

Tabelle A3: Beschreibung der Suchmöglichkeiten und -ergebnisse.
(prop.=properties)

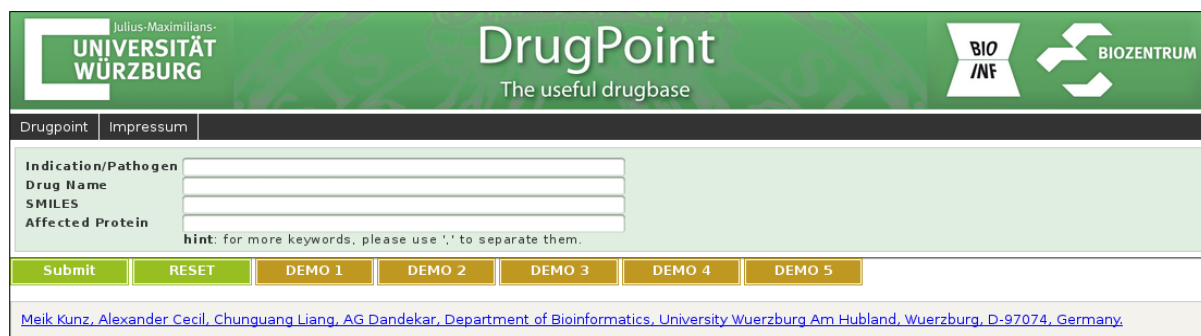
Eigenschaft	Beschreibung
<u>Suchkategorie</u>	
Indication	Diese Suchkategorie prüft alle Einträge nach der entsprechenden Indikation für ein Medikament. Diese Suche ist sehr hilfreich, um das beste Medikament für eine bestimmte pharmakologische Bedingung zu erhalten.
Pathogen	Diese Suchkategorie ist für krankheitsverursachende Organismen und findet die entsprechenden Medikamente gegen das gesuchte Pathogen.
Drug name	Eine einfache Textsuche nach dem gewünschten Medikament.
SMILES	Diese Suchkategorie benutzt den SMILES des Pharmakons. Diese Suche ist die beste Möglichkeit, um ähnliche Medikamente zu finden.
Affected Protein	Alle Medikamente der DB werden nach ihrem Effekt auf das Target durchsucht. Diese Suche ist somit sehr hilfreich, um gezielt nach allen Pharmaka für ein gewünschtes Target zu suchen.
<u>Ergebnisseite</u>	
Generic Name	Der Name des Medikaments ist angegeben.
Drugbank-ID	Die entsprechende Drugbank-ID ist angegeben.
Pharmacological prop.	Die pharmakologische Wirkung des Pharmakons ist angegeben (entsprechend der Drugbank).
Indication prop.	Informationen zur Indikation des Medikaments sind angegeben (entsprechend der Drugbank).
Structure	Die Struktur des Medikaments wird angezeigt.

SMILES and PDB	Die entsprechende SMILES-Annotation ist angegeben, eine automatisch implementierte Funktion konvertiert den SMILES in einen PDB-Strukturfile.
Chemical formula	Die chemische Formel des Medikaments wird angezeigt.
Atom count	Die Anzahl der Atome wurde berechnet.
Mass	Die molare Masse (Teil der Lipinski's rule of five) des Medikaments wurde berechnet.
H-bond donor count	Die Anzahl der H-brücken-bindenden Donore (Teil der Lipinski's rule of five) für ein Medikament wurde berechnet.
H-bond acceptor count	Die Anzahl der H-brücken-bindenden Akzeptoren (Teil der Lipinski's rule of five) eines Pharmakons wurde berechnet.
logP	Der logP-Wert (Teil der Lipinski's rule of five) des Medikaments wurde berechnet.
Ring count	Anzahl der Ringe (ringbildende Atome) eines Medikaments wurde berechnet.
Polar surface area	Die Polar surface area des Pharmakons wurde berechnet.
van-der-Waals surface	Die van-der-Waals surface area des Medikaments wurde berechnet.
Target pathways	Der Target-Pathway (Target-Signalweg) des Pharmakons ist mit einem Crosslink zur KEGG-DB (Maus über Eintrag bewegen) angegeben.
Protein binding	Die Proteinbindung in Prozent ist angegeben.
Protein Interactions	Das Target eines Medikaments ist gegeben inklusive Crosslinks zur PlateletWeb- (P-I in Blutplättchen und anderen Zellen), AnDom- (3-D Strukturvorhersage und -interaktionen) und GoSynthetic-DB (Vorhersage funktioneller Interaktionen) sowie den öffentlichen HPRD-, iHOP-, STRING- und KEGG-DB (Maus über Eintrag bewegen). Dies erlaubt eine detaillierte

	Untersuchung hinsichtlich verschiedener Aspekte und betrachtet das Medikament in seinem Interaktionskontext. Der Nutzer ist somit in der Lage, sich entsprechend seiner wissenschaftlichen Fragestellungen und Interessen individuell zu informieren.
Orthologous Group	Jedes Target wurde auf seine orthologe Gruppe untersucht. Der entsprechende COG/KOGs wird mit seiner Annotation und E-Value gezeigt. Der Nutzer kann für weiterführende Informationen über den COG/KOGs den Crosslink zur GoSynthetic- und STRING-DB nutzen (Maus über Eintrag bewegen).

