atlas Documentation

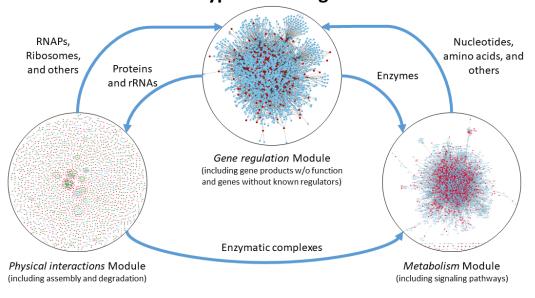
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Atlas is a small software developed to use simple text files that encode biological networks and write Rule-Based Models (RBMs). Atlas writes rules and others model components for the PySB python package PySB, PMID 23423320. The RBMs could be simulated within PySB with NFsim, PMID 26556387 (within the BioNetGen2 software, PMID 27402907), KaSim (KaSim, PMID 29950016). Models could be exported to text files in *BioNetGen* (BioNetGenLanguage) or *kappa* language (Kappa) for further calibration (BioNetFit, PMID 26556387 or pleione, PMID 31641245) and analysis (sterope for parameter sensibility and alcyone for parameter uncertainty).

Atlas: Divide-and-conquer strategy to build rule-based models from diverse types of biological networks



CONTENTS 1

2 CONTENTS

REQUIREMENTS

1. PathwayTools must be installed and running to obtain data from the BioCyc databases. Please, run `pathway-tools -lisp -python-local-only` before to obtain any data.

(Optional) The PathwayTools software could be executed in the background, with help of `nohup pathway-tools -lisp -python-local-only > /dev/null 2> /dev/null &`. Please follow instructions at http://pathwaytools.org/ to obtain a licensed copy of the software from https://biocyc.org/download-bundle.shtml. However, data could be manually formatted using a text-based editor or a spreadsheet software.

Note: If you ran into the `pathway-tools/ptools/24.0/exe/aclssl.so: undefined symbol: CRYPTO_set_locking_callback` error, please follow instructions here: https://github.com/networkbiolab/atlas/tree/master/PTools-Docker. Instructions will guide you to install a docker image that is able to run pathway tools, but does not include it, so you still need to obtain the software with a valid license.

2. (Highly recommended) Install Docker. Please follow instructions for a supported Operating System https://docs.docker.com/engine/install/:

On Ubuntu, install it with `apt-get install docker.io`.

On Win10, install Docker Desktop with WSL2 support https://docs.docker.com/docker-for-windows/wsl/.

On MacOS, install Docker Desktop https://docs.docker.com/docker-for-mac/install/.

The Docker `networkbiolab/pleiades` installs the python packages, the jupyter server, and the stochastic simulators.

- 3. (Recommended) Jupyter notebook. We recommend the use of Anaconda3 https://www.anaconda.com/products/individual because of the easier installation of the stochastic simulators from https://anaconda.org/alubbook.
- 4. (Optional) A stochastic simulator, supported by the pySB python package (BNG2, NFsim, KaSim or Stochkit). pySB requires BNG2 to simulate models with NFsim.
- 5. (Optional) Cytoscape to visualize metabolic networks and others.
- 6. (Optional) A deterministic simulator: pySB supports ODE integration via scipy.integrate.ode, BioNetGen ODE integration, and CUDA-accelerated ODE integration with Marco S. Nobile's cupSODA software (https://github.com/aresio/cupSODA). If the user feel comfortable with SBML models, pySB could export to SBML and deterministic simulation done with libRoadRunner (http://libroadrunner.org/), Tellurium (http://tellurium.analogmachine.org/), COPASI (http://copasi.org/), etc.

CHAPTER

TWO

INSTALLATION

There are different ways to install Atlas:

1. **Install the docker Pleiades (Highly recommended).** The docker container is the easiest way to obtain the software Atlas, the stochastic simulators BioNetGen and KaSim, and the Jupyter notebook.

OR

2. **Clone the Pleiades GitHub repository.** If you are familiar with git, the docker container could be obtained cloning the Pleiades repository. Further details are below.

OR

3. Install Atlas with pip3.

OR

4. **Clone the Atlas GitHub repository.** If you are familiar with git, Atlas could be obtained cloning the Atlas repository and the respective directory added to *PYTHONPATH*. Further details are below.

Note: Need Help? If you run into any problems with installation, please visit our chat room: https://gitter.im/glucksfall/pleiades

2.1 Option 1: Install the Pleiades docker container

Install the docker container is the easiest way to obtain the software Atlas.

Install the docker image "pleiades" using `docker pull networkbiolab/pleiades`. The container is based on the Anaconda3 software and it installs Atlas, and the stochastic simulators BNG2, NFsim, KaSim, and Stochkit. After building the image, please run the container with `docker run --detach --publish 10000:8888 networkbiolab/pleiades`, and go to `localhost:10000` in your preferred browser. The required password is `pleiades`.

2.2 Option 2: Clone the Pleiades repository

Download or clone the Github repository from https://github.com/networkbiolab/pleiades with `git clone https://github.com/networkbiolab/pleiades foo` (where `foo` is an absolute or relative path). Then, you could build the docker image with `docker build foo --tag pleiades` and run it with `docker run --detach --publish 10000:8888 pleiades`. Finally, go to `localhost:10000` in your preferred browser. The required password is `pleiades`.

2.3 Option 3: Install Atlas natively on your computer

The recommended approach is to use system tools, or install them if necessary. To install python packages, you could use pip, or download the package from the python package index.

1. Install with system tools

With pip, you need to execute and Atlas will be installed on \$HOME/.local/lib/python3.6/site-packages directory or similar.

```
pip3 install atlas_rbm --user
```

If you have system rights, you could install Atlas for all users with

```
sudo -H pip3 install atlas_rbm
```

2. Download from the python package index

Alternatively, you could download the package (useful when pip fails to download the package because of lack of SSL libraries) and then install with pip. For instance:

Note: Why Python3?: Atlas is intended to be used with >=python3.4 because python2.7 won't receive further development past 2020, including security updates.

Note: pip, Python, and Anaconda: Be aware which pip you invoque. You could install pip3 with sudo apt-get install python3-pip if you have system rights, or install python3 from source, and adding <python3 path>/bin/pip3 to the path, or linking it in a directory like \$HOME/bin which is commonly added to the path at login. Also be aware that, if you installed Anaconda, pip could be linked to the Anaconda specific version of pip, which will install Atlas into Anaconda's installation folder. Type which pip3 to find out the source of pip, and type python -m site or python3 -m site to find out where is more likely Atlas will be installed.

2.4 Option 4: Clone the Github repository

1. Clone with git

The source code is uploaded and maintained through Github at https://github.com/networkbiolab/atlas. Therefore, you could clone the repository locally, and then add the folder to the PYTHONPATH. Beware that you should install the *pysb* package (pysb) and others packages by any means, specially the Jupyter Notebook project (https://jupyter.org).

```
path=/opt/atlas
git clone https://github.com/networkbiolab/atlas $path
echo export PYTHONPATH="\$PYTHONPATH:\$path" >> $HOME/.profile
```

Note: Adding the path to \$HOME/.profile allows python to find the package installation folder after each user login. Similarly, adding the path to \$HOME/.bashrc allows python to find the package after each terminal invocation. Other options include setting the PYTHONPATH environmental variable in a sh file (see the example folder) or invoke python3 setup.py clean build install to install Atlas as it was downloaded from the PyPI server.

CHAPTER

THREE

MODELING

Atlas is a modular software with each script centered in a specific biological network

- 1. Metabolic Networks
- 2. Interaction Networks
 - 1. Protein-Protein Interaction Networks
 - 2. Protein-Small compounds Interaction Networks
 - 3. Protein-RNA Interaction Networks
 - 4. RNA-RNA Interaction Networks
 - 5. Transcription Factor-DNA Binding Site Interaction Networks
 - 6. Sigma Factor-Promoter Interaction Networks
- 3. Genome Graphs

3.1 Metabolic Networks

Metabolic networks have seven columns:

- 1. The 1st declares a name for the enzyme, gene, or enzymatic complex. Use *spontaneous* for non-enzymatic reactions.:
- 2. The 2nd declares the location of the enzyme, gene, or enzymatic complex: In the case of enzymatic complexes:
 - 1. If the number of locations match the number of components of the complex, each location is mapped to the component.
 - 2. If the number of locations unmatch the number of components, the first location is used for every component
 - 3. If the number of locations is one, the location is used for every component.

Valid names are: cytosol, inner membrane, periplasmic space, membrane, outer membrane, extracellular space, bacterial nucleoid, cell wall, cell projection and cytoskeleton

- 3. The 3rd declares a name for the reaction. If the name is not unique, Atlas drops the duplicated reaction;
- 4. The 4th column lists names for substrates using comma (without spaces);
- 5. The 5th column lists names for products using comma (without spaces); To declare metabolites located at a compartment, prefix the name of the metabolite (e.g. "PER-lactose"):
 - 'CYT-': 'cytosol',

- 'iMEM-': 'inner membrane',
- 'PER-': 'periplasmic space',
- 'MEM-': 'membrane',
- 'oMEM-': 'outer membrane',
- 'EX-': 'extracellular space',
- 'bNUC-': 'bacterial nucleoid',
- 'WALL-': 'cell wall',
- 'cPROJ-': 'cell projection',
- 'CYTOSK-': 'cytoskeleton'
- 6. The 6th declares the forward reaction rate; and finally
- 7. The 7th declares the reverse reaction rate.

Examples:

