

DAS for Molecular Interactions

Hagen Blankenburg



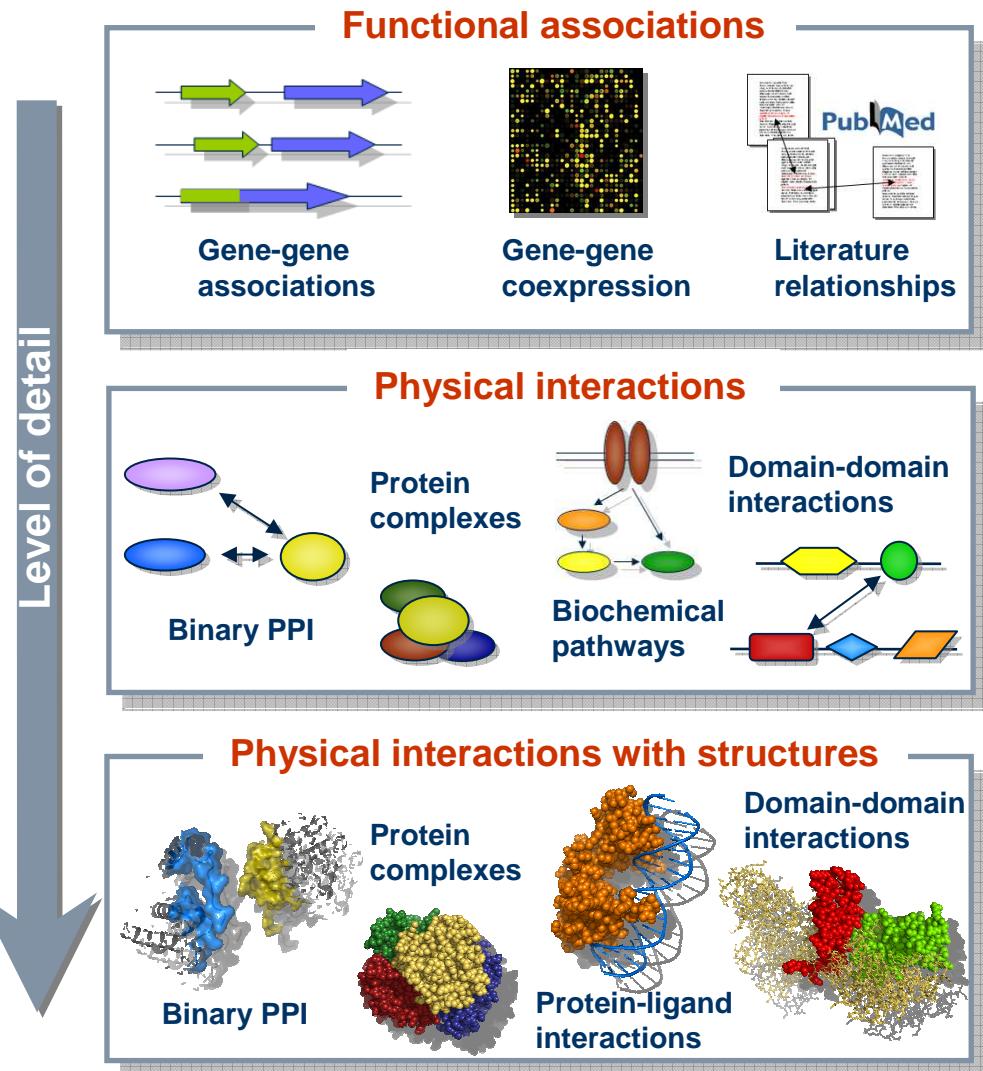
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Importance of molecular interactions

- Fundamental for understanding of cellular processes
 - Prediction of protein function
 - Importance in certain diseases
 - Essentiality of hub proteins?
- The next big thing?!
 - „Interactomics“, „network medicine“, ...



Problem I: Data abundance and distribution

Proteins Interacting in the Nucleus



Domino
domain peptide
interactions database



Bioverse



MINT a Molecular INTeractions database



Human Annotated and Predicted Protein Interaction (HAPPI)

Human protein-protein interaction network database search

Hagen Blankenburg

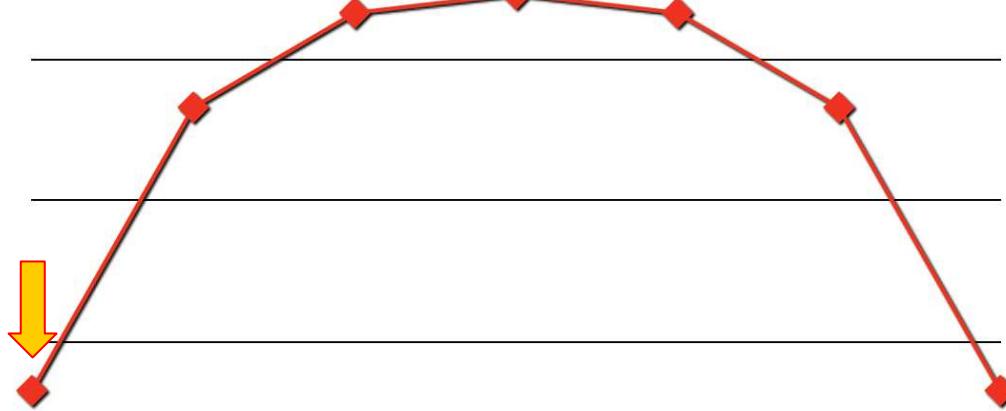
3DID - 3D interacting domains



PPID Protein-Protein Interaction Database

PIPs
Human Protein-Protein Interaction Prediction

Scientific impact



(Credit: Tim Hubbard)

