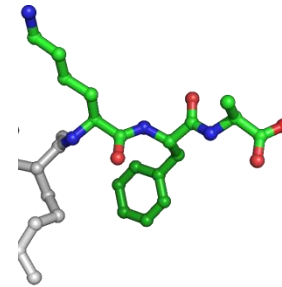


Nukleové kyseliny

5'-NCG-AAA-TTT-GCG-3'

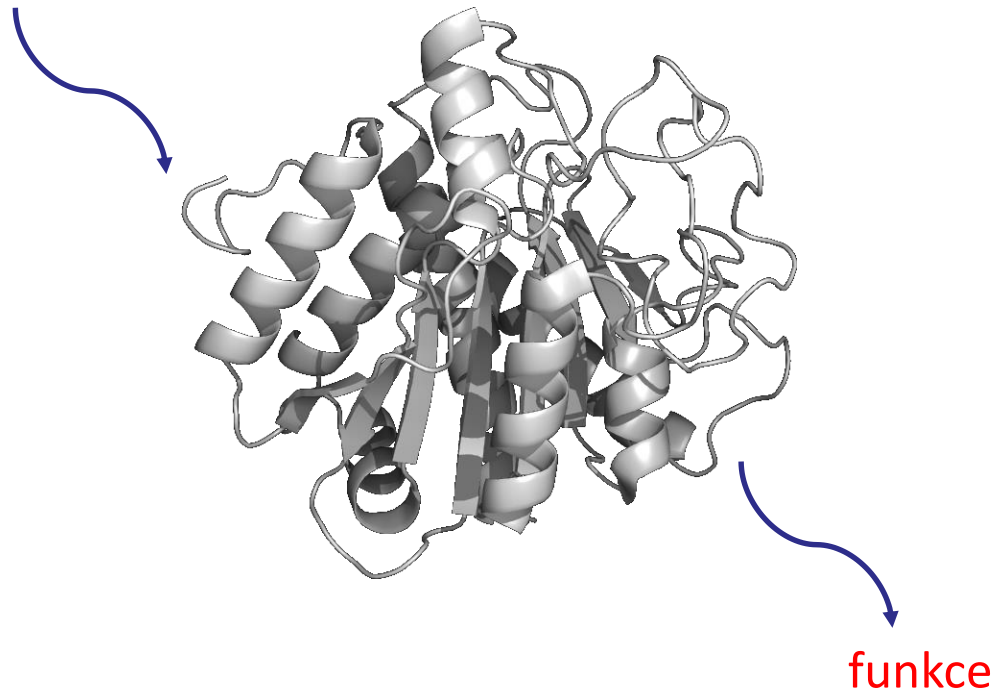


N-Lys-Phe-Ala



Proteiny

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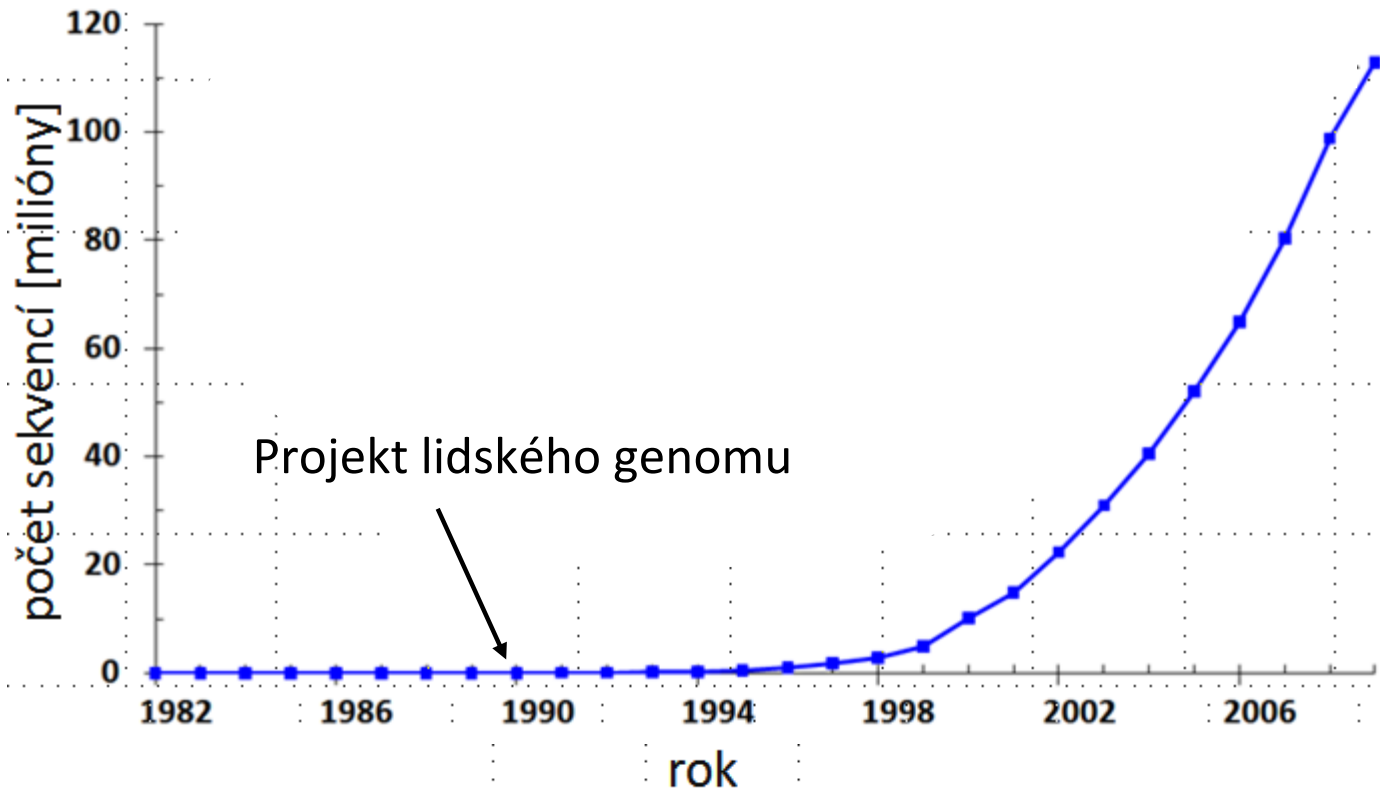