10

```
GENE OR COMPLEX ENZYME_
      →LOCATION REACTION
                                                             SUBSTRATES PRODUCTS
                                                                                                                            FWD
     →RATE RVS_RATE
    ⇒RATE RVS_RATE

spontaneous cytosol LACTOSE-MUTAROTATION alpha-

⇒lactose beta-lactose 1 1

spontaneous cytosol GALACTOSE-MUTAROTATION alpha-

⇒GALACTOSE beta-GALACTOSE 1 1

spontaneous cytosol GLUCOSE-MUTAROTATION alpha-

⇒glucose beta-glucose 1 1

LACY-MONOMER inner membrane TRANS-RXN-24 PER-PROTON, PER-alpha-

⇒lactose PROTON, alpha-lactose 1 0

LACY-MONOMER inner membrane TRANS-RXN-24-beta PER-PROTON, PER-

⇒beta-lactose PROTON, beta-lactose 1 0

LACY-MONOMER inner membrane TRANS-RXN-24-beta PER-PROTON, PER-

⇒beta-lactose PROTON, beta-lactose 1 0

LACY-MONOMER inner membrane TRANS-RXN-94 PER-PROTON, PER-

⇒MELIBIOSE PROTON, MELIBIOSE 1 0

LACY-MONOMER inner membrane RXNO-7215 PER-PROTON, PER-CPD-

⇒3561 PROTON, CPD-3561 1 0
     _{\to 3561} PROTON,CPD-3561 1 0 LACY-MONOMER inner membrane RXN0-7217 PER-PROTON,PER-CPD-
     →3785 PROTON, CPD-3785 1
                                                                             0
    LACY-MONOMER inner membrane RXN-17755 PER-PROTON, PER-CPD-
10
    →3801 PROTON, CPD-3801 1 0
BETAGALACTOSID-CPLX cytosol BETAGALACTOSID-RXN
                                                                                                                     beta-lactose,
11
     →WATER beta-GALACTOSE, beta-glucose 1 0
     BETAGALACTOSID-CPLX cytosol BETAGALACTOSID-RXN-alpha
                                                                                                                                    alpha-
    →lactose, WATER alpha-GALACTOSE, alpha-glucose 1 0

BETAGALACTOSID-CPLX cytosol RXN0-5363 alpha-lactose

→ALLOLACTOSE 1 1

BETAGALACTOSID-CPLX cytosol RXN0-5363-beta beta-

→lactose beta-ALLOLACTOSE 1 1

BETAGALACTOSID-CPLX cytosol ALLOLACTOSE-DEG-alpha alpha-
13
                                                                                                                                              alpha-
14
     →ALLOLACTOSE alpha-GALACTOSE, alpha-glucose 1 0
     BETAGALACTOSID-CPLX cytosol ALLOLACTOSE-DEG-beta beta-
    →ALLOLACTOSE beta-GALACTOSE, beta-glucose 1 0

BETAGALACTOSID-CPLX cytosol RXN-17726 CPD-3561, WATER

→GALACTOSE, Fructofuranose 1 0
    GALACTOSE, Fructofuranose

BETAGALACTOSID-CPLX

Cytosol

RXN0-7219

CPD-3785, WATER

GALACTOSE, D-ARABINOSE

1

GALACTOACETYLTRAN-CPLX

Cytosol

GALACTOACETYLTRAN-RXN-
                                                                                                                                                   bet.a-
      → galactose beta-GALACTOSE, ACETYL-COA 6-Acetyl-beta-D-Galactosa (continues on next page)
```

Chapter 3. Modeling

OR

```
GENE OR COMPLEX ENZYME 

→LOCATION REACTION
                                SUBSTRATES PRODUCTS FWD_
   \hookrightarrowRATE
              RVS_RATE
  spontaneous cytosol LACTOSE-MUTAROTATION alpha-
                 beta-lactose 1 1 cytosol GALACTOSE-MUTAROTATION
  →lactose
  spontaneous
  -GALACTOSE
                  beta-GALACTOSE 1 1
  spontaneous cytosol GLUCOSE-MUTARO

→glucose beta-glucose 1 1

lacY inner membrane TRANS-RXN-24
                  cytosol GLUCOSE-MUTAROTATION
                                                          alpha-
                                  1 1
                                                   PER-PROTON, PER-alpha-
  →lactose PROTON,alpha-lactose 1
lacY inner membrane TRANS-RXN-24-beta
                                                   0
                                                         PER-PROTON, PER-beta-
6
  →lactose PROTON, beta-lactose 1
lacY inner membrane TRANS-RXN-94
              PROTON, beta-lactose 1 0
                                                   PER-PROTON, PER-
   →MELIBIOSE PROTON, MELIBIOSE 1
  lacY inner membrane RXN0-7215
                                                PER-PROTON, PER-CPD-
  →3561 PROTON, CPD-3561

lacY inner membrane RXN0-7217

→3785 PROTON, CPD-3785 1 0

PXN-17755
                                 1 0
                                                PER-PROTON, PER-CPD-
                                 1 0
           inner membrane
                                 RXN-17755 PER-PROTON, PER-CPD-
10
             PROTON, CPD-3801 1 0
   →3801
  lacZ cytosol BETAGALACTOSID-RXN beta-lactose, WATER beta-
                          1 0
   →GALACTOSE, beta-glucose
  lacZcytosolBETAGALACTOSID-RXN-alphaalpha-lactose,→WATERalpha-GALACTOSE, alpha-glucose10lacZcytosolRXN0-5363alpha-lactosealpha-
  lacZ cytosol BETAGALACTOSID-RXN-alpha
13
   →ALLOLACTOSE
                           1
                     RXN0-5363-beta beta-lactose beta-
  lacZ cytosol
   →ALLOLACTOSE 1
                           1
  lacZ cytosol ALLOLACTOSE—DEG-alpha
                                                  alpha-ALLOLACTOSE,
             alpha-GALACTOSE, alpha-glucose 1 0
             cytosol ALLOLACTOSE-DEG-beta beta-ALLOLACTOSE, beta-GALACTOSE, beta-glucose 1 0
           cytosol ALLOLACTOSE-DEG-beta
  →WATER beta-GALACTOSE, beta-grucose -
lacZ cytosol RXN-17726 CPD-3561, WATER
                                                              beta-GALACTOSE.
  lacZ cytosol
   lacZ cytosol 0

→ARABINOSE 1 0

GALACTOACETYLTRAN-RXN-galactose

Coloctose.CO-A 1
                        RXN0-7219
                                         CPD-3785, WATER
                                                               beta-GALACTOSE, D-
  lacA cytosol
                                                              beta-GALACTOSE,
   →ACETYL-COA 6-Acetyl-beta-D-Galactose, CO-A 1
```

OR

1	GENE OR COME	PLEX ENZYME.			
-	→ LOCATION	REACTION	SUBSTRATES	PRODUCTS	FWD_
	⇔RATE	RVS_RATE			
2	spontaneous	cytosol	LACTOSE-MUTA	ROTATION	alpha-
	⇔lactose	beta-lactose	1	1	
3	spontaneous	cytosol	GALACTOSE-MU	TAROTATION	alpha-
	→GALACTOSE	beta-GALACTOSE	1	1	
4	spontaneous	cytosol	GLUCOSE-MUTA	ROTATION	alpha-
	⊶glucose	beta-glucose	1	1	
5	lacY	inner membrane	TRANS-RXN-24	PER-PRC	TON, PER-alpha-
	⇔lactose	PROTON, alpha-lact	tose 1	0	

```
lacY
                               TRANS-RXN-24-beta
            inner membrane
                                                     PER-PROTON, PER-beta-
  -lactose
               PROTON, beta-lactose
                                      1
  lacY inner membrane TRANS-RXN-94
                                               PER-PROTON, PER-
  →MELIBIOSE
                 PROTON, MELIBIOSE 1
  lacY inner membrane RXN0-7215
                                              PER-PROTON, PER-CPD-
   →3561
             PROTON, CPD-3561
                                1
                                         0
           inner membrane
                               RXN0-7217
                                              PER-PROTON, PER-CPD-
  lacY
  →3785
             PROTON, CPD-3785
                                1
                              RXN-17755
  lacY
           inner membrane
                                              PER-PROTON, PER-CPD-
10
  →3801
           PROTON, CPD-3801
                                         Ω
                              1
  [lacZ,lacZ,lacZ,lacZ] [cytosol,cytosol,cytosol]
                                                              BETAGALACTOSID-
11
  →RXN beta-lactose, WATER beta-GALACTOSE, beta-glucose
                                                              1 0
  [lacZ,lacZ,lacZ,lacZ] [cytosol,cytosol,cytosol]
                                                              BETAGALACTOSID-
  →RXN-alpha alpha-lactose, WATER alpha-GALACTOSE, alpha-
  -glucose
               1 0
  [lacZ,lacZ,lacZ,lacZ] [cytosol,cytosol,cytosol]
                                                              RXN0-
13
  →5363 alpha-lactose alpha-ALLOLACTOSE 1
                                                             1
  [lacZ,lacZ,lacZ,lacZ]
                           [cytosol, cytosol, cytosol]
                                                              RXN0-5363-
  ⇒beta beta-lactose beta-ALLOLACTOSE 1
[lacZ,lacZ,lacZ] [cytosol,cytosol,cytosol]
                                                              ALLOLACTOSE-DEG-
15
  →alpha alpha-ALLOLACTOSE, WATER alpha-GALACTOSE, alpha-
→glucose 1 0
  →glucose 1 0 [lacZ,lacZ,lacZ]
                           [cytosol, cytosol, cytosol]
                                                              ALLOLACTOSE-DEG-
  \hookrightarrowbeta beta-ALLOLACTOSE, WATER beta-GALACTOSE, beta-
  →glucose 1 0
[lacZ,lacZ,lacZ,lacZ] [cytosol,cytosol,cytosol]
                                                              RXN-
  →17726 CPD-3561, WATER beta-GALACTOSE, Fructofuranose
  [lacZ,lacZ,lacZ,lacZ] [cytosol,cytosol,cytosol]
                                                              RXN0-
18
  →7219 CPD-3785, WATER beta-GALACTOSE, D-ARABINOSE
                                                              1
  [lacA, lacA, lacA] [cytosol, cytosol] GALACTOACETYLTRAN-RXN-
                                             6-Acetyl-beta-D-Galactose,CO-
                  beta-GALACTOSE, ACETYL-COA
  -galactose
  \hookrightarrow A
```

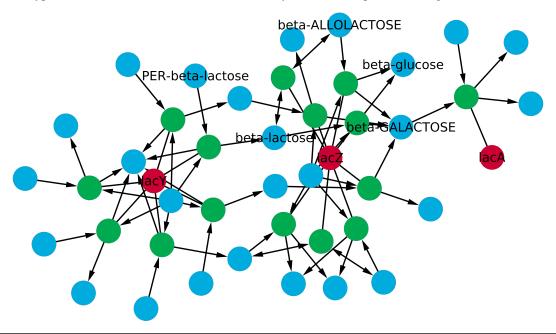
Note: Visualization in Cytoscape. Transform the input file into a Cytoscape compatible file with atlas_rbm. utils.metabolicNetwork.expand_network(network, 'output.txt') and import the network into Cytoscape.

Colors and arrows remains to the user for customization: The following image was prepared from the lactose-metabolism-cytoscape-v3.txt file, and you could reproduce it with Cytoscape:

- 1. Click on the Import Network from File System icon or click on File -> Import -> Network from File....
- 2. Navigate to the file and click on Open.
- 3. SOURCE, TARGET, and EDGE ATTRIBUTE are OK, but the 4th columns must be the SOURCE NODE ATTRIBUTE and the 5th column the TARGET NODE ATTRIBUTE. Click on the header and change it to the correct attribute. The attributes will help later to filter and to add format to nodes and edges.
- 4. Click on Filter (on the right), then on the + icon and finally on Column Filter:
- 1. On the selector, click on Edge: EDGE_ATTRIBUTE and change contains to is:
 - 1. Write NO_REVERSIBLE that will select edges that correspond to irreversible reactions. Click on Style, then Edge (in the bottom), and click on the 3rd column to bypass the format of the Target Arrow Shape and select your favorite arrow shape.
 - 2. Write REVERSIBLE and bypass the format of the Source Arrow Shape AND Target Arrow

Shape, and select your favorite arrow shape.

- 2. On the selector, click on Node: SOURCE NODE ATTRIBUTE:
 - 1. Write RXN that will select nodes enconding the reactions. Click on Style, then on Node and bypass the Fill Color. In the new window, you could set-up the color, e.g. #00AA50
 - 2. Write GENE_PROD that will select nodes encoding the gene name, protein name, or the enzyme name. Click on Style, then on Node and bypass the Fill Color. In the new window, you could set-up the color, e.g. #CC0033
 - 3. Write MET that will select nodes encoding substrate metabolites. Click on Style, then on Node and bypass the Fill Color. In the new window, you could set-up the color, e.g. #00ABDD. Also, set a shape for nodes, to differentiate substrates from products.
- 3. On the selector, click on Node: TARGET_NODE_ATTRIBUTE:
 - 1. Write MET that will select nodes encoding product metabolites. Click on Style, then on Node and bypass the Fill Color. In the new window, you could set-up the color, e.g. #00ABDD



Finally, execute atlas_rbm.construct_model_from_metabolic_network(network, verbose = False) to obtain the model.

