Bioinformatika és genomanalízis az orvostudományban

Keresés adatbázisokban

Cserző Miklós

2018

A mai előadás

- Szekvenciakeresés:
  - FASTA
  - BLAST család
  - HMMER
- Párhuzamos változatok a keresésre
- A keresési eredmények értékelése
- Szöveges keresés: eTBLAST
- Adatbányászat

Az adatbázis keresés jelentősége

- Össze tudunk hasonlítani két szekvenciát
- El tudjuk dönteni, hogy közös őstől származnak-e
- Tudunk illeszteni több, hasonló szekvenciát
- De hogyan találjuk meg a hasonlókat több millió szekvencia közt???

Mit keresünk?

- Keresés az annotációban
  - Kódok
  - Kulcsszavak
  - Azonosított funkciók
- Ez alapkövetelmény minden adatbázissal szemben
- Keresés a szekvenciában
- Ez a biológiai adatbázisok jellegzetessége

Hogy lehet gyorsan keresni?

- A szekvenciát feltördeljük rövid, összefüggő karakter-sorozatokra – *szavakra* (*wordsize, k-mer, k-tuple*)
- Az adatbázist indexeljük: elkészítjük a *k-merek* listáját és hozzárendeljük a helyüket
- Ezt csak egyszer kell megcsinálni
- A kereső szekvenciát is felbontjuk *k-merekre*
- És így keresünk az adatbázisban

GTCTGACAGCAGCCGCTGCAGCAGCTGCTGCTGCTACCAATGCAG
CTATTGCTGAAGCAA

GTC:1

GTCTGACAGCAGCCGCTGCAGCAGCTGCTGCTGCTACCAATGCAG
CTATTGCTGAAGCAA

GTC:1 TCT:2

GTCTGACAGCAGCCGCTGCAGCAGCTGCTGCTGCTACCAATGCAG
CTATTGCTGAAGCAA

GTC:1 TCT:2 CTG:3

GTCTGACAGCAGCCGCTGCAGCAGCTGCTGCTGCTACCAATGCAG
CTATTGCTGAAGCAA

Táblázatos forma (lookup table):

AAG:55, AAT:39, ACA:6, ACC:36, AGC:8:11:20:23:44:56, ATG:40, ATT:48, CAA:38:58, CAG:7:10:19:22:43, CCA:37, CCG:13, CGC:14, CTA:34:46, CTG:3:16:25:28:31:52, GAA:54, GAC:5, GCA:9:18:21:42:57, GCC:12, GCT:15:24:27:30:33:45:51, GTC:1, TAC:35, TAT:47, TCT:2, TGA:4:53, TGC:17:26:29:32:41:50, TTG:49

A FASTA család

- Honlap: http://fasta.bioch.virginia.edu/
- Szolgáltatás itt és az EBI oldalán is
- Letölthető Linuxra és Windowsra is
- Dokumentáció és tutorial is elérhető
- Az egyik legnépszerűbb kereső
- Az algoritmus régi, de azóta is folyamatosan fejlesztik a programot

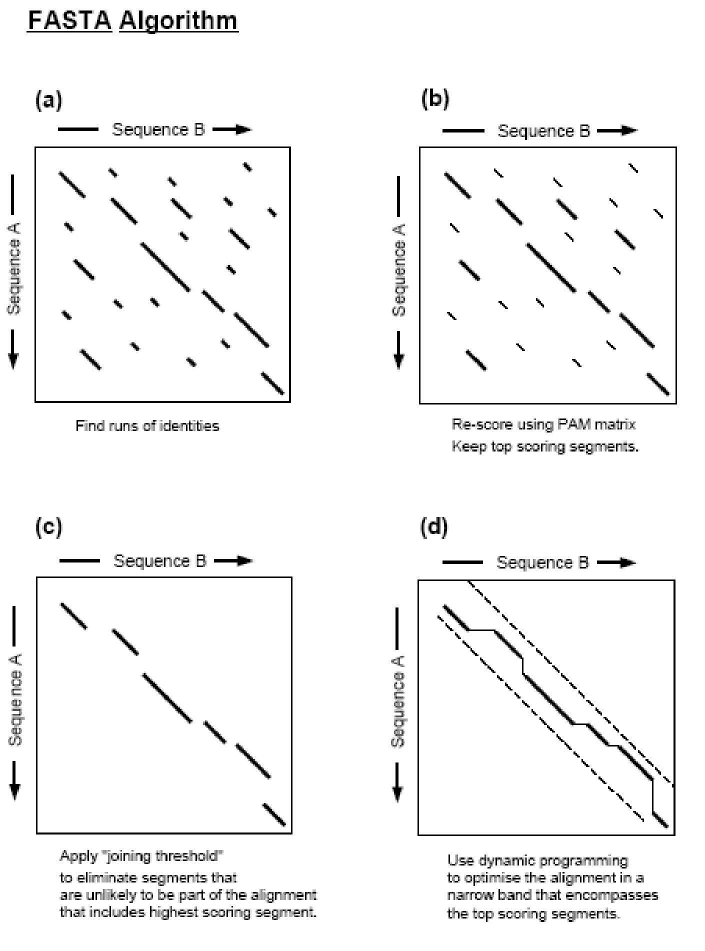
Az algoritmus négy lépése

a) Gyors keresés táblázat alapján (lookup table)

b) Pontozás mátrix alapján

c) Kiválasztás

d) S-W illesztés, végeredmény



FASTA Algorithm

Find runs of identities

Re-score using PAM matrix
Keep top scoring segments.

Apply "joining threshold"
to eliminate segments that
are unlikely to be part of the alignment
that includes highest scoring segment.

Use dynamic programming
to optimise the alignment in a
narrow band that encompasses
the top scoring segments.

A programcsalád tagjai

- A legfrissebb verzió a 3.6-os
  - „fasta”: egy szekvenciát összehasonlít egy databázis szekvenciái ellenében (fehérjét fehérjével vagy DNS-t DNS-sel), gyors algoritmust használ – táblázatos keresés
  - „ssearch”: S-W algoritmust használ a keresésre (fehérjét fehérjével vagy DNS-t DNS-sel), lassabb, de pontosabb

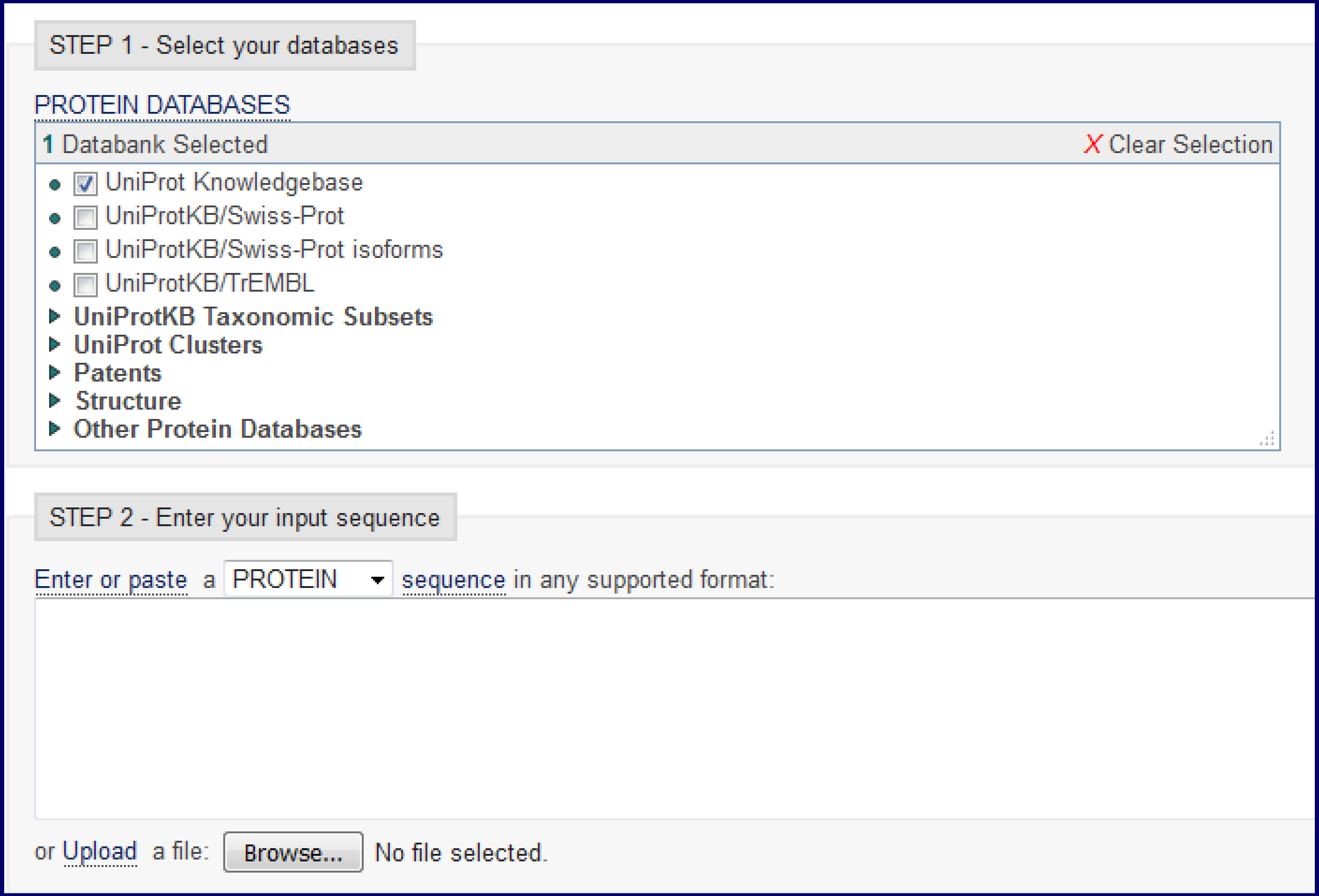
Folytatás ...

- „ggsearch”: global:global keresés (fehérje és DNS)
- „glsearch”: global:local keresés (fehérje és DNS)
- „fastx”: lefordított DNS szekvenciát keres fehérje adatbázis ellen, három frame-et fordít, toldás és frame-eltolás is megengedett
- „fasty”: mint a „fastx”, de kódonon belüli eltolás is engedett

Folytatás ...

- „tfastx”, „tfasty”: fehérje szekvenciát keres DNS adatbázis ellen
- „fastf”, „tfastf”: peptid keverék listáját keresi fehérje, illetve DNS adatbázis ellen, mintha részlegesen emésztett minta lenne
- „fasts”, „tfasts”: peptid fragmens listát keres fehérje, illetve DNS adatbázis ellen, mintha tömegspektrométerből származó minta lenne
- „lalign”: többszörös illesztő program

A FASTA felület – EBI



STEP 1 - Select your databases

PROTEIN DATABASES

1 Databank Selected — X Clear Selection

- ☑ UniProt Knowledgebase
- □ UniProtKB/Swiss-Prot
- □ UniProtKB/Swiss-Prot isoforms
- □ UniProtKB/TrEMBL
- ▸ **UniProtKB Taxonomic Subsets**
- ▸ **UniProt Clusters**
- ▸ **Patents**
- ▸ **Structure**
- ▸ **Other Protein Databases**

STEP 2 - Enter your input sequence

Enter or paste a PROTEIN ▾ sequence in any supported format:

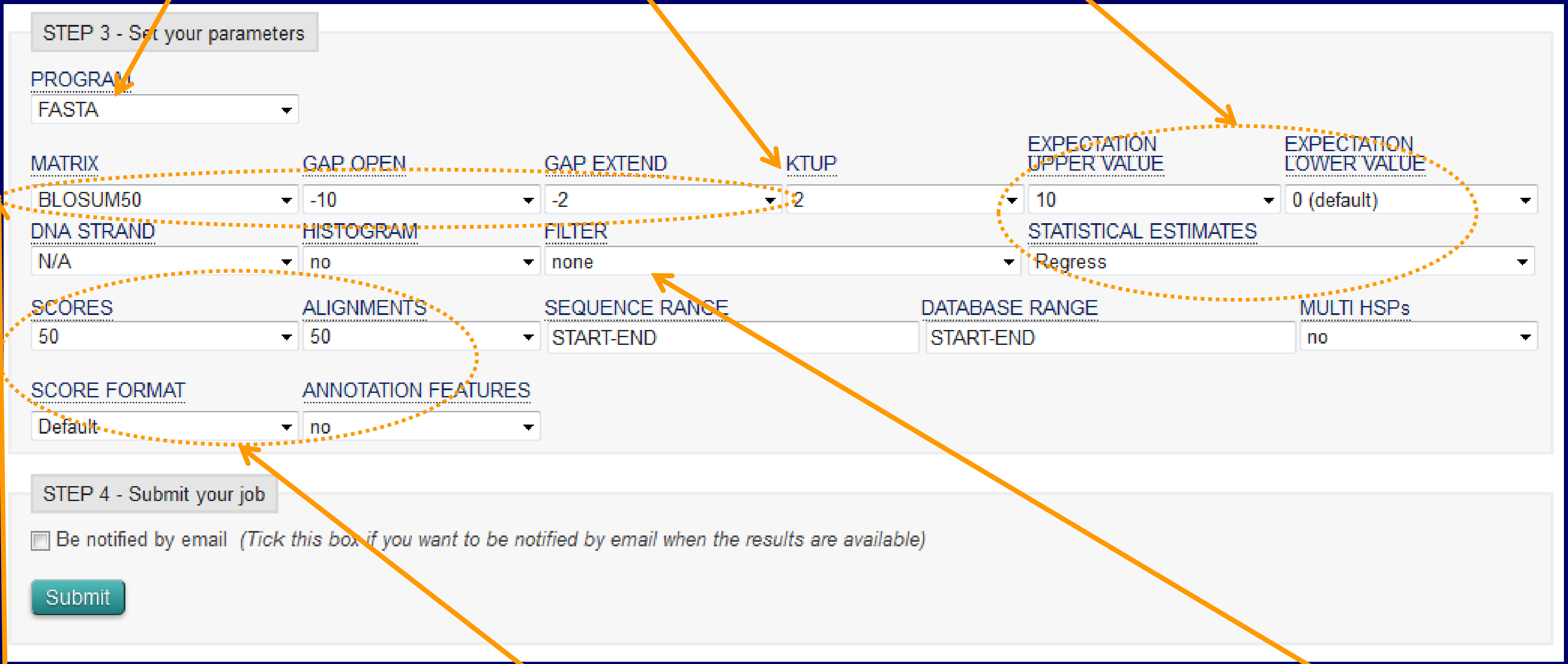
or Upload a file: Browse... No file selected.

Paraméterek

A program neve

Táblázat

Statisztika



STEP 3 - Set your parameters

PROGRAM					
FASTA					
MATRIX	GAP OPEN	GAP EXTEND	KTUP	EXPECTATION UPPER VALUE	EXPECTATION LOWER VALUE
BLOSUM50	-10	-2	2	10	0 (default)
DNA STRAND	HISTOGRAM	FILTER		STATISTICAL ESTIMATES	
N/A	no	none		Regress	
SCORES	ALIGNMENTS	SEQUENCE RANGE	DATABASE RANGE	MULTI HSPs	
50	50	START-END	START-END	no	
SCORE FORMAT	ANNOTATION FEATURES				
Default	no				

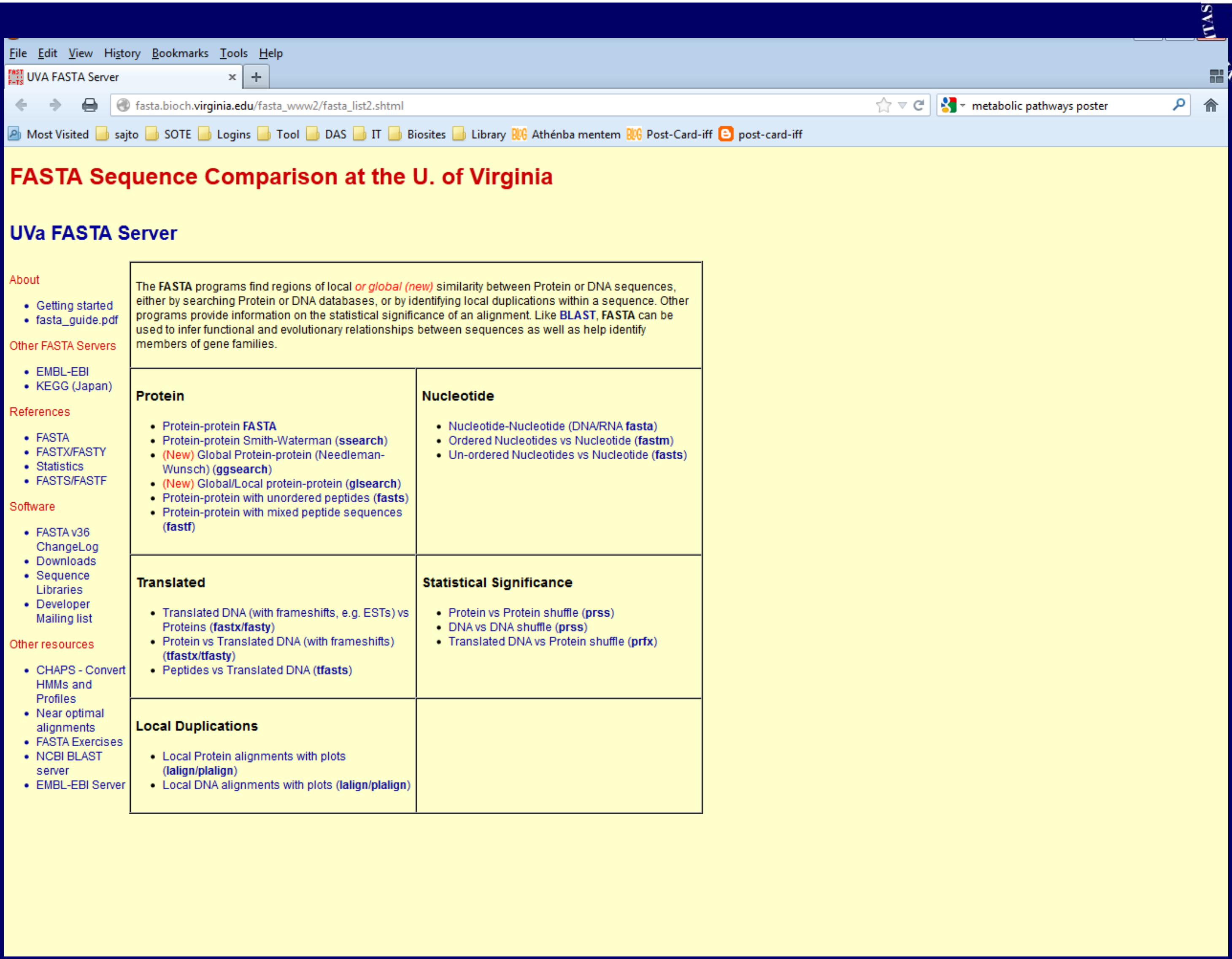
STEP 4 - Submit your job

☐ Be notified by email *(Tick this box if you want to be notified by email when the results are available)*

Mátrix paraméterek

Eredmény

Maszkolás


File Edit View History Bookmarks Tools Help
UVA FASTA Server
fasta.bioch.virginia.edu/fasta_www2/fasta_list2.shtml
metabolic pathways poster
Most Visited
sajto
SOTE
Logins
Tool
DAS
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Library
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FASTA Sequence Comparison at the U. of Virginia

UVa FASTA Server

About

- Getting started
- fasta_guide.pdf

Other FASTA Servers

- EMBL-EBI
- KEGG (Japan)

References

- FASTA
- FASTX/FASTY
- Statistics
- FASTS/FASTF

Software

- FASTA v36 ChangeLog
- Downloads
- Sequence Libraries
- Developer Mailing list

Other resources

- CHAPS - Convert HMMs and Profiles
- Near optimal alignments
- FASTA Exercises
- NCBI BLAST server
- EMBL-EBI Server

The **FASTA** programs find regions of local *or global (new)* similarity between Protein or DNA sequences, either by searching Protein or DNA databases, or by identifying local duplications within a sequence. Other programs provide information on the statistical significance of an alignment. Like **BLAST**, **FASTA** can be used to infer functional and evolutionary relationships between sequences as well as help identify members of gene families.

Protein

- Protein-protein **FASTA**
- Protein-protein Smith-Waterman (**ssearch**)
- (New) Global Protein-protein (Needleman-Wunsch) (**ggsearch**)
- (New) Global/Local protein-protein (**glsearch**)
- Protein-protein with unordered peptides (**fasts**)
- Protein-protein with mixed peptide sequences (**fastf**)

Nucleotide

- Nucleotide-Nucleotide (DNA/RNA **fasta**)
- Ordered Nucleotides vs Nucleotide (**fastm**)
- Un-ordered Nucleotides vs Nucleotide (**fasts**)

Translated

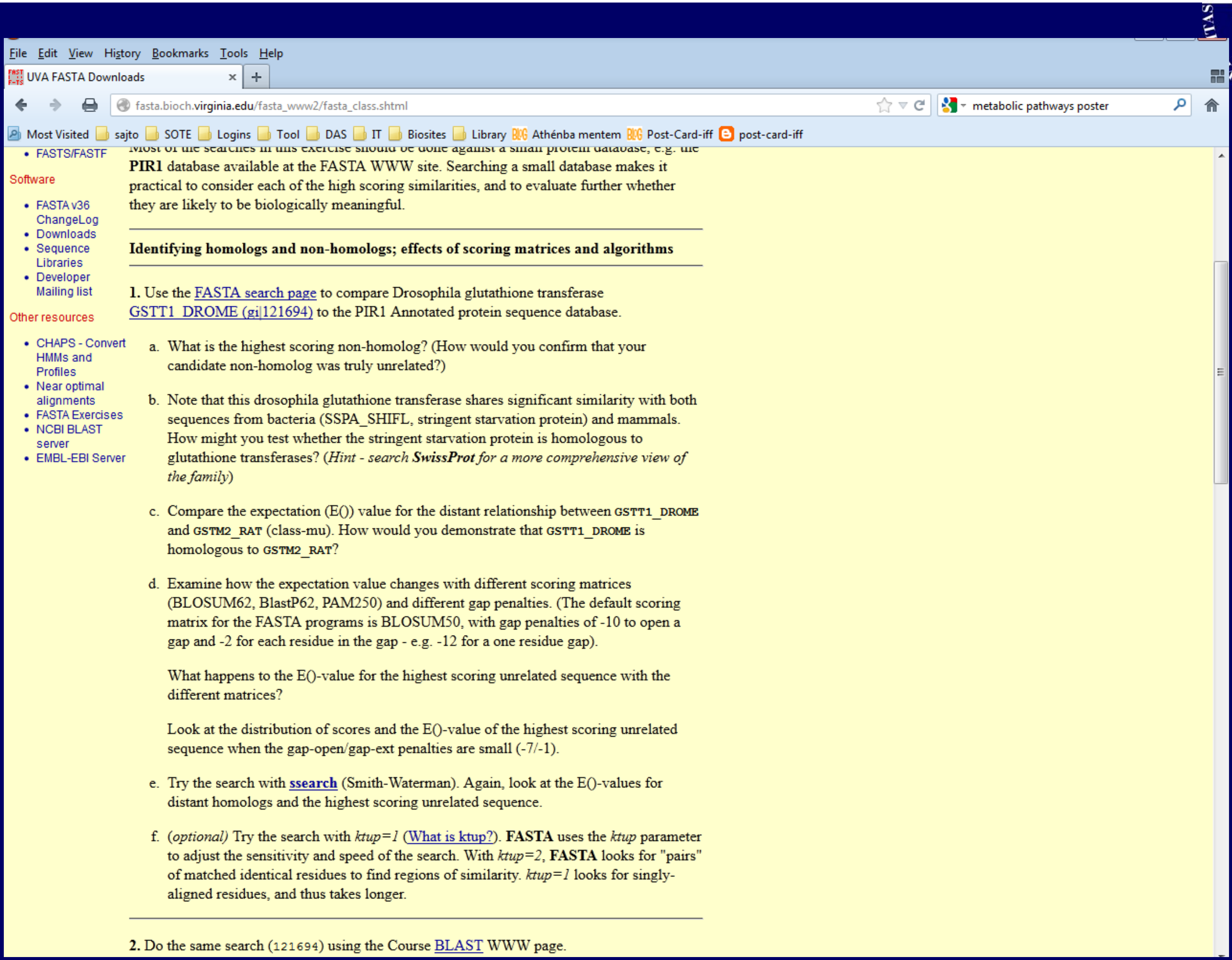
- Translated DNA (with frameshifts, e.g. ESTs) vs Proteins (**fastx**/**fasty**)
- Protein vs Translated DNA (with frameshifts) (**tfastx**/**tfasty**)
- Peptides vs Translated DNA (**tfasts**)

Statistical Significance

- Protein vs Protein shuffle (**prss**)
- DNA vs DNA shuffle (**prss**)
- Translated DNA vs Protein shuffle (**prfx**)

Local Duplications

- Local Protein alignments with plots (**lalign**/**plalign**)
- Local DNA alignments with plots (**lalign**/**plalign**)


File Edit View History Bookmarks Tools Help
UVA FASTA Downloads
fasta.bioch.virginia.edu/fasta_www2/fasta_class.shtml
metabolic pathways poster
Most Visited
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SOTE
Logins
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Biosites
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- FASTS/FASTF

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Most of the searches in this exercise should be done against a small protein database, e.g. the **PIR1** database available at the FASTA WWW site. Searching a small database makes it practical to consider each of the high scoring similarities, and to evaluate further whether they are likely to be biologically meaningful.

