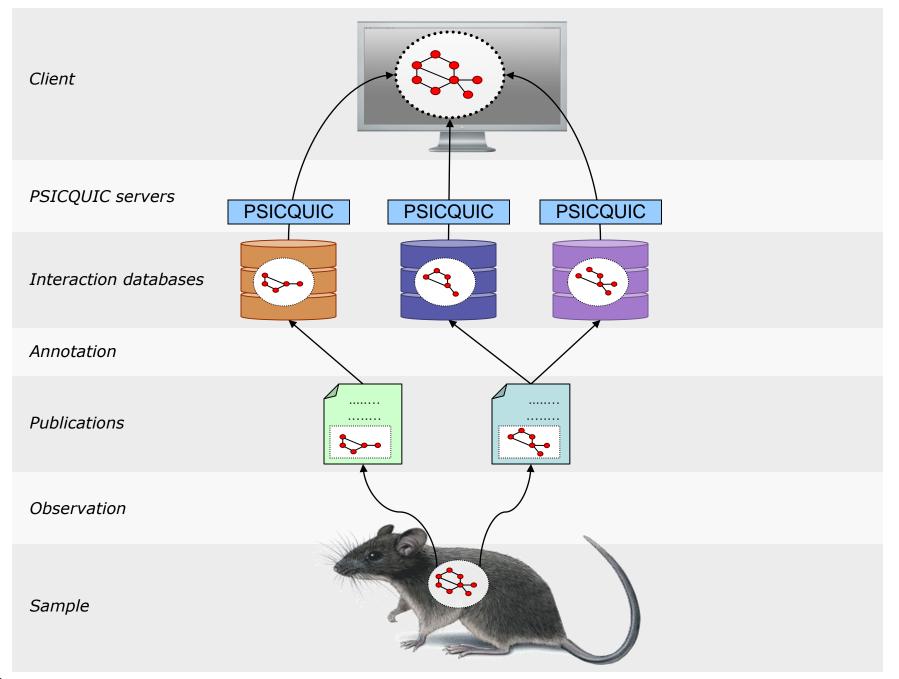
# **PSICQUIC**

A common query interface for interaction databases

Joint BSPR/EBI Conference 2010 Henning Hermjakob EBI Proteomics Services







The Molecular Interaction Standard (PSI-MI)



- •Community format for the representation of interaction data
- •XML schema
- Version 1.0: February 2004
  - The HUPO PSI Molecular Interaction Format A community standard for the representation of protein interaction data. Hermjakob, H., et al: Nature Biotechnology 2004, 22, 176-183.
- Version 2.5: October 2007
  - Quantitative parameters
  - Additional interactor types: DNA, RNA, small molecules
  - Also includes simplified tabular representation
  - Kerrien S., et al: Broadening the Horizon Level 2.5 of the HUPO-PSI Format for Molecular Interactions. BMC Biol. 2007 Oct 9;5(1):44
- •Now widely implemented by DIP, MINT, MIPS, IntAct, HPRD, ...



#### **MITAB**



- The PSI MI XML format is full-featured, but complex
- On frequent user request, we developed a simplified tabular format, MITAB 2.5
  - 15 well-defined columns to represent a molecular interaction in a database independent manner
- Now widely implemented

| 7       | FANCD1   | UniProt | DSS1<br>PR PY UN | UniProt | FANCD1; FACD;<br>Fanconi anemia<br>group D1 protein;<br>[+] | DSS1; SHFDG1; Split<br>hand/foot<br>malformation type 1<br>protein; [+] | <u>9606</u> | <u>9606</u> | <u>10373512</u> | <u>two hybrid</u>     | <u>EBI-79</u> |
|---------|----------|---------|------------------|---------|---|---|-------------|-------------|-----------------|-----------------------|---------------|
| 8       | PR BA UN |         | PR PY UN         |         |   |   |             |             | <u>10373512</u> | two hybrid            | <u>EBI-79</u> |
| 9<br>9  | PR BA UN |         | PR PY UN         |         |   |   |             |             | <u>10373512</u> | coimmunoprecipitation | <u>EBI-79</u> |
| 10<br>Q | PR PY UN |         | PR BA UN         |         |   |   |             |             | <u>10373512</u> | coimmunoprecipitation | <u>EBI-79</u> |