Note: Uniqueness of Rule names. Atlas will write *Rules* for unique metabolic reactions. Identical names will be reported for further curation.

Note: Simulation. The model can be simulated only with the instantiation of Initials:

- atlas_rbm.simulation.set_initial.cplx(model, complex_name, location, positive_number)
- atlas_rbm.simulation.set_initial.dna(model, dna_name, positive_number)
- atlas_rbm.simulation.set_initial.met(model, metabolite, location, positive_number)

3.1. Metabolic Networks

- atlas_rbm.simulation.set_initial.prot(model, prot_name, location, positive_number)
- atlas_rbm.simulation.set_initial.rna(model, rna_name, positive_number)

Note: For large models, the noObservables and the noInitials will make a faster compilation, while later you could add Initials and Observables to the model.

Use the keyword argument toFile = 'name.py' to write the model to a file (the function will return None):

```
from pysb import *
   Model()
2
   Monomer ('met',
           ['name', 'loc', 'dna', 'met', 'prot', 'rna'],
           { 'name' : [ 'ACETYL_COA', 'CO_A', 'CPD_3561', 'CPD_3785', 'CPD_3801', 'D_
   →ARABINOSE', 'Fructofuranose', 'MELIBIOSE', 'PROTON', 'WATER', '_6_Acetyl_beta_D_
   →Galactose', 'alpha_ALLOLACTOSE', 'alpha_GALACTOSE', 'alpha_glucose', 'alpha_lactose
   →', 'beta_ALLOLACTOSE', 'beta_GALACTOSE', 'beta_glucose', 'beta_lactose'],
           'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
   → 'omem']})
   Monomer ('prot',
           ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
           { 'name' : [ 'LACY_MONOMER', 'spontaneous' ],
10
           'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
11
   → 'omem']})
   Monomer ('cplx',
12
           ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
13
           { 'name' : [ 'BETAGALACTOSID_CPLX', 'GALACTOACETYLTRAN_CPLX' ],
14
           'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
   Observable('obs_met_ACETYL_COA_cyt', met(name = 'ACETYL_COA', loc = 'cyt'))
16
   Observable('obs_met_CO_A_cyt', met(name = 'CO_A', loc = 'cyt'))
17
   Observable('obs_met_CPD_3561_cyt', met(name = 'CPD_3561', loc = 'cyt'))
18
   Observable('obs_met_CPD_3785_cyt', met(name = 'CPD_3785', loc = 'cyt'))
19
   Observable('obs_met_CPD_3801_cyt', met(name = 'CPD_3801', loc = 'cyt'))
   Observable('obs_met_D_ARABINOSE_cyt', met(name = 'D_ARABINOSE', loc = 'cyt'))
21
   Observable ('obs_met_Fructofuranose_cyt', met(name = 'Fructofuranose', loc = 'cyt'))
22
   Observable('obs_met_MELIBIOSE_cyt', met(name = 'MELIBIOSE', loc = 'cyt'))
23
   Observable('obs_met_PROTON_cyt', met(name = 'PROTON', loc = 'cyt'))
24
   Observable('obs_met_WATER_cyt', met(name = 'WATER', loc = 'cyt'))
25
   Observable('obs_met__6_Acetyl_beta_D_Galactose_cyt', met(name = '_6_Acetyl_beta_D_
   Galactose', loc = 'cyt'))
   Observable('obs_met_alpha_ALLOLACTOSE_cyt', met(name = 'alpha_ALLOLACTOSE', loc = 'cyt
27
   Observable('obs_met_alpha_GALACTOSE_cyt', met(name = 'alpha_GALACTOSE', loc = 'cyt'))
28
   Observable('obs_met_alpha_glucose_cyt', met(name = 'alpha_glucose', loc = 'cyt'))
   Observable('obs_met_alpha_lactose_cyt', met(name = 'alpha_lactose', loc = 'cyt'))
30
   Observable('obs_met_beta_ALLOLACTOSE_cyt', met(name = 'beta_ALLOLACTOSE', loc = 'cyt
   Observable('obs_met_beta_GALACTOSE_cyt', met(name = 'beta_GALACTOSE', loc = 'cyt'))
32
   Observable('obs_met_beta_glucose_cyt', met(name = 'beta_glucose', loc = 'cyt'))
33
   Observable('obs_met_beta_lactose_cyt', met(name = 'beta_lactose', loc = 'cyt'))
34
   Initial(met(name = 'ACETYL_COA', loc = 'cyt', dna = None, met = None, prot = None, _
35
   →rna = None), Parameter('t0_met_ACETYL_COA_cyt', 0))
   Initial (met (name = 'CO_A', loc = 'cyt', dna = None, met = None, prot = None, rna = _
   →None), Parameter('t0_met_CO_A_cyt', 0))
```

```
Initial(met(name = 'CPD_3561', loc = 'cyt', dna = None, met = None, prot = None, rna.
37
   →= None), Parameter('t0_met_CPD_3561_cyt', 0))
   Initial (met (name = 'CPD_3785', loc = 'cyt', dna = None, met = None, prot = None, rna_
38
    →= None), Parameter('t0_met_CPD_3785_cyt', 0))
   Initial(met(name = 'CPD_3801', loc = 'cyt', dna = None, met = None, prot = None, rna_
    →= None), Parameter('t0_met_CPD_3801_cyt', 0))
   Initial(met(name = 'D_ARABINOSE', loc = 'cyt', dna = None, met = None, prot = None, _
40
   →rna = None), Parameter('t0_met_D_ARABINOSE_cyt', 0))
   Initial (met (name = 'Fructofuranose', loc = 'cyt', dna = None, met = None, prot = None,
41
   → rna = None), Parameter('t0_met_Fructofuranose_cyt', 0))
   Initial(met(name = 'MELIBIOSE', loc = 'cyt', dna = None, met = None, prot = None, rna_
   →= None), Parameter('t0_met_MELIBIOSE_cyt', 0))
   Initial(met(name = 'PROTON', loc = 'cyt', dna = None, met = None, prot = None, rna = ...)
   →None), Parameter('t0_met_PROTON_cyt', 0))
   Initial (met (name = 'WATER', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
44
   →None), Parameter('t0_met_WATER_cyt', 0))
   Initial (met (name = '_6_Acetyl_beta_D_Galactose', loc = 'cyt', dna = None, met = None, __
    →prot = None, rna = None), Parameter('t0_met__6_Acetyl_beta_D_Galactose_cyt', 0))
   Initial(met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = _
   →None, rna = None), Parameter('t0_met_alpha_ALLOLACTOSE_cyt', 0))
   Initial(met(name = 'alpha_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = _
47
   →None, rna = None), Parameter('t0_met_alpha_GALACTOSE_cyt', 0))
   Initial(met(name = 'alpha_glucose', loc = 'cyt', dna = None, met = None, prot = None, _
48
   →rna = None), Parameter('t0_met_alpha_glucose_cyt', 0))
   Initial(met(name = 'alpha_lactose', loc = 'cyt', dna = None, met = None, prot = None, __
   →rna = None), Parameter('t0_met_alpha_lactose_cyt', 0))
   Initial(met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot =...
50
   →None, rna = None), Parameter('t0_met_beta_ALLOLACTOSE_cyt', 0))
   Initial (met (name = 'beta_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = None,
51
    → rna = None), Parameter('t0_met_beta_GALACTOSE_cyt', 0))
   Initial(met(name = 'beta_glucose', loc = 'cyt', dna = None, met = None, prot = None, ...
    →rna = None), Parameter('t0_met_beta_glucose_cyt', 0))
   Initial(met(name = 'beta_lactose', loc = 'cyt', dna = None, met = None, prot = None,
53
   →rna = None), Parameter('t0_met_beta_lactose_cyt', 0))
   Initial(prot(name = 'LACY_MONOMER', loc = 'cyt', dna = None, met = None, prot = None, __
54
   →rna = None, up = None, dw = None), Parameter('t0_prot_LACY_MONOMER_cyt', 0))
   Initial (prot (name = 'spontaneous', loc = 'cyt', dna = None, met = None, prot = None,
55
   →rna = None, up = None, dw = None), Parameter('t0_prot_spontaneous_cyt', 0))
   Initial(cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
   →= None, rna = None, up = None, dw = None), Parameter('t0_cplx_BETAGALACTOSID_CPLX_
   \rightarrowcvt', 0))
   Initial(cplx(name = 'GALACTOACETYLTRAN_CPLX', loc = 'cyt', dna = None, met = None, ...
   →prot = None, rna = None, up = None, dw = None), Parameter('t0_cplx_
   →GALACTOACETYLTRAN_CPLX_cyt', 0))
   Rule ('LACTOSE_MUTAROTATION_CYT',
           met (name = 'alpha_lactose', loc = 'cyt', dna = None, met = None, prot = None, ...
   →rna = None) |
           met(name = 'beta_lactose', loc = 'cyt', dna = None, met = None, prot = None,...
60
   →rna = None),
           Parameter ('fwd_LACTOSE_MUTAROTATION_CYT', 1.000000),
61
           Parameter('rvs_LACTOSE_MUTAROTATION_CYT', 1.000000))
   Rule ('GALACTOSE_MUTAROTATION_CYT',
           met (name = 'alpha_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = ...
64
   →None, rna = None) |
           met(name = 'beta_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = None,
65
   → rna = None),
           Parameter('fwd_GALACTOSE_MUTAROTATION_CYT', 1.000000),
```

```
Parameter ('rvs_GALACTOSE_MUTAROTATION_CYT', 1.000000))
67
   Rule ('GLUCOSE_MUTAROTATION_CYT',
68
           met(name = 'alpha_glucose', loc = 'cyt', dna = None, met = None, prot = None, _
69
    →rna = None) |
           met(name = 'beta_glucose', loc = 'cyt', dna = None, met = None, prot = None,
70
    →rna = None),
           Parameter ('fwd_GLUCOSE_MUTAROTATION_CYT', 1.000000),
71
           Parameter ('rvs_GLUCOSE_MUTAROTATION_CYT', 1.000000))
72
   Rule('TRANS_RXN_24',
73
           prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
74
    → rna = None, up = None, dw = None) +
           met (name = 'PROTON', loc = 'per', dna = None, met = None, prot = None, rna = ...
75
           met(name = 'alpha_lactose', loc = 'per', dna = None, met = None, prot = None,...
76
    →rna = None) |
           prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
77
    → rna = None, up = None, dw = None) +
           met(name = 'PROTON', loc = 'cyt', dna = None, met = None, prot = None, rna = _
78
    →None) +
           met (name = 'alpha_lactose', loc = 'cyt', dna = None, met = None, prot = None, ...
79
    →rna = None),
            Parameter ('fwd_TRANS_RXN_24', 1.000000),
80
           Parameter('rvs_TRANS_RXN_24', 0.000000))
81
   Rule('TRANS_RXN_24_beta',
82
           prot (name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
83
    → rna = None, up = None, dw = None) +
           met (name = 'PROTON', loc = 'per', dna = None, met = None, prot = None, rna = ...
84
    →None) +
           met(name = 'beta_lactose', loc = 'per', dna = None, met = None, prot = None, __
85
    →rna = None) |
           prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
    → rna = None, up = None, dw = None) +
           met (name = 'PROTON', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
87
    →None) +
           met(name = 'beta_lactose', loc = 'cyt', dna = None, met = None, prot = None,...
88
    →rna = None),
           Parameter ('fwd_TRANS_RXN_24_beta', 1.000000),
89
           Parameter('rvs_TRANS_RXN_24_beta', 0.000000))
91
   Rule ('TRANS_RXN_94',
           prot (name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
92
    → rna = None, up = None, dw = None) +
           met(name = 'PROTON', loc = 'per', dna = None, met = None, prot = None, rna = __
93
    →None) +
           met(name = 'MELIBIOSE', loc = 'per', dna = None, met = None, prot = None, rna,
    →= None) |
           prot (name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
95
    → rna = None, up = None, dw = None) +
           met(name = 'PROTON', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
96
    →None) +
           met(name = 'MELIBIOSE', loc = 'cyt', dna = None, met = None, prot = None, rna_
97
    \hookrightarrow = None),
           Parameter ('fwd_TRANS_RXN_94', 1.000000),
           Parameter ('rvs_TRANS_RXN_94', 0.000000))
   Rule('RXN0_7215',
100
           prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
101
    → rna = None, up = None, dw = None) +
           met(name = 'PROTON', loc = 'per', dna = None, met = None, prot = None, rna =
102
                                                                                (continues on next page)
    →None) +
```

```
met(name = 'CPD_3561', loc = 'per', dna = None, met = None, prot = None, rna_
103
    ⇒= None) |
            prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
104
    → rna = None, up = None, dw = None) +
           met(name = 'PROTON', loc = 'cyt', dna = None, met = None, prot = None, rna = __
105
    →None) +
           met(name = 'CPD_3561', loc = 'cyt', dna = None, met = None, prot = None, rna,
106
    \rightarrow= None),
            Parameter ('fwd_RXN0_7215', 1.000000),
107
            Parameter('rvs_RXN0_7215', 0.000000))
108
    Rule('RXN0_7217',
109
            prot (name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
110
    → rna = None, up = None, dw = None) +
            met(name = 'PROTON', loc = 'per', dna = None, met = None, prot = None, rna = ...
111
    →None) +
            met(name = 'CPD_3785', loc = 'per', dna = None, met = None, prot = None, rna_
112
    →= None) |
            prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
113

→ rna = None, up = None, dw = None) +
            met(name = 'PROTON', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
114
    →None) +
            met(name = 'CPD_3785', loc = 'cyt', dna = None, met = None, prot = None, rna,
115
    \rightarrow= None),
            Parameter('fwd_RXN0_7217', 1.000000),
116
            Parameter('rvs_RXN0_7217', 0.000000))
117
   Rule('RXN_17755',
118
            prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
119
    → rna = None, up = None, dw = None) +
            met (name = 'PROTON', loc = 'per', dna = None, met = None, prot = None, rna = __
120
    →None) +
            met(name = 'CPD_3801', loc = 'per', dna = None, met = None, prot = None, rna,
121
    →= None) |
            prot (name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
122
    → rna = None, up = None, dw = None) +
           met (name = 'PROTON', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
123
    →None) +
            met(name = 'CPD_3801', loc = 'cyt', dna = None, met = None, prot = None, rna_
124
    \rightarrow= None),
125
            Parameter ('fwd_RXN_17755', 1.000000),
            Parameter ('rvs_RXN_17755', 0.000000))
126
    Rule ('BETAGALACTOSID RXN',
127
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
128
    \rightarrow= None, rna = None) +
            met(name = 'beta_lactose', loc = 'cyt', dna = None, met = None, prot = None,
129
    \rightarrowrna = None) +
            met (name = 'WATER', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
130
    →None)
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot.
131
    →= None, rna = None) +
            met(name = 'beta_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = None,
132
    → rna = None) +
           met(name = 'beta_glucose', loc = 'cyt', dna = None, met = None, prot = None,
133
    →rna = None),
            Parameter ('fwd_BETAGALACTOSID_RXN', 1.000000),
134
            Parameter ('rvs_BETAGALACTOSID_RXN', 0.000000))
135
136
   Rule ('BETAGALACTOSID_RXN_alpha',
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot
137
                                                                                 (continues on next page)
    →= None, rna = None) +
```

```
met (name = 'alpha_lactose', loc = 'cyt', dna = None, met = None, prot = None, __
138
    →rna = None) +
            met (name = 'WATER', loc = 'cyt', dna = None, met = None, prot = None, rna = __
139
    None)
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
140
    →= None, rna = None) +
            met (name = 'alpha_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = ...
141
    →None, rna = None) +
            met (name = 'alpha_glucose', loc = 'cyt', dna = None, met = None, prot = None, __
142
    →rna = None),
            Parameter ('fwd_BETAGALACTOSID_RXN_alpha', 1.000000),
143
            Parameter ('rvs_BETAGALACTOSID_RXN_alpha', 0.000000))
145
    Rule('RXN0 5363',
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
146
    →= None, rna = None) +
            met(name = 'alpha_lactose', loc = 'cyt', dna = None, met = None, prot = None, __
147
    →rna = None) |
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
148
    →= None, rna = None) +
            met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = ...
149
    →None, rna = None),
            Parameter('fwd_RXN0_5363', 1.000000),
150
            Parameter('rvs_RXN0_5363', 1.000000))
151
   Rule('RXN0_5363_beta',
152
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot.
153
    →= None, rna = None) +
           met(name = 'beta_lactose', loc = 'cyt', dna = None, met = None, prot = None,...
154
    →rna = None) |
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
155
    →= None, rna = None) +
            met (name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = ...
156
    →None, rna = None),
            Parameter ('fwd_RXN0_5363_beta', 1.000000),
157
            Parameter('rvs_RXN0_5363_beta', 1.000000))
158
   Rule ('ALLOLACTOSE_DEG_alpha',
159
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
160
    →= None, rna = None) +
161
           met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = ...
    →None, rna = None) +
            None
162
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
163
    \rightarrow= None, rna = None) +
            met(name = 'alpha_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = _
164
    →None, rna = None) +
            met(name = 'alpha_glucose', loc = 'cyt', dna = None, met = None, prot = None, _
165
    →rna = None).
            Parameter ('fwd_ALLOLACTOSE_DEG_alpha', 1.000000),
166
            Parameter ('rvs_ALLOLACTOSE_DEG_alpha', 0.000000))
167
   Rule('ALLOLACTOSE_DEG_beta',
168
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
169
    →= None, rna = None) +
            met (name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = __
170
    →None, rna = None) +
            None
171
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
172
    \rightarrow= None, rna = None) +
           met (name = 'beta_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = None,
                                                                                (continues on next page)
    → rna = None) +
```