Identifying homologs and non-homologs; effects of scoring matrices and algorithms

1. Use the FASTA search page to compare Drosophila glutathione transferase GSTT1_DROME (gi|121694) to the PIR1 Annotated protein sequence database.

a. What is the highest scoring non-homolog? (How would you confirm that your candidate non-homolog was truly unrelated?)

b. Note that this drosophila glutathione transferase shares significant similarity with both sequences from bacteria (SSPA_SHIFL, stringent starvation protein) and mammals. How might you test whether the stringent starvation protein is homologous to glutathione transferases? (*Hint - search* ***SwissProt*** *for a more comprehensive view of the family*)

c. Compare the expectation (E()) value for the distant relationship between `GSTT1_DROME` and `GSTM2_RAT` (class-mu). How would you demonstrate that `GSTT1_DROME` is homologous to `GSTM2_RAT`?

d. Examine how the expectation value changes with different scoring matrices (BLOSUM62, BlastP62, PAM250) and different gap penalties. (The default scoring matrix for the FASTA programs is BLOSUM50, with gap penalties of -10 to open a gap and -2 for each residue in the gap - e.g. -12 for a one residue gap).

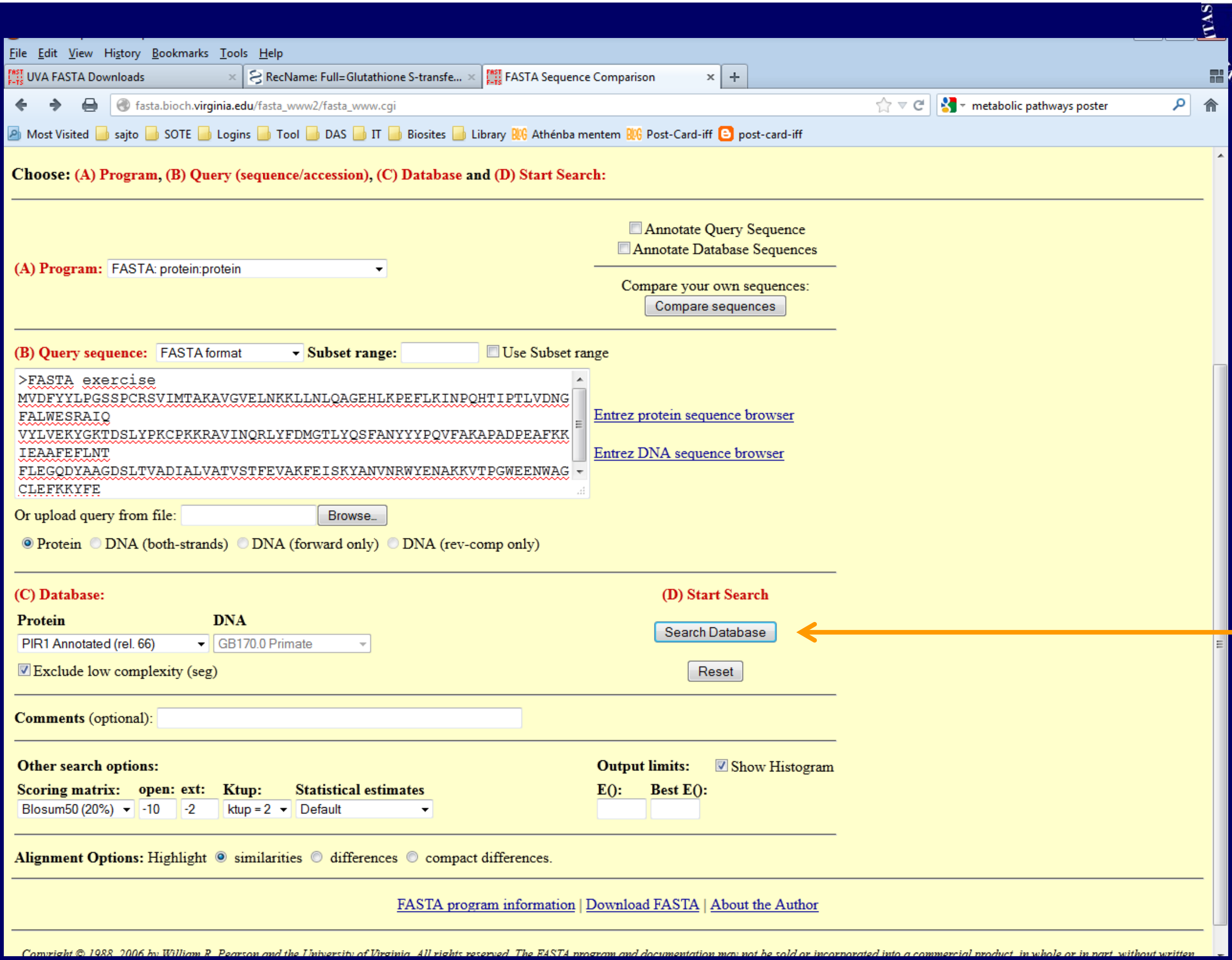
What happens to the E()-value for the highest scoring unrelated sequence with the different matrices?

Look at the distribution of scores and the E()-value of the highest scoring unrelated sequence when the gap-open/gap-ext penalties are small (-7/-1).

e. Try the search with **ssearch** (Smith-Waterman). Again, look at the E()-values for distant homologs and the highest scoring unrelated sequence.

f. (*optional*) Try the search with *ktup=1* (What is ktup?). **FASTA** uses the *ktup* parameter to adjust the sensitivity and speed of the search. With *ktup=2*, **FASTA** looks for "pairs" of matched identical residues to find regions of similarity. *ktup=1* looks for singly-aligned residues, and thus takes longer.

2. Do the same search (`121694`) using the Course BLAST WWW page.


File Edit View History Bookmarks Tools Help
UVA FASTA Downloads
RecName: Full=Glutathione S-transfe...
FASTA Sequence Comparison
fasta.bioch.virginia.edu/fasta_www2/fasta_www.cgi
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post-card-iff

Choose: (A) Program, (B) Query (sequence/accession), (C) Database and (D) Start Search:

□ Annotate Query Sequence
□ Annotate Database Sequences

(A) Program: FASTA: protein:protein

Compare your own sequences:
Compare sequences

(B) Query sequence: FASTA format **Subset range:** □ Use Subset range

```
>FASTA exercise
MVDFYYLPGSSPCRSVIMTAKAVGVELNKKLLNLQAGEHLKPEFLKINPQHTIPTLVDNG
FALWESRAIQ
VYLVEKYGKTDSLYPKCPKKRAVINQRLYFDMGTLYQSFANYYYPQVFAKAPADPEAFKK
IEAAFEFLNT
FLEGQDYAAGDSLTVADIALVATVSTFEVAKFEISKYANVNRWYENAKKVTPGWEENWAG
CLEFKKYFE
```

Entrez protein sequence browser

Entrez DNA sequence browser

Or upload query from file: Browse...

● Protein ○ DNA (both-strands) ○ DNA (forward only) ○ DNA (rev-comp only)

(C) Database:

Protein: PIR1 Annotated (rel. 66)
DNA: GB170.0 Primate

☑ Exclude low complexity (seg)

(D) Start Search

Search Database

Reset

Comments (optional):

Other search options:

Scoring matrix: Blosum50 (20%) **open:** -10 **ext:** -2 **Ktup:** ktup = 2 **Statistical estimates** Default

Output limits: ☑ Show Histogram

E(): **Best E():**

Alignment Options: Highlight ● similarities ○ differences ○ compact differences.

FASTA program information | Download FASTA | About the Author

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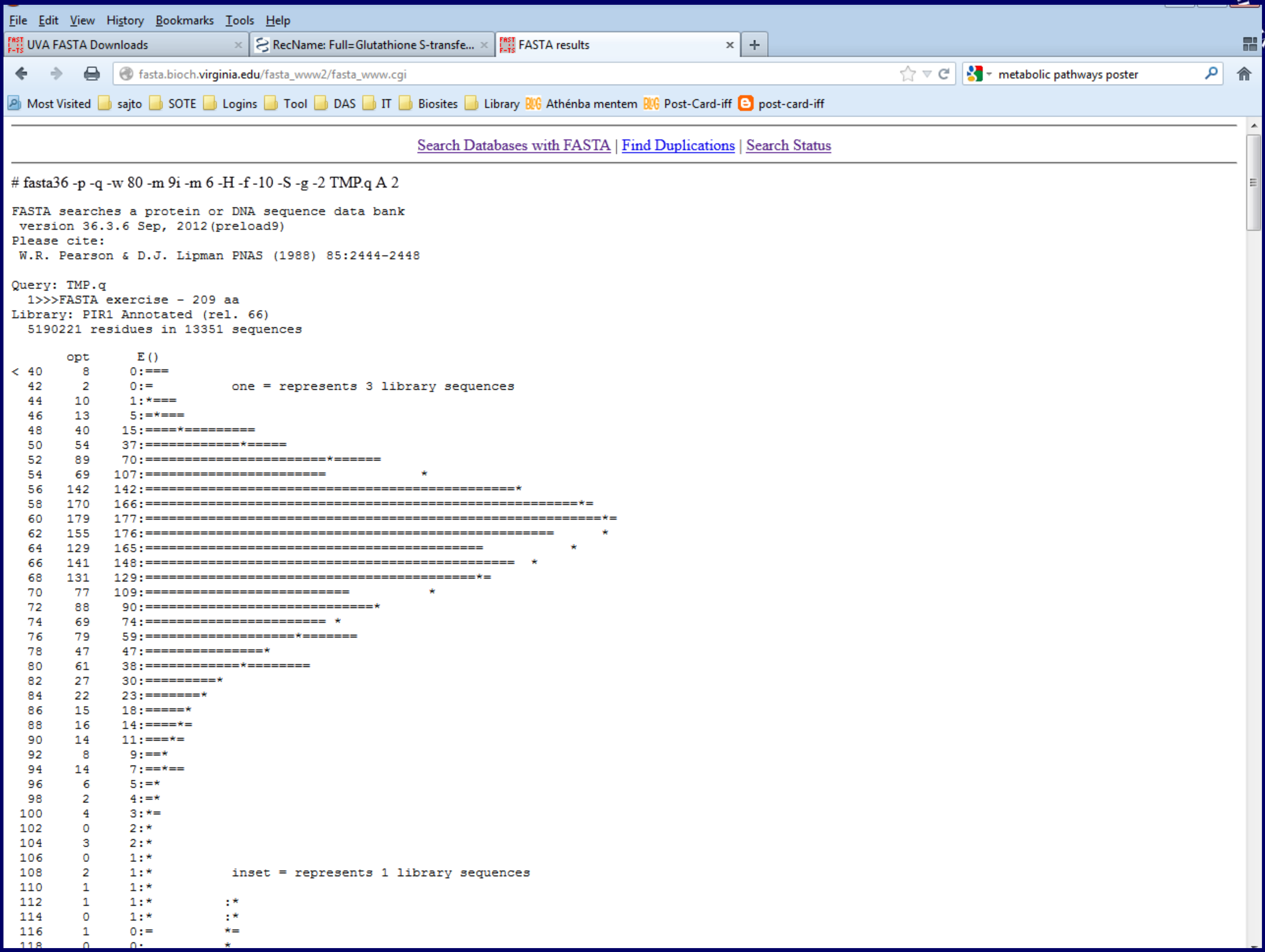

File Edit View History Bookmarks Tools Help
UVA FASTA Downloads
RecName: Full=Glutathione S-transfe...
FASTA results
fasta.bioch.virginia.edu/fasta_www2/fasta_www.cgi
metabolic pathways poster
Most Visited
sajto
SOTE
Logins
Tool
DAS
IT
Biosites
Library
Athénba mentem
Post-Card-iff
post-card-iff

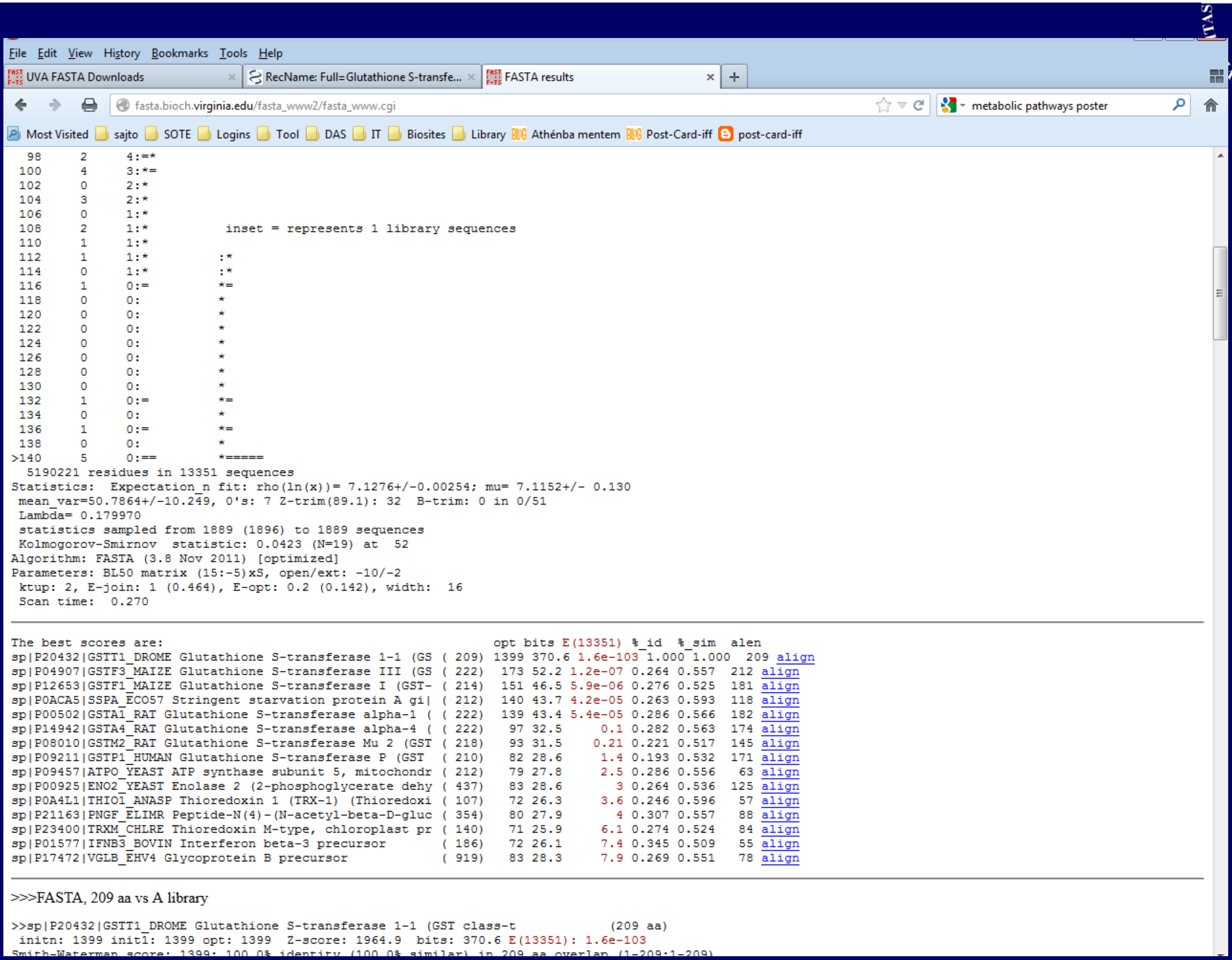
Search Databases with FASTA | Find Duplications | Search Status

```
# fasta36 -p -q -w 80 -m 9i -m 6 -H -f -10 -S -g -2 TMP.q A 2

FASTA searches a protein or DNA sequence data bank
 version 36.3.6 Sep, 2012(preload9)
Please cite:
 W.R. Pearson & D.J. Lipman PNAS (1988) 85:2444-2448

Query: TMP.q
  1>>>FASTA exercise - 209 aa
Library: PIR1 Annotated (rel. 66)
  5190221 residues in 13351 sequences

       opt      E()
< 40     8     0:===
  42     2     0:=          one = represents 3 library sequences
  44    10     1:*===
  46    13     5:=*===
  48    40    15:====*=========
  50    54    37:============*=====
  52    89    70:=======================*======
  54    69   107:=======================            *
  56   142   142:===============================================*
  58   170   166:=======================================================*=
  60   179   177:==========================================================*=
  62   155   176:====================================================      *
  64   129   165:===========================================           *
  66   141   148:===============================================  *
  68   131   129:==========================================*=
  70    77   109:==========================          *
  72    88    90:=============================*
  74    69    74:======================= *
  76    79    59:===================*=======
  78    47    47:===============*
  80    61    38:============*========
  82    27    30:=========*
  84    22    23:=======*
  86    15    18:=====*
  88    16    14:====*=
  90    14    11:===*=
  92     8     9:==*
  94    14     7:==*==
  96     6     5:=*
  98     2     4:=*
 100     4     3:*=
 102     0     2:*
 104     3     2:*
 106     0     1:*
 108     2     1:*          inset = represents 1 library sequences
 110     1     1:*
 112     1     1:*         :*
 114     0     1:*         :*
 116     1     0:=         *=
 118     0     0:          *
```


File Edit View History Bookmarks Tools Help
UVA FASTA Downloads
RecName: Full=Glutathione S-transfe...
FASTA results
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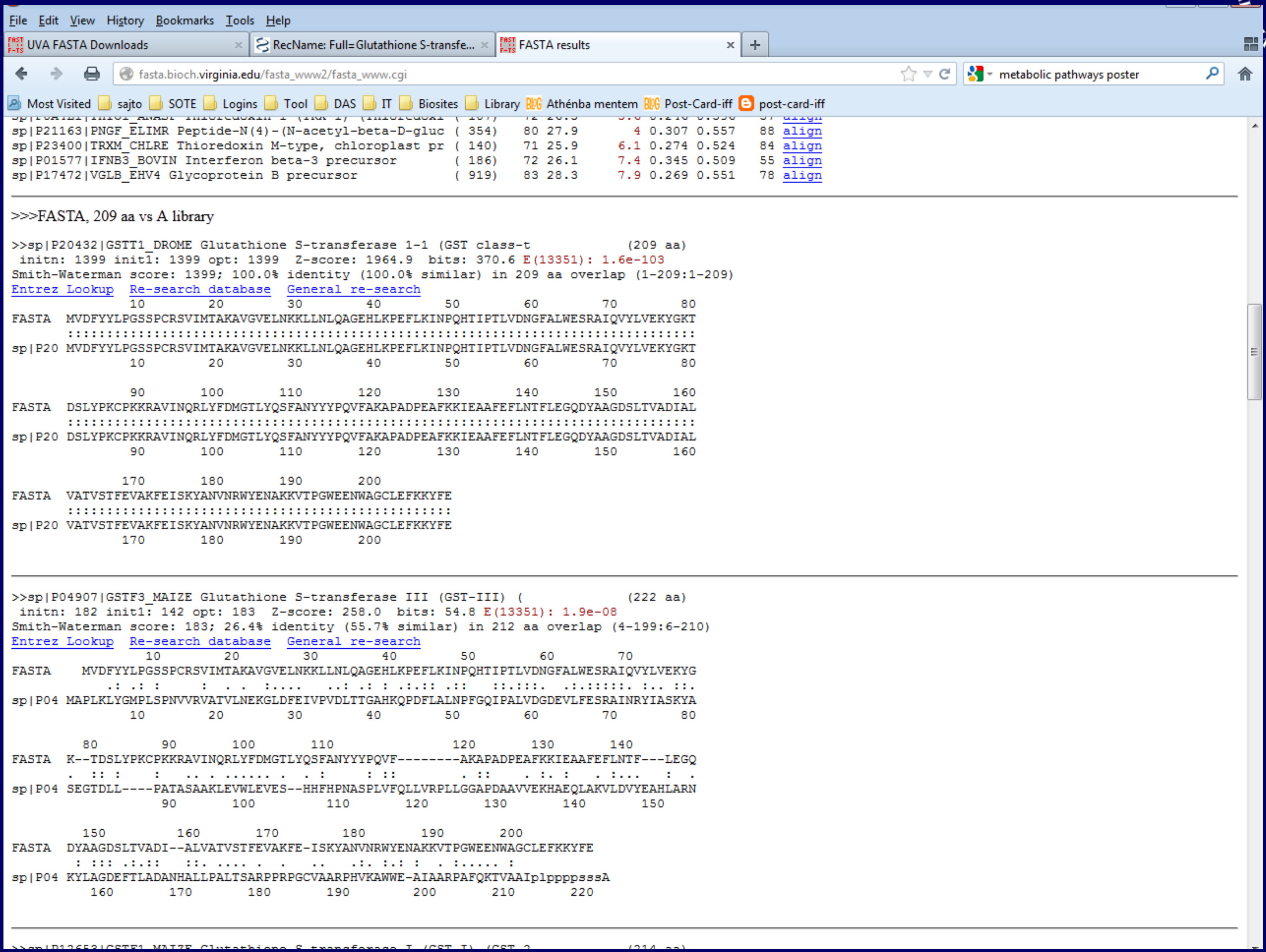
Post-Card-iff
post-card-iff

```
  98      2       4:=*
 100      4       3:*=
 102      0       2:*
 104      3       2:*
 106      0       1:*
 108      2       1:*          inset = represents 1 library sequences
 110      1       1:*
 112      1       1:*         :*
 114      0       1:*         :*
 116      1       0:=         *=
 118      0       0:          *
 120      0       0:          *
 122      0       0:          *
 124      0       0:          *
 126      0       0:          *
 128      0       0:          *
 130      0       0:          *
 132      1       0:=         *=
 134      0       0:          *
 136      1       0:=         *=
 138      0       0:          *
>140      5       0:==        *======
  5190221 residues in 13351 sequences
Statistics:  Expectation_n fit: rho(ln(x))= 7.1276+/-0.00254; mu= 7.1152+/- 0.130
 mean_var=50.7864+/-10.249, 0's: 7 Z-trim(89.1): 32  B-trim: 0 in 0/51
 Lambda= 0.179970
 statistics sampled from 1889 (1896) to 1889 sequences
 Kolmogorov-Smirnov  statistic: 0.0423 (N=19) at  52
Algorithm: FASTA (3.8 Nov 2011) [optimized]
Parameters: BL50 matrix (15:-5)xS, open/ext: -10/-2
 ktup: 2, E-join: 1 (0.464), E-opt: 0.2 (0.142), width:  16
 Scan time:  0.270
```

```
The best scores are:                                      opt bits E(13351) %_id  %_sim  alen
sp|P20432|GSTT1_DROME Glutathione S-transferase 1-1 (GS ( 209) 1399 370.6 1.6e-103 1.000 1.000  209 align
sp|P04907|GSTF3_MAIZE Glutathione S-transferase III (GS ( 222)  173 52.2 1.2e-07 0.264 0.557  212 align
sp|P12653|GSTF1_MAIZE Glutathione S-transferase I (GST- ( 214)  151 46.5 5.9e-06 0.276 0.525  181 align
sp|P0ACA5|SSPA_ECO57 Stringent starvation protein A gi| ( 212)  140 43.7 4.2e-05 0.263 0.593  118 align
sp|P00502|GSTA1_RAT Glutathione S-transferase alpha-1 ( ( 222)  139 43.4 5.4e-05 0.286 0.566  182 align
sp|P14942|GSTA4_RAT Glutathione S-transferase alpha-4 ( ( 222)   97 32.5     0.1 0.282 0.563  174 align
sp|P08010|GSTM2_RAT Glutathione S-transferase Mu 2 (GST ( 218)   93 31.5    0.21 0.221 0.517  145 align
sp|P09211|GSTP1_HUMAN Glutathione S-transferase P (GST  ( 210)   82 28.6     1.4 0.193 0.532  171 align
sp|P09457|ATPO_YEAST ATP synthase subunit 5, mitochondr ( 212)   79 27.8     2.5 0.286 0.556   63 align
sp|P00925|ENO2_YEAST Enolase 2 (2-phosphoglycerate dehy ( 437)   83 28.6       3 0.264 0.536  125 align
sp|P0A4L1|THIO1_ANASP Thioredoxin 1 (TRX-1) (Thioredoxi ( 107)   72 26.3     3.6 0.246 0.596   57 align
sp|P21163|PNGF_ELIMR Peptide-N(4)-(N-acetyl-beta-D-gluc ( 354)   80 27.9       4 0.307 0.557   88 align
sp|P23400|TRXM_CHLRE Thioredoxin M-type, chloroplast pr ( 140)   71 25.9     6.1 0.274 0.524   84 align
sp|P01577|IFNB3_BOVIN Interferon beta-3 precursor       ( 186)   72 26.1     7.4 0.345 0.509   55 align
sp|P17472|VGLB_EHV4 Glycoprotein B precursor            ( 919)   83 28.3     7.9 0.269 0.551   78 align
```

>>>FASTA, 209 aa vs A library

```
>>sp|P20432|GSTT1_DROME Glutathione S-transferase 1-1 (GST class-t          (209 aa)
 initn: 1399 init1: 1399 opt: 1399  Z-score: 1964.9  bits: 370.6 E(13351): 1.6e-103
Smith-Waterman score: 1399; 100.0% identity (100.0% similar) in 209 aa overlap (1-209:1-209)
```


