

Exploring Biological Databases

Holger Dinkel

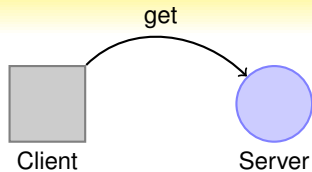
EMBO Practical Course Computational analysis of protein-protein interactions: From sequences to networks



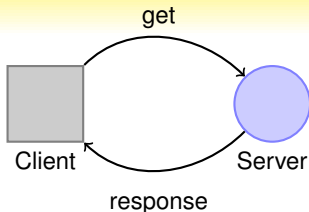
Client



Server



get: <http://www.uniprot.org/uniprot/P12931>

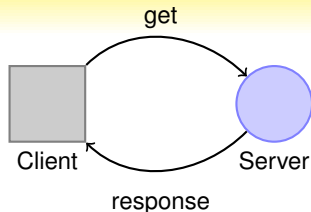


get: `http://www.uniprot.org/uniprot/P12931`
response: **HTML**

P12931 SPIC_HUMAN
Holo-photosynthetic lysine-proline kinase Bnc

Protein domain table:

Protein domain	Accession	Description	Start	End
SPIC_HUMAN	SPIC_HUMAN	SPIC_HUMAN	1	385
SPIC_HUMAN	SPIC_HUMAN	SPIC_HUMAN	1	385
SPIC_HUMAN	SPIC_HUMAN	SPIC_HUMAN	1	385
SPIC_HUMAN	SPIC_HUMAN	SPIC_HUMAN	1	385
SPIC_HUMAN	SPIC_HUMAN	SPIC_HUMAN	1	385
SPIC_HUMAN	SPIC_HUMAN	SPIC_HUMAN	1	385
SPIC_HUMAN	SPIC_HUMAN	SPIC_HUMAN	1	385
SPIC_HUMAN	SPIC_HUMAN	SPIC_HUMAN	1	385
SPIC_HUMAN	SPIC_HUMAN	SPIC_HUMAN	1	385
SPIC_HUMAN	SPIC_HUMAN	SPIC_HUMAN	1	385



get: <http://www.uniprot.org/uniprot/P12931.txt>
response: **TEXT/TSV**

```
ID SRC_HUMAN Reviewed; 536 AA.  
AC P12931; E1P5V4; Q76P87; Q86VB9; Q9H5A8;  
DT 01-OCT-1989, integrated into UniProtKB/Swiss-Prot.  
DT 23-JAN-2007, sequence version 3.  
DT 03-SEP-2014, entry version 187.  
DE RecName: Full=Proto-oncogene tyrosine-protein kinase Src;  
...
```

A RESTful application

is an application that exposes its state and functionality as a set of resources that the clients can manipulate and conforms to a certain set of principles:

- All resources are uniquely addressable, usually through URIs; other addressing can also be used, though.
- All resources can be manipulated through a constrained set of well-known actions, usually CRUD (create, read, update, delete), represented most often through the HTTP's POST, GET, PUT and DELETE; it can be a different set or a subset though - for example, some implementations limit that set to read and modify only (GET and PUT) for example
- The data for all resources is transferred through any of a constrained number of well-known representations, usually HTML, XML or JSON;
- The communication between the client and the application is performed over a *stateless* protocol that allows for multiple layered intermediaries that can reroute and cache the requests and response packets transparently for the client and the application.

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Method defines what you want to do (**GET**=retrieve, **POST**=create/update, **DELETE**=remove).

We'll be using just GET requests which can be thought of as read-only access. POST/DELETE are used to modify data on a server.

Protocol usually HTTP or HTTPS (secure)

URL defines a path to a resource

Parameters additional arguments, filters etc. usually in the form *parameter = value*; the first parameter is separated from the url by '?' while subsequent ones use '&'.

Example: searching for the term 'EMBO':

https://startpage.com/do/search?query=EMBO&with_language=lang_de

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Note:

For all these examples, any common browser can be used, however for proper 'programmatic' access tools such as 'curl' or 'wget' on the Linux/Mac commandline are much more efficient and can easily be incorporated into little scripts...

