

# BRENDA Exercises Quick Search



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- How often can you find the term "glucosidase" in enzyme names?
- How many EC classes are connected with this term?

### Exercise 2

- How many enzymes accept molybdopterin as a cofactor?
- Display the results for exact matches for molybdopterin
- To which main EC class do the enzymes belong?

### **Exercise 3**

- What is the EC number and the recommended name for the enzyme commonly termed RUBISCO?
- Display the wordmap
- RUBISCO is involved in a biological process. What is its name and what are the major metabolites of this process?
- Display the reaction diagram for RUBISCO
- How many protein sequences for RUBISCO are stored in BRENDA?





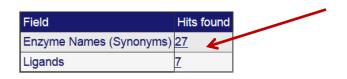


# Search with "contains"

	ybdopterin						
Cofacto	or	▼ contain	IS 🔹				
	add search field	delete search field star	t search ≪ ≪ Results 1 - 10 o				
			ew download	as CSV			
	EC Number 🔻	Recommended Name 🔻		Cofactor VA	Structure VA		
	齡心 🕅 1.1.5.6	formate dehydrogenase-N		bis(molybdopterin guanine dinucleotide)molybdenum cofactor	r 🕆 🕼 🛄		
	蒙诊 🏦 1.1.99.6	D-lactate dehydrogenase (acc	• •	molybdopterin mononucleotide	-		
	i∰ ⊚ jît 1.1.99.33	formate dehydrogenase (acce		bis(molybdopterin guanine dinucleotide)molybdenum cofactor			
	i∰ ⊘ jît 1.1.99.33	formate dehydrogenase (acce	eptor)	molybdopterin			
		formate dehydrogenase		molybdopterin			
	☆ ① 1.2.3.1   ☆ ① 1.2.3.1	aldehyde oxidase aldehyde oxidase		molybdopterin molybdopterin cytosine dinucleotide			
				molybdopterin			
<ul> <li></li></ul>							
			uctase	Imolybdopterin	YAYA Emoti 🗄		
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	Cofactor: molybdopte	erin exact organism specific information anism in taxonomic tree (slow	v e α "mammalia" for rat human we a "mammalia" or rat human we a "mammalia" for rat human we a "mammalia" for rat human we a "mammalia" for rat human we a mammalia or rat human	tungsten-molybdopterin of 51 >>> as CSV as CSV <b>Search with "exact"</b> n m Results 1 - 10 of 26 >>>> download as CSV download all results as CSV			
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Enzym	ne, Ligand	•	contains	T
	add search field dele	ete search field	start search	



≪ ≪ Results 1 - 4 of 4 ≫ ≫ and download as CSV and download all results as CSV

EC Number VA	Recommended Name VA	Synonyms 🟹 📐
齡心 🕅 2.1.1.127	[ribulose-bisphosphate carboxylase]-lysine N-methyltransferase	Rubisco large subunit epsilonN-methyltransferase; Rubisco large subunit methyltrans dimethyltransferase; Rubisco LS methyltransferase; Rubisco LSMT; Rubisco methylt
ர்ற் பிழ் 2.1.1.259	[fructose-bisphosphate aldolase]-lysine N-methyltransferase	large subunit of Rubisco methyltransferas; Rubisco methyltransferase
齡心 頎 4.1.1.39	Ribulose-bisphosphate carboxylase	archaeal Rubisco; barley rubisco; form I RubisCO; Form II Rubisco; Galdieria Rubisc red-type form I RuBisCO; Rubisco; RubisCO 1; RuBisCO 2; RubisCO redlike form I; Rubisco-LSU; RubiscoL; Tk-Rubisco; type III Rubisco
📾 👌 🕦 5.3.2.5	2,3-diketo-5-methylthiopentyl-1-phosphate enolase	RuBisCO-like protein

Sequences- 46425 protein sequences from UniProt

Reaction

Wordmap – The biological process is the photosynthesis. The main metabolites in this process are CO2, chlorophyll, 3-phosphoglycerate, and phosphoenolpyruvate