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```
met(name = 'beta_glucose', loc = 'cyt', dna = None, met = None, prot = None,...
174
    →rna = None).
            Parameter ('fwd_ALLOLACTOSE_DEG_beta', 1.000000),
175
            Parameter('rvs_ALLOLACTOSE_DEG_beta', 0.000000))
176
   Rule ('RXN_17726',
177
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
178
    →= None, rna = None) +
           met(name = 'CPD_3561', loc = 'cyt', dna = None, met = None, prot = None, rna,
179
    \rightarrow= None) +
           met(name = 'WATER', loc = 'cyt', dna = None, met = None, prot = None, rna = _
180
    →None)
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot.
181
    →= None, rna = None) +
           met (name = 'beta_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = None,
182
    → rna = None) +
            met (name = 'Fructofuranose', loc = 'cyt', dna = None, met = None, prot = None,
183
    → rna = None),
            Parameter ('fwd_RXN_17726', 1.000000),
184
            Parameter('rvs_RXN_17726', 0.000000))
185
   Rule ('RXN0_7219',
186
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot...
187
    →= None, rna = None) +
            met(name = 'CPD_3785', loc = 'cyt', dna = None, met = None, prot = None, rna_
188
    →= None) +
            met (name = 'WATER', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
189
    →None)
            cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot...
190
    \rightarrow= None, rna = None) +
           met(name = 'beta_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = None,
191
    → rna = None) +
            met(name = 'D_ARABINOSE', loc = 'cyt', dna = None, met = None, prot = None,
192
    →rna = None),
            Parameter ('fwd_RXN0_7219', 1.000000),
193
            Parameter ('rvs_RXN0_7219', 0.000000))
194
   Rule ('GALACTOACETYLTRAN_RXN_galactose',
195
           cplx(name = 'GALACTOACETYLTRAN_CPLX', loc = 'cyt', dna = None, met = None, _
196
    →prot = None, rna = None) +
           met (name = 'beta_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = None,
    → rna = None) +
           met (name = 'ACETYL_COA', loc = 'cyt', dna = None, met = None, prot = None,...
198
    →rna = None) |
            cplx(name = 'GALACTOACETYLTRAN_CPLX', loc = 'cyt', dna = None, met = None,
199
    →prot = None, rna = None) +
            met(name = '_6_Acetyl_beta_D_Galactose', loc = 'cyt', dna = None, met = None,
200
    →prot = None, rna = None) +
            met (name = 'CO_A', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
201
    →None),
            Parameter ('fwd GALACTOACETYLTRAN RXN galactose', 1.000000),
202
            Parameter ('rvs_GALACTOACETYLTRAN_RXN_galactose', 0.000000))
203
```

3.2 Protein-Protein Interaction Networks

Protein-protein interaction (PPI) networks have five columns:

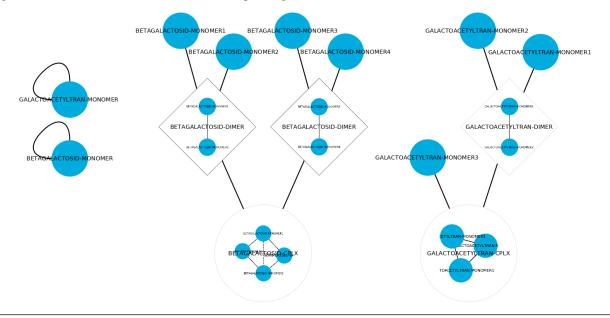
- 1. The 1st declares the SOURCE and the 2nd declares the TARGET.
 - It does not matter the order, as the two columns defines a bimolecular reaction which product is the merge of all components into one complex. *Atlas* understand components inside brackets (e.g. [lacZ,lacZ]) as a complex, therefore, the components are internally linked.
- 2. The 3rd and 4th columns declare the forward and the reverse reaction rates, respectively.
- 3. The 5th columns declares the location of the complex components:
 - 1. If the number of locations match the number of components of the complex, each location is mapped to the component.
 - 2. If the number of locations unmatch the number of components, the first location is used for every component
 - 3. If the number of locations is one, the location is used for every component.

Valid names are: cytosol, inner membrane, periplasmic space, membrane, outer membrane, extracellular space, bacterial nucleoid, cell wall, cell projection and cytoskeleton

Examples:

1	SOURCE	TARGET	FWD	_RATE	RVS_RATE	LOCATION
2	lacZ	lacZ	1.0	0.0	cytosol	
3	[lacZ,lacZ]	[1	acZ,lacZ]	1.0	0.0	cytosol
4	lacA	lacA	1.0	0.0	cytosol	
5	lacA	[lacA,lac	:A]	1.0	0.0	cytosol
6	lacI	lacI	1.0	0.0	cytosol	

Note: Visualization in Cytoscape. Cytoscape cannot import hyper-graphs. To do so, Create simple network and right-click to embed a subnetwork in the corresponding node.



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Finally, execute atlas_rbm.construct_model_from_interaction_network (network, verbose = False) to obtain the model.

Note: Uniqueness of Rule names. Atlas will write *Rules* with numbered names. Merge into one the networks (pandas.concat(list)) or use a single file to model interactions.

Note: Simulation. The model can be simulated only with the instantiation of Initials:

- atlas_rbm.simulation.set_initial.cplx(model, complex_name, location, positive_number)
- atlas_rbm.simulation.set_initial.dna(model, dna_name, positive_number)
- atlas_rbm.simulation.set_initial.met(model, metabolite, location, positive_number)
- atlas_rbm.simulation.set_initial.prot(model, prot_name, location, positive_number)
- atlas_rbm.simulation.set_initial.rna(model, rna_name, positive_number)

Note: Use the keyword argument toFile = 'name.py' to write the model to a file (the function will return None):