Historie bioinformatiky

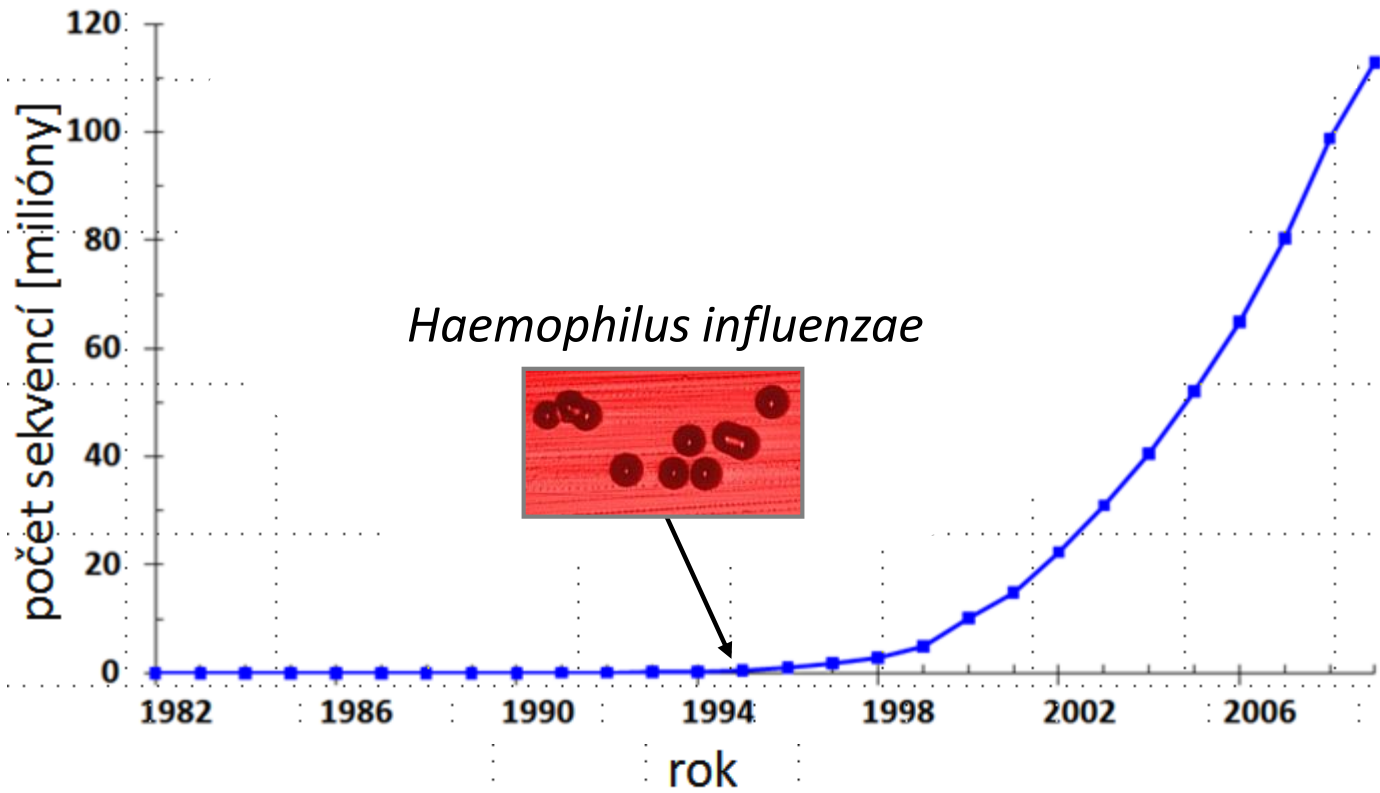
□ Revoluce



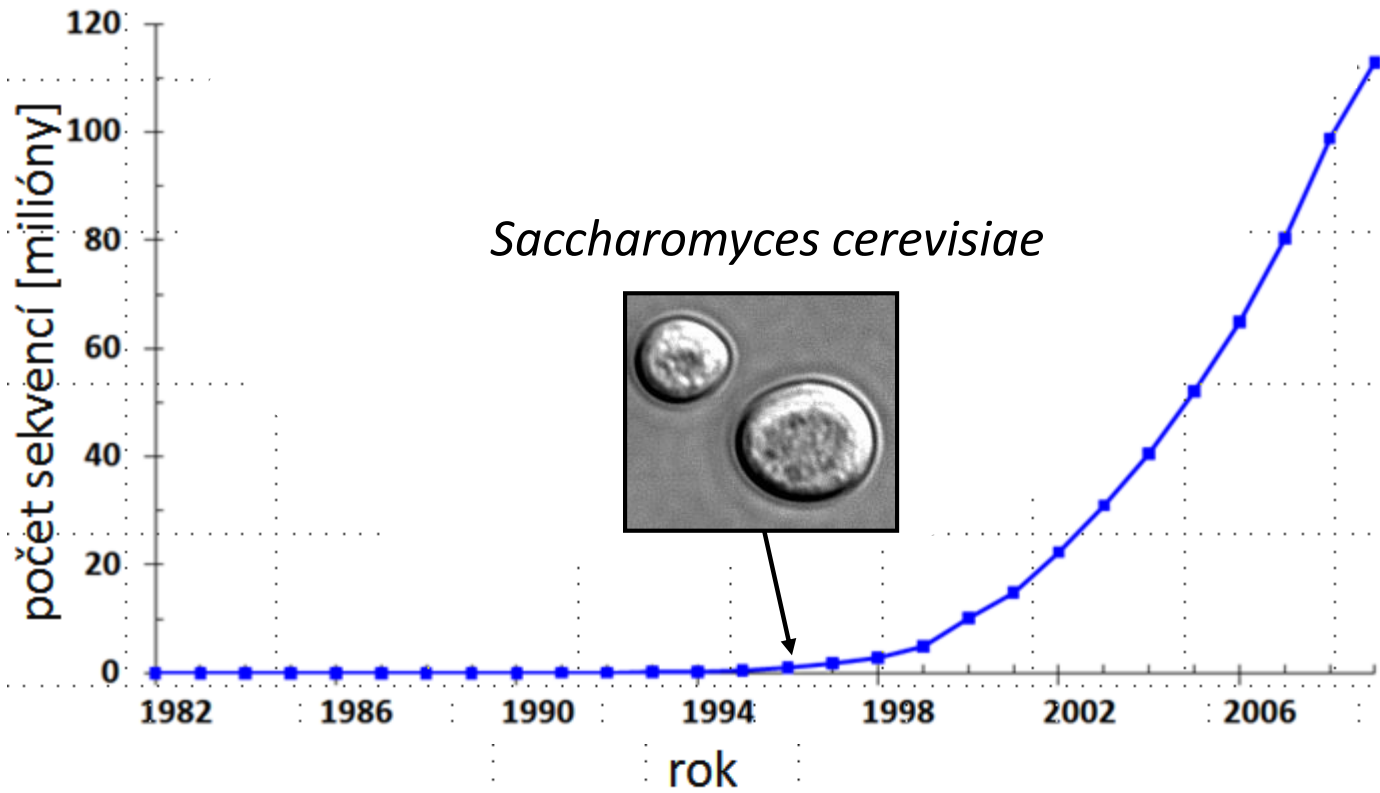
Historie bioinformatiky



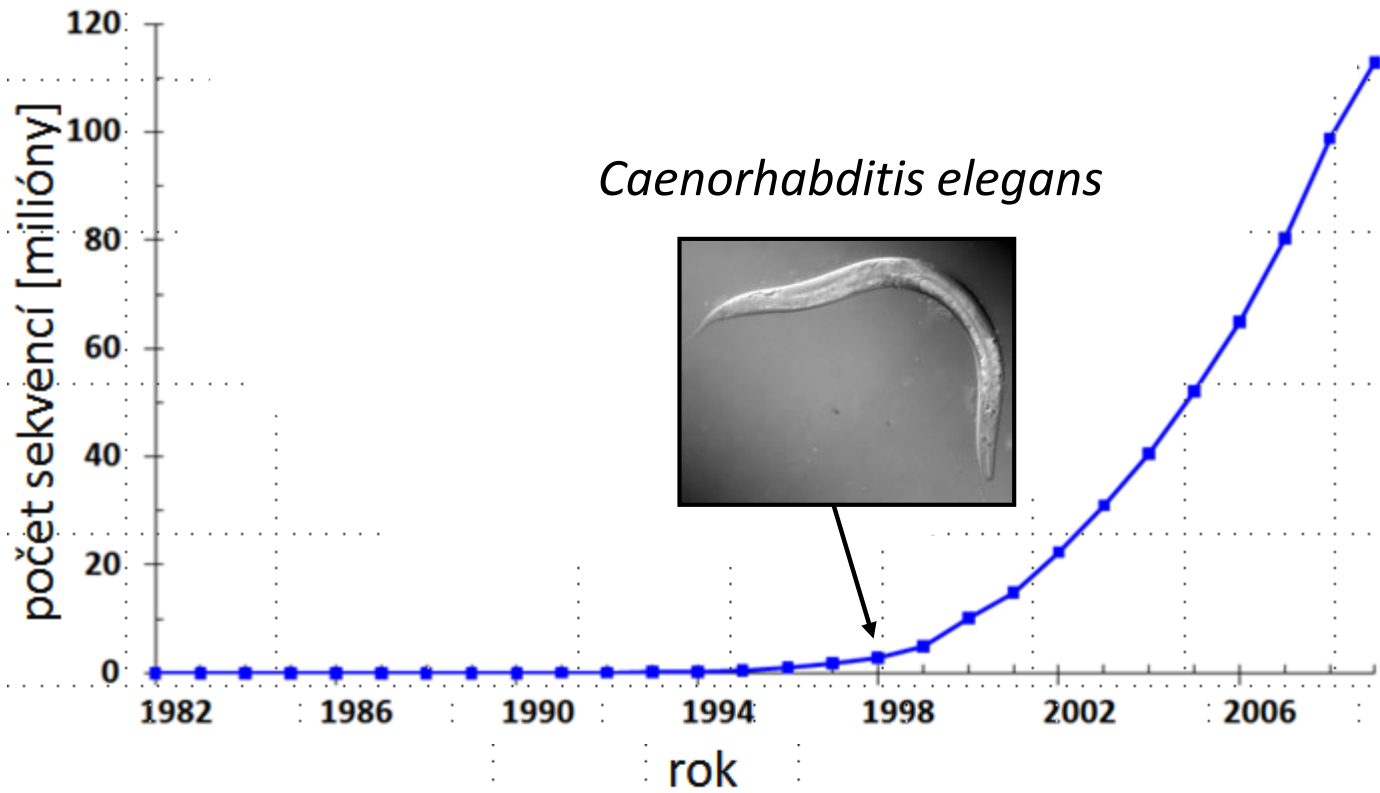
Historie bioinformatiky



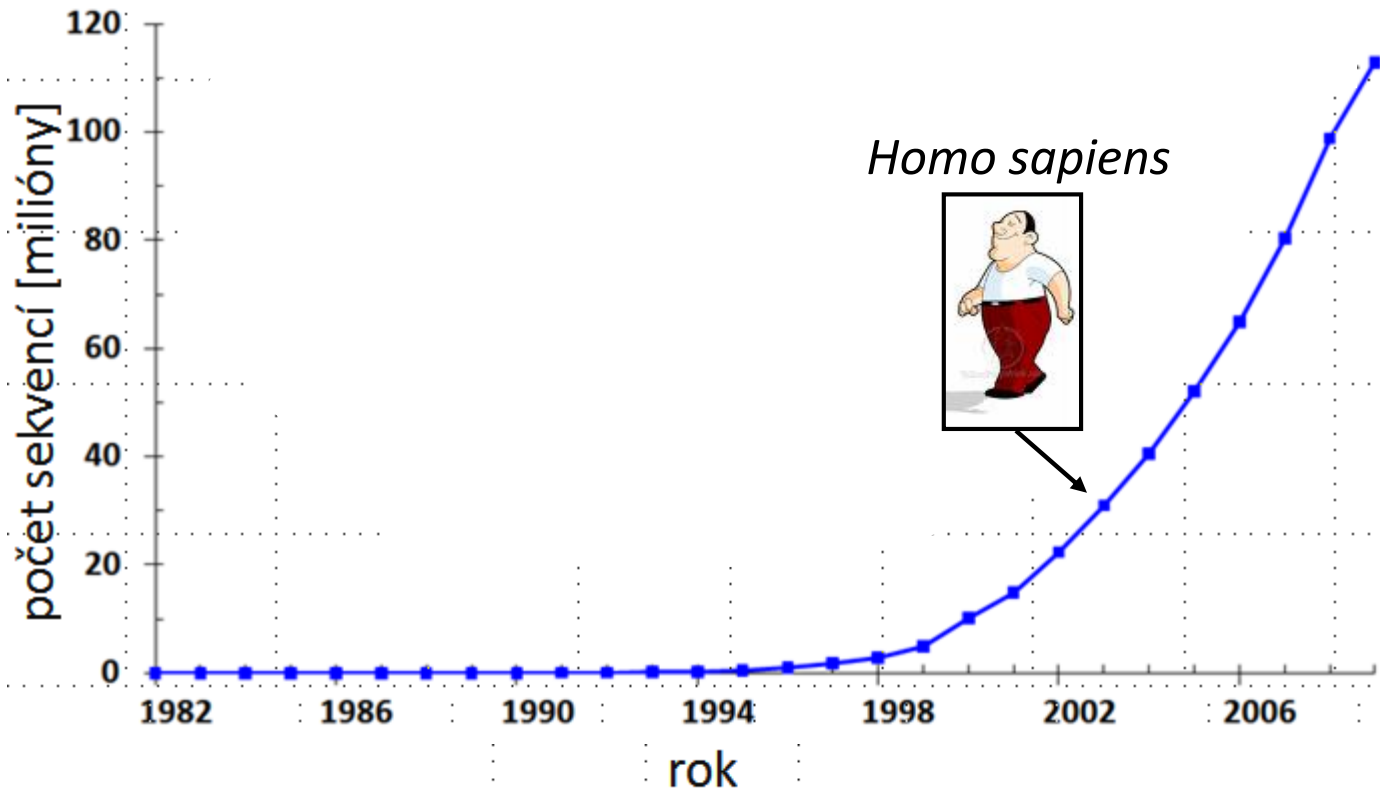
Historie bioinformatiky



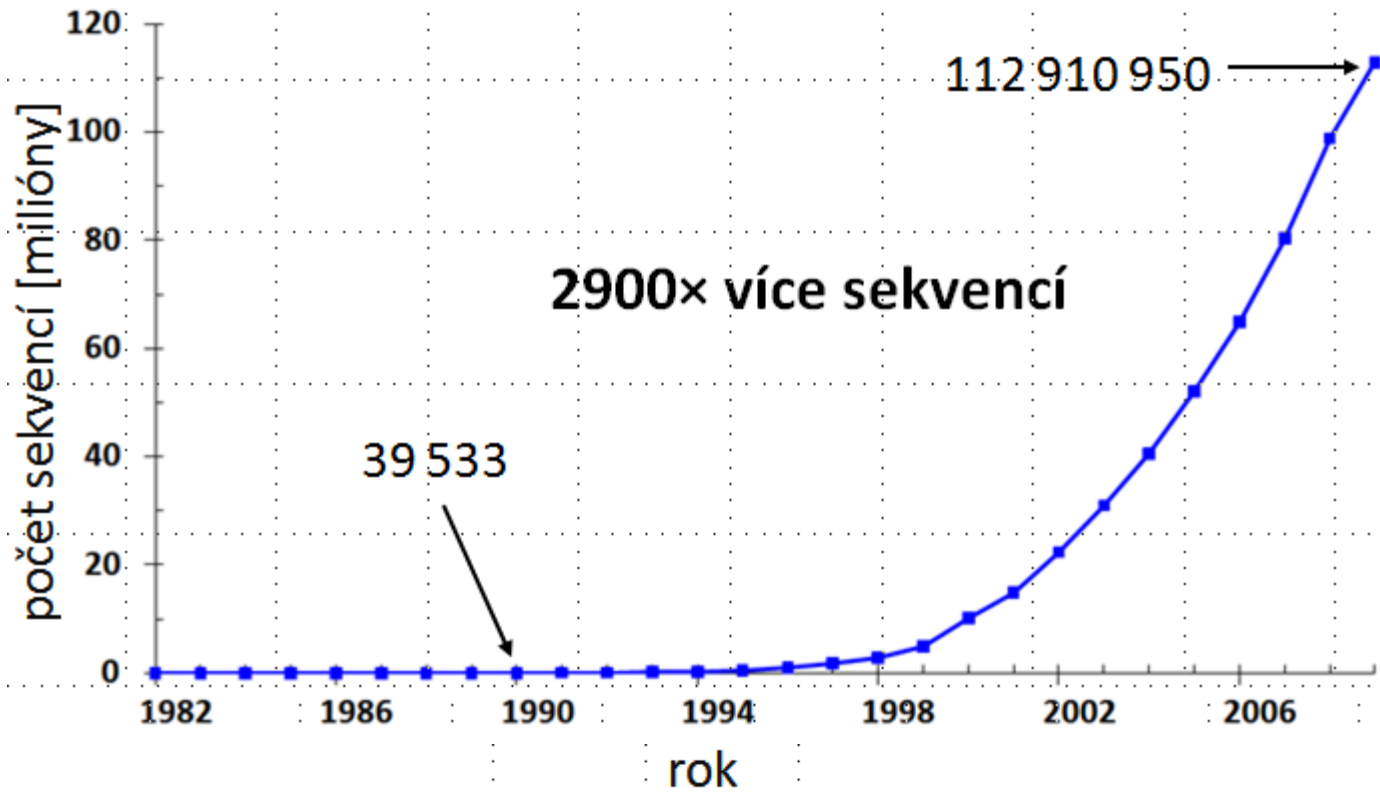
Historie bioinformatiky



Historie bioinformatiky



Historie bioinformatiky



Bioinformatické instituce

- ❑ National Center for Biotechnology Information (NCBI)
- ❑ European Bioinformatics Institute (EBI)



- National Center for Biotechnology Information (NCBI)
 - oddělení National Library of Medicine při National Institutes of Health v USA
 - Poskytuje Databáze GenBank, PubMed, OMIM, Genome dbSNP, ...
 - Informace dostupné přes vyhledávací **system Entrez**



□ National Center for Biotechnology Information (NCBI)

The screenshot shows the NCBI Entrez search engine interface. At the top left is the NCBI logo. To its right is the Entrez logo and the text "Entrez, The Life Sciences Search Engine". Below this is a navigation bar with tabs for "HOME", "SEARCH", "SITE MAP", "PubMed", "All Databases", "Human Genome", "GenBank", "Map Viewer", and "BLAST". A search bar is located below the navigation bar, with the text "Search across databases" and a "GO" button. Below the search bar is a welcome message: "Welcome to the Entrez cross-database search page". The main content area is divided into two columns of database links, each with a small icon and a description. The left column includes PubMed, PubMed Central, Site Search, Nucleotide, EST, GSS, Protein, Genome, Structure, Taxonomy, and SNP. The right column includes Books, OMIM, OMIA, dbGaP, UniGene, CDD, 3D Domains, UniSTS, PopSet, GEO Profiles, and GEO DataSets.