Too little bioinformatics



Too many databases
Too diverse interfaces

DIMA

HomoMINT: an inferred human network
domain interaction map

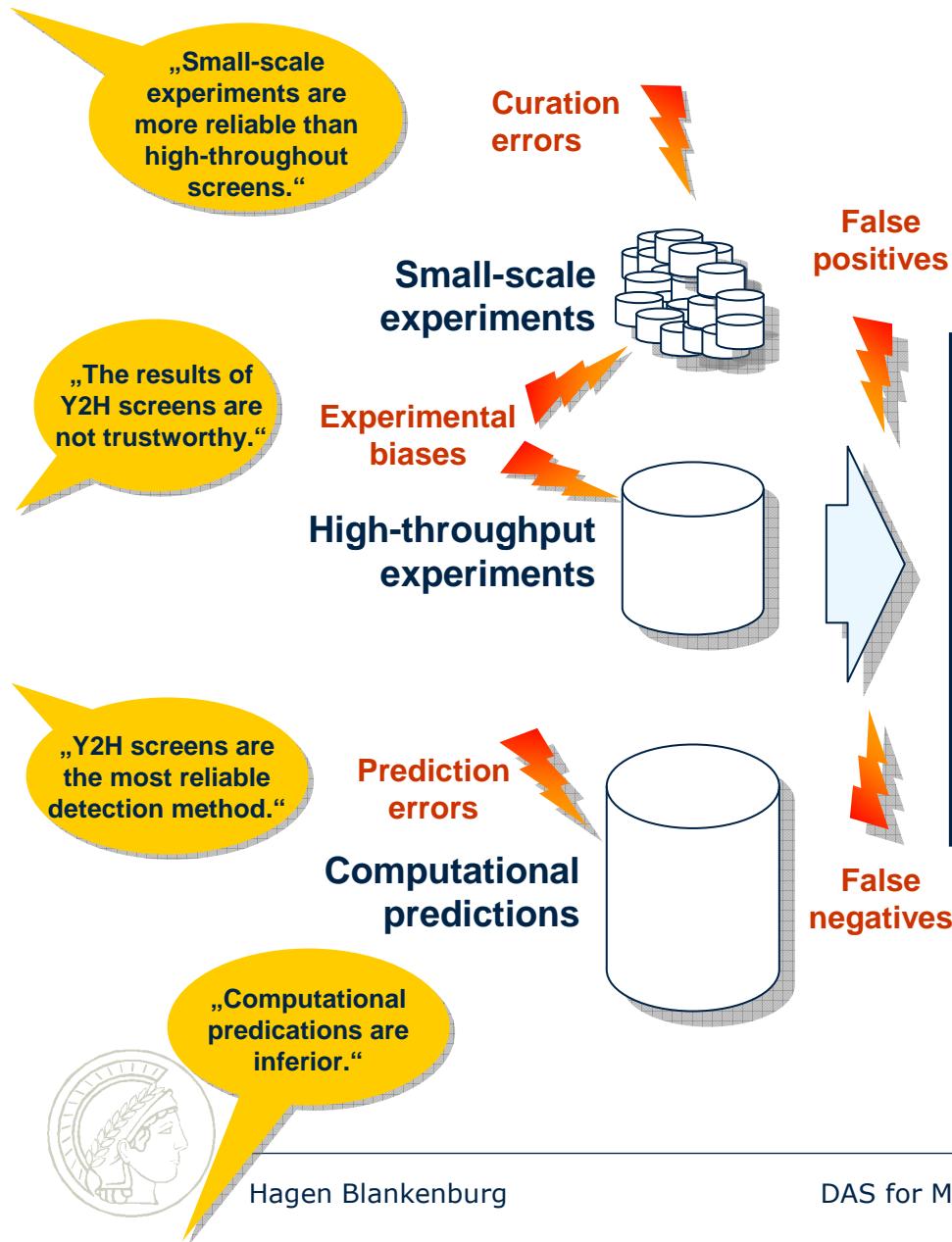
InterDom
Database of Interacting Domains

DAS for Molecular Interactions

10/03/2009

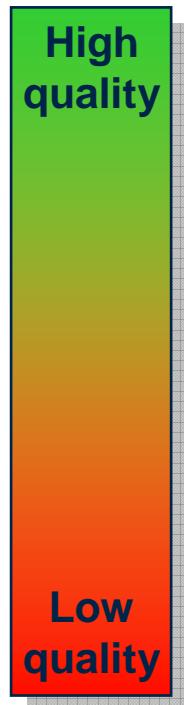
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Problem II: Data quality



Confidence measures:

- Replicate experiments
- Network topology
- Functional similarity
- Domain interactions
- Evolutionary conservation
- Co-localization
- Positive and negative standard reference sets
- ...



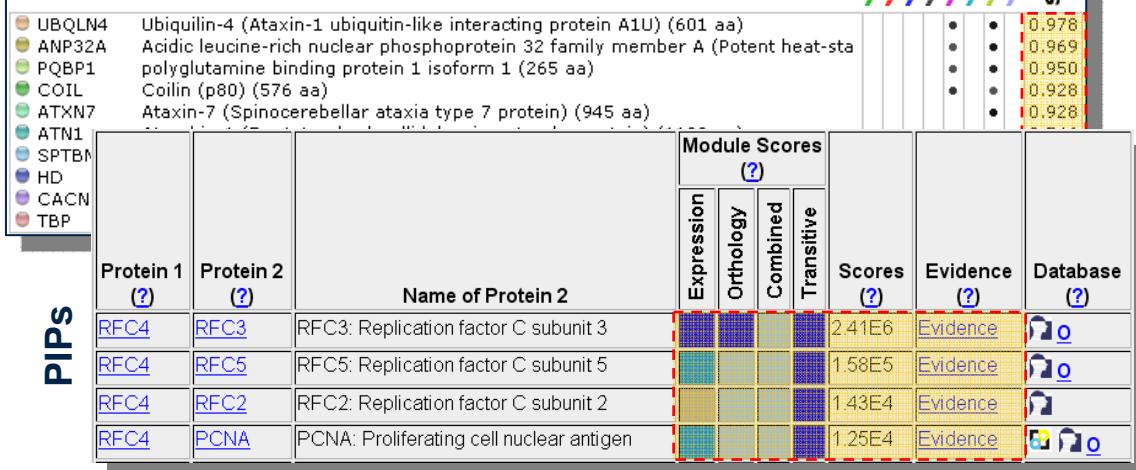
Problem II: Data quality

STRING

Your Input:

ATXN1 Ataxin-1 (Spinocerebellar ataxia type 1 protein) (815 aa)
(*Homo sapiens*)

Predicted Functional Partners:



PIPs

PROTEIN INTERACTORS		EXPERIMENTS	PROVENANCE	More Info
SERA_YEAST	APTX_YEAST	1	IntAct MINT DIP BIND	+info_inter
YNM4_YEAST	APTX_YEAST	1	IntAct	+info_inter

APID

INTERACTION FILTER AND SELECTION

Select interactions demonstrated for at least 1 experiments and with IPfam validation Select

IntAct

Description	-
Annotation	author-confidence LacZ4
Interacting molecules	Name Ac Interactor type Stoichiometry Interactor description Expression Identifier Gene Role
confidence-mapping	The authors have assigned confidence based on reporter gene activation. The Y2H interactions that can be identified by activation of three reporter genes HIS3, URA3 and lacZ were regarded as of higher confidence and classified as LacZ4 set. The Y2H interactions identified only with HIS3 and URA3 reporter genes were classified as lower confidence data set SD4.



APTX: Aprataxin (Q7Z2E3)
found to interact with 14 partner(s):

protein	interactions	score
XRCC1 Homo sapiens (P18887)	10	0.95
PARP1 Homo sapiens (P09874)	2	0.52
XRCC4 Homo sapiens (Q13426)	2	0.43
CEP350 Homo sapiens (Q5VT06)	1	0.24
CNTROB Homo sapiens (Q8N137)	1	0.24
HIVEP1 Homo sapiens (P15822)	1	0.24
HRIHFB2216 Homo sapiens (Q94799)	2	0.24
KIAA0596 Homo sapiens (Q60336)	1	0.24
P02686 Homo sapiens (P02686)	1	0.24
PICK1 Homo sapiens (Q9NRD5)	1	0.24
q53hd4_human Homo sapiens (Q53HD4)	1	0.24
SYT17 Homo sapiens (Q9BSW7)	1	0.24
TRIM37 Homo sapiens (Q94972)	2	0.24
ZNF639 Homo sapiens (Q9UID6)	2	0.24

x proteins linked to a disease.