http://www.psidev.info/MI



#### PSICQUIC: The PSI Common Query InterfaCe



- Common computational interface for querying molecular interaction databases
  - Widely implemented by independent interaction data resources
  - Simple interface, open source server implementation exists, can be "fed" from a tab-delimited file => easy to provide data
  - Not limited to protein-protein interactions, also e.g.
    - Drug-target interactions
    - Simplified pathway data

| Name  | kctive | Interactions | Version        | SOAP URL   |
|---|--------|--------------|----------------|--|
| <u>BioGrid</u>  | YES    | 241,285      | 1.1.1-SNAPSHOT | http://tyerslab.bio.ed.ac.uk:8080/psicquic-ws/webservices/psic   |
| ChEMBL  | YES    | 492,354      | 1.1.0          | http://www.ebi.ac.uk/Tools/webservices/psicquic/chembl/webse |
| <u>IntAct</u>   | YES    | 207,332      | 1.1.5          | http://www.ebi.ac.uk/Tools/webservices/psicquic/intact/webser  |
| <u>iRefIndex</u>  | YFS    | 404,453      | 1.1.5          | http://biotin.uio.no:8080/psicquic-ws/webservices/psicquic   |
| <u>MatrixDB</u>   | YES    | 520          | 1.1.6-SNAPSHOT | http://matrixdb.ibcp.fr:8080/webservices/psicquic  |
| MINT  | YES    | 116,442      | 1.1.1          | http://mint.bio.uniroma2.it/mint/psicquic/webservices/psicquic   |
| <u>MPIDB</u>  | YES    | 23,580       | 1.0-SNAPSHOT   | http://www.jcvi.org/mpidb/servlet/webservices/psicquic   |
| <u>Reactome</u>   | YES    | 74,861       | 1.1.2-SNAPSHOT | http://brie8.cshl.edu:8080/psicquic-ws-reactome/webservices/p  |
| <u>Reactome-</u><br><u>Functional-</u><br><u>Interactions</u> | YES    | 209,988      | 1.1.2-SNAPSHOT | http://brie8.cshl.edu:8090/psicquic-ws-reactome-fi/webservices   |
| STRING  | NO     | 0            | 1.0alpha       | http://string-db.org/psicquic/ws   |