# BRENDA Exercises The Enzyme Summery Page

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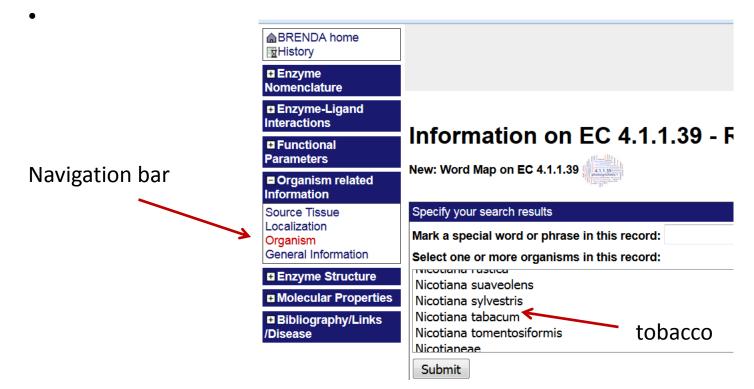


- Display the enzyme summary page for RUBISCO
- Open the menue organism-related information on the navigation bar and look at the section "organism"
- Then go back to the top of the flatfile and click Include FRENDA results (AMENDA + additional results, but less precise; more...)
- Again open the menue organism-related information on the navigation bar and look at the section "organism". What is different now?
- The optimal temperature for RUBISCO varies with the enzyme origin. What is the maximal value for optimal activity. In which organism has it been detected?
- You are only interested in RUBISCO from tobacco. How can you reduce the displayed data to show only those related to tobacco? (Note: if you do not know the scientific name for tobacco, you may need to study the tutorial on the Taxonomy Explorer first. If you know the name (or your instructor is willing to reveal it), you can go ahead with this task (2)





- Rubisco, EC 4.1.1.39
- The navigation bar is on the left side of the screen



In the organism section the BRENDA data are in dark blue. The textmining data are in light blue. The reliability of the textmining data is indicated by +, ++, +++





# BRENDA Exercises Fulltext Search





- methylmalonyl-CoA is a frequently occuring metabolite. Display a list of all BRENDA data categories where this compound is mentioned.
- How many kinetic values are stored for this compound  $(K_m, k_{cat}/K_m, K_i)$ ٠ turnover numbers)?

### Exercise 6

 What are the EC numbers for enzymes that are related to lactate dehydrogenase deficiency?





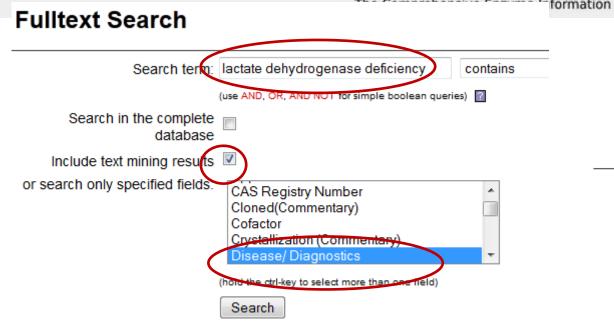
### **Fulltext Search**

Search terne: methylmalonyl-CoA contains (use AND, OR, AND NOT for simple boolean queries) Search in the complete 📝 database Include text mining results or search only specified fields: Activating Compound Ξ Amino Acid Sequence Application CAS Registry Number Cloned(Commentary) (hold the ctrl-key to select more than one field) Search

Field	Hits found
Activating Compound	1
Cloned(Commentary)	3
Crystallization (Commentary)	5
Disease/ Diagnostics	72
Enzyme Names (Synonyms)	30
Inhibitors	17
KCat/KM [mM/s]	3
Ki Value [mM]	2
KM Value [mM]	30
Ligands	118
Natural Product	5
Natural Substrate	13
Natural Substrates/ Products (Substrates)	93
Product	27
Reaction	25
Recommended Name	6
Reference by Title	329
Renatured (Commentary)	2
Substrate	60
Substrates and Products (Substrate)	390
Synonyms	19
Systematic Name	10
Turnover Number [1/s]	22







Field	Hits found
Disease/ Diagnostics	76





# **BRENDA Exercises Advanced Search**

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- Search all acetyltransferases which have been crystallized.
- How many of these have a connected pdb entry?

