

Mining Gene-Disease Associations for Drug Identification and Discovery with Open Targets

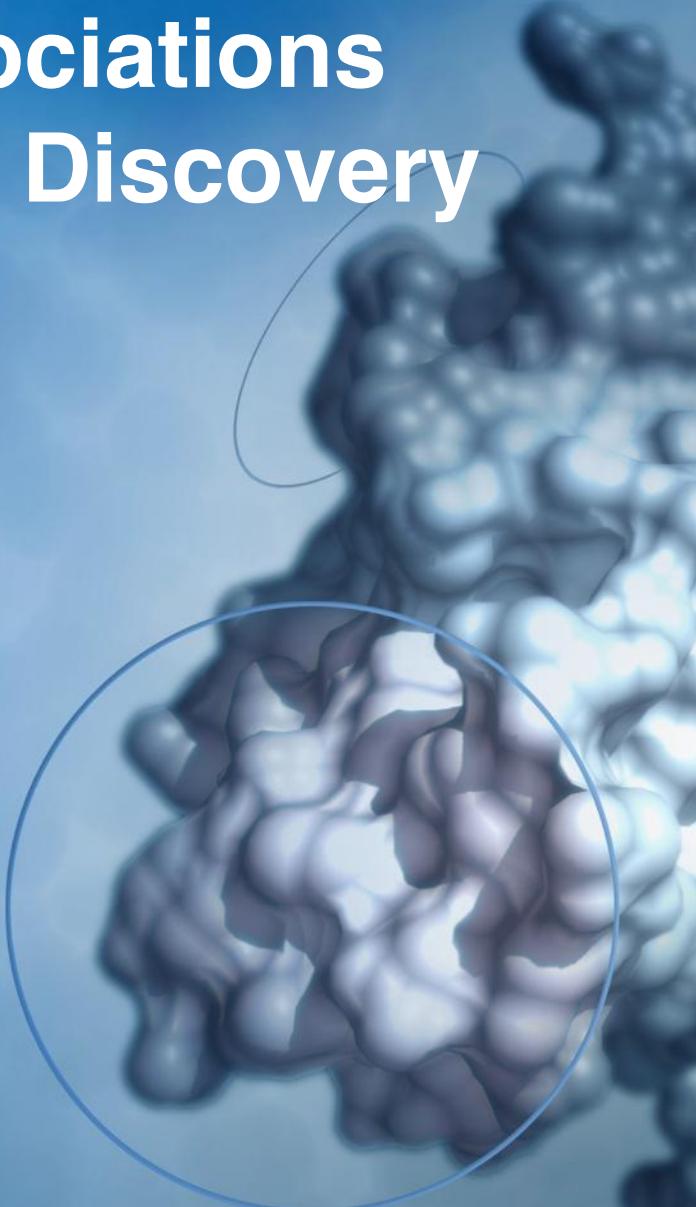
Yale School of Medicine

Denise Carvalho-Silva

Wellcome Genome Campus, United Kingdom
Open Targets Consortium
Core Bioinformatics team



Open Targets



Today 09:30-12:00

- Drug Discovery and its challenges
- The Open Targets Consortium and its Platform
- Data sources and scoring target-disease associations

Talks, demos and hands-on exercises

- Wrap up and feedback survey

Course materials

<https://github.com/deniseOme/training>



slides

Open Targets



Hands-on Workshop
Course booklet

Open Targets



Hands-on Workshop
Answer booklet

answers



Course objectives

What is the Open Targets Consortium?

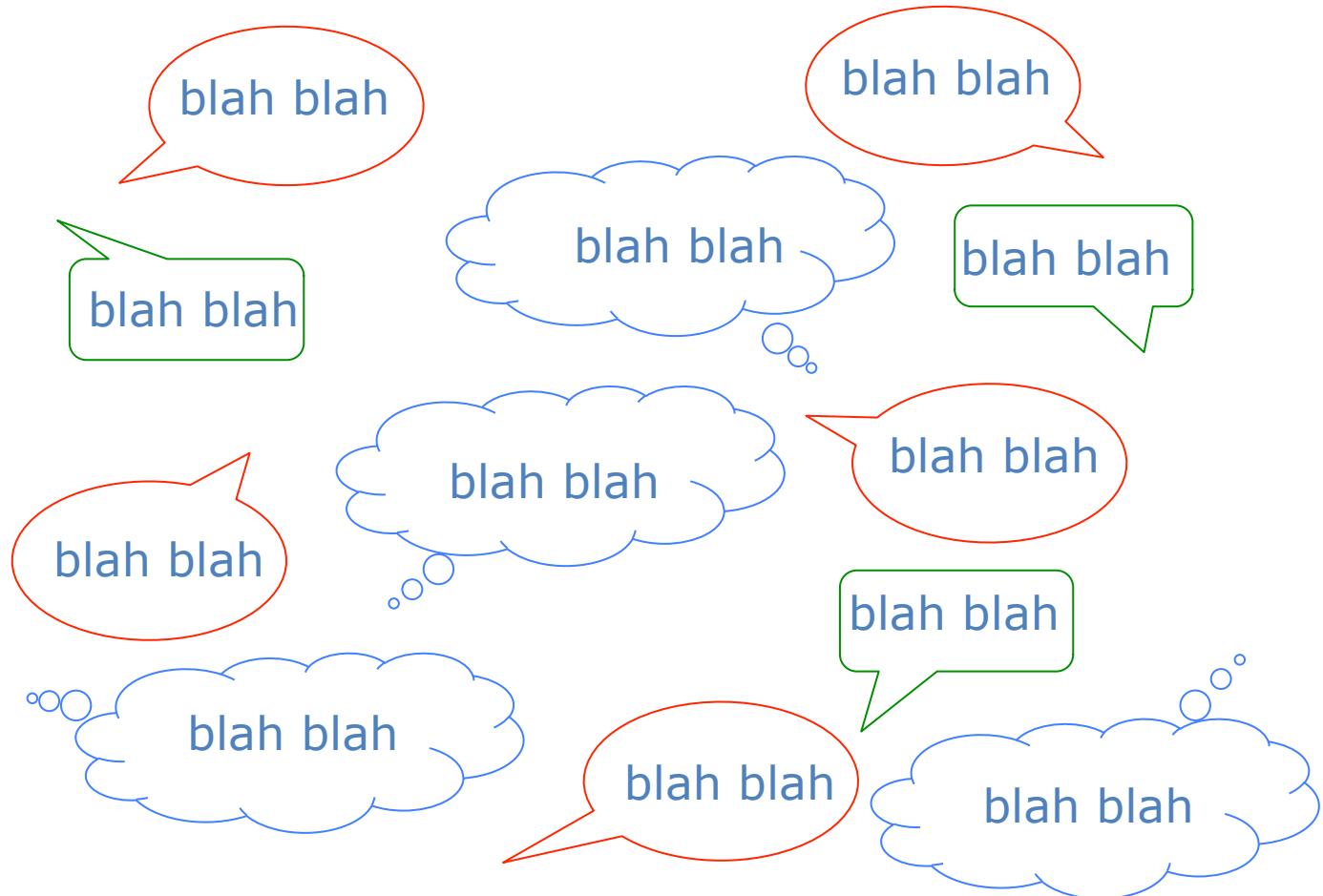
What is the Open Targets Platform?

How to navigate the Platform?

