

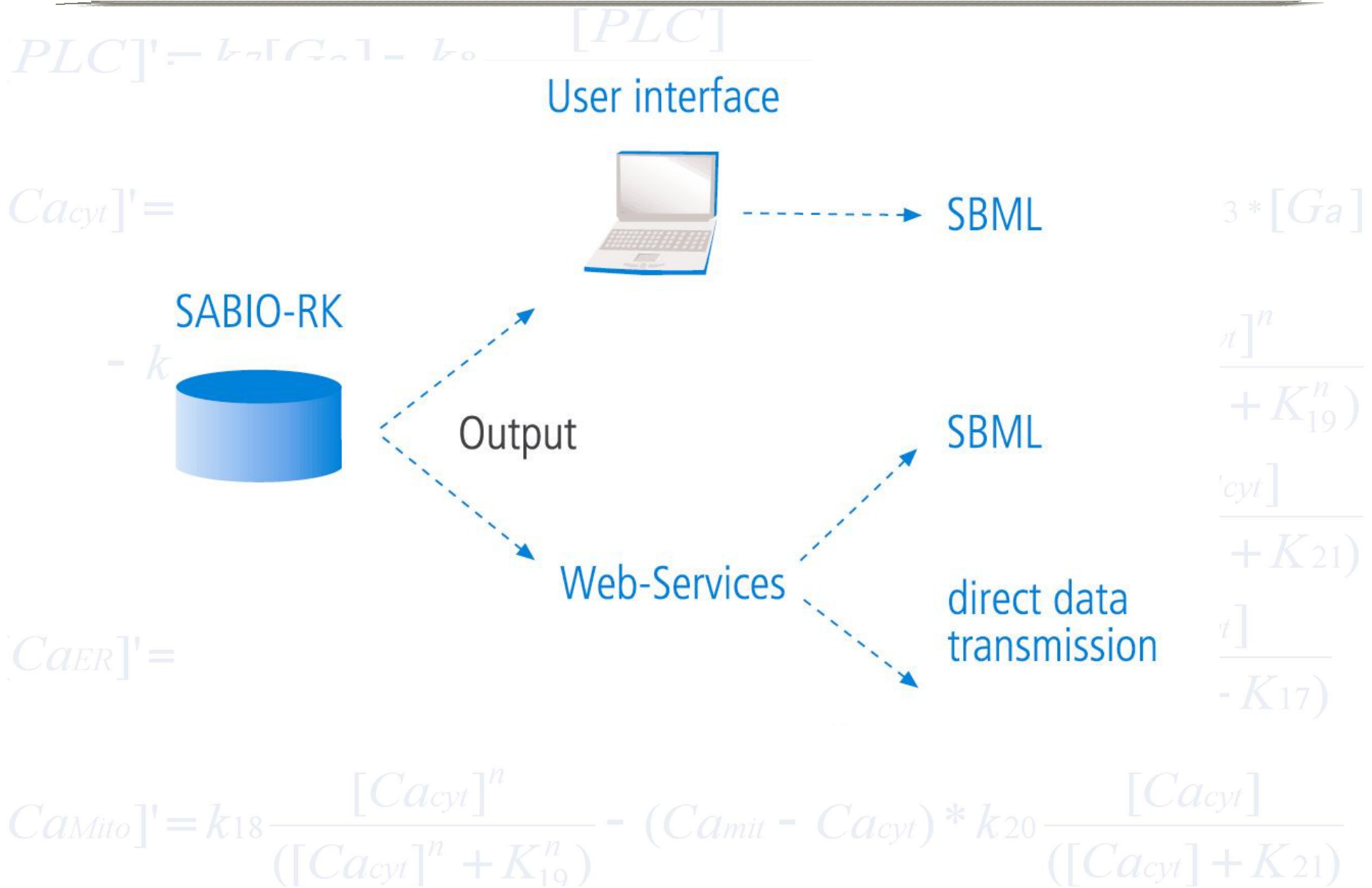
EML
Research

SABIO-RK User Interface

Ulrike Wittig

$$[Ga]' = k_1 + (k_2[Ca_{cyt}]) - k_3 \frac{[Ga][PLC]}{([Ga] + [PLC] + K_9)} - k_4 \frac{[Ga][Ca_{cyt}]}{([Ca_{cyt}] + K_{15})}$$
$$[PLC]' = k_5 \frac{[PLC]}{([PLC] + K_9)} - k_6 \frac{[PLC]^4}{([PLC]^4 + K_{16})} - k_7 \frac{[PLC]^4}{([PLC]^4 + K_{17})} + k_8 \frac{[Ca_{cyt}]^n}{([Ca_{cyt}]^n + K_{19})} - k_9 \frac{[Ca_{cyt}]^n}{([Ca_{cyt}]^n + K_{19})} + (Ca_{mit} - Ca_{cyt}) * k_{20} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{21})}$$
$$[Ca_{cyt}]' = (Ca_{ER} - Ca_{cyt}) * k_{10} * Ca_{cyt} * PLC^4 + k_{12} * PLC + k_{13} * [Ga] - k_{14} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{15})} - k_{16} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{17})} - k_{17} \frac{[Ca_{cyt}]^n}{([Ca_{cyt}]^n + K_{19})} + (Ca_{mit} - Ca_{cyt}) * k_{20} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{21})}$$
$$[Ca_{ER}]' = \frac{1}{K_{17}}$$
$$[Ca_{Mito}]' = k_{18} \frac{[Ca_{cyt}]^n}{([Ca_{cyt}]^n + K_{19})} - (Ca_{mit} - Ca_{cyt}) * k_{20} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{21})}$$