- Easy requests** The data can be requested with simple HTTP requests and returned in a variety of programatic and bioinformatical relevant formats such as JSON, XML, YAML and FASTA.
- Easy debugging** Debugging can be done in any browser. While some might not call this real programming, it surely is the first step towards programmatically querying resources.
- Reproducible** You can write all your queries into a simple script and repeat the same query later. Even just saving the URL as a bookmark in your browser helps!
 - Powerful** Any data can be made available via a REST service.
 - Bandwidth** An API allows programmatic access to some information if one does not want to download the entire dataset.
 - Standards** By using existing protocols and best-methods (HTTP), all the existing knowledge can be reused (Caching, Redirecting, ...).
- Widespread** More and more resource providers change from fat/heavy webservices to this lightweight system, for obvious reasons.

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Note:

Not meant to be a substitute for resources such as BioMART etc!

EXAMPLE: PHOSPHO.ELM

Phospho.ELM
a database of S/T/Y phosphorylation sites

Statistics:

Instances	42,575
Kinases	310
Reference	3,672
Sequences	11,223
Substrates	8,718

[Home](#) [PhosphoBlast](#) [Contribute](#) [Download](#) [Help](#) [Links](#) [About](#)

SEARCH

- for phosphorylation sites in proteins using protein name or gene name
(*eg. Paxillin, Shc, MAPK*)
- by UniPROT accession or Ensembl identifier:
(*eg. P12931 or P95211*)
- by selected kinase (List):
- by selected phospho-peptide binding domain (List):
- Choose which organisms to include
 All
 Caenorhabditis
 Drosophila
 Vertebrates
- Do not show high throughput data
- Output as Comma-Separated-Values (.csv)

<http://phospho.elm.eu.org/index.html>

Access:

The PhosphoELM database can also be accessed via URL as follows:

- by **substrate name**:
<http://phospho.elm.eu.org/bySubstrate/Paxillin.html>
- by **Uniprot ID**:
<http://phospho.elm.eu.org/byAccession/P12931.html>
- by **Uniprot ID** and **Position**
<http://phospho.elm.eu.org/byAccession/P12931/Pos17.html>
- by **ENSEMBL ID** and multiple **Positions**
<http://phospho.elm.eu.org/byAccession/ENSP00000265709/Pos216,231.html>
- by **Uniprot name**:
http://phospho.elm.eu.org/byAccession/src_human.html
- by **Kinase**:
<http://phospho.elm.eu.org/byKinase/Abl2.html>
- by **Binding domain**:
http://phospho.elm.eu.org/byDomain/CBL_SH2.html
- retrieve a **stored Sequence**:
<http://phospho.elm.eu.org/P12931.fasta>
- retrieve data **as CSV**
<http://phospho.elm.eu.org/byAccession/P12931.csv>
- retrieve data for a single position **as CSV**
<http://phospho.elm.eu.org/byAccession/P12931/Pos12.csv>
- retrieve data for **multiple** IDs **as CSV**
<http://phospho.elm.eu.org/byAccession/P12931,P55211.csv>
- using **web-services**:
<http://phospho.elm.eu.org/webservice/phosphoELMdb.wsdl>

<http://phospho.elm.eu.org/byAccession/P55211.html>

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<http://phospho.elm.eu.org/bySubstrate/Paxillin.html>
- by **Uniprot ID**:
<http://phospho.elm.eu.org/byAccession/P12931.html>
- by **Uniprot ID** and **Position**
<http://phospho.elm.eu.org/byAccession/P12931/Pos17.html>
- by **ENSEMBL ID** and multiple **Positions**
<http://phospho.elm.eu.org/byAccession/ENSP00000265709/Pos216,231.html>
- by **Uniprot name**:
http://phospho.elm.eu.org/byAccession/src_human.html
- by **Kinase**:
<http://phospho.elm.eu.org/byKinase/Abl2.html>
- by **Binding domain**:
http://phospho.elm.eu.org/byDomain/CBL_SH2.html
- retrieve a **stored Sequence**:
<http://phospho.elm.eu.org/P12931.fasta>
- retrieve data **as CSV**
<http://phospho.elm.eu.org/byAccession/P12931.csv>
- retrieve data for a single position **as CSV**
<http://phospho.elm.eu.org/byAccession/P12931/Pos12.csv>
- retrieve data for **multiple** IDs **as CSV**
<http://phospho.elm.eu.org/byAccession/P12931,P55211.csv>
- using **web-services**:
<http://phospho.elm.eu.org/webservice/phosphoELMdb.wsdl>

