

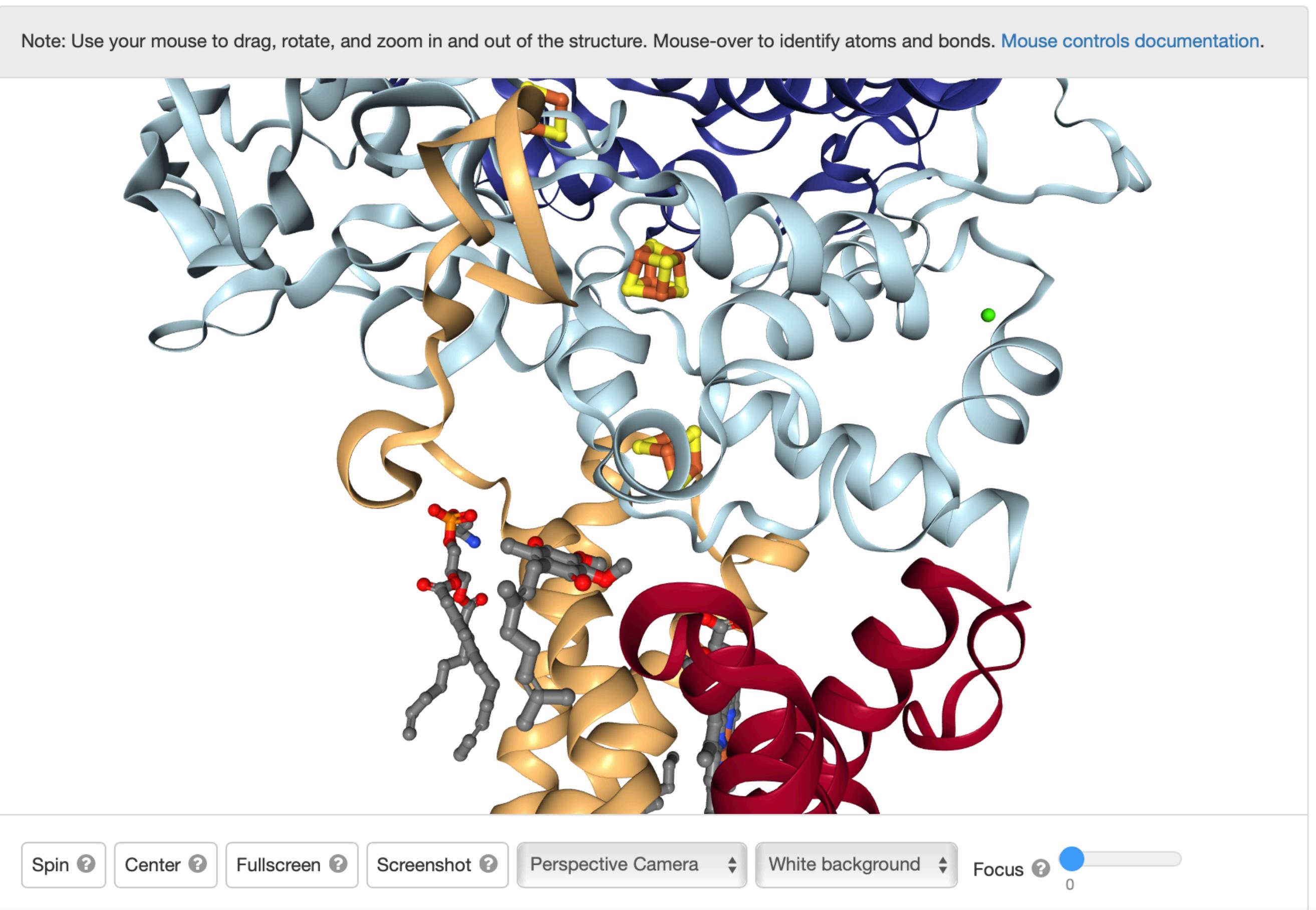
**1/16/2020 Week 1 Module 2**

**Interactive Exercise: Using Databases  
to Evaluate an SBDD Target**

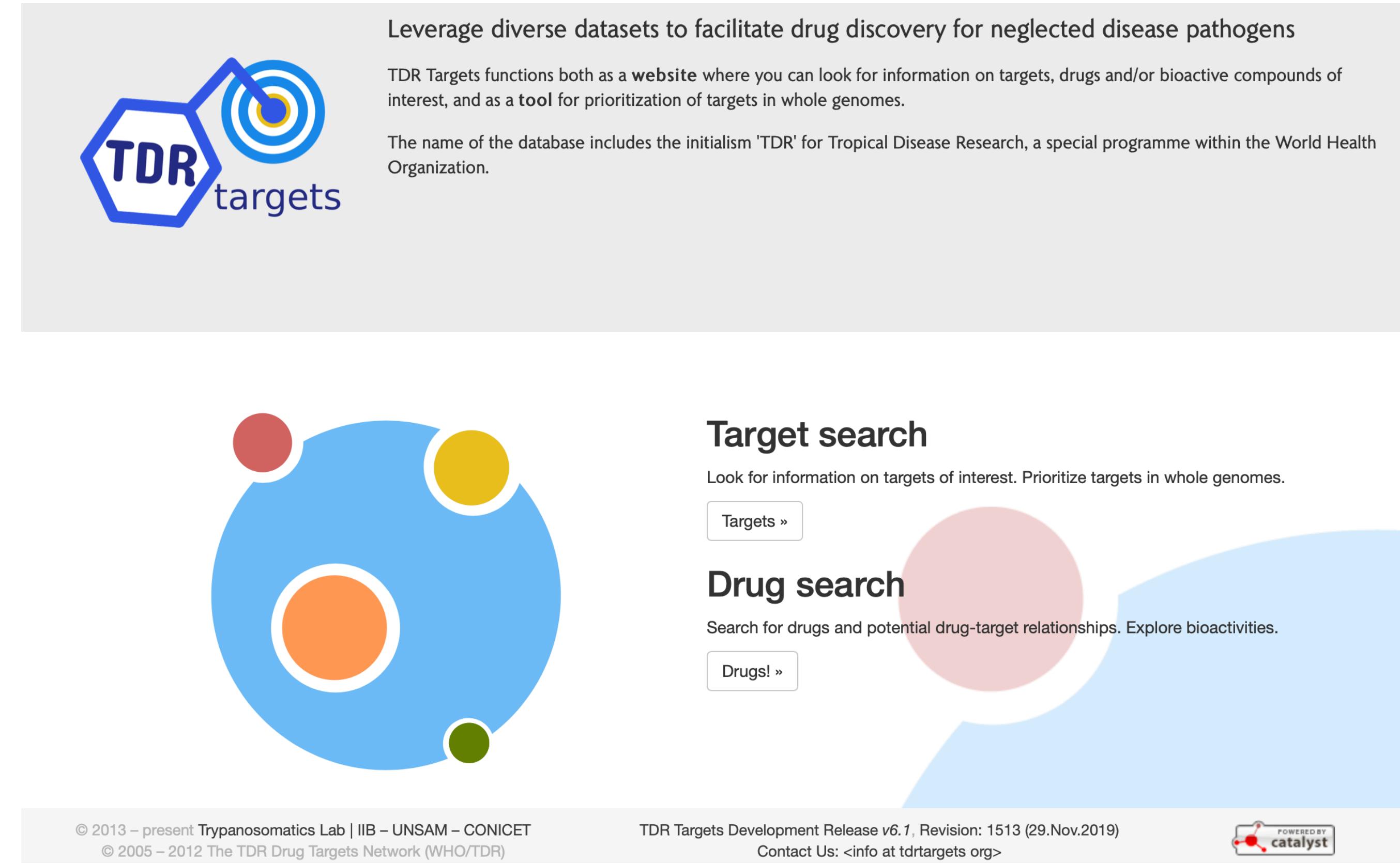
- I've been working with Oscar Juarez on discovering inhibitors for Complex II, a.k.a. Succinate Dehydrogenase (SDH), from *Pseudomonas aeruginosa*
- The structure of E. Coli SDH has been solved at a resolution of 2.6 Å
- Subunit B (cyan) has Iron-Sulfur centers
- We are targeting the ubiquinone site at the interface of subunits B, C (yellow), and D (red)

**1NEK**

Complex II (Succinate Dehydrogenase) From E. Coli with ubiquinone bound



- We think it's a good drug target but I want to see what the online databases suggest
- First, let's try TDR targets (<https://tdrtargets.org>). It is possible that an SDH drug for *P. Aeruginosa* may also work on some neglected tropical diseases.



The screenshot shows the TDR Targets homepage. At the top right, there is a logo consisting of a blue hexagon containing the letters 'TDR' and a blue circle containing a target symbol with the word 'targets' next to it. To the right of the logo, the text reads: "Leverage diverse datasets to facilitate drug discovery for neglected disease pathogens". Below this, it says: "TDR Targets functions both as a **website** where you can look for information on targets, drugs and/or bioactive compounds of interest, and as a **tool** for prioritization of targets in whole genomes." Further down, it states: "The name of the database includes the initialism 'TDR' for Tropical Disease Research, a special programme within the World Health Organization." In the center, there is a large blue circular graphic with three smaller colored circles (red, yellow, green) inside it. To the right of this graphic, under the heading "Target search", is the text: "Look for information on targets of interest. Prioritize targets in whole genomes." with a "Targets »" button. Below this, under the heading "Drug search", is the text: "Search for drugs and potential drug-target relationships. Explore bioactivities." with a "Drugs! »" button. At the bottom of the page, there is copyright information: "© 2013 – present Trypanosomatics Lab | IIB – UNSAM – CONICET © 2005 – 2012 The TDR Drug Targets Network (WHO/TDR)". On the far right, there is a small "POWERED BY catalyst" logo.