Data Access in SABIO-RK



- Search for general reaction information, kinetic laws, kinetic parameters, experimental conditions etc.
- Colour-coded representation of results

 – *Kinetic data available matching search criteria*


 – *Kinetic data available but not matching search criteria (other organism, tissues etc.)*

 – *No kinetic data available*

- Links to external databases

- Search for reactions by defining substrates /products (compound names)
- Search for reactions by defining enzymes (EC number or name)
- Search for reactions by defining proteins (UniProt identifier)
- Search for publications (author name or PubMed identifier)
- Search for reactions for a given pathway, organism, tissue, cellular location (name)
- Search for reactions containing defined kinetic parameters or laws (select from list)
- Search for reactions under defined experimental conditions (specify values)

→ **Definition of queries by the combination of all search criteria**



SABIO-RK

[CONTACT](#) | [HELP](#) | [IMPRINT](#) [Reaction Search](#)

Return only reactions having kinetic data matching all criteria (blue and grey)

- Search criteria in blue are used to define the search conditions for reactions, independently if there is or not kinetic data for these reactions.

Search Reaction


SBML Model Setup

Specify Search Criteria:

- with **Reactants(s)**
- in **Pathway(s)**
- having **Enzyme(s)**

AND or OR

- in **Publication**
- related to **Protein** (UniProtID)
- in **Organism(s)**



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Total number of reactions found for specified search criteria: **6**

[Click here to view your search criteria](#)

[Modify Search](#)

Kinetic Data Availability:

- view Kinetic data available matching the search criteria
- view Kinetic data available, but not matching all search criteria
- ⊗ No kinetic data available

Number of results per page: [Display](#)

Show only reactions having kinetic data matching the search criteria

[Send Selected Reactions to SBML File](#)

Reactions	Select Reaction(s) (De)Select All	Kinetic Data for this reaction (Click to View)	Enzyme EC#	Kinetic data for enzymes (Click to View)
L-Homocysteine + L-Serine <-> H2O + L-Cystathionine	<input type="checkbox"/>	view	4.2.1.22	view
L-Cysteine + L-Homocysteine <-> Hydrogen sulfide + L-Cystathionine	<input type="checkbox"/>	view	4.2.1.22	view
Acetate + Sulfide <-> L-Cysteine + O-Acetyl-L-serine	<input type="checkbox"/>	view	2.5.1.47 4.2.1.22	view view
L-Cysteine + 2-Mercaptoethanol <-> Hydrogen sulfide + S-(2-Hydroxyethyl)-L-	<input type="checkbox"/>	view	4.2.1.22	view

Reaction Details

Stoichiometric Equation: L-Homocysteine + L-Serine <-> H2O + L-Cystathionine

Substrates: [L-Homocysteine](#), [L-Serine](#)

Products: [H2O](#), [L-Cystathionine](#)

EC Number	in Organism	SWP/UnitProt Link	PubMedID
4.2.1.22	Homo sapiens	SWP/UnitPro	9675031
4.2.1.22	Homo sapiens	SWP/UnitPro	681363
4.2.1.22	Homo sapiens	SWP/UnitPro	15520012
4.2.1.22	Homo sapiens	SWP/UnitPro	15581573
4.2.1.22	Aeropyrum permix	SWP/UnitPro	12644499
4.2.1.22	Rattus norvegicus	SWP/UnitPro	5456996

Enzymes known to catalyse this reaction (curated information)

Pathways: [Glycine, Serine and Threonine metabolism](#), [Methionine metabolism](#)

Compound Details

[Back](#) [List of Reactions](#)

Common Name: L-Homocysteine

Synonyms: L-2-Amino-4-mercaptobutyric acid

SABIO-Compound-ID: 1950

External Links

CAS-ID	6027-13-0
KEGG-ID	C00155
PUBCHEM-ID	3455
ChEBI-ID	17588
HepatoSys-ID	C00155 (Only accessible for HepatoSys project members)

Enzyme Details

Enzyme (recommended) name	Cystathionine beta-synthase
Alternative names	L-serine hydro-lyase (adding homocysteine) Serine sulfhydrase beta-thionase Methylcysteine synthase Cysteine synthase Serine sulfhydrilase
EC Classification	4.2.1.22
Classification	Lyases Carbon-oxygen lyases Hydro-lyases
Catalyses reactions	L-Serine + Sulfide <-> L-Cysteine + H2O L-Homocysteine + L-Serine <-> H2O + Cystathionine L-Homocysteine + L-Serine <-> H2O + L-Cystathionine Selenohomocysteine + L-Serine <-> Selenocystathionine + H2O L-Cysteine + L-Homocysteine <-> Hydrogen sulfide + L-Cystathionine Acetate + Sulfide <-> L-Cysteine + O-Acetyl-L-serine L-Cysteine + 2-Mercaptoethanol <-> Hydrogen sulfide + S-(2-Hydroxyethyl)-L-cysteine
External links	Expasy KEGG IntEnz (EBI) IUBMB Reactome HepatoSys (Only accessible for HepatoSys project members)

