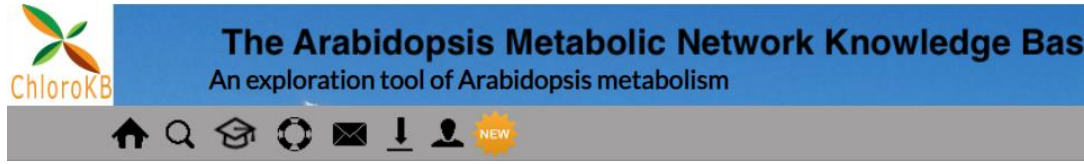
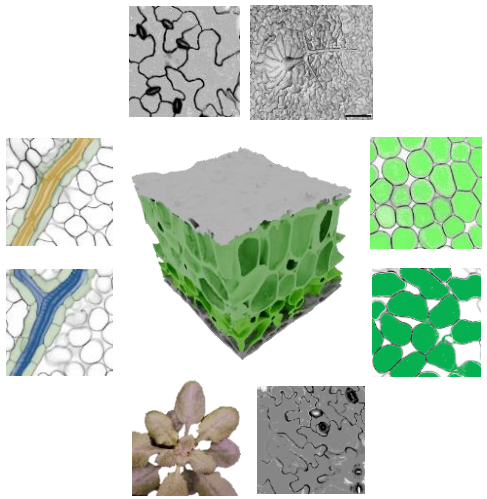
Community ressources for modelling plant metabolism



http://chlorokb.fr



The Arabidopsis leaf quantitative atlas: a cellular and subcellular mapping through unified data integration

Quantitative Plant Biology

Light Photosynthesis & Metabolism

Laboratoire de Physiologie Cellulaire & Végétale
CEA-University Grenoble Alpes-INRAE-CNRS

Gilles Curien

NETBIO, Orléans, 24-25 novembre 2025

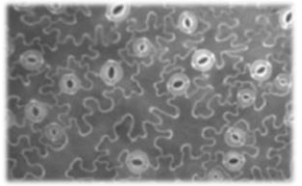
Représentation des connaissances

Comprendre: Du latin cum (« avec ») et prehensio (« saisir ») : saisir ensemble, embrasser par la pensée.

Comprendre en termes **moléculaires** comment le **système plante** se maintient et croît

en réponse à de nombreux **paramètres du milieu** très variables **au cours du temps**

Exemples: taux de CO_2, sécheresse, attaques pathogènes, stress salin, température, intensité lumineuse

Comprendre en termes moléculaires une **fonction intégrée** (exemple ouverture des stomates) 

Comprendre « ce qui » rend certaines plantes plus **robustes** que d'autres dans certaines conditions

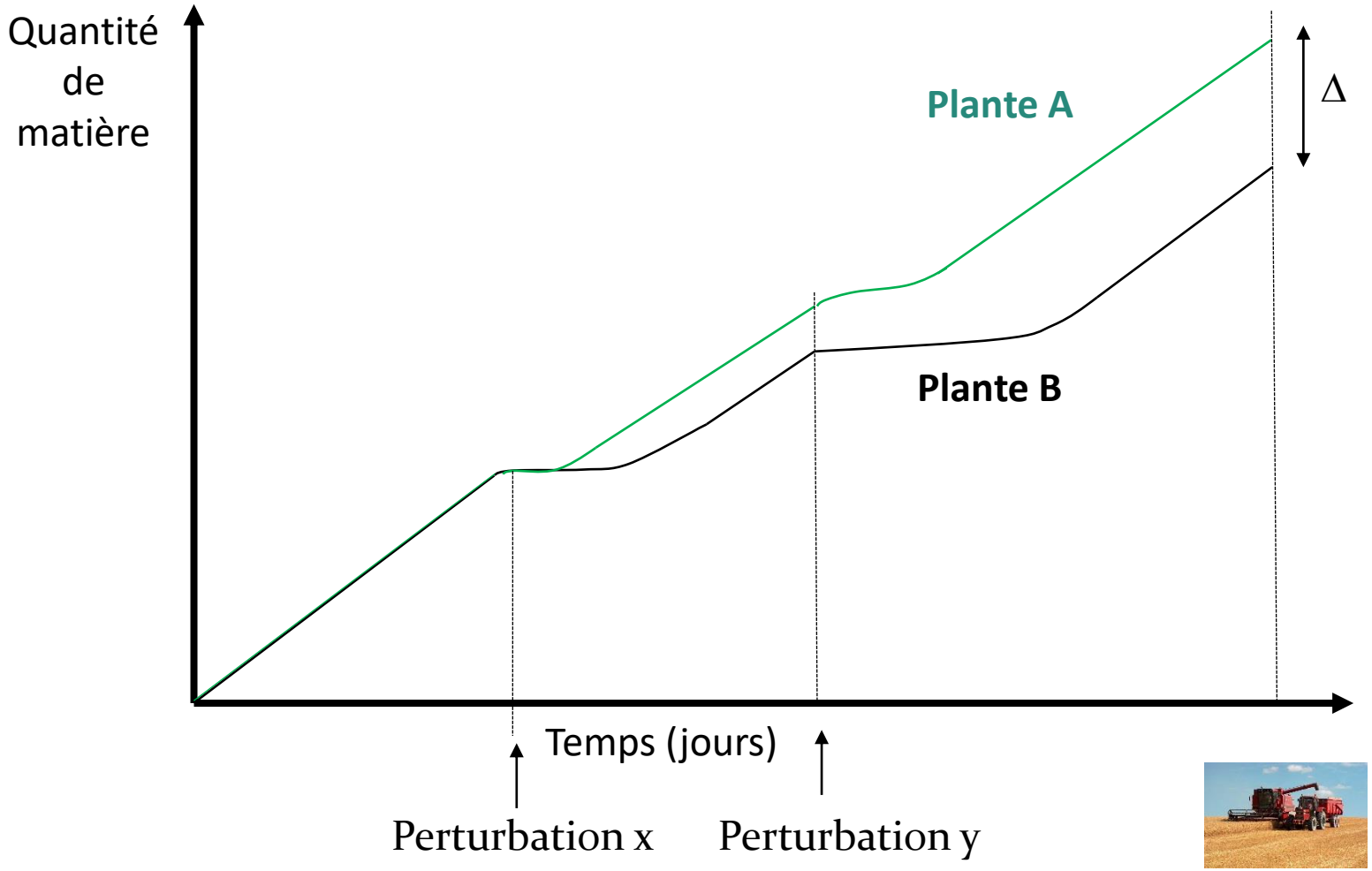
ChloroKB s'inscrit dans un **Programme de Physiologie Moléculaire**:

The study of **dynamic** (**time-dependent**) interactive processes and biochemical communications at the subcellular level

Comprendre ?

- Identifier des connexions, des entités qui contrôlent, modulent, coordonnent…

- Modéliser le comportement d'un système biologique **(quantitativement)**


Quantité de matière
Plante A
Δ
Plante B
Temps (jours)
Perturbation x
Perturbation y

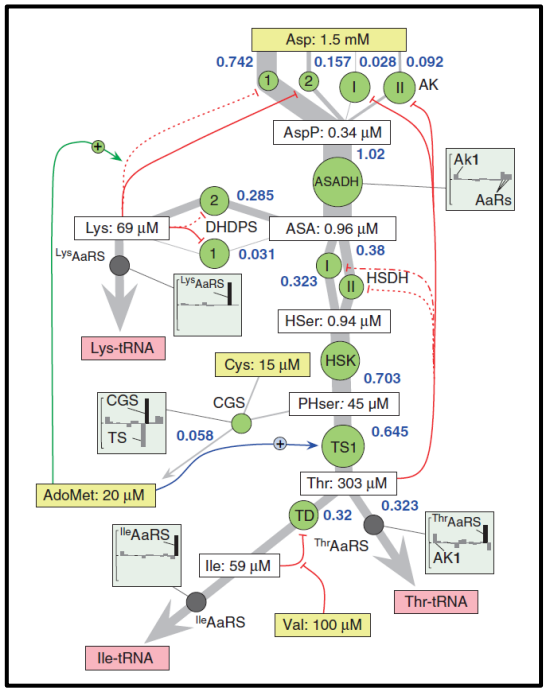
Molecular Systems Biology 5; Article number 271; doi:10.1038/msb.2009.29
Citation: *Molecular Systems Biology* 5:271

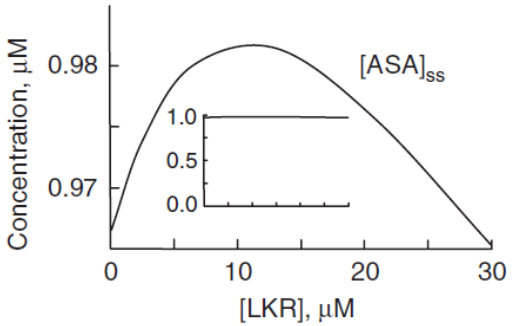
www.molecularsystemsbiology.com

molecular systems biology

Understanding the regulation of aspartate metabolism using a model based on measured kinetic parameters

Gilles Curien[1,2,3,4,*], Olivier Bastien[4], Mylène Robert-Genthon[1,2,3,4], Athel Cornish-Bowden[5], María Luz Cárdenas[5] and Renaud Dumas[1,2,3,4]





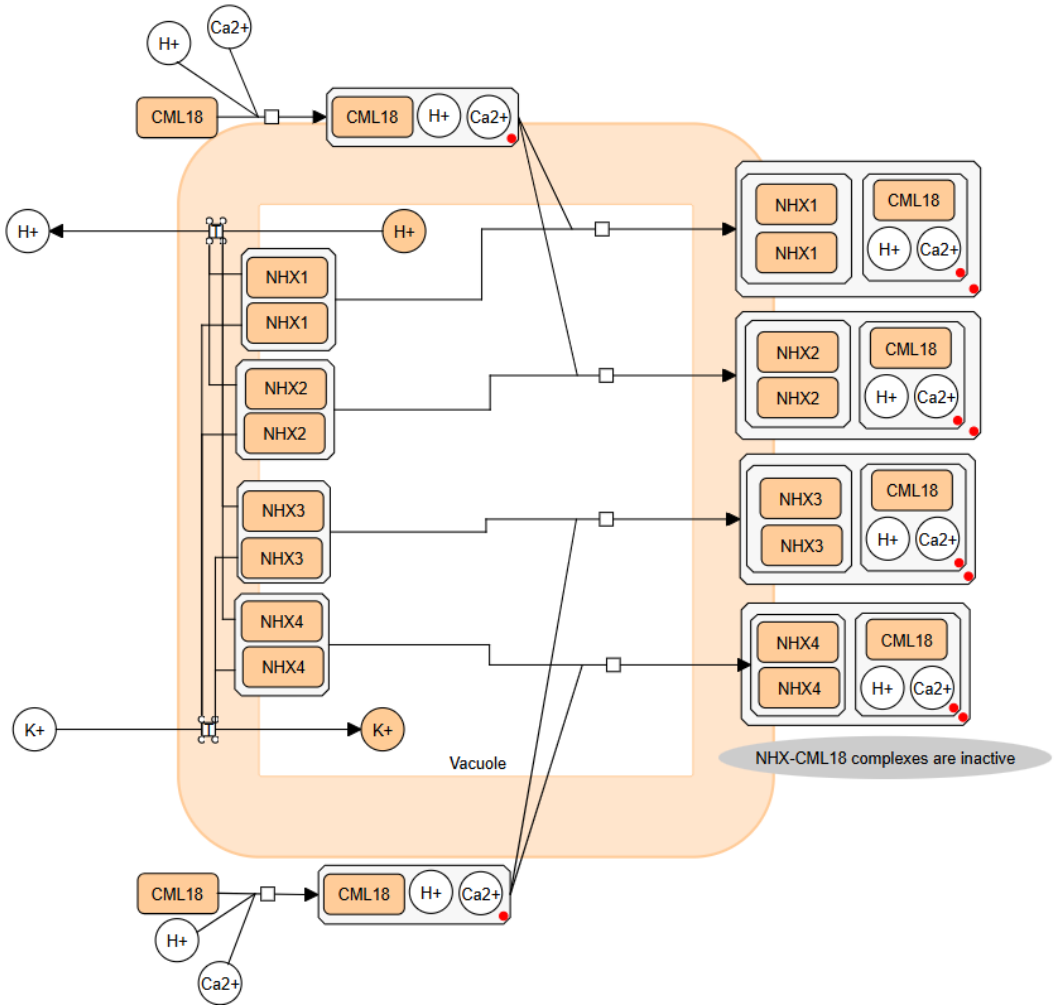
- La modélisation permet de visualiser le comportement temporel d'un système => compréhension
- La modélisation permet d'appréhender les paramètres/entités importants dans un **contexte donné** (un modèle est ancré)

ChloroKB ?