NCBI

Entrez, The Life Sciences Search Engine

HOME SEARCH SITE MAP PubMed All Databases Human Genome GenBank Map Viewer BLAST

Search across databases GO Clear Help

Welcome to the Entrez cross-database search page

| | |
|---|--|
| PubMed: biomedical literature citations and abstracts | Books: online books |
| PubMed Central: free, full text journal articles | OMIM: online Mendelian Inheritance in Man |
| Site Search: NCBI web and FTP sites | OMIA: online Mendelian Inheritance in Animals |
| Nucleotide: Core subset of nucleotide sequence records | dbGaP: genotype and phenotype |
| EST: Expressed Sequence Tag records | UniGene: gene-oriented clusters of transcript sequences |
| GSS: Genome Survey Sequence records | CDD: conserved protein domain database |
| Protein: sequence database | 3D Domains: domains from Entrez Structure |
| Genome: whole genome sequences | UniSTS: markers and mapping data |
| Structure: three-dimensional macromolecular structures | PopSet: population study data sets |
| Taxonomy: organisms in GenBank | GEO Profiles: expression and molecular abundance profiles |
| SNP: single nucleotide polymorphism | GEO DataSets: experimental sets of GEO data |

- European Bioinformatics Institute (EBI)
 - Součást European Molecular Biology Laboratory (EMBL), Wellcome Trust Genome Campus ve Velké Británii
 - Poskytuje databáze EMBL-Bank, UniProt, Ensembl, InterPro, ...
 - Informace dostupné přes vyhledávací **system SRS**



Bioinformatické instituce

□ European Bioinformatics Institute (EBI)

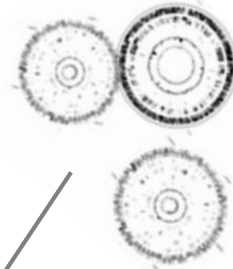
The screenshot displays the EMBL-EBI website interface. At the top, there is a search bar with the text "Nucleotide sequences" and a "Go" button. Below the search bar is the EMBL-EBI logo and the text "European Bioinformatics Institute". A navigation menu includes "EBI Home", "About EBI", "Research", "Services", "Toolbox", "Databases", "Downloads", and "Submissions". Below the menu is a "SERVICES OVERVIEW FASTLINK" section. A tree diagram on the left side of the page shows the following structure:

- Databases
 - Database Browsing
 - SRS
 - Nucleotide Databases
 - EMBL Nucleo. Sequence
 - Ensembl
 - Genomes Server
 - Genome MOT
 - EMBL-Align
 - Simple Queries
 - dbSTS Queries
 - Parasites
 - Mutations
 - IMG
 - Protein Databases
 - SWISS-PROT
 - TrEMBL
 - InterPro
 - CluSTR
 - IP
 - GOA
 - Proteome Analysis
 - HPI
 - IntEnz
- Toolbox
 - Homology & Similarity
 - Fasta
 - WU-Blast2
 - NCBI-Blast2
 - Blast2_EVEC
 - Genome/Proteome Fasta
 - MPsrch
 - Scanps2_3
 - Parasite-Blast
 - EGI-Blast
 - SNP-Fasta3 Server
 - Prot. Function. Analysis
 - CluSTR Search
 - InterProScan
 - FingerPRINTScan
 - ppsearch
 - GeneQuiz
 - Pratt
 - Radar
- Submissions
 - EMBL via WEBIN
 - EMBL-Info. Submitters
 - SWISS-PROT
 - Webin-Align
 - PDB-AutoDep
 - MIAMEpress
 - IMG/HLA
 - Sequin Software
- Downloads
 - FTP Server
 - Database Repository
 - Software Repository
 - Downloads Help Files
- Services Help

Bioinformatické databáze

- ❑ Bibliografie
- ❑ Nukleotidové sekvence
- ❑ Proteinové sekvence
- ❑ Proteinové struktury
- ❑ Genomy

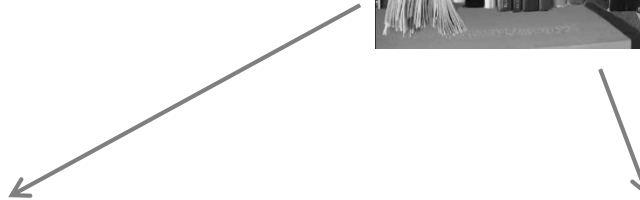
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WYKLIRTTVWHQAIVLAEIGTVVCKTQENPA
```



| Count | Icon | Database Name | Description | Searchable | None | Icon | Database Name | Description | Searchable | None |
|-------|---------------|----------------|---|------------|------|------------|---------------|--|------------|------|
| 44 | M | PubMed | biomedical literature citations and abstracts | ? | none | B | Books | online books | ? | none |
| 79 | Open Book | PubMed Central | free, full text journal articles | ? | none | Person | OMIM | online Mendelian Inheritance in Man | ? | none |
| none | W | Site Search | NCBI web and FTP sites | ? | none | Person | OMIA | Online Mendelian Inheritance in Animals | ? | none |
| 45 | DNA | Nucleotide | sequence database (includes GenBank) | ? | none | Gene | UniGene | gene-oriented clusters of transcript sequences | ? | none |
| 39 | Microscope | Protein | sequence database | ? | none | Microscope | CDD | conserved protein domain database | ? | none |
| 4 | Vertical Bars | Genome | whole genome sequences | ? | 12 | Microscope | 3D Domains | domains from Entrez Structure | ? | none |
| 12 | Microscope | Structure | three-dimensional macromolecular structures | ? | none | Microscope | UniSTS | markers and mapping data | ? | none |

Bibliografické databáze

- ❑ PubMed
- ❑ Web of Science



NCBI PubMed A service of the U.S. National Library of Medicine and the National Institutes of Health www.pubmed.gov

All Databases PubMed Nucleotide Protein Genome Structure OMIM PMC Journ

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AND in Author

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Add Another Field >>

Search Clear



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- Obsahuje více než 22 milionů citací **biomedicínské literatury**
- Integruje MEDLINE, časopisy z oblasti živých věd a online knihy
- Prohledávání možné přes **Entrez** nebo **DBGET**
- Obsahuje kromě **abstraktů** odkazy na **plné texty** dostupné přes PubMed Central nebo stránky nakladatelství



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Nat Chem Biol. 2009 Oct;5(10):727-33. Epub 2009 Aug 23.

Redesigning dehalogenase access tunnels as a strategy for degrading an anthropogenic substrate.

Pavlova M, Klvana M, Prokop Z, Chaloupkova R, Banas P, Otyepka M, Wade RC, Tsuda M, Nagata Y, Damborsky J.
Loschmidt Laboratories, Institute of Experimental Biology and National Centre for Biomolecular Research, Faculty of Science, Masaryk University, Brno, Czech Republic.

Abstract
Engineering enzymes to degrade anthropogenic compounds efficiently is challenging. We obtained *Rhodococcus rhodochrous* haloalkane dehalogenase mutants with up to 32-fold higher activity than wild type toward the toxic, recalcitrant anthropogenic compound 1,2,3-trichloropropane (TCP) using a new strategy. We identified key residues in access tunnels connecting the buried active site with bulk solvent by rational design and randomized them by directed evolution. The most active mutant has large aromatic residues at two out of three randomized positions and two positions modified by site-directed mutagenesis. These changes apparently enhance activity with TCP by decreasing accessibility of the active site for water molecules, thereby promoting activated complex formation. Kinetic analyses confirmed that the mutations improved carbon-halogen bond cleavage and shifted the rate-limiting step to the release of products. Engineering access tunnels by combining computer-assisted protein design with directed evolution may be a valuable strategy for refining catalytic properties of enzymes with buried active sites.

PMID: 19701186 [PubMed - indexed for MEDLINE]

Publication Types, MeSH Terms, Substances, Secondary Source ID

LinkOut - more resources

Full Text Sources:
[Nature Publishing Group](#)

Related citations

Biodegradation of 1,2,3-trichloropropane through directed evolution an [Appl Environ Microbiol. 2002]

Pathways and mechanisms for product release in the engineered haloalkane dehalo [J Mol Biol. 2009]

Mechanism of enhanced conversion of 1,2,3-trichloropropane b [J Comput Aided Mol Des. 2006]

Review Evolving haloalkane dehalogenases. [Curr Opin Chem Biol. 2004]

Review Alpha/Beta-hydrolase fold enzymes: structures, functions [Curr Protein Pept Sci. 2000]

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Related Citations

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Redesigning dehalogenase access tunnels as a strategy for degrading an anthropogenic substrate

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Author(s): Pavlova M (Pavlova, Martina)^{1,2}, Klvana M (Klvana, Martin)^{1,2}, Prokop Z (Prokop, Zbynek)^{1,2}, Chaloupkova R (Chaloupkova, Radka)^{1,2}, Banas P (Banas, Pavel)^{3,4}, Otyepka M (Otyepka, Michal)^{3,4}, Wade RC (Wade, Rebecca C.)⁵, Tsuda M (Tsuda, Masataka)⁶, Nagata Y (Nagata, Yuji)⁶, Damborsky J (Damborsky, Jiri)^{1,2}

Source: NATURE CHEMICAL BIOLOGY **Volume:** 5 **Issue:** 10 **Pages:** 727-733 **Published:** OCT 2009

Times Cited: 6 **References:** 50 [Citation Map](#)

Abstract: Engineering enzymes to degrade anthropogenic compounds efficiently is challenging. We obtained Rhodococcus rhodochrous haloalkane dehalogenase mutants with up to 32-fold higher activity than wild type toward the toxic, recalcitrant anthropogenic compound 1,2,3-trichloropropane (TCP) using a new strategy. We identified key residues in access tunnels connecting the buried active site with bulk solvent by rational design and randomized them by directed evolution. The most active mutant has large aromatic residues at two out of three randomized positions and two positions modified by site-directed mutagenesis. These changes apparently enhance activity with TCP by decreasing accessibility of the active site for water molecules, thereby promoting activated complex formation. Kinetic analyses confirmed that the mutations improved carbon-halogen bond cleavage and shifted the rate-limiting step to the release of products. Engineering access tunnels by combining computer-assisted protein design with directed evolution may be a valuable strategy for refining catalytic properties of enzymes with buried active sites.

Document Type: Article

Language: English

KeyWords Plus: SPHINGOMONAS-PAUCIMOBILIS UT26; HALOALKANE DEHALOGENASE; DIRECTED EVOLUTION; CYTOCHROME P450S; HETEROLOGOUS EXPRESSION; XENOBIOTIC COMPOUNDS; CATALYTIC MECHANISM; ESCHERICHIA-COLI; ENZYME; SPECIFICITY

Reprint Address: Damborsky, J (reprint author), Masaryk Univ, Fac Sci, Loschmidt Labs, Inst Expt Biol, CS-61137 Brno, Czech Republic

Cited by: 6

This article has been cited 6 times (from Web of Science).

Kourist R, Jochens H, Bartsch S, et al. [The alpha/beta-Hydrolase Fold 3DM Database \(ABHDB\) as a Tool for Protein Engineering](#) CHEMBIOCHEM 11 12 1635-1643 AUG 16 2010

Stsiapanava A, Dohnalek J, Gavira JA, et al. [Atomic resolution studies of haloalkane dehalogenases DhaA04, DhaA14 and DhaA15 with engineered access tunnels](#) ACTA CRYSTALLOGRAPHICA SECTION D-BIOLOGICAL CRYSTALLOGRAPHY 66 962-969 Part 9 SEP 2010

Brouk M, Derry NL, Shainsky J, et al. [The influence of key residues in the tunnel entrance and the active site on activity and selectivity of toluene-4-monooxygenase](#) JOURNAL OF MOLECULAR CATALYSIS B-ENZYMATIC 66 1-2 72-80 SEP 2010

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Related Records:

Databáze nukleotidových sekvencí



- ❑ GenBank
- ❑ EMBL-Bank
- ❑ DDBJ

- ❑ Anotované kolekce veřejně dostupných nukleotidových sekvencí
- ❑ Data získaná z genomových center a odborných pracovišť
- ❑ **Každodenní** vzájemná **synchronizace** nových a aktualizovaných dat
- ❑ **“Accession number”** - jedinečný identifikátor záznamu, ve všech třech databázích

Databáze nukleotidových sekvencí

□ GenBank

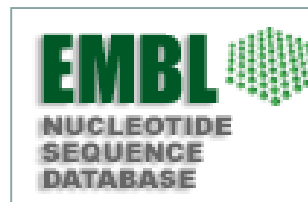
- Založena v roce 1982, provozována NCBI
- Přístupná prostřednictvím vyhledávacího systému **Entrez** nebo systému **DBGET**
- Obsahuje více než 187.000.000 sekvencí (2015)
- Nové sekvence možné vložit pomocí **BankIt** nebo **Sequin**



Databáze nukleotidových sekvencí

□ EMBL-Bank

- Založena v roce 1980, Provozována EBI
- Přístupná prostřednictvím vyhledávacího systému **SRS** či **DBGET**
- Obsahuje více než 608.000.000 sekvencí (2015)
- Nové sekvence možné vložit pomocí **Webin** nebo **Sequin**



Databáze nukleotidových sekvencí

- DNA Data Bank of Japan (DDBJ)
 - Založena v roce 1984, provozována National Institute of Genetics
 - Obsahuje více než 253.000.000 sekvencí (2015)
 - Nové sekvence možné vložit pomocí **Sakura** nebo **Sequin**



Ukázka záznamu v GenBank

□ Hlavička

- Základní informace o záznamu
- Lokus, definice, přístupový kód, klíčová slova, organizmus, reference,..

X.autotrophicus haloalkane dehalogenase (dh1A) gene, complete cds

[Comment](#) [Features](#) [Sequence](#)

LOCUS XAADHLA 3041 bp DNA linear BCT 15-FEB-1996
DEFINITION X.autotrophicus haloalkane dehalogenase (dh1A) gene, complete cds.
ACCESSION M26950
VERSION M26950.1 GI:155347
KEYWORDS haloalkane dehalogenase.
SOURCE Xanthobacter autotrophicus
ORGANISM [Xanthobacter autotrophicus](#)
Bacteria; Proteobacteria; Alphaproteobacteria; Rhizobiales;
Xanthobacteraceae; Xanthobacter.
REFERENCE 1 (bases 1 to 3041)
AUTHORS Janssen,D.B., Pries,F., van der Ploeg,J., Kazemier,B., Terpstra,P.
and Witholt,B.
TITLE Cloning of 1,2-dichloroethane degradation genes of Xanthobacter
autotrophicus GJ10 and expression and sequencing of the dh1A gene
JOURNAL J. Bacteriol. 171 (12), 6791-6799 (1989)
PUBMED [2687254](#)
COMMENT Draft entry and computer readable copy of sequence [1] kindly
provided by D.B.Janssen, 11-AUG-1989.

Ukázka záznamu v GenBank

□ Charakteristiky

- Popis jednotlivých oblastí genu
- Promotor, RBS (ribozóm vazebné místo), CDS (kódující sekvence), ...