File Edit View History Bookmarks Tools Help
UVA FASTA Downloads
RecName: Full=Glutathione S-transfe...
FASTA results
fasta.bioch.virginia.edu/fasta_www2/fasta_www.cgi
metabolic pathways poster
Most Visited
sajto
SOTE
Logins
Tool
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IT
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Library
Athénba mentem
Post-Card-iff
post-card-iff

```
sp|P21163|PNGF_ELIMR Peptide-N(4)-(N-acetyl-beta-D-gluc ( 354)   80 27.9      4 0.307 0.557   88 align
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 initn: 1399 init1: 1399 opt: 1399  Z-score: 1964.9  bits: 370.6 E(13351): 1.6e-103
Smith-Waterman score: 1399; 100.0% identity (100.0% similar) in 209 aa overlap (1-209:1-209)
Entrez Lookup  Re-search database  General re-search
               10        20        30        40        50        60        70        80
FASTA  MVDFYYLPGSSPCRSVIMTAKAVGVELNKKLLNLQAGEHLKPEFLKINPQHTIPTLVDNGFALWESRAIQVYLVEKYGKT
       ::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::
sp|P20 MVDFYYLPGSSPCRSVIMTAKAVGVELNKKLLNLQAGEHLKPEFLKINPQHTIPTLVDNGFALWESRAIQVYLVEKYGKT
               10        20        30        40        50        60        70        80

               90       100       110       120       130       140       150       160
FASTA  DSLYPKCPKKRAVINQRLYFDMGTLYQSFANYYYPQVFAKAPADPEAFKKIEAAFEFLNTFLEGQDYAAGDSLTVADIAL
       ::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::
sp|P20 DSLYPKCPKKRAVINQRLYFDMGTLYQSFANYYYPQVFAKAPADPEAFKKIEAAFEFLNTFLEGQDYAAGDSLTVADIAL
               90       100       110       120       130       140       150       160

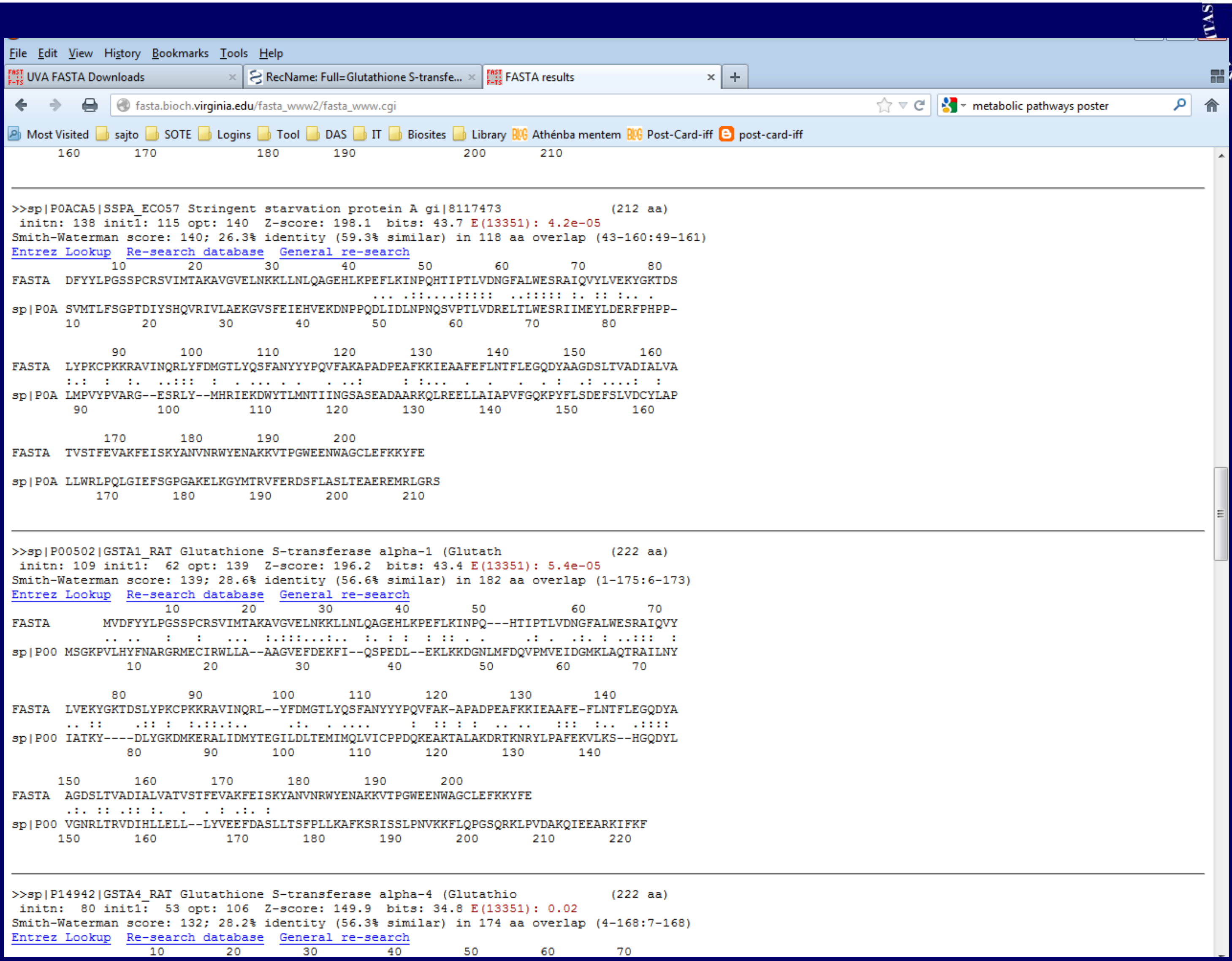
              170       180       190       200
FASTA  VATVSTFEVAKFEISKYANVNRWYENAKKVTPGWEENWAGCLEFKKYFE
       :::::::::::::::::::::::::::::::::::::::::::::::::
sp|P20 VATVSTFEVAKFEISKYANVNRWYENAKKVTPGWEENWAGCLEFKKYFE
              170       180       190       200

>>sp|P04907|GSTF3_MAIZE Glutathione S-transferase III (GST-III) (             (222 aa)
 initn: 182 init1: 142 opt: 183  Z-score: 258.0  bits: 54.8 E(13351): 1.9e-08
Smith-Waterman score: 183; 26.4% identity (55.7% similar) in 212 aa overlap (4-199:6-210)
Entrez Lookup  Re-search database  General re-search
                 10        20        30        40        50        60        70
FASTA    MVDFYYLPGSSPCRSVIMTAKAVGVELNKKLLNLQAGEHLKPEFLKINPQHTIPTLVDNGFALWESRAIQVYLVEKYG
            .: .: :     :  . .  :....   ..: .: : .:.:: .::   ::.:::.  .:.:::::. :.. ::.
sp|P04 MAPLKLYGMPLSPNVVRVATVLNEKGLDFEIVPVDLTTGAHKQPDFLALNPFGQIPALVDGDEVLFESRAINRYIASKYA
               10        20        30        40        50        60        70        80

         80        90       100       110               120       130       140
FASTA  K--TDSLYPKCPKKRAVINQRLYFDMGTLYQSFANYYYPQVF--------AKAPADPEAFKKIEAAFEFLNTF---LEGQ
       .  :: :    :   .. . ...... .  . :     : ::        . ::    . :. :   . :...   :  .
sp|P04 SEGTDLL----PATASAAKLEVWLEVES--HHFHPNASPLVFQLLVRPLLGGAPDAAVVEKHAEQLAKVLDVYEAHLARN
                  90       100         110       120       130       140       150

         150         160       170        180       190       200
FASTA  DYAAGDSLTVADI--ALVATVSTFEVAKFE-ISKYANVNRWYENAKKVTPGWEENWAGCLEFKKYFE
        : ::: .:.::   ::. .... .  .   ..   .:. :.: :  . :..... :
sp|P04 KYLAGDEFTLADANHALLPALTSARPPRPGCVAARPHVKAWWE-AIAARPAFQKTVAAIplppppsssA
          160       170       180       190        200       210       220

>>sp|P12653|GSTF1_MAIZE Glutathione S-transferase I (GST-I) (GST-2            (214 aa)
```


File Edit View History Bookmarks Tools Help
UVA FASTA Downloads
RecName: Full=Glutathione S-transfe...
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fasta.bioch.virginia.edu/fasta_www2/fasta_www.cgi
metabolic pathways poster
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SOTE
Logins
Tool
DAS
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Biosites
Library
Athénba mentem
Post-Card-iff
post-card-iff

```
      160       170             180       190              200       210

>>sp|P0ACA5|SSPA_ECO57 Stringent starvation protein A gi|8117473              (212 aa)
 initn: 138 init1: 115 opt: 140  Z-score: 198.1  bits: 43.7 E(13351): 4.2e-05
Smith-Waterman score: 140; 26.3% identity (59.3% similar) in 118 aa overlap (43-160:49-161)
Entrez Lookup  Re-search database  General re-search
             10        20        30        40        50        60        70        80
FASTA  DFYYLPGSSPCRSVIMTAKAVGVELNKKLLNLQAGEHLKPEFLKINPQHTIPTLVDNGFALWESRAIQVYLVEKYGKTDS
                                               ... .::....:::::  ..::::: :. :: :.. .
sp|P0A SVMTLFSGPTDIYSHQVRIVLAEKGVSFEIEHVEKDNPPQDLIDLNPNQSVPTLVDRELTLWESRIIMEYLDERFPHPP-
       10        20        30        40        50        60        70        80

             90       100       110       120       130       140       150       160
FASTA  LYPKCPKKRAVINQRLYFDMGTLYQSFANYYYPQVFAKAPADPEAFKKIEAAFEFLNTFLEGQDYAAGDSLTVADIALVA
       :.:  :  :.  ..:::  :  . ... . .   . ..:     : :...  .  .   .  . :  .: ....:  :
sp|P0A LMPVYPVARG--ESRLY--MHRIEKDWYTLMNTIINGSASEADAARKQLREELLAIAPVFGQKPYFLSDEFSLVDCYLAP
        90         100         110       120       130       140       150       160

            170       180       190       200
FASTA  TVSTFEVAKFEISKYANVNRWYENAKKVTPGWEENWAGCLEFKKYFE

sp|P0A LLWRLPQLGIEFSGPGAKELKGYMTRVFERDSFLASLTEAEREMRLGRS
           170       180       190       200       210

>>sp|P00502|GSTA1_RAT Glutathione S-transferase alpha-1 (Glutath              (222 aa)
 initn: 109 init1:  62 opt: 139  Z-score: 196.2  bits: 43.4 E(13351): 5.4e-05
Smith-Waterman score: 139; 28.6% identity (56.6% similar) in 182 aa overlap (1-175:6-173)
Entrez Lookup  Re-search database  General re-search
                    10        20        30        40        50           60        70
FASTA       MVDFYYLPGSSPCRSVIMTAKAVGVELNKKLLNLQAGEHLKPEFLKINPQ---HTIPTLVDNGFALWESRAIQVY
            .. ..   :   :   ...  :.:::...:..  :. : :  : :: . .     .: .  .:. : ..:::  :
sp|P00 MSGKPVLHYFNARGRMECIRWLLA--AAGVEFDEKFI--QSPEDL--EKLKKDGNLMFDQVPMVEIDGMKLAQTRAILNY
               10        20          30          40          50        60        70

             80        90         100       110       120        130        140
FASTA  LVEKYGKTDSLYPKCPKKRAVINQRL--YFDMGTLYQSFANYYYPQVFAK-APADPEAFKKIEAAFE-FLNTFLEGQDYA
       .. ::    .:: :  :.::.:..     .:.  . ....     :  :: : :  .. ..   :::  :..  .::::
sp|P00 IATKY----DLYGKDMKERALIDMYTEGILDLTEMIMQLVICPPDQKEAKTALAKDRTKNRYLPAFEKVLKS--HGQDYL
               80        90       100       110       120       130       140

      150       160       170       180       190       200
FASTA  AGDSLTVADIALVATVSTFEVAKFEISKYANVNRWYENAKKVTPGWEENWAGCLEFKKYFE
       .:. :: .:: :.  .  . : .:. :
sp|P00 VGNRLTRVDIHLLELL--LYVEEFDASLLTSFPLLKAFKSRISSLPNVKKFLQPGSQRKLPVDAKQIEEARKIFKF
      150       160         170       180       190       200       210       220

>>sp|P14942|GSTA4_RAT Glutathione S-transferase alpha-4 (Glutathio             (222 aa)
 initn:  80 init1:  53 opt: 106  Z-score: 149.9  bits: 34.8 E(13351): 0.02
Smith-Waterman score: 132; 28.2% identity (56.3% similar) in 174 aa overlap (4-168:7-168)
Entrez Lookup  Re-search database  General re-search
                  10        20        30         40        50        60        70
```

A BLAST család

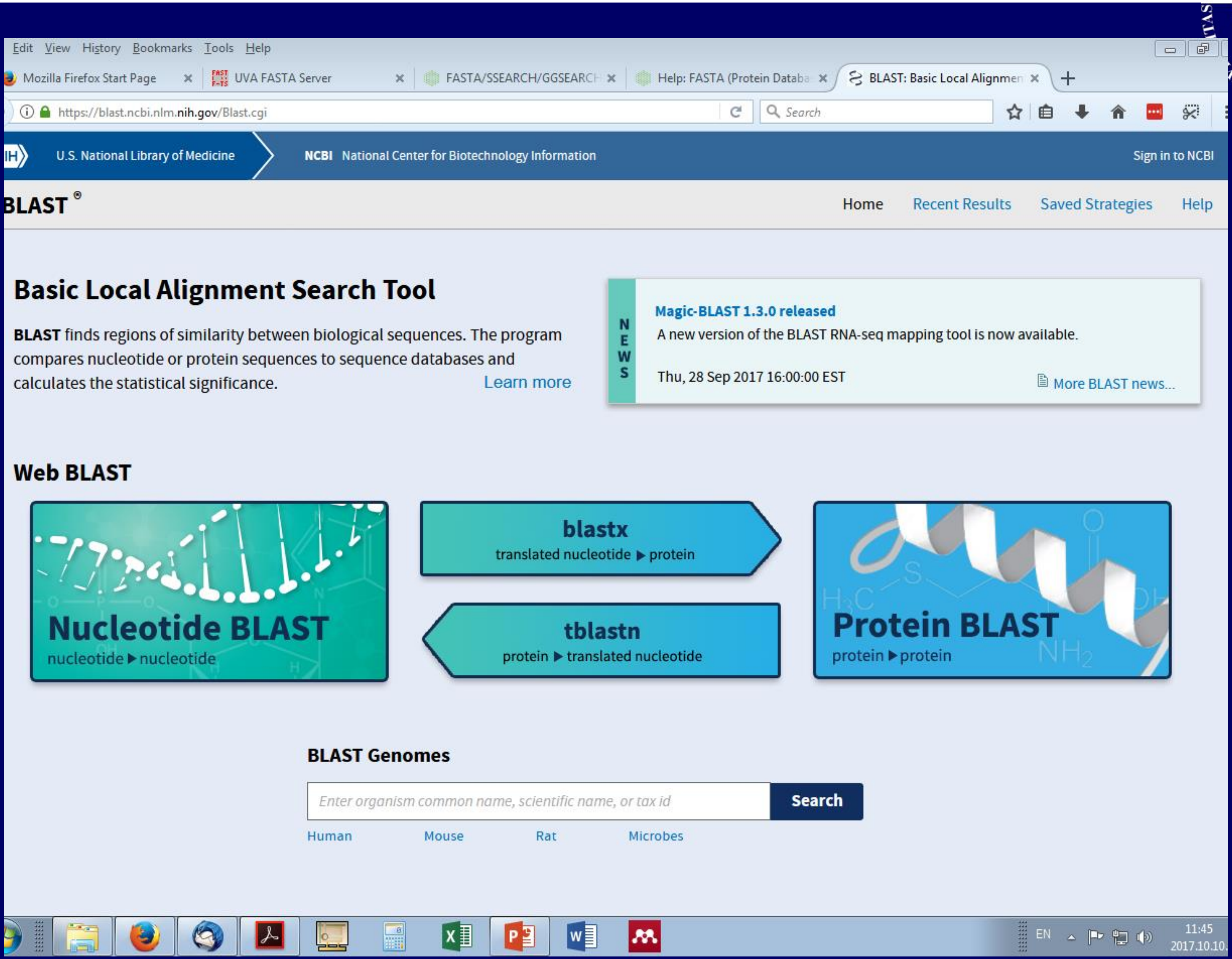
- Honlap: http://blast.ncbi.nlm.nih.gov/Blast.cgi
- Letülthető Linuxra és Windowsra is
- Web alapú szolgáltatás elérhető
- Alapos dokumentáció a honlapon
- Igen népszerű, megbízható
- Régóta van jelen az irodalomban, folyamatosan fejlesztik

Az algoritmus

1. A szekvencia maszkolása
2. A szekvencia felbontása szavakra
3. A lista szűkítése a nagy pontértékű szavakra
4. Keresés az adatbázisban a lista alapján
5. A találatok kiterjesztése (HSP – high-scoring segment pair)
6. A HSP-k statisztikus kiértékelése
7. HSP-k összefűzése hosszabb illesztéssé

A programcsomag tagjai

- „blastn”: DNS szekvencia keresése DNS adatbázis ellen
- „blastp”: fehérje szekvencia fehérje adatbázis ellen
- „psi-blast”: fehérjék iteratív keresése fehérje adatbázis ellen
- „blastx”: lefordított DNS szekvencia keresése fehérje adatbázis ellen
- „tblastx”: lefordított DNS szekvencia keresés lefordított DNS adatbázison
- „tblastn”: visszafordított fehérje keresés DNS adatbázis ellen
- „megablast”: sok szekvencia keresése egy futás során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FASTA/SSEARCH/GGSEARCH
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BLAST: Basic Local Alignmen
https://blast.ncbi.nlm.nih.gov/Blast.cgi
Search
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2017.10.10.

U.S. National Library of Medicine

NCBI National Center for Biotechnology Information

Sign in to NCBI

BLAST®

Home Recent Results Saved Strategies Help

Basic Local Alignment Search Tool

BLAST finds regions of similarity between biological sequences. The program compares nucleotide or protein sequences to sequence databases and calculates the statistical significance. Learn more

NEWS

Magic-BLAST 1.3.0 released

A new version of the BLAST RNA-seq mapping tool is now available.

Thu, 28 Sep 2017 16:00:00 EST

More BLAST news...

Web BLAST

Nucleotide BLAST
nucleotide ▶ nucleotide

blastx
translated nucleotide ▶ protein

tblastn
protein ▶ translated nucleotide

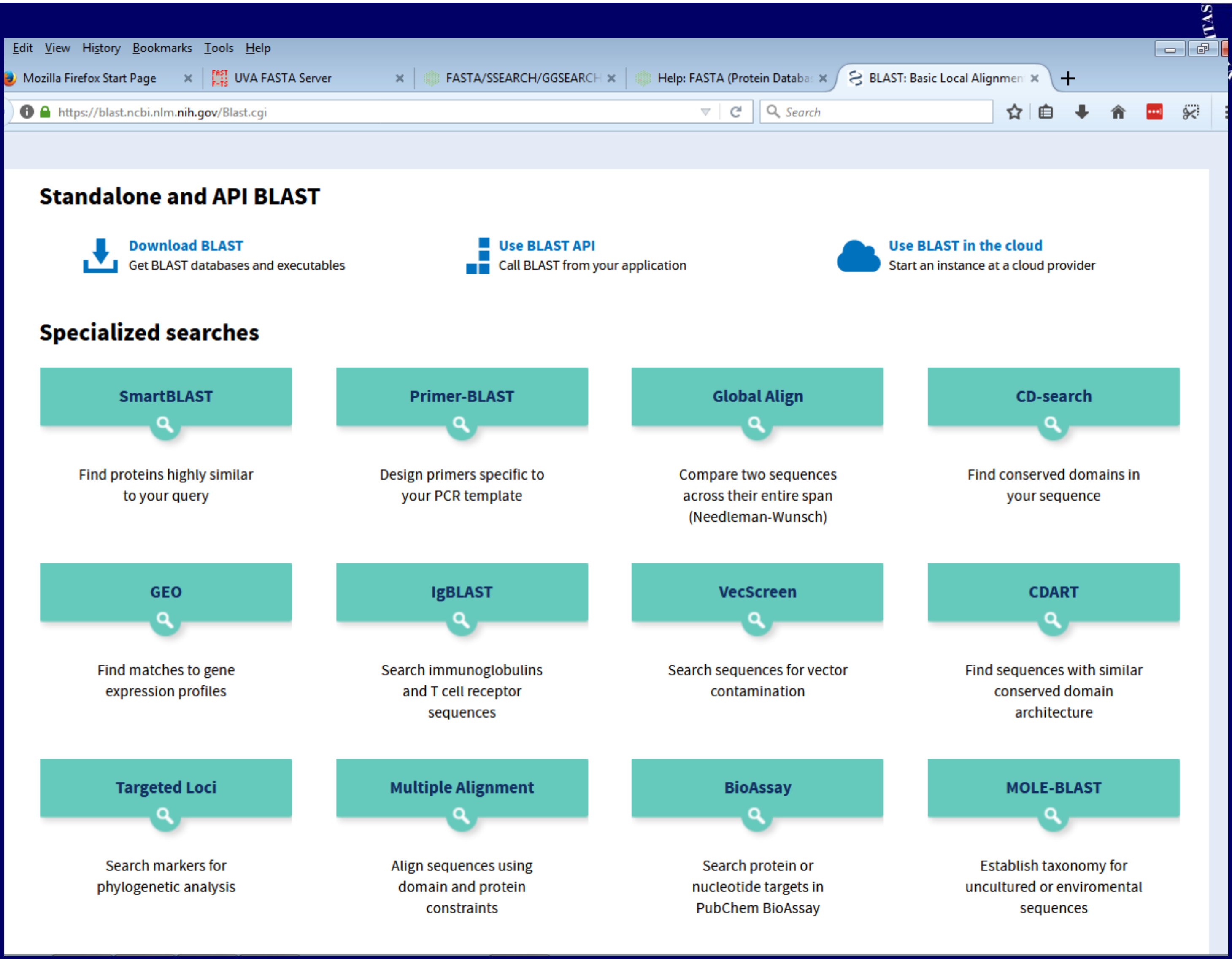
Protein BLAST
protein ▶ protein

BLAST Genomes

Enter organism common name, scientific name, or tax id

Search

Human Mouse Rat Microbes



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Mozilla Firefox Start Page
UVA FASTA Server
FASTA/SSEARCH/GGSEARCH
Help: FASTA (Protein Databa
BLAST: Basic Local Alignmen
https://blast.ncbi.nlm.nih.gov/Blast.cgi
Search

Standalone and API BLAST

Download BLAST
Get BLAST databases and executables

Use BLAST API
Call BLAST from your application

Use BLAST in the cloud
Start an instance at a cloud provider

Specialized searches

SmartBLAST
Find proteins highly similar to your query

Primer-BLAST
Design primers specific to your PCR template

Global Align
Compare two sequences across their entire span (Needleman-Wunsch)

CD-search
Find conserved domains in your sequence

GEO
Find matches to gene expression profiles

IgBLAST
Search immunoglobulins and T cell receptor sequences

VecScreen
Search sequences for vector contamination

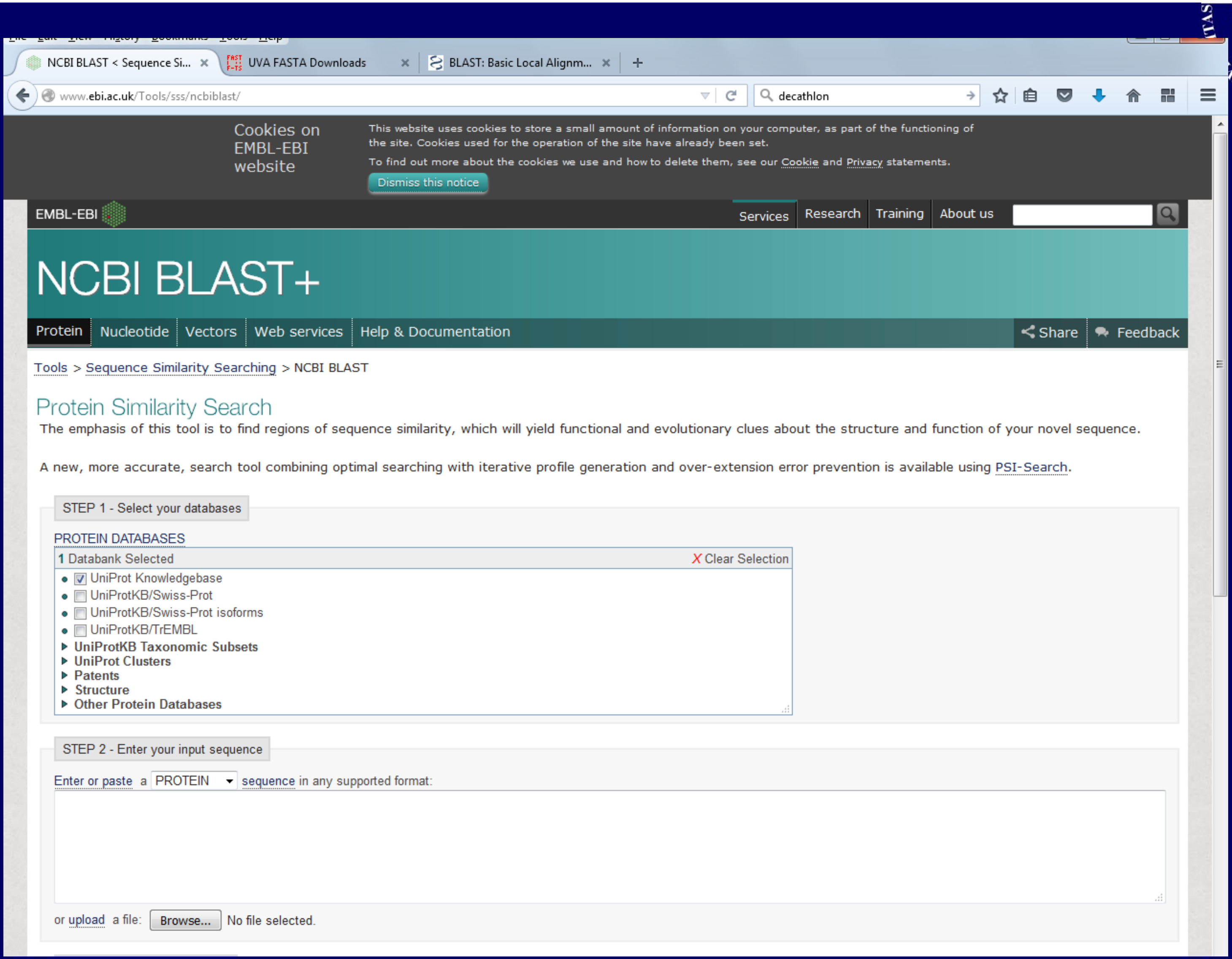
CDART
Find sequences with similar conserved domain architecture

Targeted Loci
Search markers for phylogenetic analysis

Multiple Alignment
Align sequences using domain and protein constraints

BioAssay
Search protein or nucleotide targets in PubChem BioAssay

MOLE-BLAST
Establish taxonomy for uncultured or enviromental sequences



NCBI BLAST < Sequence Si...
UVA FASTA Downloads
BLAST: Basic Local Alignm...
www.ebi.ac.uk/Tools/sss/ncbiblast/
decathlon

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To find out more about the cookies we use and how to delete them, see our Cookie and Privacy statements.