Tutorial I: Using DrugPoint database

Tutorial A)



Tutorial A illustrates the Web interface for the DrugPoint database. There are four search categories available: “Indication/Pathogen”, “Drug name”, “SMILES” and “Affected Protein”.

A query in the category “Indication/Pathogen” will check against all indications of all drugs in the database. Thus it will be helpful to find out the best possible drug against a given pathological condition. It will also check against the organisms causing those conditions and gives all drugs against the pathogens to the user.

Queries in the category “Drug name” are suitable if the generic brand names of the drugs are known to the users.

If neither the indication, nor the name nor the protein targets of a drug are known – or if the users want to check if his compound is chemically related to known drugs - the SMILES search category will be the best way to find similar drugs in the database. In order to use this function of the database, the canonical SMILES of the users' compound is mandatory.

For users searching for drugs which affect a specific protein, the query should be posted in the category “Affected Protein”. All drugs deposited in the database will be checked for their respective effects on target proteins.

Multiple queries of different in categories are also accepted and multiple keywords in one category should be separated with comma (','). Many user-friendly features have been implemented (e.g. Demo versions for each search category including a detailed description by moving the mouse above).

Tutorial B-E)

Indication/Pathogen	Hematologic disorder
Drug Name	
SMILES	
Affected Protein	

hint: for more keywords, please use ',' to separate them.

Indication/Pathogen	
Drug Name	Dexamethasone
SMILES	
Affected Protein	

hint: for more keywords, please use ',' to separate them.

Indication/Pathogen	
Drug Name	
SMILES	(C)C[C@H](O)[C@@]1(F)[C@@]2([H])CCC2=CC(=O)C=C[C@]12C
Affected Protein	

hint: for more keywords, please use ',' to separate them.

Indication/Pathogen	
Drug Name	
SMILES	
Affected Protein	Glucocorticoid receptor

hint: for more keywords, please use ',' to separate them.

Tutorial F)

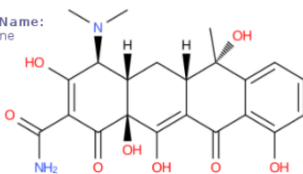
Tutorial F represents the drug Dexamethasone which is one entry the user receives for each search example in Tutorial B-E. The result page is clearly

structured and gives different outputs about general identifiers and information as well as chemical, biological, pharmacological and indication properties. The different chemical properties, e.g. the Lipinski's rule of five as important parameters for drug absorption, were calculated for all compounds in the database. Moreover, we also implemented a SMILES to PDB conversion function and users are able to download the corresponding PDB file or follow different crosslinks (see Tutorial II for more details).

Tutorial G)

Indication/Pathogen	B. burgdorferi
Drug Name	
SMILES	
Affected Protein	

hint: for more keywords, please use ',' to separate them.

Drugbank-ID: DB00759 Generic Name: Tetracycline 	chemical			pharmacological (according to DrugBank)	indication (according to DrugBank)
	Chemical formula	C22H24N2O8			
	Atom count	41			
	Mass	266,16			
	H-bond donor count	3			
	H-bond acceptor count	4			
	logP	0,43			
	Ring count	1			
	Polar surface area	84,58			
	van-der-Waals surface area	439,84			
	biological				
	Target pathways	Tetracycline Pathway			
	Protein binding	20 - 67% For more details please follow: • KEGG Search			
	Protein Interactions	16S rRNA Major prion protein 30S ribosomal protein S3 30S ribosomal protein S8 30S ribosomal protein S19 30S ribosomal protein S14 30S ribosomal protein S7			
	Orthologous Group of target protein		Group		
1		COG0199	Ribosomal protein S14	5,00E-70	
2		COG0185	Ribosomal protein S19	8,00E-64	

As mentioned in Tutorial A there is a search category for “Indications/Pathogens”. Tutorial G demonstrates the search for disease caused by the organism *B. burgdorferi* and yields tetracycline as treatment for this pathogen. Moreover, other possible indications for this drug as well as information about its mechanism of action (see column indication and pharmacological) are available here. Known drug target pathways are also presented to the users and can again be investigated by following the links provided by DrugPoint.