<http://phospho.elm.eu.org/byAccession/P55211.csv>

EXAMPLE: PHOSPHO.ELM

Query

<http://phospho.elm.eu.org/bySubstrate/cd66.html>

Output:

Substrate: CD66 (Immunoglobulin)
Seq-ID: P13688 [*Homo sapiens*]
Interaction Network(s): NetworkKIN
External Source(s): PhosphoSitePlus
MINT Interaction(s): -
GO-Terms: [\[show\]](#)
Conservation: [Click on table headers for sorting](#)

Res.	Pos.	Sequence	Kinase	PMID	Src	Cons.	ELM	Binding Domain	SMART/Pfam	IUPRED score	PDB	P3D Acc.
Y	493	DEPHHSEVY Y SLHSFEAQP	-	9967848	LTP	1.00		-	-	0.65	-	low
S	508	FEAQPTQPT S ASPLATATEI	-	11850617	LTP	1.00		-	-	0.65	-	low
Y	520	SPSLATATEI Y SEVWQ	-	9967848	LTP	1.00		-	-	0.38	-	low

Substrate: CD66 (Immunoglobulin)
Seq-ID: P31809 [*Mus musculus*]
Interaction Network(s): -
External Source(s): PHOSIDA PhosphoSitePlus
MINT Interaction(s): -
GO-Terms: [\[show\]](#)
Conservation: [Click on table headers for sorting](#)

Res.	Pos.	Sequence	Kinase	PMID	Src	Cons.	ELM	Binding Domain	SMART/Pfam	IUPRED score	PDB	P3D Acc.
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http://phospho.elm.eu.org/bySubstrate/cd66.html

■ Query by Substrate name

■ Substrate name

■ Output as HTML

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------	------	----------	--------	------	-----	-------	-----	----------------	------------	--------------	-----	----------

Query

<http://phospho.elm.eu.org/byAccession/P12931/Pos12,17.csv>

Output:

```
Acc.; Res.; Pos.; Context; Kinase; PMID; Source; ConScore; ELM; Domain; SMART; IUPRED; PDB; P3D-
P12931; S; 12; SNKSKPKDASQRRRSLEPAE; none; 2136766; 1; 0.21; ; -; ; 0.9168; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; none; 18088087; 2; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; none; 17192257; 2; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; none; 17081983; 2; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; PKA_group; 11804588; 1; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
...
```

Query

<http://phospho.elm.eu.org/byAccession/P12931/Pos12,17.csv>

- **query by Uniprot Accession**
- Protein Sequence Accession/ID
- Position / multiple Positions
- Output as CSV (character separated values)

Output:

```
Acc.; Res.; Pos.; Context; Kinase; PMID; Source; ConScore; ELM; Domain; SMART; IUPRED; PDB; P3D-
P12931; S; 12; SNKSKPKDASQRRRSLEPAE; none; 2136766; 1; 0.21; ; -; ; 0.9168; -; ;
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Acc.; Res.; Pos.; Context; Kinase; PMID; Source; ConScore; ELM; Domain; SMART; IUPRED; PDB; P3D-
P12931; S; 12; SNKSKPKDASQRRRSLEPAE; none; 2136766; 1; 0.21; ; -; ; 0.9168; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; none; 18088087; 2; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; none; 17192257; 2; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; none; 17081983; 2; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; PKA_group; 11804588; 1; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
...
```

Query

<http://phospho.elm.eu.org/byAccession/P12931/Pos12,17.csv>

- query by Uniprot Accession
- Protein Sequence Accession/ID
- **Position / multiple Positions**
- Output as CSV (character separated values)

Output:

```
Acc.; Res.; Pos.; Context; Kinase; PMID; Source; ConScore; ELM; Domain; SMART; IUPRED; PDB; P3D-
P12931; S; 12; SNKSKPKDASQRRRSLEPAE; none; 2136766; 1; 0.21; ; -; ; 0.9168; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; none; 18088087; 2; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; none; 17192257; 2; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; none; 17081983; 2; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; PKA_group; 11804588; 1; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
...
```


Query

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- query by Uniprot Accession
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Output:

```
Acc.; Res.; Pos.; Context; Kinase; PMID; Source; ConScore; ELM; Domain; SMART; IUPRED; PDB; P3D-
P12931; S; 12; SNKSKPKDASQRRRSLEPAE; none; 2136766; 1; 0.21; ; -; ; 0.9168; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; none; 18088087; 2; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; none; 17192257; 2; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; none; 17081983; 2; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
P12931; S; 17; PKDASQRRRSLEPAENVHGA; PKA_group; 11804588; 1; 0.24; MOD_PKA_1; -; ; 0.8828; -; ;
...
```