NCBI BLAST+

Tools > Sequence Similarity Searching > NCBI BLAST

Protein Similarity Search

The emphasis of this tool is to find regions of sequence similarity, which will yield functional and evolutionary clues about the structure and function of your novel sequence.

A new, more accurate, search tool combining optimal searching with iterative profile generation and over-extension error prevention is available using PSI-Search.

STEP 1 - Select your databases

PROTEIN DATABASES

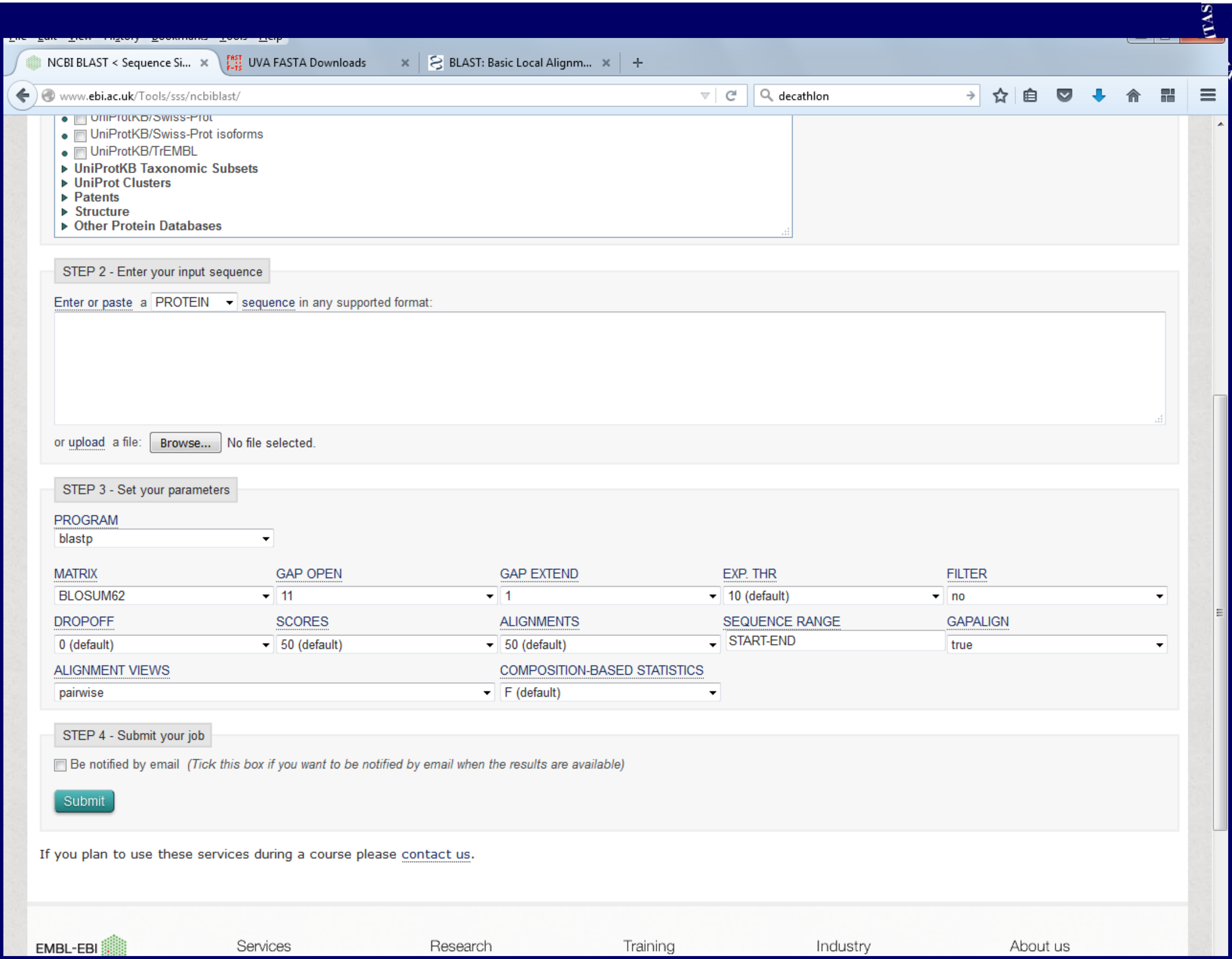
1 Databank Selected — X Clear Selection

- ☑ UniProt Knowledgebase
- □ UniProtKB/Swiss-Prot
- □ UniProtKB/Swiss-Prot isoforms
- □ UniProtKB/TrEMBL
- ▸ **UniProtKB Taxonomic Subsets**
- ▸ **UniProt Clusters**
- ▸ **Patents**
- ▸ **Structure**
- ▸ **Other Protein Databases**

STEP 2 - Enter your input sequence

Enter or paste a PROTEIN sequence in any supported format:

or upload a file: Browse... No file selected.


NCBI BLAST < Sequence Si...
UVA FASTA Downloads
BLAST: Basic Local Alignm...
www.ebi.ac.uk/Tools/sss/ncbiblast/
decathlon

- □ UniProtKB/Swiss-Prot
- □ UniProtKB/Swiss-Prot isoforms
- □ UniProtKB/TrEMBL

▸ UniProtKB Taxonomic Subsets
▸ UniProt Clusters
▸ Patents
▸ Structure
▸ Other Protein Databases

STEP 2 - Enter your input sequence

Enter or paste a PROTEIN sequence in any supported format:

or upload a file: Browse... No file selected.

STEP 3 - Set your parameters

PROGRAM: blastp

MATRIX	GAP OPEN	GAP EXTEND	EXP. THR	FILTER
BLOSUM62	11	1	10 (default)	no
DROPOFF	**SCORES**	**ALIGNMENTS**	**SEQUENCE RANGE**	**GAPALIGN**
0 (default)	50 (default)	50 (default)	START-END	true
ALIGNMENT VIEWS		**COMPOSITION-BASED STATISTICS**		
pairwise		F (default)		

STEP 4 - Submit your job

□ Be notified by email *(Tick this box if you want to be notified by email when the results are available)*

Submit

If you plan to use these services during a course please contact us.

Paraméterek

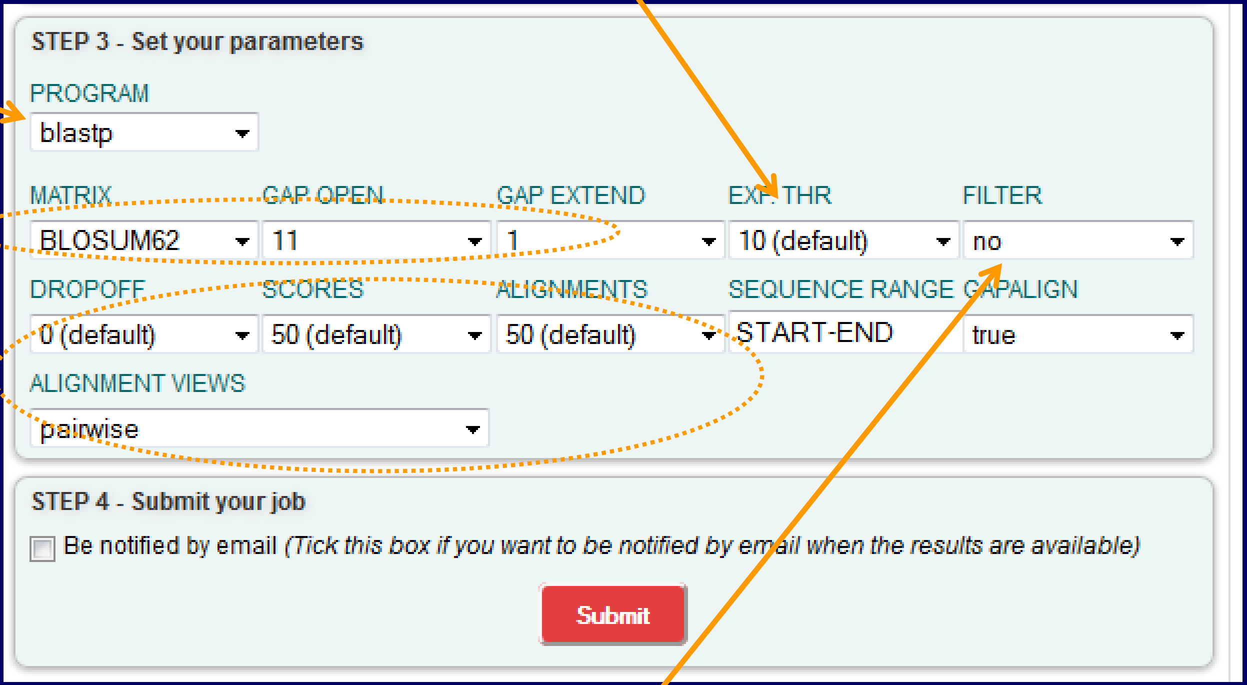
A program neve

Mátrix paraméterek

Eredmény

Statisztika

Maszkolás



STEP 3 - Set your parameters

PROGRAM: blastp

MATRIX	GAP OPEN	GAP EXTEND	EXP. THR	FILTER
BLOSUM62	11	1	10 (default)	no
DROPOFF	SCORES	ALIGNMENTS	SEQUENCE RANGE	GAPALIGN
0 (default)	50 (default)	50 (default)	START-END	true

ALIGNMENT VIEWS: pairwise

STEP 4 - Submit your job

☐ Be notified by email *(Tick this box if you want to be notified by email when the results are available)*

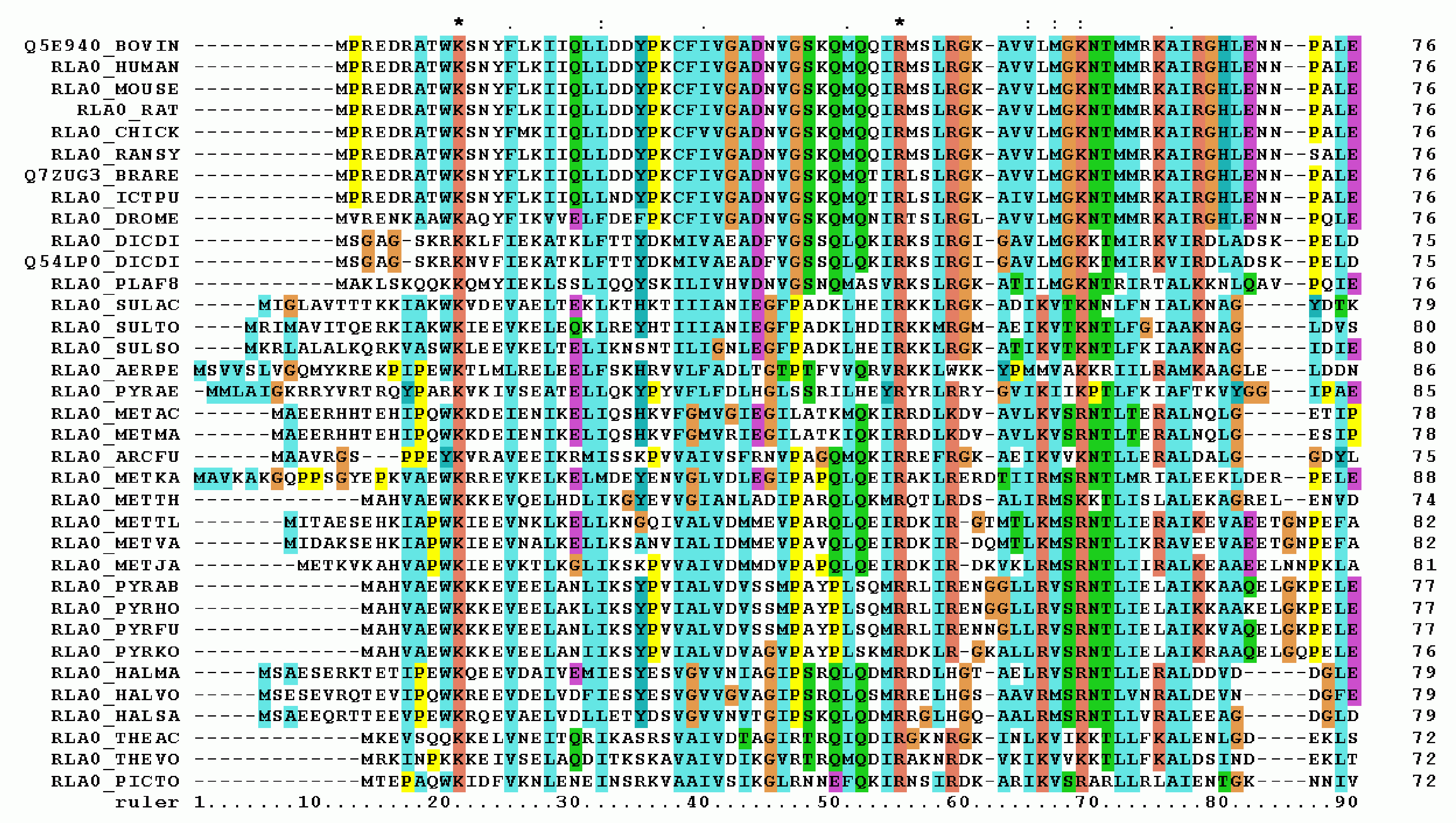
Egy további változat

BLAT:

- A cél a további gyorsítás
- Az ár: rosszabb érzékenység
  - Csak a nagyon hasonló szegmenseket talalálja meg: 95% egyezés DNS-re, 80% fehérjére
  - Rövid egyezéseket nem talál meg
- Új generációs szekvenálásnál igen hasznos

Profilkeresés

- Az aminósavak helyettesítési hajlandósága függ a pozíciótól
- Egy jó többszörös illesztés megadja ezt az információt
- A többszörös illesztést közvetlenül „profillá” alakítjuk
- Ezt használjuk a kereséshez
- Megnő az eljárás érzékenysége