- Représenter la connaissance du réseau moléculaire d'*Arabidopsis thaliana* dans un objectif de modélisation (horizon)

Enjeux de représentation des connaissances en biologie

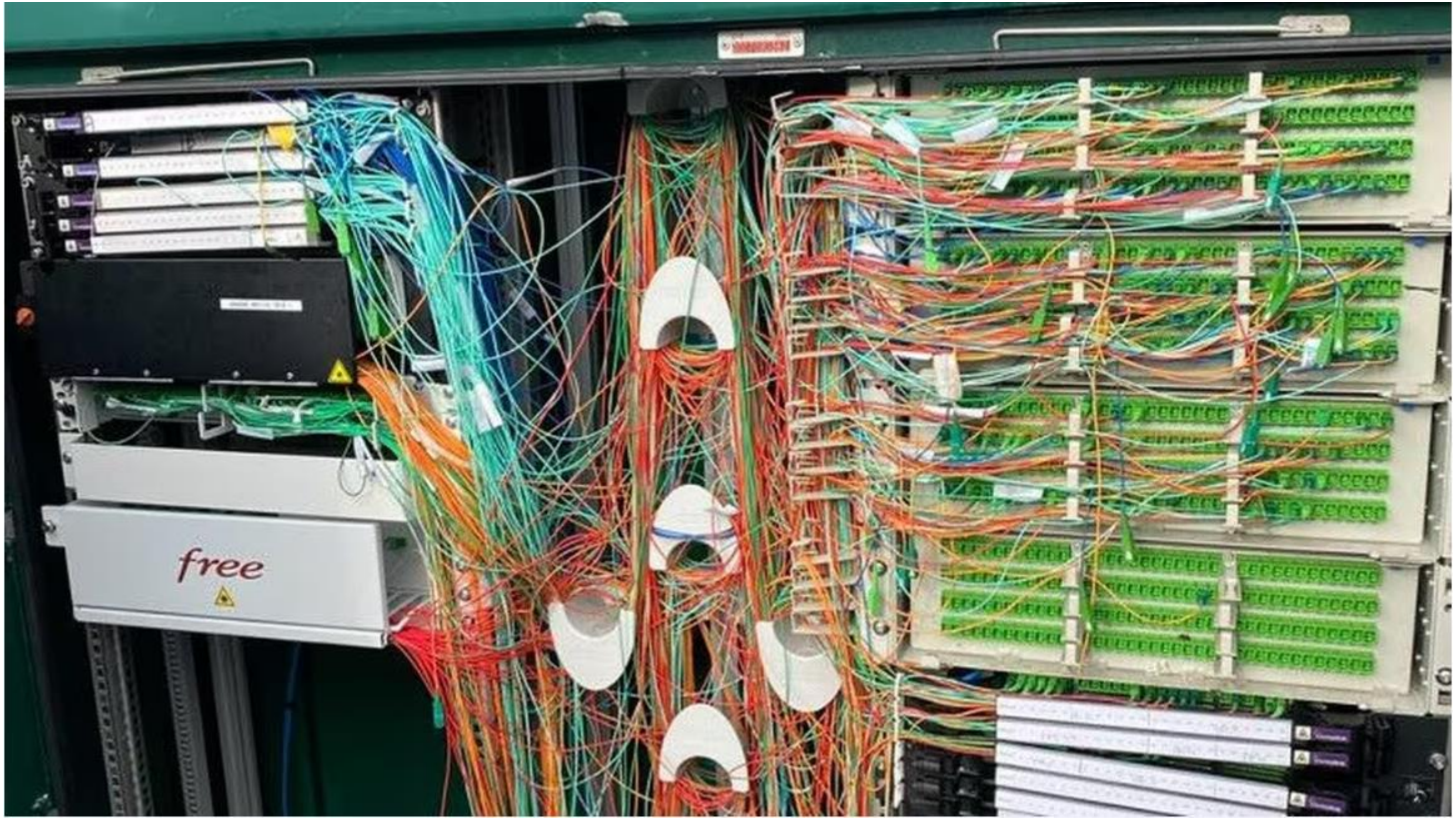
1. Lisible et compréhensible par un être humain (non-expert)



Enjeux de représentation des connaissances en biologie

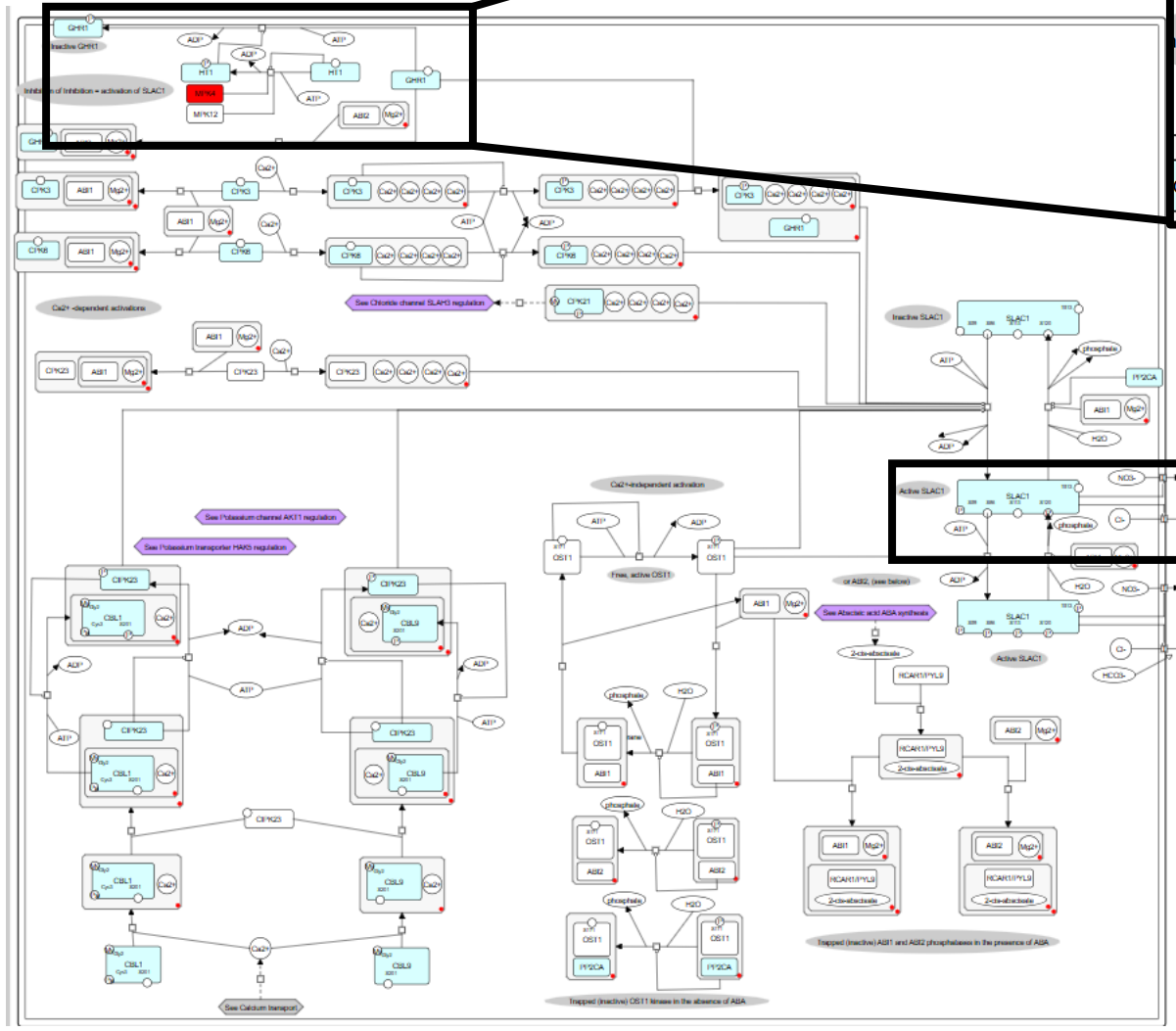
1. Lisible et compréhensible par un être humain

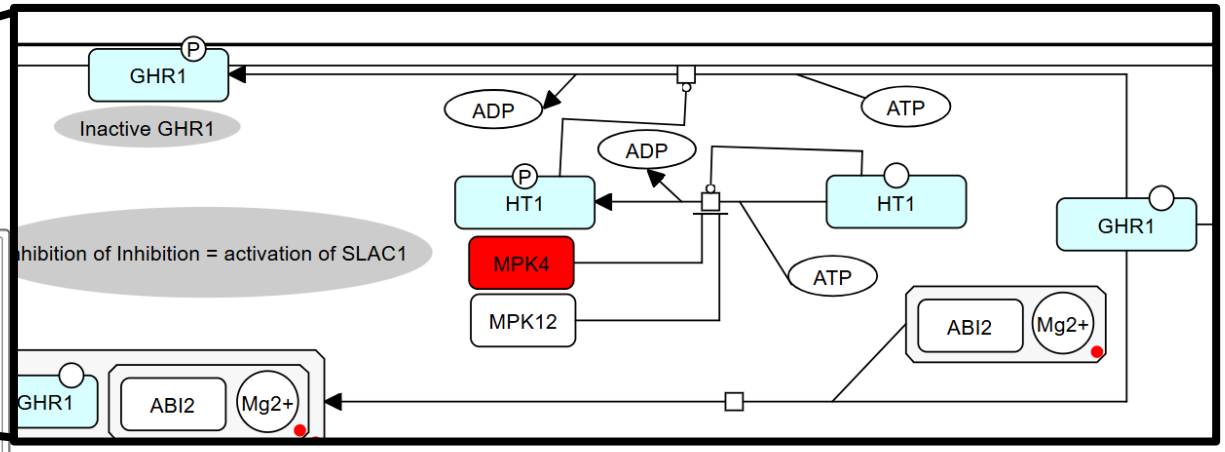
BIN2 also phosphorylates and destabilizes WRKY54 (Chen et al., 2017). In turn, BIN2 is dephosphorylated and inhibited by ABA INSENSITIVE 1 (ABI1, one of nine clade A PP2C members) and ABI2, while the phosphorylation of BIN2 is promoted by the inhibition of ABI1 and/or ABI2 via their interactions with ABA-bound ABA receptors when ABA accumulates under stress conditions (Wang et al., 2018a). BRI1-ASSOCIATED RECEPTOR KINASE1 (BAK1; also known as SOMATIC EMBRYOGENESIS RECEPTOR-LIKE KINASE 3, SERK3), a member of the SERK subfamily (which comprises the Leucine Rich Repeats Receptor-Like protein Kinases [LRR-RLKs] SERK1–SERK5), is a co-receptor of many different

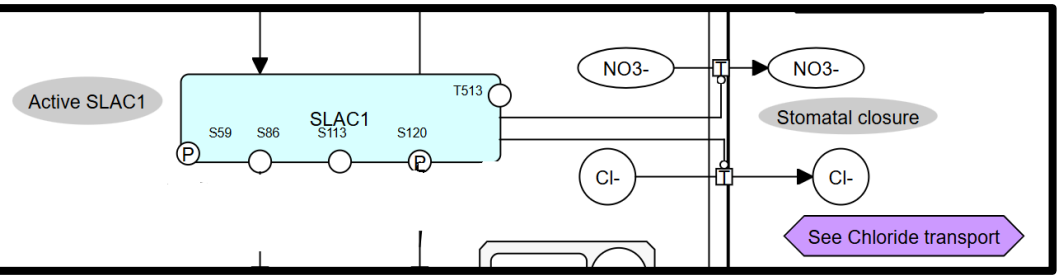

free

PLoS Biol. 2016 Dec 6;14(12):e2000322. doi: 10.1371/journal.pbio.2000322. eCollection 2016 Dec.

Natural Variation in Arabidopsis Cvi-0 Accession Reveals an Important Role of MPK12 in Guard Cell CO2 Signaling

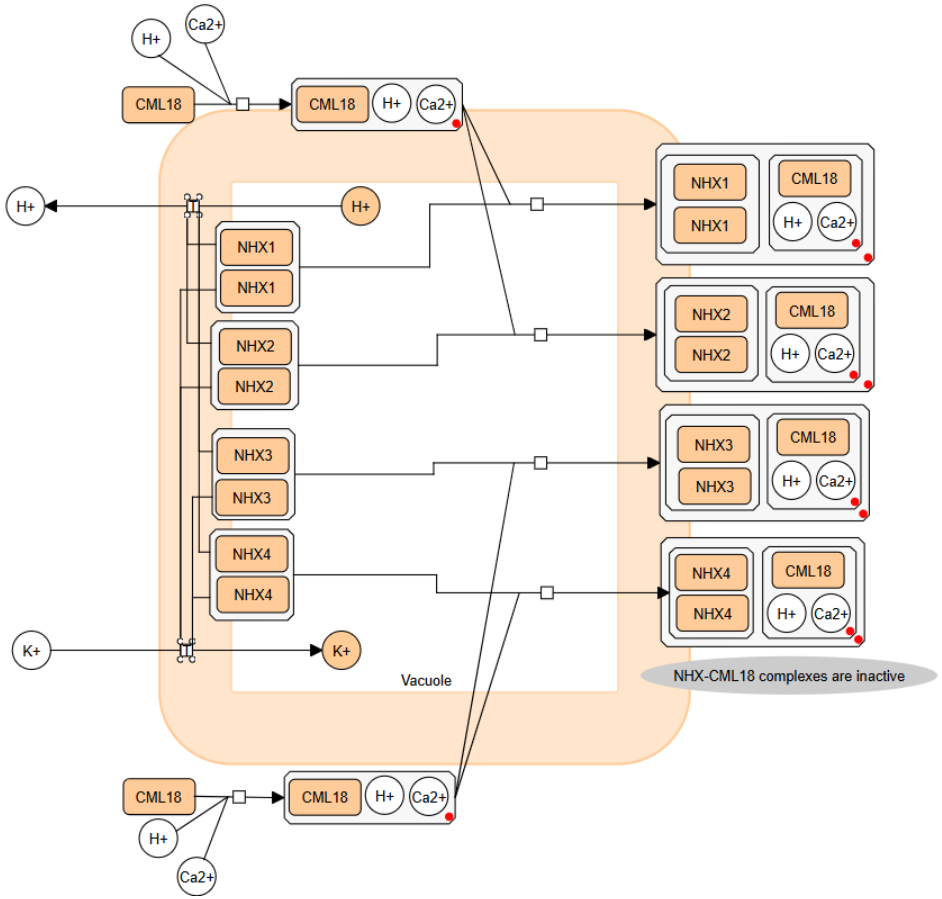


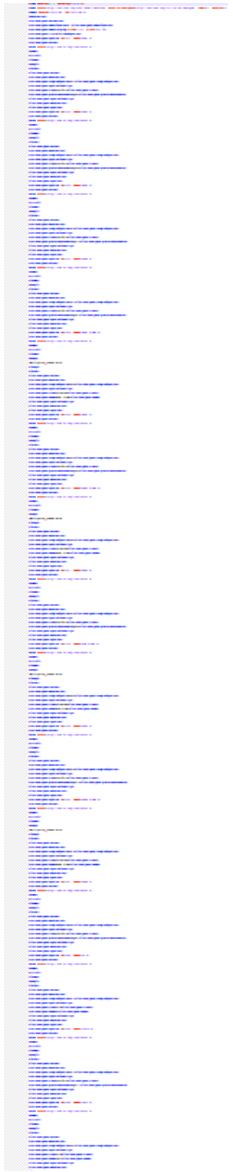




Enjeux de représentation des connaissances en biologie

2. Structuration (lisibles par une machine)





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Enjeux de représentation des connaissances en biologie