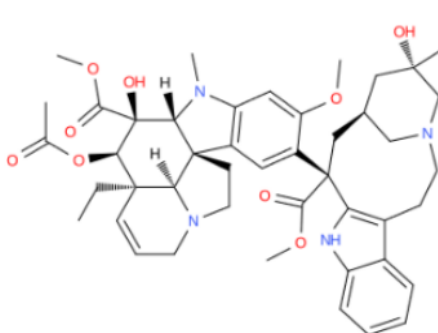
Tutorial H) Query concatenation

Indication/Pathogen	Lymphomas
Drug Name	
SMILES	
Affected Protein	Tubulin

hint: for more keywords, please use ',' to separate them.

Drugbank-ID:
DB00570

Generic Name:
Vinblastine



Tutorial H illustrates how queries joining more search categories at the same time (Example: “Lymphomas” in the category “Indication/Pathogen” and “Tubulin” in the category “Affected Protein”). In this example, DrugPoint yields only one result (the drug: Vinblastine). However, DrugPoint generated six entries for Lymphomas and twelve when searching Tubulin (both not shown). In this case, query with more searching categories successfully reduces the output number and locates a better appropriate drug.

Tutorial II: Putting the drug into its Protein Interaction context

In the DrugPoint database the drug targets and their protein interactions place the drug into its interaction context. For each drug target we thus display the protein

interactions according to the perspective of a number of databases and prediction software, giving a detailed view on involved protein interactions around a drug and its principal target and how to judge and compare these.

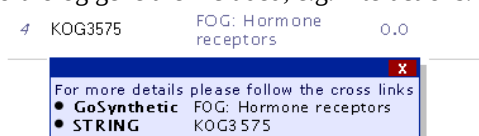
Protein binding	70,00%																					
Protein Interactions	Glucocorticoid receptor Annexin A1 Nitric oxide synthase Nuclear receptor DB1 For more details: • PlateletWeb Search • AnDom Search • GoSynthetic Search • HPRD Search • iHOP Search • STRING Search • KEGG Search																					
Orthologous Group of target protein	<table><thead><tr><th>Group</th><th>Annotation</th><th>E-Value</th></tr></thead><tbody><tr><td>1 KOG1158</td><td>NADP/FAD dependent oxidoreductase</td><td>0.0</td></tr><tr><td>2 COG4362</td><td>Nitric oxide synthase, oxygenase domain</td><td>1,00E-107</td></tr><tr><td>3 COG0369</td><td>Sulfite reductase, alpha subunit (flavoprotein)</td><td>4,00E-65</td></tr><tr><td>4 KOG3575</td><td>FOG. Hormone receptors</td><td>0.0</td></tr><tr><td>5 KOG0819</td><td>Annexin</td><td>0.0</td></tr><tr><td>6 KOG4215</td><td>Hepatocyte nuclear factor 4 and similar</td><td>5,00E-26</td></tr></tbody></table> For more details please follow the cross links • GoSyntheticHepatocyte nuclear factor 4 and similar steroid hormone receptors • STRING KOG4215	Group	Annotation	E-Value	1 KOG1158	NADP/FAD dependent oxidoreductase	0.0	2 COG4362	Nitric oxide synthase, oxygenase domain	1,00E-107	3 COG0369	Sulfite reductase, alpha subunit (flavoprotein)	4,00E-65	4 KOG3575	FOG. Hormone receptors	0.0	5 KOG0819	Annexin	0.0	6 KOG4215	Hepatocyte nuclear factor 4 and similar	5,00E-26
	Group	Annotation	E-Value																			
	1 KOG1158	NADP/FAD dependent oxidoreductase	0.0																			
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	4 KOG3575	FOG. Hormone receptors	0.0																			
	5 KOG0819	Annexin	0.0																			
6 KOG4215	Hepatocyte nuclear factor 4 and similar	5,00E-26																				

Tutorial J) Analyzing drug effects with COG/KOGs

DrugPoint warehoused the orthologous group in MySQL. In the example given, the group identified is the KOG3575 gene and protein family (one of the hormone receptors, found with high significant E-Value 0.0). The table available from DrugPoint shows for the KOG 3575 receptor family its distribution in different organism. The drug can act on all these receptors (e.g. Estrogen related receptor in mouse) and the user gets an overview on these multiple effects mediated by the COG family if the drug is given.