### PSICQUIC: Simple PSICQUIC viewer





# http://www.ebi.ac.uk/Tools/webservices/psicquic/view



### PSICQUIC: Simple PSICQUIC viewer



| ψ  | Proteomics<br>Standards<br>Initiative   | SICQ      | UIC VI                       | ew                          |  |  |             |                          |                       |                       |                          |                                  |                                  |  |  |
|----|---|-----------|------------------------------|-----------------------------|--|--|-------------|--------------------------|-----------------------|-----------------------|--------------------------|----------------------------------|----------------------------------|--|--|
| S  | earch: abl*/  | AND speci | es:9606                      |                             |  | Se   | arch C      | lear <mark>Fiel</mark> d | ls »                  |                       |                          | MQL                              | <u>syntax reference</u>          |  |  |
|    |   |           |                              |                             |  |  |             |                          |                       |                       |                          |                                  | Total: 2,712 binary interactions |  |  |
|    | ck on the links below to display the results for each service ( <u>refresh</u> )  |           |                              |                             |  |  |             |                          |                       |                       |                          |                                  |                                  |  |  |
|    | ■ <u>APID</u> - 481 ■ <u>InnateDB</u> - 9 ■ <u>MINT</u> - 352 ■ STRING<br>■ <u>BioGrid</u> - 205 ■ IntAct - 335 ■ MPIDB - 0 |           |                              |                             |  |  |             |                          |                       |                       |                          |                                  |                                  |  |  |
|    | <u>BIUGHU</u> - 205<br>ChEMBL - 799   | )         |                              | intact - 33:<br>iRefIndex - |  |  | eactome - 0 |                          |                       |                       |                          |                                  |                                  |  |  |
|    | DIP - 0   |           |                              | MatrixDB - 🛛                |  | <u> </u>   | eactome-F   | <u>ls</u> -179           |                       |                       |                          |                                  |                                  |  |  |
| 19 | CHEBI:49840;<br>EBI-1380990   | Schebi    | <u>P00519;</u><br>EBI-375543 | UniProt                     | purvalanol b   | ABL;<br>Abelson<br>murine<br>leukemia viral<br>oncogene<br>homolog 1;<br>Proto-<br>oncogene<br>c-Abl;<br>p150; JTK7;<br>abl1_human |             | ABL1                     |                       | Human ( <u>9606</u> ) | Bantscheff et al. (2007) | <u>17721511</u>                  | association                      |  |  |
| 20 | P00519;<br>EBI-375543   | UNING ST  | EBI-1550568                  |                             | ABL;<br>Abelson<br>murine<br>leukemia viral<br>oncogene<br>homolog 1;<br>Proto-<br>oncogene<br>c-Abl;<br>p150; JTK7;<br>abl1_human |  | ABL1        |                          | Human ( <u>9606</u> ) | -2                    | Lin et al. (2007)        | <u>17486070</u>                  | enzymatic reaction               |  |  |
| 21 | <u>Q9UJV9;</u><br>EBI-1046350   |           | <u>P00519;</u><br>EBI-375543 | UniProt                     | DEAD box<br>protein 41;<br>DEAD box<br>protein<br>abstrakt<br>homolog;   | ABL;<br>Abelson<br>murine<br>leukemia viral<br>oncogene<br>homolog 1;  | DDX41       | ABL1                     | Human ( <u>9606</u> ) | Human ( <u>9606</u> ) | Wu et al. (2007)         | <u>17474147</u><br>imex:IM-11903 | physical association             |  |  |



#### **PSICQUIC:**

#### **Pointing to other resources**



EBI > Databases > Pathways & Networks > IntAct > View

| 8      | Search: BRCA2 Search Clear Show Advanced Fields »   |       |                 |        |  |            |                   |                          |                 |                              |    |  |
|--------|---|-------|-----------------|--------|--|------------|-------------------|--------------------------|-----------------|------------------------------|----|--|
|        | Home       Search       Interactions (89)       Browse       Lists       Interaction Details       Molecule View       Graph  |       |                 |        |  |            |                   |                          |                 |                              |    |  |
| > [0   | <b>89</b> binary interactions were found in IntAct. <b>23</b> of them are one inated from <u>spoke expanded co-complexes</u> and you may want to <u>filter</u> them. [Counting results in other databases] Previous 1-30 of 89 Vext 30 Export to: Select format Vexport Change Columns Displayed Previous |       |                 |        |  |            |                   |                          |                 |                              |    |  |
| Pre    | Name  | Links | Name            | Links  | Aliases  | Aliases    | Export<br>Species | _                        | Publication     | Interaction Detection Method | In |  |
|        |   |       | molecule B      |        |  | molecule B |                   | Species<br>molecule<br>B |                 | Interaction Detection Method |    |  |
| 1      | FANCD1  |       | atp<br>SM NE EN | SCHEBI | FANCD1;<br>FACD;<br>Fanconi<br>anemia group<br>D1 protein; [+] | atp        | <u>9606</u>       |                          | <u>19303847</u> | <u>atpase assay</u>          | EE |  |
| 2      | PR NE IN  |       | SM NE EN        |        |  |            |                   |                          | <u>19303847</u> | atpase assay                 | EE |  |
| 3<br>Q | PR NE IN  |       | SM NE EN        |        |  |            |                   |                          | <u>19303847</u> | atpase assay                 | EE |  |
| 4      | PR NE IN  |       | SM NE EN        |        |  |            |                   |                          | <u>19303847</u> | atpase assay                 | EE |  |
| 5      | PR NE IN  |       |                 |        |  |            |                   |                          | <u>19303847</u> | atpase assay                 | EE |  |