3-Rendre compte de la réalité biologique

Lumière

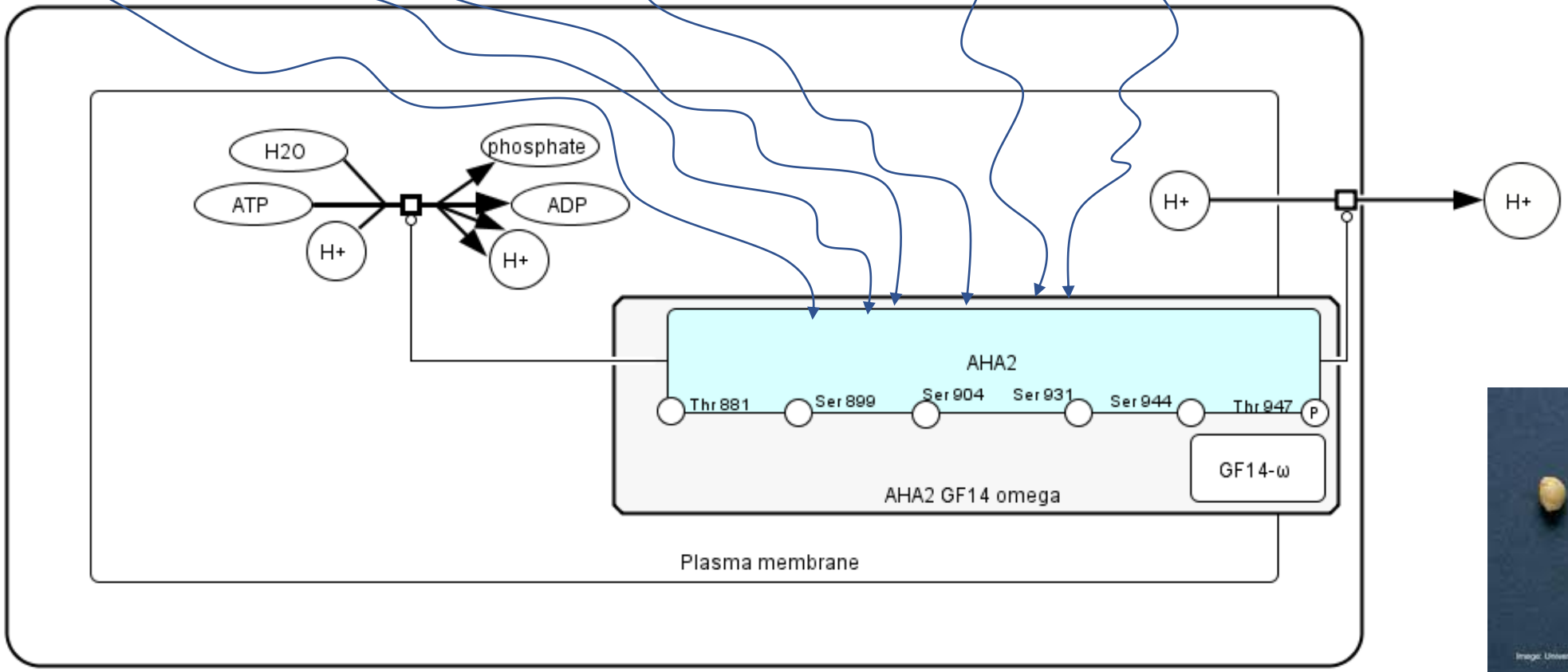
Energy charge

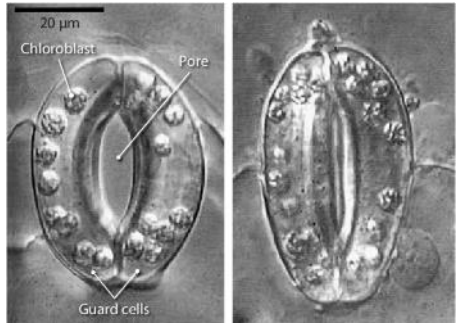
CO_2

Hormones

Abscissic acid
Auxins
Brassinosteroids

Pathogènes

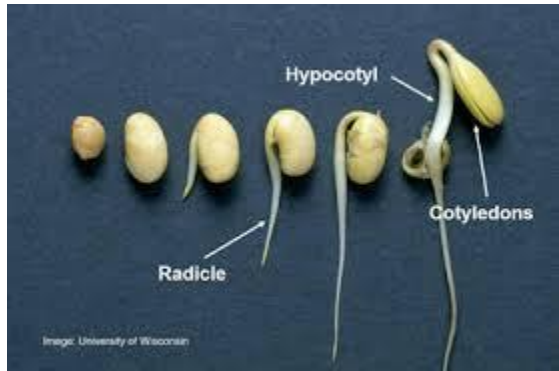




Ouverture/fermeture des stomates

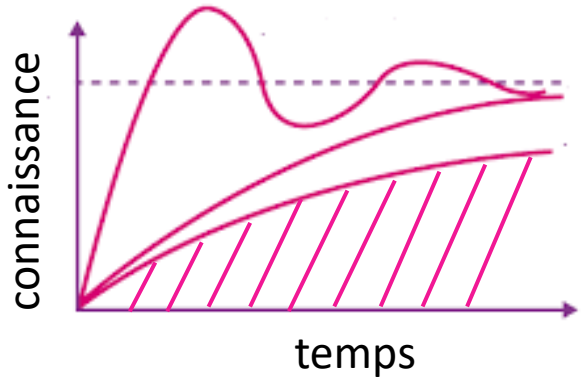
Contexte ?

Croissance



Enjeux de représentation des connaissances en biologie

4-Intégrer le degré de certitude-gérer les données conflictuelles



5-Intégrer les nouvelles informations/corriger

6-Généricité:

- permettre de répondre à de nombreuses questions
- Utilisation à différents fins (ex : modélisation sous contrainte, analyse de données omics…)
- Intégration d'autres types de données

ChloroKB en quelques slides –intérêts et limites

Arabidopsis thaliana

10 m

280 cartes

3 cm

Online since 2016

http://chlorokb.fr

ChloroKB **network metrics** in 2025

2270 proteins

400 proteins without gene ID

1480 complexes

1424 metabolites-ions

5500 pages

The Arabidopsis Chloroplast Knowledge Base

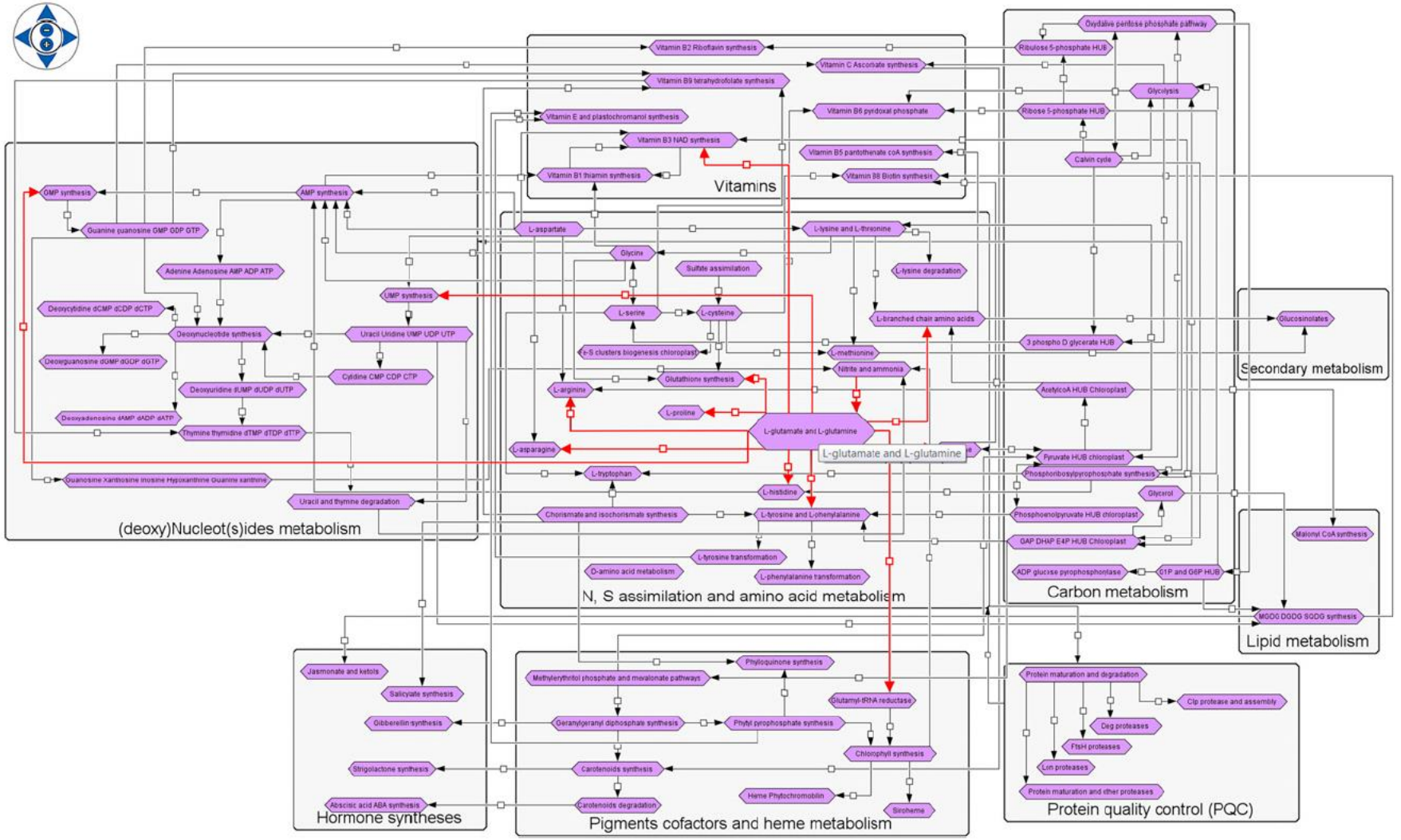
An exploration tool for chloroplast metabolism connected with other cell compartments