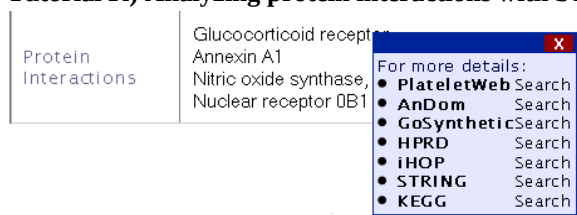
protein	start_position	end_position	orthologous_group	protein_annotation
10090.ENSMUSP00000000450	1	505	KOG3575	peroxisome proliferator activated receptor gamma Gene; Receptor that binds peroxisome prolif ...
10090.ENSMUSP000000002177	1	445	KOG3575	nuclear receptor subfamily 1, group H, member 3 Gene; Orphan receptor. Interaction with RXR ...
10090.ENSMUSP000000002320	28	440	KOG3575	peroxisome proliferator activator receptor delta Gene; Ligand-activated transcription factor ...
10090.ENSMUSP000000002466	1	390	KOG3575	nuclear receptor subfamily 2, group F, member 6 Gene
10090.ENSMUSP000000005820	10	358	KOG3575	nuclear receptor subfamily 1, group I, member 3 Gene
10090.ENSMUSP000000019938	1	385	KOG3575	nuclear receptor subfamily 2, group E, member 1 Gene; Orphan receptor that binds DNA as a mo ...
10090.ENSMUSP000000022304	108	475	KOG3575	thyroid hormone receptor beta Gene; High affinity receptor for triiodothyronine
10090.ENSMUSP000000023119	1	422	KOG3575	vitamin D receptor Gene; Nuclear hormone receptor. Transcription factor that mediates the ac ...
10090.ENSMUSP000000023504	1	429	KOG3575	nuclear receptor subfamily 1, group I, member 2 Gene; Nuclear receptor that binds and is act ...
10090.ENSMUSP000000026036	1	472	KOG3575	nuclear receptor subfamily 0, group B, member 1 Gene; Orphan nuclear receptor. Component of ...
10090.ENSMUSP000000027906	1	458	KOG3575	estrogen-related receptor gamma Gene; Orphan receptor that acts as transcription activator I ...

For analyzing drug effects with COG/KOGs, users can also follow the links in DrugPoint to STRING or GoSynthetic. There, further information about the ortholog gene are included, e.g. interactions.



Regarding to the ortholog groups analysis of DrugPoint, users get all relevant COG/KOGs and organisms for a drug and the option to find out the corresponding proteins as well as prediction of effects in different organisms, e.g. if antibiotic, which organisms have the target protein family (potential antibiotic action of the drugs) and which other not (prediction: no main target effects). Another alternative is also the estimate of binding opportunities and Quantitative structure-activity relationship (QSAR), in particular, if the analysis is coupled to structure files available via the AnDom link (see below).

Tutorial K) Analyzing protein interactions with STRING



The STRING-database specializes on predicting protein interactions combining a number of large-scale experimental data as well as different interaction prediction tools (homology, text mining, co-expression, co-occurrence and neighborhood). Therefore, users get for a drug target further interactions by moving the mouse above to the corresponding DrugPoint output (e.g. Glucocorticoid receptor). Furthermore, users can select an organisms or search against all organism (auto-detect).

search by name search by protein sequence multiple names multiple sequences

protein name: (examples: #1 #2 #3)
 Glucocorticoid receptor

(STRING understands a variety of protein names and accessions; you can also try a [random entry](#))

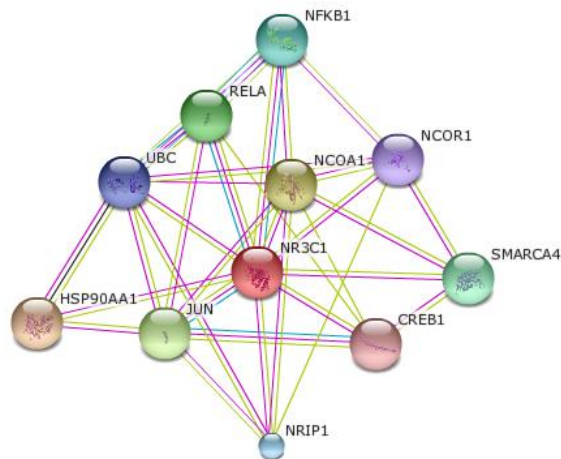
organism:
 auto-detect ▼

interactors wanted:
☐ COGs ☒ Proteins

After clicking to the Go button, query results are shown (here only two) and users can follow the entry of interest (here for NR3C1 in human).

organism	protein
☒ Homo sapiens	NR3C1 - nuclear receptor subfamily 3, group C, member 1 (glucocorticoid receptor); Receptor for glucocorticoids (GC). Has a dual mode of action: as a transcription factor that binds to glucocorticoid response elements (GRE) and as a modulator of other transcription factors. Affects inflammatory responses, cellular proliferation and differentiation in target tissues. Could act as a coactivator for STAT5-dependent transcription upon growth hormone (GH) stimulation and could reveal an essential role of hepatic GR in the control of body growth. Involved in chromatin remodeling. Plays a significant [...]
☐ Mus musculus	Nr3c1 - nuclear receptor subfamily 3, group C, member 1 Gene; Receptor for glucocorticoids (GC). Has a dual mode of action: as a transcription factor that binds to glucocorticoid response elements (GRE) and as a modulator of other transcription factors. Affects inflammatory responses, cellular proliferation and differentiation in target tissues. Could act as a coactivator for STAT5-dependent transcription upon growth hormone (GH) stimulation and could reveal an essential role of hepatic GR in the control of body growth. Involved in chromatin remodeling. Plays a significant role in transactivat [...]