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 © 2005 – 2012 The TDR Drug Targets Network (WHO/TDR)

TDR Targets Development Release v6.1, Revision: 1513 (29.Nov.2019)  
 Contact Us: <info at tdrtargets.org>

POWERED BY catalyst

- Try a “Quick Search...” for “succinate dehydrogenase”. This yields many results that are various subunits of the enzyme from different species
- Compared to the ubiquinone binding site, the “flavoprotein subunit” is on the opposite side of the complex

## Target list

Search results for query: #2 (succinate dehydrogenase)

Show query parameters

Convert this list of targets into a list of drugs: [More information?](#)

Retrieve: [All Associations \(Curated and Predicted\)](#) [Curated Associations](#) [Target Putative Associations \(predicted\) ▾](#)

Organism	Name ▾	Ortholog group	Product
<i>B. malayi</i>	<a href="#">Bm1_17325</a>	<a href="#">OG5_126927</a>	succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
<i>B. malayi</i>	<a href="#">Bm1_17330</a>	<a href="#">OG5_126927</a>	succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
<i>B. malayi</i>	<a href="#">Bm1_17690</a>	<a href="#">OG5_126893</a>	succinate dehydrogenase [ubiquinone] iron-sulfur protein, mitochondrial
<i>B. malayi</i>	<a href="#">Bm1_30090</a>	<a href="#">OG5_129614</a>	Succinate dehydrogenase cytochrome b560 subunit, mitochondrialprecursor
<i>B. malayi</i>	<a href="#">Bm1_35660</a>	<a href="#">OG5_129488</a>	Succinate dehydrogenase
<i>C. trachomatis</i>	<a href="#">CT_591</a>	<a href="#">OG5_126893</a>	succinate dehydrogenase iron sulfur subunit
<i>C. trachomatis</i>	<a href="#">CT_592</a>	<a href="#">OG5_126927</a>	succinate dehydrogenase flavoprotein subunit
<i>E. granulosus</i>	<a href="#">EgrG_000416000</a>	<a href="#">No group</a>	succinate dehydrogenase ubiquinone iron sulfur

- A few of the hits had “iron-sulfur subunit” in the name. The iron-sulfur subunit is B, one of those next to the ubiquinone binding site.
- Try a “Quick Search...” for “succinate dehydrogenase iron-sulfur”.

### Search results for query: #7 (succinate dehydrogenase iron-sulfur)

Show query parameters

Convert this list of targets into a list of drugs: [More information?](#)

Retrieve: [All Associations \(Curated and Predicted\)](#) [Curated Associations](#) [Target Putative Associations \(predicted\) ▾](#)

9 records found   Showing page 1 of 1 (records 1-9)   Number of records to display 25 <input type="button" value="Find orthologs in select species"/>			
Organism	Name ▾	Ortholog group	Product
<i>L. Loa</i> (eye worm)	LOAG_10155	OG5_126893	succinate dehydrogenase iron-sulfur protein
<i>M. ulcerans</i>	MUL_1370	OG5_126893	succinate dehydrogenase iron-sulfur subunit
<i>S. mansoni</i>	Smp_089640.2	OG5_126893	succinate dehydrogenase iron-sulfur protein
<i>S. mansoni</i>	Smp_089640.3	OG5_126893	succinate dehydrogenase iron-sulfur protein
<i>T. brucei</i>	Tb927.8.3380	OG5_126893	succinate dehydrogenase iron-sulfur subunit
<i>T. brucei</i>	Tb927.9.5960	OG5_126893	succinate dehydrogenase iron-sulfur subunit, putative
<i>T. cruzi</i>	TcCLB.504949.30	OG5_126893	succinate dehydrogenase iron-sulfur subunit
<i>T. cruzi</i>	TcCLB.509769.60	OG5_126893	succinate dehydrogenase iron-sulfur subunit
<i>W. endosymbiont of Brugia malayi</i>	Wbm0600	OG5_126893	succinate dehydrogenase iron-sulfur subunit

- Click on Tb927.8.3380 and scroll down to Essentiality Data
- Suppose that we discover a SDH inhibitor in our SBDD campaign against the ubiquinone binding site of *P. Aeruginosa*. Based on these data, which other species would be most worth testing its efficacy against? Which would be least worth testing?

Essentiality			
<b>Tb927.8.3380 has direct evidence of essentiality</b>			
Gene/Ortholog	Organism	Phenotype	Source Study
mtu1581	Mycobacterium tuberculosis	non-essential	nmpdr
mtu3379	Mycobacterium tuberculosis	non-essential	nmpdr
Tb09.160.4380	Trypanosoma brucei	no significant loss or gain of fitness in bloodstream forms (3 days)	alsford
Tb09.160.4380	Trypanosoma brucei	significant gain of fitness in bloodstream forms (6 days)	alsford
Tb09.160.4380	Trypanosoma brucei	no significant loss or gain of fitness in procyclic forms	alsford
Tb09.160.4380	Trypanosoma brucei	significant gain of fitness in differentiation of procyclic to bloodstream forms	alsford
Tb927.8.3380 <span style="background-color: orange; border: 1px solid black; padding: 2px;">this record</span>	Trypanosoma brucei	significant loss of fitness in bloodstream forms (3 days)	alsford
Tb927.8.3380 <span style="background-color: orange; border: 1px solid black; padding: 2px;">this record</span>	Trypanosoma brucei	significant loss of fitness in bloodstream forms (6 days)	alsford
Tb927.8.3380 <span style="background-color: orange; border: 1px solid black; padding: 2px;">this record</span>	Trypanosoma brucei	significant loss of fitness in procyclic forms	alsford
Tb927.8.3380 <span style="background-color: orange; border: 1px solid black; padding: 2px;">this record</span>	Trypanosoma brucei	significant loss of fitness in differentiation of procyclic to bloodstream forms	alsford
b0724	Escherichia coli	non-essential	goodall
b4153	Escherichia coli	non-essential	goodall