Entry Nr. 3101		Tissue:	liver
Organism:		EC Class: 4.2.1.22	wildtype
Tissue:		Recombinant	Expressed in Escherichia coli
EC Class: 4.2.1.22		Substrates	
Organism:		name	location
Tissue:		L-Homocysteine	-
EC Class: 4.2.1.22		L-Serine	-
Organism:		Products	
Tissue:		name	location
EC Class: 4.2.1.22		H2O	-
Organism:		L-Cystathionine	-
Tissue:		Modifiers	
EC Class: 4.2.1.22		name	location
Organism:		Cystathionine beta-synthase(Enzyme)	-
Tissue:		effect	Modifier-Catalyst
EC Class: 4.2.1.22		comment	(P35520)*4;
Organism:		protein complex	
Tissue:		Enzyme (protein data)	
EC Class: 4.2.1.22		UniProt-ID	name
Organism:		subunit	-
Tissue:		complex	-
EC Class: 4.2.1.22		mol. weight (kDa)	252.0
Organism:		deviation (kDa)	-
Tissue:		Kinetic Law	
EC Class: 4.2.1.22		type	formula
Organism:		Michaelis-Menten	$E * k_{cat} * S / (K_m + S)$
Tissue:		Parameters	
EC Class: 4.2.1.22		name	species
Organism:		E	Enzyme
Tissue:		S	L-Serine
EC Class: 4.2.1.22		type	start value
Organism:		A	L-Homocysteine
Tissue:		Km	L-Serine
EC Class: 4.2.1.22		concentration	end value
Organism:		kcat_Km	L-Serine
Tissue:		kcat	-
EC Class: 4.2.1.22		concentration	deviation
Organism:		kcat	-
Tissue:		unit	comment
EC Class: 4.2.1.22		-	-
Organism:		0.005	6.4
Tissue:		5	-
EC Class: 4.2.1.22		3	-
Organism:		2	-
Tissue:		6	-
EC Class: 4.2.1.22		unit	comment
Organism:		mM	-
Tissue:		mM	-
EC Class: 4.2.1.22		mM	-
Organism:		mM ⁽⁻¹⁾ *s ⁽⁻¹⁾	-
Tissue:		s ⁽⁻¹⁾	-
EC Class: 4.2.1.22		Experimental conditions	
Organism:		start value	end value
Tissue:		pH	8.6
EC Class: 4.2.1.22		temperature	37
Organism:		buffer: 10 mM Tris/HCl	- °C
Tissue:		General comment:	-
EC Class: 4.2.1.22		PUBMEDID:	9675031
Organism:		Entry Nr. 8224	

$$[PLC]' = k_7[Ga] - k_8 \frac{[PLC]}{([PLC] + K_9)}$$

Search for general compounds/ compound classes

$$[Ca_{cyt}]' = (Ca_{ER} - Ca_{cyt}) * \frac{k_{10} * Ca_{cyt} * PLC^4}{PLC^4 + K_{11}^4} + k_{12} * PLC + k_{13} * [Ga]$$

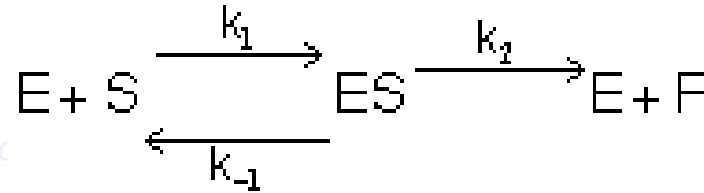
Example: Amino acid

→ search result gives all reactions with any amino acid as substrate or product

$$- k_{14} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{15})} - k_{16} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{17})} - k_{18} \frac{[Ca_{cyt}]^n}{([Ca_{cyt}]^n + K_{19}^n)} + (Ca_{mit} - Ca_{cyt}) * k_{20} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{21})}$$

$$[Ca_{ER}]' = - (Ca_{ER} - Ca_{cyt}) * \frac{k_{10} * Ca_{cyt} * PLC^4}{PLC^4 + K_{11}^4} + k_{16} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{17})}$$

$$[Ca_{Mito}]' = k_{18} \frac{[Ca_{cyt}]^n}{([Ca_{cyt}]^n + K_{19}^n)} - (Ca_{mit} - Ca_{cyt}) * k_{20} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{21})}$$



- For simulation experiments detailed information about the reaction mechanism and kinetic parameters for the steps are necessary

- No quantitative data for mechanism steps available in structured format

- Relation of the reaction mechanism data to the overall reaction

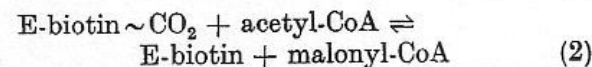
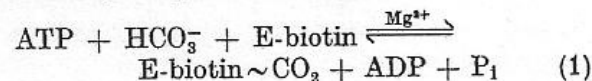
$$[Ca_{ER}]' = -(Ca_{ER} - Ca_{cyt}) * \frac{k_{10} * Ca_{cyt} * PLC^4}{PLC^4 + K_{11}^4} + k_{16} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{17})}$$

$$[Ca_{Mito}]' = k_{18} \frac{[Ca_{cyt}]^n}{([Ca_{cyt}]^n + K_{19}^n)} - (Ca_{mit} - Ca_{cyt}) * k_{20} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{21})}$$