After this, a protein interaction network is given as well as further information about the proteins and the interaction type (e.g. violet Kanten are experimental and light green text mining; here only interaction for NR3C1 is shown).



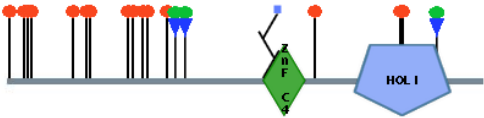
Tutorial L) Analyzing protein interactions and drug effects with HPRD

Protein Interactions	Glucocorticoid receptor Annexin A1 Nitric oxide synthase, Nuclear receptor OB1
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For more details:
 • [PlateletWeb](#) Search
 • [AnDom](#) Search
 • [GoSynthetic](#) Search
 • [HPRD](#) Search
 • [iHOP](#) Search
 • [STRING](#) Search
 • [KEGG](#) Search

To find out which interactions occur really in the patient users can follow the crosslink to HPRD. The HPRD database assembles hand curated data on verified human protein-protein interactions (see above). By moving the mouse above to the corresponding output (e.g. Glucocorticoid receptor) users can follow the crosslink to HPRD by clicking Search and the query results are shown in a new window. For the Glucocorticoid receptor users get two entries including an overview.

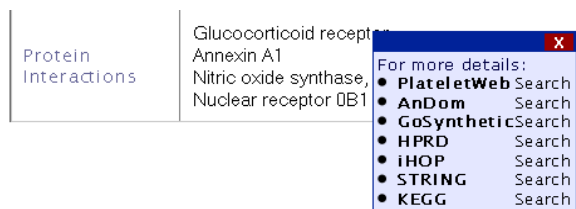
Your search for **Glucocorticoid receptor** in **Protein** reports **2** matches.
Results are sorted by relevance, indicating the number of occurrences of items searched for.
Showing matches **1** to **2**

	↓ Sort by	Relevance	Number of PTMs	Protein Length	Number of Interactions
1	Name : Glucocorticoid receptor		Molecule Function : Ligand-dependent nuclear receptor activity		
					
Number of Interactions : 90					
2	Name : Glucocorticoid receptor DNA binding factor 1		Molecule Function : Ligand-dependent nuclear receptor activity		
					
Number of Interactions : 2					

By clicking to Name (Glucocorticoid receptor, first entry) a detailed list of the protein interactions as well as further information (e.g. experimental type) of the corresponding entry is given. Therefore, DrugPoint allows analyzing and prediction of drug effects as well as side-effects.

ALTERNATE NAMES	DISEASES	PTMs & SUBSTRATES	EXTERNAL LINKS
SUMMARY	SEQUENCE	INTERACTIONS	EXTERNAL LINKS
Protein Interactions			
PROTEIN INTERACTORS		Experiment Type	Type
Name of Interactor			
14-3-3.Eta		In Vitro ; Yeast 2 Hybrid	Direct
Active transcription factor CREB		In Vitro	Direct
Adenosine deaminase		In Vitro	Direct
C/EBP alpha		In Vivo ; In Vitro	Direct
Calmodulin 1		In Vitro ; In Vivo	Direct

Tutorial M) Analyzing protein interactions and drug effects with PlateletWeb



Tissue-specific protein interactions as well as known drug effects on any protein in the interaction network are available from the PlateletWeb crosslink. The database thus includes tissue-specific expression datasets and many cardiovascular drugs including knowledge on cardiovascular side-effects. Tissue specific protein interactions allow minimizing side-effects, in particular platelet versus other tissues. Moreover, interaction predictions for all human tissues are implemented as well as concrete Phosphorylation-information and all known drug interactions for all human proteins are incorporated. Clicking in DrugPoint to the PlateletWeb Search, query results are shown in a new window (here five for the Glucocorticoid receptor). For each entry an overview is given (e.g. about the detection level and the number of interactions) and users can follow the interactions of interest by clicking to the number of total interacting proteins in the Description column (7 for the entry glucocorticoid receptor DNA binding factor 1).