```
from pysb import *
   Model()
2
   Monomer ('prot',
            ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
5
            { 'name' : [ 'lacA', 'lacI', 'lacZ' ],
6
            'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
   → 'omem']})
   Observable('obs_prot_lacA_cyt', prot(name = 'lacA', loc = 'cyt', dna = None, met = _
   →None, prot = None, rna = None, up = None, dw = None))
   Initial(prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
   →None, up = None, dw = None), Parameter('t0_prot_lacA_cyt', 0))
   Observable('obs_prot_lacI_cyt', prot(name = 'lacI', loc = 'cyt', dna = None, met = _
10
   →None, prot = None, rna = None, up = None, dw = None))
   Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna =_
    →None, up = None, dw = None), Parameter('t0_prot_lacI_cyt', 0))
   Observable('obs_prot_lacZ_cyt', prot(name = 'lacZ', loc = 'cyt', dna = None, met = _
12
   →None, prot = None, rna = None, up = None, dw = None))
   Initial(prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =_
13
   →None, up = None, dw = None), Parameter('t0_prot_lacZ_cyt', 0))
   Initial(prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = _
   \rightarrowNone, up = None, dw = 1) %
           prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = __
15
   \rightarrowNone, up = 1, dw = 2) %
           prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
16
   \rightarrowNone, up = 2, dw = None),
           Parameter('t0_cplx_lacAx3_cyt', 0))
   Observable('obs_cplx_lacAx3_cyt',
18
           prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = __
   \rightarrowNone, up = None, dw = 1) %
           prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
20
    \rightarrowNone, up - 1, dw - 2) %
                                                                                (continues on next page)
```

```
prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = _
21
    \rightarrowNone, up = 2, dw = None))
   Initial(prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = __
22
    \rightarrowNone, up = None, dw = 1) %
            prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = _
23
    \rightarrowNone, up = 1, dw = None),
            Parameter('t0_cplx_lacAx2_cyt', 0))
24
   Observable('obs_cplx_lacAx2_cyt',
25
            prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = _
26
    \rightarrowNone, up = None, dw = 1) %
            prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = __
27
    \rightarrowNone, up = 1, dw = None))
   Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna = ...)
28
    \rightarrowNone, up = None, dw = 1) %
            prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna = _
29
    \rightarrowNone, up = 1, dw = None),
            Parameter('t0_cplx_lacIx2_cyt', 0))
   Observable('obs_cplx_lacIx2_cyt',
31
            prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna = _
32
    \rightarrowNone, up = None, dw = 1) %
            prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna = __
33
    \rightarrowNone, up = 1, dw = None))
   Initial(prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = _
34
    \rightarrowNone, up = None, dw = 1) %
            prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = _
    \rightarrowNone, up = 1, dw = 2) %
            prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
36
    \rightarrowNone, up = 2, dw = 3) %
            prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = __
37
    \rightarrowNone, up = 3, dw = None),
            Parameter('t0_cplx_lacZx4_cyt', 0))
   Observable('obs_cplx_lacZx4_cyt',
39
            prot (name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
40
    \rightarrowNone, up = None, dw = 1) %
            prot (name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
41
    \rightarrowNone, up = 1, dw = 2) %
            prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = _
42
    \rightarrowNone, up = 2, dw = 3) %
            prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = __
    \rightarrowNone, up = 3, dw = None))
   Initial(prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
44
    \rightarrowNone, up = None, dw = 1) %
            prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = _
45
    \rightarrowNone, up = 1, dw = None),
            Parameter('t0_cplx_lacZx2_cyt', 0))
47
   Observable('obs_cplx_lacZx2_cyt',
            prot(name = 'lacz', loc = 'cyt', dna = None, met = None, prot = None, rna = _
48
    \rightarrowNone, up = None, dw = 1) %
            prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = _
49
    \rightarrowNone, up = 1, dw = None))
   Rule ('PhysicalInteractionRule_1',
            prot (name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna = __
51
    \rightarrowNone, up = None, dw = None) +
            prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
52
    →None, up = None, dw = None)
            prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
53
    \rightarrowNone, up = None, dw = 1) %
```

```
prot (name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna = _
54
    \rightarrowNone, up = 1, dw = None),
            Parameter('fwd_PhysicalInteractionRule_1', 1.000000),
55
            Parameter('rvs_PhysicalInteractionRule_1', 0.000000))
   Rule('PhysicalInteractionRule_2',
57
            prot (name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna = _
58
    \rightarrowNone, up = None, dw = 1) %
            prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna = _
59
    \rightarrowNone, up = 1, dw = None) +
            prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna = _
60
    \rightarrowNone, up = None, dw = 2) %
            prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna = _
61
    \rightarrowNone, up = 2, dw = None)
            prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
62
    \rightarrowNone, up = None, dw = 1) %
            prot (name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna = _
63
    \rightarrowNone, up = 1, dw = 2) %
            prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna = __
    \rightarrowNone, up = 2, dw = 3) %
            prot (name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
65
    \rightarrowNone, up = 3, dw = None),
            Parameter ('fwd_PhysicalInteractionRule_2', 1.000000),
66
            Parameter('rvs_PhysicalInteractionRule_2', 0.000000))
67
   Rule ('PhysicalInteractionRule_3',
            prot(name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna = _
    \rightarrowNone, up = None, dw = None) +
            prot (name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
70
    →None, up = None, dw = None)
            prot (name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna = _
71
    \rightarrowNone, up = None, dw = 1) %
            prot(name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
72
    \rightarrowNone, up = 1, dw = None),
            Parameter ('fwd_PhysicalInteractionRule_3', 1.000000),
73
            Parameter ('rvs_PhysicalInteractionRule_3', 0.000000))
74
   Rule('PhysicalInteractionRule_4',
75
            prot(name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna = _
76
    →None, up = None, dw = None) +
            prot (name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
    \rightarrowNone, up = None, dw = 1) %
            prot (name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
78
    \rightarrowNone, up = 1, dw = None)
            prot(name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna = _
79
    \rightarrowNone, up = None, dw = 1) %
            prot (name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
    \rightarrowNone, up = 1, dw = 2) %
            prot(name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
81
    \rightarrowNone, up = 2, dw = None),
            Parameter ('fwd_PhysicalInteractionRule_4', 1.000000),
82
            Parameter('rvs_PhysicalInteractionRule_4', 0.000000))
83
84
   Rule('PhysicalInteractionRule_5',
            prot (name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
    →None, up = None, dw = None) +
            prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
86
    →None, up = None, dw = None)
            prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = __
87
    \rightarrowNone, up = None, dw = 1) %
            prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
                                                                                   (continues on next page)
    →None, up = 1, dw = None),
```

```
Parameter('fwd_PhysicalInteractionRule_5', 1.000000),
Parameter('rvs_PhysicalInteractionRule_5', 0.000000))
```

3.3 Protein-Small compounds Interaction Networks

Protein-small compound interaction networks have five columns:

- 1. The 1st declares the SOURCE and the 2nd declares the TARGET.
 - It does not matter the order, as the two columns defines a bimolecular reaction which product is the merge of all components into one complex. *Atlas* understand components inside brackets (e.g. <code>[lacZ, SMALL-alpha-ALLOLACTOSE]</code>) as a complex, therefore, the components are internally linked.
- 2. The 3rd and 4th columns declare the forward and the reverse reaction rates, respectively.
- 3. The 5th columns declares the location of the complex components:
 - 1. If the number of locations match the number of components of the complex, each location is mapped to the component.
 - 2. If the number of locations unmatch the number of components, the first location is used for every component
 - 3. If the number of locations is one, the location is used for every component.

Valid names are: cytosol, inner membrane, periplasmic space, membrane, outer membrane, extracellular space, bacterial nucleoid, cell wall, cell projection and cytoskeleton

Example, and note the use of the prefix SMALL- to tell Atlas the component is a metabolite:

```
SOURCE
               TARGET
                             FWD RATE
                                            RVS_RATE
                                                           LOCATION
                                                             0.0001
2
  [lacI,lacI]
                   SMALL-alpha-ALLOLACTOSE
                                                 10.0
                                                                          cytosol
  [lacI, lacI, SMALL-alpha-ALLOLACTOSE] SMALL-alpha-ALLOLACTOSE
                                                                         10.
           0.0001
                         cytosol
  [lacI,lacI]
                    SMALL-beta-ALLOLACTOSE
                                                           0.0001
                                                                          cytosol
                                               10.0
  [lacI, lacI, SMALL-beta-ALLOLACTOSE] SMALL-beta-ALLOLACTOSE
                                                                       10.0
                                                                                  0.
  →0001
              cytosol
```

Finally, execute atlas_rbm.construct_model_from_interaction_network(network, verbose = False) to obtain the model.

Note: Uniqueness of Rule names. Atlas will write *Rules* with numbered names. Merge into one the networks (pandas.concat(list)) or use a single file to model interactions.

Note: Simulation. The model can be simulated only with the instantiation of Initials:

- atlas_rbm.simulation.set_initial.cplx(model, complex_name, location, positive_number)
- atlas_rbm.simulation.set_initial.dna(model, dna_name, positive_number)
- atlas_rbm.simulation.set_initial.met(model, metabolite, location, positive_number)

- atlas_rbm.simulation.set_initial.prot(model, prot_name, location, positive_number)
- atlas_rbm.simulation.set_initial.rna(model, rna_name, positive_number)

Note: Use the keyword argument toFile = 'name.py' to write the model to a file (the function will return None):