3DID

PDB ID	chain 1	residues	chain 2	residues	score	Z-score	more information	RasMol
1ibr	D	318-359	C	12-170	7.85	3.38228	1ibr	
1ibr	B	318-359	A	12-170	6.32	3.01999	1ibr	
1ibr	D	214-248	C	12-170	3.35	2.82048	1ibr	

Dissociation constant (Kd) M

-

Solution: Distributed System



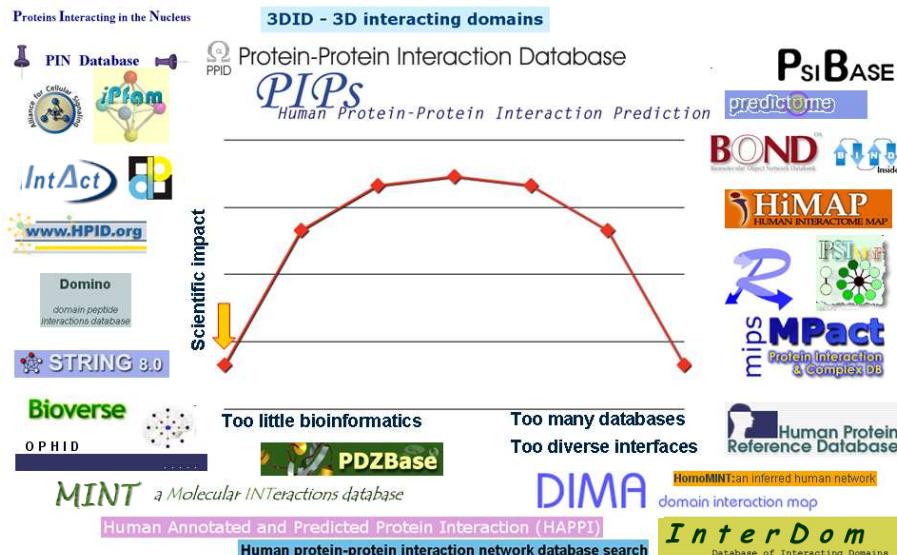
Interaction data servers



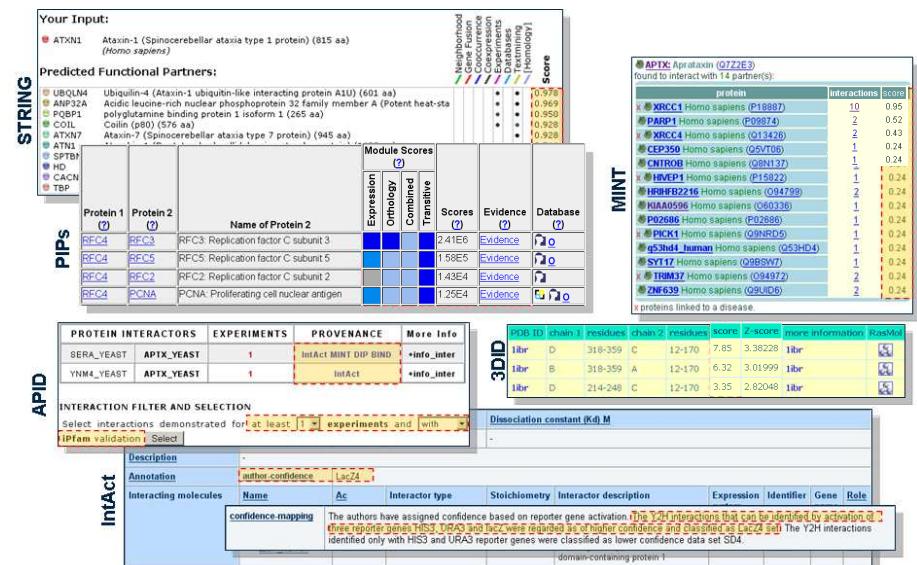
Interaction confidence scoring servers



Problem I: Data abundance and distribution



Problem II: Data quality



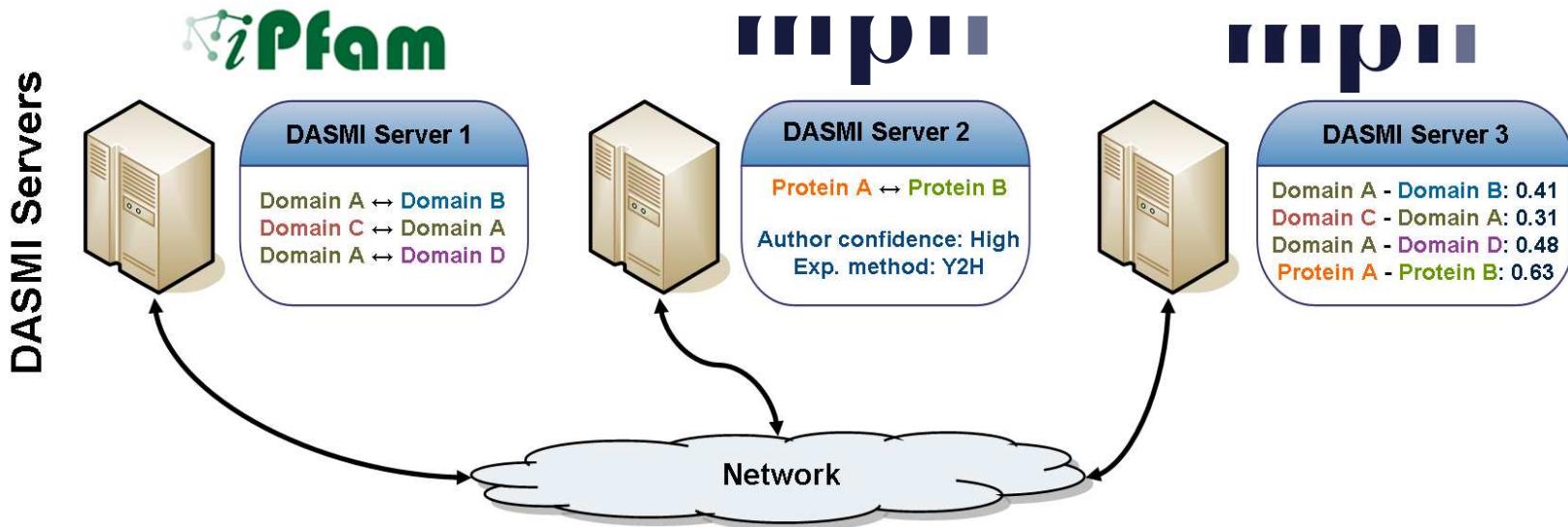
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DAS for Molecular Interactions (DASMI) - Servers