How to connect with us

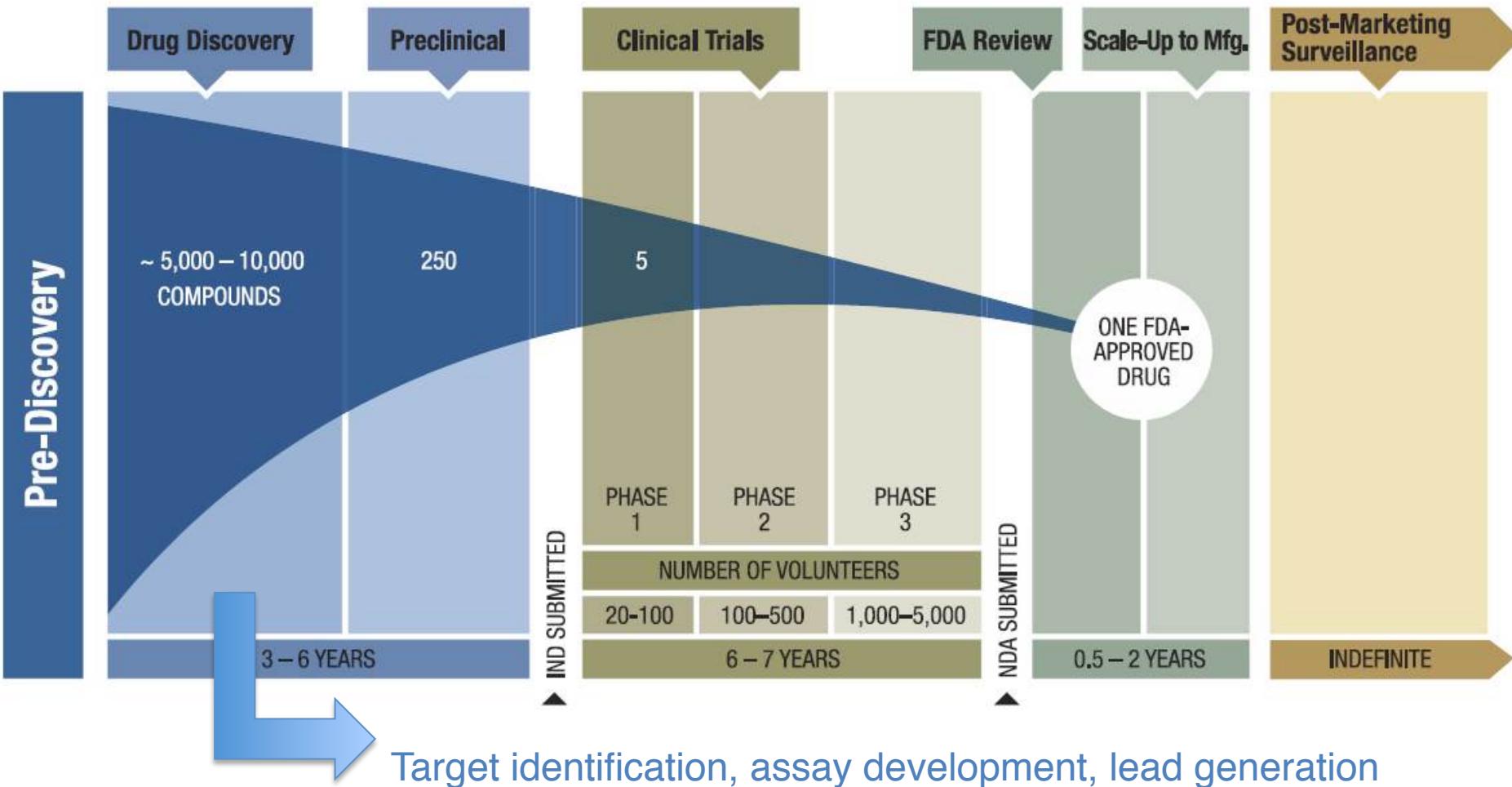


Open Targets

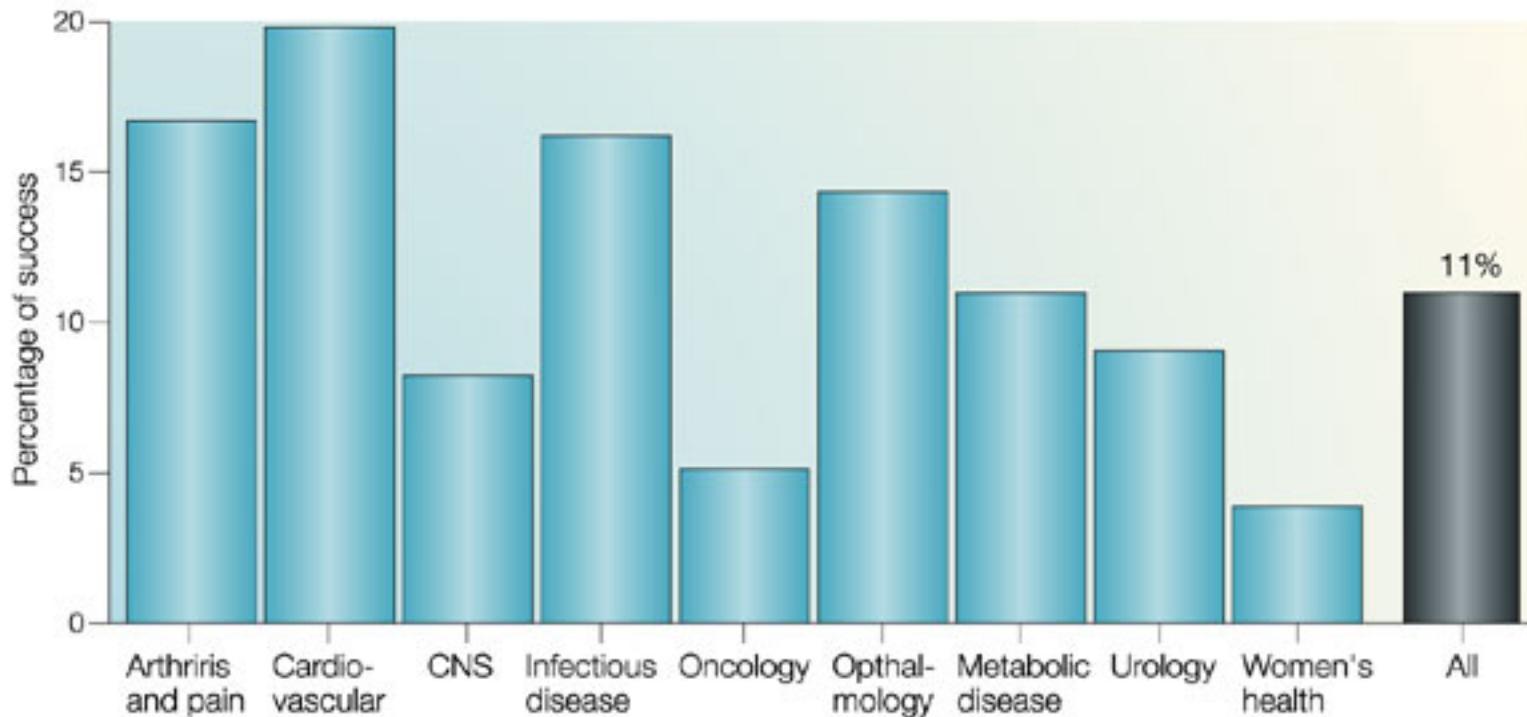


Open Targets

Drug discovery path: timeline



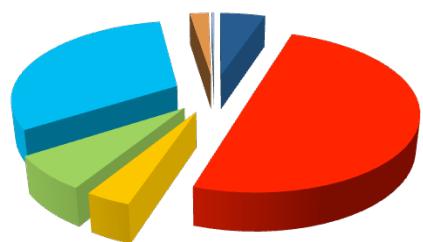
Drug discovery: the challenges



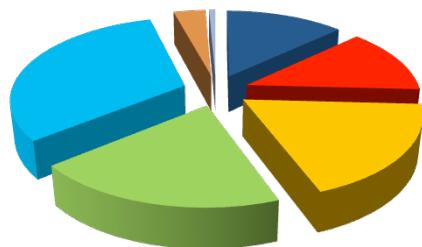
Lengthy, costly, low success rate, **high attrition rate**

What are the causes for the attrition?

Pre-clinical



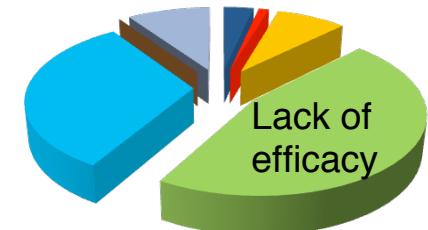
Phase I



Phase II



Phase III



- Pharmacokinetics/bioavailability
- Clinical safety
- Commercial
- Regulatory

- Non-clinical toxicology
- Efficacy
- Technical



*Professor Sir
Mike Stratton
Director, Sanger Institute*

Can we improve
target identification?



*Patrick Vallance, President
Pharmaceuticals R&D
GlaxoSmithKline*



*Professor Dame
Janet Thornton
former Director, EMBL-EBI*

Yes, we can!
And we should.

But one institution
can not do it alone.



Open Targets Consortium*



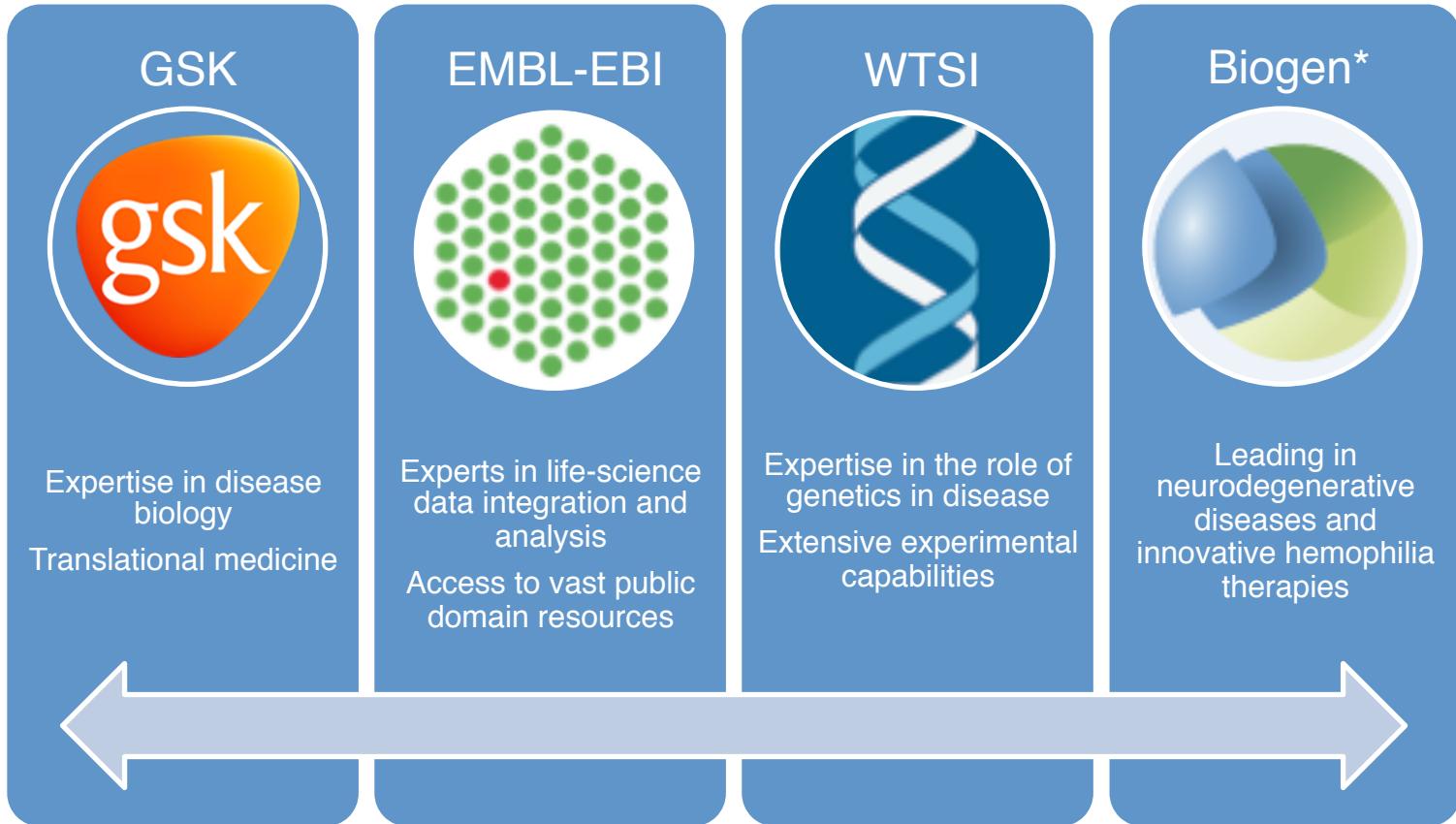
* Launched in March 2014
Three founding partners