```
from pysb import *
   Model()
2
   Monomer ('met',
4
            ['name', 'loc', 'dna', 'met', 'prot', 'rna'],
            { 'name' : [ 'alpha_ALLOLACTOSE', 'beta_ALLOLACTOSE' ],
6
            'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
   → 'omem']})
   Monomer('prot',
           ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
Q
            { 'name' : [ 'lacI' ],
10
           'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
11
   Observable('obs_met_alpha_ALLOLACTOSE_cyt', met(name = 'alpha_ALLOLACTOSE', loc = 'cyt
12
   Initial (met (name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = _
13
   →None, rna = None), Parameter('t0_met_alpha_ALLOLACTOSE_cyt', 0))
   Observable('obs_met_beta_ALLOLACTOSE_cyt', met(name = 'beta_ALLOLACTOSE', loc = 'cyt
   Initial (met (name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = __
15
   →None, rna = None), Parameter('t0_met_beta_ALLOLACTOSE_cyt', 0))
   Observable('obs_prot_lacI_cyt', prot(name = 'lacI', loc = 'cyt', dna = None, met = _
16
   →None, prot = None, rna = None, up = None, dw = None))
   Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna = _
17
   →None, up = None, dw = None), Parameter('t0_prot_lacI_cyt', 0))
   Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
18
   \rightarrow up = None, dw = 1) %
           prot(name = 'lacI', loc = 'cyt', dna = None, met = 3, prot = None, rna = None,
19
   \rightarrow up = 1, dw = None) %
           met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 3,
20
   → rna = None) %
           met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2,
21
   → rna = None),
           Parameter('t0_cplx_lacIx2_alpha_ALLOLACTOSEx2_cyt', 0))
22
   Observable('obs_cplx_lacIx2_alpha_ALLOLACTOSEx2_cyt',
23
           prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
24
   \rightarrow up = None, dw = 1) %
           prot(name = 'lacI', loc = 'cyt', dna = None, met = 3, prot = None, rna = None,
25
   \rightarrow up = 1, dw = None) %
           met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 3,
26
   → rna = None) %
           met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2,
27
   → rna = None))
   Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
   \rightarrow up = None, dw = 1) %
           prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna = __
29
   \rightarrowNone, up = 1, dw = None) %
           met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2,
30
      rna = None),
```

```
Parameter('t0_cplx_lacIx2_alpha_ALLOLACTOSEx1_cyt', 0))
31
   Observable('obs_cplx_lacIx2_alpha_ALLOLACTOSEx1_cyt',
32
            prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
33
    \rightarrow up = None, dw = 1) %
            prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna = __
34
    \rightarrowNone, up = 1, dw = None) %
           met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2,
35
    → rna = None))
   Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
36
    \rightarrow up = None, dw = 1) %
           prot(name = 'lacI', loc = 'cyt', dna = None, met = 3, prot = None, rna = None,
37
    \rightarrow up = 1, dw = None) %
           met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 3,...
    →rna = None) %
           met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2,_
    \rightarrowrna = None),
40
            Parameter('t0_cplx_lacIx2_beta_ALLOLACTOSEx2_cyt', 0))
   Observable('obs_cplx_lacIx2_beta_ALLOLACTOSEx2_cyt',
41
            prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
42
    \rightarrow up = None, dw = 1) %
            prot(name = 'lacI', loc = 'cyt', dna = None, met = 3, prot = None, rna = None,
43
    \rightarrow up = 1, dw = None) %
            met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 3,_
44
    →rna = None) %
            met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2,_
    →rna = None))
   Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
46
    → up = None, dw = 1) %
            prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna = __
47
    \rightarrowNone, up = 1, dw = None) %
           met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2,...
    →rna = None),
            Parameter('t0_cplx_lacIx2_beta_ALLOLACTOSEx1_cyt', 0))
49
   Observable ('obs_cplx_lacIx2_beta_ALLOLACTOSEx1_cyt',
50
            prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
51
    \rightarrow up = None, dw = 1) %
            prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna = __
52
    \rightarrow None, up = 1, dw = None) %
           met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2, ...
    →rna = None))
   Rule ('PhysicalInteractionRule_1',
54
            prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = __
55
    \rightarrowNone, up = None, dw = 1) %
            prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
    \rightarrowNone, up = 1, dw = None) +
            met (name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, prot = None, met = ...
57
    →None, rna = None) |
            prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 2, rna = None,
58
    \rightarrow up = None, dw = 1) %
            prot (name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = _
    \rightarrowNone, up = 1, dw = None) %
           met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 2, met = None,
    → rna = None),
            Parameter ('fwd_PhysicalInteractionRule_1', 10.000000),
61
62
            Parameter('rvs_PhysicalInteractionRule_1', 0.000100))
63
   Rule('PhysicalInteractionRule_2',
            prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 2, rna = None,
                                                                                  (continues on next page)

→ up = None, dw = 1) %
```

26

```
prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = __
65
    \rightarrowNone, up = 1, dw = None) %
           met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 2, met = None,
66
    → rna = None) +
           met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, prot = None, met = ...
67
   →None, rna = None)
           prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 2, rna = None,
68
   \rightarrow up = None, dw = 1) %
           prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 3, rna = None,
69
   \rightarrow up = 1, dw = None) %
           met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 3, met = None,
    → rna = None) %
71
           met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 2, met = None,
   → rna = None),
            Parameter ('fwd_PhysicalInteractionRule_2', 10.000000),
72.
            Parameter('rvs_PhysicalInteractionRule_2', 0.000100))
73
   Rule('PhysicalInteractionRule_3',
74
            prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
75
    \rightarrowNone, up = None, dw = 1) %
            prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = _
76
    \rightarrowNone, up = 1, dw = None) +
           met (name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = None, met = ...
77
   →None, rna = None) |
           prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 2, rna = None,
    \rightarrow up = None, dw = 1) %
           prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = ___
   \rightarrowNone, up = 1, dw = None) %
           met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 2, met = None,...
80
   →rna = None),
           Parameter('fwd_PhysicalInteractionRule_3', 10.000000),
81
           Parameter('rvs_PhysicalInteractionRule_3', 0.000100))
   Rule('PhysicalInteractionRule_4',
83
           prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 2, rna = None,
84
   \rightarrow up = None, dw = 1) %
           prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = __
85
   \rightarrowNone, up = 1, dw = None) %
           met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 2, met = None, __
    →rna = None) +
           met (name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = None, met = __
   →None, rna = None)
           prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 2, rna = None,
88
    \rightarrow up = None, dw = 1) %
           prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 3, rna = None,
    → up = 1, dw = None) %
           met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 3, met = None,_
    →rna = None) %
           met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 2, met = None,...
91
   \rightarrowrna = None),
            Parameter ('fwd_PhysicalInteractionRule_4', 10.000000),
92
           Parameter ('rvs_PhysicalInteractionRule_4', 0.000100))
```

3.4 Transcription Factor-DNA Binding Site Interaction Networks

The transcription factor-DNA binding site network represents the physical interaction bewteen proteins and DNA. The network have five columns:

1. The 1st declares the SOURCE and the 2nd declares the TARGET.

It does not matter the order, as the two columns defines a bimolecular reaction which product is the merge of all components into one complex. *Atlas* understand components inside brackets (e.g. [lacI,lacI]) as a complex, therefore, the components are internally linked.

- 2. The 3rd and 4th columns declare the forward and the reverse reaction rates, respectively.
- 3. The 5th columns declares the location of the complex components:
 - 1. If the number of locations match the number of components of the complex, each location is mapped to the component.
 - If the number of locations unmatch the number of components, the first location is used for every component
 - 3. If the number of locations is one, the location is used for every component.

Valid name is: cytosol.

Example, and note the use of the prefix BS- to tell *Atlas* the component is a DNA binding site followed by a name and two coordinates:

1	SOURCE	TARGET	FWD_RATE	RVS_	RATE	LOCATION	
2	# lacZYA						
3	[lacI,lacI]	BS-la	cI-422-402	1.0	0.01	cytosol	
4	[lacI,lacI]	BS-la	cI-21-1	1.0	0.01	cytosol	
5	[lacI,lacI]	BS-la	cI-72-92	1.0	0.01	cytosol	

Finally, execute atlas_rbm.construct_model_from_interaction_network (network, verbose = False) to obtain the model.

Note: Uniqueness of Rule names. Atlas will write *Rules* with numbered names. Merge into one the networks (pandas.concat(list)) or use a single file to model interactions.

Note: Simulation. The model can be simulated only with the instantiation of Initials:

- atlas_rbm.simulation.set_initial.cplx(model, complex_name, location, positive_number)
- atlas_rbm.simulation.set_initial.dna(model, dna_name, positive_number)
- atlas_rbm.simulation.set_initial.met(model, metabolite, location, positive_number)
- atlas_rbm.simulation.set_initial.prot(model, prot_name, location, positive number)
- atlas_rbm.simulation.set_initial.rna(model, rna_name, positive_number)

Note: Use the keyword argument toFile = 'name.py' to write the model to a file (the function will return None):

```
from pysb import *
1
   Model()
2
3
   Monomer ('prot',
            ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
            { 'name' : [ 'lacI' ],
            'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
   → 'omem']})
   Monomer('dna',
            ['name', 'type', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
            { 'name' : [ 'lacI_21_1', 'lacI_422_402', 'lacI_72_92' ],
10
            'type' : ['BS'],
11
            'loc' : ['cyt']})
12
   Observable('obs_prot_lacI_cyt', prot(name = 'lacI', loc = 'cyt', dna = None, met = _
13
   →None, prot = None, rna = None, up = None, dw = None))
   Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna = _
14
   →None, up = None, dw = None), Parameter('t0_prot_lacI_cyt', 0))
   Rule ('PhysicalInteractionRule_1',
15
           prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = __
   \rightarrowNone, up = None, dw = 1) %
           prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
17
   \rightarrowNone, up = 1, dw = None) +
           dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, prot = None,
18
   \hookrightarrowmet = None, rna = None, up = WILD, dw = WILD) |
           prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = __
   \rightarrowNone, up = None, dw = 1) %
           prot(name = 'lacI', loc = 'cyt', dna = 2, prot = None, met = None, rna = None,
20
   \rightarrow up = 1, dw = None) %
           dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, prot = 2,...
21
   →met = None, rna = None, up = WILD, dw = WILD),
           Parameter('fwd_PhysicalInteractionRule_1', 1.000000),
22
           Parameter('rvs_PhysicalInteractionRule_1', 0.010000))
23
   Rule('PhysicalInteractionRule_2',
24
           prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = ...
25
   \rightarrowNone, up = None, dw = 1) %
           prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = _
26
   \rightarrowNone, up = 1, dw = None) +
            dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, prot = None, __
    →met = None, rna = None, up = WILD, dw = WILD) |
            prot (name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = _
28
    \rightarrowNone, up = None, dw = 1) %
           prot(name = 'lacI', loc = 'cyt', dna = 2, prot = None, met = None, rna = None,
29
   \rightarrow up = 1, dw = None) %
            dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, prot = 2, met = _
   →None, rna = None, up = WILD, dw = WILD),
            Parameter('fwd_PhysicalInteractionRule_2', 1.000000),
31
           Parameter('rvs_PhysicalInteractionRule_2', 0.010000))
32
   Rule('PhysicalInteractionRule_3',
33
           prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = _
34
   \rightarrowNone, up = None, dw = 1) %
            prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = _
    \rightarrowNone, up = 1, dw = None) +
            dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, prot = None,
36
   →met = None, rna = None, up = WILD, dw = WILD)
           prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = _ ...
37
   \rightarrowNone, up = None, dw = 1) %
           prot(name = 'lacI', loc = 'cyt', dna = 2, prot = None, met = None, rna = None,
      up = 1, dw = None) %
                                                                                 (continues on next page)
```