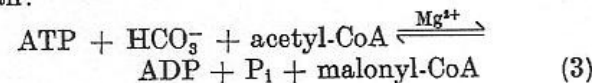
Literature

- no standard representation
- manual information extraction

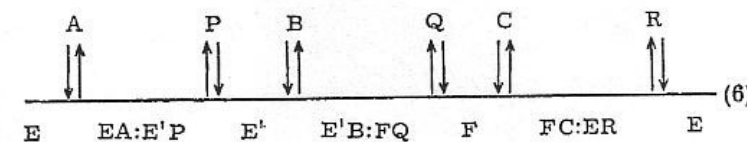
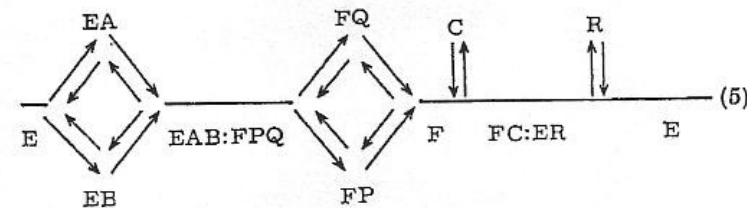
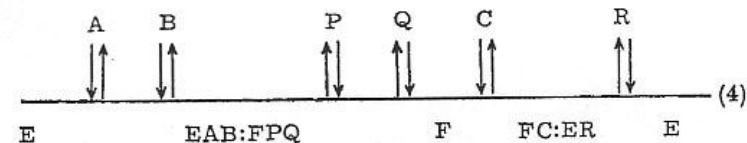
isolated the carboxylated enzyme, which was capable of transferring its carboxyl to acetyl-CoA. The active carboxyl in the carboxylated enzyme was shown to be bound to the 1'-N-atom of biotin linked to the ε-amino group of a lysine residue in the enzyme. These results support the following reaction mechanism involving two partial reactions.



Overall:



Enzymes. Acetyl-CoA carboxylase or acetyl-CoA:CO₂ ligase (ADP) (EC 6.4.1.2); pyruvate kinase or ATP: pyruvate phosphotransferase (EC 2.7.1.40); lactate dehydrogenase or L-lactate:NAD oxidoreductase (EC 1.1.1.27); hexokinase or ATP: D-hexose 6-phosphotransferase (EC 2.7.1.1); glucose-6-phosphate dehydrogenase or D-glucose-6-phosphate:NADP oxidoreductase (EC 1.1.1.49); citrate synthase or citrate oxaloacetate-lyase (CoA-acetylating) (EC 4.1.3.7); malate dehydrogenase or L-malate:NAD oxidoreductase (EC 1.1.1.37).



A, B, P and Q represent substrates and products of the first partial reaction [Eqn. (1)], and C and R acetyl-CoA and malonyl-CoA, respectively. E and F represent two forms of the enzyme, *i.e.* enzyme-

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Stopped-flow Kinetic Analysis of the Reaction Catalyzed by the Full-length Yeast Cystathionine β -Synthase*

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Shinichi Taoka and Ruma Banerjee‡

From the Biochemistry Department, University of Nebraska, Lincoln, Nebraska 68588-0664

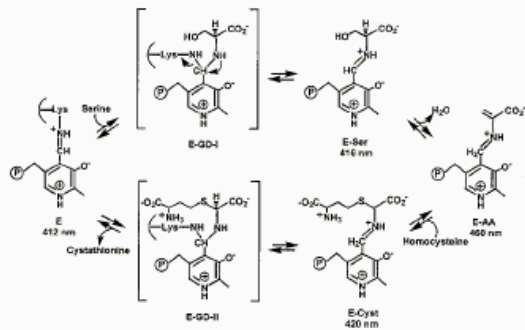
Cystathionine β -synthase found in yeast catalyzes a pyridoxal phosphate-dependent condensation of homocysteine and serine to form cystathionine. Unlike the homologous mammalian enzymes, yeast cystathionine β -synthase lacks a second cofactor, heme, which facilitates detailed kinetic studies of the enzyme because the different pyridoxal phosphate-bound intermediates can be followed by their characteristic absorption spectra. We conducted a rapid reaction kinetic analysis of the

catalyzes the condensation of serine and homocysteine to give cystathionine in a pyridoxal phosphate (PLP)¹-dependent reaction. Cystathionine is subsequently cleaved in the trans-sulfuration pathway by another PLP-dependent enzyme, γ -cystathionase, to give cysteine and α -ketoglutarate.

Cystathionine β -synthases from *Trypanosoma cruzi*, *Saccharomyces cerevisiae*, and humans have highly homologous sequences. All are predicted to belong to the β or Fold II family of PLP-dependent enzymes (6, 7). This similarity is borne out in

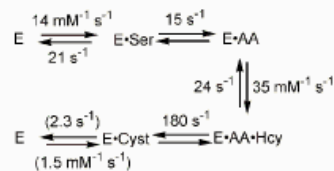
Cystathionine beta-synthase (EC 4.2.1.22) L-Serine + L-Homocysteine = Cystathionine + H₂O

L-Serine + L-Homocysteine = Cystathionine + H₂O

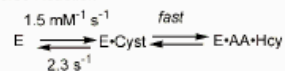


SCHEME I. Intermediates in the reaction catalyzed by cystathionine β -synthase and their absorption maxima as determined in this study. The two gem-diamine intermediates (*GD-I* and *GD-II*), shown in *square brackets*, were not observed in the pre-steady-state kinetic analysis of the full-length yeast enzyme. *AA* and *Cyst* denote aminoacrylate and cystathionine, respectively.

A. Forward Reaction



B. Reverse Reaction



SCHEME II. Minimal kinetic scheme for reaction catalyzed by yeast cystathionine β -synthase in the forward and reverse directions. The values shown in *parentheses* in *A* are taken from *B*, where the reaction was followed in the reverse direction.