EMBL-EBI



Who is Open Targets?



*Biogen joined the consortium in February 2016

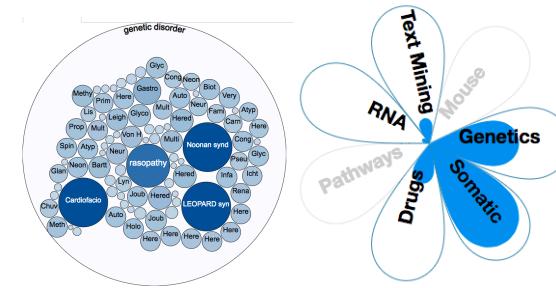
The two major areas of work* within Open Targets

Experimental projects



Generate new evidence
CRISPR
Organoids
Single cell RNASeq
Cell line fusion analyses
Metabolite GWAS

Core bioinformatics pipelines

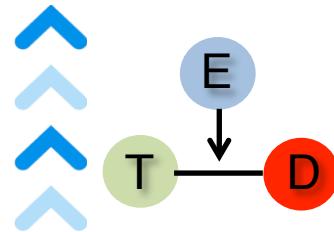


Database for data integration
Web portal
REST API
Python client (fully supported)
R client (community)
Data dumps

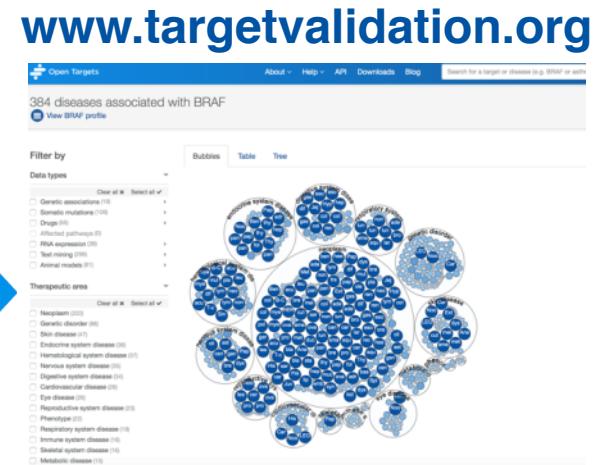
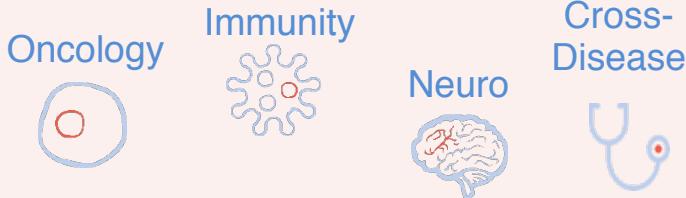
* Concurrent
www.opentargets.org/projects

Integration of existing and new data

Public Databases and Pipelines



Open Targets experimental data: NEW
Physiologically relevant and at scale



Graphical user interface

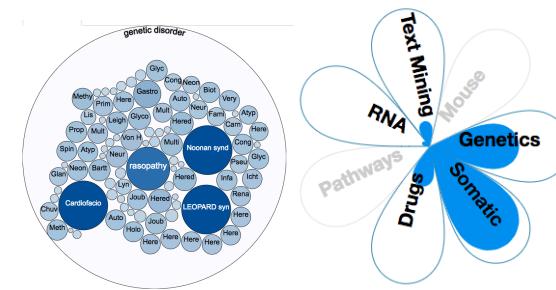
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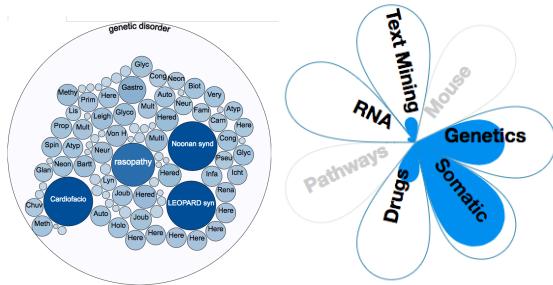


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Open Targets Platform*

- Developed by the Core Bioinformatics team at EMBL-EBI
- Allow scientists to identify target–disease associations
- Frequent updates: new data, new web features
- Improvements driven by our user communities

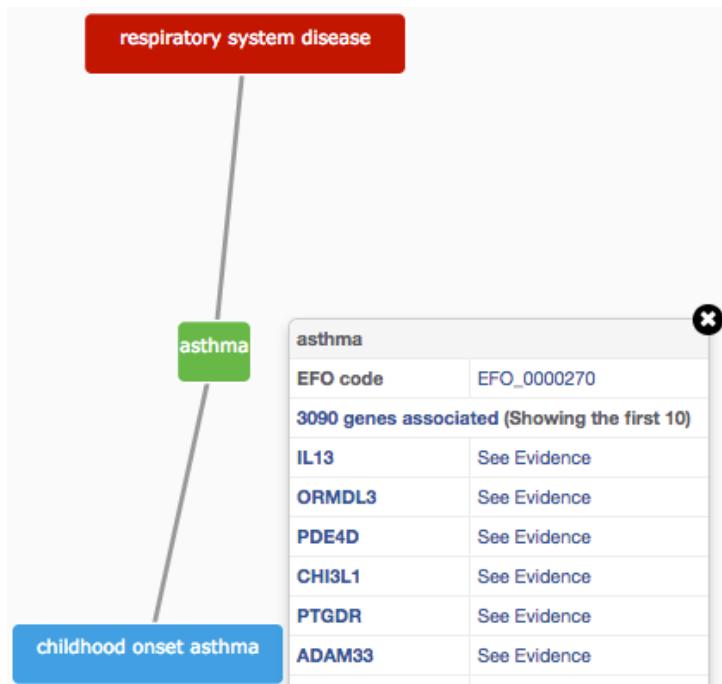
<https://www.targetvalidation.org/>



* First release: December 2015

Experimental Factor Ontology* (EFO)

- Ontology: smart dictionary → relationships between entities
- EFO: way to organise experimental variables (e.g. diseases)



controlled vocabulary
+
hierarchy (relationship)

* <https://www.ebi.ac.uk/efo/>

Increases the richness of annotation
Promotes consistency
Allow for easier and automatic integration

How do we associate diseases and phenotypes w/ targets?

- 1 ChEMBL, UniProt, EVA (w/ ClinVar) curate diseases and phenotypes
- 2 Map disease/phenotypes to an ontology using EFO and HPO terms
- 3 Use genes as proxies for our targets
- 4 Create target-disease evidence JSON objects
- 5 Calculate for each supporting evidence the likelihood of gene A being associated with disease B
- 6 Compute integrated target-disease scores at the levels of data source, data type and overall score

A possible use case



[Am J Hum Genet.](#) 2006 Jun; 78(6): 1011–1025.

Published online 2006 Apr 25. doi: [10.1086/504300](https://doi.org/10.1086/504300)

PMCID: PMC1474084

Reconstruction of a Functional Human Gene Network, with an Application for Prioritizing Positional Candidate Genes

[Lude Franke](#),¹ [Harm van Bakel](#),¹ [Like Fokkens](#),¹ [Edwin D. de Jong](#),² [Michael Egmont-Petersen](#),³ and [Cisca Wijmenga](#)¹

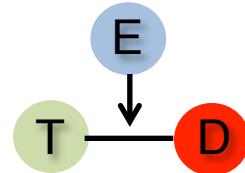
- Detect disease genes from a functional gene network
- 96 diseases (Mendelian and complex inheritance, cancer)
- 345 unique disease genes
- e.g. renal cell carcinoma (papillary) and *MET*, Alzheimer's and ENSG00000091513

Tutorial 1*: Renal cell carcinoma

- How many targets are associated with this disease?
- Which data sources were used to support this association?
- Which targets are based on “Genetic association” evidence only?
- Which drugs are known to be in clinical trials for this disease?
- Which diseases are related to renal cell carcinoma?