#### **PSICQUIC:**

#### **Pointing to other resources**



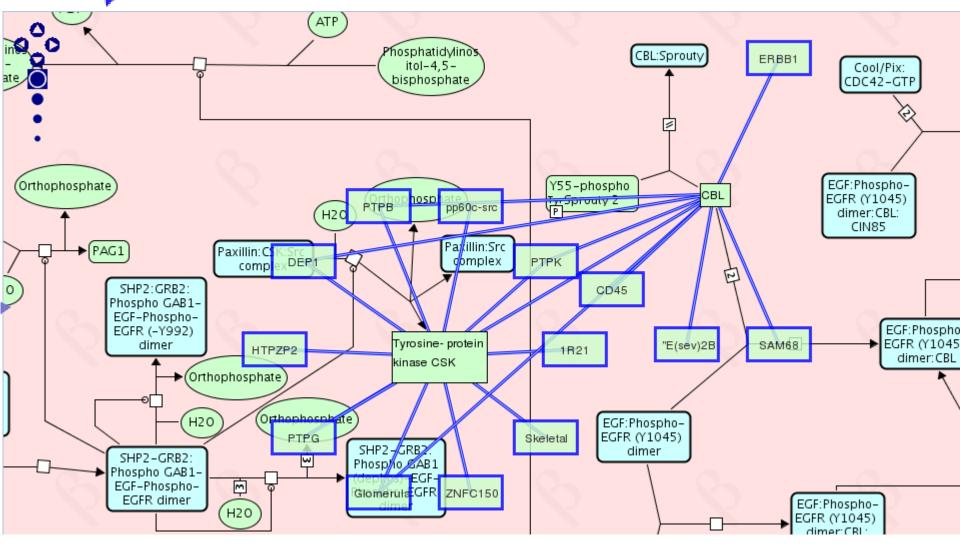
EBI > Databases > Pathways & Networks > IntAct > View

| S      | Search: BRCA2 Search Clear Show Advanced Fields »  |            |                |           |  |                          |                          |                           |                              |   |     |  |
|--------|--|------------|----------------|-----------|--|--------------------------|--------------------------|---------------------------|------------------------------|---|-----|--|
|        | Home       Search       Interactions (89)       Browse       Lists       Interaction Details       Molecule View       Graph |            |                |           |  |                          |                          |                           |                              |   |     |  |
| > Y(   |  | so matches | 82 interaction | evidences |  | databases. 💿             |                          |                           | nplexes  and y               | rou may want to <u>filter</u> them.<br>ed Previ | ous |  |
|        | Name Links Name Links Aliases Alias  |            |                |           | Aliases<br>molecule B  | Species<br>molecule<br>A | Species<br>molecule<br>B | Publication<br>Identifier | Interaction Detection Method | ction Detection Method In                       |     |  |
| 1      | FANCD1   | UniProt    | atp            | SCHEBI    | FANCD1;<br>FACD;<br>Fanconi<br>anemia group<br>D1 protein; [+] | atp                      | <u>9606</u>              |                           | <u>19303847</u>              | <u>atpase assay</u>                             | EE  |  |
| 2<br>Q | PR NE (IN)   |            | SM NE EN       |           |  |                          |                          |                           | <u>19303847</u>              | atpase assay                                    | EE  |  |
| 3<br>Q | PR NE (IN)   |            | SM NE EN       |           |  |                          |                          |                           | <u>19303847</u>              | atpase assay                                    | EE  |  |
| 4      | PR NE [IN]   |            | SM NE EN       |           |  |                          |                          |                           | <u>19303847</u>              | atpase assay                                    | EE  |  |
| 5<br>Q | PR NE IN   |            | SM NE EN       |           |  |                          |                          |                           | <u>19303847</u>              | atpase assay                                    | EE  |  |