ChloroKB

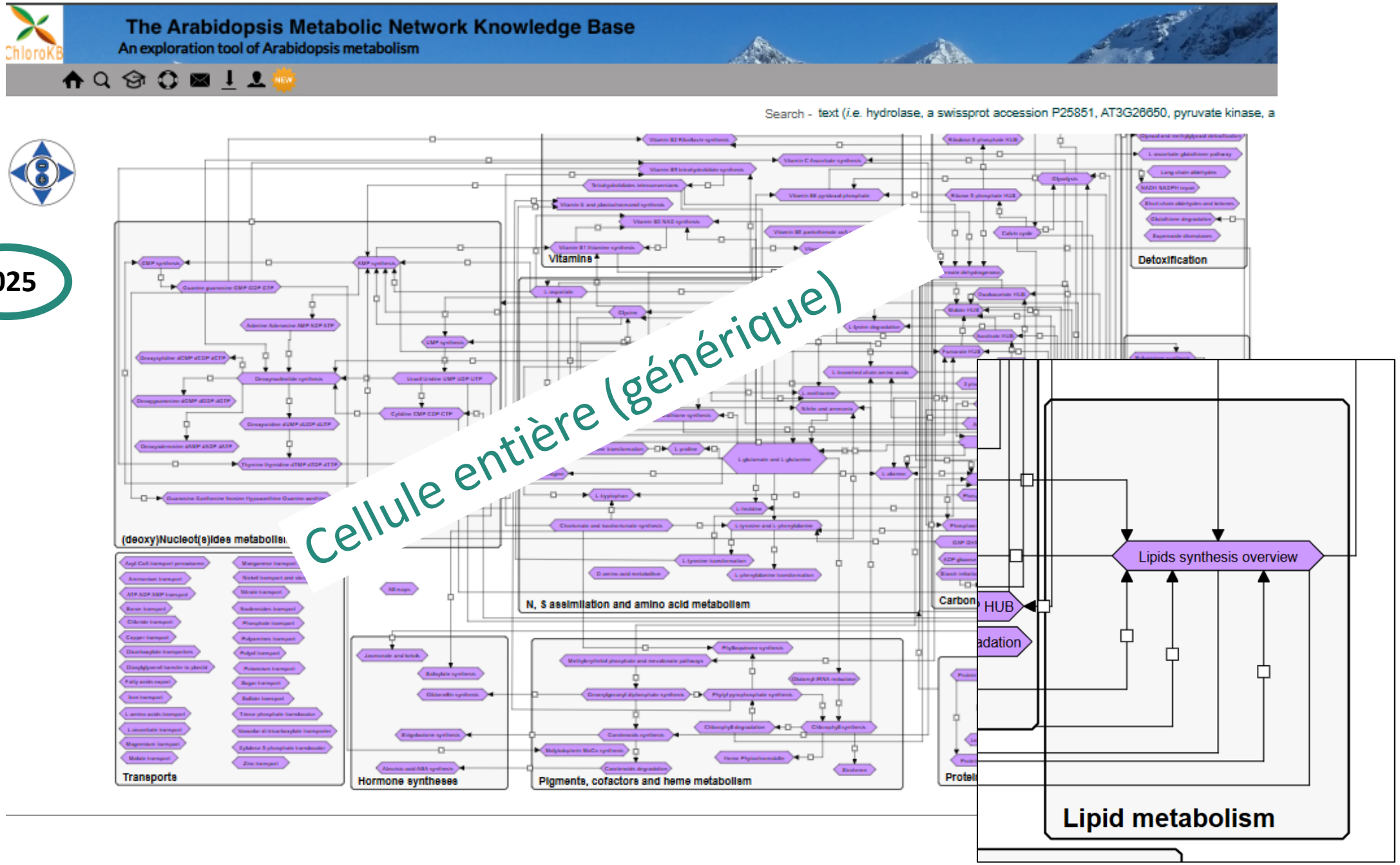
Show/Hide Legend

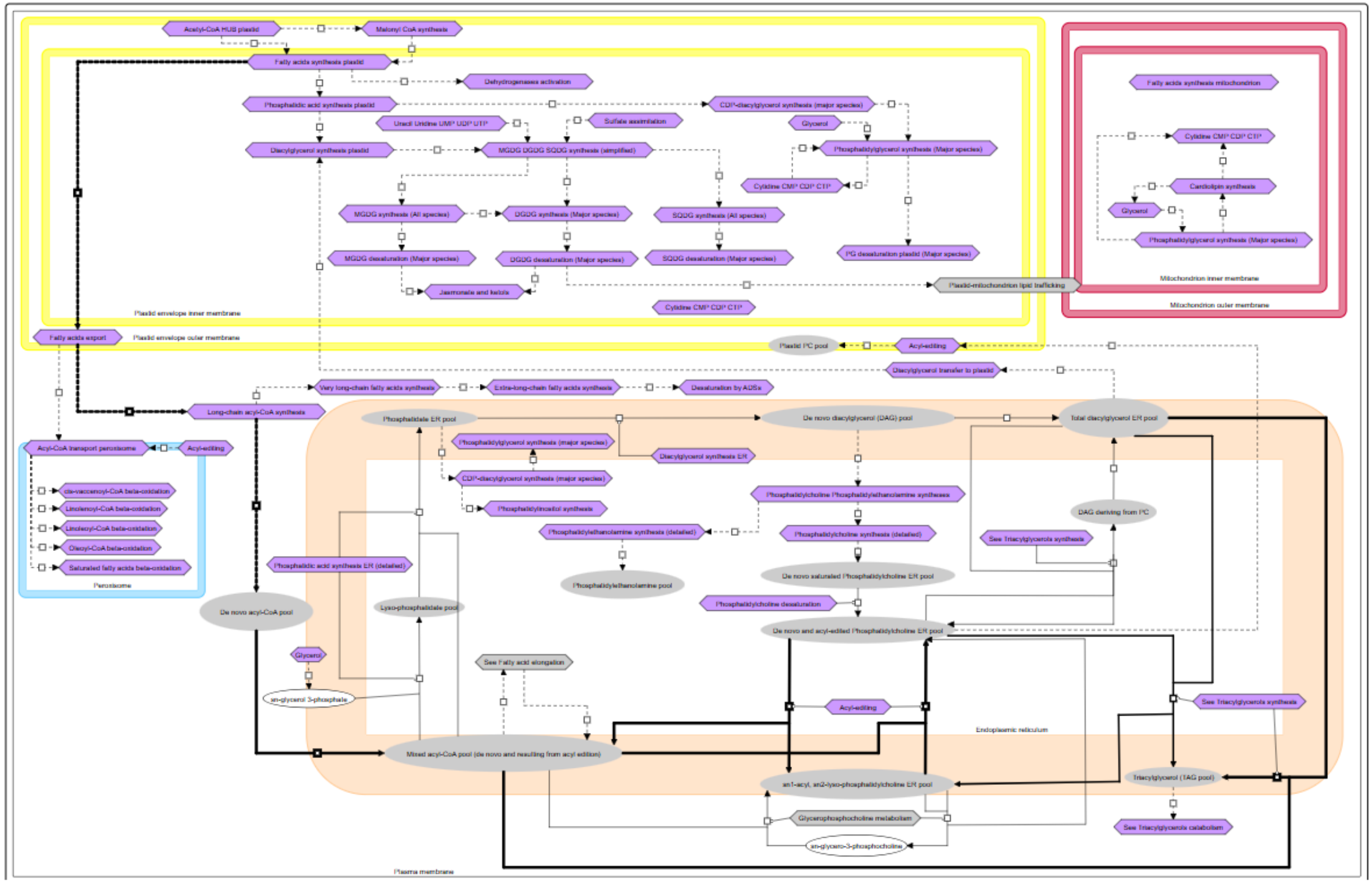
Search - text (*i.e.* hydrolase, a swissprot accession P25851, AT3G26650, pyruvate kinase, a first author name, a PubMed accession) Search

2017

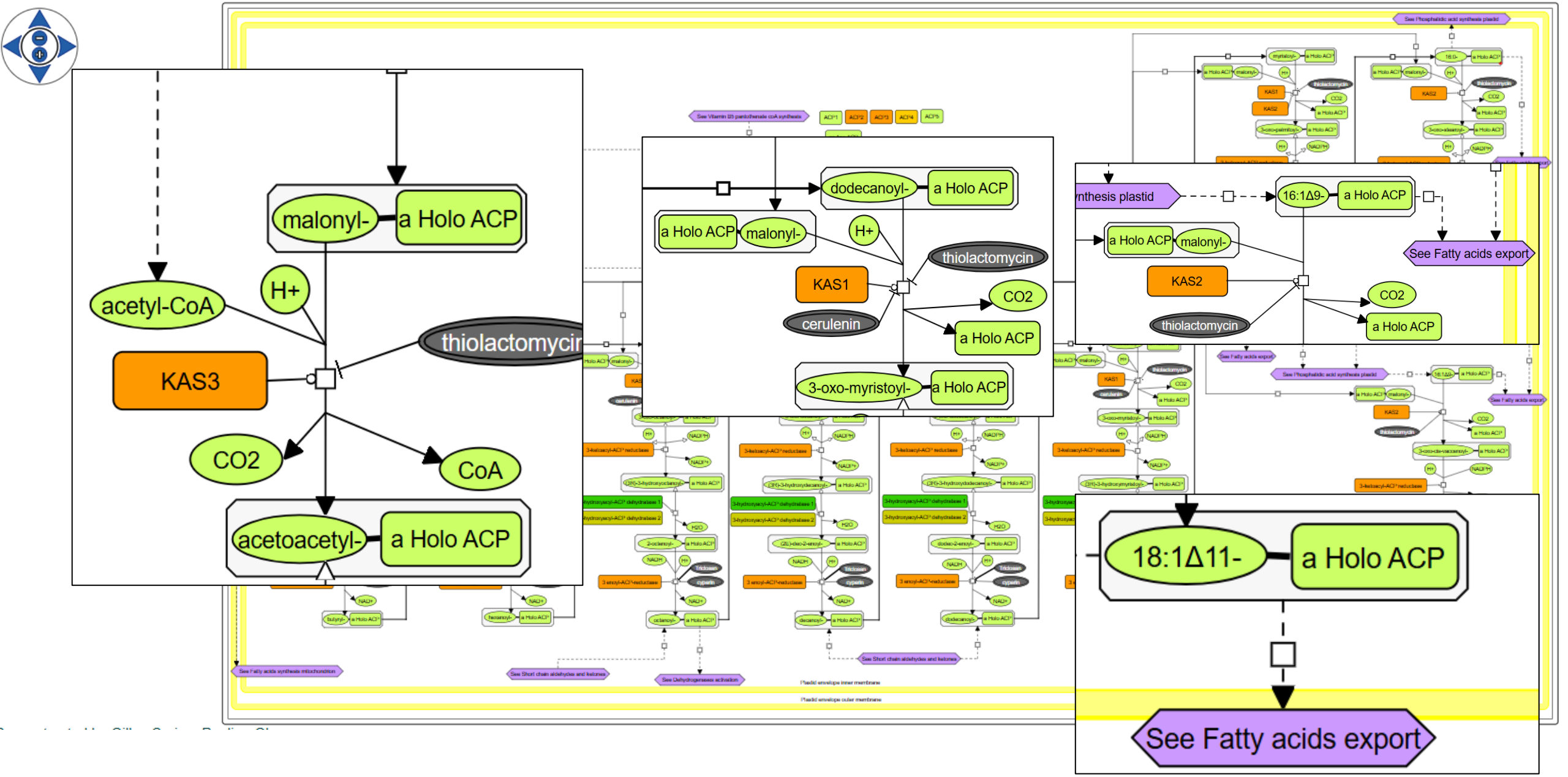


prabi
Pôle Rhône-Alpes de Bioinformatique

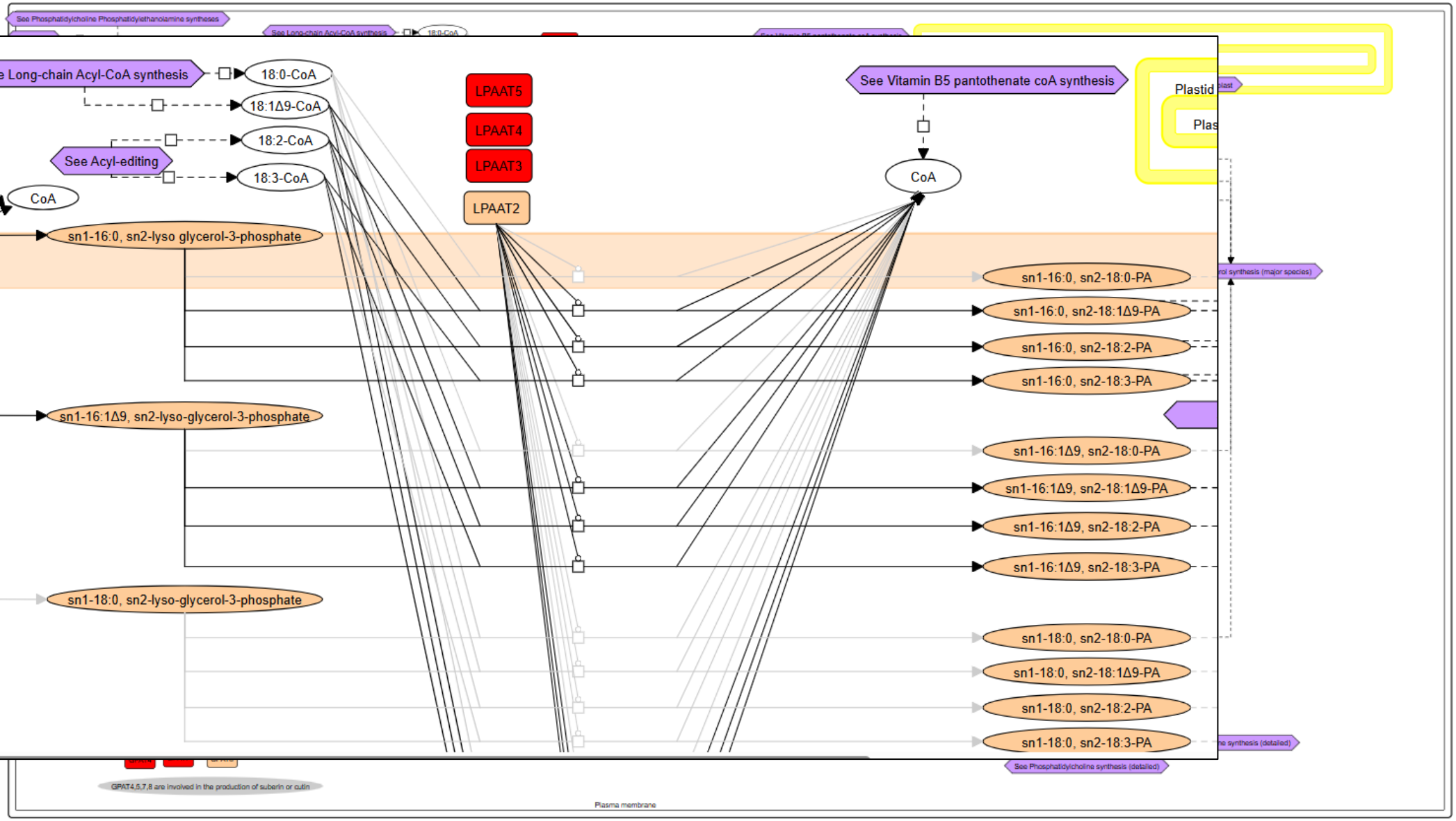

The Arabidopsis Metabolic Network Knowledge Base
An exploration tool of Arabidopsis metabolism
Search - text (i.e. hydrolase, a swissprot accession P25851, AT3G26650, pyruvate kinase, a
2025
Cellule entière (générique)
Vitamins
Detoxification
(deoxy)Nucleot(e)ides metabolism
N, S assimilation and amino acid metabolism
Carbon
Transports
Hormone syntheses
Pigments, cofactors and heme metabolism
Lipids synthesis overview
HUB
Lipid metabolism


Acetyl-CoA HUB plastid
Malonyl CoA synthesis
Fatty acids synthesis plastid
Dehydrogenases activation
Phosphatidic acid synthesis plastid
CDP-diacylglycerol synthesis (major species)
Uracil Uridine UMP UDP UTP
Sulfide assimilation
Glycerol
Diacylglycerol synthesis plastid
MGDG DGDG SQDG synthesis (simplified)
Phosphatidylglycerol synthesis (Major species)
Cytidine CMP CDP CTP
MGDG synthesis (All species)
DGDG synthesis (Major species)
SQDG synthesis (All species)
MGDG desaturation (Major species)
DGDG desaturation (Major species)
SQDG desaturation (Major species)
PG desaturation plastid (Major species)
Jasmonate and ketols
Plastid-mitochondrion lipid trafficking
Cytidine CMP CDP CTP
Plastid envelope inner membrane
Plastid envelope outer membrane
Fatty acids export
Plastid PC pool
Acyl-editing
Diacylglycerol transfer to plastid
Very long-chain fatty acids synthesis
Extra-long-chain fatty acids synthesis
Desaturation by ADSs
Long-chain acyl-CoA synthesis
Fatty acids synthesis mitochondrion
Cytidine CMP CDP CTP
Cardiolipin synthesis
Glycerol
Phosphatidylglycerol synthesis (Major species)
Mitochondrion inner membrane
Mitochondrion outer membrane
Acyl-CoA transport peroxisome
Acyl-editing
cis-vaccenoyl-CoA beta-oxidation
Linolenoyl-CoA beta-oxidation
Linoleoyl-CoA beta-oxidation
Oleoyl-CoA beta-oxidation
Saturated fatty acids beta-oxidation
Peroxisome
Phosphatidate ER pool
De novo diacylglycerol (DAG) pool
Total diacylglycerol ER pool
Phosphatidylglycerol synthesis (major species)
Diacylglycerol synthesis ER
CDP-diacylglycerol synthesis (major species)
Phosphatidylinositol synthesis
Phosphatidylcholine Phosphatidylethanolamine synthases
Phosphatidylethanolamine synthesis (detailed)
Phosphatidylcholine synthesis (detailed)
DAG deriving from PC
See Triacylglycerols synthesis
Phosphatidylethanolamine pool
De novo saturated Phosphatidylcholine ER pool
Phosphatidic acid synthesis ER (detailed)
Phosphatidylcholine desaturation
De novo acyl-CoA pool
Lyso-phosphatidate pool
De novo and acyl-edited Phosphatidylcholine ER pool
Glycerol
sn-glycerol 3-phosphate
See Fatty acid elongation
Acyl-editing
See Triacylglycerols synthesis
Endoplasmic reticulum
Mixed acyl-CoA pool (de novo and resulting from acyl edition)
sn1-acyl, sn2-lyso-phosphatidylcholine ER pool
Triacylglycerol (TAG pool)
Glycerophosphocholine metabolism
See Triacylglycerols catabolism
sn-glycero-3-phosphocholine
Plasma membrane