```
gene          918..1931
              /gene="dh1A"
promoter      918..946
              /gene="dh1A"
              /note="putative"
promoter      945..974
              /gene="dh1A"
              /note="putative"
RBS           986..998
              /gene="dh1A"
CDS           999..1931
              /gene="dh1A"
              /codon_start=1
              /transl_table=11
              /product="haloalkane dehalogenase"
              /protein_id="AAA88691.1"
              /db_xref="GI:155348"
              /translation="MINAIRTPDQRFSNLDQYFPSPNYLDDLPGYPLRAHYLDEGNS
DAEDVFLCLHGPTWSYLYRKMIPVFAESGARVIAPDFFGFGKSDKPVDEEDYTTFEFH
RNFLALALIERLDLRNITLVVQDWGGFLGLTLPMDPSRFKRLIIMNACLMTDPVTQPA
FSAFVTQPADGFTA WKYDLVTPSDLRLDQFMKRWAPT LTEAEASAYAAPFPDTSYQAG
```

Ukázka záznamu v GenBank



□ Charakteristiky

| FEATURES | Location/Qualifiers |
|--------------------------|---|
| source | 1..3041 /organism="Xanthobacter autotrophicus" /mol_type="genomic DNA" /strain="GJ10" /db_xref="taxon:280" |
| CDS | complement(316..924) /note="ORF 1; putative" /codon_start=1 /transl_table=11 /product="unknown protein" /protein_id="AAA88690.1" /db_xref="GI:1197026" /translation="MSTFFEPENGMKQNAKTERILDVALELLETEGEFGLTMRQVATQ ADMSLSNVQYYFKSEDLVAMADRYFQRCCLTMAEHPPLSAGRDOHAQLRALLRELL GHGLEISEMCRIFREYWAIAIATRNETHVHGLKSYRDLAEVMAEKLAPLASSEKALAVA VSLVPIYVEGYSVTAIAMPESIDTISETLTNVVLEQLRISNS" |
| gene | 918..1931 /gene="dh1A" |
| promoter | 918..946 /gene="dh1A" /note="putative" |
| promoter | 945..974 /gene="dh1A" /note="putative" |
| RBS | 986..998 /gene="dh1A" |
| CDS | 999..1931 /gene="dh1A" /codon_start=1 /transl_table=11 /product="haloalkane dehalogenase" /protein_id="AAA88691.1" /db_xref="GI:155348" /translation="MINAIRTPDQRFNSLDQYFSPNYLDDLPGYPLRAHYLDEGNS DAEDVFLCLHGEPWYSYLKMLPVFAESGARVIAPDFFGFKSDKPVDEEDYTFEFH RNFLALIERLDRNITLVVQDWGGFLGLTLPMDPSRFKRLIIMNACLMTDPVTPQPA FSAFVTQPADGFTAWKYDLVTPSDLRLDQFMKRWAPTLTEAEASAYAAPPDTSYQAG VRKFPKMVAQRDQACIDISTEALISFWQNDWNGQTFMAIGMKDKLLGPDVMPKALIN GCEPELEIADAGHFVQEFGEQVAREALKHFAETE" |

Ukázka záznamu v GenBank

□ Sekvence

```
ORIGIN      1 bp upstream of BamHI site.
      1 atgataaatg caattcgcac cccggaccaa cgcttcagca atctcgatca gtatccgttc
     61 agccccaact acctggacga cctccccggc taccgggat  tgcgggcaca ctacctcgac
    121 gagggcaatt ctgacgctga agacgttttt ctctgccttc atggcgagcc cacctggagt
    181 tacctgtatc gcaagatgat cccggtatth gctgaatcag gcgcacgagt tattgcgcca
    241 gacttttttg gattcggaaa atccgacaag ccagtagacg aagaagacta caccttcgaa
    301 tttcaccgca acttcctgct tgcactaatc gaacggcttg acttgcgcaa cattacgctg
    361 gtcgttcagg actggggcgg atttttgggg ctgaccttac cgatggccga cccttcccgc
    421 ttcaagcgcc tgatcatcat gaacgcctgc ttgatgaccg acccggtcac ccagcctgcg
    481 tttagcgcct ttgtcaccca gcctgcggat ggctttaccg cctggaaata cgatctggtt
    541 acgccatcag acctgcgcct tgaccagttc atgaagcgtt gggcgcccac actgaccgaa
    601 gctgaggcct ccgcgtatgc tgcgcctttc cctgacactt cctatcaggc tgggtgtacgc
    661 aagtttccca agatggtcgc gcaacgcgac caggcctgca tcgacatttc aaccgaagcg
    721 atttcgttct ggcagaacga ctggaatggc cagaccttca tggccattgg catgaaagac
    781 aaattgctgg gaccggacgt catgtatcct atgaaggcgc tcattaatgg ctgcccggaa
    841 ccctcgaaa tagcggacgc tggccatttc gtacaggagt ttggcgagca agtggctcgc
    901 gaggcctga  aacactttgc cgagacagaa tag
```

//

Databáze proteinových sekvencí

- UniProtKB
- nr Protein Database



Databáze proteinových sekvencí

□ UniProtKB

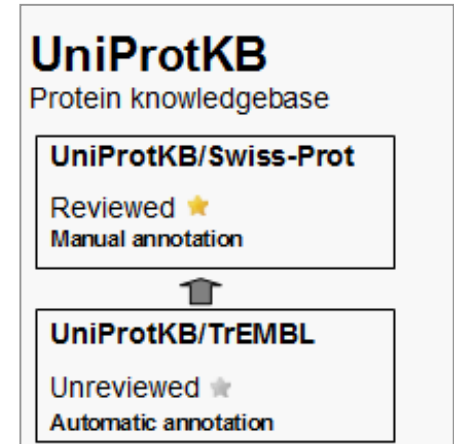
- Spolupráce EBI, Swiss Institute of Bioinformatics a Protein Information Resource
- Centrální úložiště proteinových sekvencí a funkčních informací
- **Kvalitní anotace** - informace o funkci proteinu a jednotlivých aminokyselin, experimentální informace, biologické ontologie, klasifikace, odkazy do dalších databází
- **Indikace kvality** anotace (**manuální** vs. **automatická**)



Databáze proteinových sekvencí

□ UniProtKB/Swiss-Prot

- Vysoká kvalita manuálních anotací
- 😊 Manuální anotace – **spolehlivé informace**
- 😞 549.000 sekvencí (2015)



□ UniProtKB/TrEMBL

- Sekvence konceptuální translací kódujících sekvencí EMBL-Bank
- 😞 Automatická anotace – **nižší kvalita, možnosti chyb**
- 😊 50.825.000 sekvencí (2015)



Ukázka záznamu v UniProtKB

- ❑ Názvy a zdroj proteinu
- ❑ Vlastnosti proteinu

| Names and origin | | Hide Top |
|----------------------|---|------------|
| Protein names | <i>Recommended name:</i> Haloalkane dehalogenase EC=3.8.1.5 <i>Alternative name(s):</i> 1,3,4,6-tetrachloro-1,4-cyclohexadiene hydrolase 1,4-TCDN chlorohydrolase | |
| Gene names | Name: linB | |
| Organism | Pseudomonas paucimobilis (Sphingomonas paucimobilis) | |
| Taxonomic identifier | 13689 [NCBI] | |
| Taxonomic lineage | Bacteria › Proteobacteria › Alphaproteobacteria › Sphingomonadales › Sphingomonadaceae › Sphingomonas | |
| Protein attributes | | Hide Top |
| Sequence length | 296 AA. | |
| Sequence status | Complete. | |
| Sequence processing | The displayed sequence is further processed into a mature form. | |
| Protein existence | Evidence at protein level. | |

Ukázka záznamu v UniProtKB

□ Obecná anotace

| General annotation (Comments) Hide Top | |
|---|--|
| Function | Catalyzes hydrolytic cleavage of carbon-halogen bonds in halogenated aliphatic compounds, leading to the formation of the corresponding primary alcohols, halide ions and protons. Has a broad substrate specificity since not only monochloroalkanes (C3 to C10) but also dichloroalkanes (> C3), bromoalkanes, and chlorinated aliphatic alcohols were good substrates. Shows almost no activity with 1,2-dichloroethane, but very high activity with the brominated analog. Is involved in the degradation of the important environmental pollutant gamma-hexachlorocyclohexane (lindane) as it also catalyzes conversion of 1,3,4,6-tetrachloro-1,4-cyclohexadiene (1,4-TCDN) to 2,5-dichloro-2,5-cyclohexadiene-1,4-diol (2,5-DDOL) via the intermediate 2,4,5-trichloro-2,5-cyclohexadiene-1-ol (2,4,5-DNOL). HAMAP MF_01231 |
| Catalytic activity | 1-haloalkane + H ₂ O = a primary alcohol + halide. HAMAP MF_01231 1,4-TCDN + 2 H ₂ O = 2,5-DDOL + 2 chloride. HAMAP MF_01231 |
| Enzyme regulation | Competitively inhibited by the key pollutants 1,2-dichloroethane (1,2-DCE) and 1,2-dichloropropane (1,2-DCP). HAMAP MF_01231 |
| Pathway | Xenobiotic degradation; gamma-hexachlorocyclohexane degradation. HAMAP MF_01231 |
| Subunit structure | Monomer. HAMAP MF_01231 |
| Subcellular location | Periplasm. Ref.4 |
| Induction | Constitutively expressed. HAMAP MF_01231 |
| Miscellaneous | Is not N-terminally processed during export, so it may be secreted into the periplasmic space via a hitherto unknown mechanism. HAMAP MF_01231 |
| Sequence similarities | Belongs to the haloalkane dehalogenase family, Type 2 subfamily. |
| Biophysicochemical properties | pH dependence: Optimum pH is 8.2. HAMAP MF_01231 |

Ukázka záznamu v UniProtKB

□ Ontologie

| Ontologies | |
|---|---|
| Keywords | |
| Biological process | Detoxification |
| Cellular component | Periplasm |
| Molecular function | Hydrolase |
| Technical term | 3D-structure Direct protein sequencing |
| Gene Ontology (GO) | |
| Biological process | response to toxin <small>Inferred from electronic annotation. Source: UniProtKB-KW</small> |
| Cellular component | periplasmic space <small>Inferred from electronic annotation. Source: UniProtKB-SubCell</small> |
| Molecular function | haloalkane dehalogenase activity <small>Inferred from electronic annotation. Source: HAMAP</small> |
| Complete GO annotation... | |
















Ukázka záznamu v UniProtKB

□ Anotace sekvence

| Sequence annotation (Features) | | | | | | |
|-------------------------------------|----------------------|-------------|--------|--|----------------|--------------------|
| | Feature key | Position(s) | Length | Description | Graphical view | Feature identifier |
| Molecule processing | | | | | | |
| <input checked="" type="checkbox"/> | Initiator methionine | 1 | 1 | Removed (Ref.4) (Ref.1) | | |
| <input type="checkbox"/> | Chain | 2 – 296 | 295 | Haloalkane dehalogenase (HAMAP MF_01231) | | PRO_0000216778 |
| Sites | | | | | | |
| <input checked="" type="checkbox"/> | Active site | 108 | 1 | Nucleophile (HAMAP MF_01231) | | |
| <input checked="" type="checkbox"/> | Active site | 132 | 1 | Proton donor (HAMAP MF_01231) | | |
| <input checked="" type="checkbox"/> | Active site | 272 | 1 | Proton acceptor (HAMAP MF_01231) | | |
| <input checked="" type="checkbox"/> | Binding site | 38 | 1 | Halide (HAMAP MF_01231) | | |
| <input checked="" type="checkbox"/> | Binding site | 109 | 1 | Halide (HAMAP MF_01231) | | |
| Natural variations | | | | | | |
| <input checked="" type="checkbox"/> | Natural variant | 81 | 1 | A → T in strain: B90. | | |
| <input checked="" type="checkbox"/> | Natural variant | 112 | 1 | A → V in strain: B90. | | |
| <input checked="" type="checkbox"/> | Natural variant | 134 – 135 | 2 | IA → VT in strain: B90. | | |
| <input checked="" type="checkbox"/> | Natural variant | 138 | 1 | I → L in strain: B90. | | |
| <input checked="" type="checkbox"/> | Natural variant | 247 | 1 | A → H in strain: B90. | | |
| <input checked="" type="checkbox"/> | Natural variant | 253 | 1 | M → I in strain: B90. | | |

Ukázka záznamu v UniProtKB

□ Anotace sekvence

| Natural variations | | | | | |
|--------------------|-----------------|-----------|---|--|---|
| ■ | Natural variant | 81 | 1 | A → T in strain: B90. |  |
| ■ | Natural variant | 112 | 1 | A → V in strain: B90. |  |
| ■ | Natural variant | 134 – 135 | 2 | IA → VT in strain: B90. |  |
| ■ | Natural variant | 138 | 1 | I → L in strain: B90. |  |
| ■ | Natural variant | 247 | 1 | A → H in strain: B90. |  |
| ■ | Natural variant | 253 | 1 | M → I in strain: B90. |  |
| Experimental info | | | | | |
| ■ | Mutagenesis | 38 | 1 | N → D, E, F or Q: Loss of activity. Ref.7 |  |
| ■ | Mutagenesis | 108 | 1 | D → A: Loss of activity. Ref.6 |  |
| ■ | Mutagenesis | 108 | 1 | D → N: 58% of wild-type activity. Ref.6 |  |
| ■ | Mutagenesis | 109 | 1 | W → L: Loss of activity. Ref.7 |  |
| ■ | Mutagenesis | 132 | 1 | E → Q: Loss of activity. Ref.6 |  |
| ■ | Mutagenesis | 151 | 1 | F → L, W or Y: Increase in activity. Ref.7 |  |
| ■ | Mutagenesis | 169 | 1 | F → L: 31% of wild-type activity. Ref.7 |  |
| ■ | Mutagenesis | 244 | 1 | E → Q: 38% of wild-type activity. Ref.6 |  |
| ■ | Mutagenesis | 272 | 1 | H → A: Loss of activity. Ref.6 |  |

Ukázka záznamu v UniProtKB

□ Sekvence

Sequences

| Sequence | Length | Mass (Da) | Tools | |
|--|--------|-----------|--------|--|
| <input type="checkbox"/> P51698-1 [UniParc]. | FASTA | 296 | 33,108 | <input type="text" value="Blast"/> <input type="button" value="go"/> |

Last modified January 23, 2007. Version 4.
Checksum: 6EEE011B157DBAE1