- Click on Tb927.8.3380 and scroll down to Essentiality Data
- Suppose that we discover a SDH inhibitor in our SBDD campaign against the ubiquinone binding site of *P. Aeruginosa*. Based on these data, which other species would be most worth testing its efficacy against? Which would be least worth testing?
- The inhibitor should be tested against *T. brucei* and *T. gondii*. It probably won't be effective against *M. tuberculosis* and *P. berghei*.

Essentiality			
Tb927.8.3380 has direct evidence of essentiality			
Gene/Ortholog	Organism	Phenotype	Source Study
mtu1581	Mycobacterium tuberculosis	non-essential	nmpdr
mtu3379	Mycobacterium tuberculosis	non-essential	nmpdr
Tb09.160.4380	Trypanosoma brucei	no significant loss or gain of fitness in bloodstream forms (3 days)	alsford
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Tb927.8.3380 <span style="background-color: orange; border: 1px solid black; padding: 2px;">this record</span>	Trypanosoma brucei	significant loss of fitness in procyclic forms	alsford
Tb927.8.3380 <span style="background-color: orange; border: 1px solid black; padding: 2px;">this record</span>	Trypanosoma brucei	significant loss of fitness in differentiation of procyclic to bloodstream forms	alsford
b0724	Escherichia coli	non-essential	goodall
b4153	Escherichia coli	non-essential	goodall

- Also take a look at “Structural information”
- There is no crystal structures and the homology models from Modbase are not high quality. The homology model could be a guide, but I would not base an SBDD campaign against a *T. brucei* homology model.

**Structural information**

**Modbase 3D models:**

There are 3 models calculated for this protein. More info on these models, including the models themselves is available at: [Modbase](#)

Target Beg	Target End	Template	Template Beg	Template End	Identity	Evalue	Model Score	MPQS	zDope
32	156	<a href="#">1zoy</a> (B)	16	151	46.00	0	1	0.950829	0.33
32	156	<a href="#">4ysx</a> (B)	40	175	46.00	0	0.99	0.956829	0.26
168	229	<a href="#">5i9f</a> (A)	348	409	23.00	0.53	0.98	0.708498	-1.37

[+ Help me make sense of these data.](#)

**Target Beg:** first modeled residue  
**Target End:** last modeled residue  
**Template:** template structure used for modelling (PDB accession and chain)  
**Template Beg:** first template residue in target-template alignment  
**Template End:** last template residue in target-template alignment  
**Identity:** sequence identity  
**Evalue:** E value for target-template hit  
**Model Score:** GA341 score (>0.7 for reliable model)  
**MPQS:** ModPipe Quality Score (>1.1 for reliable model)

- The structure we have used as a basis for modeling studies has been 1NEK. I tried this in the PockeTome (<http://ablab.ucsd.edu/POCKETOME/>). There was no record for it.
- Try a search for “succinate”. Did you find SDH?

The screenshot shows the PockeTome web interface. At the top left, there are two search boxes: one for "Search for 1nek" in "PDB codes", and another for "Search for succinate" in "Pocketome". Below these are links for "About", "Browse All", "Find chemical", "Access and format", "Downloads", and "Citation". A sidebar on the left lists "Molsoft Browser Free Download" and "Disclaimer" (© 2011–2020 Abagyan Lab). The main content area is titled "Search Results" and displays a list of protein entries. Each entry includes the protein name, family, domains/regions, PDB codes, and HET codes. A color-coded bar indicates domain regions: blue for R (Receptor-binding), green for S1 (Peptidase S1), red for D (Peptidase D), and grey for other regions.