*coursebook: pages 8 -15

Publicly available data



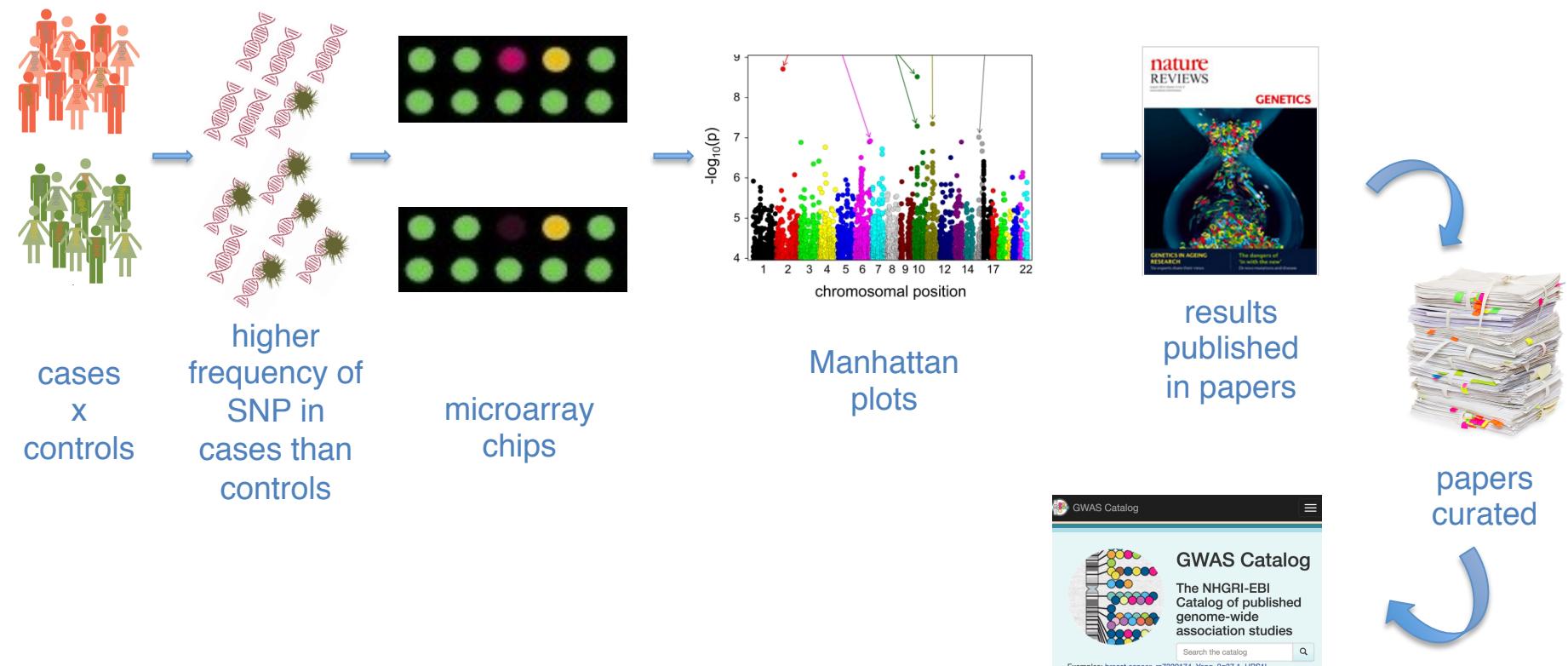
- Similar data sources are grouped into data types

Data sources	Data types
GWAS catalog, UniProt, EVA, G2P	Genetic associations
Cancer Gene Census, EVA, IntOgen	Somatic mutations
Expression Atlas	RNA expression
ChEMBL	Drugs
Reactome	Affected pathways
Europe PMC	Text mining
PhenoDigm	Animal models
Your favourite data?	Let us know!

<http://tinyurl.com/platform-your-say>

Data sources: GWAS catalog

- GenomeWide Association Studies (www.nature.com/nrg/series/gwas/index.html)
- Array-based chips → genotyping 100,000 SNPs genomewide



<https://www.ebi.ac.uk/gwas/>

SNP-trait associations
Published in the GWAS catalog

Data sources: UniProt* and UniProt literature**

- Catalog of protein information (sequence, annotation, function)



* Manual curation of variants in the coding region, seen in patients

** Associations between target and disease, no specific mutation

Data sources: EVA

- Catalog of genetic variants (SNPs, CNVs; germline or somatic)
- Clinical information from ClinVar available: rare diseases

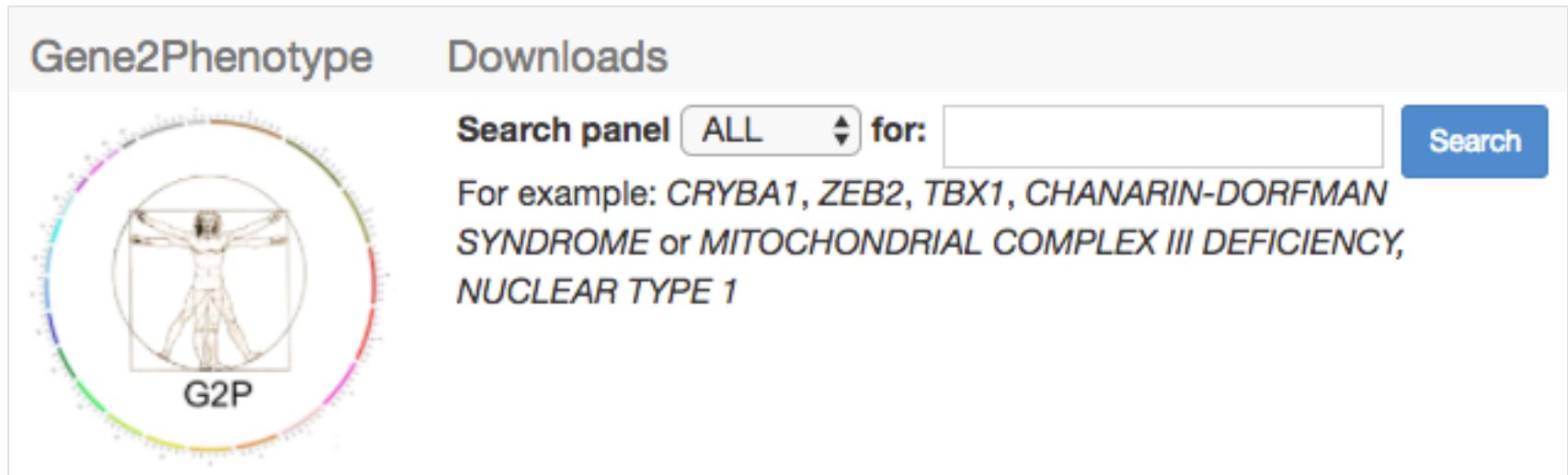
The screenshot shows the European Variation Archive (EVA) website. The header features the EVA logo and the text "European Variation Archive". Below the header is a navigation bar with links: Home, Submit Data, Study Browser, Variant Browser, Clinical Browser (which is highlighted in blue), GA4GH, API, FAQ, and Feedback.

The main content area is titled "ClinVar Browser" with a help icon. On the left, there is a "Filter" sidebar. The "Position" filter is set to "Assembly : GRCh37". The "Filter By:" dropdown is set to "Chromosomal", and the "Chromosome" dropdown shows "2:48000000-49000000". The "Consequence" filter has a "search" input field.

The main table displays 10 records out of 960, showing clinical variant details:

...	Posi...	Affecte... i	A...	Most Severe Consequence...	Trait	Clinical Significance	ClinVar ...
2	480...	MSH6	T/G	upstream_gen...	Lynch synd...	Benign	RCV000...
2	480...	MSH6	G/A	upstream_gen...	Lynch synd...	Benign	RCV000...
2	480...	MSH6	C/T	upstream_gen...	Lynch synd...	Benign	RCV000...
2	480...	MSH6	C/T	upstream_gen...	Lynch synd...	Benign	RCV000...
2	480...	MSH6	G/T	5_prime_UTR...	Lynch synd...	Uncertain s...	RCV000...
2	480...	MSH6	G/T	5_prime_UTR...	Hereditary ...	conflicting ...	RCV000...
2	480...	MSH6	C/T	5_prime_UTR...	Lynch synd...	Uncertain s...	RCV000...
2	480...	MSH6	C/T	5_prime_UTR...	Hereditary ...	conflicting ...	RCV000...
2	480...	MSH6	G/T	5_prime_UTR...	Hereditary ...	Benign	RCV000...
2	480...	MSH6	G/T	5_prime_UTR...	Hereditary ...	conflicting ...	RCV000...