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                                 *   .      :       .          .   *         : : :      .
Q5E940_BOVIN -----------MPREDRATWKSNYFLKIIQLLDDYPKCFIVGADNVGSKQMQQIRMSLRGK-AVVLMGKNTMMRKAIRGHLENN--PALE     76
  RLA0_HUMAN -----------MPREDRATWKSNYFLKIIQLLDDYPKCFIVGADNVGSKQMQQIRMSLRGK-AVVLMGKNTMMRKAIRGHLENN--PALE     76
  RLA0_MOUSE -----------MPREDRATWKSNYFLKIIQLLDDYPKCFIVGADNVGSKQMQQIRMSLRGK-AVVLMGKNTMMRKAIRGHLENN--PALE     76
    RLA0_RAT -----------MPREDRATWKSNYFLKIIQLLDDYPKCFIVGADNVGSKQMQQIRMSLRGK-AVVLMGKNTMMRKAIRGHLENN--PALE     76
  RLA0_CHICK -----------MPREDRATWKSNYFMKIIQLLDDYPKCFVVGADNVGSKQMQQIRMSLRGK-AVVLMGKNTMMRKAIRGHLENN--PALE     76
  RLA0_RANSY -----------MPREDRATWKSNYFLKIIQLLDDYPKCFIVGADNVGSKQMQQIRMSLRGK-AVVLMGKNTMMRKAIRGHLENN--SALE     76
Q7ZUG3_BRARE -----------MPREDRATWKSNYFLKIIQLLDDYPKCFIVGADNVGSKQMQTIRLSLRGK-AVVLMGKNTMMRKAIRGHLENN--PALE     76
  RLA0_ICTPU -----------MPREDRATWKSNYFLKIIQLLNDYPKCFIVGADNVGSKQMQTIRLSLRGK-AIVLMGKNTMMRKAIRGHLENN--PALE     76
  RLA0_DROME -----------MVRENKAAWKAQYFIKVVELFDEFPKCFIVGADNVGSKQMQNIRTSLRGL-AVVLMGKNTMMRKAIRGHLENN--PQLE     76
  RLA0_DICDI -----------MSGAG-SKRKKLFIEKATKLFTTYDKMIVAEADFVGSSQLQKIRKSIRGI-GAVLMGKKTMIRKVIRDLADSK--PELD     75
Q54LP0_DICDI -----------MSGAG-SKRKNVFIEKATKLFTTYDKMIVAEADFVGSSQLQKIRKSIRGI-GAVLMGKKTMIRKVIRDLADSK--PELD     75
  RLA0_PLAF8 -----------MAKLSKQQKKQMYIEKLSSLIQQYSKILIVHVDNVGSNQMASVRKSLRGK-ATILMGKNTRIRTALKKNLQAV--PQIE     76
  RLA0_SULAC -----MIGLAVTTTKKIAKWKVDEVAELTEKLKTHKTIIIANIEGFPADKLHEIRKKLRGK-ADIKVTKNNLFNIALKNAG-----YDTK     79
  RLA0_SULTO ----MRIMAVITQERKIAKWKIEEVKELEQKLREYHTIIIANIEGFPADKLHDIRKKMRGM-AEIKVTKNTLFGIAAKNAG-----LDVS     80
  RLA0_SULSO ----MKRLALALKQRKVASWKLEEVKELTELIKNSNTILIGNLEGFPADKLHEIRKKLRGK-ATIKVTKNTLFKIAAKNAG-----IDIE     80
  RLA0_AERPE MSVVSLVGQMYKREKPIPEWKTLMLRELEELFSKHRVVLFADLTGTPTFVVQRVRKKLWKK-YPMMVAKKRIILRAMKAAGLE---LDDN     86
  RLA0_PYRAE -MMLAIGKRRYVRTRQYPARKVKIVSEATELLQKYPYVFLFDLHGLSSRILHEYRYRLRRY-GVIKIIKPTLFKIAFTKVYGG---IPAE     85
  RLA0_METAC ------MAEERHHTEHIPQWKKDEIENIKELIQSHKVFGMVGIEGILATKMQKIRRDLKDV-AVLKVSRNTLTERALNQLG-----ETIP     78
  RLA0_METMA ------MAEERHHTEHIPQWKKDEIENIKELIQSHKVFGMVRIEGILATKIQKIRRDLKDV-AVLKVSRNTLTERALNQLG-----ESIP     78
  RLA0_ARCFU ------MAAVRGS---PPEYKVRAVEEIKRMISSKPVVAIVSFRNVPAGQMQKIRREFRGK-AEIKVVKNTLLERALDALG-----GDYL     75
  RLA0_METKA MAVKAKGQPPSGYEPKVAEWKRREVKELKELMDEYENVGLVDLEGIPAPQLQEIRAKLRERDTIIRMSRNTLMRIALEEKLDER--PELE     88
  RLA0_METTH -------------MAHVAEWKKKEVQELHDLIKGYEVVGIANLADIPARQLQKMRQTLRDS-ALIRMSKKTLISLALEKAGREL--ENVD     74
  RLA0_METTL -------MITAESEHKIAPWKIEEVNKLKELLKNGQIVALVDMMEVPARQLQEIRDKIR-GTMTLKMSRNTLIERAIKEVAEETGNPEFA     82
  RLA0_METVA -------MIDAKSEHKIAPWKIEEVNALKELLKSANVIALIDMMEVPAVQLQEIRDKIR-DQMTLKMSRNTLIKRAVEEVAEETGNPEFA     82
  RLA0_METJA --------METKVKAHVAPWKIEEVKTLKGLIKSKPVVAIVDMMDVPAPQLQEIRDKIR-DKVKLRMSRNTLIIRALKEAAEELNNPKLA     81
  RLA0_PYRAB -------------MAHVAEWKKKEVEELANLIKSYPVIALVDVSSMPAYPLSQMRRLIRENGGLLRVSRNTLIELAIKKAAQELGKPELE     77
  RLA0_PYRHO -------------MAHVAEWKKKEVEELAKLIKSYPVIALVDVSSMPAYPLSQMRRLIRENGGLLRVSRNTLIELAIKKAAKELGKPELE     77
  RLA0_PYRFU -------------MAHVAEWKKKEVEELANLIKSYPVVALVDVSSMPAYPLSQMRRLIRENNGLLRVSRNTLIELAIKKVAQELGKPELE     77
  RLA0_PYRKO -------------MAHVAEWKKKEVEELANIIKSYPVIALVDVAGVPAYPLSKMRDKLR-GKALLRVSRNTLIELAIKRAAQELGQPELE     76
  RLA0_HALMA -----MSAESERKTETIPEWKQEEVDAIVEMIESYESVGVVNIAGIPSRQLQDMRRDLHGT-AELRVSRNTLLERALDDVD-----DGLE     79
  RLA0_HALVO -----MSESEVRQTEVIPQWKREEVDELVDFIESYESVGVVGVAGIPSRQLQSMRRELHGS-AAVRMSRNTLVNRALDEVN-----DGFE     79
  RLA0_HALSA -----MSAEEQRTTEEVPEWKRQEVAELVDLLETYDSVGVVNVTGIPSKQLQDMRRGLHGQ-AALRMSRNTLLVRALEEAG-----DGLD     79
  RLA0_THEAC -------------MKEVSQQKKELVNEITQRIKASRSVAIVDTAGIRTRQIQDIRGKNRGK-INLKVIKKTLLFKALENLGD----EKLS     72
  RLA0_THEVO -------------MRKINPKKKEIVSELAQDITKSKAVAIVDIKGVRTRQMQDIRAKNRDK-VKIKVVKKTLLFKALDSIND----EKLT     72
  RLA0_PICTO -------------MTEPAQWKIDFVKNLENEINSRKVAAIVSIKGLRNNEFQKIRNSIRDK-ARIKVSRARLLRLAIENTGK----NNIV     72
       ruler 1.......10........20........30........40........50........60........70........80........90
```

	1	2	3	4	5	6	7	8	9	…
A	a_1									
C										
D										
E										
F										
…										

	1	2	3	4	5	6	7	8	9	…
A	a_1									
C	c_1									
D										
E										
F										
…										

	1	2	3	4	5	6	7	8	9	…
A	a_1									
C	c_1									
D	d_1									
E	e_1									
F	f_1									
…										

	1	2	3	4	5	6	7	8	9	…
A	a_1	a_2								
C	c_1	c_2								
D	d_1	d_2								
E	e_1	e_2								
F	f_1	f_2								
…										

	1	2	3	4	5	6	7	8	9	…
A	a_1	a_2	a_3	a_4	a_5	a_6	a_7	a_8	a_9	
C	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8	c_9	
D	d_1	d_2	d_3	d_4	d_5	d_6	d_7	d_8	d_9	
E	e_1	e_2	e_3	e_4	e_5	e_6	e_7	e_8	e_9	
F	f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8	f_9	
…										

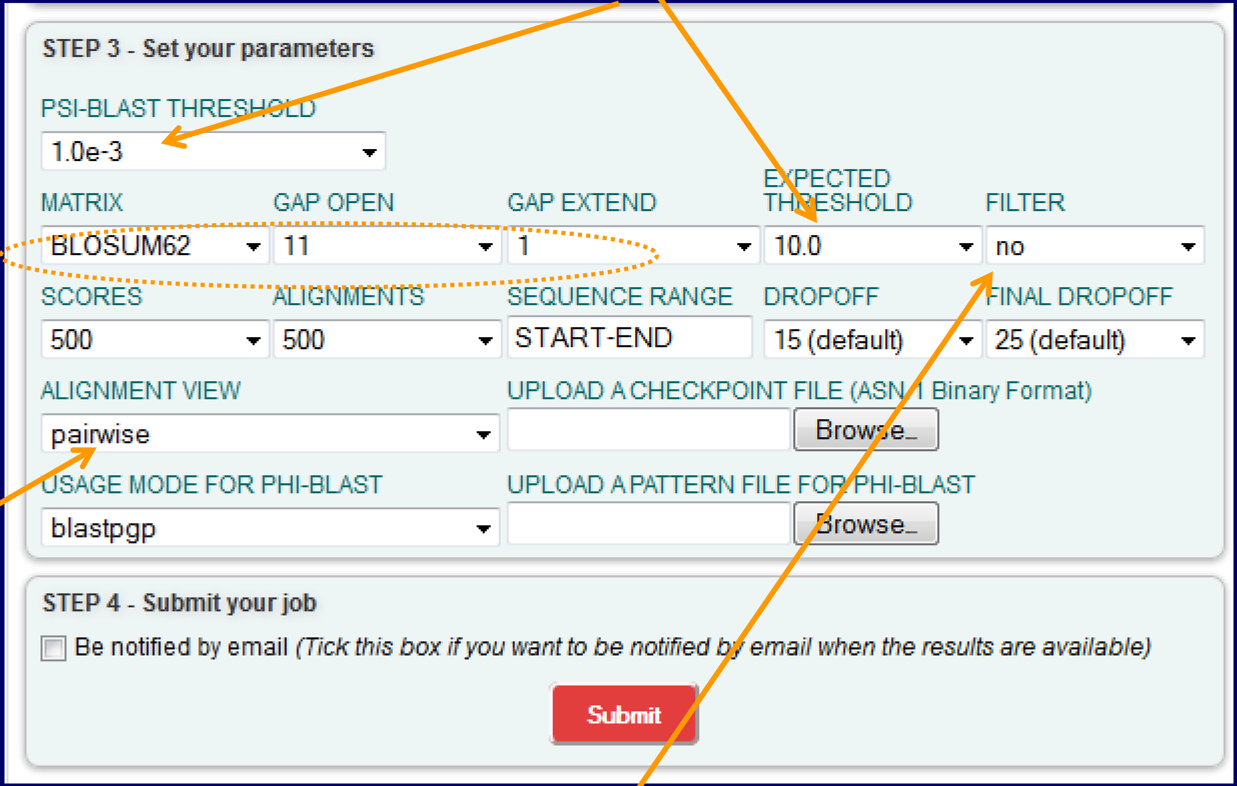
Megvalósítás: PSI-BLAST

- Egy BLAST kereséssel megtaláljuk a közeli homológokat
- Ezekből többszörös illesztést készítünk
- Ebből származtatjuk a kerső profilt a következő BLAST kereséshez
- Ezzel bővül a homológok listája a távolabbi rokonokkal
- Az eljárást ismételjük

Paraméterek

Statisztika

Mátrix paraméterek



STEP 3 - Set your parameters

PSI-BLAST THRESHOLD: 1.0e-3

MATRIX	GAP OPEN	GAP EXTEND	EXPECTED THRESHOLD	FILTER
BLOSUM62	11	1	10.0	no
SCORES	ALIGNMENTS	SEQUENCE RANGE	DROPOFF	FINAL DROPOFF
500	500	START-END	15 (default)	25 (default)

ALIGNMENT VIEW: pairwise

UPLOAD A CHECKPOINT FILE (ASN.1 Binary Format)

USAGE MODE FOR PHI-BLAST: blastpgp

UPLOAD A PATTERN FILE FOR PHI-BLAST

STEP 4 - Submit your job

□ Be notified by email *(Tick this box if you want to be notified by email when the results are available)*

Eredmény

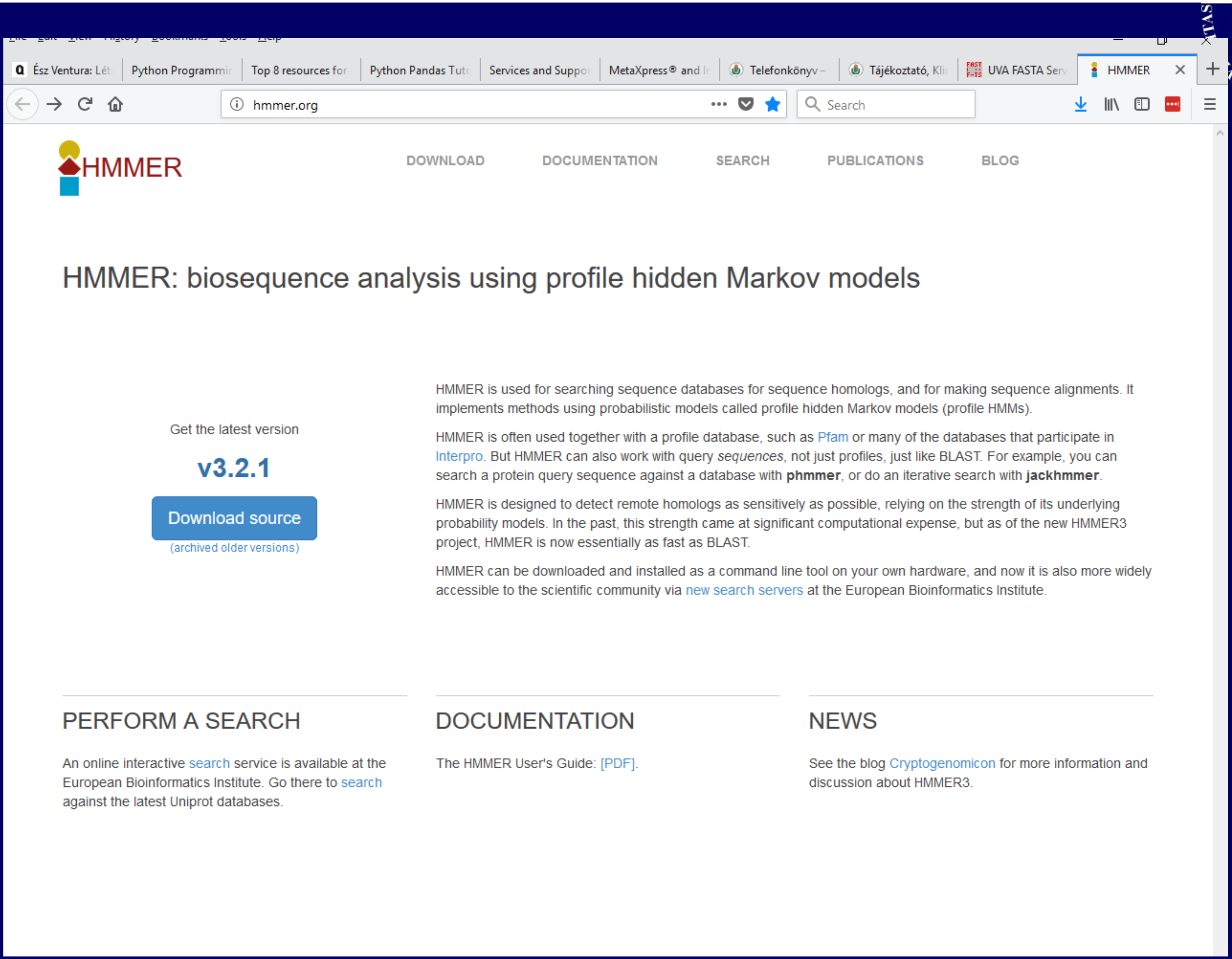
Maszkolás

Másik lehetőség HMMER

- Honlap: http://hmmer.org/
- Letölthető Linux és Windows verzióban
- Bőséges dokumentáció a honlapon
- Fehérje szekvenciákat kezel
- Egyszerre gyors és pontos módszer
- Egy hatékony statisztikai modellen alapul – „Markov modell”

A programcsalád tagjai

- „phmmer”: egy vagy több fehérje szekvenciát keres a fehérje adatbázis ellenében
- „hmmscan”: fehérje szekvenciákat keres profil adatbázis ellen
- „hmmsearch”: profilokat keres fehérje adatbázis ellenében
- “jackhmmer”: interaktív változat



HMMER: biosequence analysis using profile hidden Markov models

Get the latest version

v3.2.1

Download source

(archived older versions)

HMMER is used for searching sequence databases for sequence homologs, and for making sequence alignments. It implements methods using probabilistic models called profile hidden Markov models (profile HMMs).

HMMER is often used together with a profile database, such as Pfam or many of the databases that participate in Interpro. But HMMER can also work with query *sequences*, not just profiles, just like BLAST. For example, you can search a protein query sequence against a database with **phmmer**, or do an iterative search with **jackhmmer**.

HMMER is designed to detect remote homologs as sensitively as possible, relying on the strength of its underlying probability models. In the past, this strength came at significant computational expense, but as of the new HMMER3 project, HMMER is now essentially as fast as BLAST.

HMMER can be downloaded and installed as a command line tool on your own hardware, and now it is also more widely accessible to the scientific community via new search servers at the European Bioinformatics Institute.

PERFORM A SEARCH

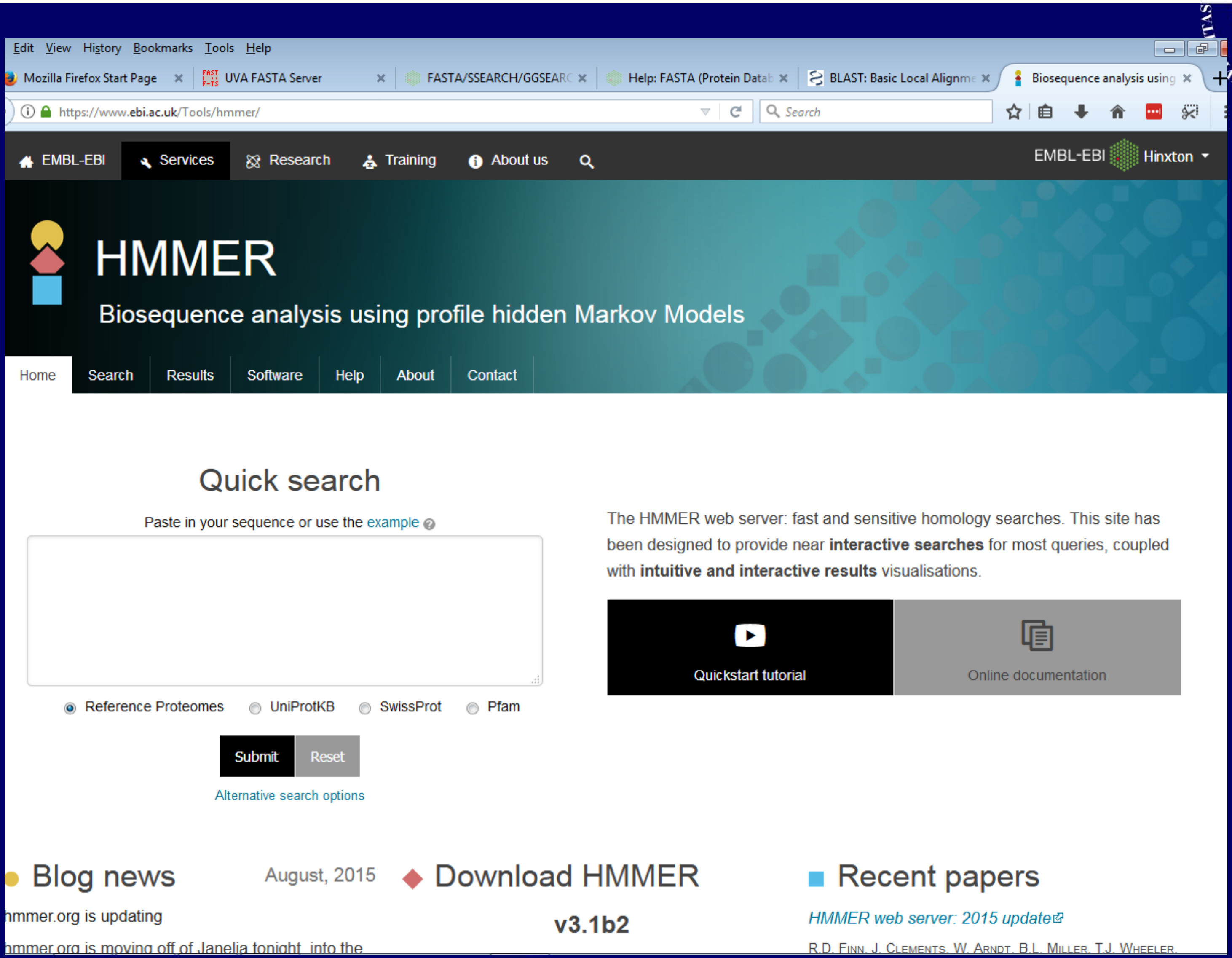
An online interactive search service is available at the European Bioinformatics Institute. Go there to search against the latest Uniprot databases.

DOCUMENTATION

The HMMER User's Guide: [PDF].

NEWS

See the blog Cryptogenomicon for more information and discussion about HMMER3.



https://www.ebi.ac.uk/Tools/hmmer/

HMMER

Biosequence analysis using profile hidden Markov Models

Quick search

Paste in your sequence or use the example

◉ Reference Proteomes ○ UniProtKB ○ SwissProt ○ Pfam

Alternative search options

The HMMER web server: fast and sensitive homology searches. This site has been designed to provide near **interactive searches** for most queries, coupled with **intuitive and interactive results** visualisations.

Blog news

August, 2015

hmmer.org is updating

hmmer.org is moving off of Janelia tonight, into the

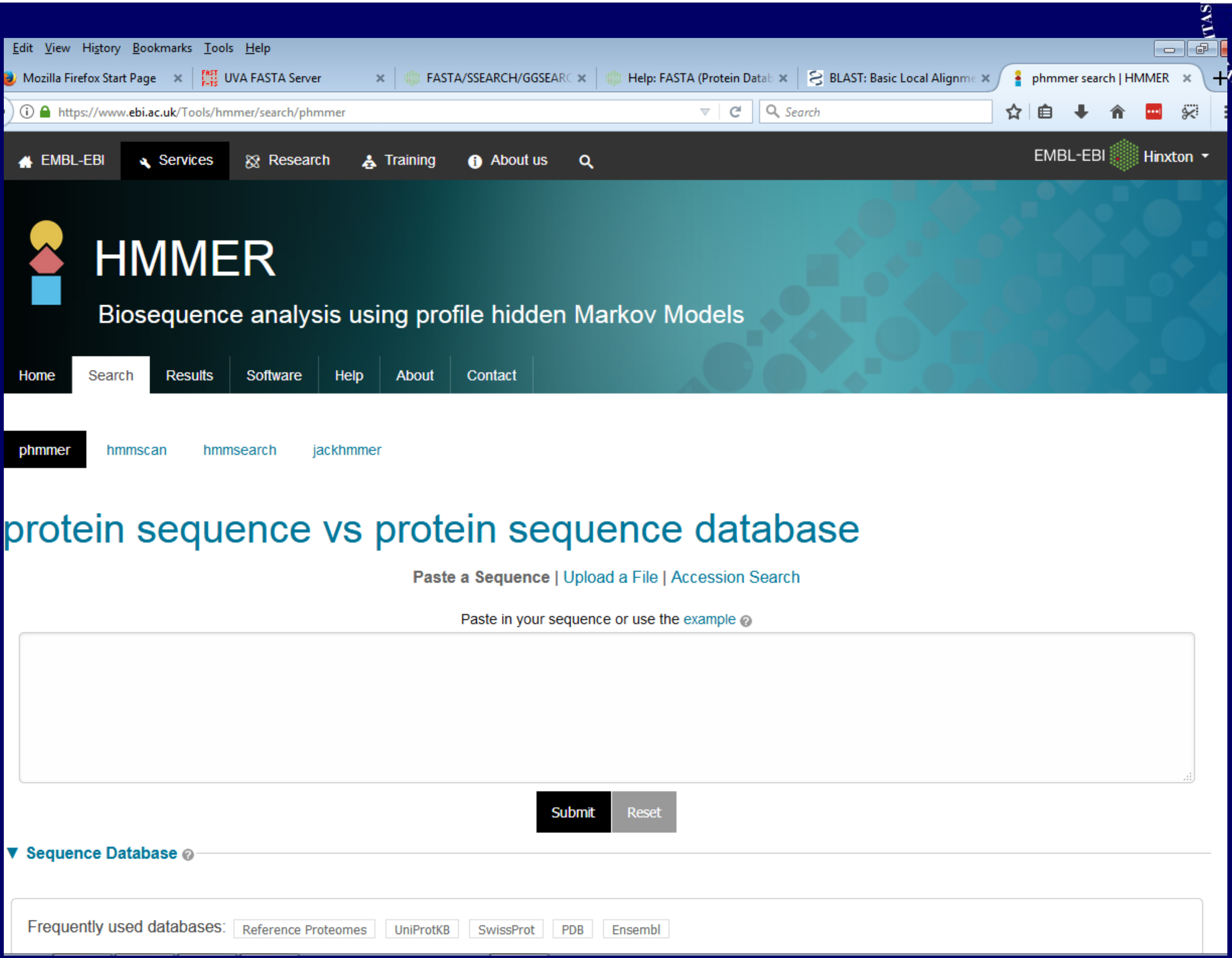
Download HMMER

v3.1b2

Recent papers

HMMER web server: 2015 update

R.D. Finn, J. Clements, W. Arndt, B.L. Miller, T.J. Wheeler,



HMMER

Biosequence analysis using profile hidden Markov Models

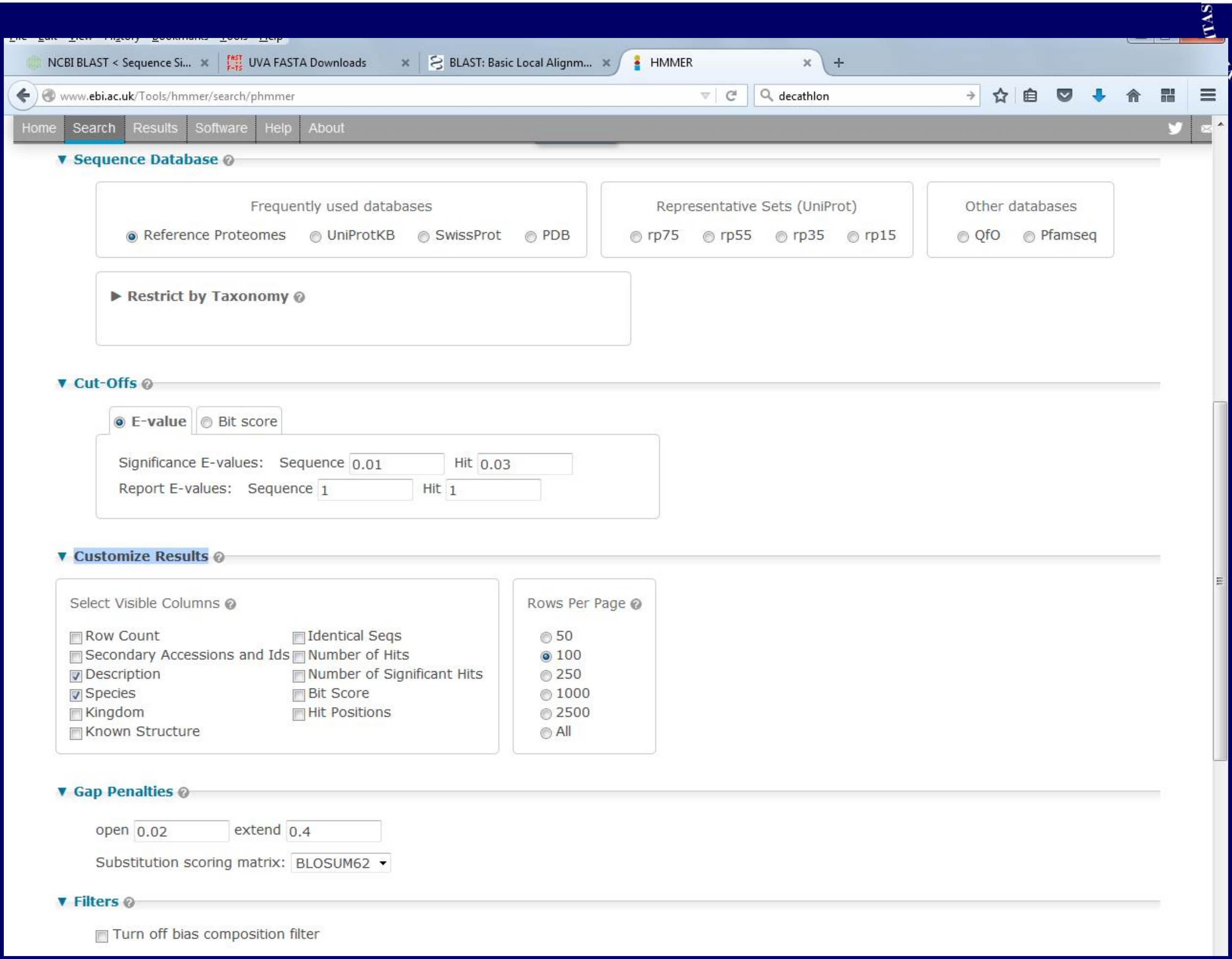
protein sequence vs protein sequence database

Paste a Sequence | Upload a File | Accession Search

Paste in your sequence or use the example

▼ Sequence Database

Frequently used databases: Reference Proteomes UniProtKB SwissProt PDB Ensembl


NCBI BLAST < Sequence Si...
UVA FASTA Downloads
BLAST: Basic Local Alignm...
HMMER
www.ebi.ac.uk/Tools/hmmer/search/phmmer
decathlon
Home
Search
Results
Software
Help
About

▼ Sequence Database

Frequently used databases
● Reference Proteomes ○ UniProtKB ○ SwissProt ○ PDB

Representative Sets (UniProt)
○ rp75 ○ rp55 ○ rp35 ○ rp15

Other databases
○ QfO ○ Pfamseq

▶ Restrict by Taxonomy

▼ Cut-Offs

● E-value ○ Bit score

Significance E-values: Sequence 0.01 Hit 0.03
Report E-values: Sequence 1 Hit 1

▼ Customize Results

Select Visible Columns

- □ Row Count
- □ Secondary Accessions and Ids
- ☑ Description
- ☑ Species
- □ Kingdom
- □ Known Structure
- □ Identical Seqs
- □ Number of Hits
- □ Number of Significant Hits
- □ Bit Score
- □ Hit Positions

Rows Per Page

- ○ 50
- ● 100
- ○ 250
- ○ 1000
- ○ 2500
- ○ All

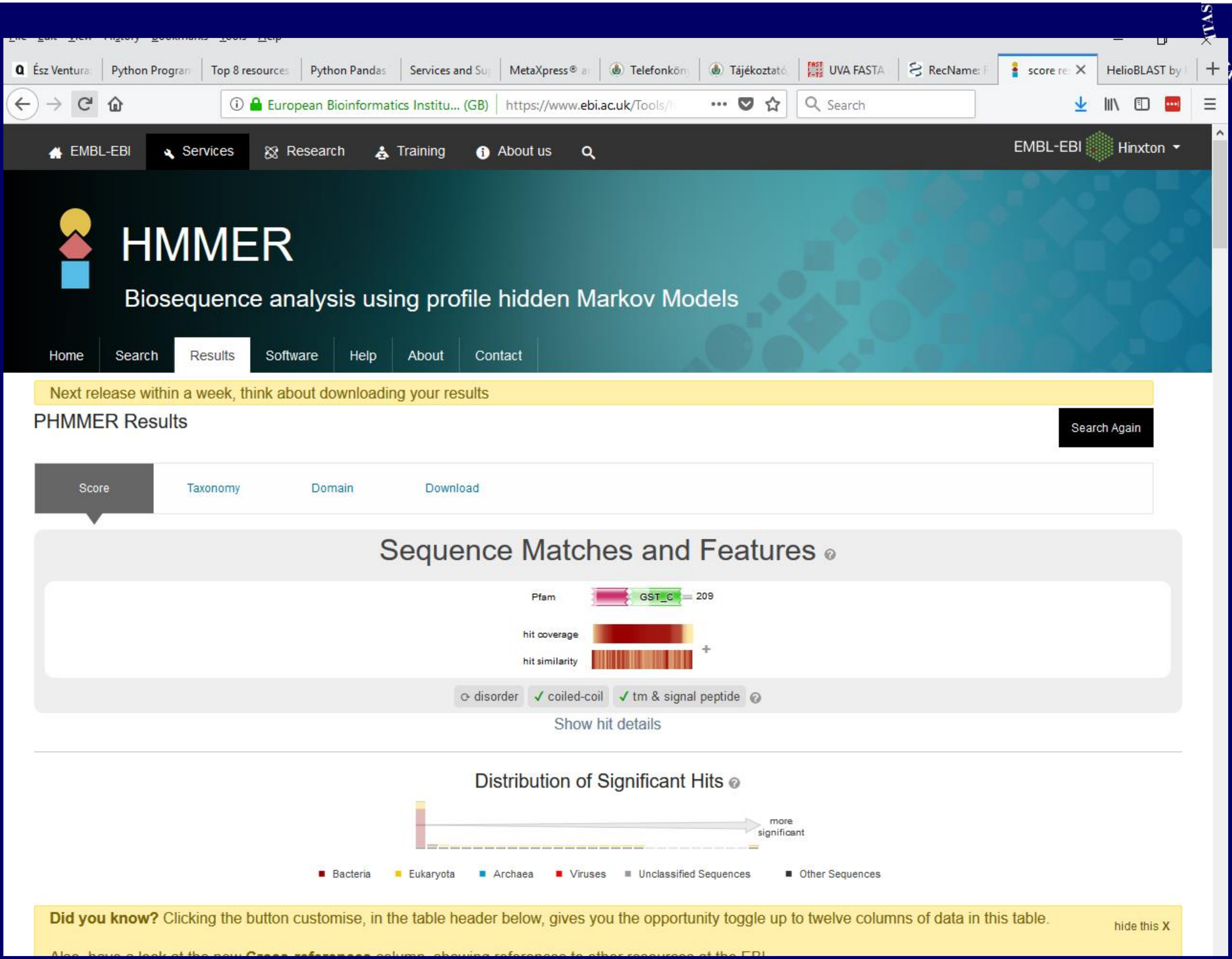
▼ Gap Penalties

open 0.02 extend 0.4

Substitution scoring matrix: BLOSUM62

▼ Filters

□ Turn off bias composition filter



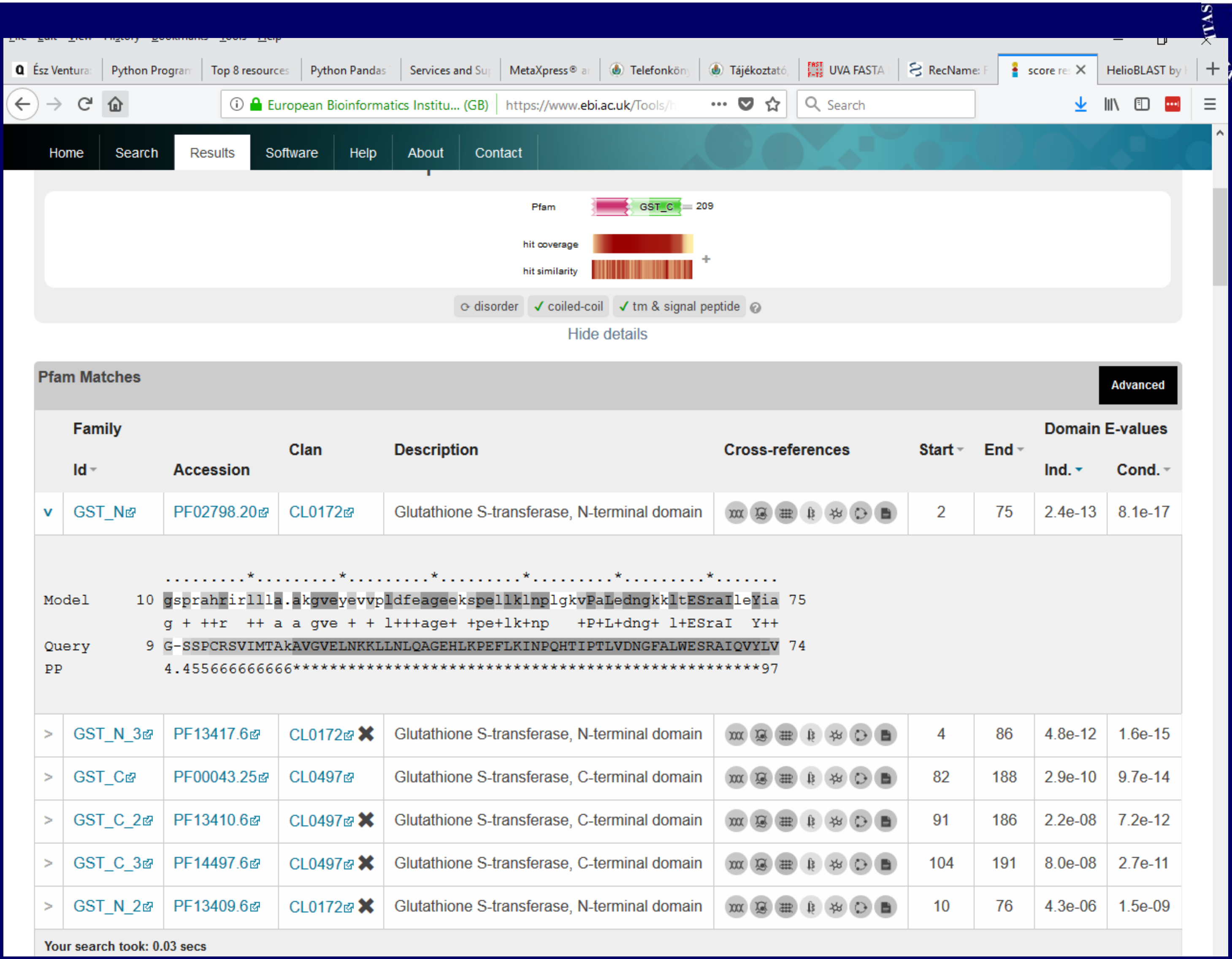
Next release within a week, think about downloading your results

PHMMER Results

Sequence Matches and Features

Distribution of Significant Hits

Did you know? Clicking the button customise, in the table header below, gives you the opportunity toggle up to twelve columns of data in this table.



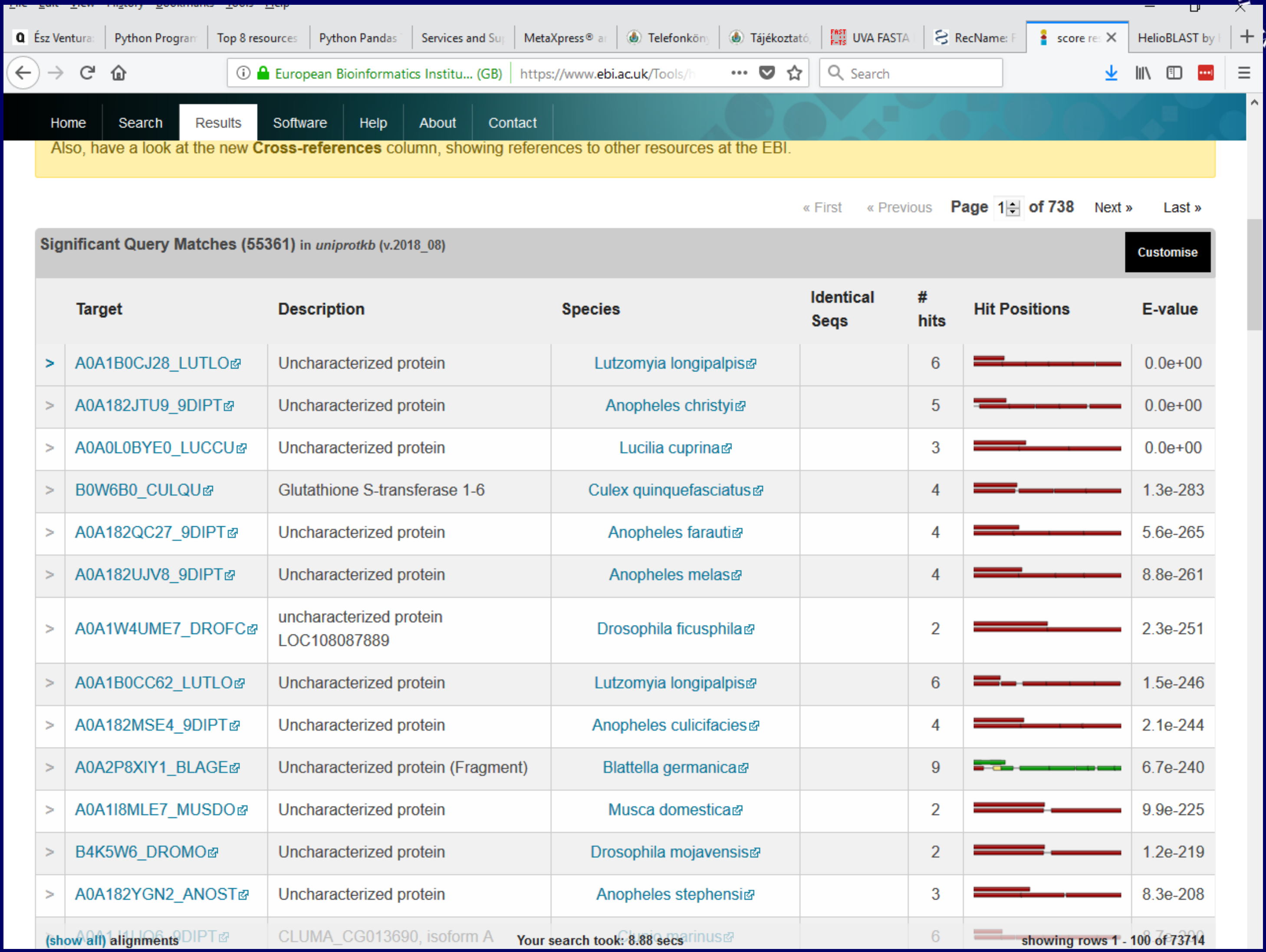
Pfam Matches

	Family							Domain E-values	
	Id	Accession	Clan	Description	Cross-references	Start	End	Ind.	Cond.
v	GST_N	PF02798.20	CL0172	Glutathione S-transferase, N-terminal domain		2	75	2.4e-13	8.1e-17