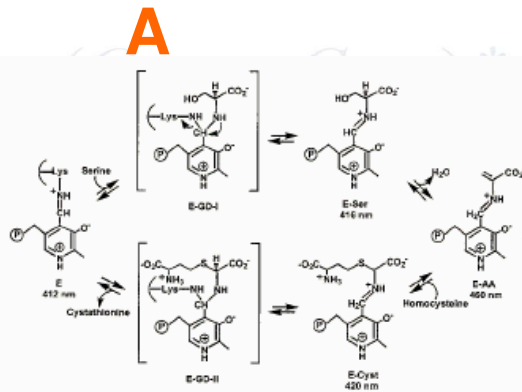


Not useful for the storage
in the SABIO-RK database



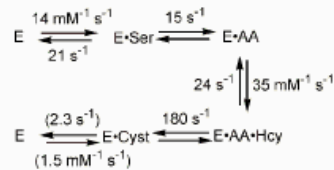
Useful for the storage
in the SABIO-RK database

L-Serine + L-Homocysteine = Cystathionine + H₂O

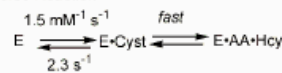


SCHEME I. Intermediates in the reaction catalyzed by cystathionine β -synthase and their absorption maxima as determined in this study. The two gem-diamine intermediates (*GD-I* and *GD-II*), shown in square brackets, were not observed in the pre-steady-state kinetic analysis of the full-length yeast enzyme. AA and Cyst denote aminoacrylate and cystathionine, respectively.

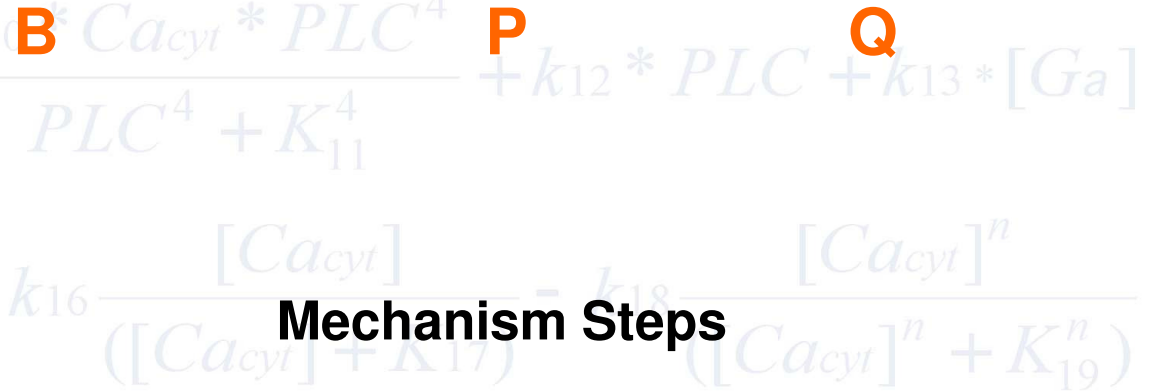
A. Forward Reaction



B. Reverse Reaction



SCHEME II. Minimal kinetic scheme for reaction catalyzed by yeast cystathionine β -synthase in the forward and reverse directions. The values shown in parentheses in A are taken from B, where the reaction was followed in the reverse direction.