```
      10      20      30      40      50      60
MSLGAKPFGE KKFIEIKGRR MAYIDEGTGD PILFQHGMPY SSYLWRNIMP HCAGLGRLIA
      70      80      90     100     110     120
CDLIGMGDSD KLDPSGPERY AYAHRDYLD ALWEALDLGD RVVLVVHDWG SALGFDWARR
     130     140     150     160     170     180
HRERVQGIAY MEAIAMPIEW ADFPEQDRDL FQAFRSQAGE ELVLQDNVAV EQVLPGLILR
     190     200     210     220     230     240
PLSEAEMAAV REPFLAAGEA RRPTLSWPRQ IPIAGTPADV VAIARDYAGW LSESPIPKLF
     250     260     270     280     290
INAEPGALTT GRMRDFCRTW PNQTEITVAG AHFIQEDSPD EIGAAIAAFV RRLRPA
```

[« Hide](#)

Ukázka záznamu v UniProtKB

□ Reference

| References | | Hid |
|------------|---|-----|
| [1] | <p>"Cloning and sequencing of a dehalogenase gene encoding an enzyme with hydrolase activity involved in the degradation of gamma-hexachlorocyclohexane in <i>Pseudomonas paucimobilis</i>." Nagata Y., Nariya T., Ohtomo R., Fukuda M., Yano K., Takagi M. J. Bacteriol. 175:6403-6410(1993) [PubMed: 7691794] [Abstract] <u>Cited for:</u> NUCLEOTIDE SEQUENCE [GENOMIC DNA], PROTEIN SEQUENCE OF 2-16. <u>Strain:</u> UT26.</p> | |
| [2] | <p>Nagata Y., Nariya T., Ohtomo R., Fukuda M., Yano K., Takagi M. Submitted (MAR-1999) to the EMBL/GenBank/DDBJ databases <u>Cited for:</u> SEQUENCE REVISION.</p> | |
| [3] | <p>"Cloning and characterization of lin genes responsible for the degradation of hexachlorocyclohexane isomers by <i>Sphingomonas paucimobilis</i> strain B90." Kumari R., Subudhi S., Suar M., Dhingra G., Raina V., Dogra C., Lal S., van der Meer J.R., Holliger C., Lal R. Appl. Environ. Microbiol. 68:6021-6028(2002) [PubMed: 12450824] [Abstract] <u>Cited for:</u> NUCLEOTIDE SEQUENCE [GENOMIC DNA]. <u>Strain:</u> B90.</p> | |
| [4] | <p>"Two different types of dehalogenases, LinA and LinB, involved in gamma-hexachlorocyclohexane degradation in <i>Sphingomonas paucimobilis</i> UT26 are localized in the periplasmic space without molecular processing." Nagata Y., Futamura A., Miyauchi K., Takagi M. J. Bacteriol. 181:5409-5413(1999) [PubMed: 10464214] [Abstract] <u>Cited for:</u> PROTEIN SEQUENCE OF 2-10, SUBCELLULAR LOCATION.</p> | |
| [5] | <p>"Purification and characterization of a haloalkane dehalogenase of a new substrate class from a gamma-hexachlorocyclohexane-degrading bacterium, <i>Sphingomonas paucimobilis</i> UT26." Nagata Y., Miyauchi K., Damborsky J., Manova K., Ansorgova A., Takagi M. Appl. Environ. Microbiol. 63:3707-3710(1997) [PubMed: 9293022] [Abstract] <u>Cited for:</u> CHARACTERIZATION. <u>Strain:</u> UT26.</p> | |

Databáze proteinových sekvencí

□ nr Protein Database

- Databáze proteinových sekvencí NCBI
- Kolekce sekvencí získaných konceptuální translací kódujících oblastí GenBank/EMBL-Bank/DDBJ a dále sekvencí z UniProtKB, PRF a RCSB PDB
- ☹ většinou automatická anotace – nižší kvalita, možnost chyb
- ☹ chybí indikace původu anotace
- 😊 více než 25.000.000 sekvencí (2015)

Formáty sekvencí

- Prostá sekvence

```
DQLTEEQIAEFKEAFSLFDK
```

Formáty sekvencí

- Prostá sekvence
- GenBank

```
LOCUS      AAU03518      237 bp      DNA                PLN      04-FEB-1995
DEFINITION Aspergillus awamori internal transcribed spacer 1 (ITS1) and 18S
           rRNA and 5.8S rRNA genes, partial sequence.
ACCESSION  U03518
BASE COUNT      41 a      77 c      67 g      52 t
ORIGIN
      1 aacctgcgga aggatcatta ccgagtgcgg gtcctttggg cccaacctcc catccgtgtc
     61 tattgtaccg tgttgcttcg gcgggcccgc cgcttgctcg ccgcgggggg ggcgcctctg
    121 cccccggggc ccgtgcccgc cggagacccc aacacgaaca ctgtctgaaa gcgtgcagtc
    181 tgagttgatt gaatgcaatc agttaaactt ttcaacaatg gatctcttgg ttccggc
//
```

Formáty sekvencí

- Prostá sekvence
- GenBank
- EMBL