### **Exercise 8**

 Xylose from hydrolyzed wood components might be a good material for energy production or biofuel production. Find enzymes that may be useful in these processes.







### **Advanced Search results**

New advanced search



pyruvate dehydrogenase (acetyl-transferring) (EC 1.2.4.1) from *Homo sapiens* 

Crystallization (Commentary)

Crystallization	Reference
recombinant enzyme, orthorhombic crystals in polyethylene glycol 3350 by vapor-diffusion method, space group P222	348993
vapour diffusion method with 14-18% PEG 3350, 0.1 mM sodium azide, and 200 mM NaSCN in 50 mM potassium phosphate (pH 8.0)	685160

#### pyruvate dehydrogenase (acetyl-transferring)

(EC 1.2.4.1) from *Escherichia coli* Crystallization (Commentary)

#### Crystallization

in complex with phosphonolactylthiamine diphosphate as structural and electrostatic analogue of alpha-lactylthiamin diphosphate. Presence of phosp

preparation of catalytic subunit E1 of pyruvate dehydrogenase complex, without cofactors thiamine diphosphate and Mg2+, no evidence of disorder/c complex with thiamine 2-thiazolone diphosphate

purified enzyme E1 in complex with inhibitor thiamine thiazolone diphosphate and Mg2+, sitting drop vapour diffusion method, reservoir solution: 15-:

### **Advanced Search results**

#### New advanced search

#### pyruvate dehydrogenase (acetyl-transferring)

(EC 1.2.4.1) from *Homo sapiens* Crystallization (Commentary)



Crystallization	Reference
recombinant enzyme, orthorhombic crystals in polyethylene glycol 3350 by vapor-diffusion method, space group P222	348993
vapour diffusion method with 14-18% PEG 3350, 0.1 mM sodium azide, and 200 mM NaSCN in 50 mM potassium phosphate (pH 8.0)	685160

#### PDB ID

PDB ID	Chain	UniProt (1st accession)
1ni4	А	P08559
1ni4	С	P08559
1ni4	В	P08559



EC Number:	exact	•		use * as a wildcard
Organism:	exact	•		use * as a wildcard (* in
Enzyme Name:	exact	•		]
Search in text fields				
٥				
1. Application	-	contains •	production	
2. Ligands	•	contains -	xylose	
•				

### glucose 1-dehydrogenase (PQQ, quinone)

(EC 1.1.5.2) from *Pyrobaculum aerophilum* Application

Application	Commentary
biofuel	construction of a long-life biofuel cell using a hyperthermophilic enzyme. For the cathode, the mul
production	glucose dehydrogenase from Pyrobaculum aerophilum is used. When the enzymes are used as e

### Ligands

Role	Ligand	Structure	inchi	chebilD	Reference
KM Value	D-xylose				711018
Substrate	D-xylose				711018
Turnover Number	D-xylose				711018

### acetylxylan esterase

(EC 3.1.1.72) from Trichoderma reesei
 Application



# **BRENDA Exercises EC Explorer**

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- You are looking for enzymes that transfer methyl groups
- There are several search modes which you might use for this search.
- However this time use the EC Explorer for this search
- Start with using the search mode of the EC Explorer
- try using a part-name
- try using a compound which is able to donate a methyl group
- Then use the browse mode
- Look at the various links and display the information provided there
- Now try other search modes for this tasks (your instructor will appreciate your feedback)





### **EC Explorer**

owse EC tree] - [search]					
ease use AND or OR in combin	natio	n with <b>NOT</b> to re	efine y	you query	
EC number	<b>v</b>	begins with	•		
Common name	<b>√</b>	contains	•		First thing you may guess that these enzymes
Reaction	✓	contains	•		are called "methyltransferase" and enter the
Systematic name		contains	•		term into "synonyms"
Comment		contains	•		
CAS registry number		contains	•		
Synonyms	<b>√</b>	contains	•	methyltransferase	
History		contains	•		
clude 🔲 class (x.) 🔲 subclass	(x.x.	) 🔲 sub-subcla	iss (x.	x.x.) 🗹 serial number (	x.x.x.x)
	sea	arch 10 🔻	resu	Its	