Overall Reaction



A

B

P

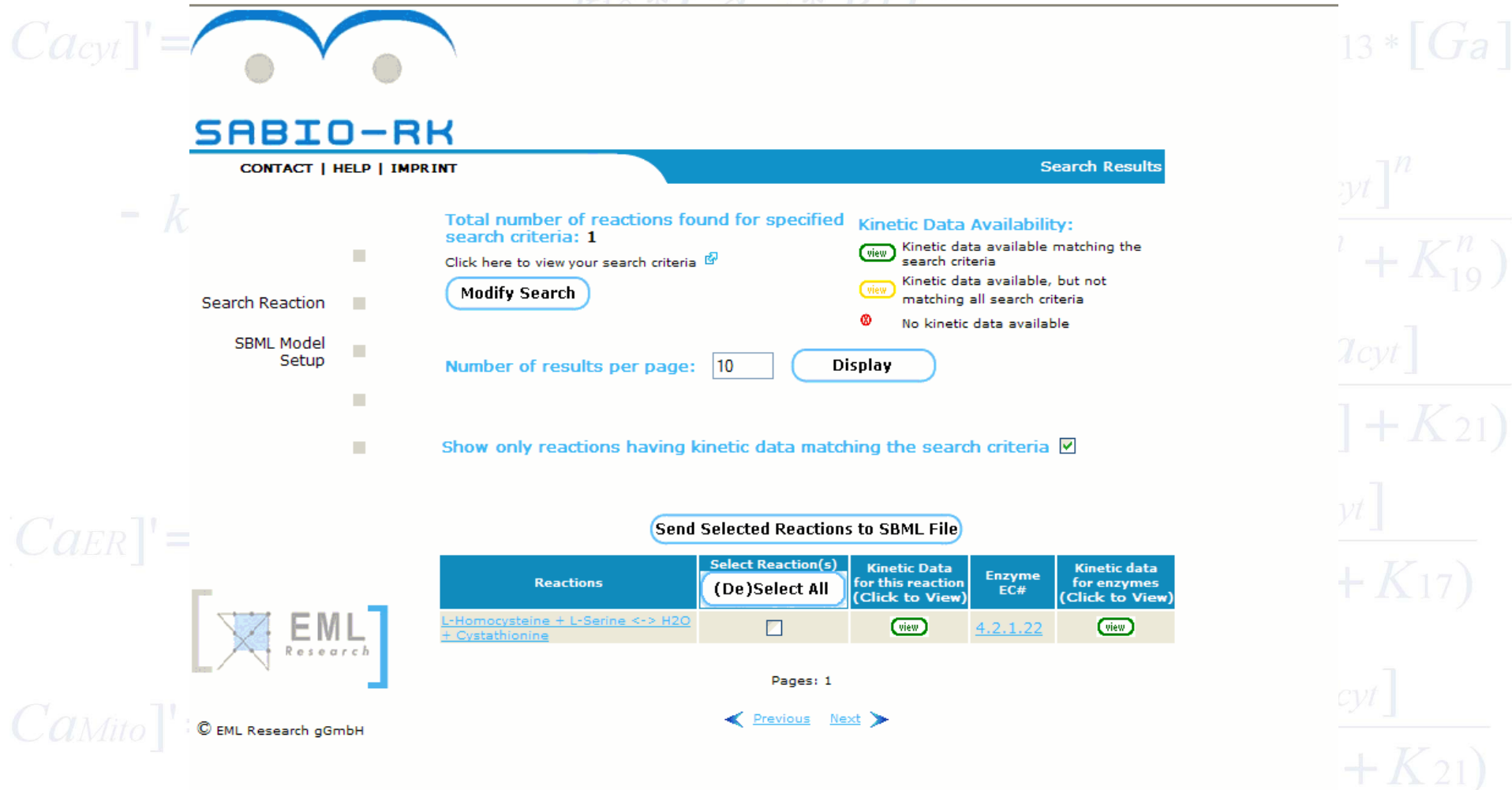
Q

Mechanism Steps



**Insertion using the
SABIO-RK Input Interface**

L-Serine + L-Homocysteine = Cystathionine + H2O



SABIO-RK
CONTACT | HELP | IMPRINT Search Results

Total number of reactions found for specified search criteria: **1**
 Click here to view your search criteria [🔗](#)

Modify Search

Number of results per page: **Display**

Show only reactions having kinetic data matching the search criteria

Send Selected Reactions to SBML File

Reactions	Select Reaction(s) (De)Select All	Kinetic Data for this reaction (Click to View)	Enzyme EC#	Kinetic data for enzymes (Click to View)
L-Homocysteine + L-Serine <-> H2O + Cystathionine	<input type="checkbox"/>	view	4.2.1.22	view

Pages: 1
[← Previous](#) [Next →](#)

L-Serine + L-Homocysteine = Cystathionine + H2O

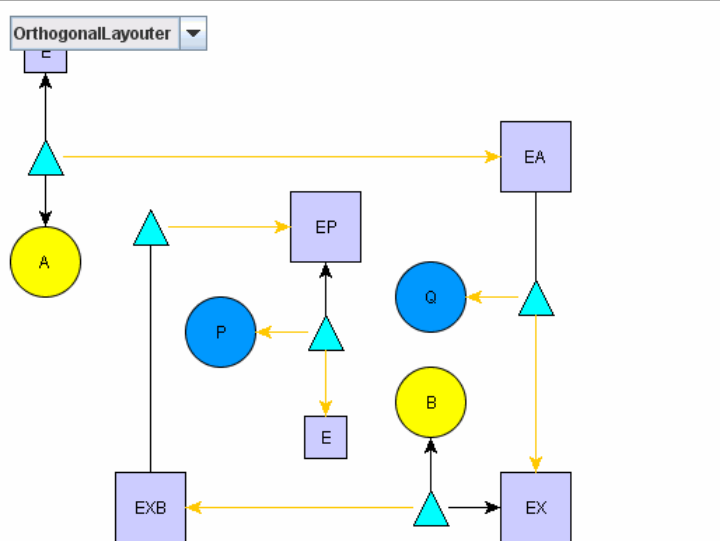
Entry Nr. 20619		[⊕][⊖]		Select	Show Mechanism		
Organism:	Saccharomyces cerevisiae						
Tissue:	unknown						
EC Class:	4.2.1.22						
	wildtype						
Substrates							
name	location	comment					
L-Serine	-	-					
L-Homocysteine	-	-					
Products							
name	location	comment					
H2O	-	-					
Cystathionine	-	-					
Modifiers							
name	location	effect	comment	protein complex			
Cystathionine beta-synthase(Enzyme)	-	Modifier-Catalyst	-	P32582;			
Enzyme (protein data)							
	UniProt-ID	name	mol. weight (kDa)	deviation (kDa)			
subunit	-	-	-	-			
complex	-	-	56.0	-			
Kinetic Law							
type	formula						
-	-						
Parameters							
name	species	type	start value	end value	deviation	unit	comment
Kd	L-Serine	Kd	1.5	-	0.3	mM	-
E	Enzyme	concentration	18	-	-	μM	-
A	L-Serine	concentration	0	20	-	mM	-
kcat	-	kcat	1.7	-	-	s ⁻¹	-
Experimental conditions							
	start value	end value	unit				
pH	8	-	-				
temperature	14	16	°C				
buffer: 0.2 mM Tris							
General comment: -							
PUBMEDID: 11948191							

Mechanism for Reaction:
L-Homocysteine + L-Serine = H2O + Cystathionine
EntriesID: 20619

■ Substrate
 ■ Product
 ■ Activator
 ■ Inhibitor
 Enzyme/Enzyme-Complex
 Molecule
 ▲ Reaction Details

Mechanism step details

OrthogonalLayouter



Legend


Name	Description
A	L-Serine
B	L-Homocysteine
E	Enzyme
EA	Enzyme-Serine
EP	Enzyme-Cystathionine
EX	Enzyme-Aminoacrylate
EXB	Enzyme-Aminoacrylate-Homocysteine
P	Cystathionine
Q	H2O