Proteins matching 'GLUCOCORTICOID RECEPTOR'					
Detection Level	Gene Symbol	Description	Platelet Phosphosites	Human Phosphosites	
Both	EEF1A1	eukaryotic translation elongation factor 1 alpha 1 99 total interacting proteins 38 platelet interacting proteins		ST Y	
None	BAG1	BCL2-associated athanogene 22 total interacting proteins 8 platelet interacting proteins		ST	
Both	GRLF1	glucocorticoid receptor DNA binding factor 1 7 total interacting proteins 6 platelet interacting proteins	ST	ST Y	
None	NCOA2	nuclear receptor coactivator 2 57 total interacting proteins 19 platelet interacting proteins		ST	
None	BTBD6	BTB (POZ) domain containing 6 -			

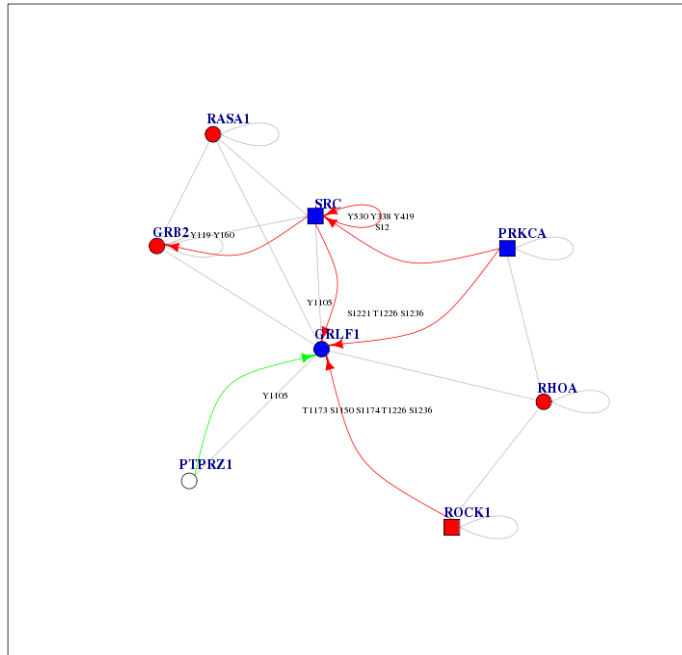
Now, users get all interaction partners including their interactions and can also view the interactions in different network formats (network download, e.g. as pdf or cytoscape session, is available).

Interaction partners for GRLF1						
 >>> To view in Network format, click here						
Detection Level	Gene Symbol	Description	Platelet Phosphosites	Human Phosphosites	Reference	Experiment Type
Proteome	GRB2	growth factor receptor-bound protein 2 271 total interacting proteins 131 platelet interacting proteins		ST Y	1 study	

>>> Click here to download the Compressed file for Cytoscape

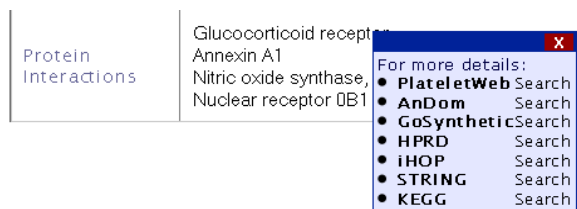
>>> Click here to download the file in pdf format

>>> Click here to view the picture in high (1600 x 1600) resolution



Tutorial N) Analyzing drug effects with GoSynthetic

With DrugPoint users can follow also the crosslink to the GoSynthetic database.



There, analyzing of drug effects including the hierarchical functional and gene ontology categories help to better analyze a drug target and its functional interactions according to gene ontology and gene functions. With GoSynthetic users can search systematically for protein targets with a specific function in mind and analyze a protein interaction network around a drug regarding involved functions. Moreover, these categories help also to reveal side-effects and make a prediction of affected subnetworks and of drug combination effects. A bridging function is implemented in DrugPoint such that also the corresponding target sequence of the target sequence of interest is analyzed by GoSynthetic. A model organism (in this example Homo sapiens) of choice can be specified, next functional hierarchy, interaction networks and clustering of involved functions is examined.