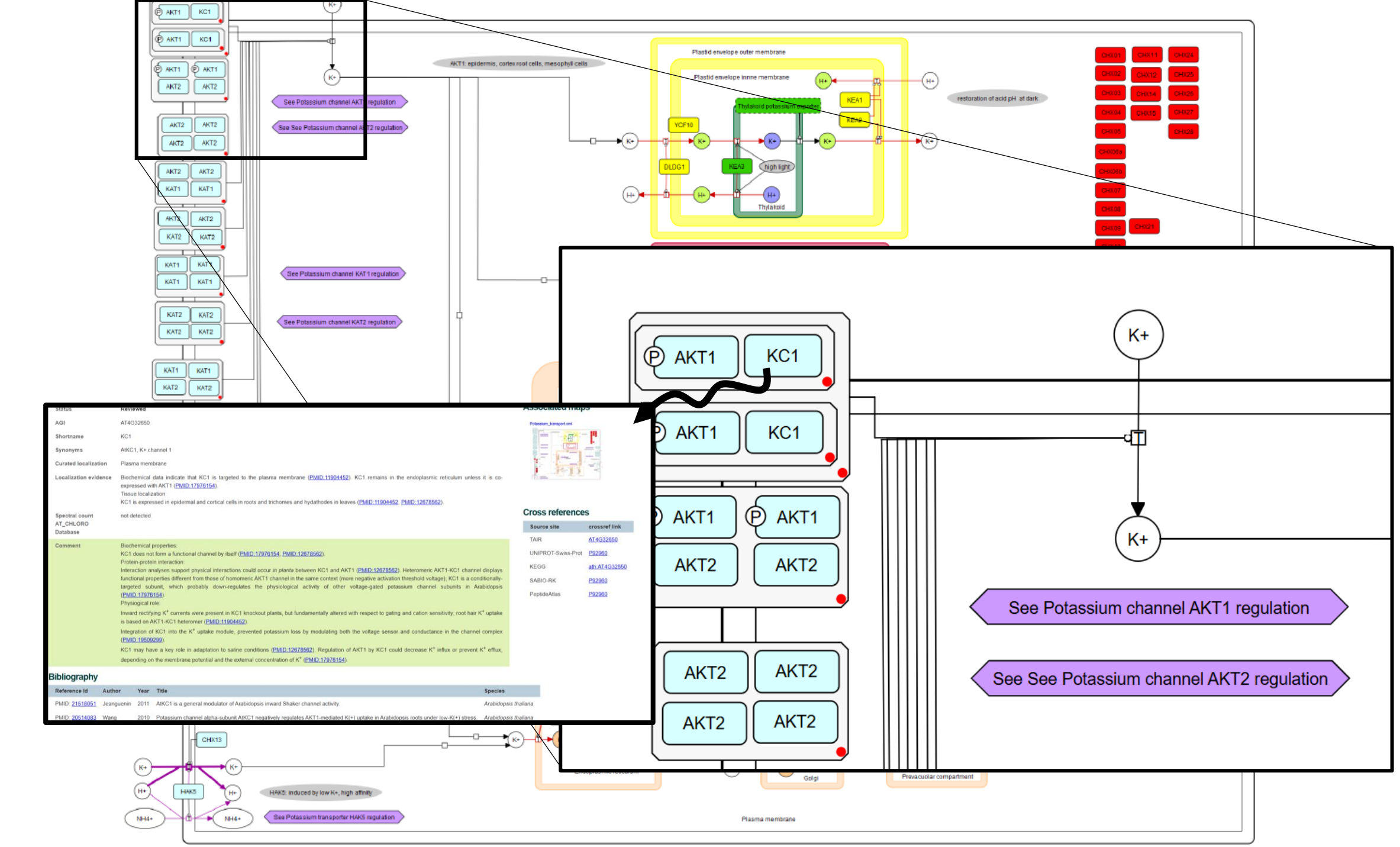
Fatty_acids_synthesis_plastid

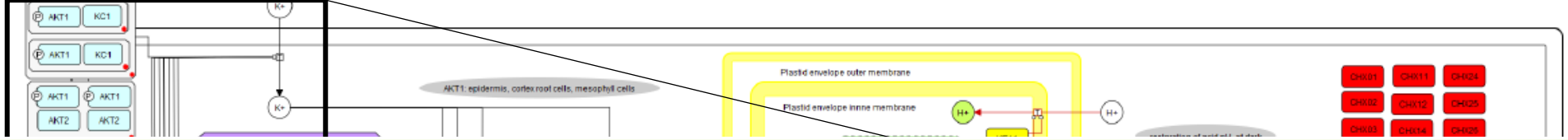


Phosphatidic_acid_synthesis_ER_(detailed)



Reconstructed by Gilles Curien


AKT1
KC1
AKT2
KAT1
KAT2
See Potassium channel AKT1 regulation
See See Potassium channel AKT2 regulation
See Potassium channel KAT1 regulation
See Potassium channel KAT2 regulation
AKT1: epidermis, cortex root cells, mesophyll cells
Plastid envelope outer membrane
Plastid envelope inner membrane
Thylakoid potassium transporter
KEA1
KEA2
YCF10
DLDG1
high light
Thylakoid
restoration of acid pH at dark
CHX01
CHX02
CHX03
CHX04
CHX05
CHX05a
CHX05b
CHX07
CHX08
CHX09
CHX11
CHX12
CHX14
CHX15
CHX21
CHX24
CHX25
CHX26
CHX27
CHX28
Status Reviewed
AGI AT4G32650
Shortname KC1
Synonyms AtKC1, K+ channel 1
Curated localization Plasma membrane
Localization evidence Biochemical data indicate that KC1 is targeted to the plasma membrane (PMID:11904452). KC1 remains in the endoplasmic reticulum unless it is co-expressed with AKT1 (PMID:17976154)
Tissue localization:
KC1 is expressed in epidermal and cortical cells in roots and trichomes and hydathodes in leaves (PMID:11904452, PMID:12678562)
Spectral count AT_CHLORO Database not detected
Comment
Biochemical properties:
KC1 does not form a functional channel by itself (PMID:17976154, PMID:12678562).
Protein-protein interaction:
Interaction analyses support physical interactions could occur in planta between KC1 and AKT1 (PMID:12678562). Heteromeric AKT1-KC1 channel displays functional properties different from those of homomeric AKT1 channel in the same context (more negative activation threshold voltage); KC1 is a conditionally-targeted subunit, which probably down-regulates the physiological activity of other voltage-gated potassium channel subunits in Arabidopsis (PMID:17976154).
Physiological role:
Inward rectifying K+ currents were present in KC1 knockout plants, but fundamentally altered with respect to gating and cation sensitivity; root hair K+ uptake is based on AKT1-KC1 heteromer (PMID:11904452).
Integration of KC1 into the K+ uptake module, prevented potassium loss by modulating both the voltage sensor and conductance in the channel complex (PMID:19509299).
KC1 may have a key role in adaptation to saline conditions (PMID:12678562). Regulation of AKT1 by KC1 could decrease K+ influx or prevent K+ efflux, depending on the membrane potential and the external concentration of K+ (PMID:17976154).
Associated maps
Potassium_transport.xml
Cross references
Source site crossref link
TAIR AT4G32650
UNIPROT-Swiss-Prot P92960
KEGG ath:AT4G32650
SABIO-RK P92960
PeptideAtlas P92960
Bibliography
Reference Id Author Year Title Species
PMID: 21518051 Jeanguenin 2011 AtKC1 is a general modulator of Arabidopsis inward Shaker channel activity. Arabidopsis thaliana
PMID: 20514083 Wang 2010 Potassium channel alpha-subunit AtKC1 negatively regulates AKT1-mediated K(+) uptake in Arabidopsis roots under low-K(+) stress Arabidopsis thaliana
CHX13
HAK5
HAK5: induced by low K+, high affinity
See Potassium transporter HAK5 regulation
NH4+
Golgi
Prevacuolar compartment
Plasma membrane
See Potassium channel AKT1 regulation
See See Potassium channel AKT2 regulation



Comment

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Interaction analyses support physical interactions could occur *in planta* between KC1 and AKT1 (PMID:12678562). Heteromeric AKT1-KC1 channel displays functional properties different from those of homomeric AKT1 channel in the same context (more negative activation threshold voltage); KC1 is a conditionally-targeted subunit, which probably down-regulates the physiological activity of other voltage-gated potassium channel subunits in Arabidopsis (PMID:17976154).

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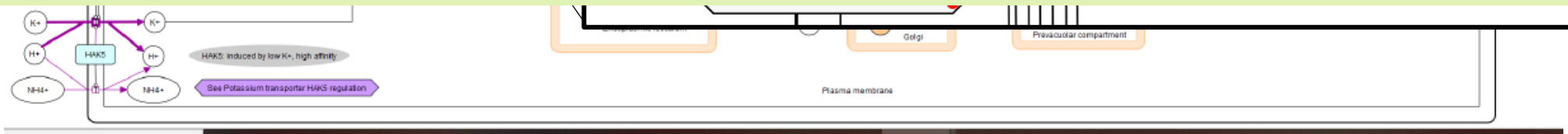
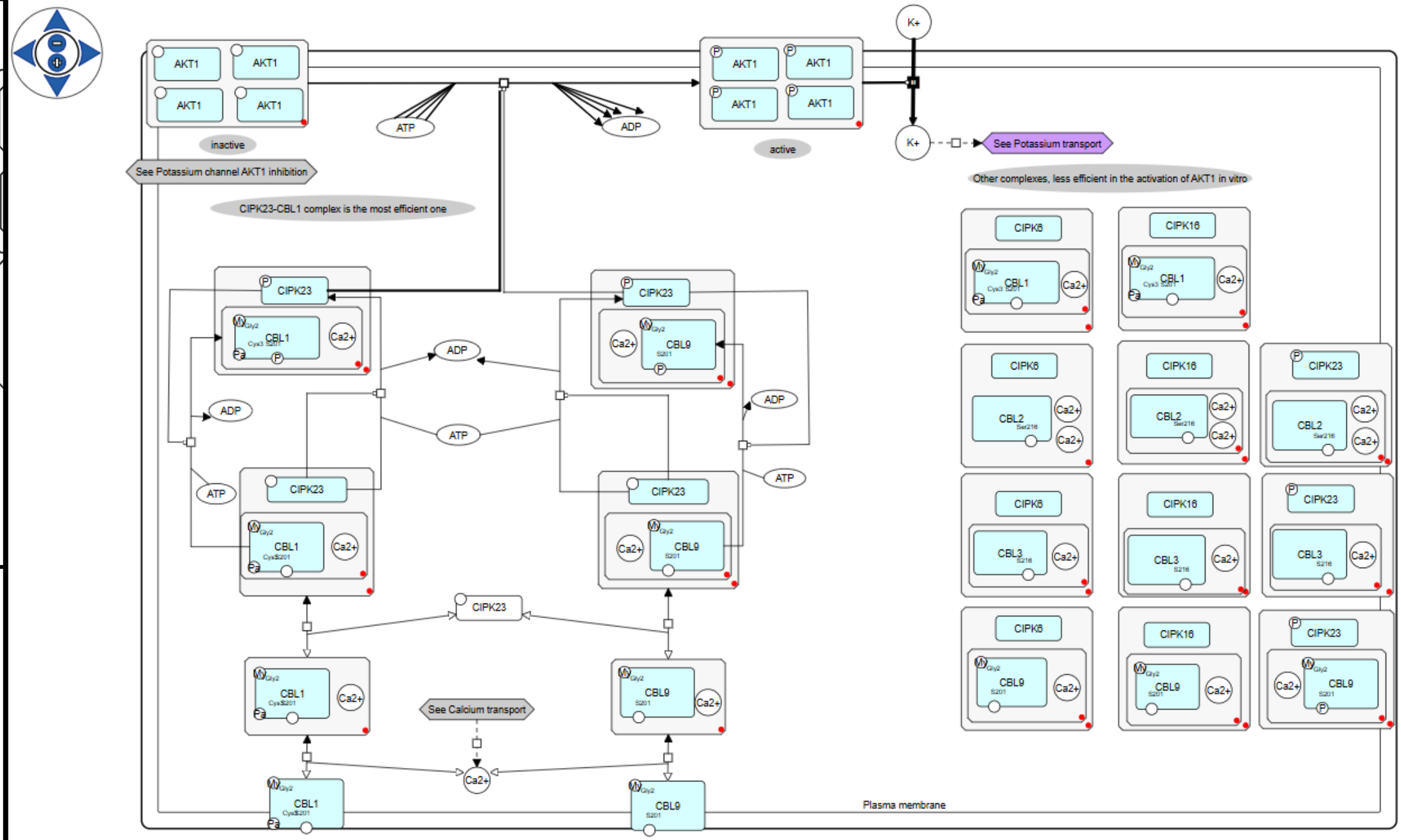
Integration of KC1 into the K^+ uptake module, prevented potassium loss by modulating both the voltage sensor and conductance in the channel complex (PMID:19509299).

KC1 may have a key role in adaptation to saline conditions (PMID:12678562). Regulation of AKT1 by KC1 could decrease K^+ influx or prevent K^+ efflux, depending on the membrane potential and the external concentration of K^+ (PMID:17976154).



Potassium_channel_AKT1_regulation



Reconstructed by Gilles Curien

Phosphorylated active AK1 tetramer

Shortname	none
Curated localization	Plasma membrane
Localization evidence	
Spectral count AT_CHLORO Database	not detected
Comment	Regulation: CIPK23/CBL1 or CIPK23/CBL9 pairs activate AKT1 upon a signal elicited by K^+ starvation (PMID:16814720). CIPK23 kinase in complex with Ca^{2+}-CBL1 or Ca^{2+}-CBL9 phosphorylates and activates AKT1 (PMID:16814720, PMID:16895985). CIPK6 and CIPK16 in combination with CBL1, CBL2, CBL3 or CBL9 are also able to activate AKT1 channel though CIPK23/CBL1 couple is the most efficient one (PMID:17898163). AKT1 channel activity is negatively regulated by a complicated interplay between PP2C phosphatases (AIP1, AIP1H, AHG1) and CBLs as analysed in (PMID:21596690).