EXAMPLE: ELM

Search ELM Instances

Full-Text Search (use "*" to get all instances)

P12931

Filter by instance Logic

Filter by organism



submit












Reset

export 5 instances as:

[gff](#) [pir](#) [fasta](#) [tsv](#)

5 Instances for search term 'P12931':

(click table headers for sorting; Notes column: =Number of Switches, =Number of Interactions)

ELM identifier	Acc., Gene-, Name	Start	End	Subsequence	Logic	#Ev.	Organism	Notes
LIG_SH2_SRC	 P12931 SRC SRC_HUMAN	530	533	AFLEDYFTSTEFQIQPGENL	TP	1	 Homo sapiens (Human)	1 
LIG_SH3_4	 P12931 SRC SRC_HUMAN	252	259	TVCPZSRPQIQGLAKDAKEI	TP	0	 Homo sapiens (Human)	
MOD_CDK_1	 P12931 SRC SRC_HUMAN	72	78	GFNSSDTYXSPQAGPLAGG	TP	1	 Homo sapiens (Human)	
MOD_NMyristoyl	 P12931 SRC SRC_HUMAN	1	7	HGSRKSRPKDASQRKSLRP	TP	0	 Homo sapiens (Human)	
MOD_TYR_CSK	 P12931 SRC SRC_HUMAN	526	534	AFLEDYFTSIRPQIQPGENL	TP	1	 Homo sapiens (Human)	

Please cite: The Eukaryotic Linear Motif Resource ELM: 10 Years and Counting (PMID:  24214962)

feedback@elm.eu.org

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EXAMPLE: ELM

Search ELM Instances

Full-Text Search (use *** to get all instances)

P12931

Filter by Instance Logic

Filter by organism

submit

Reset

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5 Instances for search term 'P12931':

(click table headers for sorting; Notes column: =Number of Switches, =Number of Interactions)

ELM identifier	Acc., Gene-, Name	Start	End	Subsequence	Logic	#Ev.	Organism	Notes
LIG_SH2_SRC	P12931 SRC SRC_HUMAN	530	533	AFLEDVFTSTEFQIQPSEKL	TP	1	Homo sapiens (Human)	1
LIG_SH3_4	P12931 SRC SRC_HUMAN	252	259	TVCPFRSPQVQGLAKDAHEI	TP	0	Homo sapiens (Human)	
MOD_CDK_1	P12931 SRC SRC_HUMAN	72	78	GFNSDDYVZSPQAGVLAGG	TP	1	Homo sapiens (Human)	
MOD_NMyristoyl	P12931 SRC SRC_HUMAN	1	7	HGGKASFPKDAQRRKLEP	TP	0	Homo sapiens (Human)	
MOD_TYR_CSK	P12931 SRC SRC_HUMAN	526	534	AFLEDVFTSREFQIQPSEKL	TP	1	Homo sapiens (Human)	

Please cite: The Eukaryotic Linear Motif Resource ELM: 10 Years and Counting (PMID: 24214962)

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ELM Downloads

Below you'll find examples of the different ways that can be used to query ELM programmatically. No special client is needed for this just a browser or maybe "curl"/"wget" for scripted access. By using these access methods you implicitly agree to using/distributing this data according to the [ELM Software License Agreement](#).

Classes

Last modified on: Aug. 14, 2015, 1:19 p.m.












Here you can download a list of ELM classes, either all at once or limit the list by providing a query term "q".

Name	Example	URL
all	 html /elms/elm_index.html	
all	 tsv /elms/elms_index.tsv	
by query term	 tsv /elms/elms_index.tsv?q=PCSK	
by ELM id	 html /ELME00012.html	

Instances

Last modified on: Aug. 13, 2015, 2:09 p.m.

Annotated ELM instances can be queried in a variety of ways. You are encouraged to use the **search form** to get a feeling for the parameters. Common examples include limiting the query by either instance logic or taxon.