Entry	Family	Domains/regions	PDB	HET
ARLY2_ANAPL_4_468	Argininosuccinate lyase [Lyase 1 family. Argininosuccinate lyase subfamily]	[R] Substrate binding	1auw, 1dcn, 1hy1, 1k7w, 1tju, 1tjv, 1tjw	as1
ASSY_THET8_1_400	Argininosuccinate synthase [Argininosuccinate synthase family. Type 1 subfamily]	[R] Substrate binding	1j1z, 1j20, 1j21, 1kh1, 1kh2, 1kh3, 1kor	amp, anp, as1, atp, cir
PURA_ECOLI_2_432	Adenylosuccinate synthetase [Adenylosuccinate synthetase family]	[R] IMP binding	1ade, 1adi, 1cg0, 1cg1, 1cg3, 1cg4, 1ch8, 1cib, 1gim, 1gin, 1hon, 1hoo, 1hop, 1juy, ...	amp, doi, dpo, gcp, gdp, gnh, gnp, gpx, h5p, hda, imo, imp, pgs, rpd, rpl
DRAA_ECOLX_22_160	Dr hemagglutinin structural subunit [Dr-adhesin family]	[R] Receptor-binding	1usq, 1ut1, 2jkl, 2jkn, 2w5p	brx, cl8, clm
GTR3_HUMAN_1_489	Solute carrier family 2, facilitated glucose transporter member 3 [Major facilitator superfamily. Sugar transporter (TC 2.A.1.1) family. Glucose transporter subfamily]	[R] Important for selectivity against fructose, [R] Monosaccharide binding	4zw9, 4zwb, 4zwc, 5c65	y01
NCZS_STRCZ_35_147	Neocarzinostatin [Neocarzinostatin family]	[R] Substrate binding	1nco, 1noa, 2cbm, 2cbo, 2cbq, 4jw3	chr, mrd, th2
TRY1_BOVIN_66_246	Cationic trypsin [Peptidase S1 family]	[D] Peptidase S1, [R] Substrate binding	1aq7, 1auj, 1az8, 1bju, 1bjv, 1btp, 1btv, 1btw, 1btx, 1bty, 1btz, 1c1n, 1c1o, 1c1p, 1c1q, 1c1r, 1c...	0ca, 0cb, 123, 124, 12u, 132, 13u, 169, 22m, 23m, 312, 334, 3yh, 49u, 607, 623, 653, 655...

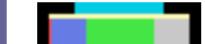
- The structure we have used as a basis for modeling studies has been 1NEK. I tried this in the PockeTome (<http://ablab.ucsd.edu/POCKETOME/>). There was no record for it.
- Try a search for “succinate”. Did you find SDH?
- I didn’t find it either

The screenshot shows the PockeTome web interface. At the top left, there is a search bar with "1nek" in the "Search for" field and "PDB codes" in the "in" dropdown. Below this is another search bar with "succinate" in the "Search for" field and "Pocketome" in the "in" dropdown. To the right of these search fields is a large logo featuring the word "PockeTome" in a stylized font where the letters are composed of molecular structures. The background of the page features a repeating pattern of blue and white cylinders, resembling test tubes or molecular structures.

**Search Results**

Show only:  Human;  Other mammals;  Gram-positive bacteria;  Gram-negative bacteria;  Archaea;  Virus;  Other.

ARLY2\_ANAPL\_4\_468 Argininosuccinate lyase [Lyase 1 family. Argininosuccinate lyase subfamily]

 Domains/regions: [R] Substrate binding  
PDB: 1auw, 1dcn, 1hy1, 1k7w, 1tju, 1tjv, 1tjw  
HET: as1

ASSY\_THET8\_1\_400 Argininosuccinate synthase [Argininosuccinate synthase family. Type 1 subfamily]

 Domains/regions: [R] Substrate binding  
PDB: 1j1z, 1j20, 1j21, 1kh1, 1kh2, 1kh3, 1kor  
HET: amp, anp, as1, atp, cir

PURA\_ECOLI\_2\_432 Adenylosuccinate synthetase [Adenylosuccinate synthetase family]

 Domains/regions: [R] IMP binding  
PDB: 1ade, 1adi, 1cg0, 1cg1, 1cg3, 1cg4, 1ch8, 1cib, 1gim, 1gin, 1hon, 1hoo, 1hop, 1juy, ...  
HET: amp, doi, dpo, gcp, gdp, gnh, gnp, gpx, h5p, hda, imo, imp, pgs, rpd, rpl

DRAA\_ECOLX\_22\_160 Dr hemagglutinin structural subunit [Dr-adhesin family]

 Domains/regions: [R] Receptor-binding  
PDB: 1usq, 1ut1, 2jkl, 2jkn, 2w5p  
HET: brx, cl8, clm

GTR3\_HUMAN\_1\_489 Solute carrier family 2, facilitated glucose transporter member 3 [Major facilitator superfamily. Sugar transporter (TC 2.A.1.1) family. Glucose transporter subfamily]

 Domains/regions: [R] Important for selectivity against fructose, [R] Monosaccharide binding  
PDB: 4zw9, 4zwb, 4zwc, 5c65  
HET: y01

NCZS\_STRCZ\_35\_147 Neocarzinostatin [Neocarzinostatin family]

 Domains/regions: [R] Monosaccharide binding  
PDB: 1nco, 1noa, 2cbm, 2 cbo, 2cbq, 4jw3  
HET: chr, mrd, th2