```
              .........*.........*.........*.........*.........*.........*.......
Model      10 gsprahrirllla.akgveyevvpldfeageekspellklnplgkvPaLedngkkltESraIleYia 75
              g + ++r  ++ a a gve + + l+++age+ +pe+lk+np   +P+L+dng+ l+ESraI  Y++
Query       9 G-SSPCRSVIMTAkAVGVELNKKLLNLQAGEHLKPEFLKINPQHTIPTLVDNGFALWESRAIQVYLV 74
PP            4.45566666666****************************************************97
```

	Id	Accession	Clan	Description	Cross-references	Start	End	Ind.	Cond.
>	GST_N_3	PF13417.6	CL0172 ✖	Glutathione S-transferase, N-terminal domain		4	86	4.8e-12	1.6e-15
>	GST_C	PF00043.25	CL0497	Glutathione S-transferase, C-terminal domain		82	188	2.9e-10	9.7e-14
>	GST_C_2	PF13410.6	CL0497 ✖	Glutathione S-transferase, C-terminal domain		91	186	2.2e-08	7.2e-12
>	GST_C_3	PF14497.6	CL0497 ✖	Glutathione S-transferase, C-terminal domain		104	191	8.0e-08	2.7e-11
>	GST_N_2	PF13409.6	CL0172 ✖	Glutathione S-transferase, N-terminal domain		10	76	4.3e-06	1.5e-09

Your search took: 0.03 secs



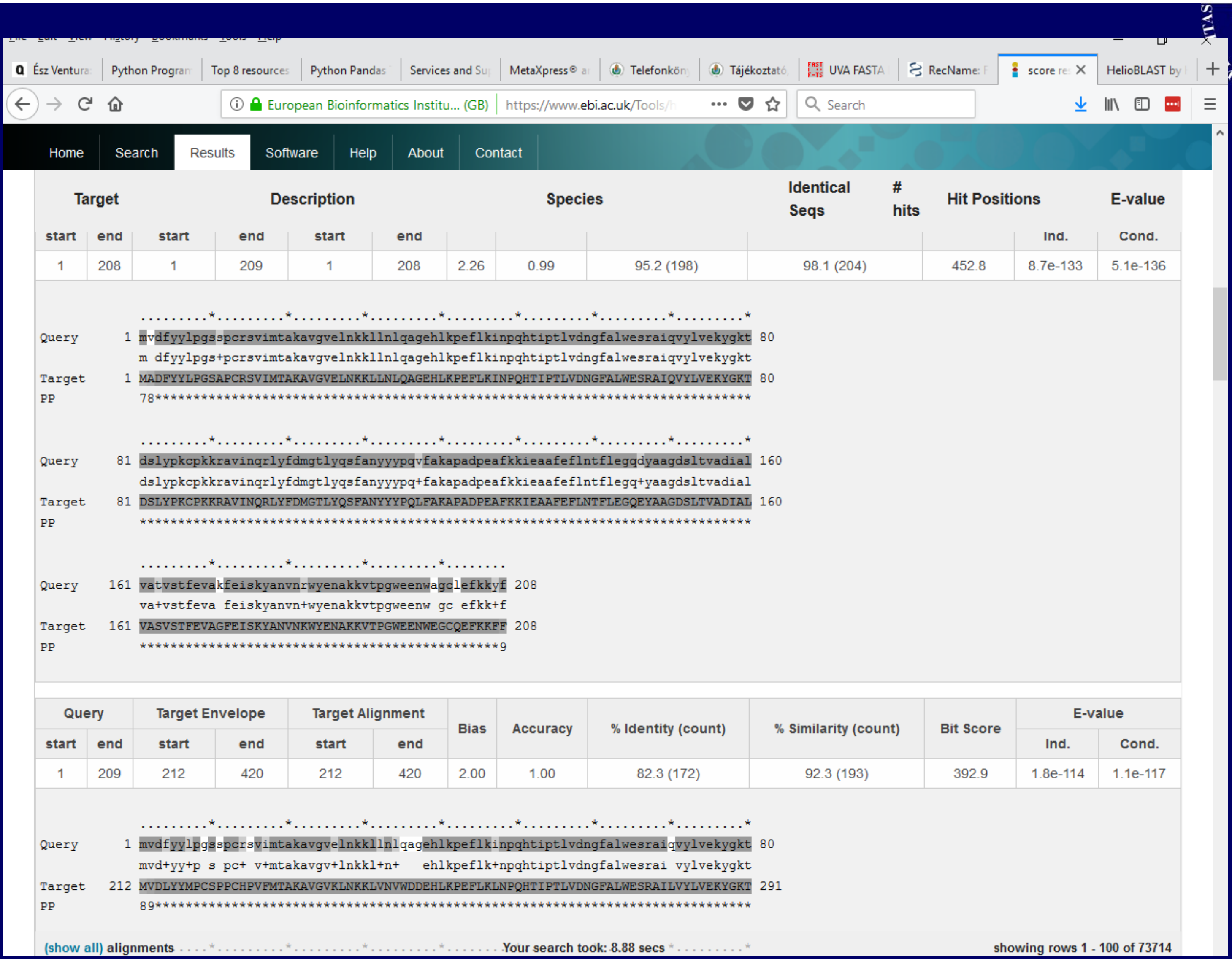
Also, have a look at the new **Cross-references** column, showing references to other resources at the EBI.

« First « Previous **Page** 1 **of 738** Next » Last »

Significant Query Matches (55361) in ***uniprotkb*** **(v.2018_08)**

	Target	Description	Species	Identical Seqs	# hits	Hit Positions	E-value
>	A0A1B0CJ28_LUTLO	Uncharacterized protein	Lutzomyia longipalpis		6		0.0e+00
>	A0A182JTU9_9DIPT	Uncharacterized protein	Anopheles christyi		5		0.0e+00
>	A0A0L0BYE0_LUCCU	Uncharacterized protein	Lucilia cuprina		3		0.0e+00
>	B0W6B0_CULQU	Glutathione S-transferase 1-6	Culex quinquefasciatus		4		1.3e-283
>	A0A182QC27_9DIPT	Uncharacterized protein	Anopheles farauti		4		5.6e-265
>	A0A182UJV8_9DIPT	Uncharacterized protein	Anopheles melas		4		8.8e-261
>	A0A1W4UME7_DROFC	uncharacterized protein LOC108087889	Drosophila ficusphila		2		2.3e-251
>	A0A1B0CC62_LUTLO	Uncharacterized protein	Lutzomyia longipalpis		6		1.5e-246
>	A0A182MSE4_9DIPT	Uncharacterized protein	Anopheles culicifacies		4		2.1e-244
>	A0A2P8XIY1_BLAGE	Uncharacterized protein (Fragment)	Blattella germanica		9		6.7e-240
>	A0A1I8MLE7_MUSDO	Uncharacterized protein	Musca domestica		2		9.9e-225
>	B4K5W6_DROMO	Uncharacterized protein	Drosophila mojavensis		2		1.2e-219
>	A0A182YGN2_ANOST	Uncharacterized protein	Anopheles stephensi		3		8.3e-208
>	A0A1J1IJQ6_9DIPT	CLUMA_CG013690, isoform A	Clunio marinus		6		[illegible]

(show all) alignments Your search took: 8.88 secs showing rows 1 - 100 of 73714



Target			Description					Species	Identical Seqs	# hits	Hit Positions	E-value
start	end	start	end	start	end						Ind.	Cond.
1	208	1	209	1	208	2.26	0.99	95.2 (198)	98.1 (204)	452.8	8.7e-133	5.1e-136

```
                .........*.........*.........*.........*.........*.........*.........*.........*
Query        1 mvdfyylpgsspcrsvimtakavgvelnkkllnlqagehlkpeflkinpqhtiptlvdngfalwesraiqvylvekygkt 80
               m dfyylpgs+pcrsvimtakavgvelnkkllnlqagehlkpeflkinpqhtiptlvdngfalwesraiqvylvekygkt
Target       1 MADFYYLPGSAPCRSVIMTAKAVGVELNKKLLNLQAGEHLKPEFLKINPQHTIPTLVDNGFALWESRAIQVYLVEKYGKT 80
PP             78******************************************************************************

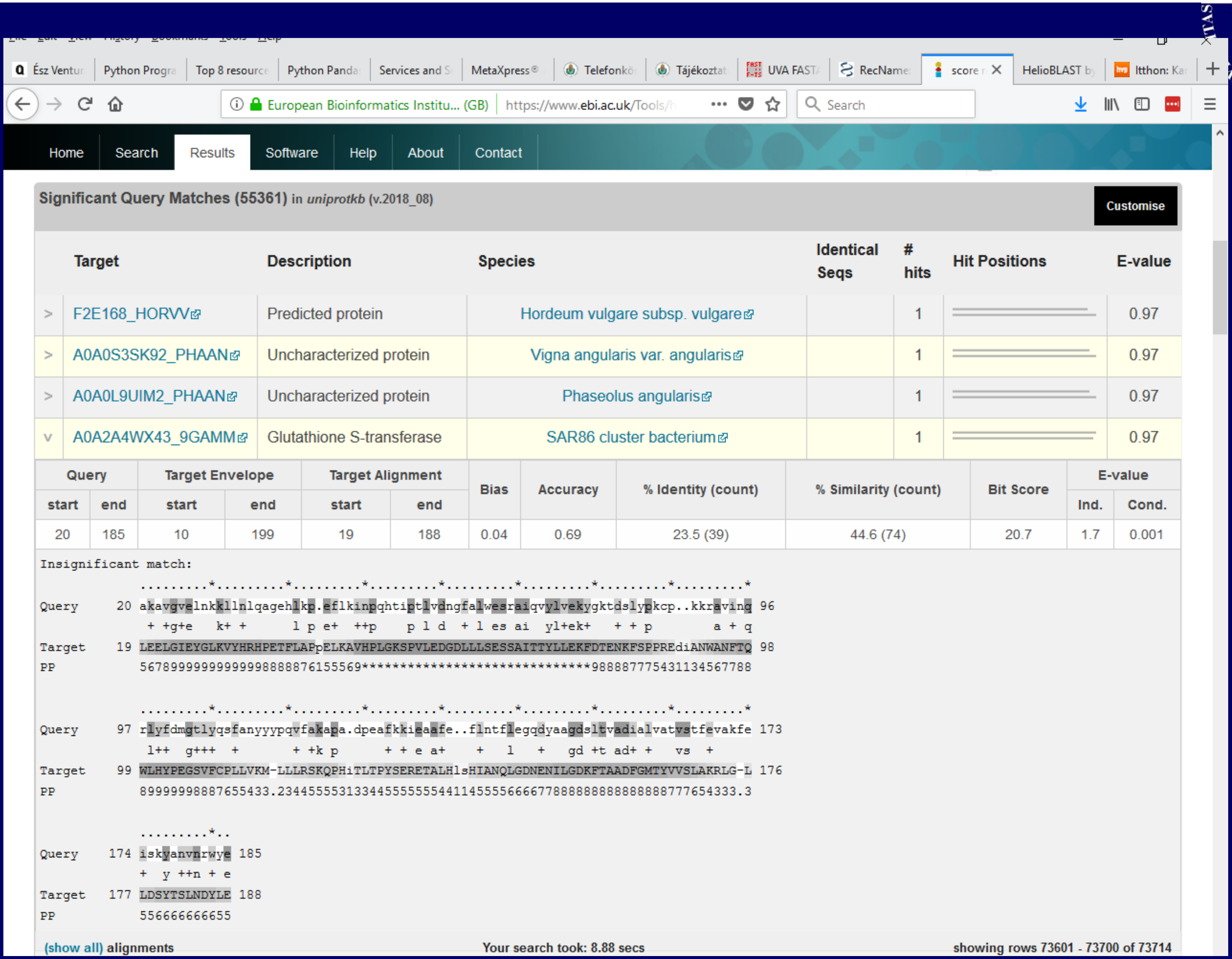
                .........*.........*.........*.........*.........*.........*.........*.........*
Query       81 dslypkcpkkravinqrlyfdmgtlyqsfanyyypqvfakapadpeafkkieaafeflntflegqdyaagdsltvadial 160
               dslypkcpkkravinqrlyfdmgtlyqsfanyyypq+fakapadpeafkkieaafeflntflegq+yaagdsltvadial
Target      81 DSLYPKCPKKRAVINQRLYFDMGTLYQSFANYYYPQLFAKAPADPEAFKKIEAAFEFLNTFLEGQEYAAGDSLTVADIAL 160
PP             ********************************************************************************

                .........*.........*.........*.........*........
Query      161 vatvstfevakfeiskyanvnrwyenakkvtpgweenwagclefkkyf 208
               va+vstfeva feiskyanvn+wyenakkvtpgweenw gc efkk+f
Target     161 VASVSTFEVAGFEISKYANVNKWYENAKKVTPGWEENWEGCQEFKKFF 208
PP             ***********************************************9
```

Query		Target Envelope		Target Alignment		Bias	Accuracy	% Identity (count)	% Similarity (count)	Bit Score	E-value	
start	end	start	end	start	end						Ind.	Cond.
1	209	212	420	212	420	2.00	1.00	82.3 (172)	92.3 (193)	392.9	1.8e-114	1.1e-117

```
                .........*.........*.........*.........*.........*.........*.........*.........*
Query        1 mvdfyylpgsspcrsvimtakavgvelnkkllnlqagehlkpeflkinpqhtiptlvdngfalwesraiqvylvekygkt 80
               mvd+yy+p s pc+ v+mtakavgv+lnkkl+n+   ehlkpeflk+npqhtiptlvdngfalwesrai vylvekygkt
Target     212 MVDLYYMPCSPPCHPVFMTAKAVGVKLNKKLVNVWDDEHLKPEFLKLNPQHTIPTLVDNGFALWESRAILVYLVEKYGKT 291
PP             89******************************************************************************
```

(show all) alignments   Your search took: 8.88 secs   showing rows 1 - 100 of 73714



Significant Query Matches (55361) in *uniprotkb* (v.2018_08)

	Target	Description	Species	Identical Seqs	# hits	Hit Positions	E-value
>	F2E168_HORVV	Predicted protein	Hordeum vulgare subsp. vulgare		1		0.97
>	A0A0S3SK92_PHAAN	Uncharacterized protein	Vigna angularis var. angularis		1		0.97
>	A0A0L9UIM2_PHAAN	Uncharacterized protein	Phaseolus angularis		1		0.97
v	A0A2A4WX43_9GAMM	Glutathione S-transferase	SAR86 cluster bacterium		1		0.97

Query		Target Envelope		Target Alignment		Bias	Accuracy	% Identity (count)	% Similarity (count)	Bit Score	E-value	
start	end	start	end	start	end						Ind.	Cond.
20	185	10	199	19	188	0.04	0.69	23.5 (39)	44.6 (74)	20.7	1.7	0.001

```
Insignificant match:
             .........*.........*.........*.........*.........*.........*.........*.........*
Query     20 akavgvelnkkllnlqagehlkp.eflkinpqhtiptlvdngfalwesraiqvylvekygktdslypkcp..kkravinq 96
              + +g+e   k+ +      l p e+  ++p    p l d  + l es ai  yl+ek+   + + p        a + q
Target    19 LEELGIEYGLKVYHRHPETFLAPpELKAVHPLGKSPVLEDGDLLLSESSAITTYLLEKFDTENKFSPPREdiANWANFTQ 98
PP           56789999999999998888876155569******************************988887775431134567788

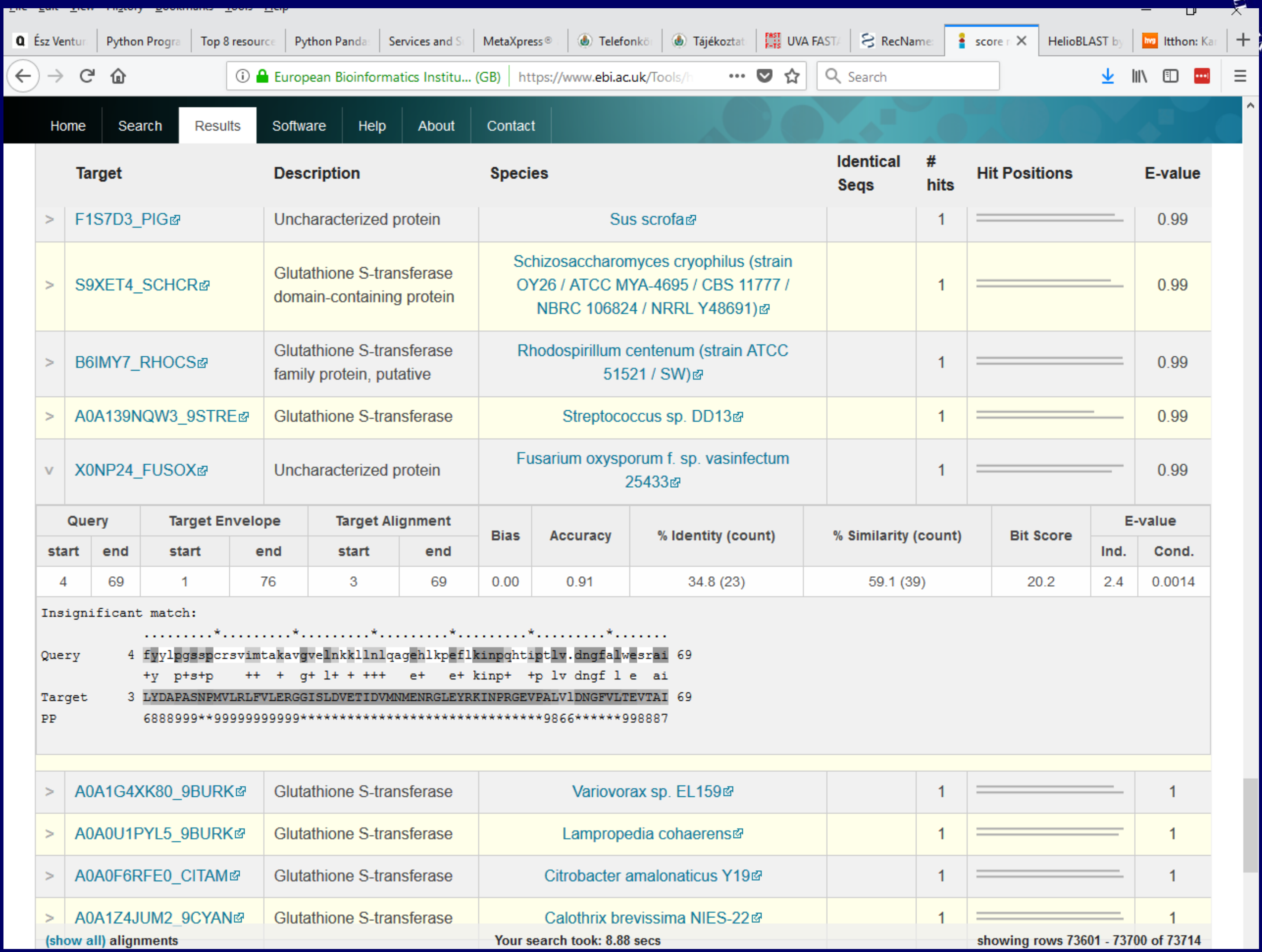
             .........*.........*.........*.........*.........*.........*.........*.........*
Query     97 rlyfdmgtlyqsfanyyypqvfakapa.dpeafkkieaafe..flntflegqdyaagdsltvadialvatvstfevakfe 173
              l++  g+++  +       + +k p      + + e a+    +   l   +   gd +t ad+ +   vs  +
Target    99 WLHYPEGSVFCPLLVKM-LLLRSKQPHiTLTPYSERETALHlsHIANQLGDNENILGDKFTAADFGMTYVVSLAKRLG-L 176
PP           89999998887655433.23445555313344555555441145555666677888888888888888777654333.3