## PSICQUIC: Overlay of molecular interactions on Reactome pathways (beta)

Proteomics

Services





### PSICQUIC Query Language: MIQL



 Based on Lucene, with specific field names

 Example: ppx AND species:"Escheri chia coli" AND pubauth:"Scott"

| Field Name       | Searches on  | Implicit* | Example                       |
|------------------|--|-----------|-------------------------------|
| idA              | IdentifierA  | No        | idA:P74565                    |
| id               | Identifiers (A or B)   | No        | <u>id:P74565</u>              |
| alias            | Aliases (A or B)   | No        | alias:(KHDRBS1 HCK)           |
| identifiers      | Identifiers and Aliases undistinctively  | Yes       | identifier:P74565             |
| pubauth          | Publication 1 st author(s)   | Yes       | pubauth:scott                 |
| pubid            | Publication Identifier(s) OR   | Yes       | pubid:(10837477<br>12029088)  |
| taxidA           | Tax ID interactor A: be it the tax ID or the species name  | No        | taxidA:mouse                  |
| taxidB           | Tax ID interactor B: be it the tax ID or species name  | No        | <u>taxidB:9606</u>            |
| species          | Species. Tax ID A and Tax ID B   | Yes       | <u>species:human</u>          |
| type             | Interaction type(s)  | Yes       | type:"physical interaction"   |
| detmethod        | Interaction Detection method(s)  | Yes       | detmethod:"two hybrid*"       |
| interaction_id   | Interaction identifier(s)  | Yes       | interaction_id:EBI-<br>761050 |
| annotation       | Annotations Interactor A or B  | No        | annotation:experimental       |
| properties       | Properties of Interactor A or B (note that this field also contains parent terms of ontology terms of GO, InterPro and PSI-MI) | Yes       | properties:"1GQ5"             |
| expansion        | Expansion method(s)  | Yes       | <u>expansion:spoke</u>        |
| dataset          | Dataset name(s)  | Yes       | dataset:Apoptosis             |
| experimentalRole | Experimental role(s) interactor A or interactor B  | No        | experimentalRole:prey         |
| biologicalRole   | Biological role(s) interactor A or interactor B  | No        | biologicalRole:enzyme         |
| hostOrganism     | Host organism in which the interaction was detected  | Yes       | <u>hostOrganism:human</u>     |