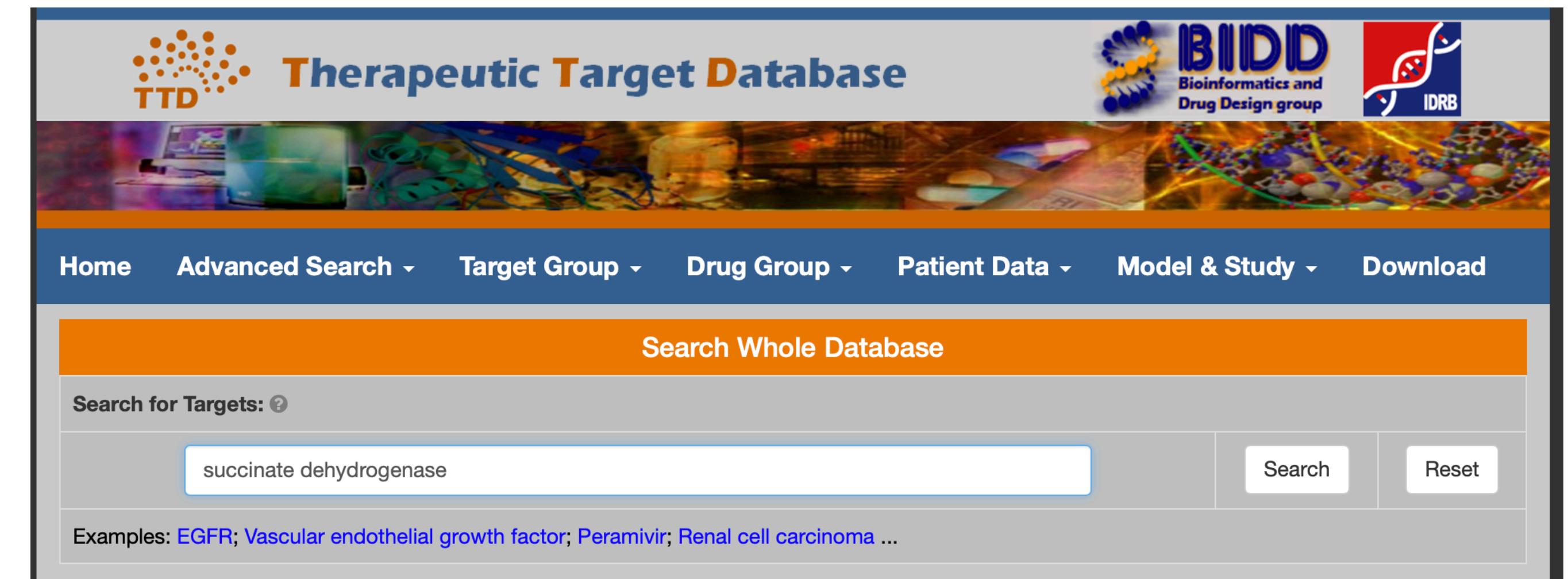
TRY1\_BOVIN\_66\_246 Cationic trypsin [Peptidase S1 family]

 Domains/regions: [D] Peptidase S1, [R] Substrate binding  
PDB: 1aq7, 1auj, 1az8, 1bju, 1bjv, 1btp, 1btv, 1btw, 1btz, 1btz, 1c1n, 1c1o, 1c1p, 1c1q, 1c1r, 1c...  
HET: 0ca, 0cb, 123, 124, 12u, 132, 13u, 169, 22m, 23m, 312, 334, 3yh, 49u, 607, 623, 653, 655...

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Lab

- Now try “NADH ubiquinone” in the Therapeutic Target Database (<http://idrblab.net/ttd/>)
- Did you find SDH?



The screenshot shows the Therapeutic Target Database (TTD) homepage. At the top, there's a banner with the TTD logo (orange dots), the text "Therapeutic Target Database", the BIDD logo (Bioinformatics and Drug Design group), and the IDRB logo (red and blue stylized letters). Below the banner is a navigation bar with links: Home, Advanced Search, Target Group, Drug Group, Patient Data, Model & Study, and Download. The main content area has a search bar with the placeholder "Search for Targets: ?" and a text input field containing "succinate dehydrogenase". To the right of the input field are two buttons: "Search" and "Reset". Below the search bar, there's a note: "Examples: EGFR; Vascular endothelial growth factor; Peramivir; Renal cell carcinoma ...".

- Now try “NADH ubiquinone” in the Therapeutic Target Database (<http://idrblab.net/ttd/>)
- Did you find SDH?
- Looks like it is there, as T39811.



The screenshot shows the homepage of the Therapeutic Target Database (TTD). At the top, there's a banner with the TTD logo, the text "Therapeutic Target Database", and logos for BIDD (Bioinformatics and Drug Design group) and IDRB. Below the banner is a navigation bar with links for Home, Advanced Search, Target Group, Drug Group, Patient Data, Model & Study, and Download. The main content area has a search bar with the placeholder "Search for Targets: ?" and a text input field containing "succinate dehydrogenase". To the right of the input field are "Search" and "Reset" buttons. Below the search bar, there's a note with examples of search terms: EGFR; Vascular endothelial growth factor; Peramivir; Renal cell carcinoma ...

- Are there currently any drugs that target SDH?