```
ID    AA03518      standard; DNA; FUN; 237 BP.
XX
AC    U03518;
XX
DE    Aspergillus awamori internal transcribed spacer 1 (ITS1) and 18S
DE    rRNA and 5.8S rRNA genes, partial sequence.
XX
SQ    Sequence 237 BP; 41 A; 77 C; 67 G; 52 T; 0 other;
aacctgcgga aggatcatta ccgagtgcgg gtcctttggg cccaacctcc catccgtgtc          60
tattgtaccc tgttgcttcg gcgggcccgc cgcttgtcgg ccgccggggg ggcgcctctg          120
ccccccgggc ccgtgccgcg cggagacccc aacacgaaca ctgtctgaaa gcgtgcagtc          180
tgagttgatt gaatgcaatc agttaaactt ttcaacaatg gatctcttgg ttccggc          237
//
```

Formáty sekvencí



- ❑ Prostá sekvence
- ❑ GenBank
- ❑ EMBL
- ❑ **FASTA**

➔ `>gi|155348|gb|AAA88691.1| haloalkane dehalogenase
...INAI RTPDQRF SNLDQY PFS PNYLDDLP GYPGLRAHYLDEGN SDAEDVF
AESGARVIAPDFFGFGKSDKPVDEEDYTFEFHRNELLALIERL DLRNITL
FKRLIIMNACLMTDPVTQPAFSAFVTQPADGFTAWKYDLVTPSDLRLDQF
PDTSYQAGVRKFKPMVAQRDQACIDISTEAI SFWQNDWNGQTFMAIGMKD
PLEIADAGHFVQEFGEQVAREALKHFAETE`

Nejčastěji používaný formát

Databáze proteinových struktur

- Worldwide Protein Data Bank (wwPDB)
 - Světový depositář proteinových struktur, obsahuje rovněž struktury nukleových kyselin a biomolekulárních komplexů
 - Research Collaboratory for Structural Bioinformatics (RCSB PDB), Protein Data Bank Europe (PDBe), Protein Data Bank Japan (PDBj), Biological Magnetic Resonance Data Bank (BioMagResBank)
 - Obsahuje více než 84.000 struktur (2012)
 - Struktury získané rentgenovou krystalografií (88%) a nukleární magnetickou rezonancí (11 %)



Databáze genomů

- ❑ Entrez Genome
- ❑ Ensembl
- ❑ Genomes OnLine Database GOLD

- ❑ Informace o zdrojovém organizmu
- ❑ Nukleotidové a proteinové sekvence
- ❑ Geny v kontextu genomu
- ❑ Anotace a analýza genomů

Ukázka záznamu v Entrez Genome

☐ Přehled prokaryotických genomů

Overview [8348] Eukaryotes [2215] Prokaryotes [14202] Viruses [3212]

| First | Previous | Shown: 1 - 100 out of 1309 items | | | | Next | Last | Download selected records | | | | | | |
|---|--------------------------|----------------------------------|----------------|-----------|-------|-------------|------------|---------------------------|-----------|------|---------|--------------|-------------|----------------------|
| Organism/Name | BioProject | Group | SubGroup | Size (Mb) | GC% | Chromosomes | | WGS | Scaffolds | Gene | Protein | Release Date | Modify Date | Status |
| | | Actinobacte ▾ | — All Actinc ▾ | | | RefSeq | INSDC | | | | | | | All ▾ |
| Acaricomes phytoseiuli DSM 14247 | PRJNA174970 | Actinobacteria | Actinobacteria | - | - | - | - | - | - | - | - | - | - | No data |
| Acidimicrobium ferrooxidans DSM 10331 | PRJNA59215 PRJNA29525 | Actinobacteria | Actinobacteria | 2.16 | 68.30 | NC_013124.1 | CP001631.1 | - | - | 2089 | 1964 | 2009/08/18 | 2012/01/30 | Complete |
| Acidothermus cellulolyticus 11B | PRJNA58501 PRJNA16097 | Actinobacteria | Actinobacteria | 2.44 | 66.90 | NC_008578.1 | CP000481.1 | - | - | 2217 | 2157 | 2006/11/09 | 2012/01/24 | Complete |
| Actinoalloteichus spitiensis RMV-1378 | PRJNA76807 | Actinobacteria | Actinobacteria | 5.71 | 72.40 | - | - | AGVX01 | - | - | - | 2011/12/20 | 2012/05/31 | Scaffolds or contigs |
| Actinobaculum sp. oral taxon 183 str. F0552 | PRJNA173932 | Actinobacteria | Actinobacteria | - | - | - | - | - | - | - | - | - | - | No data |
| Actinobaculum massiliae ACS-171-V-CoI2 | PRJNA52091 | Actinobacteria | Actinobacteria | - | - | - | - | - | - | - | - | - | - | SRA or Traces |
| Actinobaculum schaalii | PRJNA52093 | Actinobacteria | Actinobacteria | - | - | - | - | - | - | - | - | - | - | No data |

Ukázka záznamu v Entrez Genome

☐ Přehled prokaryotických genomů

Overview [8348] Eukaryotes [2215] Prokaryotes [14202] Viruses [3212]

First Previous **Shown: 1 - 100 out of 1309 items** Next Last Download selected records

| Organism/Name | BioProject | Group | SubGroup | Size (Mb) | GC% | Chromosomes | | WGS | Scaffolds | Gene | Protein | Release Date | Modify Date | Status |
|---|--------------------------|----------------|----------------|-----------|-------|-------------|------------|--------|-----------|------|---------|--------------|-------------|----------------------|
| | | Actinobacte ▾ | — All Actinc ▾ | | | RefSeq | INSDC | | | | | | | All ▾ |
| Acaricomes phytoseiuli DSM 14247 | PRJNA174970 | Actinobacteria | Actinobacteria | - | - | - | - | - | - | - | - | - | - | No data |
| Acidimicrobium ferrooxidans DSM 10331 | PRJNA59215 PRJNA29525 | Actinobacteria | Actinobacteria | 2.16 | 68.30 | NC_013124.1 | CP001631.1 | - | - | 2089 | 1964 | 2009/08/18 | 2012/01/30 | Complete |
| Acidothermus cellulolyticus 11B | PRJNA58501 PRJNA16097 | Actinobacteria | Actinobacteria | 2.44 | 66.90 | NC_008578.1 | CP000481.1 | - | - | 2217 | 2157 | 2006/11/09 | 2012/01/24 | Complete |
| Actinoalloteichus spitiensis RMV-1378 | PRJNA76807 | Actinobacteria | Actinobacteria | 5.71 | 72.40 | - | - | AGVX01 | - | - | - | 2011/12/20 | 2012/05/31 | Scaffolds or contigs |
| Actinobaculum sp. oral taxon 183 str. F0552 | PRJNA173932 | Actinobacteria | Actinobacteria | - | - | - | - | - | - | - | - | - | - | No data |
| Actinobaculum massiliae ACS-171-V-CoI2 | PRJNA52091 | Actinobacteria | Actinobacteria | - | - | - | - | - | - | - | - | - | - | SRA or Traces |
| Actinobaculum schaalii | PRJNA52093 | Actinobacteria | Actinobacteria | - | - | - | - | - | - | - | - | - | - | No data |

Ukázka záznamu v Entrez Genome

□ Informace o genomu

[Organism Overview](#) ; [Genome Project Report](#) ; [Genome Annotation Report](#)

Acidothermus cellulolyticus 11B

Thermotolerant cellulolytic organism

Lineage: [Bacteria](#)[3351]; [Actinobacteria](#)[547]; [Actinobacteria](#)[547]; [Actinobacteridae](#)[502]; [Actinomycetales](#)[485]; [Frankineae](#)[11]; [Acidothermaceae](#)[1]; [Acidothermus](#)[1]; [Acidothermus cellulolyticus](#)[1]; [Acidothermus cellulolyticus 11B](#)[0]

Acidothermus cellulolyticus strain 11B. This strain (11B; ATCC 43068) is the type strain for the species. The genome sequence from this organism will provide information on the regulation and production of potentially useful enzymes.

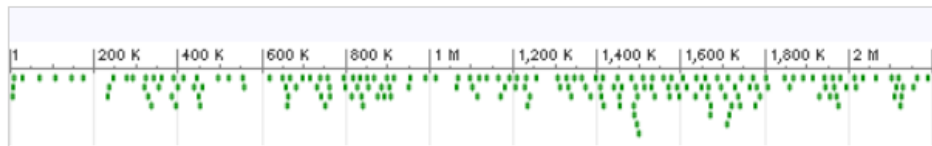
▾ Genome Sequencing Projects

◆ Chromosomes [1] ◆ Scaffolds or contigs [0] ◆ SRA or Traces [0] ◆ No data [0]

| Organism | BioProject | Assembly | Status | Chrs | Size (Mb) | GC% | Gene | Protein |
|---|---|-----------|--------|------|-----------|------|-------|---------|
| Acidothermus cellulolyticus 11B | PRJNA58501 , PRJNA16097 | ASM1502v1 | ◆ | 1 | 2.44 | 66.9 | 2,217 | 2,157 |

▾ Genome Region

[Go to nucleotide](#) [Graphics](#) [FASTA](#) [GenBank](#)



Ukázka záznamu v Entrez Genome

□ Informace o genomu

[Organism Overview](#) ; [Genome Project Report](#) ; [Genome Annotation Report](#)

Acidothermus cellulolyticus 11B

Thermotolerant cellulolytic organism

Lineage: [Bacteria](#)[3351]; [Actinobacteria](#)[547]; [Actinobacteria](#)[547]; [Actinobacteridae](#)[502]; [Actinomycetales](#)[485]; [Frankineae](#)[11]; [Acidothermaceae](#)[1]; [Acidothermus](#)[1]; [Acidothermus cellulolyticus](#)[1]; [Acidothermus cellulolyticus 11B](#)[0]

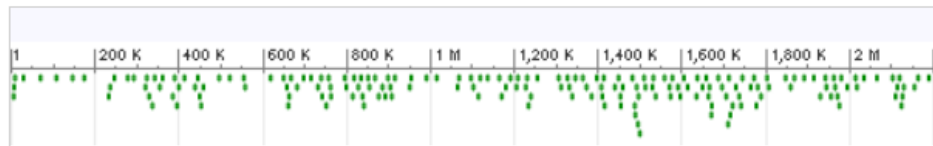
Acidothermus cellulolyticus strain 11B. This strain (11B; ATCC 43068) is the type strain for the species. The genome sequence from this organism will provide information on the regulation and production of potentially useful enzymes.

▾ Genome Sequencing Projects

◆ Chromosomes [1] ◆ Scaffolds or contigs [0] ◆ SRA or Traces [0] ◆ No data [0]

| Organism | BioProject | Assembly | Status | Chrs | Size (Mb) | GC% | Gene | Protein |
|---|--|-----------|--------|------|-----------|------|-------|---------|
| Acidothermus cellulolyticus 11B | PRJNA58501, PRJNA16097 | ASM1502v1 | ◆ | 1 | 2.44 | 66.9 | 2,217 | 2,157 |

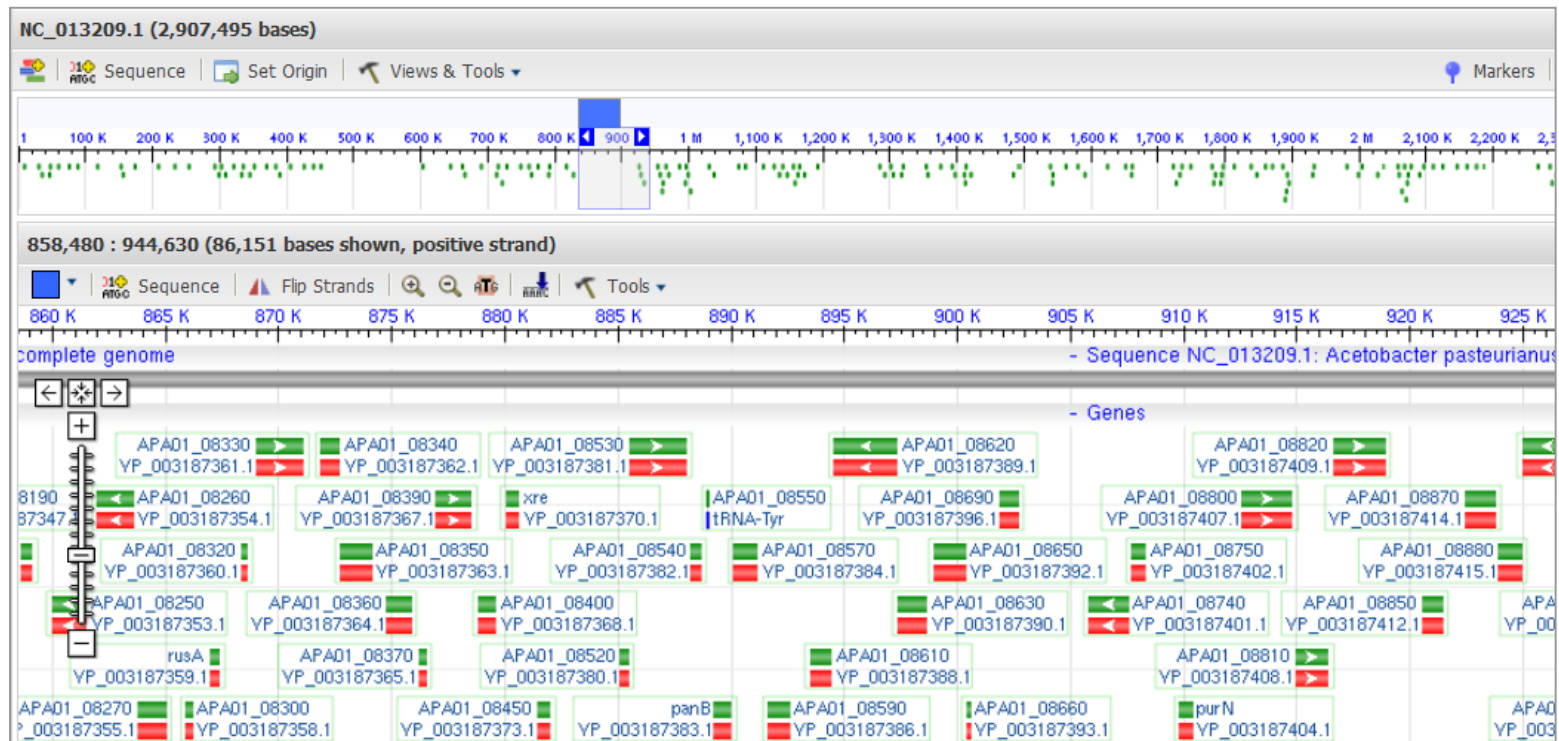
▾ Genome Region



Go to nucleotide [Graphics](#) [FASTA](#) [GenBank](#)

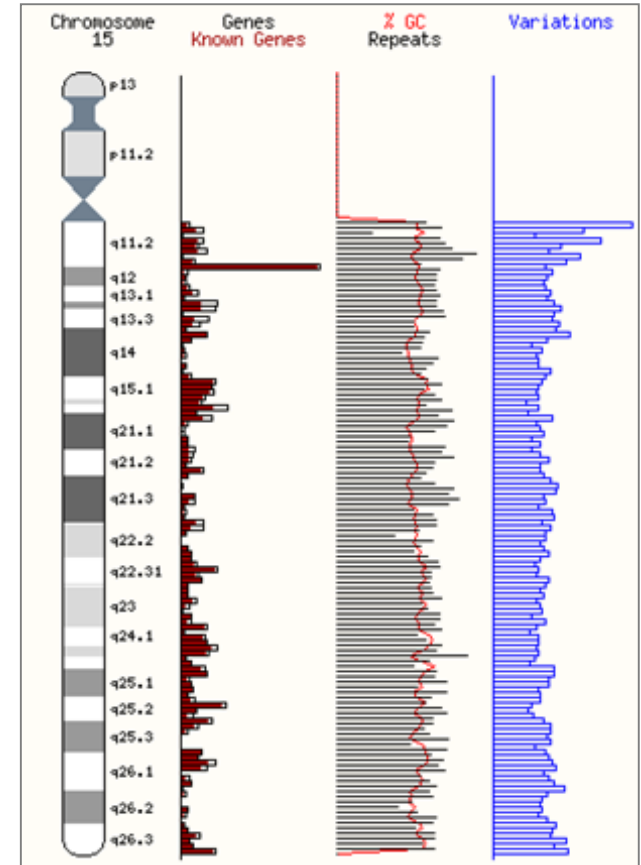
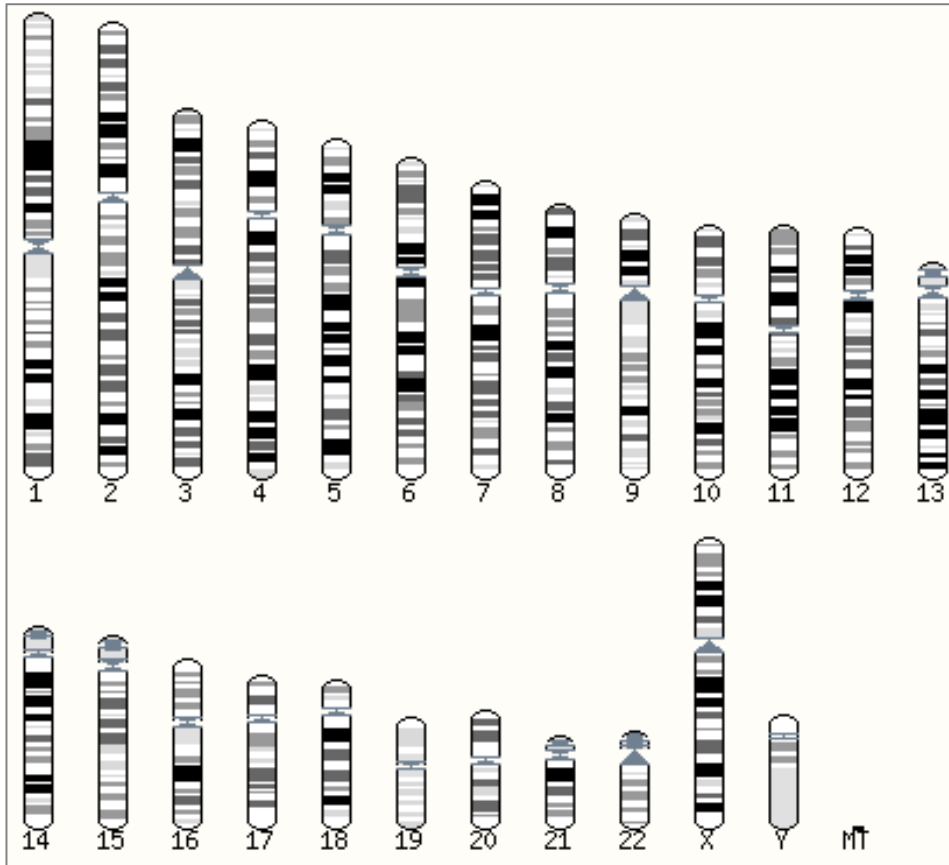
Ukázka záznamu v Entrez Genome

- Grafické znázornění genomu



Ukázka záznamu v Ensembl

- Anotace eukaryotických genomů



Ukázka záznamu v GOLD

Seznam dokončených a probíhajících genomových projektů

| Complete Published Genome Projects: 1375 | | | | | | | | | | | | |
|--|---|---------------------------------------|--|---|---------|---------|-------|---------------------------|---|-----------------------------------|--|---------------------------|
| A Archaeal: 94 B Bacterial: 1148 E Eukaryal: 133 | | | | | | | | | | | | |
| << first < prev 1 2 3 4 5 next > last >> 100 | | | | | | | | | | | | |
| GOLD ID | ORGANISM | DOMAIN | INFORMATION | SIZE | CHROM # | PLASM # | GC % | DATA | SEQUENCING CENTER | GENOME DATABASE | PUBLICATION | CONTACT |
| Gc01325 | Saccharomyces cerevisiae S288c | E | FUNGI-ASCOMYCOTA Taxonomy Entrez | | 16 | | | | Saccharomyces Genome Database | | | |
| Gc01378 | Ferrimonas balearica PAT, DSM 9799 | B | PROTEOBACTERIA-GAMMA Taxonomy Entrez GEBA | 4279 Kb 3947 orfs | 1 | | 50% | CP002209 | DOE Joint Genome Institute DSMZ | IMG-GEBA | Unpublished 2010-09-24 | Wovke T |
| Gc01374 | Vulcanisaeta distributa IC-017, DSM 14429 | A | CRENARCHAEOTA-THERMOPROTEI Taxonomy Entrez Isolation GEBA | 2374 Kb 2592 orfs MAP | 1 | | 45.4% | NC_014537 | DOE Joint Genome Institute DSMZ | NCBI | Unpublished 2010-09-22 | Bruce D |
| Gc01375 | Halomonas elongata DSM 2581 | B | PROTEOBACTERIA-GAMMA Taxonomy Entrez | 4061 Kb 3556 orfs MAP | 1 | | 63% | NC_014532 | Max-Planck Institute | NCBI | Environmental Microbiology in press 2010-09-17 | Kunte,H.J |
| Gc01372 | Methanoplanus petrolearius SEBR 4847, DSM 11571 | A | EURYARCHAEOTA-METHANOMICROBIA Taxonomy Entrez Isolation GEBA | 2843 Kb 2881 orfs MAP | 1 | | 50% | NC_014507 | DOE Joint Genome Institute DSMZ | NCBI | Unpublished 2010-09-17 | Bruce D |
| Gc01373 | Sulfurimonas autotrophica OK10, DSM 16294 | B | PROTEOBACTERIA-EPSILON Taxonomy Entrez Isolation | 2153 Kb 2220 orfs | 1 | | 35.2% | CP002205 | DOE Joint Genome Institute DSMZ | IMG-GEBA | 2010-09-15 | Bruce D |
| Gc01376 | Spirochaeta thermophila DSM 6192 | B | SPIROCHAETES Taxonomy Entrez | 2472 Kb | 1 | | 52% | CP001698 | Goettingen Genomics Laboratory | | Unpublished 2010-09-10 | Liebl,W |
| Gc01377 | Dickeya dadantii 3937 | B | PROTEOBACTERIA-GAMMA Taxonomy Entrez Plant Pathogen Article | 4922 Kb | 1 | | | CP002038 | J. Craig Venter Institute Univ of Wisconsin | Univ of Wisconsin | Unpublished 2010-09-10 | Perna N |

PROJECT TYPE DISTRIBUTION

SEQUENCING STATUS DISTRIBUTION

PHYLOGENETIC DISTRIBUTION

Problémy bioinformatických databází

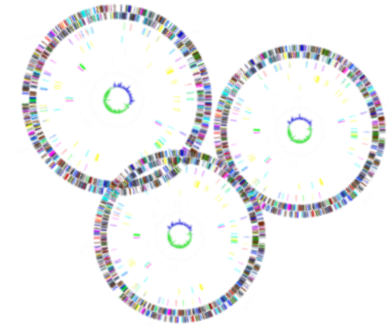


- ❑ Vysoká **redundance** dat
- ❑ **Chyby** v sekvencích
- ❑ **Chyby** a nepřesnosti v anotacích
- ❑ Propagace **chyb** během automatických anotací

Prohledávání databází

- ❑ Textové prohledávání
- ❑ Sekvenční prohledávání

vložení dat



prohledání databáze

NCBI Entrez, The Life Sciences Search Engine

HOME SEARCH SITE MAP PubMed All Databases Human Genome GenBank Map Viewer BLAST

Search across databases GO CLEAR Help

| | | | |
|------|--|------|--|
| 44 | PubMed: biomedical literature citations and abstracts | none | Books: online books |
| 79 | PubMed Central: free, full text journal articles | none | OMIM: online Mendelian Inheritance |
| none | Site Search: NCBI web and FTP sites | none | OMIA: Online Mendelian Inheritance |
| 45 | Nucleotide: sequence database (includes GenBank) | none | UniGene: gene-oriented clusters of sequences |
| 39 | Protein: sequence database | none | CDD: conserved protein domain data |
| 4 | Genome: whole genome sequences | 12 | 3D Domains: domains from Entrez |
| 12 | Structure: three-dimensional macromolecular structures | none | UniSTS: markers and mapping data |

1: [ABI93216](#). Report: LinB [Xanthomonas...[gi:115291795]]
>gi|115291795|gb|ABI93216.1| LinB [Xanthomonas sp. ICHL2]
MILG&NPFGENQFIIEIKGRM&YIDEQTDLPILFQHG&NPTS&SL&NRNIMPH&C&GL&GLI&CDLI&MGD&D
KLD&P&GPER&TY&A&HR&D&LD&L&M&E&ALD&L&D&R&V&L&V&H&D&G&V&L&G&F&D&A&R&R&R&E&V&Q&G&I&A&M&E&A&V&M&P&L&E&D
A&D&F&E&Q&R&D&L&F&Q&A&F&S&Q&G&E&L&V&L&Q&D&M&F&V&E&Q&L&P&G&L&L&R&E&L&S&E&A&M&A&Y&R&E&P&L&A&G&E&A&R&R&P&L&J&O&P&R&Q
I&P&I&A&G&T&P&A&D&V&A&I&A&R&D&A&G&L&S&E&S&P&I&P&K&L&F&I&N&E&P&G&L&T&G&M&R&D&F&C&T&W&P&M&Q&T&E&I&T&V&A&G&A&F&I&Q&E&S&P&D
E&I&G&A&I&A&F&V&K&R

2: [AAR05978](#). Report: LinB [Sphingomonas...[gi:37963683]]
>gi|37963683|gb|AAR05978.1| LinB [Sphingomonas paucimobilis]
MSL&A&M&P&F&G&E&N&Q&F&I&E&I&K&G&R&M&A&Y&I&D&E&Q&T&D&L&P&I&L&F&Q&H&G&N&P&T&S&S&L&M&R&N&I&M&P&H&C&A&G&L&G&L&I&A&C&D&L&I&M&G&D&S&D
KLD&P&G&P&E&R&T&Y&A&E&H&R&D&L&D&A&M&E&A&L&D&L&D&R&V&L&V&H&D&G&V&L&G&F&D&A&R&R&R&E&V&Q&G&I&A&M&E&A&V&M&P&L&E&D
A&D&F&E&Q&R&D&L&F&Q&A&F&S&Q&G&E&L&V&L&Q&D&M&F&V&E&Q&L&P&G&L&L&R&E&L&S&E&A&M&A&Y&R&E&P&L&A&G&E&A&R&R&P&L&J&O&P&R&Q
I&P&I&A&G&T&P&A&D&V&A&I&A&R&D&A&G&L&S&E&S&P&I&P&K&L&F&I&N&E&P&G&L&T&G&M&R&D&F&C&T&W&P&M&Q&T&E&I&T&V&A&G&A&F&I&Q&E&S&P&D
E&I&G&A&I&A&F&V&K&R&L&P&A

Textové prohledávání databází



- ❑ Entrez
- ❑ SRS
- ❑ DBGET

- ❑ **Integrují** data z různých databází
- ❑ Umožňují prohledání mnoha databází **současně**
- ❑ Umožňují formulaci dotazů pomocí **logických operátorů**

Textové prohledávání databází



□ Entrez

- Vyhledávací systém pro databáze **NCBI**
- Integruje data ze 40 různých databází, **pouze NCBI**

NCBI

Entrez, The Life Sciences Search Engine

HOME | SEARCH | SITE MAP | PubMed | All Databases | Human Genome | GenBank | Map Viewer | BLAST

Search across databases [Help](#)

| | | | | | | | |
|------|--|--|--|------|--|--|--|
| 44 | | PubMed: biomedical literature citations and abstracts | | none | | Books: online books | |
| 79 | | PubMed Central: free, full text journal articles | | none | | OMIM: online Mendelian Inheritance in Man | |
| none | | Site Search: NCBI web and FTP sites | | none | | OMIA: Online Mendelian Inheritance in Animals | |
| 45 | | Nucleotide: sequence database (includes GenBank) | | none | | UniGene: gene-oriented clusters of transcript sequences | |
| 39 | | Protein: sequence database | | none | | CDD: conserved protein domain database | |
| 4 | | Genome: whole genome sequences | | 12 | | 3D Domains: domains from Entrez Structure | |

Textové prohledávání databází



□ SRS

- Vyhledávací systém pro databáze **EBI**
- Umožňuje prohledávat i databáze **jiných** institucí, databáze **uživatelů** či databáze **výsledků** vybraných výpočetních nástrojů

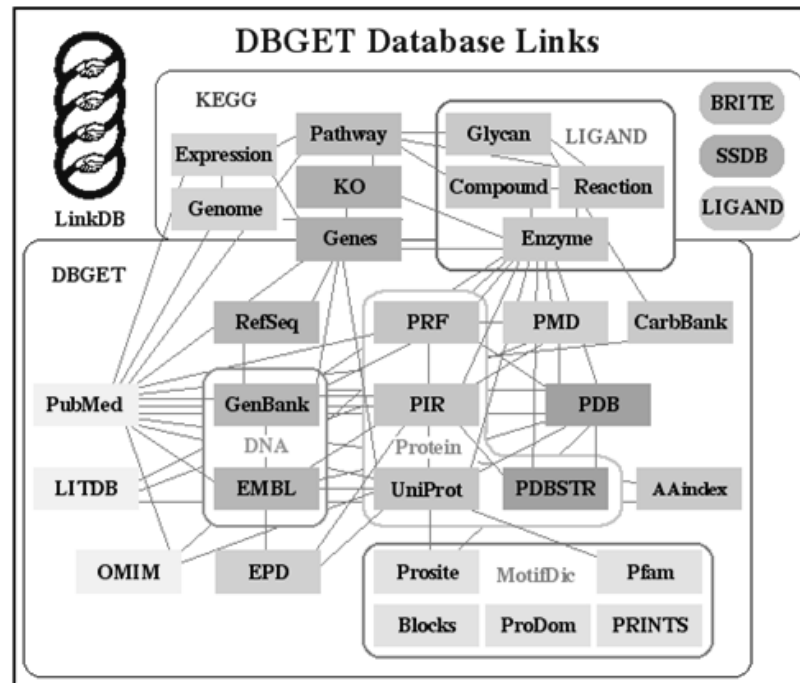
The screenshot shows the EMBL-EBI SRS search interface. At the top, there is a navigation bar with the EMBL-EBI logo, 'EB-eye Search', a dropdown menu set to 'All Databases', a search input field containing 'Enter Text Here', a 'Go' button, a 'Reset ? Advanced Search' link, and a 'Give us feedback' button. Below this is a secondary navigation bar with links for 'Databases', 'Tools', 'EBI Groups', 'Training', 'Industry', 'About Us', 'Help', 'Site Index', and social media icons. A third bar contains tabs for 'Quick Search', 'Library Page', 'Query Form', 'Tools', 'Results', 'Projects', 'Views', and 'Databanks'. The main content area features the 'SRS' logo and a link to 'Start a Permanent Project'. A 'Quick Text Search' section is highlighted, containing a 'Find' dropdown menu set to 'Nucleotides', a 'matching' label, and a search input field with 'Enter Text Here'. A 'Search Tips' link is also present.

Textové prohledávání databází



□ DBGET

- Vyhledávací systém pro databáze **LinkDB**
- Umožňuje mj. prohledávat databázi **metabolických drah KEGG**



Ukázka textového prohledávání

□ Vyhledávání na základě klíčových slov

Search across databases [Help](#)

■ - Result counts displayed in gray indicate one or more terms not found

| | | |
|-------------|---|---|
| 1258 | PubMed: biomedical literature citations and abstracts | Books: online books |
| 312 | PubMed Central: free, full text journal articles | 703 OMIM: online Mendelian Inheritance in Man |
| 4 | Site Search: NCBI web and FTP sites | none OMIA: online Mendelian Inheritance in Animals |
| 152 | Nucleotide: Core subset of nucleotide sequence records | none dbGaP: genotype and phenotype |
| | 1 EST: Expressed Sequence Tag records | 1 UniGene: gene-oriented clusters of transcript sequences |
| | 12 GSS: Genome Survey Sequence records | none CDD: conserved protein domain database |
| 96 | 96 Protein: sequence database | none 3D Domains: domains from Entrez Structure |

Ukázka sekvenčního prohledávání

□ Vyhledávání na základě sekvenční podobnosti