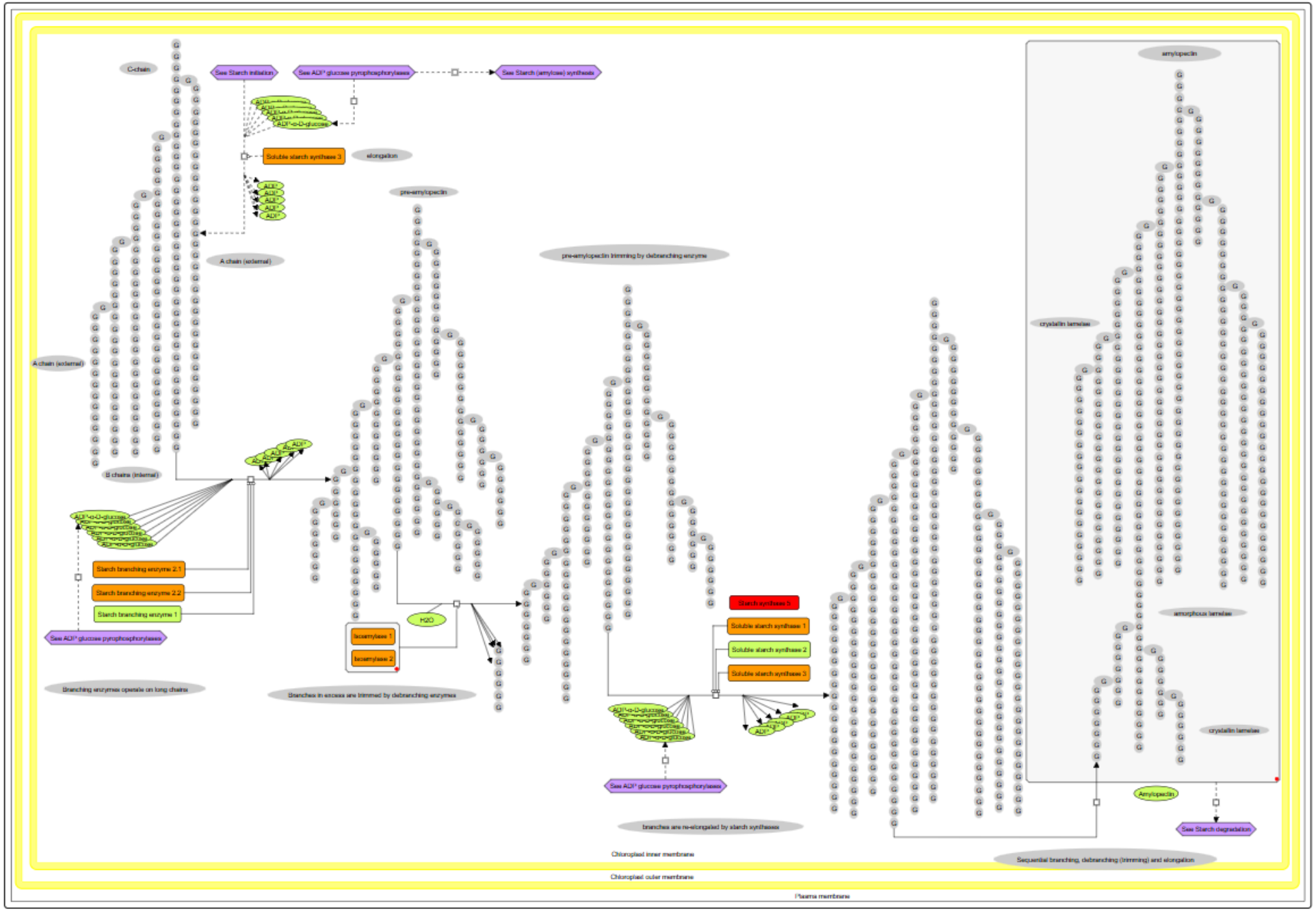
Reactions

Source	Reactions
TRANSPORT	"K+(extracellular)"-> "K+(cytosol)"

Bibliography

Reference Id	Author	Year	Title	Species
PMID: 21596690	Lan	2011	Mechanistic analysis of AKT1 regulation by the CBL-CIPK-PP2CA interactions.	*Arabidopsis thaliana*
PMID: 17898163	Lee	2007	A protein phosphorylation/dephosphorylation network regulates a plant potassium channel.	*Arabidopsis thaliana*
PMID: 16895985	Li	2006	A Ca(2)+ signaling pathway regulates a K(+) channel for low-K response in Arabidopsis.	*Arabidopsis thaliana*
PMID: 16814720	Xu	2006	A protein kinase, interacting with two calcineurin B-like proteins, regulates K+ transporter AKT1 in Arabidopsis.	*Arabidopsis thaliana*

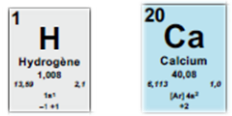
Starch_(amylopectin)_synthesis



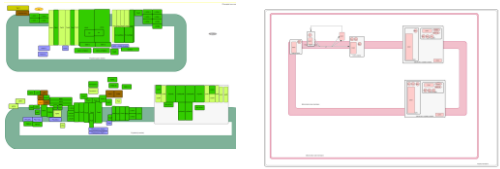
Reconstructed by Gilles Curien

Ce que ne contient pas (encore) ChloroKB:

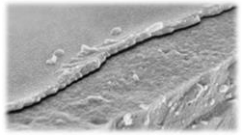
-transport et régulation du transport des Protons et du Calcium



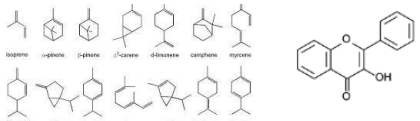
-chaines de transfert d'électrons (photosynthèse et respiration)



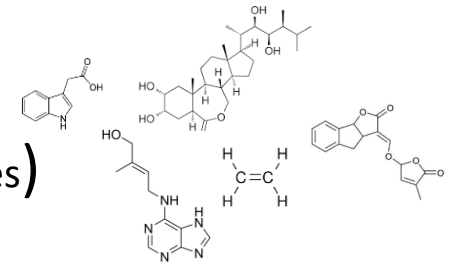
-métabolisme de la paroi



-métabolisme des terpènes & flavonoïdes



-métabolisme d'hormones (auxine, brassinosteroides, cytokinines, ethylène, strigolactones)



-synthèse et transport des protéines

-synthèse/dégradation d'ARN et d'ADN

-signalisation/contrôle de l'expression des gènes

Quelles utilisations de ChloroKB ?

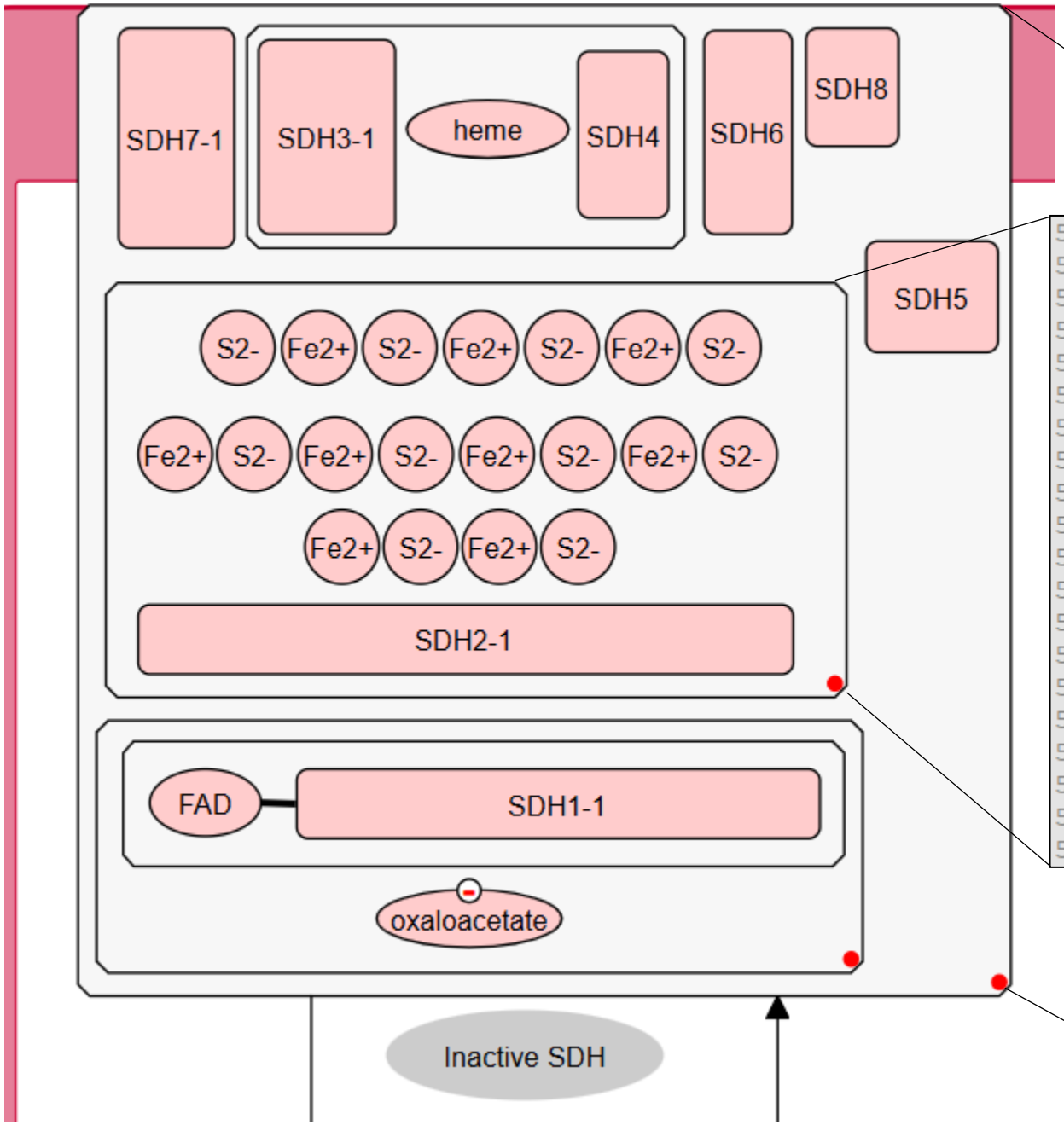
-Explorer-vérifier-compléter des modèles (gain de temps)

-communiquer avec des experts (améliorer les représentations)

-Extraire des données

-extraction automatique de matrice de stoichiométrie => modélisation sous contrainte

Molecule/Reaction	(R)-mevalonate 5-phosphate_transport_perox(direction 1)	(R)-mevalonate 5-phosphate_transport_perox(direction 2)	1.1.1.34-RXN(3-hydroxy-3-methylglutaryl-coenzyme A reductase 2)	1.1.1.34-RXN(3-hydroxy-3-methylglutaryl-coenzyme A reductase 1)	
(R)-mevalonate 5-phosphate(cytosol)	-1	1	0	0	
(R)-mevalonate 5-phosphate(peroxisome)	1	-1	0	0	
(S)-3-hydroxy-3-methylglutaryl-CoA(cytosol)	0	0	-1	-1	
(R)-mevalonate(cytosol)	0	0	1	1	
NADPH(cytosol)	0	0	-2	-2	
H+(cytosol)	0	0	-2	-2	
NADP+(cytosol)	0	0	2	2	

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-Composition de complexes protéines-protéines
Ou protéines-métabolites
- identifiants uniques
-stoichiométrie des composants

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Possibilités d'exports

Map_ID Gene_ID Name(s) Etc….

global_matrix.xml ChloroKBexport.json


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Projets

Améliorer la compréhension des réseaux d'Arabidopsis en spécialisant ChloroKB

32 Stades développementaux

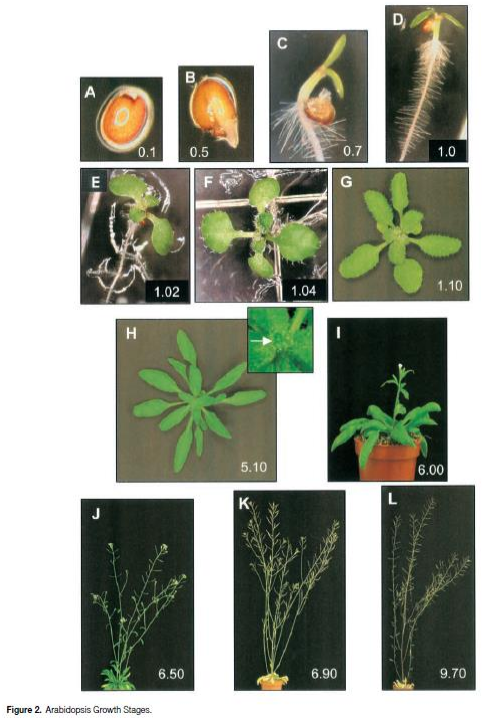
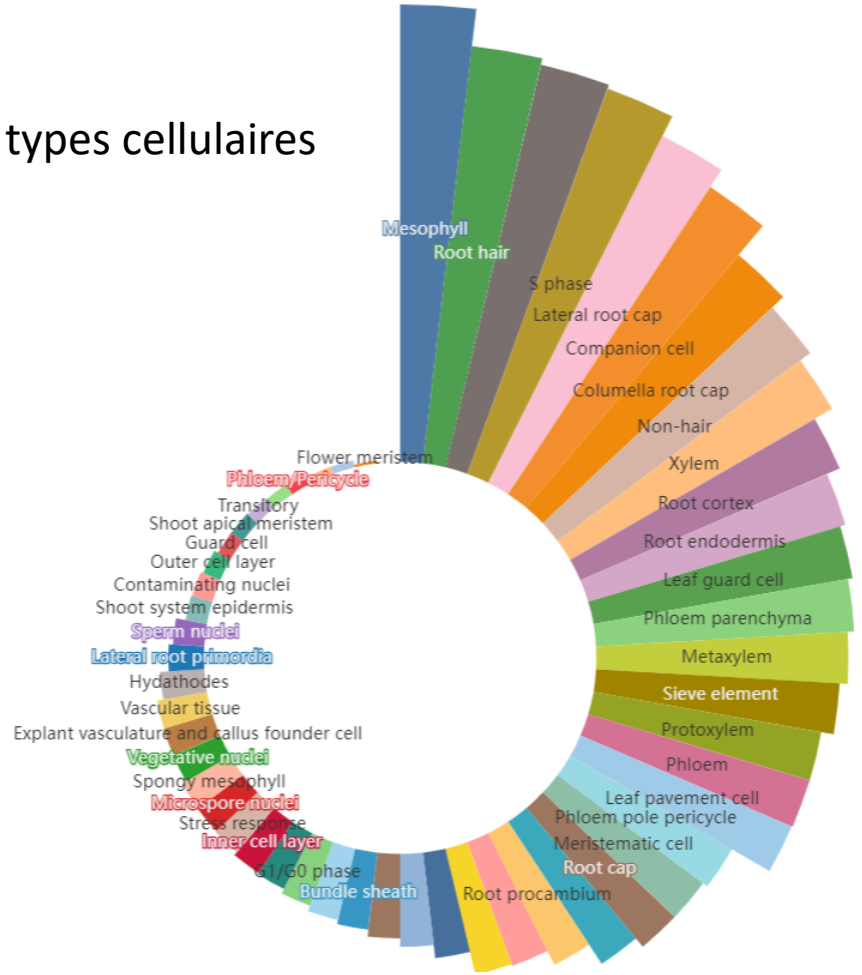


Figure 2. Arabidopsis Growth Stages.

Boyes_2001_PMID_11449047

Associer représentation de réseau
et
Single cell transcriptomics ?