11

#### PSICQUIC: SOAP and REST interfaces

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|------------------------|--------------------------------|---|--|
|                        | http://www.ebi.ac.             | uk/Tools/webservices/psicquic/intact/webservices/current/searc              | niyqueryypubaun:gavinynrstResuit=o@naxResuits=1000                         |
| 😇 Google Calendar [ TT | 🛛 🚼 Google Docs 🛛 🔀 Proteomics | [ LEO \phantom W Wikipedia 🛠 Independent 🚯 CiteXplore 🚯                     | 🕽 EBI Staff 📷 W 流 Systems Group News 🚯 PSICQUI                             |
| 😇 Google Calendar      | 🖂 🚺 IntAct                     | 🖂 🚺 PSICQUIC View 🖂   | 🚯 Ontology Lookup Service (OLS) 🔤 🚯 PSICQUI                                |
| uniprotkb:P53859       | intact:EBI-1731                | uniprotkb:Q02821 intact:EBI-1797  | uniprotkb:YNL232W(locus name) uni  |
| uniprotkb:P53859       | intact:EBI-1731                | uniprotkb:P40579 intact:EBI-1804  | uniprotkb:YNL232W(locus name) uni  |
| uniprotkb:P53859       | intact:EBI-1731                | uniprotkb:P53859 intact:EBI-1731  | uniprotkb:YNL232W(locus name) uni  |
| uniprotkb:P53859       | intact:EBI-1731                | uniprotkb:Q08162 intact:EBI-1740  | uniprotkb:YNL232W(locus name) uni  |
| uniprotkb:P53859       | intact:EBI-1731                | uniprotkb:P48240 intact:EBI-1749  | uniprotkb:YNL232W(locus name) uni  |
| uniprotkb:P53859       | intact:EBI-1731                | uniprotkb:P38792 intact:EBI-1757  | uniprotkb:YNL232W(locus name) uni  |
| uniprotkb:P53859       | intact:EBI-1731                | uniprotkb:Q12277 intact:EBI-1765  | uniprotkb:YNL232W(locus name) uni  |
| uniprotkb:P53859       | intact:EBI-1731                | uniprotkb:P25359 intact:EBI-1773  | uniprotkb:YNL232W(locus name) uni  |
| uniprotkb:P53859       | intact:EBI-1731                | uniprotkb:Q12149 intact:EBI-1782  | uniprotkb:YNL232W(locus name) uni  |
| uniprotkb:P53859       | intact:EBI-1731                | uniprotkb:P46948 intact:EBI-1788  | uniprotkb:YNL232W(locus name) uni  |
| uniprotkb:P53859       | intact:EBI-1731                | uniprotkb:Q08491 intact:EBI-1389  | uniprotkb:YNL232W(locus name) uni  |
| uniprotkb:Q05636       | intact:EBI-1810                | uniprotkb:Q05636 intact:EBI-1810  | uniprotkb:YDR280W(locus name) uni  |
| uniprotkb:Q05636       | intact:EBI-1810                | uniprotkb:P53859 intact:EBI-1731  | uniprotkb:YDR280W(locus name) uni  |
| uniprotkb:Q05636       | intact:EBI-1810                | uniprotkb:Q08162 intact:EBI-1740  | uniprotkb:YDR280W(locus name) uni  |
| uniprotkb:Q05636       | intact:EBI-1810                | uniprotkb:Q04217 intact:EBI-1820  | uniprotkb:YDR280W(locus name) uni  |
| uniprotkb:Q05636       | intact:EBI-1810                | uniprotkb:P48240 intact:EBI-1749  | uniprotkb:YDR280W(locus name) uni  |
| uniprotkb:Q05636       | intact:EBI-1810                | uniprotkb:P38792 intact:EBI-1757  | uniprotkb:YDR280W(locus name) uni  |
| uniprotkb:Q05636       | intact:EBI-1810                | uniprotkb:Q08285 intact:EBI-1831  | uniprotkb:YDR280W(locus name) uni  |
| uniprotkb:Q05636       | intact:EBI-1810                | uniprotkb:P25359 intact:EBI-1773  | uniprotkb:YDR280W(locus name) uni  |

#### http://code.google.com/p/psicquic/



**PSICQUIC:** 



#### The challenge

#### FROM:

| Click on the links below to di | isplay the results for each service (re | etresh)            |        |  |
|--------------------------------|---|--------------------|--------|--|
| APID - 481                     | InnateDB - 9                            | MINT - 352         | STRING |  |
| BioGrid - 205                  | IntAct - 335                            | MPIDB - 0          |        |  |
| ChEMBL - 799                   | iRefindex - 352                         | Reactome - 0       |        |  |
| 🔵 DIP - 0                      | 🔵 MatrixDB - 🛛                          | Reactome-FIS - 179 |        |  |

|   |   |             |         |            |         |              | _              |      |                       |                          |          |             |
|---|---|-------------|---------|------------|---------|--------------|----------------|------|-----------------------|--------------------------|----------|-------------|
| 1 |   |             |         |            | UniProt | purvalanol b | ABL;           | ABL1 | Human ( <u>9606</u> ) | Bantscheff et al. (2007) | 17721511 | association |
|   | ! | EBI-1380990 | <u></u> | EBI-375543 |         |              | Abelson        |      |                       |                          |          |             |
|   |   |             |         |            |         |              | murine         |      |                       |                          |          |             |
|   |   |             |         |            |         |              | leukemia viral |      |                       |                          |          |             |
|   |   |             |         |            |         |              | oncogene       |      |                       |                          |          |             |
|   |   |             |         |            |         |              | homolog 1;     |      |                       |                          |          |             |
|   |   |             |         |            |         |              | Proto-         |      |                       |                          |          |             |
|   |   |             |         |            |         |              | oncogene       |      |                       |                          |          |             |
|   |   |             |         |            |         |              | c-Abl;         |      |                       |                          |          |             |
|   |   |             |         |            |         |              | p150; JTK7;    |      |                       |                          |          |             |
|   |   |             |         |            |         |              | abl1_human     |      |                       |                          |          |             |
|   |   |             |         |            |         |              |                |      |                       |                          |          |             |