#### 

EC 🔺 👻	Common name 🔺 👻	Reaction 🔺 🔫	Synonyms 🔺 👻
	[methionine synthase] reductase	2 [methionine synthase]-methylcob(I)alamin + 2 <i>S</i> -adenosylhomocysteine + NADP <sup>+</sup> = 2 [methionine synthase]-cob(II)alamin + NADPH + H <sup>+</sup> + 2 <i>S</i> -adenosyl-L-methionine	methionine synthase cob(II)alamin reducta synthase]-cobalamin methyltransferase (co
	nicotinamide <i>N</i> -methyltransferase	S-adenosyl-L-methionine + nicotinamide = S-adenosyl-L-homocysteine + 1-methylnicotinamide	nicotinamide methyltransferase
	guanidinoacetate	S-adenosyl-L-methionine + guanidinoacetate = S-adenosyl-L-homocysteine + creatine	GA methylpherase; guanidinoacetate meth



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### **EC Explorer**

[browse EC tree] - [search] back to top EC Browser 1 Oxidoreductases (7908 organisms) 🖕 2 Transferases (5546 organisms) 📑 🖬 👘 🧖 🖕 2.1 Transferring one-carbon groups (1114 organisms) 📑 📼 🧖 🖕 2.1.1 Methyltransferases (963 organisms) 📑 💷 🦻 2.1.1.1 nicotinamide N-methyltransferase (6 organisms) 🛆 📑 📾 🦻 2.1.1.2 guanidinoacetate N-methyltransferase (9 organisms) 🚡 📑 🔤 🦻 2.1.1.3 thetin-homocysteine S-methyltransferase (1 organism) A Frame Frame 2.1.1.4 acetylserotonin O-methyltransferase (15 organisms) 🛆 📑 🛲 · 2.1.1.5 betaine—homocysteine S-methyltransferase (13 organisms) 🛆 📑 🛲 📑 📼 2.1.1.6 catechol O-methyltransferase (22 organisms) 🛆 🎫 – 2.1.1.7 nicotinate N-methyltransferase (5 organisms) 🛆 📑 📼 📑 2.1.1.8 histamine N-methyltransferase (9 organisms) 🛆 📑 2.1.1.9 thiol S-methyltransferase (19 organisms) 🛆 Press - 2.1.1.10 homocysteine S-methyltransferase (13 organisms) 🛽 📑 🏧 – 2.1.1.11 magnesium protoporphyrin IX methyltransferase (14 organisms) 🛆 📑 🛲 👘 – 2.1.1.12 methionine S-methyltransferase (15 organisms) 🛆 📑 🛲 📑 🚥 2.1.1.13 methionine synthase (28 organisms) 🛆 📑 📾 🦻 2.1.1.14 5-methyltetrahydropteroyltriglutamate—homocysteine S-methyltransferase (23 organisms) 🛆 📑 🛲 2.1.1.15 fatty-acid O-methyltransferase (4 organisms) 🛆 📑 🔤 2.1.1.16 methylene-fatty-acyl-phospholipid synthase (1 organism) 🛆 📑 📾 2.1.1.17 phosphatidylethanolamine 2.1.1.18 polysaccharide O-methyltr You can systematically click through the tree 2.1.1.19 trimethylsulfonium-tetrah until you reach the desired enzyme class. 2.1.1.20 glycine N-methyltransferas Sequences, reaction, flatfils can be displayed







# BRENDA Exercises Taxonomic Tree





- Search the scientific name for yeast
- How many EC numbers and amino acid sequences are stored in BRENDA for this organism?
- How many synonyms are reported for this organism?