Data sources: Gene2Phenotype



Gene2Phenotype

Downloads

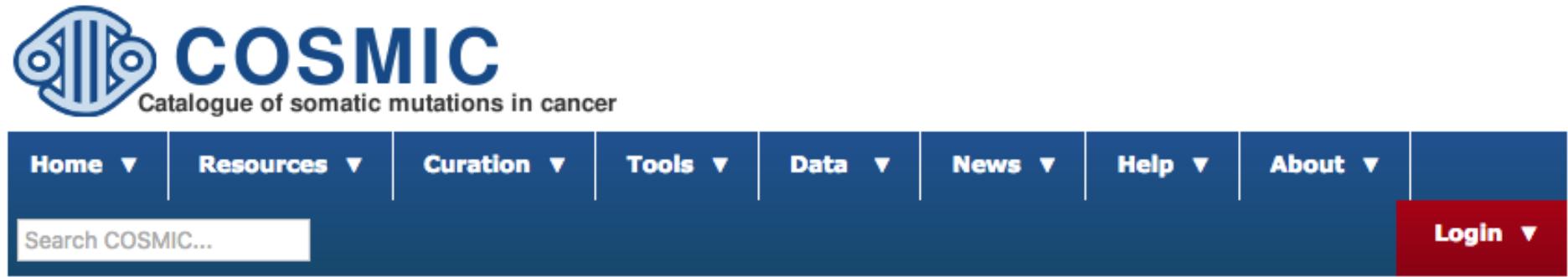
Search panel ALL for: Search

For example: *CRYBA1, ZEB2, TBX1, CHANARIN-DORFMAN SYNDROME or MITOCHONDRIAL COMPLEX III DEFICIENCY, NUCLEAR TYPE 1*

G2P

- Catalog of variants, genes, phenotypes
- Developmental disorders
- Literature curation → consultant clinical geneticists in the UK

Data sources: The Cancer Gene Census



The screenshot shows the COSMIC website homepage. At the top left is the COSMIC logo, which consists of a stylized blue eye-like icon followed by the word "COSMIC" in a bold, blue, sans-serif font. Below the logo is the tagline "Catalogue of somatic mutations in cancer". A horizontal navigation bar follows, featuring eight items: "Home ▾", "Resources ▾", "Curation ▾", "Tools ▾", "Data ▾", "News ▾", "Help ▾", and "About ▾". To the right of this bar is a red "Login ▾" button. Below the navigation bar is a search bar containing the placeholder text "Search COSMIC...".

- catalog of genes for which mutations have been causally implicated in cancer
- genes associated with specific plus other cancers associated with that gene

Data sources: IntOGen

The screenshot shows the homepage of the IntOGen website. At the top is a navigation bar with links for Search, Downloads, Analysis, and About. On the far right is a Sign In button. Below the navigation bar is the IntOGen logo, which consists of a stylized orange 'i' icon followed by the word 'intOGen' in lowercase. To the right of the logo is the text 'Integrative Onco Genomics'. Below the logo is a search bar containing the placeholder text 'e.g. Mutation frequency of VHL'. To the right of the search bar is a microphone icon. Below the search bar are links for 'Search example' and 'Show more examples'.

intOGen

Search Downloads Analysis About

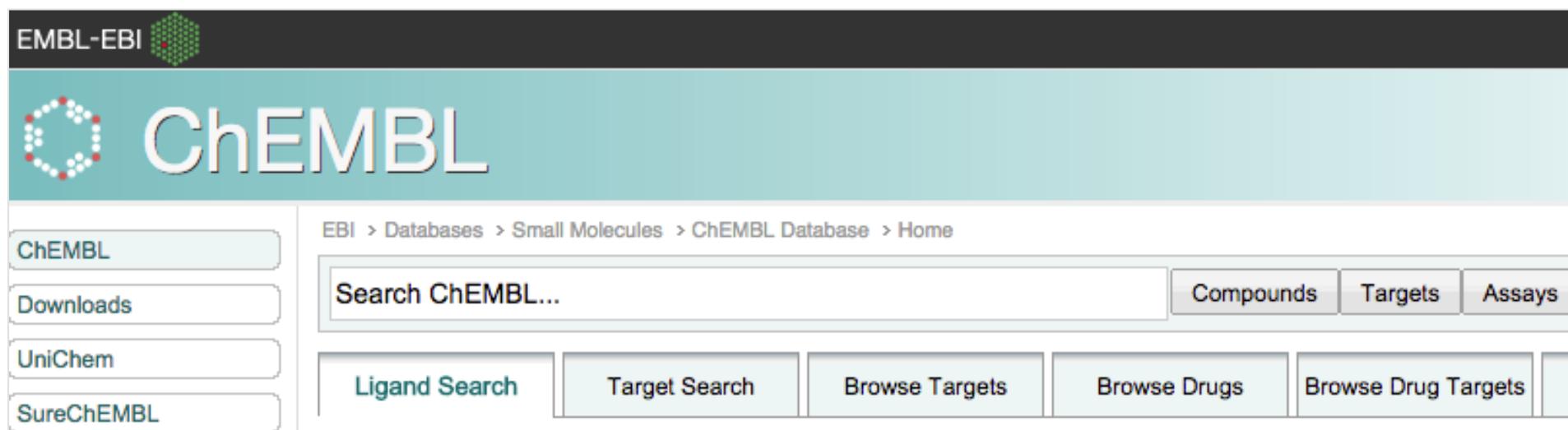
Sign In

e.g. Mutation frequency of VHL

Search example | Show more examples

- catalog of genes and somatic (driver) mutations
- involvement in cancer biology

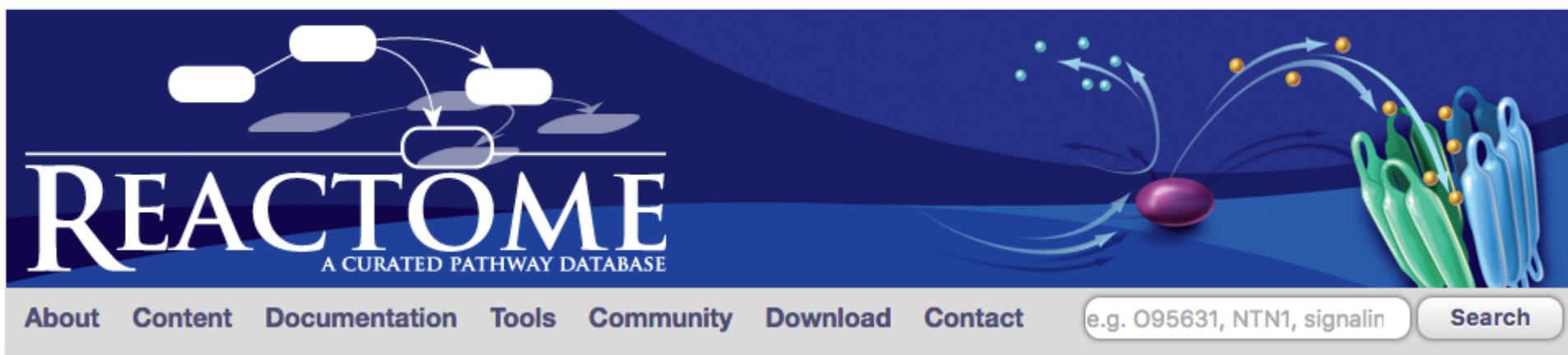
Data sources: ChEMBL



The screenshot shows the ChEMBL database homepage. At the top left is the EMBL-EBI logo. The main header features the ChEMBL logo (a stylized circular pattern) and the word "ChEMBL". Below the header is a navigation bar with links to "ChEMBL", "Downloads", "UniChem", and "SureChEMBL". To the right of the navigation bar is a search bar containing the placeholder "Search ChEMBL...". Above the search bar is a breadcrumb trail: "EBI > Databases > Small Molecules > ChEMBL Database > Home". To the right of the search bar are three buttons: "Compounds", "Targets", and "Assays". Below the search bar are five buttons: "Ligand Search", "Target Search", "Browse Targets", "Browse Drugs", and "Browse Drug Targets".

- Catalog of known drugs linked to a disease and a known target
- Drugs → FDA approved for marketing or clinical trials

Data sources: Reactome

The image shows the Reactome homepage. At the top, there is a blue banner featuring a molecular interaction diagram with nodes and arrows. Below the banner, the word "REACTOME" is written in large, white, serif capital letters, with "A CURATED PATHWAY DATABASE" in smaller letters underneath. Below the title, there is a navigation bar with links: "About", "Content", "Documentation", "Tools", "Community", "Download", and "Contact". To the right of the navigation bar is a search bar containing the placeholder text "e.g. O95631, NTN1, signalin" and a "Search" button.

- Catalog of biochemical reactions and pathways
- Manual curation of pathways affected by mutations

Data sources: Expression Atlas

EMBL-EBI 

Services Research Training About us

 Expression Atlas

Enter gene query...
Examples: [ASPM](#), [Apoptosis](#), [ENSMUSG00000021789](#), [zinc finger](#)

Search

Home Release notes FAQ Download Help Licence About Feedback

Expression Atlas: Differential and Baseline Expression

The Expression Atlas provides information on gene expression patterns under different biological conditions. Gene expression data is re-analysed in-house to detect genes showing interesting baseline and differential expression patterns. [Read more about Expression Atlas.](#)

- Catalog of patterns of gene expression
- Baseline expression for human genes
- Differential expression (healthy versus diseases tissues)

Data sources: Europe PMC

The screenshot shows the Europe PMC homepage. At the top, there is a navigation bar with links for "About", "Tools", "Developers", "Help", and "Europe PMC plus". To the left of the navigation bar is the Europe PMC logo, which consists of three overlapping colored circles (blue, green, and red) followed by the text "Europe PMC". Below the navigation bar is a search bar with the placeholder text "Search worldwide, life-sciences literature". To the right of the search bar is a blue "Search" button with a magnifying glass icon. Below the search bar, there is an example search query: "E.g. "breast cancer" HER2 Smith J".