```
>gb|AAT70109.1 CurN [Lyngbya majuscula]  
Length=341
```

```
Score = 303 bits (777), Expect = 8e-81, Method: Composition-based stats.  
Identities = 148/297 (49%), Positives = 188/297 (63%), Gaps = 8/297 (2%)
```

```
Query 2 SEIGTGFPPDPHYVEVLGERMHYVDVGRDGTPLVFLFHGNPTSSYLWRNIIPHV-APSHR 60  
I + FPF VEV G + YVD G G PVLFLFHGNPTSSYLWRNIIPV A +R  
Sbjct 41 LPISSEFPFAKRTVEVEGATIAIYVDEG--SGQPVLFLFHGNPTSSYLWRNIIPYVVAAGYR 98  
  
Query 61 CIAPDLIGMGKSDKPDLDYFFDDHVRYLDAFIEALGLEEVVLVIHDWGSALGFHWAKRNP 120  
+APDLIGMG S KPD++Y DHV Y+D FI+ALGL+++VLVIHDWGS +G A+ NP  
Sbjct 99 AVAPDLIGMGDSAKPDIEYRLQDHVAYMDGFIDALGLDDMVLVIHDWGSVIGMRHARLNP 158  
  
Query 121 ERVKGCIACMEFIRPI----PTWDEWPEFARETFQAFRTADVGRELIIDQNAFIEGVLPK- 175  
+RV +A ME + P P+++ F+ RTADVG ++++D N F+E +LP+  
Sbjct 159 DRVAAVAEMEALVPPALPMPSEYAMGPQLGLPFRDLRTADVGEKMLVDGNFFVETILPEM 218  
  
Query 176 CVVRPLTEVEMDHYREPFLLKPVDRPLWRFNEIPIAGEPANIVALVEAYMNWLHQSPVP 235  
VVR L+E EM YR PF R P ++P E+PI GEPA A V WL SP+P  
Sbjct 219 GVVRSLSEAEEMAAYRAPFPTRQSRPLPTLQWPREVPIGGEPAFAEAEVLKNGEWLMA SPIP 278  
  