### Tax Tree Explorer

browse taxonomy tree] - [sear	ch] - 🔓 [Example]	
Scientific name or synony	m: exact 🔹 yeast	(use AND, OR, AN
type of synonym (optiona	al): all types of synonyms 🔹	
NCBI Taxonomy I	D: = •	
Rar	nk: all types of ranks ▼	
	Search	
1 different results found		
1: yeast (Saccharomyces cere	evisiae) 🔻	
cerevisiae            û         î         1405 aa sequences of Saccharomyces cerevisiae             NCBI 4932             Found 2518 enzymes for Saccharomyces cerevisiae             1.1.1.1             Show enzyme             Synonyms             1. Candida robusta 2. Saccaromyces	└ cellular organisms └ Eukaryota I (superkingdom) └ Opisthokonta I └ Fungi I (kingdom) └ Dikarya I (subkingdom) └ Ascomycota I (phylum) └ saccharomyceta I └ Saccharomyceta I └ Saccharomyceta I └ Saccharomyceta └ Saccharomyceta └ Saccharomyceta └ Saccharomyceta	፪ (class) les ፪ (order) taceae ፪ (family)

7405 amino acid sequences2518 EC classes15 synonyms

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# BRENDA Exercises BTO





- How many terms in the BTO contain "skin"?
- How many EC numbers are stored in BRENDA for skin cancer cells?
- What is the definition of this term?







### **Ontology explorer**

- BTO (BRENDA Tissue Or	itology)	
Change ontology:	BTO (BRENDA Tissue Ontology)	✓ Version 2015-04-30
Term:	contains 🔻 skin	use AND (NOT) or OR
Synonym:	contains 🔻	use AND (NOT) or OR
Definition:	contains 🔹	use AND (NOT) or OR
restrict to BRENDA links:		
Tissue		
	search	
12 different search results foun	d	
<ul> <li>3: foreskin keratinocyte cell lin</li> <li>4: foreskin melanocyte cell lin</li> <li>5: skin</li> <li>6: skin cancer cell</li> </ul> Details for skin cancer cell	e -	Tree view
	- tissues, cell types and enzyme sources t	issues, cell types and enzyme sources
cell	└ animal <b>1</b> └ whole body <b>1</b>	占 tissues, cell types and enzyme sources fmm 占 animal fmm
BTO (BRENDA Tissue Ontology) ID	L integument	占 whole body 111
BTO:0001286	└ skin <b>⑤</b> └ <mark>skin cancer cell</mark>	│
BTO:0001286 is linked to 150 enzymes:		
1.1.1.42 -		│
Show enzyme		🖶 cancer stem cell 🚱 🗂 🗂 👘
Definition		
The two most common forms		



# BRENDA Exercises Ligands



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- How many enzymes are affected by promethazine?
- Which enzymes are inhibited by this compound?
- Which enzyme can metabolize this compound and what is the product?
- What happens to the enzyme after the product is formed?

## Exercise 13

- How many enzymes can metabolize cellobiose in an oxidative manner?
- How many enzyme can hydrolyze this compounds?

## Exercise 14

- Display the structure of cellopentaose.
- What are the products of cellopentaose hydrolysis?



Substrates and Products (Substrate)	celloplose	contains -	show 10 - results			
	Don't snow organism sp	ecific information	(fast!)			
	Search organism in taxonomic tree (slow, e.g. "mammalia" for rat,human,monkey,)					
	(Not possible to combine with the	ne first option)				
Refine your search						
Recommended Name: 🗵		contains -	]			
EC Number	1.	ber ins with 👻	]			
Commentary Substrates:		contains -	]			
Organism:		contains -	]			
Products:		contains -	]			
Commentary (Products):		contains -				
Reversibility:		contains -	]			
	Search					

Tip: unclick all options for this search EC number begins with 1. gives 45 results

EC number begins with 3. (for hydrolases) gives 65 results

#### Search term: cellobiose



EC Number 🔨	Recommended Name	
蒙诊 🌐 1.1.1.121	aldose 1-dehydrogenase (NAD+)	
<b>診</b> 诊 fft 1.1.1.47	glucose 1-dehydrogenase [NAD(P)+]	

# Exercise 14: cellooligosaccharides and D-glucose





# BRENDA Exercises Pathways



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- How many enzymes are part of the BRENDA pyrimidine metabolism?
- How many enzymes are part of the KEGG pyrimidine metabolism? •

### Exercise 16

- Display the BRENDA interactive benzoyl-CoA degradation pathway ٠
- What is the final metabolite in this pathway?
- Show the molecule diagram, the molecular formula and the INChI key for this metabolite.