```
dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, prot = 2, met_

None, rna = None, up = WILD, dw = WILD),

Parameter('fwd_PhysicalInteractionRule_3', 1.000000),

Parameter('rvs_PhysicalInteractionRule_3', 0.010000))
```

3.5 Sigma Factor-Promoter Interaction Networks

The Sigma Factor-Promoter network have five columns:

1. The 1st declares the SOURCE and the 2nd declares the TARGET.

It does not matter the order, as the two columns defines a bimolecular reaction which product is the merge of all components into one complex. *Atlas* understand components inside brackets (e.g. [rpoA, rpoA, rpoB, rpoC, rpoD]) as a complex, therefore, the components are internally linked.

- 2. The 3rd, 4th, and 5th columns declare rates:
 - The FWD_DOCK_RATE and the RVS_DOCK_RATE define the rates of the binding of the RNAP to the promoter and its separation, respectively.
 - The FWD_SLIDE_RATE defines the rate of the transition from the promoter to the following DNA feature declared in the genome graph.

Note the name of the promoter: name of the gene followed by \propto and a number.

Examples:

1	SOURCE TARGET	FWD_DOCK_RATE	RVS_DOCK_RATE		FWD_SLIDE_RATE	
2	#Docking to promoters					
3	[rpoA,rpoA,rpoB,rpoC,rpoD]	lacZ-pro4	1.0	1.0	1.0	
4	[rpoA,rpoA,rpoB,rpoC,rpoD]	lacZ-pro3	1.0	1.0	1.0	
5	[rpoA,rpoA,rpoB,rpoC,rpoD]	lacZ-pro2	1.0	1.0	1.0	
6	[rpoA,rpoA,rpoB,rpoC,rpoD]	lacZ-pro1	1.0	1.0	1.0	
7	[rpoA,rpoA,rpoB,rpoC,rpoD]	lacY-pro1	1.0	1.0	1.0	

Finally, execute atlas_rbm.construct_model_from_sigma_specificity_network(interaction_network, genome_graph, verbose = False) to obtain the model.

Note: Simulation. The model can be simulated only with the instantiation of Initials:

- atlas_rbm.simulation.set_initial.cplx(model, complex_name, location, positive_number)
- atlas_rbm.simulation.set_initial.dna(model, dna_name, positive_number)
- atlas_rbm.simulation.set_initial.met(model, metabolite, location, positive_number)
- atlas_rbm.simulation.set_initial.prot(model, prot_name, location, positive_number)
- atlas_rbm.simulation.set_initial.rna(model, rna_name, positive_number)

Note: Use the keyword argument toFile = 'name.py' to write the model to a file (the function will return None):

```
from pysb import *
   Model()
2
3
   Monomer ('dna',
4
           ['name', 'type', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
            { 'name' : ['lacA', 'lacI_21_1', 'lacI_422_402', 'lacI_72_92', 'lacY', 'lacZ
   'type': ['BS', 'cds', 'pro1', 'pro2', 'pro3', 'pro4', 'rbs', 'ter1', 'ter2'],
            'loc' : ['cyt']})
8
   Monomer('rna',
9
            ['name', 'type', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
10
            { 'name' : ['lacA', 'lacI_21_1', 'lacI_422_402', 'lacI_72_92', 'lacY', 'lacZ
11
    \hookrightarrow '],
            'type': ['BS', 'cds', 'pro1', 'pro2', 'pro3', 'pro4', 'rbs', 'ter1', 'ter2'],
12
            'loc' : ['cyt']})
13
   Monomer ('prot',
14
           ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
15
            { 'name' : ['lacA', 'lacI_21_1', 'lacI_422_402', 'lacI_72_92', 'lacY', 'lacZ
   'loc' : ['cyt', 'mem']})
17
   Monomer ('cplx',
18
            ['name', 'loc', 'dna', 'met', 'prot', 'rna'],
19
            { 'name' : ['RIBOSOME_CPLX'],
20
           'loc' : ['cyt']})
21
   Rule('docking_1_lacZ_pro4',
22
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
23
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
24
           prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
25
           prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
26
           prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = 4, dw = None) +
27
           dna(name = 'lacZ', type = 'pro4', loc = 'cyt', prot = None, up = WILD, dw = _
    →WILD)
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
29
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
30
           prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
31
           prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
32
           prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
33
           dna(name = 'lacz', type = 'pro4', loc = 'cyt', prot = 5, up = WILD, dw =_
34
    →WILD),
           Parameter ('fwd_docking_1_lacZ_pro4', 1.000000),
35
           Parameter ('rvs_docking_1_lacZ_pro4', 1.000000))
36
   Rule('docking_2_lacZ_pro3',
37
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
38
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
39
           prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
           prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
41
           prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = 4, dw = None) +
42
           dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = None, up = WILD, dw = _
43
   \hookrightarrow WTT_iD)
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
44
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
45
           prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
46
           prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
47
           prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
48
           dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = 5, up = WILD, dw =__
49
    →WILD),
           Parameter('fwd_docking_2_lacZ_pro3', 1.000000),
```

```
Parameter ('rvs_docking_2_lacZ_pro3', 1.000000))
51
   Rule('docking_3_lacZ_pro2',
52
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
53
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
54
           prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
55
           prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
56
           prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = 4, dw = None) +
57
           dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = None, up = WILD, dw = ...
58
    \hookrightarrow WTI_D)
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
59
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
           prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
62
           prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
           prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
63
           dna(name = 'lacz', type = 'pro2', loc = 'cyt', prot = 5, up = WILD, dw =_
64
    →WITD).
           Parameter('fwd_docking_3_lacZ_pro2', 1.000000),
65
           Parameter('rvs_docking_3_lacZ_pro2', 1.000000))
66
   Rule('docking_4_lacZ_pro1',
67
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
68
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2)
69
           prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
70
           prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
71
           prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = 4, dw = None) +
72
           dna(name = 'lacZ', type = 'prol', loc = 'cyt', prot = None, up = WILD, dw = _
73
    →WILD) |
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
74
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
75
           prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
76
           prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
77
           prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
78
           dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = 5, up = WILD, dw =_
79
    →WITID).
           Parameter ('fwd_docking_4_lacZ_pro1', 1.000000),
80
           Parameter('rvs_docking_4_lacZ_pro1', 1.000000))
81
   Rule('docking_5_lacY_pro1',
82
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
83
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
           prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
           prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
86
           prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = 4, dw = None) +
87
           dna(name = 'lacY', type = 'prol', loc = 'cyt', prot = None, up = WILD, dw = _
88
    →WILD)
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
89
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
90
           prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
91
           prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
92
           prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
93
           dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = 5, up = WILD, dw =_
94
    \hookrightarrowWILD),
           Parameter ('fwd_docking_5_lacY_pro1', 1.000000),
           Parameter('rvs_docking_5_lacY_pro1', 1.000000))
   Rule('sliding_1_lacZ_pro4_pro3_holoenzyme',
97
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
98
           prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
99
           prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
100
           prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
```

```
prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
102
            dna(name = 'lacz', type = 'pro4', loc = 'cyt', prot = 5, up = WILD, dw =_
103
    \rightarrow WTI.D) +
            dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = None, up = WILD, dw = _
104
    →WILD) +
            None >>
105
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
106
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
107
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
108
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
109
            prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = None, dw = __
110
    →None) %
            dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = 4, up = WILD, dw = ...
111
    →WILD) +
            dna(name = 'lacZ', type = 'pro4', loc = 'cyt', prot = None, up = WILD, dw = _
112
    →WIID) +
            rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot = _
113
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_1_lacZ_pro4_pro3_holoenzyme', 1.000000))
114
   Rule('sliding_2_lacZ_pro3_pro2_holoenzyme',
115
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
116
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
117
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
118
            prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
119
            prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
120
121
            dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = 5, up = WILD, dw = ...
    →WILD) +
            dna(name = 'lacz', type = 'pro2', loc = 'cyt', prot = None, up = WILD, dw = ...
122
    →WIID) +
            None >>
123
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
124
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
125
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
126
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
127
            prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = None, dw = _
128
    →None) %
            dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = 4, up = WILD, dw =
129
    →WTT<sub>1</sub>D) +
            dna(name = 'lacz', type = 'pro3', loc = 'cyt', prot = None, up = WILD, dw = __
    →WIID) +
            rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = _
131
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_2_lacZ_pro3_pro2_holoenzyme', 1.000000))
132
   Rule('sliding_3_lacZ_pro2_92_holoenzyme',
133
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
134
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
135
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
136
            prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
137
            prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
138
            dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = 5, up = WILD, dw =_
139
    →WILD) +
            dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = None, up = WILD, dw_
140
    →= WILD) +
            None >>
141
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
142
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
143
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
```

```
prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
145
            prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = None, dw = ...
146
    →None) %
            dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = 4, up = WILD, dw =_
147
    →WILD) +
            dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = None, up = WILD, dw = _
148
    →WILD) +
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,...
149
    →prot = None, rna = None, up = None, dw = None),
           Parameter('fwd_sliding_3_lacZ_pro2_92_holoenzyme', 1.000000))
150
   Rule ('sliding_4_lacZ_pro1_rbs_holoenzyme',
151
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
152
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
153
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
154
            prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
155
            prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
156
            dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = 5, up = WILD, dw =_
157
    →WILD) +
            dna (name = 'lacZ', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw = _
158
    →WILD) +
           None >>
159
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
160
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
161
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
162
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
163
           prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = None, dw = ...
164
    →None) %
            dna(name = 'lacz', type = 'rbs', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
165
            dna(name = 'lacZ', type = 'prol', loc = 'cyt', prot = None, up = WILD, dw = _
166
    →WILD) +
167
           rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
    →None, rna = None, up = None, dw = None),
           Parameter ('fwd_sliding_4_lacZ_pro1_rbs_holoenzyme', 1.000000))
168
   Rule ('sliding_5_lacY_pro1_rbs_holoenzyme',
169
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
170
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
171
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
            prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
            prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
174
            dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = 5, up = WILD, dw = ...
175
    →WILD) +
            dna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw = _
176
    →WILD) +
177
            None >>
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
178
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
179
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
180
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
181
            prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = None, dw = _
182
    →None) %
            dna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
183
            dna(name = 'lacY', type = 'prol', loc = 'cyt', prot = None, up = WILD, dw = ...
184
    →WILD) +
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
185
    →None, rna = None, up = None, dw = None),
```