53 types cellulaires



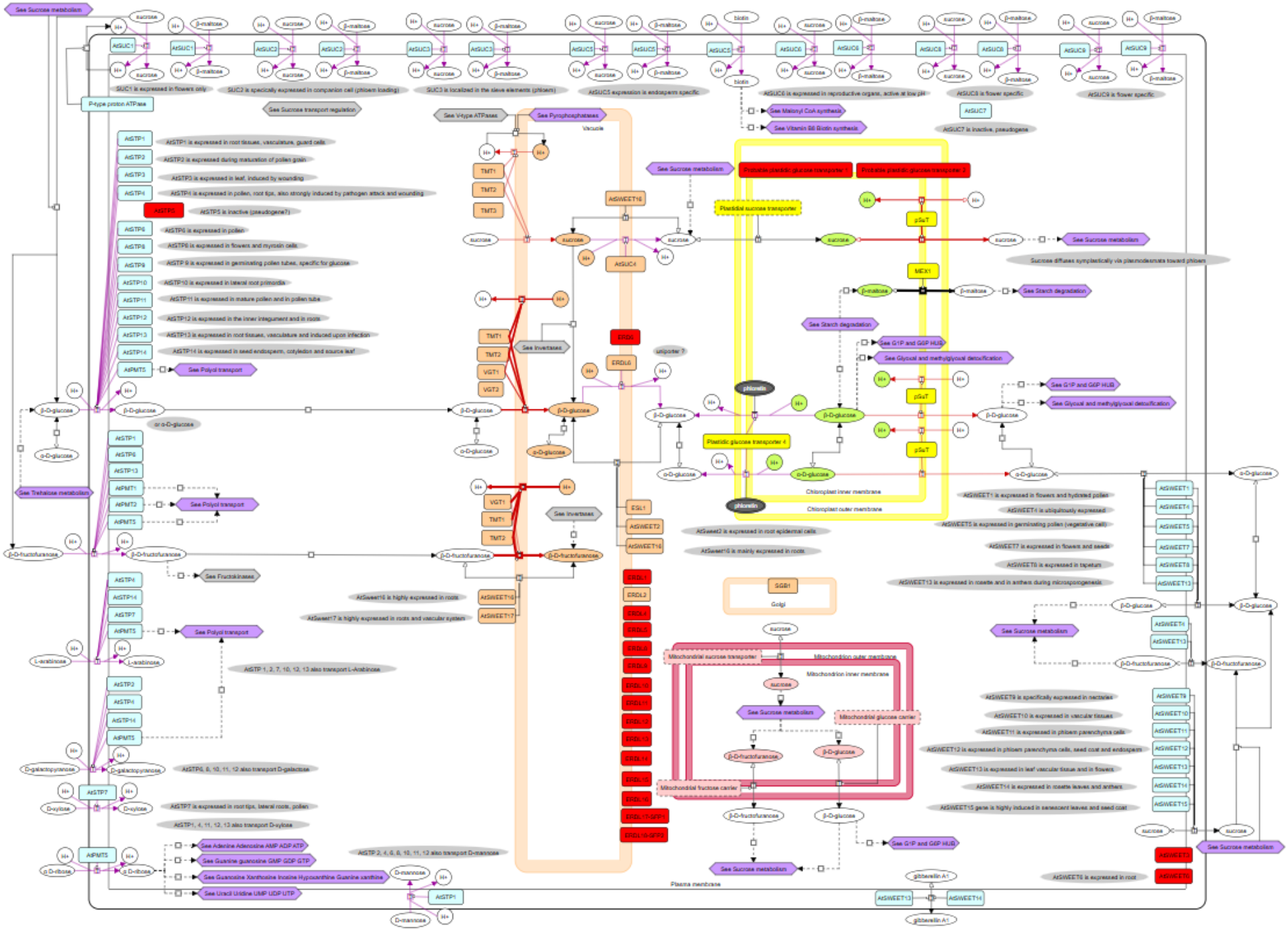
https://biobigdata.nju.edu.cn/scplantdb/marker?species=arabidopsis_thaliana

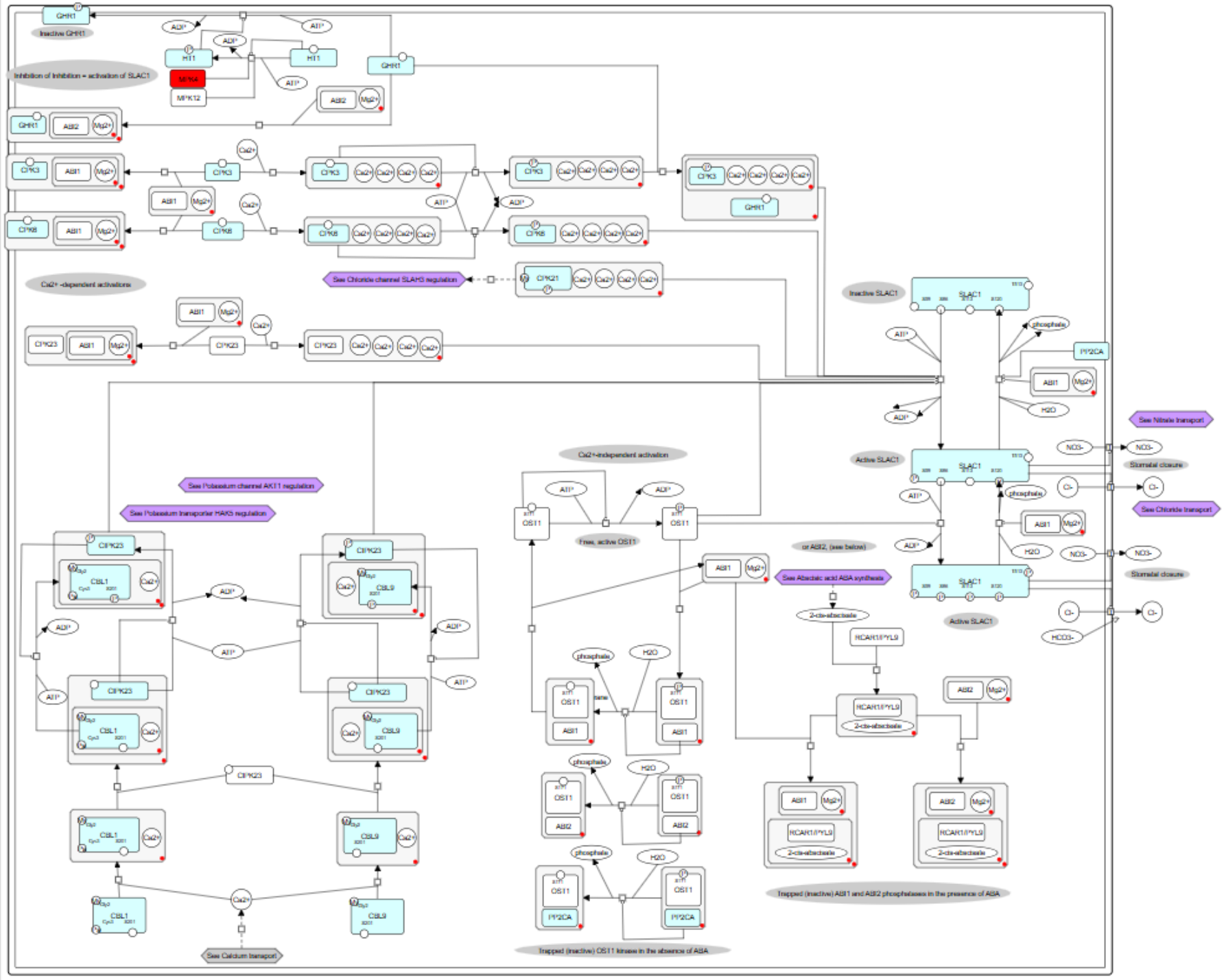
He_2024_PMID_37638765 : Sc PlantDB

Sugar_transport

Cellule générique

Déconvolution pour chaque type cellulaire

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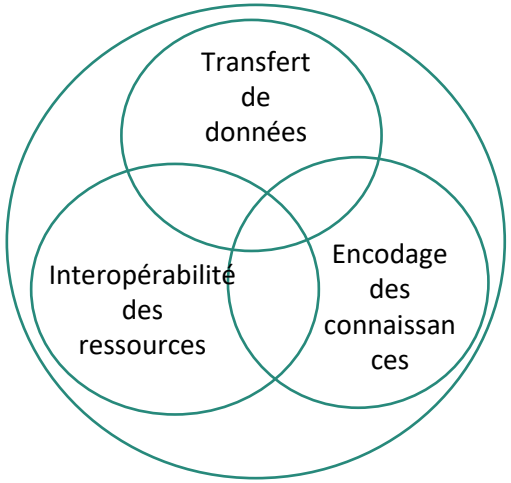
Inactive GHR1
ADP
ATP
HT1
MPK4
MPK12
Inhibition of Inhibition = activation of SLAC1
ABI2
Mg2+
CIPK3
ABI1
Ca2+
CIPK8
CIPK21
See Chloride channel SLAH3 regulation
Ca2+ -dependent activations
CIPK23
See Potassium channel AKT1 regulation
See Potassium transporter HAK5 regulation
CBL1
CBL9
See Calcium transport
Ca2+-independent activation
OST1
Free, active OST1
or ABI2, (see below)
See Abscisic acid ABA synthesis
2-cis-xanthoxalin
HCAR1/PYL9
Trapped (inactive) OST1 kinase in the absence of ABA
PP2CA
Trapped (inactive) ABI1 and ABI2 phosphatases in the presence of ABA
Inactive SLAC1
SLAC1
phosphate
H2O
See Nitrate transport
NO3-
Stomatal closure
Active SLAC1
Cl-
See Chloride transport
HCO3-

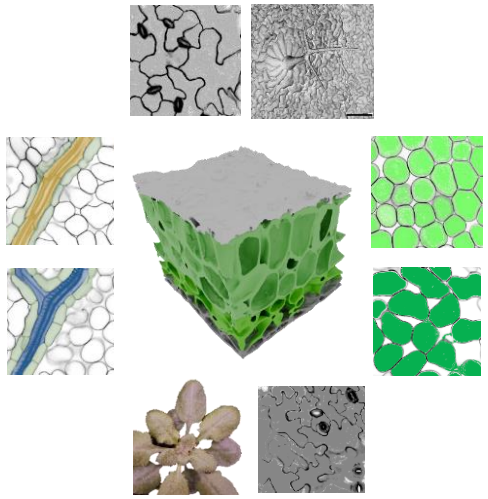
Projets

Sauvetage du site web

Consortium KOMOD (DIGIT-BIO)



http://chlorokb.fr



The Arabidopsis leaf quantitative atlas: a cellular and subcellular mapping through unified data integration

Quantitative Plant Biology

Merci pour votre attention

Light Photosynthesis & Metabolism

Laboratoire de Physiologie Cellulaire & Végétale
CEA-University Grenoble Alpes-INRAE-CNRS

Gilles Curien

NETBIO, Orléans, 24-25 novembre 2025

Le quantitatif fait la différence

-Changes in gene promoter strength
-DNA accessibility (epigenetics)
-mRNA stability
-post-translational modifications

$$v = \frac{k_{cat}[E]\cdot[S]}{\left(1+\frac{[I]}{K_i}\right)K_M + [S]}$$

Punctual mutations

Regulatory properties

Protein	K_m (*P*-pyruvate) − Glc6*P*	K_m (*P*-pyruvate) + Glc6*P*	$I_{0.5}$ (L-malate)	V_{max}
	µM			U/mg protein
FT966	652	362	1200	29
FP966	61	21	80	27

Le quantitatif fait la différence

Maximal activity

$$v = \frac{k_{cat} \cdot [E][S]}{K_M + [S]}$$




$$V = \frac{k_{cat} \cdot [E] \cdot [S]}{K_M + [S]}$$

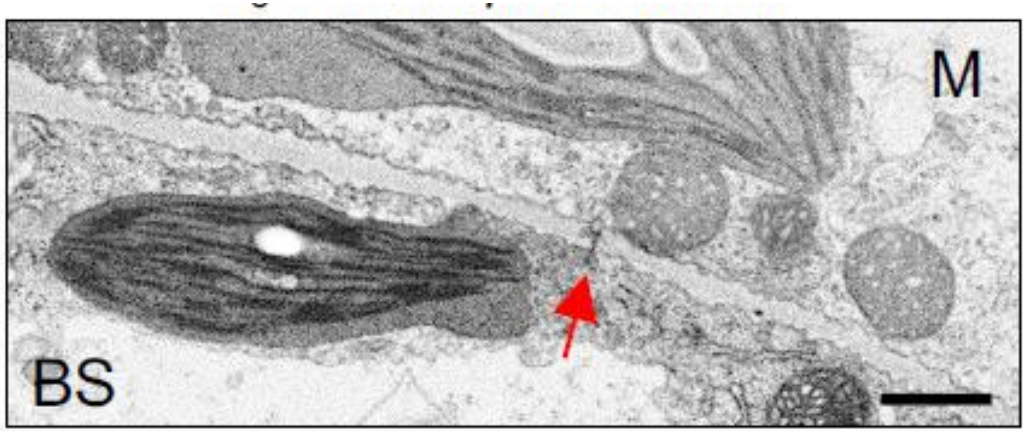
Table 1
C4 photosynthesis in the genus *Flaveria*: a stepwise evolution of a quantitative trait [32]

Parameter	*F. pringlei*	*F. linearis*	*F. pubescens*	*F. brownii*	*F. trinervia*
Kranz leaf anatomy	No	Poorly developed		Well developed	
CO_2 compensation point [µbar]	62	27	21	6	3
PEPC activity [µmol/mg Chl•h]	24	123	207	460	900
C4 cycle	-	+	++	+++	++++
Photosynthesis type	C3	C3-C4	C3-C4	C4-like	C4

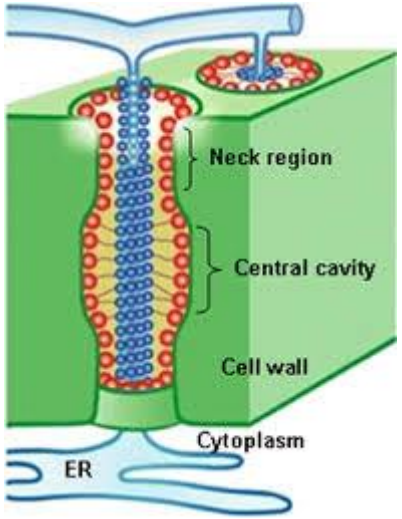
C4 Photosynthesis

Svensson_2003_PMID_12781769(PEPC)