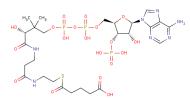


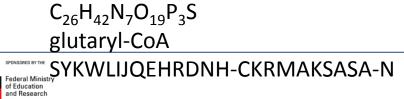
Search Pathway		32 EC classes in the BRENDA
Patheav: pyrimidine meta Refine your search	bolism exact how 100 - results	pyrimidine metabolism
Recommended Name: Z	contains	61 EC classes in the KEGG
KEGG Link: 🗵	contains ▼	pyrimidine metabolism
Source Data ase: V BRENDA	contains	

#### Search term: pyrimidine metabolism

end download all results as CSV							
EC Number VA	Recommended Name	Pathway 🔨	KEGG Link	MetaCyc Link 🔨 📥	Source Database		
≇ு் நி 1.3.1.2	dihydropyrimidine dehydrogenase (NADP+)	pyrimidine metabolism	-	-	BRENDA		
<b>診</b> 合 fft 1.3.1.14	dihvdroorotate dehvdrogenase (NAD+)	pvrimidine metabolism	-	-	BRENDA		

Results 1 - 32 of 32 
 N





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# BRENDA Exercises Sequences, Genomes





- Search for amino acid sequences of RUBISCO from soybean (if you can't remember the EC number or the recommened name for RUBISCO or the scientific name for the soybean you might try to find it in BRENDA by yourself. Of course your instructor can give valuable tips)
- Perform a BLAST with entry P00865 and find out how many other sequences can be matched with 100% identity.
- Find out the molecular weight and a literature reference for P00865.

### **Exercise 18**

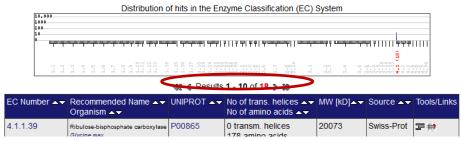
- Search for transferases in the genomes of the genus Solanum.
- Select 5 entries for visualization and look for enzyme details





#### Amino acid sequence search

Amino acid Sequence:	contains •
No. of results:	10 🗸
Recommended name: (of enzyme)	contains -
EC Number:	exact 🗸 4.1.1.39
1st Accession Code: (UniProt)	contains -
Organism:	colitains - glycine max
Number of amino acids:	
Molecular weight [Da]:	
Transmembrane helices:	
N-terminus:	inside outside
Source:	SwissProt TREMBL
	search reset