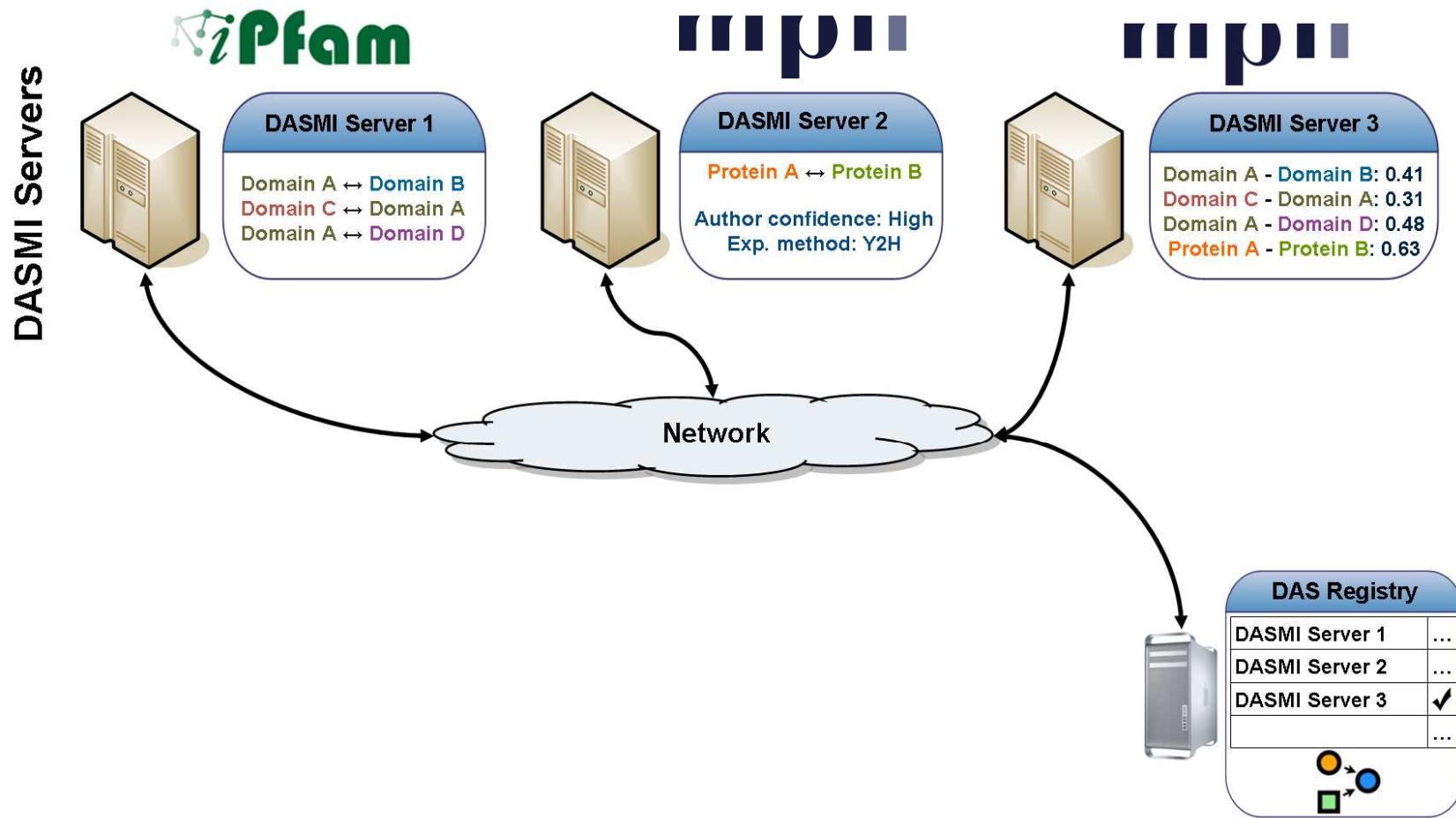


- Servers have coordinate / identifier systems

UniProtKB:	P51587, BRCA2_HUMAN
Entrez Gene:	675
GeneInfo:	119395734, 28400649, 1177438, 14424438, 2315186, 27065822, 37675289, 1161384, 16116616,
RefSeq:	NP_000050.2, NM_000059
IPI:	IPI00412408
Ensembl:	ENSG00000139618



DAS for Molecular Interactions (DASMI) - Registry



DAS registry – <http://www.dasregistry.org>

All DAS servers with interaction capability

available DAS services

organism:	authority:	type:
any	any	any

capability: label:
interaction any display

[1 - 10 | 28] next > last >> | show all

pos	id	clients	nickname	status	capabilities	coordinateSystem	description	project
1	DS_529	ldsc-core		interaction	Pfam,Protein Sequence		show >	
							go to site	
2	DS_527	interdom		interaction	Pfam,Protein Sequence		show >	
							go to site	
3	DS_526	3dId		interaction	Pfam,Protein Sequence		show >	
							go to site	
4	DS_531	apmm2		interaction	Pfam,Protein Sequence		show >	
							go to site	
5	DS_530	apmm1		interaction	Pfam,Protein Sequence		show >	
							go to site	
6	DS_528	ldsc		interaction	Pfam,Protein Sequence		show >	
							go to site	
7	DS_498	homomint		interaction	Entrez, Gene_ID		show >	
							go to site	
8	DS_499	ccsb-hi1		interaction	Entrez, Gene_ID		show >	
							go to site	
9	DS_500	sanger		interaction	Entrez, Gene_ID		show >	
							go to site	
10	DS_501	sanger-core		interaction	Entrez, Gene_ID		show >	
							go to site	

[1 - 10 | 28] next > last >> | show all

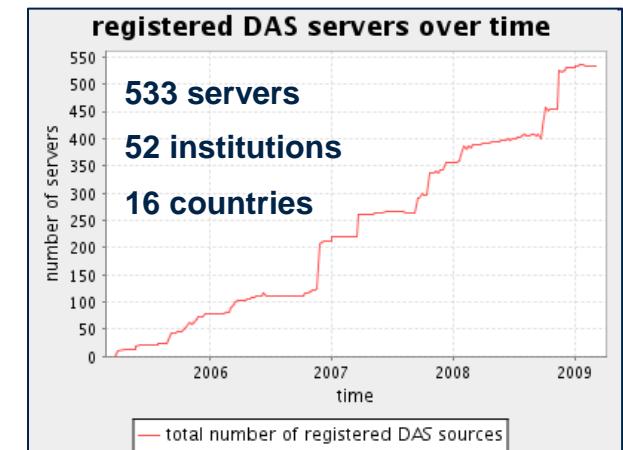
DAS - client legend:

- ... SPICE
- ... Ensembl
- ... Dasty

[home | list sources | validate | register new | statistics | history | docu] © 2008