             .........*..
Query    174 iskyanvnrwye 185
             +  y ++n + e
Target   177 LDSYTSLNDYLE 188
PP           556666666655
```

(show all) alignments

Your search took: 8.88 secs

showing rows 73601 - 73700 of 73714



	Target	Description	Species	Identical Seqs	# hits	Hit Positions	E-value
>	F1S7D3_PIG	Uncharacterized protein	Sus scrofa		1		0.99
>	S9XET4_SCHCR	Glutathione S-transferase domain-containing protein	Schizosaccharomyces cryophilus (strain OY26 / ATCC MYA-4695 / CBS 11777 / NBRC 106824 / NRRL Y48691)		1		0.99
>	B6IMY7_RHOCS	Glutathione S-transferase family protein, putative	Rhodospirillum centenum (strain ATCC 51521 / SW)		1		0.99
>	A0A139NQW3_9STRE	Glutathione S-transferase	Streptococcus sp. DD13		1		0.99
v	X0NP24_FUSOX	Uncharacterized protein	Fusarium oxysporum f. sp. vasinfectum 25433		1		0.99

Query		Target Envelope		Target Alignment		Bias	Accuracy	% Identity (count)	% Similarity (count)	Bit Score	E-value	
start	end	start	end	start	end						Ind.	Cond.
4	69	1	76	3	69	0.00	0.91	34.8 (23)	59.1 (39)	20.2	2.4	0.0014

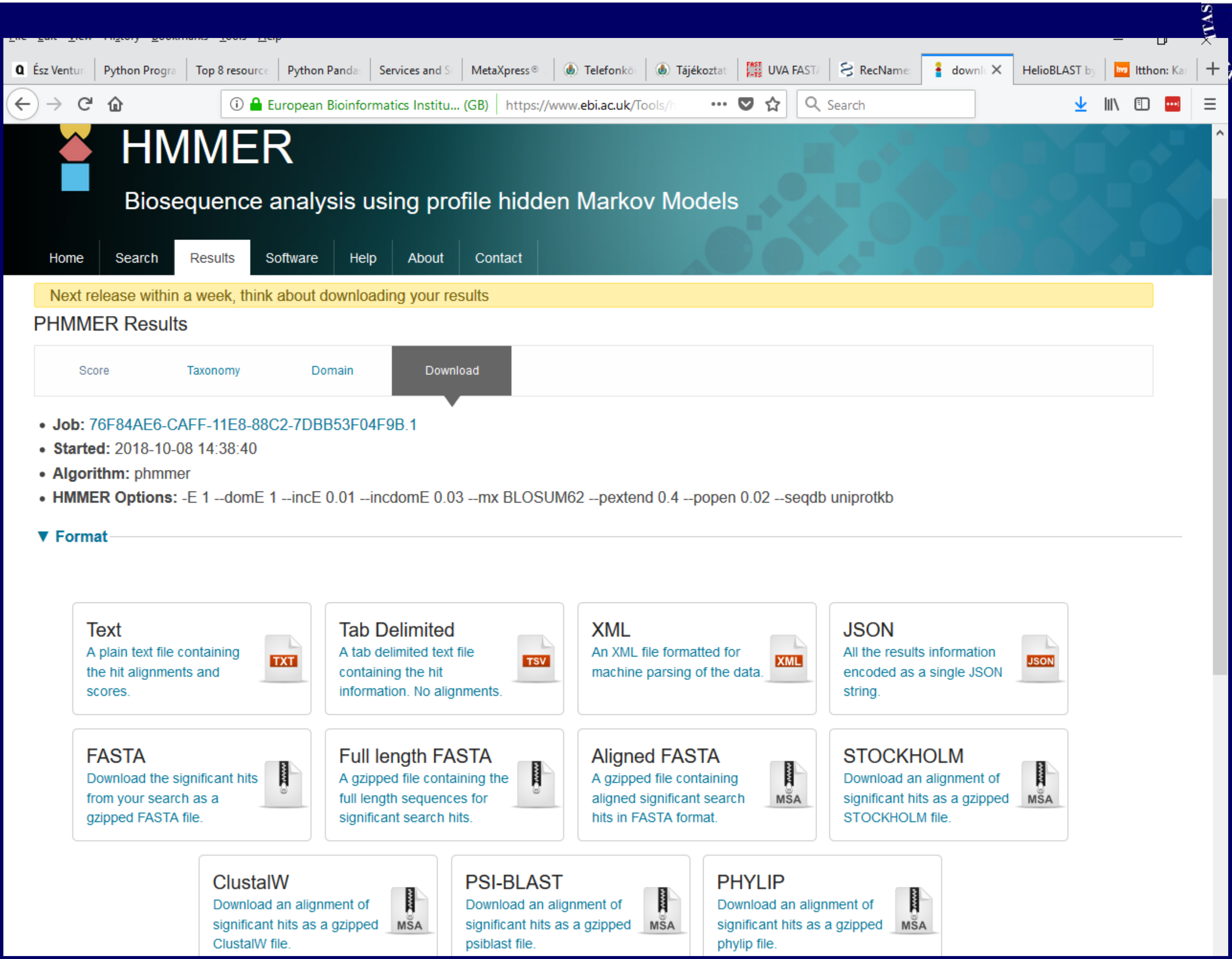
```
Insignificant match:
           .........*.........*.........*.........*.........*.........*.......
Query    4 fyylpgsspcrsvimtakavgvelnkklln1qagehlkpeflkinpqhtiptlv.dngfalwesrai 69
           +y  p+s+p    ++  +  g+ l+ + +++   e+   e+ kinp+  +p lv dngf l e  ai
Target   3 LYDAPASNPMVLRLFVLERGGISLDVETIDVMNMENRGLEYRKINPRGEVPALVlDNGFVLTEVTAI 69
PP         6888999**99999999999*******************************9866******998887
```

	Target	Description	Species	Identical Seqs	# hits	Hit Positions	E-value
>	A0A1G4XK80_9BURK	Glutathione S-transferase	Variovorax sp. EL159		1		1
>	A0A0U1PYL5_9BURK	Glutathione S-transferase	Lampropedia cohaerens		1		1
>	A0A0F6RFE0_CITAM	Glutathione S-transferase	Citrobacter amalonaticus Y19		1		1
>	A0A1Z4JUM2_9CYAN	Glutathione S-transferase	Calothrix brevissima NIES-22		1		1

(show all) alignments

Your search took: 8.88 secs

showing rows 73601 - 73700 of 73714



HMMER

Biosequence analysis using profile hidden Markov Models

Next release within a week, think about downloading your results

PHMMER Results

Score | Taxonomy | Domain | Download

- **Job:** 76F84AE6-CAFF-11E8-88C2-7DBB53F04F9B.1
- **Started:** 2018-10-08 14:38:40
- **Algorithm:** phmmer
- **HMMER Options:** -E 1 --domE 1 --incE 0.01 --incdomE 0.03 --mx BLOSUM62 --pextend 0.4 --popen 0.02 --seqdb uniprotkb

▼ **Format**

Text — A plain text file containing the hit alignments and scores. (TXT)

Tab Delimited — A tab delimited text file containing the hit information. No alignments. (TSV)

XML — An XML file formatted for machine parsing of the data. (XML)

JSON — All the results information encoded as a single JSON string. (JSON)

FASTA — Download the significant hits from your search as a gzipped FASTA file.

Full length FASTA — A gzipped file containing the full length sequences for significant search hits.

Aligned FASTA — A gzipped file containing aligned significant search hits in FASTA format. (MSA)

STOCKHOLM — Download an alignment of significant hits as a gzipped STOCKHOLM file. (MSA)

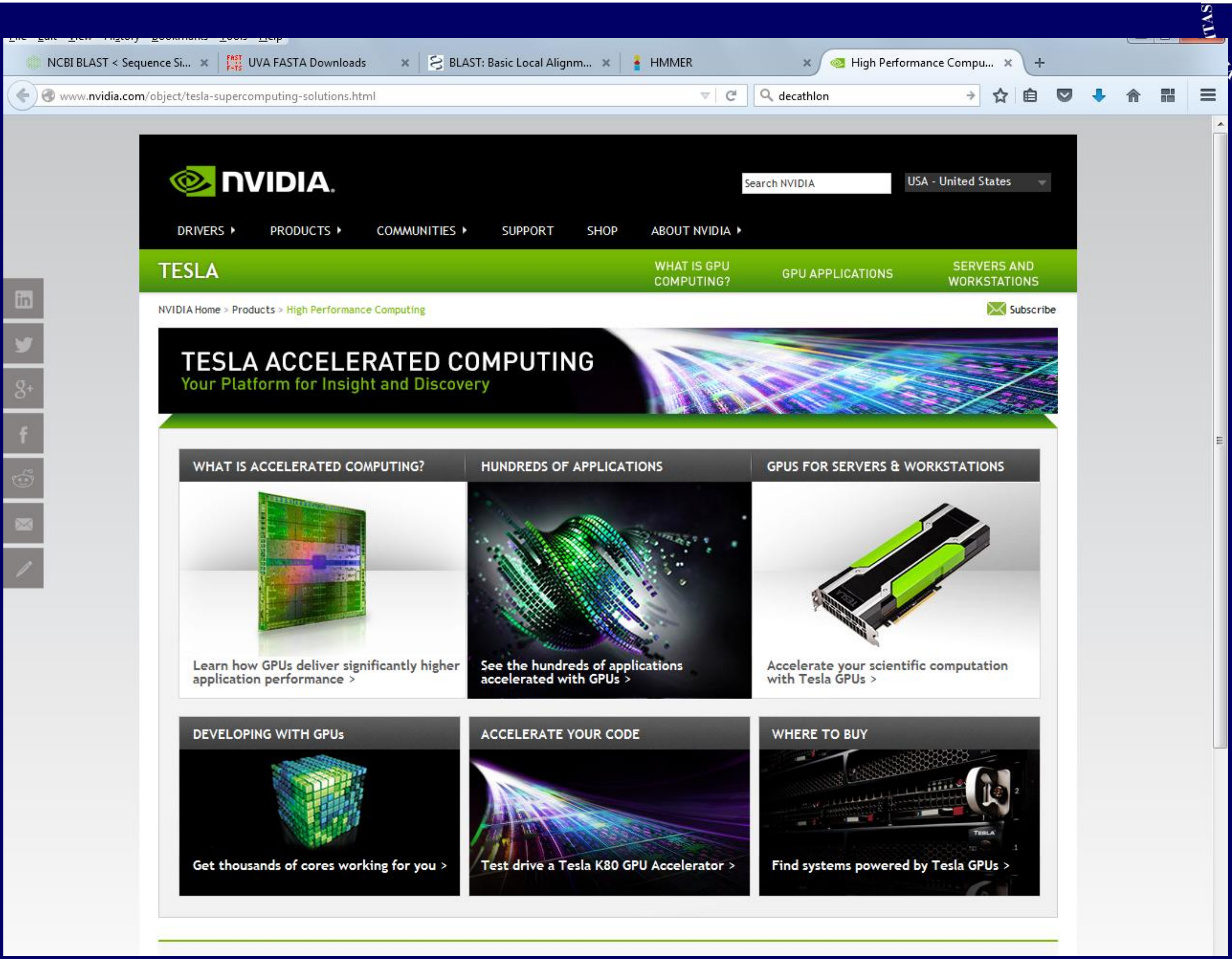
ClustalW — Download an alignment of significant hits as a gzipped ClustalW file. (MSA)

PSI-BLAST — Download an alignment of significant hits as a gzipped psiblast file. (MSA)

PHYLIP — Download an alignment of significant hits as a gzipped phylip file. (MSA)

Paralell keresés

- A szekvenciák sorrendje egy adatbázisban esetleges
- Nem kell sorban haladni a keresés során
- Több processzoros, több magos architekturán párhuzamosan lehet futtatni a keresést – GPU computing
- A párhuzamos futtatáshoz nemcsak a kódot kell átírni, de az algoritmust is



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UVA FASTA Downloads
BLAST: Basic Local Alignm...
HMMER
High Performance Compu...

www.nvidia.com/object/tesla-supercomputing-solutions.html

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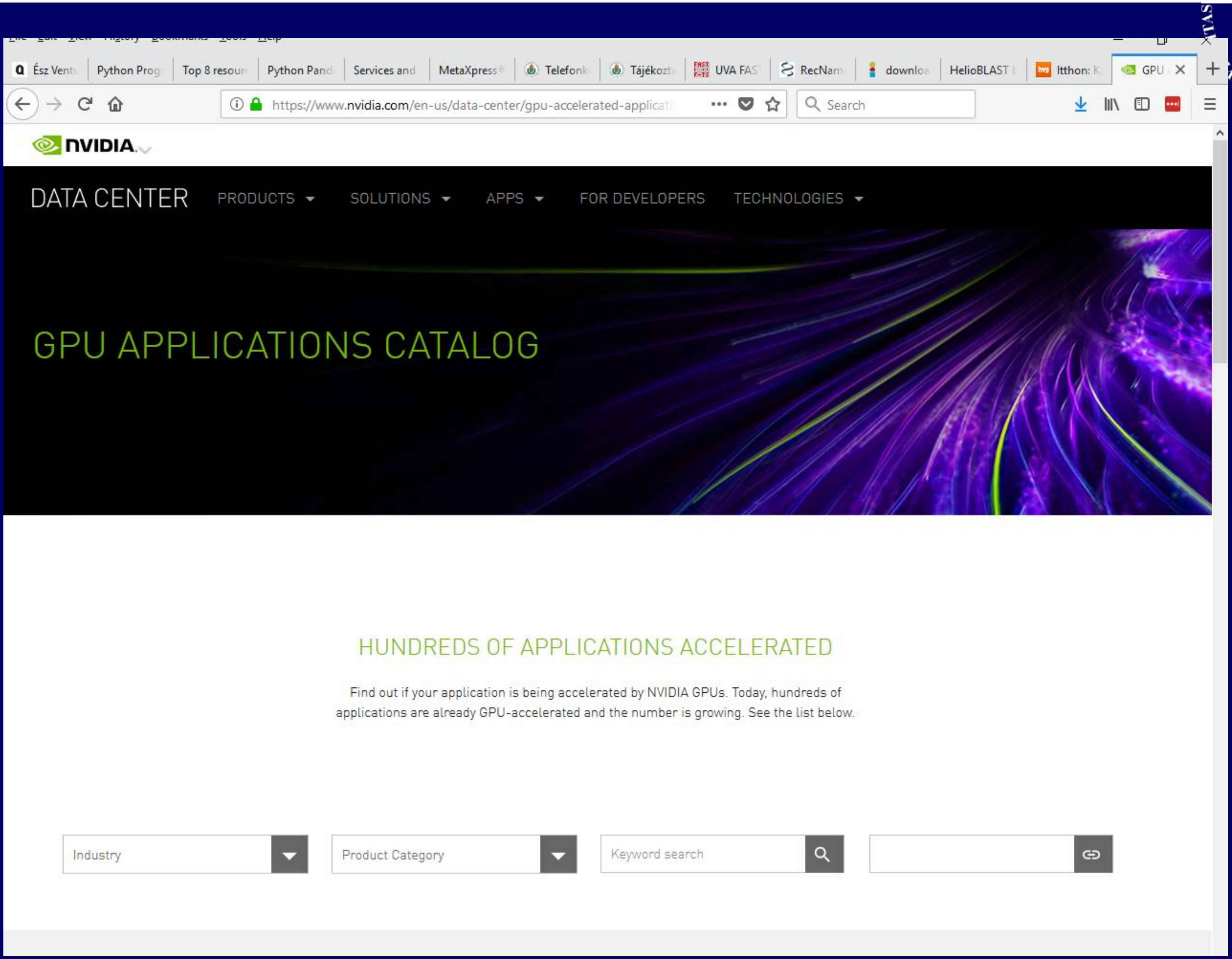
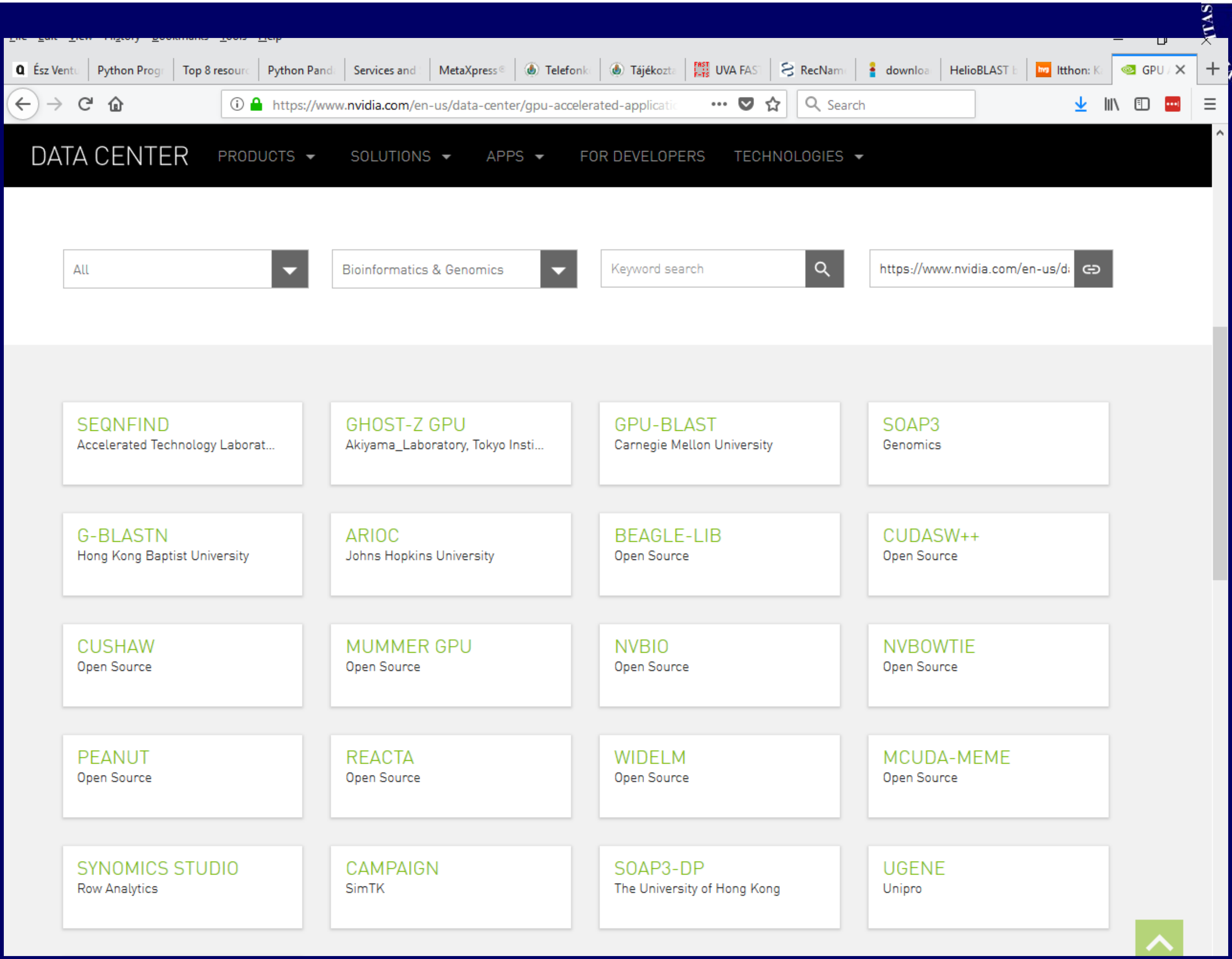


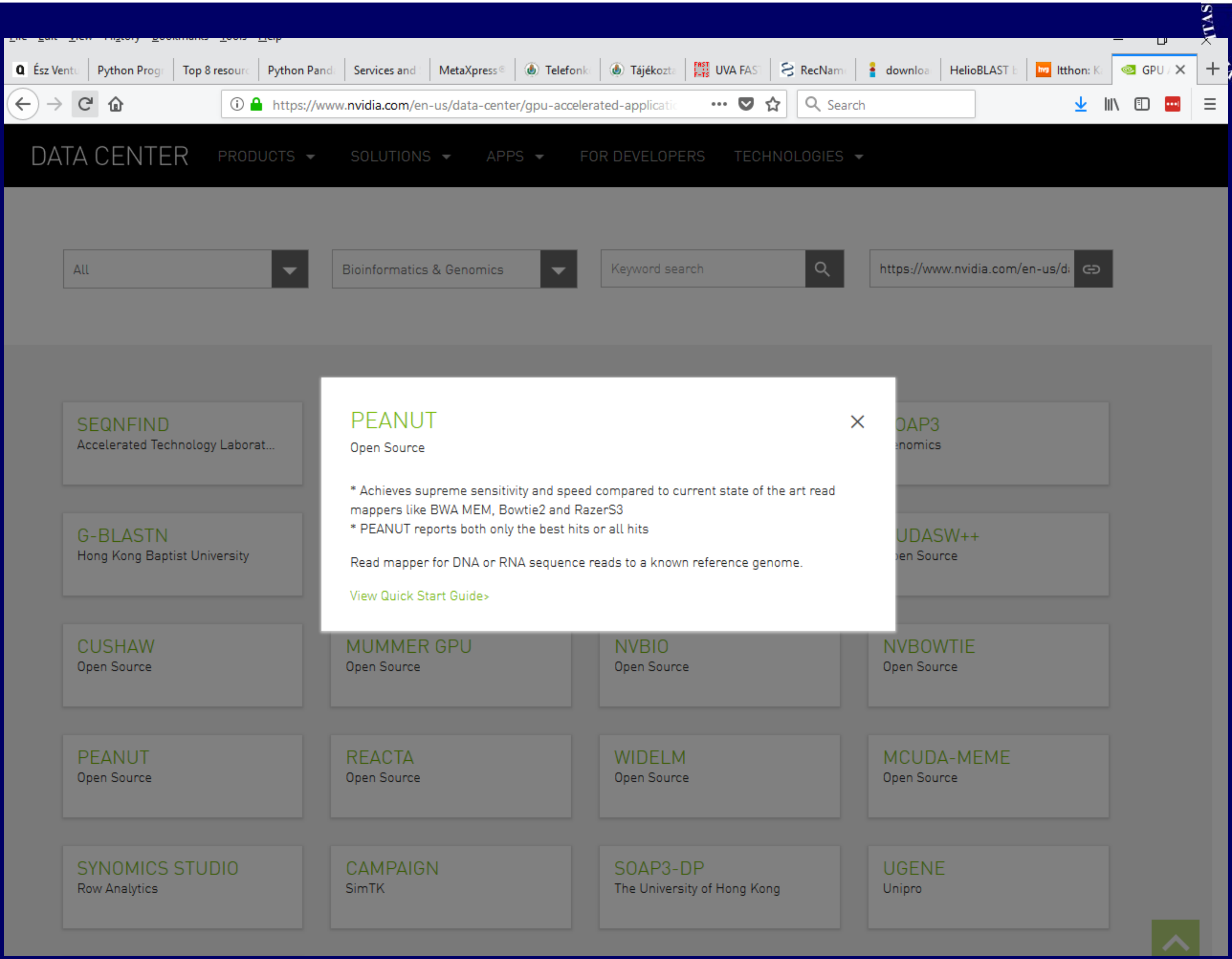
GPU APPLICATIONS CATALOG

HUNDREDS OF APPLICATIONS ACCELERATED

Find out if your application is being accelerated by NVIDIA GPUs. Today, hundreds of applications are already GPU-accelerated and the number is growing. See the list below.



SEQNFIND Accelerated Technology Laborat...	GHOST-Z GPU Akiyama_Laboratory, Tokyo Insti...	GPU-BLAST Carnegie Mellon University	SOAP3 Genomics
G-BLASTN Hong Kong Baptist University	ARIOC Johns Hopkins University	BEAGLE-LIB Open Source	CUDASW++ Open Source
CUSHAW Open Source	MUMMER GPU Open Source	NVBIO Open Source	NVBOWTIE Open Source
PEANUT Open Source	REACTA Open Source	WIDELM Open Source	MCUDA-MEME Open Source
SYNOMICS STUDIO Row Analytics	CAMPAIGN SimTK	SOAP3-DP The University of Hong Kong	UGENE Unipro



PEANUT
Open Source

* Achieves supreme sensitivity and speed compared to current state of the art read mappers like BWA MEM, Bowtie2 and RazerS3
* PEANUT reports both only the best hits or all hits

Read mapper for DNA or RNA sequence reads to a known reference genome.

View Quick Start Guide>

SEQNFIND
Accelerated Technology Laborat...

OAP3
enomics

G-BLASTN
Hong Kong Baptist University

UDASW++
pen Source

CUSHAW
Open Source

MUMMER GPU
Open Source

NVBIO
Open Source

NVBOWTIE
Open Source

PEANUT
Open Source

REACTA
Open Source

WIDELM
Open Source

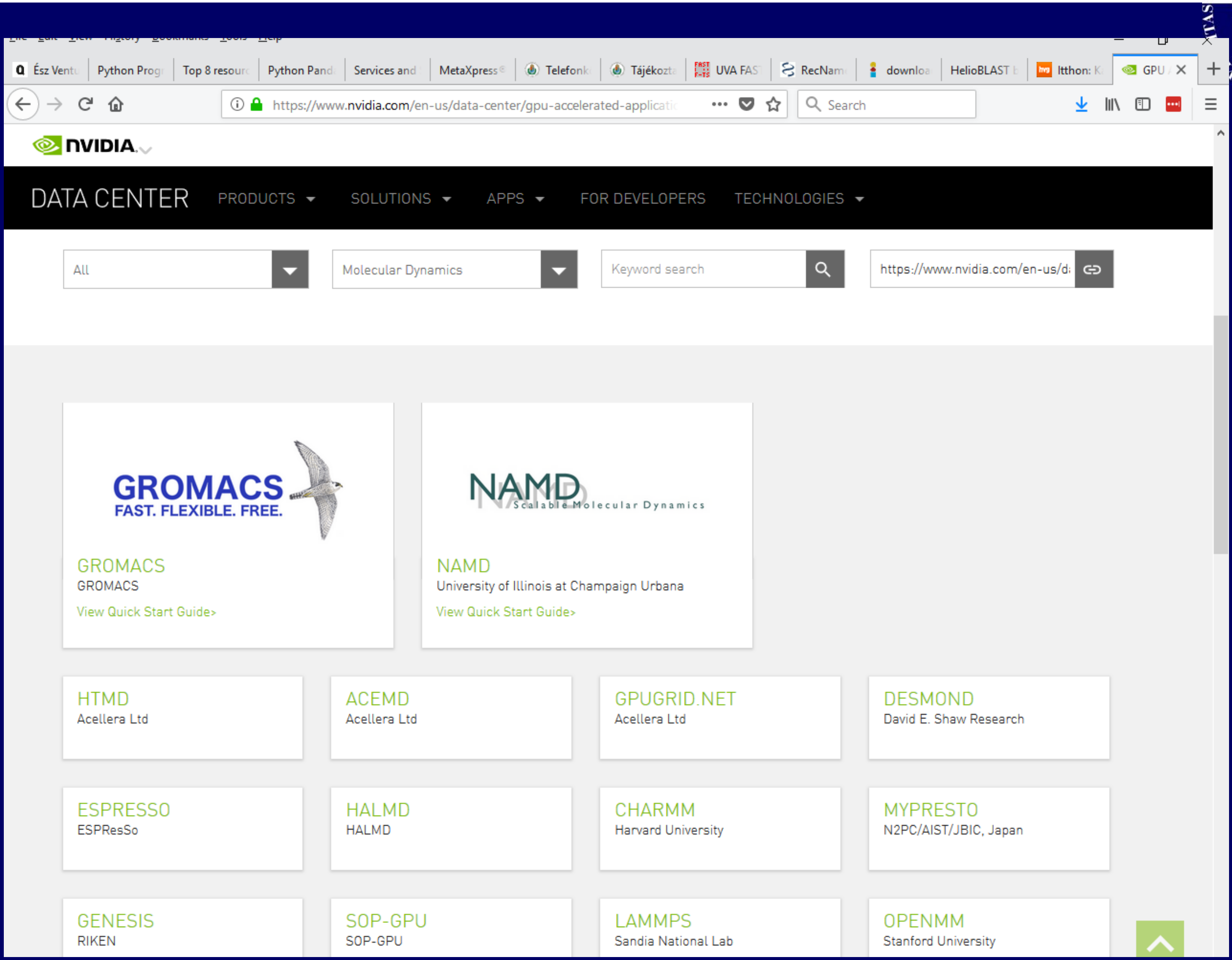
MCUDA-MEME
Open Source

SYNOMICS STUDIO
Row Analytics

CAMPAIGN
SimTK

SOAP3-DP
The University of Hong Kong

UGENE
Unipro



Molecular Dynamics

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University of Illinois at Champaign Urbana
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HALMD

CHARMM
Harvard University

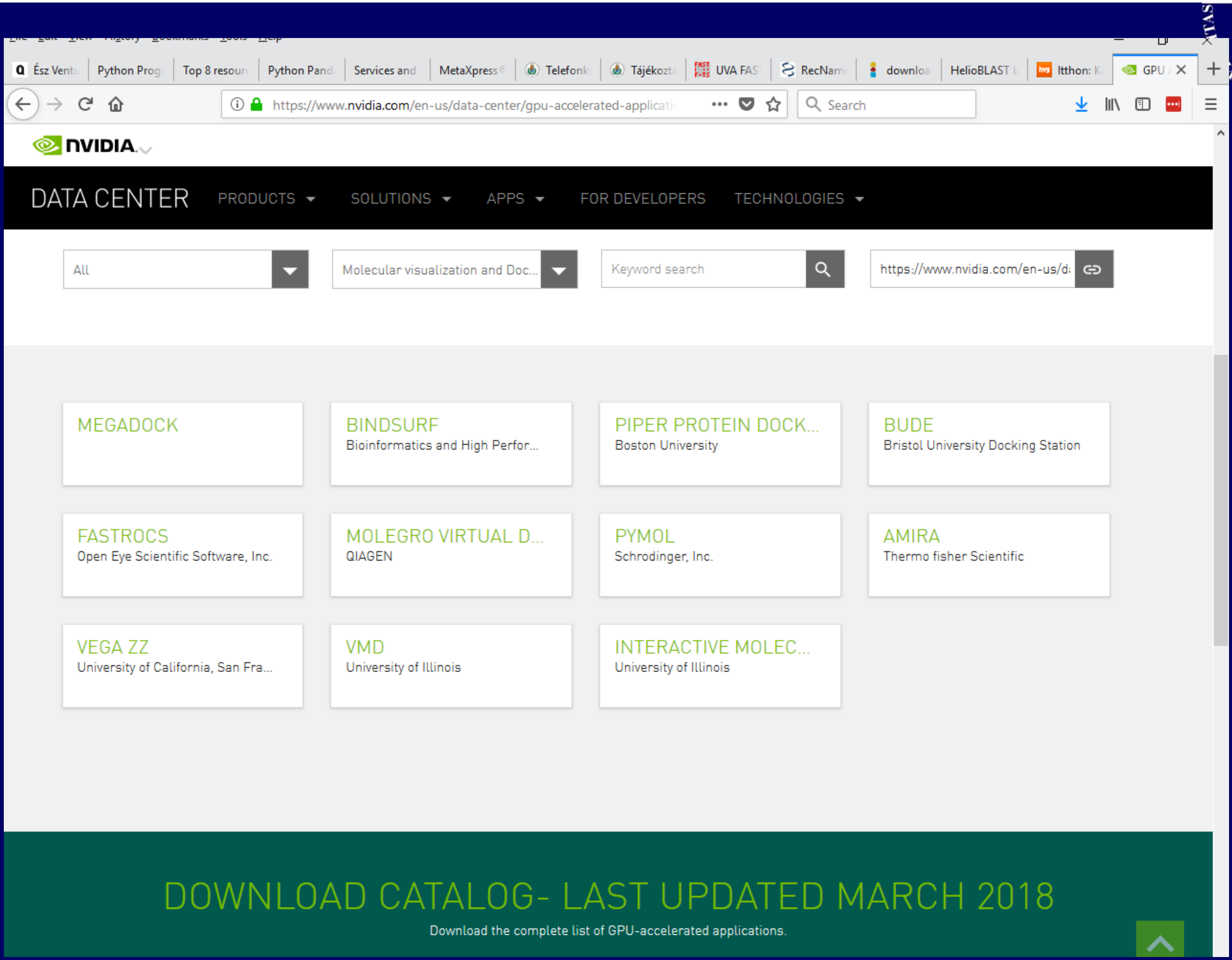
MYPRESTO
N2PC/AIST/JBIC, Japan

GENESIS
RIKEN

SOP-GPU
SOP-GPU

LAMMPS
Sandia National Lab

OPENMM