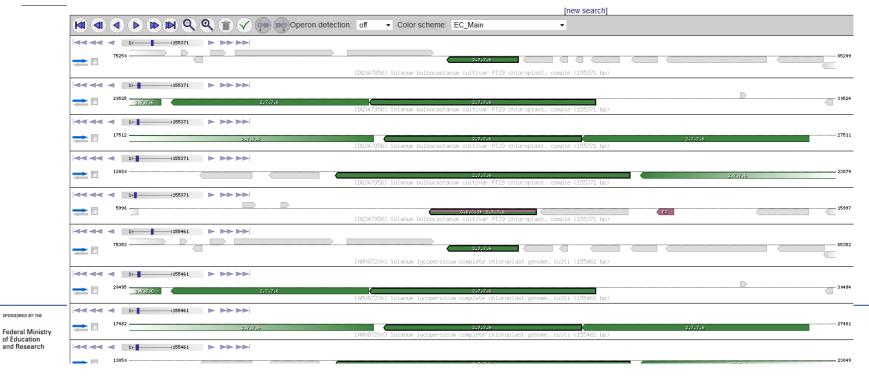








		honeive Fre	une a bufe see able a	e	the set		
Available genomes: down CTRL or SHIFT to select multiple genomes)	Elkaryota     Solanum bulbocastanum cultivar PT29 chloroplast     Solanum lycopersicum chromosome ch01     Solanum lycopersicum chromosome ch02     Solanum lycopersicum chromosome ch04     Solanum lycopersicum chromosome ch04     Solanum lycopersicum chromosome ch05	Please select one or more genomes from below for vis Visualize selected Visualize selecte			e or more genomes from below for visualization. isualize selected Visualize i Results r - 20 of 85 C	alization. EC Number Accession	
Organism:	Solanum lycopersicum chromosome ch06		Solanum bulbocastanum	rpoA	RNA polymerase alpha subunit DNA-directed RNA polymerase subunit alpha Plastid-encoded RNA polymerase subunit alpha	2.7.7.6	Q2MIF6
Taxonomy:	begins with		Solanum bulbocastanum	rpoB	RNA polymerase beta subunit DNA-directed RNA polymerase subunit beta PEP Plastid-encoded RNA polymerase subunit beta	<mark>2.</mark> 7.7.6	Q2MIJ5
EC Number- UniProt Accession:	exact		Solanum bulbocastanum	rpoC1	RNA polymerase beta subunit DNA-directed RNA polymerase subunit beta' PEP Plastid-encoded RNA polymerase subunit beta'	<mark>2.</mark> 7.7.6	Q2MIJ6
Protein Name: Max. number of results:	exact		Solanum bulbocastanum	rpoC2	RNA polymerase beta' subunit DNA-directed RNA polymerase subunit beta'' PEP Plastid-encoded RNA polymerase subunit beta''	<mark>2.</mark> 7.7.6	Q2MIJ7
	□ Display homolog proteins with min. ○ 50% ○ 90% ○	10	Solanum bulbocastanum	atpA		3.6.3.14 <mark>2.</mark> 7.7.6	Q2MIK2
Genome	Explorer						





# BRENDA Exercises Exploring more Features



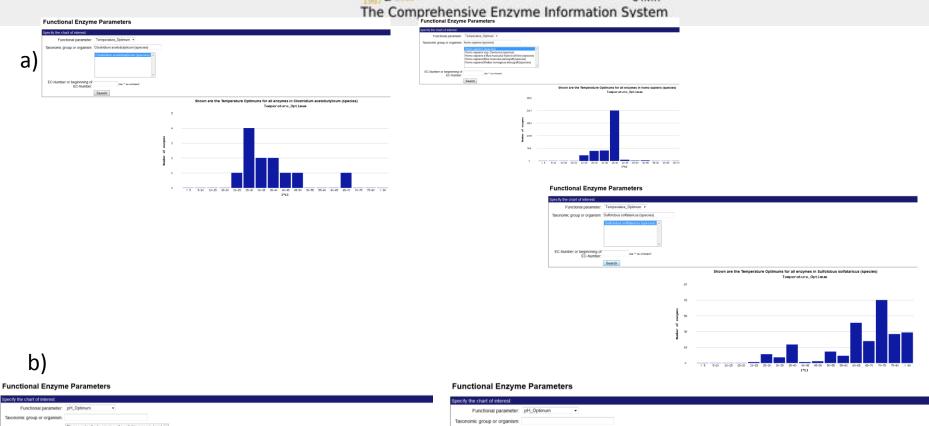


### Extra Exercises

- a) Organisms and their enzymes are adapted to the environment in which they live. Use the search option **Functional Parameters** to display the temperature optimum for the enzymes of Clostridium acetobutylicum, Homo sapiens, and Sulfolobus solfataricus to display the optimal temperatures. Can you detect differences?
- b) The pH optima of enzyme-catalyzed reactions often depends on the type of reaction. Redox reactions are catalyzed best at neutral pH-values. Hydrolytic reactions require different conditions. Display the pH optima for oxidoreductases acting on C-OH bond with NAD(P)+ as cofactors. Then display the pH optima for serine endopeptidases. (Note: you may have to consult the EC Explorer to find out the EC subclasses for these enzymes)



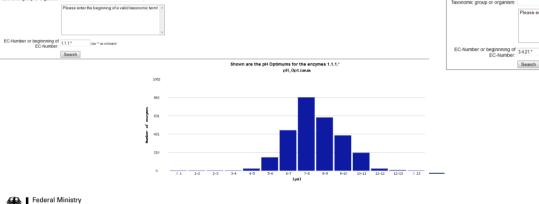




Please enter the beginning of a valid taxonomic term! -

Use \*\* as wildcard!

Search



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#### Shown are the pH Optimums for the enzymes 3.4.21.\* pH\_Optimum 377 302 226 Ja Ja 151 < 1 1-2 2-3 0 11-12 12-13 > 13 3-4 4-5 7-8 8-9 9-10 5-6 6-7

[pH]