**Therapeutic Target Database**

**BIDD**  
Bioinformatics and  
Drug Design group

**IDRB**

Home Advanced Search ▾ Target Group ▾ Drug Group ▾ Patient Data ▾ Model & Study ▾ Download

### Target Information

Target General Information	
Target ID	T39811 (Former ID: TTDI01376)
Target Name	Succinate dehydrogenase (SDHD)
Synonyms	Succinate-ubiquinone reductase membrane anchor subunit; Succinate-ubiquinone oxidoreductase cytochrome b small subunit; Succinate dehydrogenase complex subunit D; Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial; SDH4; QPs3; CybS; CII-4
Gene Name	SDHD
Target Type	Literature-reported target
Function	Membrane-anchoring subunit of succinate dehydrogenase (SDH) that is involved in complex II of the mitochondrial electron transport chain and is responsible for transferring electrons from succinate to ubiquinone (coenzyme Q).
UniProt ID	DHSD_HUMAN <a href="#">🔗</a>
Sequence	MAVLWRLSAVCAGALGGRALLRTPVVRPAHISAFLQDRPIPEWCVGQHIHLSPSHSGSK AASLHWTSERVVSVLLGLPAAYLNPCSAMDYSLAAALTGHGWL GQVVTDYVHDAL QKAAKAGLLALSALTFAGLCYFNYHDVGICKAVMLWKL

### References

REF 1	Succinate dehydrogenase is a direct target of sirtuin 3 deacetylase activity. PLoS One. 2011;6(8):e23295. <a href="#">🔗</a>
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If you find any error in data or bug in web service, please kindly report it to [Dr. Wang](#) and [Dr. Li](#).

- Are there currently any drugs that target SDH?
- No

**Therapeutic Target Database**

Home Advanced Search ▾ Target Group ▾ Drug Group ▾ Patient Data ▾ Model & Study ▾ Download

### Target Information

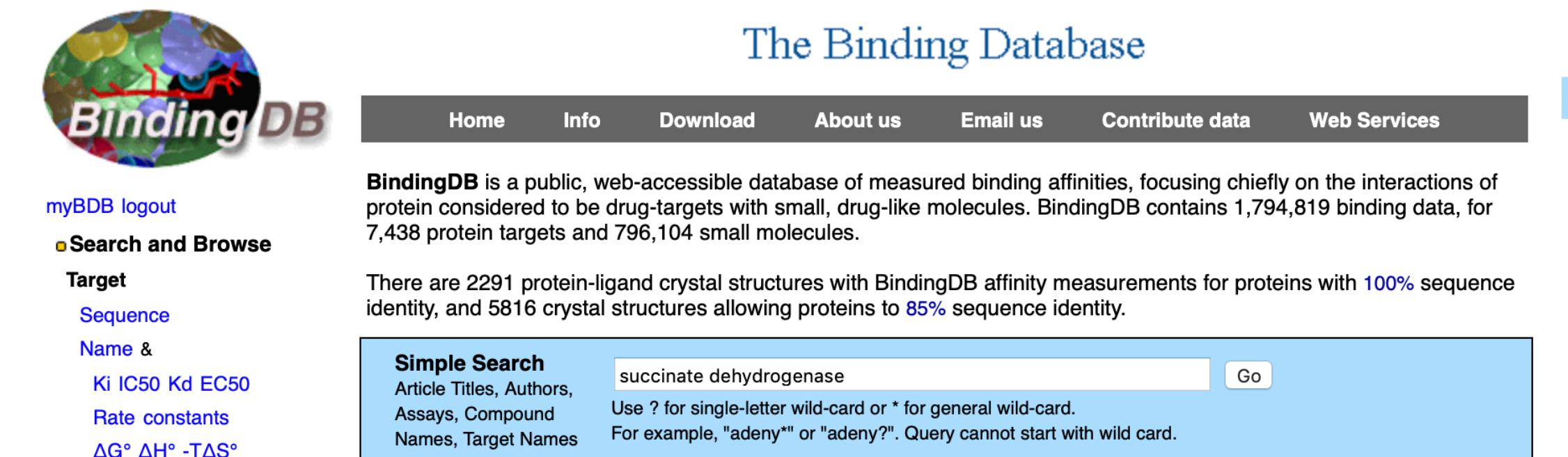
Target General Information	
Target ID	T39811 (Former ID: TTDI01376)
Target Name	Succinate dehydrogenase (SDHD)
Synonyms	Succinate-ubiquinone reductase membrane anchor subunit; Succinate-ubiquinone oxidoreductase cytochrome b small subunit; Succinate dehydrogenase complex subunit D; Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial; SDH4; QPs3; CybS; CII-4
Gene Name	SDHD
Target Type	Literature-reported target
Function	Membrane-anchoring subunit of succinate dehydrogenase (SDH) that is involved in complex II of the mitochondrial electron transport chain and is responsible for transferring electrons from succinate to ubiquinone (coenzyme Q).
UniProt ID	DHSD_HUMAN <a href="#">🔗</a>
Sequence	MAVLWRLSAVCAGALGGRALLRTPVVRPAHISAFLQDRPIPEWCVGQHIHLSPSHSGSK AASLHWTSERVVSVLLGLPAAYLNPCSAMDYSLAAALTGHGWL GQVVTDYVHDAL QKAAKAGLLALSALTFAGLCYFNYHDVGICKAVMLWKL

### References

REF 1	Succinate dehydrogenase is a direct target of sirtuin 3 deacetylase activity. PLoS One. 2011;6(8):e23295. <a href="#">🔗</a>
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If you find any error in data or bug in web service, please kindly report it to [Dr. Wang](#) and [Dr. Li](#).