- 1 A+E-->EA
- 2 EA-->A+E
- 3 EA-->EX+Q
- 4 B+EX-->EXB
- 5 EXB-->B+EX
- 6 EXB-->EP
- 7 EP-->E+P
- 8 E+P-->EP

$$Ca_{Mito}]' = k_{18} \frac{[Ca_{cyt}]}{([Ca_{cyt}]^n + K_{19}^n)} - (Ca_{mit} - Ca_{cyt}) * k_{20} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{21})}$$

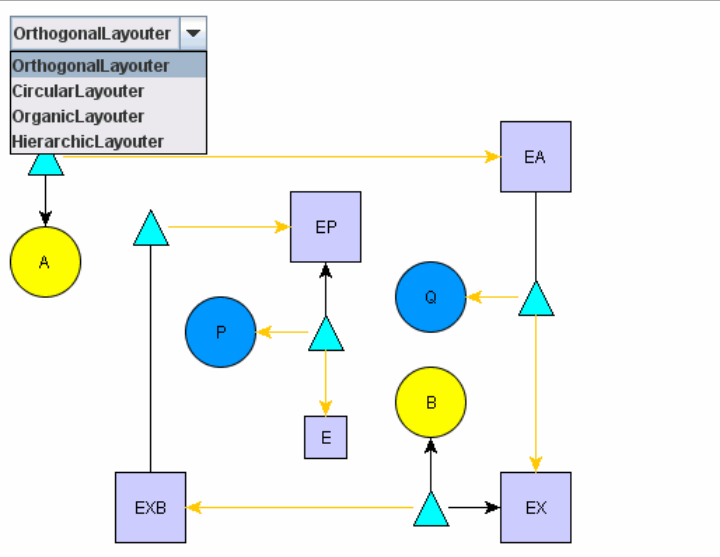
Mechanism for Reaction:
L-Homocysteine + L-Serine = H2O + Cystathionine
EntriesID: 20619

■ Substrate
 ■ Product
 ■ Activator
 ■ Inhibitor
 Enzyme/Enzyme-Complex
 Molecule
 ▲ Reaction Details



OrthogonalLayouter

- OrthogonalLayouter
- CircularLayouter
- OrganicLayouter
- HierarchicLayouter



Legend

Name	Description
A	L-Serine
B	L-Homocysteine
E	Enzyme
EA	Enzyme-Serine
EP	Enzyme-Cystathionine
EX	Enzyme-Aminoacrylate
EXB	Enzyme-Aminoacrylate-Homocysteine
P	Cystathionine
Q	H2O

Mechanism step details

- 1 A+E-->EA ⊕ ⊖
- 2 EA-->A+E ⊕ ⊖
- 3 EA-->EX+Q ⊕ ⊖
- 4 B+EX-->EXB ⊕ ⊖
- 5 EXB-->B+EX ⊕ ⊖
- 6 EXB-->EP ⊕ ⊖
- 7 EP-->E+P ⊕ ⊖
- 8 E+P-->EP ⊕ ⊖

$$[PLC]' = k_7[Ga] - k_8 \frac{[PLC]}{([PLC] + K_9)}$$

Mechanism for Reaction:
L-Homocysteine + L-Serine = H2O + Cystathionine
EntriesID: 20619

■ Substrate
 ■ Product
 ■ Activator
 ■ Inhibitor
 Enzyme/Enzyme-Complex
 Molecule
 ▲ Reaction Details

OrthogonalLayouter

Legend

Name	Description
A	L-Serine
B	L-Homocysteine
E	Enzyme
EA	Enzyme-Serine
EP	Enzyme-Cystathionine
EX	Enzyme-Aminoacrylate
EXB	Enzyme-Aminoacrylate-Homocysteine
P	Cystathionine
Q	H2O

Mechanism step details

Expand All
Close All

1 A+E-->EA

Substrates	
name	description
E	Enzyme
A	L-Serine

Products	
name	description
EA	Enzyme-Serine

Kinetic law	
type	formula
-	-

Parameter						
name	species	type	start value	end value	dev.	unit
A	L-Serine	concentration	0.0	20.0	-	mM
E	Enzyme	concentration	18.0	-	-	µM
k1		rate const.	14.0	-	-	mM ⁽⁻¹⁾ s ⁽⁻¹⁾

Experimental conditions			
	start value	end value	unit
temperature	14	16	°C
pH	8	-	
buffer	0.2 mM Tris		

General comment: -

2 EA-->A+E

$$[Ca_{Mito}]' = k_{18} \frac{[Ca_{cyt}]}{([Ca_{cyt}]^n + K_{19}^n)} - (Ca_{mit} - Ca_{cyt}) * k_{20} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{21})}$$

$$[PLC]' = k_7[Ga] - k_8 \frac{[PLC]}{([PLC] + K_9)}$$

Mechanism for Reaction:
L-Homocysteine + L-Serine = H2O + Cystathionine
EntriesID: 20619

■ Substrate
 ■ Product
 ■ Activator
 ■ Inhibitor
 Enzyme/Enzyme-Complex
 Molecule
 ▲ Reaction Details

OrthogonalLayouter

Legend

Name	Description
A	L-Serine
B	L-Homocysteine
E	Enzyme
EA	Enzyme-Serine
EP	Enzyme-Cystathionine
EX	Enzyme-Aminoacrylate
EXB	Enzyme-Aminoacrylate-Homocysteine
P	Cystathionine
Q	H2O