Le quantitatif fait la différence



Plasmodesmata



Plasmodesmata density

C4 plants

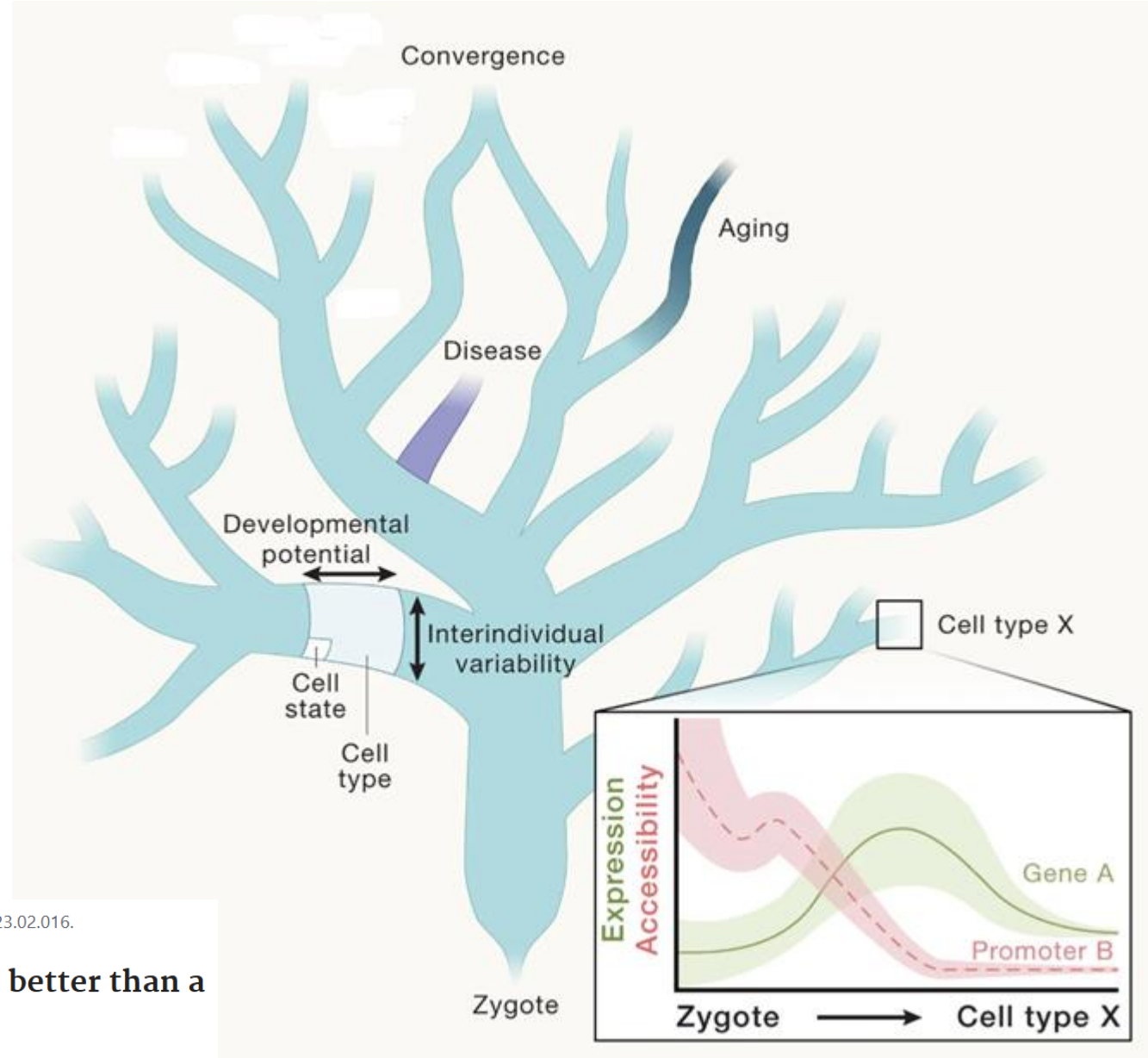
Setaria viridis, **9.3 /µm²**

maize, **7.5 /µm²**

C3 plants

Rice **1.0 / µm²**

Wheat **2.6 /mm²**



Review > Cell. 2023 Mar 16;186(6):1103-1114. doi: 10.1016/j.cell.2023.02.016.

A reference cell tree will serve science better than a reference cell atlas

Silvia Domcke [1], Jay Shendure [2]

Affiliations + expand

PMID: 36931241 DOI: 10.1016/j.cell.2023.02.016

PMID: 36931241

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Metabolites

ID_Map | ID_in ChloroKB | Name (s) | Localisation(s) | Record_ID (one per localization)

global_matrix.xml | ChloroKBexport.json | ChloroKBmolecularspeciesexport.json | ChloroKBreactionsexport.json


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Reactions

global_matrix.xml | ChloroKBexport.json | ChloroKBmolecularspeciesexport.json | ChloroKBreactionsexport.json


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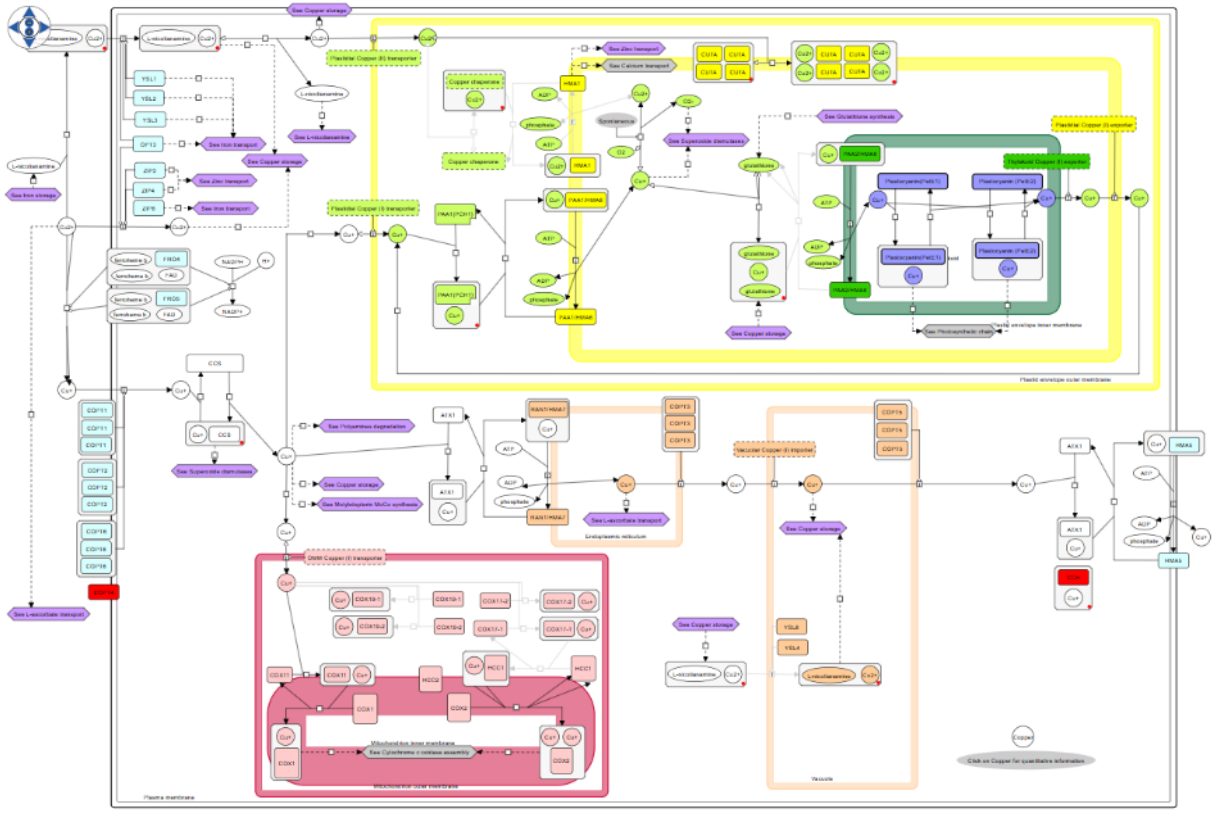
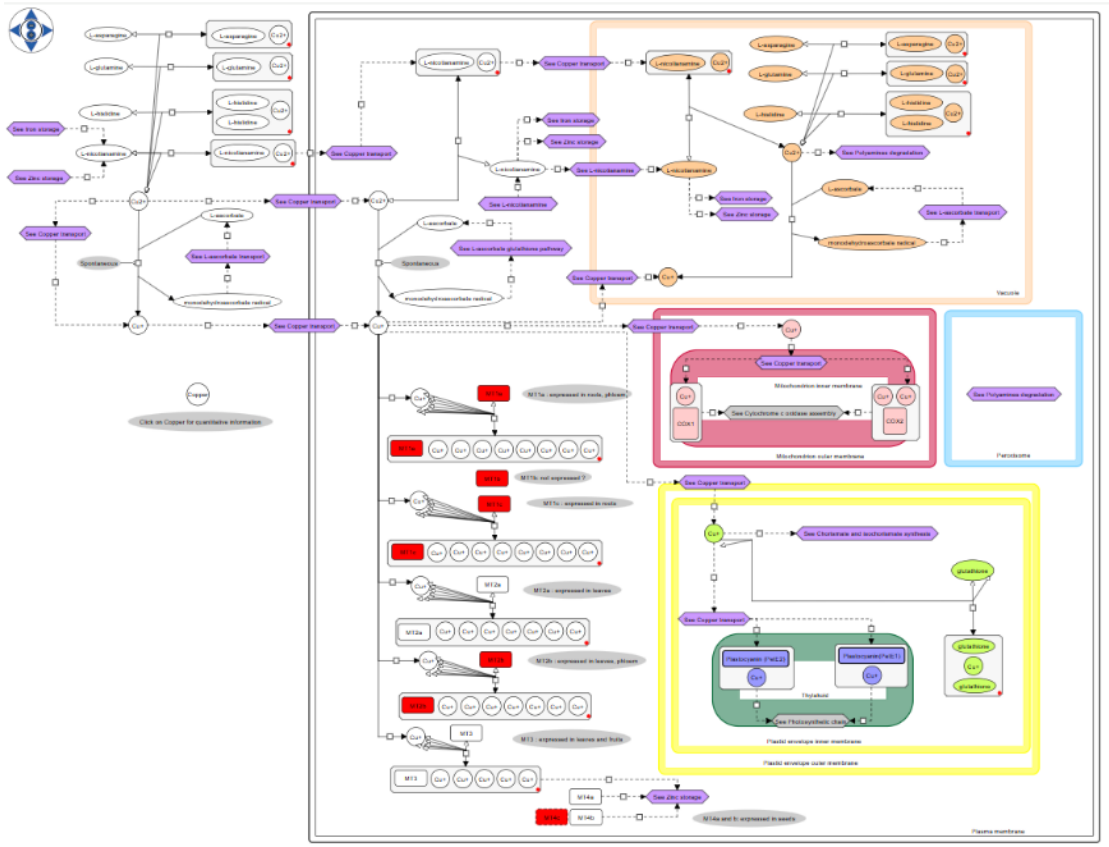
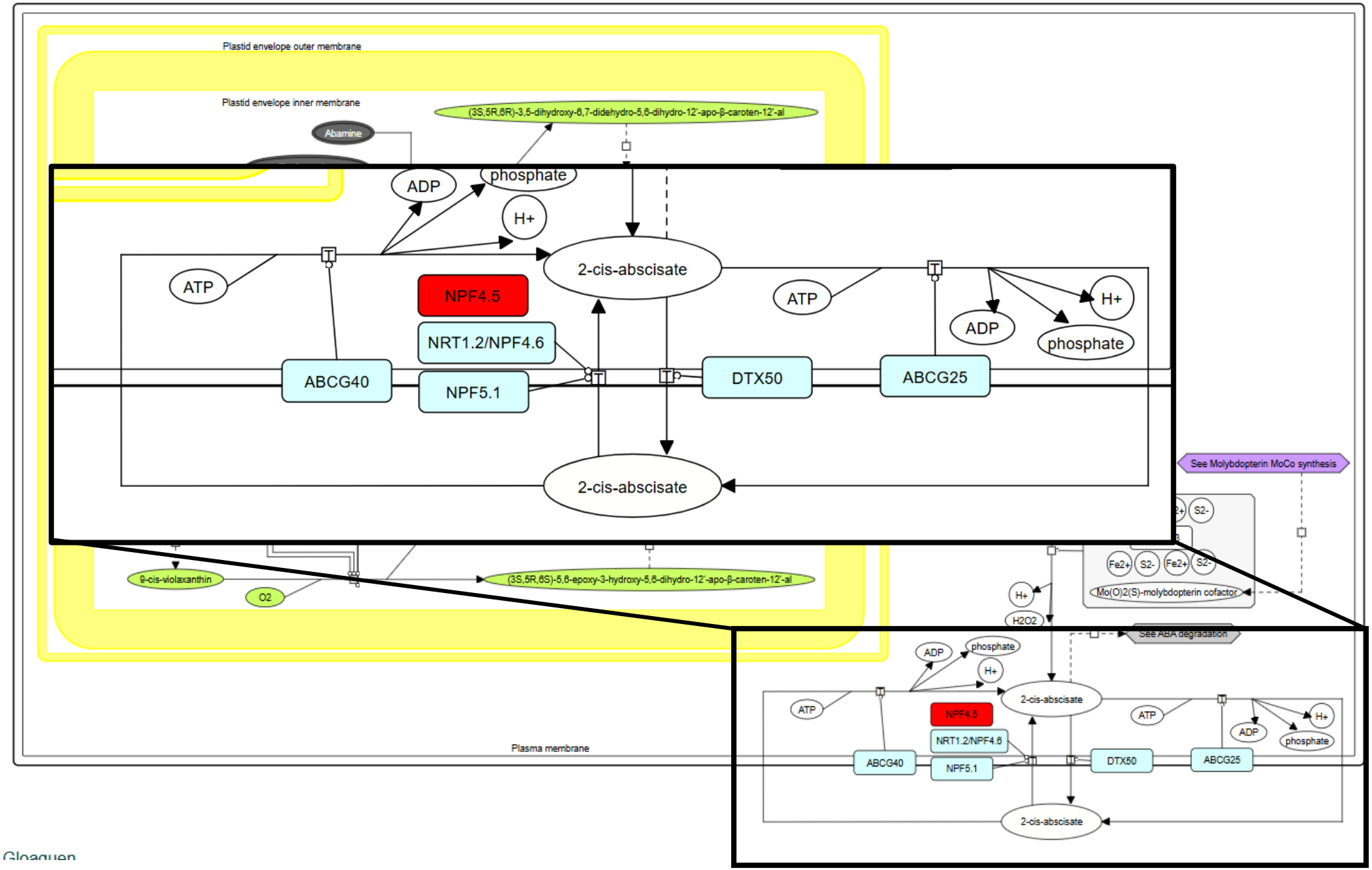
Copper transport and Copper storage

130 publications





Abscisic_acid_ABA_synthesis



Reconstructed by Gilles Curien, Pauline Gloaguen

Starch_degradation