Search

GoSynthetic Sequence Searching

Sequence

```
MDSKESLTGPGREENPSSVLAQERGDVMDFYKTLRGGATVKVSASSPFLAVASQSDSKORELLVDFFPKGSVSNAAQFDLSKAVLSMGLIMGE
TETKVMGNDLGFPQQQISSLSSGETDLKLLSESIANLNRSVTPENPKSSASTAVSAAPTEKEFPKTHSDVSSQQHLKGQTGTNGGVNKLKY
TTDQSTFD ILQDLFFSSGSGKETNESPMRSDLL IDENCLLSPLAGEDDSFLLEGNSNEDCKPL ILPDTKPKIKD MGDVLVLSSPSNVTL PQV
KTEKEDF IELCTPGVIGKQELGTVYCCASFPGANIIIGNKMSAISVHGVSSTSGGQMHYDMNTASLSQQQDKP IFNVIPP IPVGSSEMMNRQ
GSGDDNLTSLGTLNFFGRVTFVSNGYSSPMRFDVSSPPSSSTATTGFPFKLCLVCSDEASGCHYGVLTGSGCKVFFKRAVEGQHNYLCAGR
NDCIIDKIRKNCPCACRYRKLQAGMNLKARKTKKKIKIGIQOATTGVSQETS ENPKNKTIVFATLPQLTPTLVSLLEVI EPEVL YAGYDSSV
PDSTWRIMITLNM LGGQVIAAVKAKAIPGFNHLHDDQMTLLQYSMMFLMAFALGWRSTFGSSANLLCFAPDLIINEQRM LPCM YDQCK
HMLVYSSSELHRLQVSYREYLCMKTL LLSVFKDGLKSQELPDEIRMTYIKELGKAIVKREGNSSQNWQRFYQLTKLLDSMHEVVENMLNYC
PQTFLDKIMSIEFFPEMLAEIITNQIPKYSNGNIKLLFHQK
```

Model Org.

(specify a model organism which is closest related to your sequence please)

Results including different parameters, e.g. GO-ID, Description and a pie chart view, are given, lists of descriptions list all functions involved in the sub-network analyzed (here for glucocorticoid receptor activity).

ID: P04150 Model: Glucocorticoid receptor OS=Homo sapiens GN=NR3C1 PE=1 SV=1	
List	
GoSynPointer	Description
GO:0016020	membrane
GO:0005759	mitochondrial matrix
GO:0005634	nucleus
GO:0007165	signal transduction
GO:0006111	regulation of gluconeogenesis
GO:0005622	intracellular
GO:0004883	glucocorticoid receptor activity
GO:0030325	adrenal gland development
GO:0003700	transcription factor activity
GO:0005496	steroid binding
Search result	
Network Transmitter Adjuvant Receiver Linear Active Whole complex Information storage Regulation Barrier	
Piechart view, process type summary Back to Query page	

In the example given, users obtain the functional relation (biological function as Controller and technical function as Receiver) including interactions and can also download the interaction network file for Cytoscape.

View

View: switch to
Biological Terms

+ "Controller" --- (isa) ---> Controller NR3C1, NR3C1, NR3C1, NR3C1

View

View: switch to
Technical Terms

+ "Receiver" --- (isa) ---> Receiver NR3C1, NR3C1, NR3C1, NR3C1

proteins:

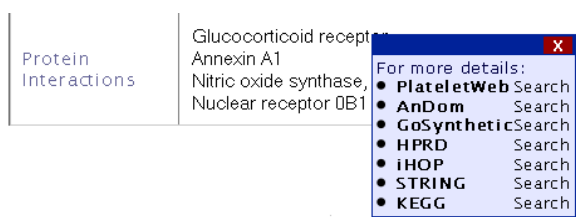
Intact

Interaction network file for Cytoscape : [Download](#), you could load the network file using the import function in Cytoscape.

Another option is the usage of the VRelations view with GoSynthetic, showing all interactions graphically including their functional clustering. This allows to scan for side-effects and to optimize the function profile of the drug.

Tutorial O) Analyzing drug effects with AnDom

For a given target in DrugPoint, users can identify all domains including structure information as well as the PDB file for docking and drug optimization. Furthermore, the finding of a potential structure for a drug is also feasible in this context. This works for every protein target sequence which has at least little fact with 3D homology.



The AnDom crosslink opens a new window and the implemented bridging function put the sequence (in this example for Glucocorticoid receptor) into the search field.

Protein-Identifier:

(e.g. KPYK1_ECOLI or P0AD61 or AAB47952)