Query 236 KLLFWGTPGVLIPPAEAAARLAESLPNCKTVDIGPGLHYLQEDNPDLIGSEIARWLPG 292  
KLLF PG L P L+E++PN + +G G H+LQED+P LIG IA WL  
Sbjct 279 KLLFHAEPGALAPKPVVDYLSENVNLEVRVFGAGTHFLQEDHPHLIGQGIADWLR 335
```

Sequences producing significant alignments:

| | | | Score (Bits) | E Value | |
|--|--|--------------------------------------|---|---------------------|--------|
| | | sp P59336 DHAA_RHOSD | Haloalkane dehalogenase >pdb 1BN6 A Chai... | 429 | 1e-118 |
| | | sp POA3G2 DHAA_RHORH | Haloalkane dehalogenase >sp POA3G3 DHAA_... | 424 | 3e-117 |
| | | pdb 1CQW A | Chain A, Nai CocrySTALLISED With Haloalkane Dehalo... | 424 | 4e-117 |
| | | sp Q9Z0R0 DHAA_MYCSX | Haloalkane dehalogenase >emb CAA10076.1 ... | 422 | 1e-116 |
| | | gb AAV70825.1 | HT2 [Expression vector pHT2] | 415 | 1e-114 |
| | | ref YP_001675030.1 | alpha/beta hydrolase fold [Shewanella hal... | 320 | 8e-86 |
| | | ref YP_734675.1 | alpha/beta hydrolase fold [Shewanella sp. MR... | 318 | 3e-85 |
| | | ref YP_001473250.1 | alpha/beta hydrolase fold [Shewanella sed... | 317 | 6e-85 |
| | | ref ZP_01736514.1 | alpha/beta hydrolase [Marinobacter sp. ELB... | 317 | 6e-85 |
| | | ref YP_738656.1 | alpha/beta hydrolase fold [Shewanella sp. MR... | 316 | 9e-85 |
| | | ref YP_001502590.1 | alpha/beta hydrolase fold [Shewanella pea... | 316 | 9e-85 |
| | | ref NP_717353.1 | hydrolase, alpha/beta hydrolase fold family ... | 315 | 2e-84 |
| | | ref YP_750057.1 | alpha/beta hydrolase fold [Shewanella frigid... | 315 | 2e-84 |
| | | ref YP_268879.1 | hydrolase, alpha/beta hydrolase fold family ... | 315 | 2e-84 |
| | | ref YP_001761524.1 | alpha/beta hydrolase fold [Shewanella woo... | 315 | 3e-84 |
| | | ref ZP_01841154.1 | alpha/beta hydrolase fold [Shewanella bait... | 315 | 3e-84 |
| | | ref YP_870347.1 | alpha/beta hydrolase fold [Shewanella sp. AN... | 314 | 4e-84 |
| | | ref YP_129676.1 | putative haloalkane dehalogenase [Photobacte... | 314 | 7e-84 |
| | | ref ZP_01221858.1 | putative haloalkane dehalogenase [Photobac... | 313 | 8e-84 |
| | | ref YP_001365757.1 | alpha/beta hydrolase fold [Shewanella bal... | 313 | 9e-84 |
| | | ref YP_562379.1 | alpha/beta hydrolase fold [Shewanella denitr... | 313 | 9e-84 |
| | | ref ZP_01897865.1 | putative haloalkane dehalogenase [Moritell... | 313 | 1e-83 |
| | | ref YP_001049934.1 | alpha/beta hydrolase fold [Shewanella bal... | 313 | 1e-83 |
| | | ref YP_943362.1 | alpha/beta hydrolase fold [Psychromonas ingr... | 313 | 1e-83 |
| | | ref YP_001182970.1 | alpha/beta hydrolase fold [Shewanella put... | 312 | 2e-83 |
| | | ref YP_001554014.1 | alpha/beta hydrolase fold [Shewanella bal... | 312 | 2e-83 |
| | | ref ZP_01706252.1 | alpha/beta hydrolase fold [Shewanella putr... | 310 | 7e-83 |
| | | ref YP_964030.1 | alpha/beta hydrolase fold [Shewanella sp. W3... | 310 | 9e-83 |
| | | ref YP_510562.1 | haloalkane dehalogenase [Jannaschia sp. CCS1... | 308 | 3e-82 |
| | | ref ZP_01216824.1 | hydrolase, alpha/beta hydrolase fold famil... | 307 | 8e-82 |
| | | ref YP_001093840.1 | alpha/beta hydrolase fold [Shewanella loi... | 306 | 1e-81 |
| | | ref NP_106032.1 | haloalkane dehalogenase [Mesorhizobium loti ... | 303 | 8e-81 |
| | | gb AAT70109.1 | CurN [Lyngbya majuscula] | 303 | 8e-81 |
| | | ref ZP_01055470.1 | haloalkane dehalogenase [Roseobacter sp. M... | 303 | 1e-80 |
| | | ref ZP_01617455.1 | haloalkane dehalogenase [marine gamma prot... | 302 | 2e-80 |
| | | ref ZP_01592200.1 | alpha/beta hydrolase fold [Geobacter lovle... | 300 | 7e-80 |
| | | ref ZP_01911259.1 | alpha/beta hydrolase [Plesiocystis pacific... | 300 | 9e-80 |
| | | ref YP_001230772.1 | alpha/beta hydrolase fold [Geobacter uran... | 300 | 9e-80 |

Problémy prohledávání databází



□ Textové vyhledávání

- ☹ chybné, nepřesné či obecné anotace
- ☹ synonyma
- ☹ velký počet falešně pozitivních a falešně negativních výsledků

□ Sekvenční vyhledávání

- ☹ podmínka evoluční příbuznosti
- ☹ větší nároky na uživatele
- ☹ potenciálně falešně pozitivní i falešně negativní výsledky

□ Vhodné je oba přístupy **kombinovat**

Reference

- ❑ Claverie, J-M., & Notredame, C. (2006) **Bioinformatics for Dummies** (2nd ed.) Wiley Publishing, Hoboken, p. 436.
- ❑ Xiong, J. (2006) **Essential Bioinformatics**, Cambridge University Press, New York, p. 352.

- ❑ **ENTREZ tutorial:** <http://www.ncbi.nlm.nih.gov/Entrez/tutor.html>
- ❑ **SRS documentation:** <http://srs.ebi.ac.uk/srs/doc/index.html>
- ❑ **NCBI handbook:** <http://www.ncbi.nlm.nih.gov/books/NBK21101/>
- ❑ **UniProtKB manual:** <http://www.uniprot.org/manual/>

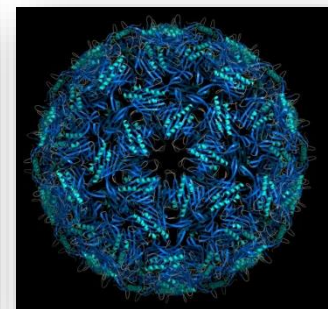
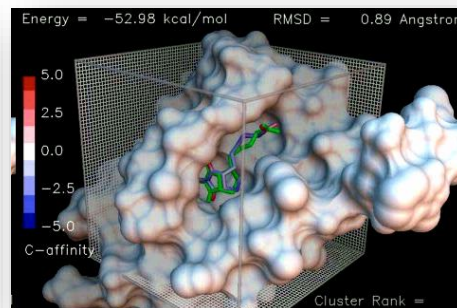
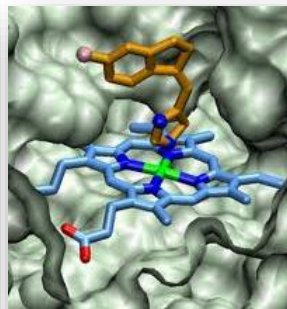
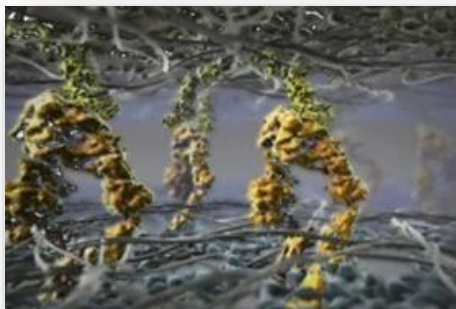
- ❑ **NCBI:** <http://www.ncbi.nlm.nih.gov/>
- ❑ **EBI:** <http://www.ebi.ac.uk/>
- ❑ **Pubmed:** <http://www.ncbi.nlm.nih.gov/pubmed>
- ❑ **Web of Science:** <http://apps.isiknowledge.com>

Reference

- ❑ **GenBank:** <http://www.ncbi.nlm.nih.gov/genbank/>
- ❑ **EMBL-EBI:** <http://www.ebi.ac.uk/embl/>
- ❑ **DDBJ:** <http://www.ddbj.nig.ac.jp/>
- ❑ **UniProt:** <http://www.uniprot.org/>
- ❑ **nrdb:** <http://www.ncbi.nlm.nih.gov/protein/>
- ❑ **wwPDB:** <http://www.wwpdb.org/>
- ❑ **Entrez Genome:** <http://www.ncbi.nlm.nih.gov/genome>
- ❑ **Ensembl:** <http://www.ensembl.org>
- ❑ **GOLD:** <http://www.genomesonline.org/>
- ❑ **Entrez:** <http://www.ncbi.nlm.nih.gov/sites/gquery>
- ❑ **SRS:** <http://srs.ebi.ac.uk>
- ❑ **DBGET:** <http://www.genome.jp/dbget/>

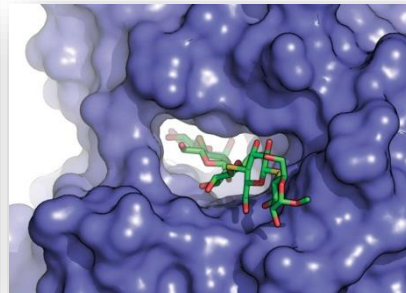
Strukturní biologie Bi9410+9410c

- Období: podzim
- Rozsah: přednáška 2 hodiny/týden, cvičení 2 hodiny/týden
- Vyučující: Mgr. Jan Brezovský, Ph.D.
- Osnova:
 - struktura, stabilita a dynamika biologických makromolekul
 - makromolekulární interakce a komplexy
 - stanovení a předpověď struktury, identifikace důležitých oblastí
 - stanovení vlivu mutace na strukturu a funkci proteinu
 - aplikace v biologickém výzkumu, návrhu léčiv a biokatalyzátorů



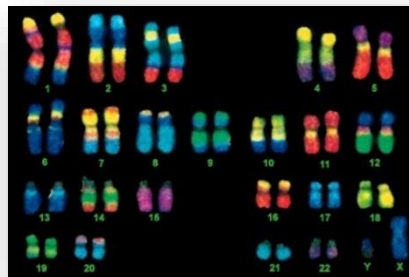
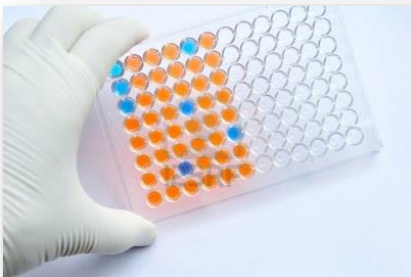
Proteinové inženýrství Bi7410

- Období: jaro
- Rozsah: přednáška 1 hodina/týden
- Vyučující: Mgr. Radka Chaloupková, Ph.D.
- Osnova:
 - **strukturně-funkční vztahy proteinů**
 - **metody exprese a purifikace rekombinantních proteinů**
 - **metody strukturní a funkční analýzy proteinů**
 - **racionální design, semi-racionální design a řízená evoluce**
 - **příklady využití proteinového inženýrství**



Molekulární biotechnologie Bi7430

- Období: podzim (každoročně)
- Rozsah: přednáška 2 hodiny/týden, cvičení 2 hodiny/týden
- Přednášky: Doc. Prokop, Dr. Dvořák, Dr. Bidmanová
- Cvičení: Dr. Bidmanová, Dr. Beerens, Dr. Štěpánková, Mgr. Buryška, Mgr. Chrást
- Osnova:
 - **proteinové a metabolické inženýrství**
 - **molekulární diagnostika a moderní vakcíny**
 - **buněčná a genová terapie a regenerativní medicína**
 - **molekulární biotechnologie v průmyslu a zemědělství**



Mikrobiologické exkurze Bi6161

- Období: jaro
- Rozsah: 4 dvou až pěti hodinové exkurze
- Vyučující: Mgr. Šárka Bidmanová, Ph.D.
- Exkurze:
 - Pivovar Starobrnno – <http://www.starobrnno.cz/>
 - Erba Lachema – <https://www.eralachema.com/>
 - Čistírna odpadních vod – <http://www.vodarenska.cz/>
 - Kompostárna – <http://www.kompostarna-blansko.cz/>



Biotechnologické exkurze Bi7171

- Období: podzim
- Rozsah: 4 jednodenní exkurze (8.2.-11.2.2015)
- Vyučující: Mgr. Šárka Bidmanová, Ph.D.
- Exkurze:
 - [Biotechnologické centrum INBIT](http://www.jic.cz/inbit) – www.jic.cz/inbit
 - [Bioveta](http://www.bioveta.cz) – www.bioveta.cz
 - [BioVendor](http://www.biovendor.cz) – www.biovendor.cz
 - [Contipro Group](http://www.contipro.com) – www.contipro.com