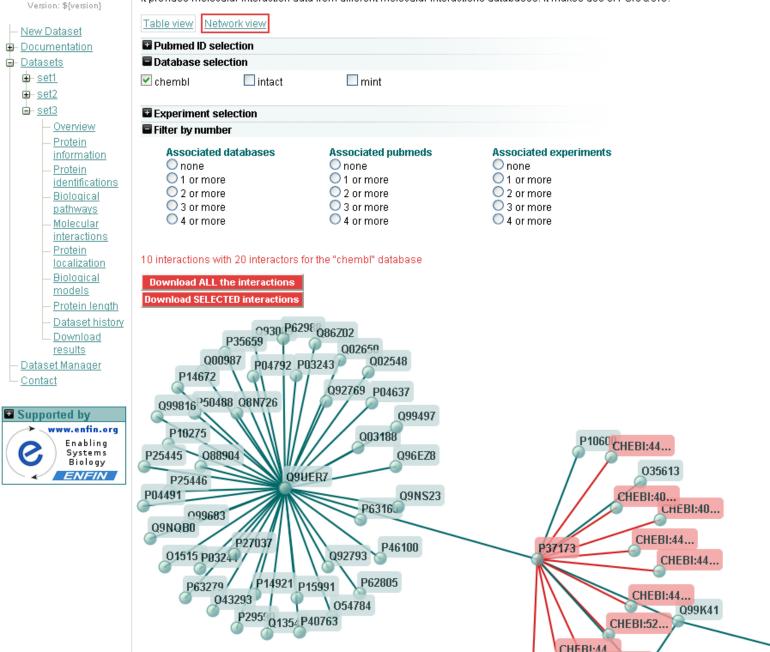
#### TO:

| PR PY UN  | PR BA UN |          |             |             | Marston et al. (1999) | <u>10373512</u> | <u>coimmunoprecipitation</u>   |        | EBI-79852  |
|-----------|----------|----------|-------------|-------------|-----------------------|-----------------|--------------------------------|--------|------------|
| At4g00020 |          |          | <u>3702</u> | <u>3702</u> | Siaud et al. (2004)   | <u>15014444</u> | two hybrid                     | MINT   | EBI-307726 |
| PR BA UN  | PR PY UN | (Lasty Z |             |             | Dray et al. (2006)    | <u>16415210</u> | two hybrid                     | IntAct | EBI-930902 |
| PR BA UN  | PR PY UN |          |             |             | Siaud et al. (2004)   | <u>15014444</u> | two hybrid                     | MINT   | EBI-930747 |
| PR BA UN  | PR PY UN |          |             |             | Dray et al. (2006)    | <u>16415210</u> | anti taq coimmunoprecipitation | IntAct | EBI-930779 |

EBI > Databases > Proteomics

#### Molecular Interactions - Dataset: set3

It provides molecular interaction data from different molecular interactions databases. It makes use of PSICQUIC.



Q13131





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Antonio Fabregat Mundo Visitor

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Curator

cientific Database Curator



**Bijay Jassal** 

Curator

Gustavo A. Salazar

Visitor

Sarala Wimalaratne

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**Bioinformatician** 

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Visitor



Steven Jupe Knowledge Database Curator/Developer



Florian Reisinger Software Developer



Rui Wang Bioinformatician



Jyoti Khadake Senior Database Curator



Andreas Schoenegger Trainee























Gavin O'Kelly



















Bernard de Bono

T.B.A.

Bruno Aranda

Software Engineer

















































**Thank you!** 

**Questions?** 

**ALL PSI CONTRIBUTORS!** 

IntAct team:

**Funding** 

 Bruno Aranda Samuel Kerrien Rafael Jimenez

•EU FW6 Enfin

•EU FW7 PSIMEx

**All PSICQUIC implementors!** 