- Text mining → association between targets and diseases
- Titles, abstracts, full text (but supplementary tables) are mined
- Co-occurrence in the same sentence of target and disease names (or synonyms)

Data sources: PhenoDigm

The screenshot shows the homepage of the PhenoDigm database. At the top, there is a dark header bar with the Wellcome Trust Sanger Institute logo on the left. To the right of the logo is a blue navigation bar containing links for "ABOUT" (with a dropdown arrow), "Who we are", "Careers", "Study", "Sex in Science", "Groups", and "Campus". On the far right of the blue bar is a magnifying glass icon representing a search function. Below the header, the main title "Welcome to PhenoDigm (PHENOtype comparisons for Disease and Gene Models)" is displayed in large, bold, black font. Underneath the title, there is a horizontal menu bar with three items: "Diseases" (which is highlighted in blue and underlined), "Tissue phenotype associations", and "Secondary phenotypes". Below this menu, a large, bold, black subtitle reads "Analyzing curated phenotype annotations to associate animal models with human diseases".

Welcome to PhenoDigm (PHENOtype comparisons for Disease and Gene Models)

Diseases Tissue phenotype associations Secondary phenotypes

Analyzing curated phenotype annotations to associate animal models with human diseases

- Semantic approach to map between clinical features observed in humans and annotations of phenotypes in mouse models
- PMID: 23660285

<http://www.sanger.ac.uk/resources/databases/phenodigm/>

Coffee break

Tutorial 2*: Evidence supporting the MET-papillary renal cell carcinoma association

- Which genetic evidence supports this association?
- Can you view this in a genome browser display?
- Are there any drugs in clinical trials for this disease?
- Is there a mouse model that mimics this disease?
- Which tissue has the highest RNA expression from GTEx?
- Are there other kidney diseases associated with this target? Can you export the table with this information? How strong is this association?

Exercises

Pages 29-32

<https://github.com/deniseOme/training>

How confident can you be of the target-disease associations in Open Targets?

Statistical integration, aggregation and scoring*

- A) per evidence (e.g. lead SNP from a GWAS paper)
- B) per data source (e.g. GWAS catalog)
- C) per data type (e.g. Genetic associations)
- D) overall

*https://github.com/opentargets/association_score_methods

Factors affecting the relative strength of an evidence

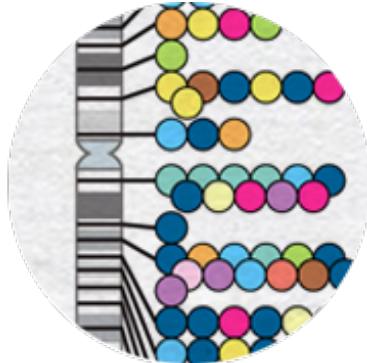
e.g. *GWAS Catalog*

$$S = f * s * c$$

f, relative occurrence of a target-disease evidence

s, strength of the effect described by the evidence

c, confidence of the observation for the target-disease evidence



f= sample size (cases versus controls)

s = predicted functional consequence

c = *p*-value reported in the paper

Aggregating scores across the data

- Using a mathematical function, the harmonic sum*

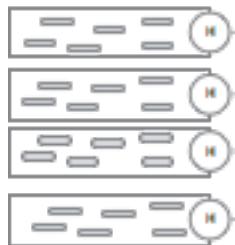
$$S_{1..i} = S_1 + \frac{S_2}{2^2} + \frac{S_3}{3^2} + \frac{S_4}{4^2} \dots + \frac{S_i}{i^2}$$

where S_1, S_2, \dots, S_i are the individual sorted evidence scores in descending order

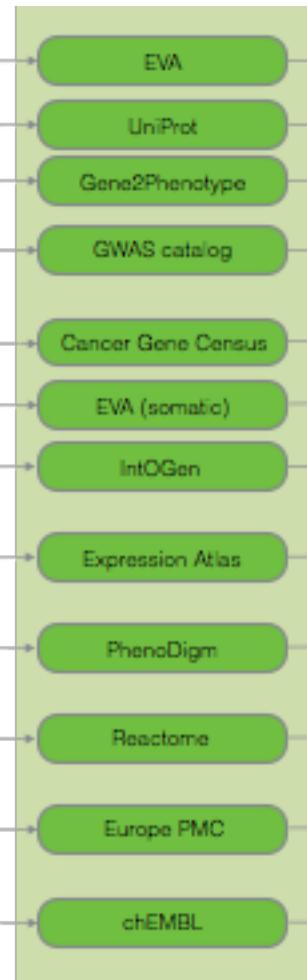
- Advantages:
 - A) account for replication
 - B) deflate the effect of large amounts of data e.g. text mining

* PMID: 19107201, PMID: 20118918

Pieces of evidence



Data sources



Data types

Genetic association

Somatic mutation

RNA expression

Animal models

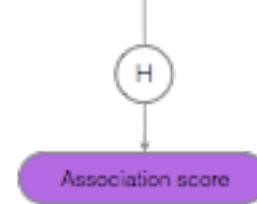
Affected pathways

Text mining

Drugs

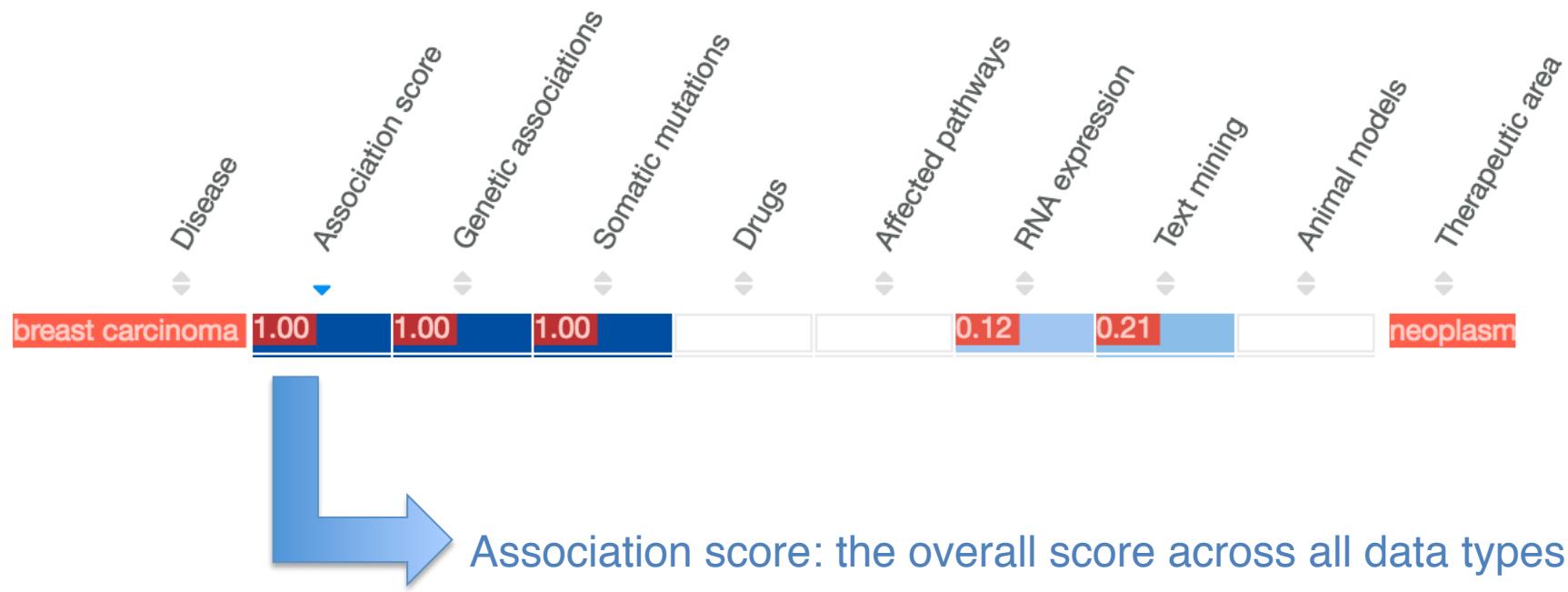


Harmonic sum



Open Targets

Ranking the target-disease association



- Based on the data sources
- Different weight applied:

genetic association = drugs = mutations = pathways > RNA expression > animal models = text mining

Disclaimer: score, dos and don'ts

- It's a ranking of target-disease associations
- It shows how confident we are in the association
- It's based on data sources, publicly available



- It can help you to design your null hypothesis
- It can help you to decide which target to pursue
- It is NOT sufficient on its own (use it in combination with...)

Tutorial 3*: your list of targets for a disease

Franke et al (2006) described seven genes associated with Alzheimer's disease: ENSG00000091513, ENSG00000175899, ENSG00000143801, ENSG00000142192, ENSG00000130203, ENSG00000010704, ENSG00000080815.

