Exploring Biological Databases

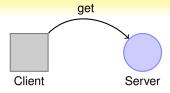
Holger Dinkel

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

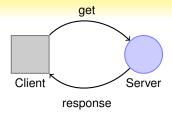




Client



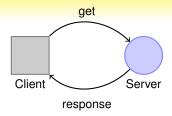
get: http://www.uniprot.org/uniprot/P12931



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

response: HTML





 $\underline{\underline{get}}: \texttt{http://www.uniprot.org/uniprot/P12931.txt}$

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;
...
```

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.

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.
- Reproducable 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!



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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- 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
- **w** 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

Query

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

Output:



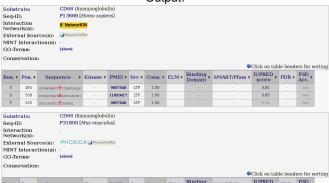
Exploring Biological Database

Query

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

- Query by Substrate name
- Substrate name
- Output as HTML

Output:

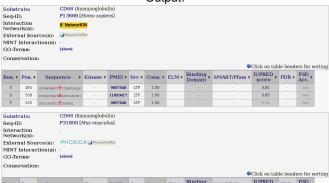


Exploring Biological Database

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

- Query by Substrate name
- Substrate name
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http://phospho.elm.eu.org/bySubstrate/cd66.html

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Query

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

```
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; -; ; ...
```

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)

```
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; -; ; ...
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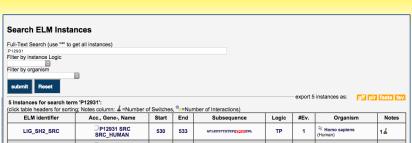
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ш	LEM Identifier	Addit delic , Hame	- Cturt		Gubbequenoc	Logio	,	O garnom	110100
į	LIG_SH2_SRC	⊋P12931 SRC SRC_HUMAN	530	533	AFLEDYFISTEPQ <u>YOPG</u> ENL	TP	1	S Homo sapiens (Human)	14
	LIG_SH3_4	P12931 SRC SRC_HUMAN	252	259	TVCPTS <u>KPOTOGLA</u> KDAWEI	TP	0	S Homo sapiens (Human)	
1	MOD_CDK_1	P12931 SRC SRC_HUMAN	72	78	GPNSSD <u>TYTSPOR</u> AGPLAGG	TP	1	S Homo sapiens (Human)	
	MOD_NMyristoyl	P12931 SRC SRC_HUMAN	1	7	MGSNKSKPKDASQRRRSLEP	TP	0	S Homo sapiens (Human)	
	MOD_TYR_CSK	P12931 SRC SRC_HUMAN	526	534	APLEDYPTSTEPQYOPGENL	TP	1	[≳] Homo sapiens (Human)	
- 1									

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

feedback@elm.eu.org

ELM data can be downloaded & distributed for non-commercial use according to the ELM Software License Agreement

EXAMPLE: ELM

Search ELM Instances

gff pir fasta tsv

(click table headers for sortin	g; Notes column: 🕹 =Number o	f Switches	, 🐂=Nur	nber of Interactions)				
ELM identifier	Acc., Gene-, Name	Start	End	Subsequence	Logic	#Ev.	Organism	Notes
LIG_SH2_SRC	P12931 SRC SRC_HUMAN	530	533	AFLEDYFISTEP <u>OYOPG</u> ENL	TP	1	€ Homo sapiens (Human)	14
LIG_SH3_4	P12931 SRC SRC_HUMAN	252	259	TVCPTS <u>KPOTOGLA</u> KDANEI	TP	0	€ Homo sapiens (Human)	
MOD_CDK_1	P12931 SRC SRC_HUMAN	72	78	GPNSSD <u>TVTSPOR</u> AGPLAGO	TP	1	€ Homo sapiens (Human)	
MOD_NMyristoyl	P12931 SRC SRC_HUMAN	1	7	MGSNKSK PKDASQRRRSLEP	TP	0	8 Homo sapiens (Human)	
MOD_TYR_CSK	P12931 SRC SRC_HUMAN	526	534	APLEDYPTSTEPQYOPGENL	TP	1	€ Homo sapiens (Human)	

Please cite: The Eukaryotic Linear Motif Resource ELM: 10 Years and Counting (PMID: 8 24214962)

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 "cur1"/"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
- Instances
- Interactions
 Interaction Domains
- Methods
 PDBs
- GOTerms
 Renamed ELM classes
- Media / Files

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		/imi /elms/elm_index.html	
all		lov /elms/elms_index.tsv	
by query term		<pre>lsv /elms/elms_index.tsv?q=PCSK</pre>	
by ELM id		html /ELME000012.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		

ELM Downloads

Below you'll find examples of the different ways that can be used to query ELM programmatically. No special clier is needed for this just a browser or maybe "ourl"/"wget" for scripted access. <u>By using these access methods yo</u> implicitly agree to using/distributing this data according to the ELM Software License Agreement.

Classes

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

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_ir	ndex.html
all		tsv /elms/elms_	index.tsv
by query terr	m	tsv /elms/elms_	index.tsv?q=PCSK
		html /ELME0000	12.html

Instances

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

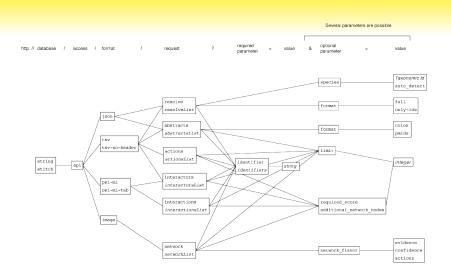
Annotated ELM instances can be queried in a variety of ways. You are encouraged to use the search form to get feeling for the parameters. Common examples include limiting the query by either instance logic or taxon.

Name	Example	
all	html /elms/in	stances.html?q=*
by Uniprot acc	fasta instance	es.fasta?q=P12931
by Uniprot name	gff instance	es.gff?q=SRC_HUMAN
by Uniprot acc	tsv instance	es.tsv?q=P12931
by query term	pir instance	es.pir?q=PCSK
by query term	tsv instance	es.tsv?q=src
by query term	mitab instance	es.mitab?q=src
by query term	xml instance	es.psimi?q=src
by query term using additional parameter "instance logic"	tsv instance	es.tsv?q=src&instance_logic=true+positive
by Instance id	li him /ELMI0	00123.html
All docking motifs annotated in taxon		

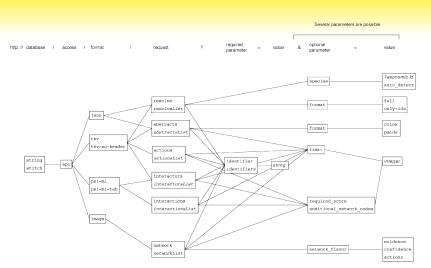
- Classos
- Instances
 - Interactions
- Methods
- PDBs
 - Renamed FLM classe
 - Media / Files

Exploring Biological Databases

EXAMPLE: STRING / STITCH



EXAMPLE: STRING / STITCH



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

EXAMPLE: UNIPROT



EXAMPLE: UNIPROT



Questions?



EVERY TIME YOU ASK A STUPID QUESTION...
God kills a kitten.