- Maintained at Sanger Institute

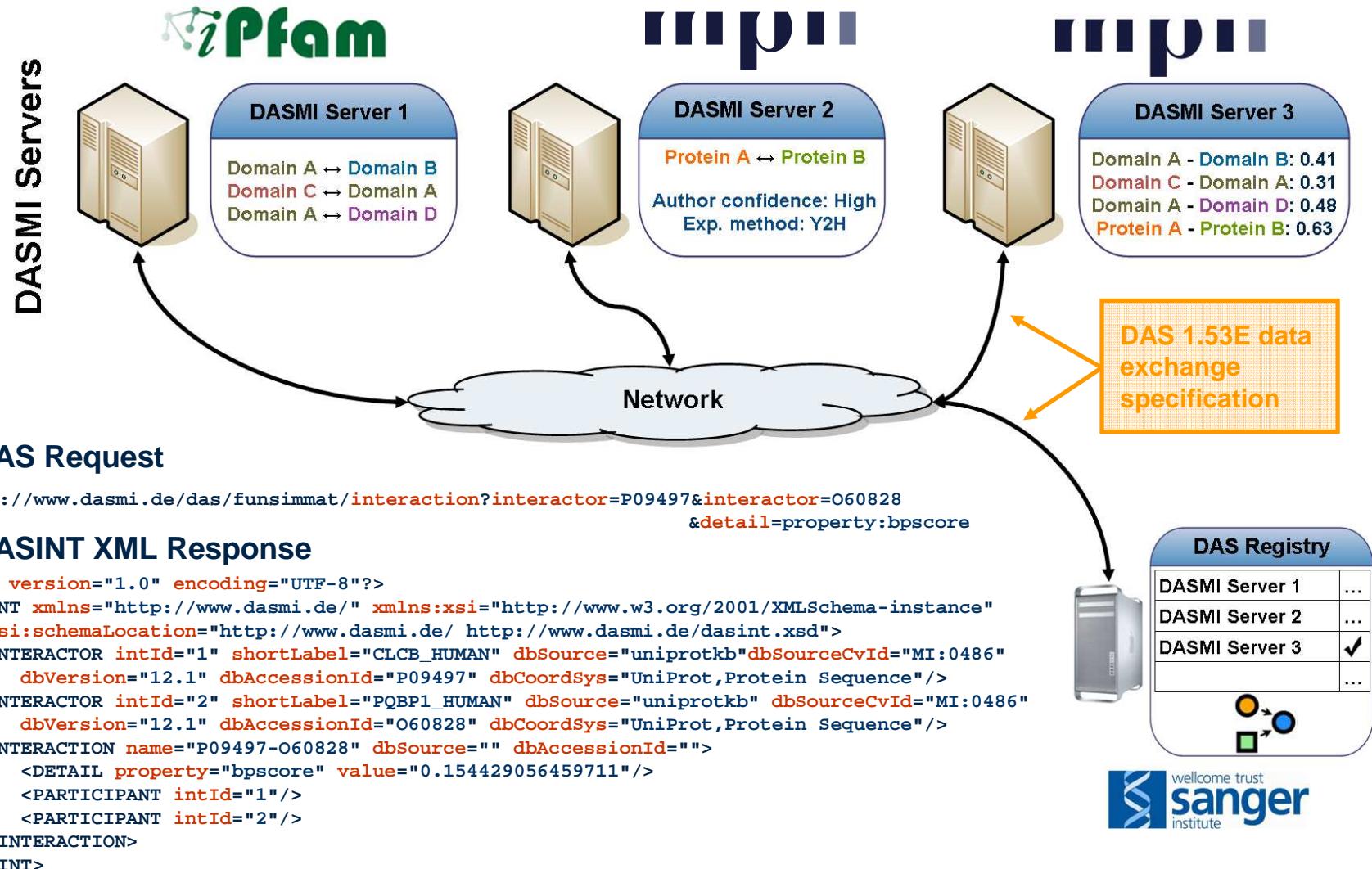


Domain interactions

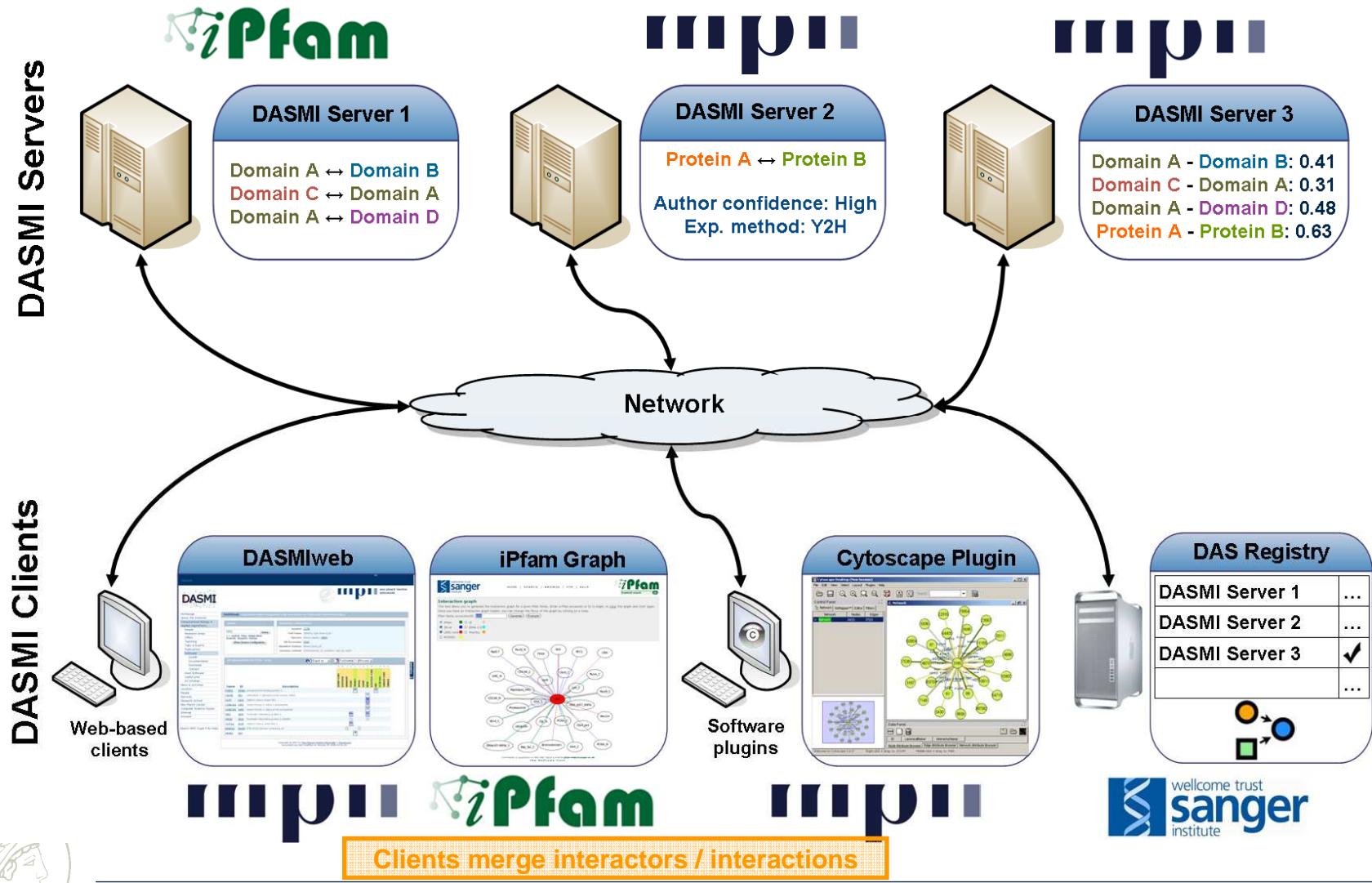
Protein interactions



DAS for Molecular Interactions (DASMI) - Data exchange



DAS for Molecular Interactions (DASMI) - Clients



iPfam graphical domain interaction browser



HOME | SEARCH | BROWSE | FTP | HELP



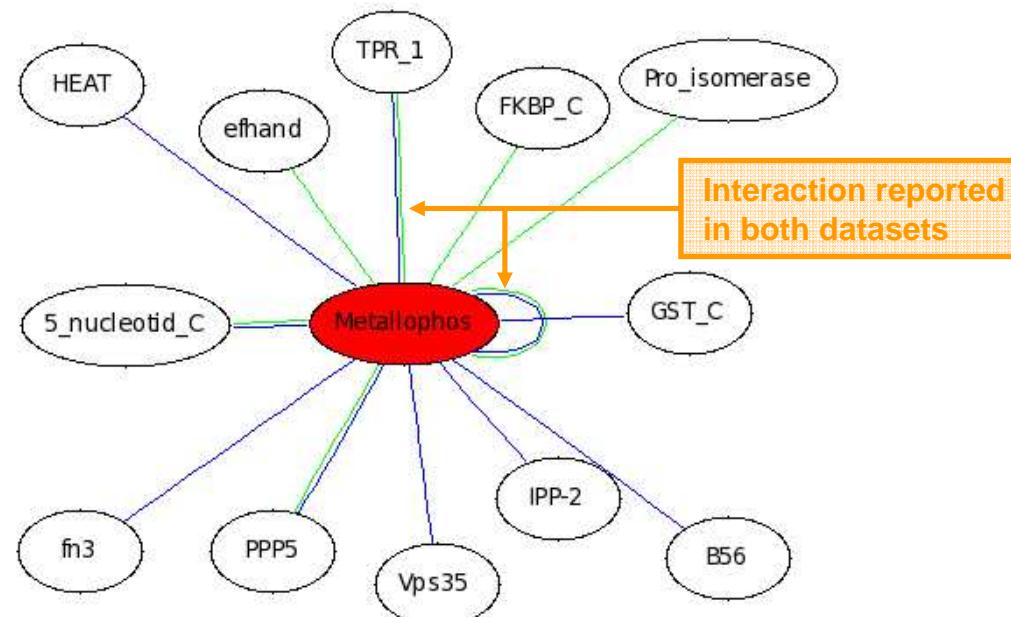
Interaction graph

This tool allows you to generate the interaction graph for a given Pfam family. Enter a Pfam accession or ID to begin, or [clear](#) this graph and start again. Once you have an interaction graph loaded, you can change the focus of the graph by clicking on a node.

Pfam family accession/ID:

- iPfam LP
- 3D-id DIMA 2.0
- LDSC core Wuchty
- RCDPSO

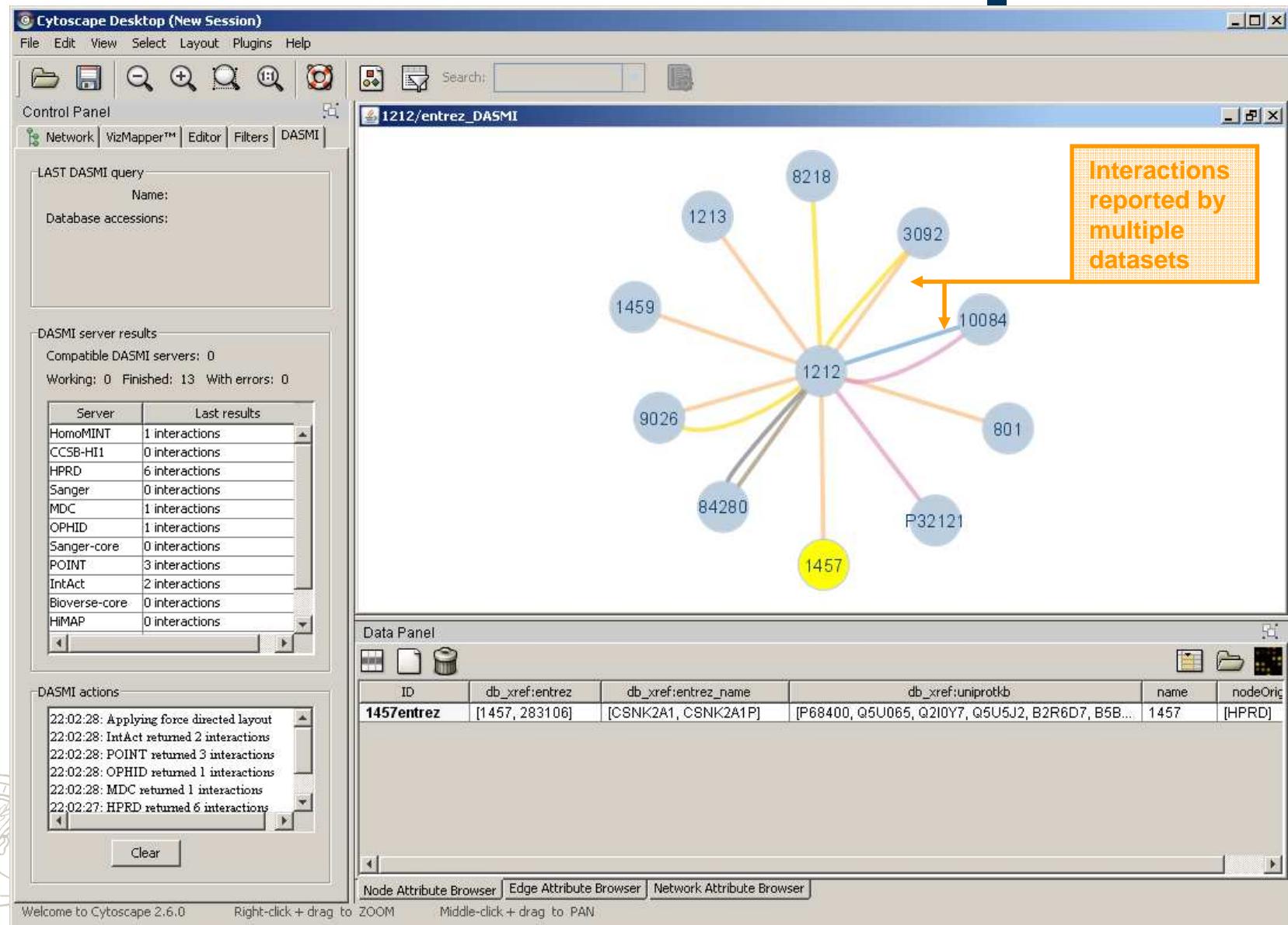
Selected domain
interaction servers



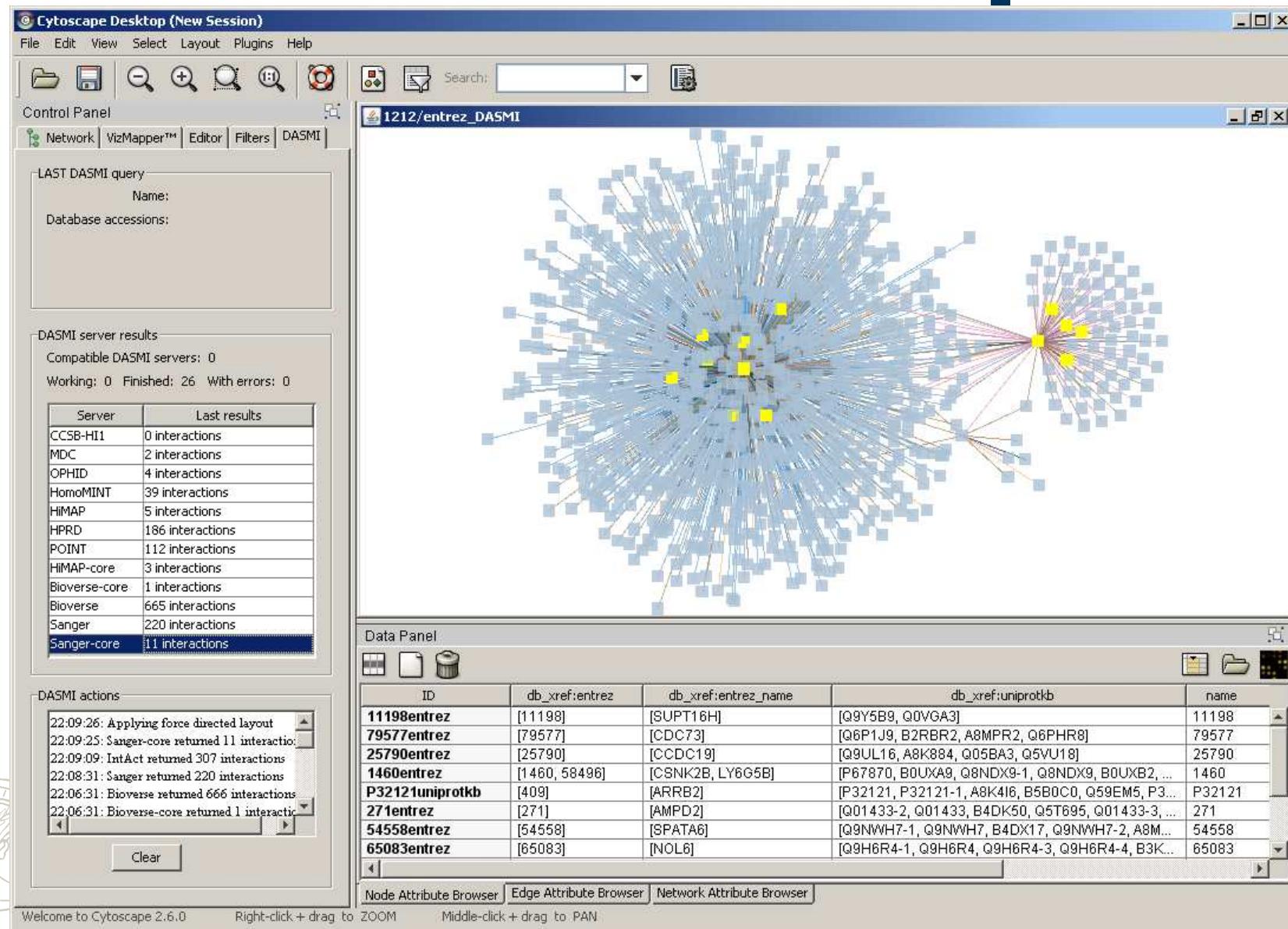
Comments or questions on the site? Send a mail to pfam-help@sanger.ac.uk

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DASMI Cytoscape Client





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DASMIweb - dynamic online integration and annotation of molecular interaction data

Query

Query

e.g. Ensembl, Entrez Gene, Genelinfo, Pfam, RefSeq, UniProtKB

Show Source Configuration

Interactor Information

Identifier:	961 (Entrez Gene) (Leukocyte surface antigen CD47 precursor (Integrin-associated protein)(IAP) (Antigenic surface determinant protein OA3) (Protein MER6).) (CD47 molecule)
UniProtKB	CD47_HUMAN, A8K198_HUMAN, Q71A41_HUMAN,
UniGene	Hs.446414,
Entrez Gene	961,
UniParc	UPI0000049C6C, UPI00001BDF2Z,

22 interactions (showing 11 to 20) [previous](#) [next](#)

Export as ... Select confidence measure ...

Name	ID	Description	Predictions	Literature curation / experiments	Interaction reported by multiple datasets
P2RY2	5029	P2Y purinoceptor 2 (P2Y2) (P2U purinoceptor 1) (P2U1) (ATP receptor)(Purinergic receptor).			
EPB42	2038	Erythrocyte membrane protein band 4.2 (Erythrocyte protein 4.2)(P4.2).			
THBS1	7057	Hypothetical protein (Fragment).			
UBQLN1	29979	Ubiquilin-1 (Protein linking IAP with cytoskeleton 1) (PLIC-1) (hPLIC-1).			
RHAG	6005	Rhesus blood group-associated glycoprotein (Rhesus blood group-associated ammonia channel) (Erythrocyte plasma membrane 50 kDaglycoprotein) (Rh50A) (CD241 antigen).			
PTK2	5747	Focal adhesion kinase 1 (EC 2.7.10.2) (FADK 1) (pp125FAK) (Protein-tyrosine kinase 2).			
ITGA6	3655	Integrin alpha-6 variant (Fragment).			
COMP	1311	Cartilage oligomeric matrix protein variant (Fragment).			
THBS2	7058	Hypothetical protein DKFZp686G02190 (Fragment).			
THBS3	7059	Thrombospondin 3 variant (Fragment).			
THBS4	7060	Thrombospondin-4 precursor.			

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[Entrez Gene](#) 961,

[UniParc](#) UPI0000049C6C, UPI00001BDF2Z,

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All confidence scoring methods that returned results for the current interactions

Name	ID	Description	Select confidence measure ...					