- Which of these have the strongest association w/ Alzheimer's?
- Are there any targets, which are membrane receptors?
- Which amino acids of this membrane receptor (putative drug target) correspond to the extracellular domain?

Wrap up

Open Targets Platform is the place:

For drug target ID and selection in drug discovery

Rank target-disease associations: different sources

Integrated information on target and diseases

Oh Yes!
And all is 100% free
and open source



Open Targets

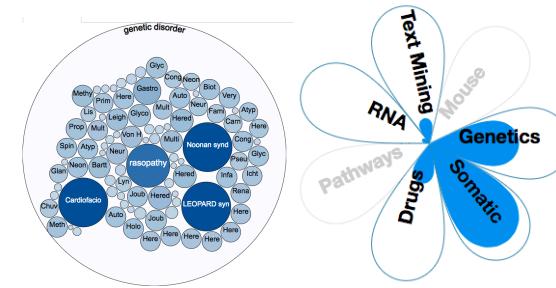
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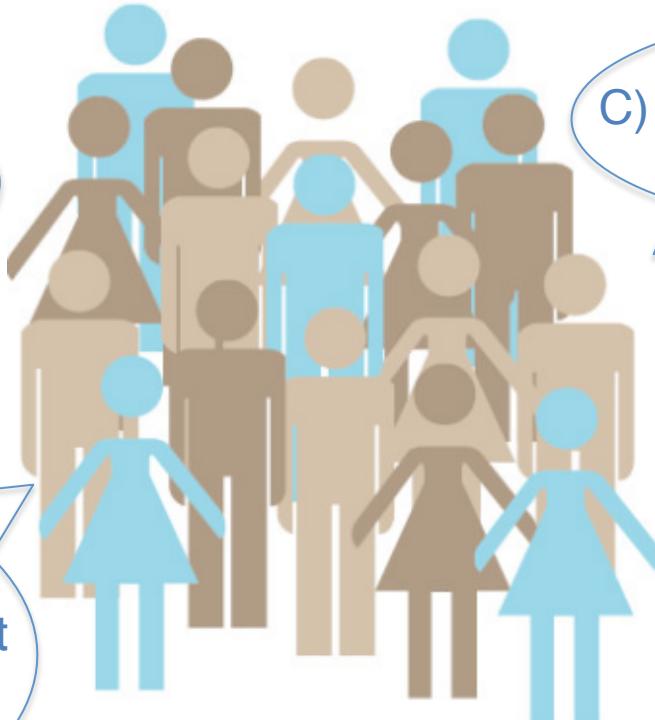
* Concurrent
www.opentargets.org/projects

We support decision-making

A) Which targets are associated with a disease?

B) What evidence supports this target-disease association?

F) What else can I find out about my drug target?



E) If this target is associated with other diseases, can I get the association for diseases from different therapeutic areas?

C) Are there FDA drugs for this association?

D) For a given target, are there other diseases associated with it?



Open Targets

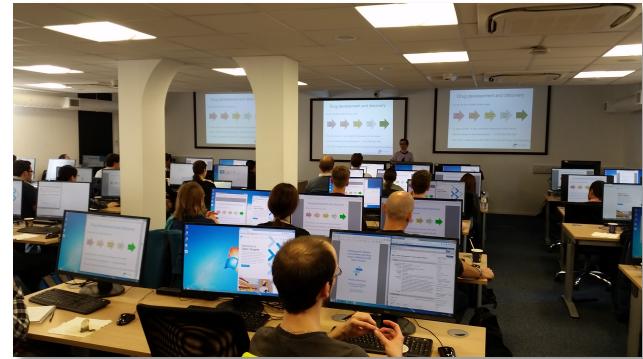
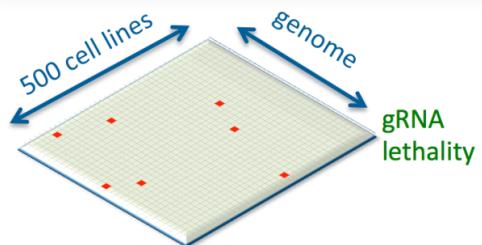
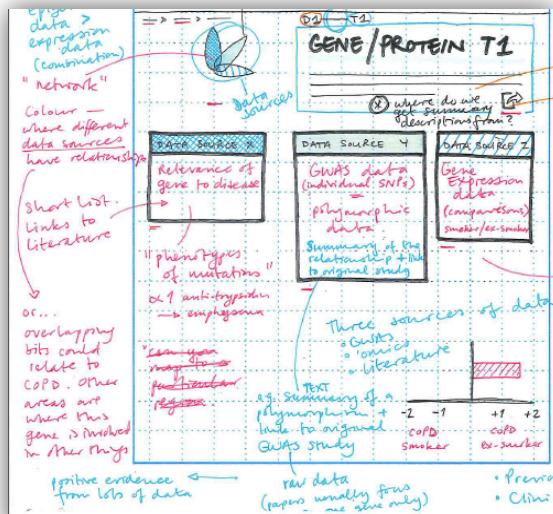
What makes Open Targets unique?

Addressing all areas of human disease

Putting our users first

Working genome wide

Bringing the partners together



ets

How to cite us

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doi: 10.1093/nar/gkw1055

Open Targets: a platform for therapeutic target identification and validation

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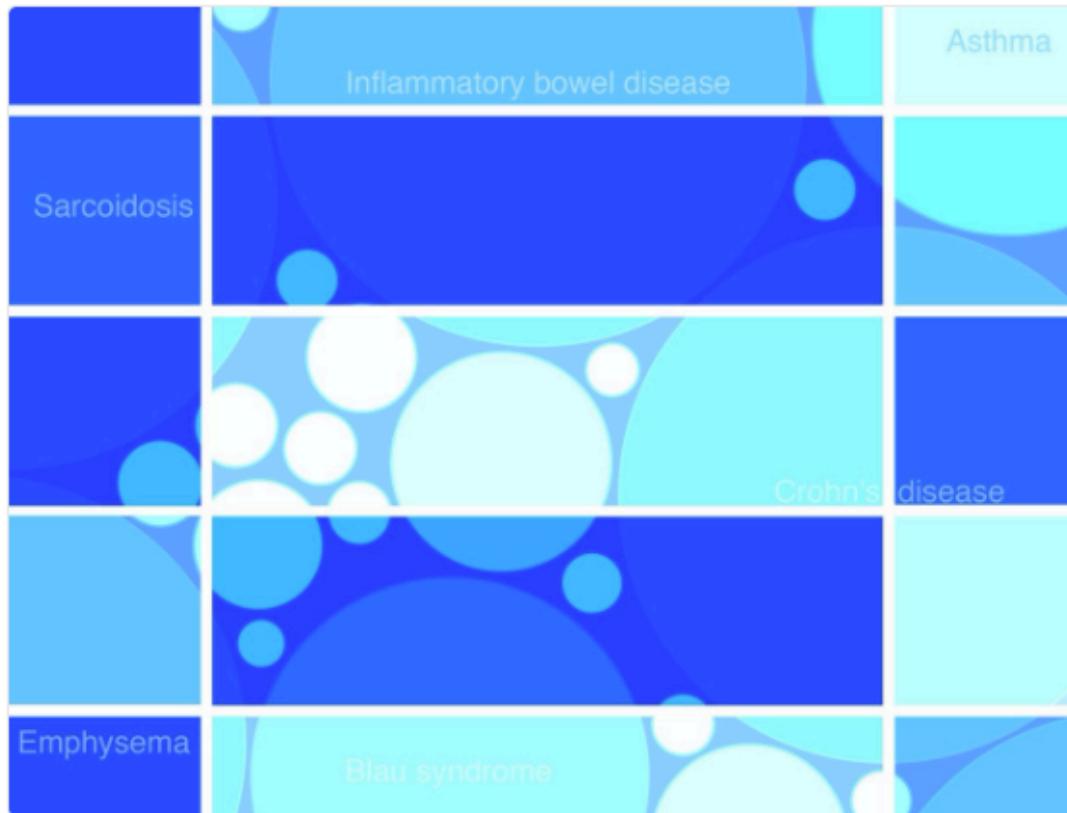
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<http://www.narbreakthrough.com/>



...And the 2017 Breakthrough Articles Award goes to...