Stanford University



MEGADOCK	BINDSURF Bioinformatics and High Perfor...	PIPER PROTEIN DOCK... Boston University	BUDE Bristol University Docking Station
FASTROCS Open Eye Scientific Software, Inc.	MOLEGRO VIRTUAL D... QIAGEN	PYMOL Schrodinger, Inc.	AMIRA Thermo fisher Scientific
VEGA ZZ University of California, San Fra...	VMD University of Illinois	INTERACTIVE MOLEC... University of Illinois	

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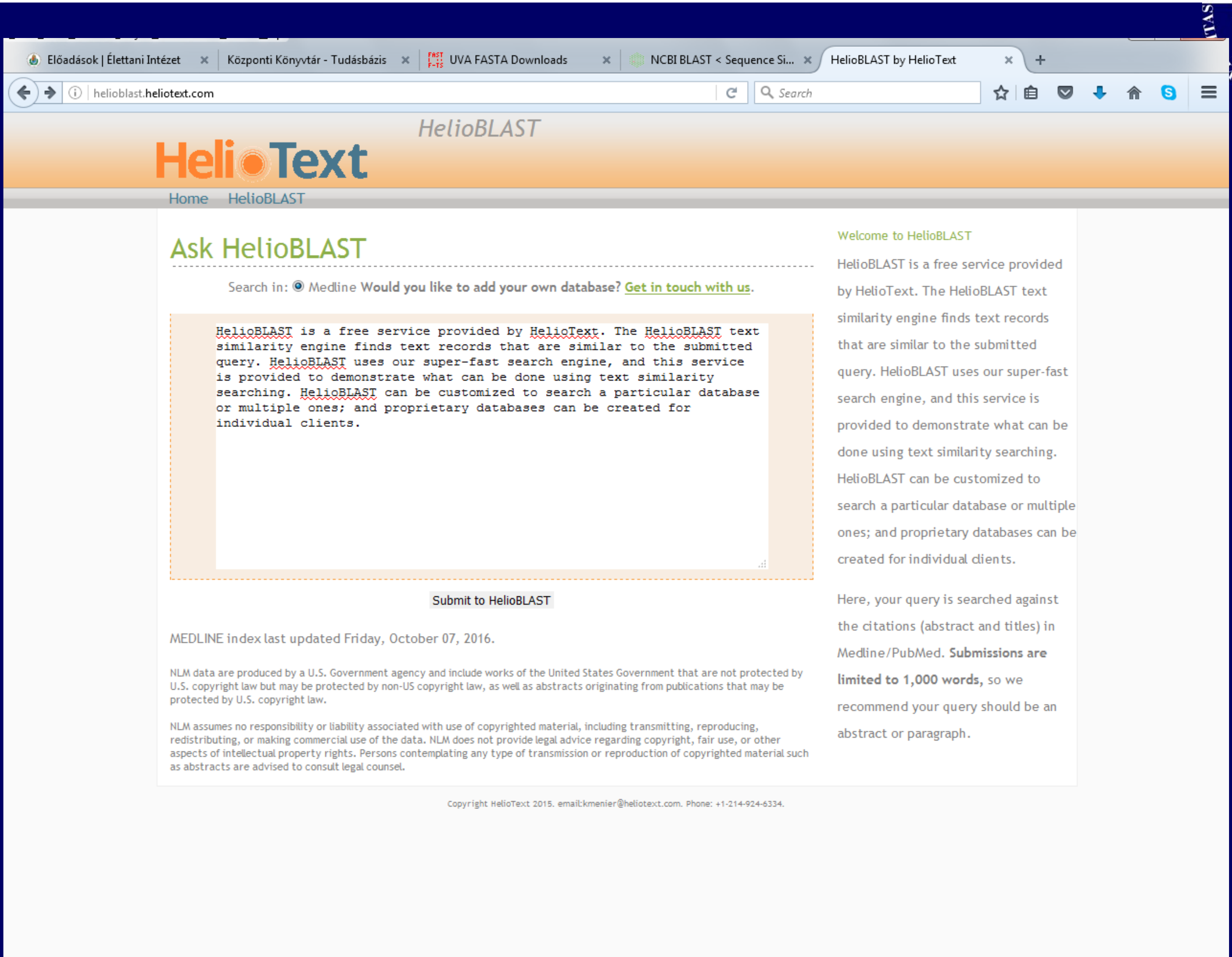
Adatbányászat

- Keresés szöveges adatbázisokban
- MEDLINE: tudományos szövegek kivonatai
- Ez is elsődleges adatbázis
- Igen nagy és ingyenesen elérhető
- Egy cikk mennyire hasonlít egy másikra?
- „számítógépes nyelvészet” – adatbányászat

eTBLAST

- Első fázis: súlyozott kulcsszó keresés
- Ez gyors, de nem túl érzékeny
- Második fázis: „mondat illesztő” lépés
- Ez az érzékenyebb
- Tartalmuk szerint hasonló cikkeket talál
- Javaslatot tesz a megfelelő újságra
- Hasonló érdeklődésű kutatókat azonosít
- http://helioblast.heliotext.com/



Ask HelioBLAST

Search in: ● Medline **Would you like to add your own database?** Get in touch with us.

HelioBLAST is a free service provided by HelioText. The HelioBLAST text similarity engine finds text records that are similar to the submitted query. HelioBLAST uses our super-fast search engine, and this service is provided to demonstrate what can be done using text similarity searching. HelioBLAST can be customized to search a particular database or multiple ones; and proprietary databases can be created for individual clients.

Submit to HelioBLAST

MEDLINE index last updated Friday, October 07, 2016.

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Here, your query is searched against the citations (abstract and titles) in Medline/PubMed. **Submissions are limited to 1,000 words,** so we recommend your query should be an abstract or paragraph.

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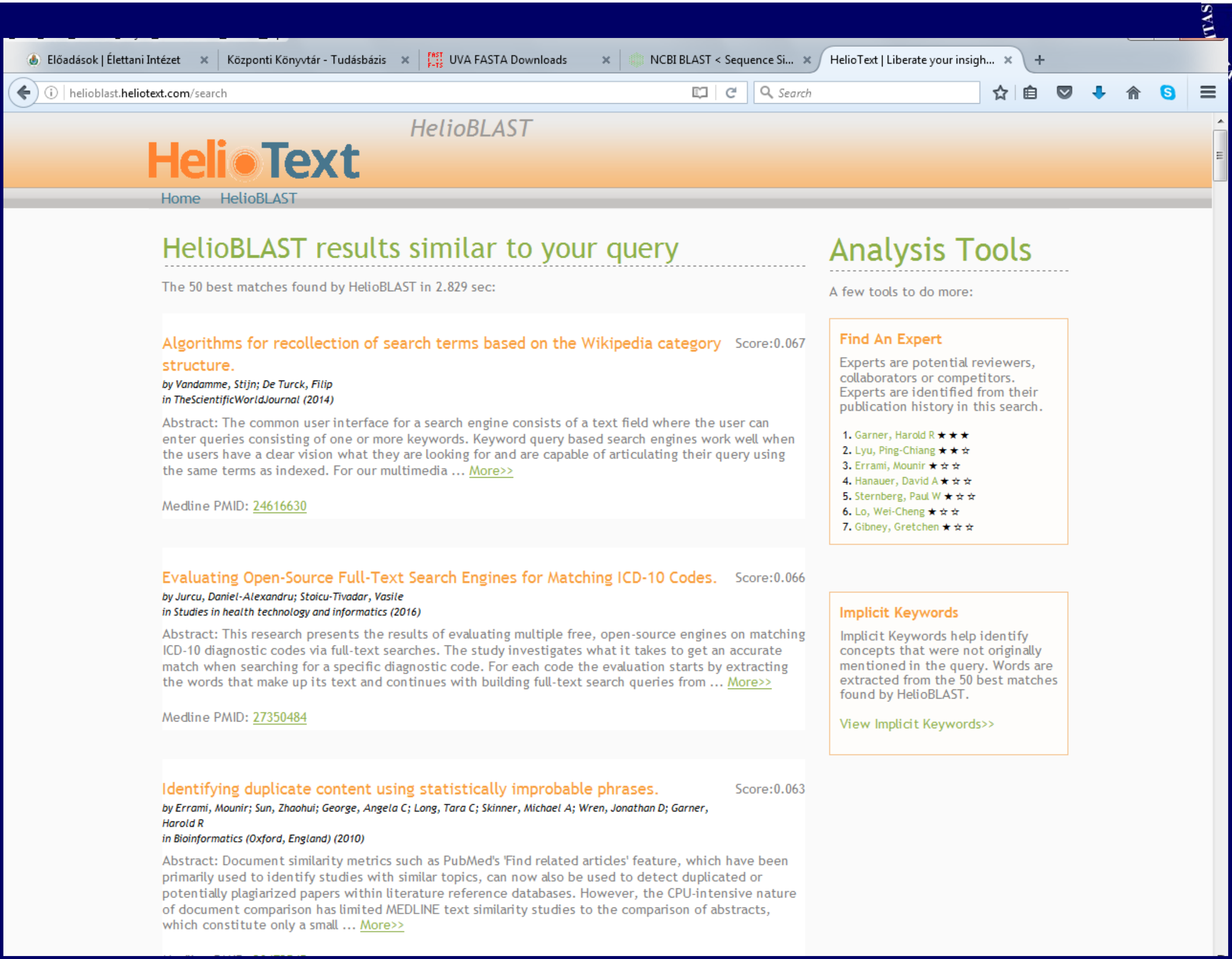
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HelioBLAST results similar to your query

The 50 best matches found by HelioBLAST in 2.829 sec:

Algorithms for recollection of search terms based on the Wikipedia category structure. Score:0.067

by Vandamme, Stijn; De Turck, Filip
in TheScientificWorldJournal (2014)

Abstract: The common user interface for a search engine consists of a text field where the user can enter queries consisting of one or more keywords. Keyword query based search engines work well when the users have a clear vision what they are looking for and are capable of articulating their query using the same terms as indexed. For our multimedia ... More>>

Medline PMID: 24616630

Evaluating Open-Source Full-Text Search Engines for Matching ICD-10 Codes. Score:0.066

by Jurcu, Daniel-Alexandru; Stoicu-Tivadar, Vasile
in Studies in health technology and informatics (2016)

Abstract: This research presents the results of evaluating multiple free, open-source engines on matching ICD-10 diagnostic codes via full-text searches. The study investigates what it takes to get an accurate match when searching for a specific diagnostic code. For each code the evaluation starts by extracting the words that make up its text and continues with building full-text search queries from ... More>>

Medline PMID: 27350484

Identifying duplicate content using statistically improbable phrases. Score:0.063

by Errami, Mounir; Sun, Zhaohui; George, Angela C; Long, Tara C; Skinner, Michael A; Wren, Jonathan D; Garner, Harold R
in Bioinformatics (Oxford, England) (2010)

Abstract: Document similarity metrics such as PubMed's 'Find related articles' feature, which have been primarily used to identify studies with similar topics, can now also be used to detect duplicated or potentially plagiarized papers within literature reference databases. However, the CPU-intensive nature of document comparison has limited MEDLINE text similarity studies to the comparison of abstracts, which constitute only a small ... More>>

Analysis Tools

A few tools to do more:

Find An Expert

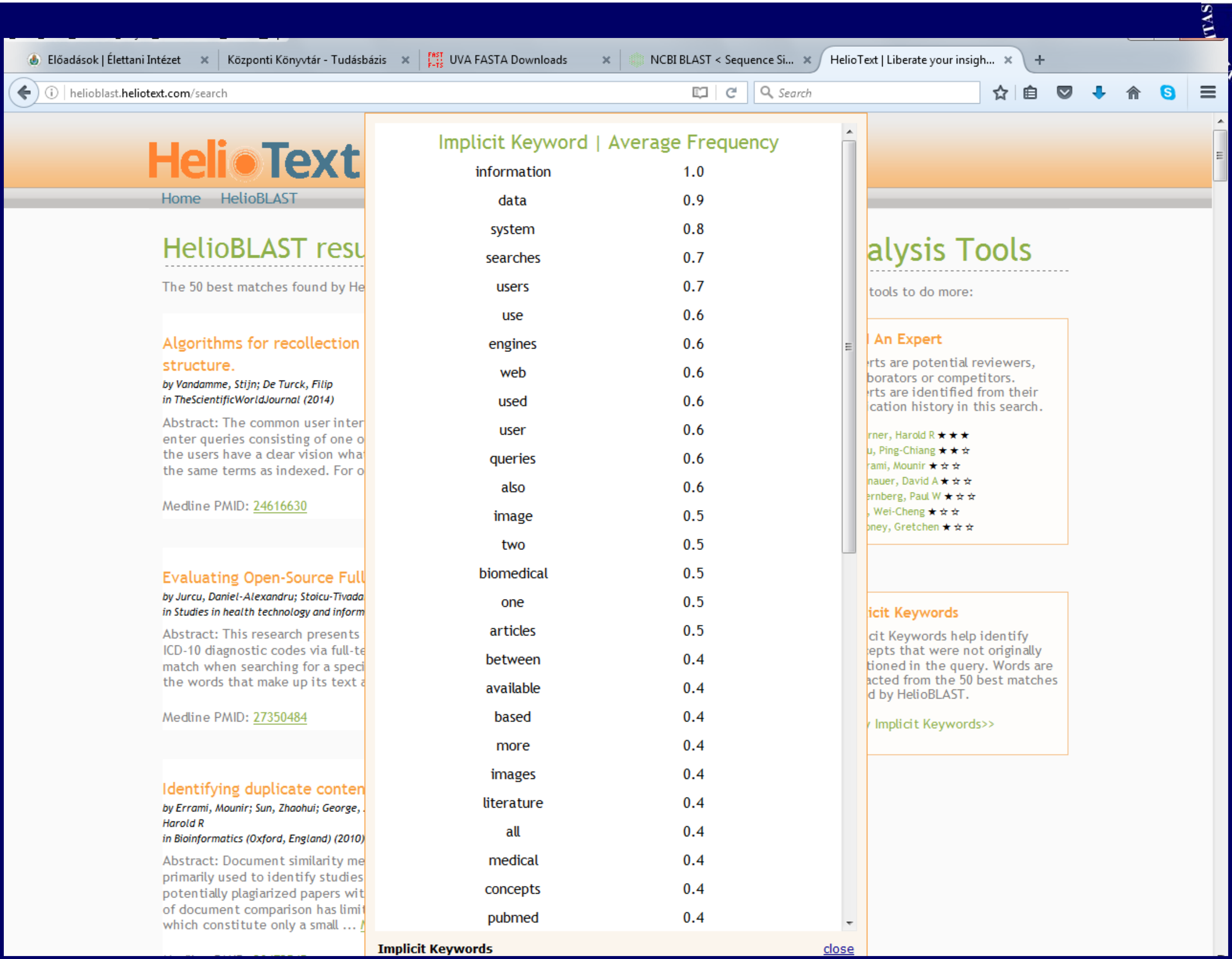
Experts are potential reviewers, collaborators or competitors. Experts are identified from their publication history in this search.

1. Garner, Harold R ★★★
2. Lyu, Ping-Chiang ★★☆
3. Errami, Mounir ★☆☆
4. Hanauer, David A ★☆☆
5. Sternberg, Paul W ★☆☆
6. Lo, Wei-Cheng ★☆☆
7. Gibney, Gretchen ★☆☆

Implicit Keywords

Implicit Keywords help identify concepts that were not originally mentioned in the query. Words are extracted from the 50 best matches found by HelioBLAST.

View Implicit Keywords>>



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The 50 best matches found by He

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Implicit Keyword	Average Frequency
information	1.0
data	0.9
system	0.8
searches	0.7
users	0.7
use	0.6
engines	0.6
web	0.6
used	0.6
user	0.6
queries	0.6
also	0.6
image	0.5
two	0.5
biomedical	0.5
one	0.5
articles	0.5
between	0.4
available	0.4
based	0.4
more	0.4
images	0.4
literature	0.4
all	0.4
medical	0.4
concepts	0.4
pubmed	0.4

Implicit Keywords close

alysis Tools

tools to do more:

An Expert

rts are potential reviewers, borators or competitors. rts are identified from their cation history in this search.

rner, Harold R ★★★
u, Ping-Chiang ★★☆
rami, Mounir ★☆☆
nauer, David A ★☆☆
rnberg, Paul W ★☆☆
, Wei-Cheng ★☆☆
oney, Gretchen ★☆☆

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Implicit Keywords>>

Mit tanultunk ma?

- Az adatbázis keresés lényegében nagyléptékű szekvenciaillesztés.
- Nagyon kiforrott technika.
- Gyakran a bioinformatikai vizsgálódás kiindulópontja.

Feladat 5.

- Válassz ki egy érdekes cikket és a kivonatával keress hasonlókat az et-blast rendszerben. Mennyire hatékony a szolgáltatás?
- Esetleg fogalmazd meg egy néhány mondatos kivonatban a téged érdeklő problémát és azzal keress.