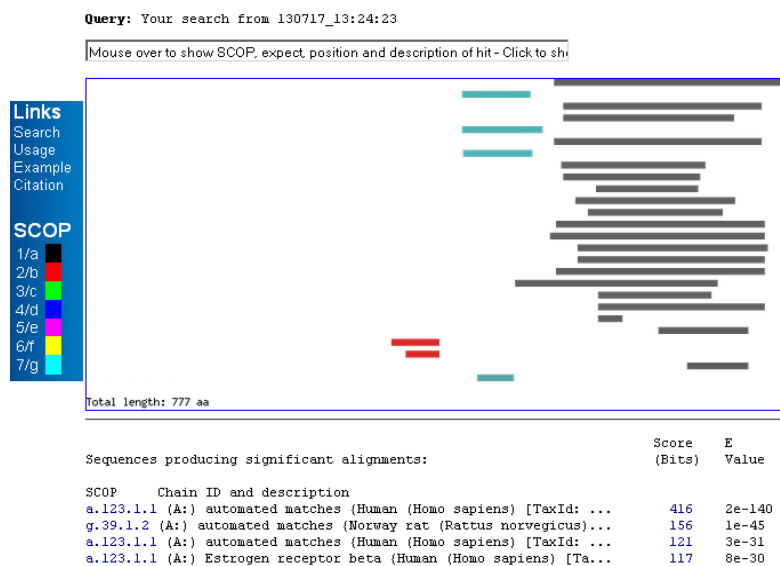
Protein-Sequence: (in FASTA-format or raw sequence - digits will be ignored)

```
MDSKESLTPGREENPSSVLAQERGDVMDFYKTLRGGATVKVSASSPSLAVASQSDSKQRLLVDFPKGSVSNAAQQPDLSK
AVSLSMGLYMGETETKVMGNDLGFPQQGQISLSSGETDLKLEESIANLNRSTSVPENPKSSASTAVSAAPTEKEFPKTH
SDVSSEQQHLKGQTGTNGGNVKLYTTDQSTFDILQDLEFSSGSPGKETNESPWRSDDLIDENCLLSPLAGEDDSFLLGN
SNEDCKPLILPDTKPKIKDNGDLVLSSPSNVTLQVKTEDFIELCTPGVIKQKELGTVYCOASFPGANIIGNKMSAIS
VHGVSSTGGQMYHYDMNTASLSQQQDQKPIFNVIPIPVGSENNWRCQSGDDMLTSLGTLNFPGRIVFSNGYSSPSMRP
DVSSPPSSSTATTGPPPKLCLVCSDEASGCHYGVLTCGSCKVFFKRAVEGQHNYLCAGRNDICIIDKIRKNCPCACRYRK
CLQAGMNLKARKTKKKIKGIQQATTGVSQETSENPENKTIIVPATLPOLPTLVSLLEVIEPEVLYAGYDSSVPDSTWRIM
TTLNMLGGRQVIAAVKWAIPAIFRNHLDDQMILLQYSWMFLMAFALGWSYRQSSANLLCFAPDLIINEQRMILPCMY
DQCKHMLYVSSSELHRLQVSYEEYLCMKITLLLSVFPKDGLKSQELFDEIRMTYIKELGKAIKREGNSSQNWRQFYQLTK
```

Parameters:

Method:
Database:
Expect:
Filter: ☒ Low complexity (SEG)
Show: ☒ Index List

Users can select between different parameters (e.g. Method and Database) and click to the Search button for analyzing the sequence. The Search result will be immediately displayed including structural classification information, e.g. SCOP identification, description and E-Value (please note, here only four results shown).



Users get the alignment by scroll down or clicking to the Score value (here for Estrogen receptor beta is presented).

```
> a.123.1.1 (A:) Estrogen receptor beta (Human (Homo sapiens) [TaxId:
9606]}
Length=237

Score = 117 bits (295), Expect = 8e-30
Identities = 57/198 (29%), Positives = 92/198 (46%), Gaps = 10/198 (5%)

Query 532 LVSLLEVIEPEVLYAGYDSSVPDSTWRIMTTLNMLGGRQVIAAVKAKAIPGFRNLHLDD 591
          LV L EP + S P + +M +L L +++ + WAK IPGF L L D
Sbjct 7 LVLTLLAEPPHVLIS-RPSAPFTEASMMMSLTKLADKELVHMISWAKKIPGFVLSLFD 65

Query 592 QMTLLQYSWMFLMAFALGWRSYRQSSANLLCFAPDLIIN-EQRMTLPCMYDQCKHMLYVS 650
          Q+ LL+ WM ++ L WRS L FAPDL+++ ++ + + + +L +
Sbjct 66 QVRLLESCWMEVLMMLMWSRIDHPGK--LIFAPDLVLDREDEGKCEGILEIFDMLLAT 123

Query 651 SELHRLQVSYYEYLCMKTLTLLSSVPKDGKLSQELFDEIRM-----TYIKELGKAIVKR 704
          S L++ ++EYLC+K ++LL+S + + + D R L I K
Sbjct 124 SRFRELKLQHKYLCVKAMILLNSSMYPLVTATQDADSSRKLALLNAVTDALVWVIAKS 183

Query 705 EGNSSQNWRQFYQLTKLL 722
          +S Q R L LL
Sbjct 184 GISSQQQSMRLANLLMLL 201
```

By clicking to the corresponding SCOP-ID, structural information also available and makes further domain investigations easily possible (here about the Nuclear receptor ligand-binding domain not shown).

Modellierung und Simulation von Protein-Interaktionen
am Beispiel von Wirts-Pathogen-Interaktionen

Kunz, M.

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