#OpenTargets, as well as @MonarchInit & @denovodb! @NAR_Open buff.ly/2iGMXlc



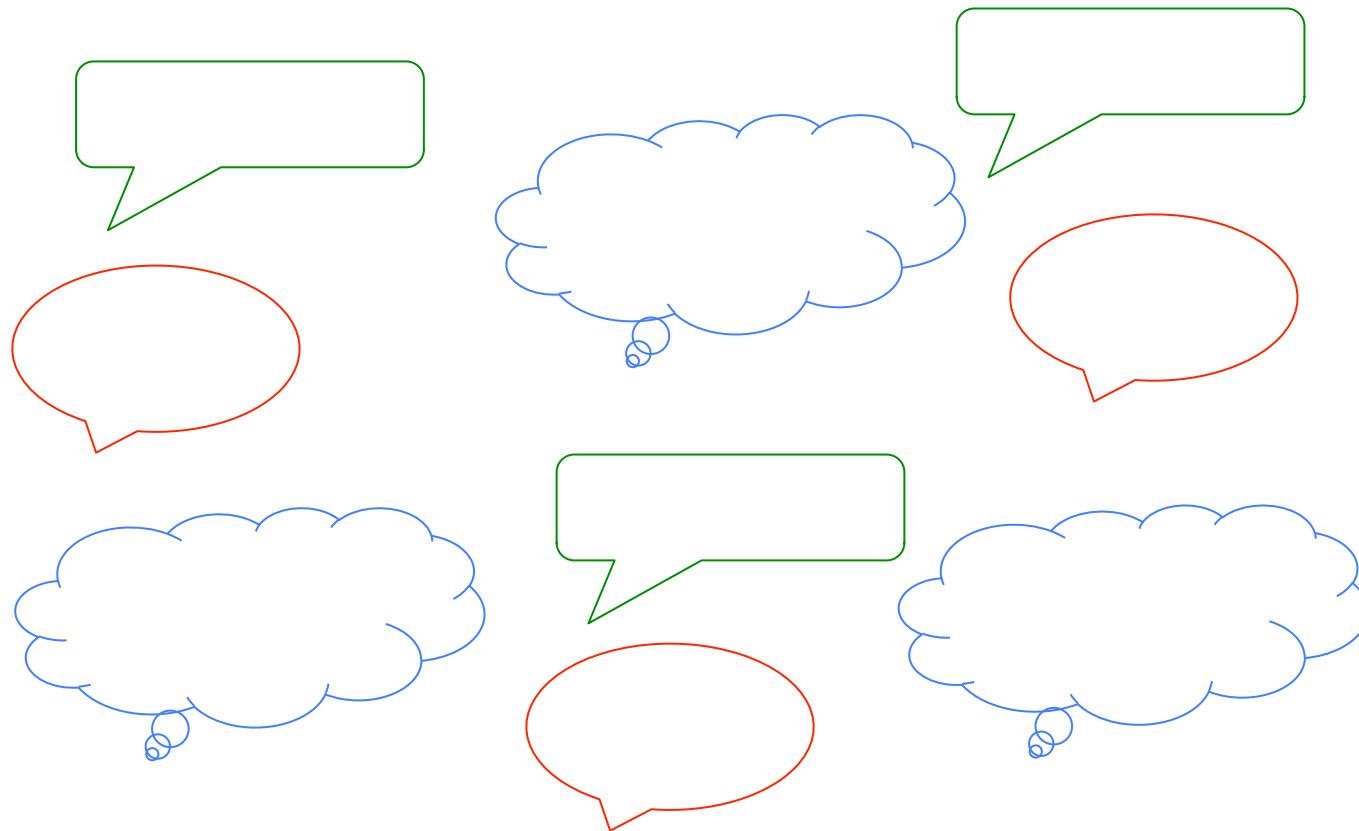
RETWEETS
10

LIKES
8



Open Targets

Your take home message

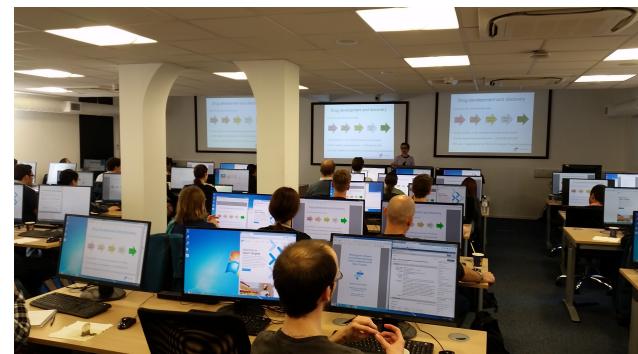
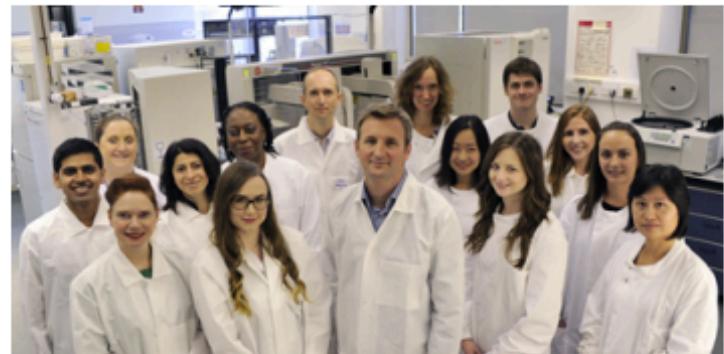


Open Targets

Short feedback survey

<http://tinyurl.com/yale-090217>

Acknowledgements



support@targetvalidation.org



Open Targets

Get in touch



@targetvalidate



support@targetvalidation.org



www.facebook.com/OpenTargets/



blog.opentargets.org/



<http://tinyurl.com/opentargets-in>

Extra slides

Alternative ways to access the data

Looking for our entire datasets?

<https://www.targetvalidation.org/downloads/data>

- All target-disease associations: 215 MB
- All evidence: 4.35 GB

Looking for extracts of our datasets?

- API: REST calls, Python client
- R client: maintained by the community



Open Targets

REST API endpoints



public : Publicly supported stable API.

Open/Hide | List operations | Expand operations

GET /public/evidence

POST /public/evidence

GET /public/evidence/filter

POST /public/evidence/filter

GET /public/association

GET /public/association/filter

POST /public/association/filter

GET /public/search

GET /public/auth/request_token

GET /public/auth/validate_token

GET /public/utils/ping

GET /public/utils/version

GET /public/utils/stats

- Query association and evidence by gene identifiers and diseases
- Filter by type of evidence

<https://www.targetvalidation.org/documentation/api>



Open Targets

GET

/public/association



Implementation notes

After integrating all evidence connecting a target to a specific disease, we compute an association score by mean of an harmonic sum. This association score provides an indication of how strong the evidence behind each connection is and can be used to rank genes in order of likelihood as drug targets. The association id is constructed by using the ensembl id of the gene and the EFO id for the disease (eg. ENSG00000073756-EFO_0003767). The method returns an association object, which contain data and summary on each evidence type included in the calculation of the score, as well as the score itself.

Parameters

Parameter	Value	Description	Parameter type	Data type
id	ENSG00000073756-EFO_0003767	an association ID usually in the form of TARGET_ID-DISEASE_ID	query	string

Response messages

HTTP status code	Reason	Model
200	Successful response	

[Try it out!](#)[Hide response](#)

Request URL

https://www.targetvalidation.org/api/latest/public/association?id=ENSG00000073756-EFO_0003767



Response body

```
{  
  "from": 0,  
  "facets": null,  
  "took": 6,  
  "therapeutic_areas": [],  
  "total": 1,  
  "data": [  
    {  
      "target": {  
        "gene_info": {  
          "symbol": "PTGS2",  
          "ensembl_id": "ENSG00000073756",  
          "name": "PTGS2",  
          "chromosome": 12, "start": 123456789, "end": 123456789},  
        "evidence": [{"source": "Ensembl", "score": 100, "type": "Gene"}, {"source": "EFO", "score": 100, "type": "Disease"}]  
      }  
    }  
  ]  
}
```

- Paste the URL in a location bar in a browser
- Use the terminal window (e.g. with CURL)
- Use one of our clients (i.e. R and Python)

Python and R clients for the REST API

opentargets
latest

Search docs

Tutorial
High Level API
Low Level API
Code Documentation
Changelog

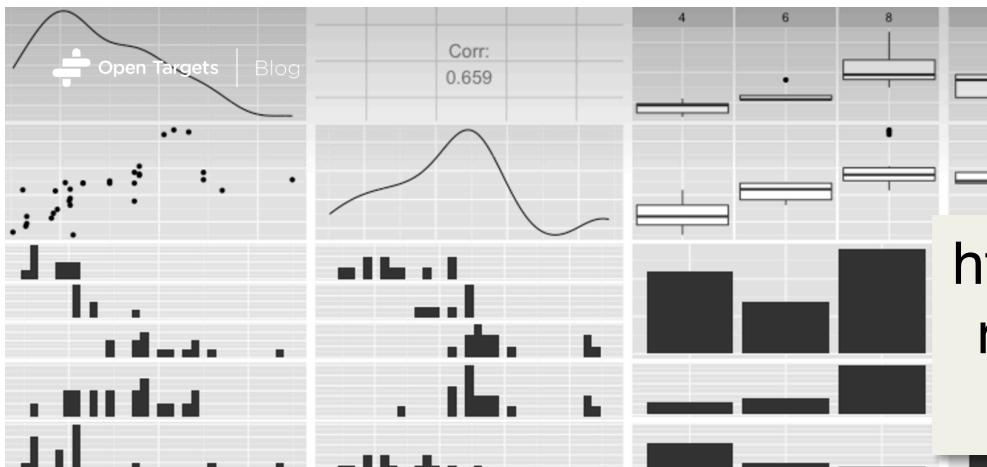
Docs » opentargets - Python client for targetvalidation.org

Edit on GitHub

opentargets - Python client for targetvalidation.org

opentargets is the official python client for the [Open Targets REST API](#) at [targetvalidation.org](#)

<http://opentargets.readthedocs.io>



[https://blog.opentargets.org/
rest-api-exploration-using-
an-r-client/](https://blog.opentargets.org/rest-api-exploration-using-an-r-client/)

How to access Open Targets
with R