Name	Example	URL
all	 html /elms/instances.html?q=*	
by Uniprot acc	 fasta instances.fasta?q=P12931	
by Uniprot name	 gff instances.gff?q=SRC_HUMAN	
by Uniprot acc	 tsv instances.tsv?q=P12931	
by query term	 pir instances.pir?q=PCSK	
by query term	 tsv instances.tsv?q=src	
by query term	 mitab instances.mitab?q=src	
by query term	 xml instances.psimi?q=src	
by query term using additional parameter "instance logic"	 tsv instances.tsv?q=src&instance_logic=true+positive	
by Instance id	 html /ELMI000123.html	
All docking motifs annotated in taxon	 fasta instances.fasta?taxon=PCSK	

- [Classes](#)
- [Instances](#)
- [Interactions](#)
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- [Methods](#)
- [PDBs](#)
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Classes

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Here you can download a list of ELM classes, either all at once or limit the list by providing a query term "q".

Name	Example	URL
all	 html /elms/elm_index.html	
all	 tsv /elms/elms_index.tsv	
by query term	 tsv /elms/elms_index.tsv?q=PCSK	
by ELM id	 html /ELME00012.html	

Instances

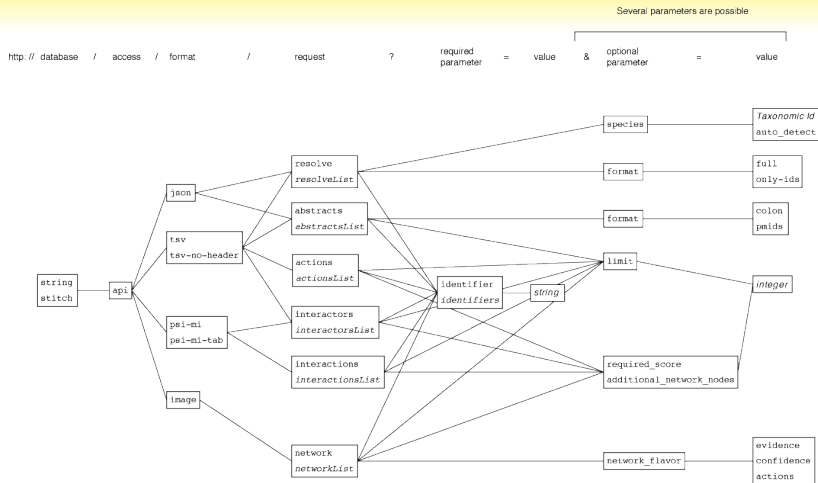
Last modified on: Aug. 13, 2015, 2:09 p.m.

Annotated ELM instances can be queried in a variety of ways. You are encouraged to use the [search form](#) to get a feeling for the parameters. Common examples include limiting the query by either instance logic or taxon.

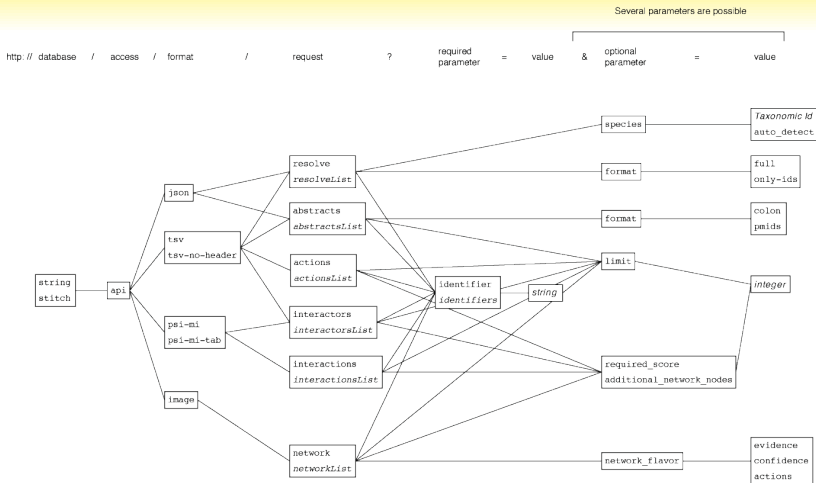
Name	Example	URL
all	 html /elms/instances.html?q=*	
by Uniprot acc	 fasta instances.fasta?q=P12931	
by Uniprot name	 gff instances.gff?q=SRC_HUMAN	
by Uniprot acc	 tsv instances.tsv?q=P12931	
by query term	 pir instances.pir?q=PCSK	
by query term	 tsv instances.tsv?q=src	
by query term	 mitab instances.mitab?q=src	
by query term	 xml instances.psimi?q=src	
by query term using additional parameter "instance logic"	 tsv instances.tsv?q=src&instance_logic=true+positive	
by Instance id	 html /ELMI000123.html	
All docking motifs annotated in taxon	 fasta instances.fasta?taxon=PCSK	