P2RY2	5029	P2Y purinoceptor 2 (P2Y2) (P2U purinoceptor 1) (P2U1) (ATP receptor) (Purinergic receptor).	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
EPB42	2038	Erythrocyte membrane protein band 4.2 (Erythrocyte protein 4.2)(P4.2).	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
THBS1	7057	Hypothetical protein (Fragment).	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
UBQLN1	29979	Ubiquilin-1 (Protein linking IAP with cytoskeleton 1) (PLIC-1) (hPLIC-1).	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
RHAG	6005	Rhesus blood group-associated glycoprotein (Rhesus blood group-associated ammonia channel) (Erythrocyte plasma membrane 50 kDaglycoprotein) (Rh50A) (CD241 antigen).	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
PTK2	5747	Focal adhesion kinase 1 (EC 2.7.10.2) (FADK 1) (pp125FAK) (Protein-tyrosine kinase 2).	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
ITGA6	3655	Integrin alpha-6 variant (Fragment).	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
COMP	1311	Cartilage oligomeric matrix protein variant (Fragment).	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
THBS2	7058	Hypothetical protein DKFZp686G02190 (Fragment).	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
THBS3	7059	Thrombospondin 3 variant (Fragment).	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
THBS4	7060	Thrombospondin-4 precursor.	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

POINT OPHID HPIDB HOC DIP BIOVERSE-CORE

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961

e.g. Ensembl, Entrez Gene, Genelinfo, Pfam, RefSeq, UniProtKB

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[UniGene](#) Hs.446414,

[Entrez Gene](#) 961,

[UniParc](#) UPI0000049C6C, UPI00001BDF2Z,

22 interactions (showing 11 to 20) [previous](#) [next](#) Export as ... Bioverse (originalConfidenceScore) [Query Confidence Sources](#)

Name	ID	Description	SANGER-CORE	INTACT	CCSB-H11	HPRD	BIOVERSE	SANGER	MINT	HOMOMINT	HIMAP-CORE	POINT	OPHIID	HPTDB	HDC	DIP	BIOVERSE-CORE
P2RY2	5029	P2Y purinoceptor 2 (P2Y2) (P2U purinoceptor 1) (P2U1) (ATP receptor) (Purinergic receptor).															
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THBS3	7059	Thrombospondin 3 variant (Fragment).															
THBS4	7060	Thrombospondin-4 precursor.															