Mechanism step details

Expand All
Close All

1 A+E-->EA

Substrates	
name	description
E	Enzyme
A	L-Serine

Products	
name	description
EA	Enzyme-Serine

Kinetic law	
type	formula
-	-

Parameter						
name	species	type	start value	end value	dev.	unit
A	L-Serine	concentration	0.0	20.0	-	mM
E	Enzyme	concentration	18.0	-	-	µM
k1		rate const.	14.0	-	-	mM ⁽⁻¹⁾ s ⁽⁻¹⁾

Experimental conditions			
	start value	end value	unit
temperature	14	16	°C
pH	8	-	
buffer	0.2 mM Tris		

General comment: -

2 EA-->A+E

$$[Ca_{Mito}]' = k_{18} \frac{[Ca_{cyt}]}{([Ca_{cyt}]^n + K_{19}^n)} - (Ca_{mit} - Ca_{cyt}) * k_{20} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{21})}$$

Mechanism for Reaction:
L-Homocysteine + L-Serine = H2O + Cystathionine
EntriesID: 20619

■ Substrate
 ■ Product
 ■ Activator
 ■ Inhibitor
 Enzyme/Enzyme-Complex
 Molecule
 ▲ Reaction Details

OrthogonalLayouter

Legend

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A	L-Serine
B	L-Homocysteine
E	Enzyme
EA	Enzyme-Serine
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EX	Enzyme-Aminoacrylate
EXB	Enzyme-Aminoacrylate-Homocysteine
P	Cystathionine
Q	H2O

Mechanism step details

1 A+E-->EA

Substrates	
name	description
E	Enzyme
A	L-Serine

Products	
name	description
EA	Enzyme-Serine

Kinetic law	
type	formula
-	-

Parameter						
name	species	type	start value	end value	dev.	unit
A	L-Serine	concentration	0.0	20.0	-	mM
E	Enzyme	concentration	18.0	-	-	µM
k1		rate const.	14.0	-	-	mM ⁽⁻¹⁾ *s ⁽⁻¹⁾

Experimental conditions			
	start value	end value	unit
temperature	14	16	°C
pH	8	-	
buffer	0.2 mM Tris		

General comment: -


2 EA-->A+E

Equation of Reaction

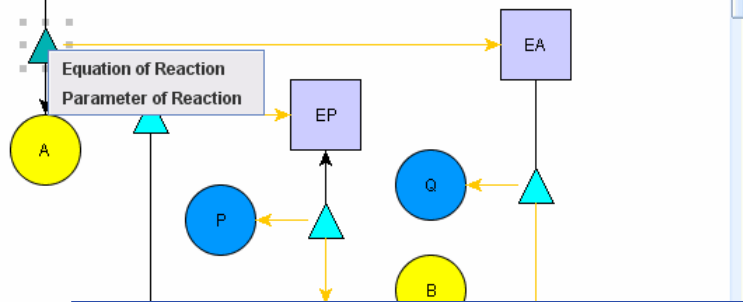
A+E<=>EA

Mechanism for Reaction:
L-Homocysteine + L-Serine = H2O + Cystathionine
EntriesID: 20619

■ Substrate
 ■ Product
 ■ Activator
 ■ Inhibitor
 Enzyme/Enzyme-Complex
 Molecule
 ▲ Reaction Details



OrthogonalLayouter



Legend

Name	Description
A	L-Serine
B	L-Homocysteine
E	Enzyme
EA	Enzyme-Serine
EP	Enzyme-Cystathionine
EX	Enzyme-Aminoacrylate
EXB	Enzyme-Aminoacrylate-Homocysteine
P	Cystathionine
Q	H2O

Parameter of Reaction

Name	Species	Type	Start Value	End Value	Deviation	Unit	Comment
A	L-Serine	concentrati...	0.0	20.0		mM	
E	Enzyme	concentrati...	18.0			μM	
k1		rate const.	14.0			mM ⁻¹ *s ⁻¹ ...	
k_minus1		rate const.	21.0			s ⁻¹	

Close

Mechanism step details

Expand All Close All

1 A+E-->EA

Substrates	
name	description
E	Enzyme
A	L-Serine

Products	
name	description
EA	Enzyme-Serine

Kinetic law	
type	formula
-	-

Parameter						
name	species	type	start value	end value	dev.	unit
A	L-Serine	concentration	0.0	20.0	-	mM
E	Enzyme	concentration	18.0	-	-	μM
k1		rate const.	14.0	-	-	mM ⁻¹ *s ⁻¹

Experimental conditions			
	start value	end value	unit
temperature	14	16	°C
pH	8	-	
buffer	0.2 mM Tris		

General comment: -

2 EA-->A+E

- expansion of compound classification
- classification of organisms, tissues/ cell types, cell locations
- search for mechanism
- search for modifiers: inhibitor/ activator/ cofactor

- less reaction oriented search

Examples:

→ search for all enzymes in a tissue/ organism etc.

→ search for all organisms containing specific enzyme

$$[Ca_{ER}]' = - (Ca_{ER} - Ca_{cyt}) * \frac{k_{10} * Ca_{cyt} * PLC^4}{PLC^4 + K_{11}^4} + k_{16} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{17})}$$

$$[Ca_{Mito}]' = k_{18} \frac{[Ca_{cyt}]^n}{([Ca_{cyt}]^n + K_{19}^n)} - (Ca_{mit} - Ca_{cyt}) * k_{20} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{21})}$$