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- [Methods](#)
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- [GOTerms](#)
- [Renamed ELM classes](#)
- [Media / Files](#)

EXAMPLE: STRING / STITCH



EXAMPLE: STRING / STITCH



http://string-db.org/api/psi-mi-tab/interactions?identifier=YOL086C&additional_network_nodes=2

EXAMPLE: UNIPROT

UniProtKB Advanced

BLAST Align Retrieve/ID mapping Help Contact

UniProtKB results

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Filter by ¹

- Reviewed (54)
- Unreviewed (70)

Popular organisms

- Human (25)
- Mouse (21)
- Rat (10)
- Bovine (3)
- Zebrafish (2)

Other organisms

1 to 25 of 124

Entry	Entry name	Protein names	Gene names	Organism	Length
<input type="checkbox"/> P42684	ABL2_HUMAN	Abelson tyrosine-protein kinase 2	ABL2, ABL, ARG	Homo sapiens (Human)	1,182
<input type="checkbox"/> Q4JIM5	ABL2_MOUSE	Abelson tyrosine-protein kinase 2	Abl2, Arg	Mus musculus (Mouse)	1,182
<input type="checkbox"/> F8VQH0	F8VQH0_MOUSE	Non-specific protein-tyrosine kinas...	Abl2	Mus musculus (Mouse)	1,182
<input type="checkbox"/> B2RQ57	B2RQ57_MOUSE	Non-specific protein-tyrosine kinas...	Abl2	Mus musculus (Mouse)	1,078
<input type="checkbox"/> F1M0N1	F1M0N1_RAT	Non-specific protein-tyrosine kinas...	Abl2, Abl2_mapped, rCG_46463	Rattus norvegicus (Rat)	1,208
<input type="checkbox"/> A0A087WQB7	A0A087WQB7_MOUSE	Abelson tyrosine-protein kinase 2	Abl2	Mus musculus (Mouse)	269
<input type="checkbox"/> B0UXN7	B0UXN7_DANRE	Non-specific protein-tyrosine kinas...	abl2	Danio rerio (Zebrafish) (Brachydanio rerio)	1,135
<input type="checkbox"/> G1SVS3	G1SVS3_RABIT	Non-specific protein-tyrosine kinas...	ABL2	Oryctolagus cuniculus (Rabbit)	1,047

EXAMPLE: UNIPROT

UniProtKB Advanced

BLAST Align Retrieve/ID mapping Help Contact

UniProtKB results

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Swiss-Prot
- Unreviewed (70)
TrEMBL

Popular organisms

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- Rat (10)
- Bovine (3)
- Zebrafish (2)

Other organisms

BLAST Align 1 to 25 of 124 Show 25

Entry	Gene names	Organism	Length
<input type="checkbox"/> P42684	ABL2, ABL, ARG	Homo sapiens (Human)	1,182
<input type="checkbox"/> Q4JIM5	Abl2, Arg	Mus musculus (Mouse)	1,182
<input type="checkbox"/> FBVQH0	Abl2	Mus musculus (Mouse)	1,182
<input type="checkbox"/> B2RQ57	Abl2	Mus musculus (Mouse)	1,078
<input type="checkbox"/> F1M0N1	Non-specific protein-tyrosine kinases...	Rattus norvegicus (Rat)	1,208
<input type="checkbox"/> A0A087WQB7	Abelson tyrosine-protein kinase 2	Mus musculus (Mouse)	269
<input type="checkbox"/> B0UXN7	Non-specific protein-tyrosine kinases...	Danio rerio (Zebrafish) (Brachydanio rerio)	1,135
<input type="checkbox"/> G1SVS3	Non-specific protein-tyrosine kinases...	Oryctolagus cuniculus (Rabbit)	1,047

Download selected (0) Download all (124)

Format

- FASTA (canonical)
- FASTA (canonical & isoform)
- Tab-separated
- Text
- Excel
- GFF
- XML
- RDF/XML
- List

Questions?



EVERY TIME YOU ASK A STUPID QUESTION..

God kills a kitten.

motifake.com