- Finally let's try BindingDB (<http://www.bindingdb.org/bind/index.jsp>)
- Search for “succinate dehydrogenase”. Then click on “succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial”.
- How many hits do you get?



The screenshot shows the main page of the BindingDB website. At the top right, there is a "BindingDB News" section with a blue header and white text. Below it, the main content area has a title "The Binding Database". On the left, there is a sidebar with links: "myBDB logout", "Search and Browse", "Target", "Sequence", "Name & ID", "Ki IC<sub>50</sub> Kd EC<sub>50</sub>", "Rate constants", and "ΔG° ΔH° -TΔS°". The main content area contains a brief description of the database, stating it is a public, web-accessible database of measured binding affinities focusing on drug-target interactions. It mentions 1,794,819 binding data for 7,438 protein targets and 796,104 small molecules. Below this, there is a "Simple Search" form with a text input field containing "succinate dehydrogenase", a "Go" button, and some usage instructions.

- Finally let's try BindingDB (<http://www.bindingdb.org/bind/index.jsp>)
- Search for “succinate dehydrogenase”. Then click on “succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial”.
- How many hits do you get?
- I see 57!

The Binding Database

myBDB logout

Search and Browse

Target

Sequence  
Name &  
Ki IC50 Kd EC50  
Rate constants  
 $\Delta G^\circ \Delta H^\circ - T\Delta S^\circ$   
pH (Enzymatic Assay)  
pH (ITC)  
Substrate or Competitor  
Compound Mol. Wt:  
Chemical Structure

Pathways

Source Organism

Number of Compounds  
Monomer List in csv  
Het List in SDF

Compound

FDA Drugs  
Important Compounds  
Chemical Structure  
Name  
SMILES  
Number of Data / Targets

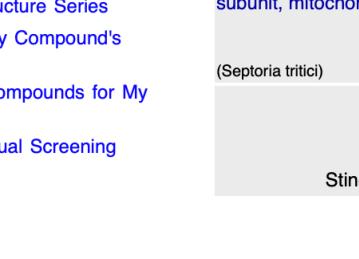
Special tools

3D Structure Series  
Find My Compound's Targets  
Find Compounds for My Targets  
Do Virtual Screening  
SCOP

E-MAIL

Compile Data Set for Download or QSAR  
Add this page Add all pages Clear Selection Make Data Set

Found 57 hits

Target/Host (Institution)	Ligand	Target/Host Links	Ligand Links	Trg + Lig Links	Ki nM	$\Delta G^\circ$ kJ/mole	IC50 nM	Kd nM	EC50/IC50 nM	$k_{off}$ s <sup>-1</sup>	$k_{on}$ M <sup>-1</sup> s <sup>-1</sup>	pH	Temp °C
Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial ( <i>Septoria tritici</i> )	BDBM50191588  (2R,3S,6S,7R,8R)-3-((3-formamido-2-hydroxybenzoyl)...) Show SMILES Show InChI	UniProtKB/SwissProt GoogleScholar	Purchase CHEBI CHEMBL KEGG PC cid PC sid PDB UniChem	Article PubMed	n/a	n/a	2	n/a	n/a	n/a	n/a	n/a	
Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial ( <i>Septoria tritici</i> )	BDBM50411095  (CHEMBL439507) Show SMILES Show InChI	UniProtKB/SwissProt GoogleScholar	CHEMBL PC cid PC sid UniChem	Article PubMed	n/a	n/a	5	n/a	n/a	n/a	n/a		
Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial ( <i>Septoria tritici</i> )	BDBM50411096 	UniProtKB/SwissProt GoogleScholar	CHEMBL PC cid PC sid UniChem	Article PubMed	n/a	n/a	26	n/a	n/a	n/a	n/a		

Assay Description  
Inhibition of *Septoria nodorum* succinate dehydrogenase and Qi site of mitochondrial respiratory chain complex 3 by FMET2-3 assay  
Article DOI: [10.1021/jm060408s](https://doi.org/10.1021/jm060408s)  
BindingDB Entry DOI: [10.7270/Q2TD9ZJC](https://doi.org/10.7270/Q2TD9ZJC)

More data for this Ligand-Target Pair

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# What do I learn from the BindingDB hits?

- The relatively large number of compounds that bind to SDH suggests that the site is druggable
- The results are from two studies, one that tested inhibition for a bacterium *Septoria tritici*, and another for humans. The fact that many compounds bind to the human enzyme means that specificity could be an issue.
- It may be worth trying some of the compounds against *P. Aeruginosa*.