Original confidence score provided by the authors

SANGER-CORE	0	1	0	11	5	0	0	1	1	0	6	2	0	0	0	1
INTACT																
CCSB-H11																
HPRD																
BIOVERSE																
SANGER																
MINT																
HOMOMINT																
HIMAP																
POINT																
OPHIID																
HPTDB																
HDC																
DIP																
BIOVERSE-CORE																

Details for Bioverse (originalConfidenceScore)

The confidence score as reported in the original publication.
Range: 0-1
<http://nar.oxfordjournals.org/cgi/content/abstract/31/13/3736>

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[UniGene](#) Hs.446414,
[Entrez Gene](#) 961,
[UniParc](#) UPI0000049C6C, UPI00001BDF2Z,

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 Domain support (predicted)

Protein interactions supported by underlying domain interactions
1

Name	ID	Description
P2RY2	5029	P2Y purinoceptor 2 (P2Y2) (P2U purinoceptor 1) (P2U1) (ATP receptor) (Purinergic receptor).
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THBS3	7059	Thrombospondin 3 variant (Fragment).
THBS4	7060	Thrombospondin-4 precursor.

Domain support (predicted)

This measure indicates protein-protein interactions that are supported by underlying domain-domain interactions. The domain-domain interaction datasets used in the predicted subset are based on diverse computational predication algorithms. Please see the respective interaction details for more information on the datasets.

Range: 1

<http://www.dasmi.de>



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 Query

e.g. Ensembl, Entrez Gene, Genelinfo, Pfam, RefSeq UniProtKB

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UniProtKB [CD47_HUMAN](#), [A8K198_HUMAN](#), [Q71A41_HUMAN](#),
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Entrez Gene [961](#),
UniParc [UPI0000049C6C](#), [UPI00001BDF27](#),

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[Domain support \(predicted\)](#)
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Name	ID	Description	SANGER-CORE	INTACT	CCSB-H11	HPRD	BIOVERSE	SANGER	MINT	HOMOMINT	HLMP	HLMP-CORE	POINT	OPIOD	HPIDB	MDIC	DIP	BIOVERSE-CORE
P2RY2	5029	P2Y purinoceptor 2 (P2Y2) (P2U purinoceptor 1) (P2U1) (ATP receptor)(Purinergic receptor).	0	1	0	11	5	0	0	1	1	0	6	2	0	0	0	1
EPB42	2038	Erythrocyte membrane protein band 4.2 (Erythrocyte protein 4.2)(P4.2).																
			Details from source HPRD															
			link http://www.hprd.org/interactions?protein=01517&isoform_id=01517_1&isoform_name= link http://www.hprd.org/interactions?protein=03017&isoform_id=03017_1&isoform_name= DAS query string http://dasmi.bioinf.mpi-inf.mpg.de/das/hprd/interaction?interactor=008722&interactor=A8K198&interactor=Q71A41&operation=union															
			Details from source Domain support															
			predicted PF00927-PF04549: IPPRI core (0.03977) predicted PF00927-PF08204: IPPRI core (0.03977) predicted PF00868-PF04549: IPPRI core (0.061411) predicted PF00868-PF08204: IPPRI core (0.061411) predicted PF01841-PF04549: IPPRI core (0.061411) predicted PF01841-PF08204: IPPRI core (0.061411)															
			Details from source FunSimMat2.1															
			MFScore 0.976656009021968 CCscore 0.846404924988201															
			Details on domain interactions															
			Details for Domain support (predicted)															
			<p>This measure indicates protein-protein interactions that are supported by underlying domain-domain interactions. The domain-domain interaction datasets used in the predicted subset are based on diverse computational predication algorithms. Please see the respective interaction details for more information on the datasets.</p> <p>Range: 1</p> <p>http://www.dasmi.de</p>															

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Search MPII (type ? for help)

DASMIweb - dynamic online integration and annotation of molecular interaction data

Query

 Query

e.g. Ensembl, Entrez Gene, Genelinfo, Pfam, RefSeq, UniProtKB

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Interactor Information

Identifier: [961 \(Entrez Gene\)](#) (Leukocyte surface antigen CD47 precursor (Integrin-associated protein)(IAP) (Antigenic surface determinant protein OA3) (Protein MER6.)) (CD47 molecule)

[UniProtKB](#) [CD47_HUMAN](#), [A8K198_HUMAN](#), [Q71A41_HUMAN](#),
[UniGene](#) [Hs.446414](#),
[Entrez Gene](#) [961](#),
[UniParc](#) [UPI0000049C6C](#), [UPI00001BDF2Z](#),

22 interactions (showing 11 to 20) [previous](#) [next](#)
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Functional similarity based on GO annotation of interactors

Name	ID	Description
P2RY2	5029	P2Y purinoceptor 2 (P2Y2) (P2U purinoceptor 1) (P2U1) (ATP receptor) (Purinergic receptor).
EPB42	2038	Erythrocyte membrane protein band 4.2 (Erythrocyte protein 4.2) (P4.2).
THBS1	7057	Hypothetical protein (Fragment).
UBQLN1	29979	Ubiquilin-1 (Protein linking IAP with cytoskeleton 1) (PLIC-1) (hPLIC-1).
RHAG	6005	Rhesus blood group-associated glycoprotein (Rhesus blood group-associated ammonia channel) (Erythrocyte plasma membrane 50 kDa glycoprotein) (Rh50A) (CD241 antigen).
PTK2	5747	Focal adhesion kinase 1 (EC 2.7.10.2) (FADK 1) (pp125FAK) (Protein-tyrosine kinase 2).
ITGA6	3655	Integrin alpha-6 variant (Fragment).
COMP	1311	Cartilage oligomeric matrix protein variant (Fragment).
THBS2	7058	Hypothetical protein DKFZp686G02190 (Fragment).
THBS3	7059	Thrombospondin 3 variant (Fragment).
THBS4	7060	Thrombospondin-4 precursor.

Details for FunSimMat2.1 (BPscore)

The BPscore is based on biological process annotation of the Gene Ontology.
Range: 0-1
<http://funsimmat.bioinf.mpi-inf.mpg.de/help.php>

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Conclusions & Outlook



- Usage of DASMI servers and clients surprisingly good, but more external DASMI servers are desirable
- DAS client and server libraries (Dazzle, ProServer, (MyDAS), Dasobert, Bio-DAS-lite) support DASMI
- Considerable overlap with HUPO-PSI initiatives for distributed interaction data retrieval (PSICQUIC) and confidence scoring (PSISCORE)
- Develop methods for combining different interaction confidence scoring schemas in DASMI clients

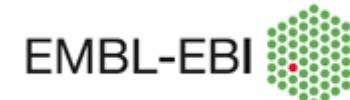


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