```
Parameter ('fwd sliding 5 lacY pro1 rbs holoenzyme', 1.000000))
186
    Rule('sliding_1_lacZ_pro3_to_lacZ_pro2',
187
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
188
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
189
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
190
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
191
            dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = 4, up = WILD, dw = ...
192
    →WILD)
            dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = None, up = WILD, dw = _
193
    \hookrightarrowWILD) +
            None >>
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
195
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
197
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
198
            dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = 4, up = WILD, dw =_
199
    \hookrightarrow WTI_iD) +
            dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = None, up = WILD, dw = _
200
    →WILD) +
            rna (name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = ...
201
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_1_lacZ_pro3_to_lacZ_pro2', 1.000000))
202
    Rule('sliding_2_lacZ_pro2_to_BS_lacI_72_92',
203
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
204
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
207
            dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = 4, up = WILD, dw =_
208
    →WIID) +
            dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = None, up = WILD, dw_
209
    →= WILD) +
            None >>
210
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
211
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
212
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
213
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
214
            dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = 4, up = WILD, dw =_
    →WTID) +
            dna(name = 'lacz', type = 'pro2', loc = 'cyt', prot = None, up = WILD, dw = __
    →WIID) +
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
217
    →prot = None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_2_lacZ_pro2_to_BS_lacI_72_92', 1.000000))
218
    Rule('sliding_3_BS_lacI_72_92_to_BS_lacI_21_1',
219
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
220
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
221
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3)
222
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
223
            dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = 4, up = WILD, dw =_
224
    →WILD) +
            dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', prot = None, up = WILD, dw.,
225
    →= WILD) +
            None >>
226
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
227
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
228
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
229
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
                                                                                (continues on next page)
```

```
dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', prot = 4, up = WILD, dw = _
231
    →WIID) +
            dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = None, up = WILD, dw_
232
    \rightarrow = WILD) +
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, _
233
    ⇒prot = None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_3_BS_lacI_72_92_to_BS_lacI_21_1', 1.000000))
234
    Rule('sliding_4_BS_lacI_21_1_to_lacZ_pro1',
235
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
236
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
237
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
238
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
            dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', prot = 4, up = WILD, dw = ...
    →WILD) +
            dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = None, up = WILD, dw = _
241
    \hookrightarrowWTID) +
242
            None >>
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
243
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
244
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
245
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
246
            dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = 4, up = WILD, dw =_
247
    \hookrightarrow WTI_iD) +
            dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', prot = None, up = WILD, dw_
    →= WILD) +
            rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = ...
249
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_4_BS_lacI_21_1_to_lacZ_pro1', 1.000000))
250
251
    Rule('sliding_5_lacZ_pro1_to_lacZ_rbs',
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
252
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
253
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
254
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
255
            dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = 4, up = WILD, dw = __
256
    →WILD) +
            dna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw =_
257
    →WILD) +
            None >>
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
260
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
261
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
262
            dna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
263
            dna(name = 'lacz', type = 'prol', loc = 'cyt', prot = None, up = WILD, dw =_
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
265
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_5_lacZ_pro1_to_lacZ_rbs', 1.000000))
266
267
    Rule('sliding_6_lacZ_rbs_to_lacZ_cds',
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
270
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
271
            dna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
272
            dna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = None, up = WILD, dw =
                                                                                (continues on next page)
    →WILD) +
```

```
None >>
274
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
275
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
276
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
277
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
278
            dna(name = 'lacz', type = 'cds', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
279
            dna (name = 'lacZ', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw =
280
    →WILD) +
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
281
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_6_lacZ_rbs_to_lacZ_cds', 1.000000))
282
    Rule('sliding_7_lacZ_cds_to_BS_lacI_422_402',
283
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
284
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
285
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
286
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
287
            dna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
288
            dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', prot = None, up = WILD,...
289
    \rightarrow dw = WILD) +
            None >>
290
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
291
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
292
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
293
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
            dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', prot = 4, up = WILD, dw.,
295
    →= WILD) +
            dna (name = 'lacZ', type = 'cds', loc = 'cyt', prot = None, up = WILD, dw =_
296
    \hookrightarrow WTI_iD) +
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,...
297
    ⇒prot = None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_7_lacZ_cds_to_BS_lacI_422_402', 1.000000))
298
    Rule('sliding_8_BS_lacI_422_402_to_lacY_pro1',
299
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
300
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
301
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
302
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
            dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', prot = 4, up = WILD, dw_
            dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = None, up = WILD, dw = ...
305
    →WILD) +
            None >>
306
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
308
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
309
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
310
            dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = 4, up = WILD, dw =_
311
    →WILD) +
            dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', prot = None, up = WILD,
312
    \rightarrow dw = WILD) +
            rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = __
313
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_8_BS_lacI_422_402_to_lacY_pro1', 1.000000))
314
315
   Rule('sliding_9_lacY_pro1_to_lacY_rbs',
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
316
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
                                                                                (continues on next page)
```

```
prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3)
318
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
319
            dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = 4, up = WILD, dw = _
320
    →WILD) +
            dna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw = _
321
    →WILD) +
            None >>
322
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
323
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
324
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
325
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) % = 1000
            dna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
327
            dna(name = 'lacY', type = 'prol', loc = 'cyt', prot = None, up = WILD, dw = _
328
    →WILD) +
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
329
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_9_lacY_pro1_to_lacY_rbs', 1.000000))
330
    Rule('sliding_10_lacY_rbs_to_lacY_cds',
331
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
332
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
333
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
334
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
335
            dna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
337
            dna(name = 'lacY', type = 'cds', loc = 'cyt', prot = None, up = WILD, dw = ...
    →WILD) +
            None >>
338
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
339
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
340
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
341
342
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
            dna(name = 'lacY', type = 'cds', loc = 'cyt', prot = 4, up = WILD, dw = WILD)...
343
            dna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw =
344
    →WILD) +
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
345
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_10_lacY_rbs_to_lacY_cds', 1.000000))
    Rule('sliding_11_lacY_cds_to_lacA_rbs',
347
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
348
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
349
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
350
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
351
352
            dna(name = 'lacY', type = 'cds', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
            dna (name = 'lacA', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw = __
353
    →WILD)
            None >>
354
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
355
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
357
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
358
            dna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = 4, up = WILD, dw = WILD)...
359
            dna(name = 'lacY', type = 'cds', loc = 'cyt', prot = None, up = WILD, dw =
360
    →WILD)
```

```
rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
361
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_11_lacY_cds_to_lacA_rbs', 1.000000))
362
   Rule('sliding_12_lacA_rbs_to_lacA_cds',
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
366
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
367
            dna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
368
            dna (name = 'lacA', type = 'cds', loc = 'cyt', prot = None, up = WILD, dw = _
    →WILD) +
           None >>
370
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
371
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
372
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
373
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
374
            dna(name = 'lacA', type = 'cds', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
375
            dna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw = ...
376
    →WILD)
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
377
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_12_lacA_rbs_to_lacA_cds', 1.000000))
378
   Rule('sliding_13_lacA_cds_to_lacA_ter1',
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
380
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
381
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
382
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
383
            dna(name = 'lacA', type = 'cds', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
384
            dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = None, up = WILD, dw =_
385
    →WILD) >>
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
386
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
387
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
388
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
389
            dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = 4, up = WILD, dw =_
    →WILD) +
            dna(name = 'lacA', type = 'cds', loc = 'cyt', prot = None, up = WILD, dw = ...
391
    →WILD),
           Parameter('fwd_sliding_13_lacA_cds_to_lacA_ter1', 1.000000))
392
   Rule('sliding_14_lacA_ter1_to_lacA_ter2',
393
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
395
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
396
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
397
            dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = 4, up = WILD, dw =_
398
    →WTT<sub>1</sub>D) +
            dna(name = 'lacA', type = 'ter2', loc = 'cyt', prot = None, up = WILD, dw =_
    →WILD) >>
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
401
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
402
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
403
            dna(name = 'lacA', type = 'ter2', loc = 'cyt', prot = 4, up = WILD, dw = _
404
    →WILD) +
```

```
dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = None, up = WILD, dw = ...
405
    →WILD),
            Parameter('fwd_sliding_14_lacA_ter1_to_lacA_ter2', 1.000000))
406
    Rule('falloff_from_lacA_ter1',
407
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3)
410
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
411
            dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = 4, up = WILD, dw =_
412
    \hookrightarrow WTT_iD) >>
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
413
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
415
            prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = None) +
416
            dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = None, up = WILD, dw =_
417
    →WITD).
            Parameter('fwd_falloff_from_lacA_ter1', 1.000000))
418
    Rule('falloff_from_lacA_ter2',
419
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
420
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
421
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3)
422
            prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
423
            dna(name = 'lacA', type = 'ter2', loc = 'cyt', prot = 4, up = WILD, dw =_
424
    →WILD) >>
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
425
            prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
426
            prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
427
            prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = None) +
428
            dna(name = 'lacA', type = 'ter2', loc = 'cyt', prot = None, up = WILD, dw = _
429
    →WILD),
            Parameter('fwd_falloff_from_lacA_ter2', 1.000000))
430
    Rule('dr_lacZ_rbs',
431
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
432
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = None) |
433
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
434
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = 1),
435
            Parameter ('fwd_dr_lacZ_rbs', 1.000000),
436
            Parameter('rvs_dr_lacZ_rbs', 1.000000))
    Rule('dr_lacY_rbs',
438
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
439
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = None) |
440
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
441
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = 1),
442
            Parameter ('fwd_dr_lacY_rbs', 1.000000),
443
444
            Parameter('rvs_dr_lacY_rbs', 1.000000))
    Rule ('dr_lacA_rbs',
445
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
446
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = None) |
447
448
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = 1),
449
            Parameter ('fwd_dr_lacA_rbs', 1.000000),
            Parameter('rvs_dr_lacA_rbs', 1.000000))
451
    Rule('sr_lacZ_rbs',
452
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
453
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = 1) +
454
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = None) +
455
            None >>
```

```
cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
457
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = 1) +
458
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = None) +
459
            prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = _
460
    →None, up = None, dw = None),
            Parameter('fwd_sr_lacZ_rbs', 1.000000))
461
   Rule('sr_lacY_rbs',
462
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
463
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = 1) +
464
            rna(name = 'lacY', type = 'cds', loc = 'cyt', prot = None) +
465
            None >>
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', prot = 1) +
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = None) +
469
            prot(name = 'lacY', loc = 'cyt', dna = None, met = None, prot = None, rna = _
470
    →None, up = None, dw = None),
            Parameter('fwd_sr_lacY_rbs', 1.000000))
471
   Rule('sr_lacA_rbs',
472
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
473
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = 1) +
474
            rna(name = 'lacA', type = 'cds', loc = 'cyt', prot = None) +
475
            None >>
476
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
477
            rna(name = 'lacA', type = 'cds', loc = 'cyt', prot = 1) +
478
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = None) +
            prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
480
    →None, up = None, dw = None),
            Parameter('fwd_sr_lacA_rbs', 1.000000))
481
   Rule('fr_lacZ_cds',
482
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
483
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = 1) >>
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
485
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = None),
486
            Parameter('fwd_fr_lacZ_cds', 1.000000))
487
   Rule('fr_lacY_cds',
488
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
489
            rna(name = 'lacY', type = 'cds', loc = 'cyt', prot = 1) >>
490
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
            rna(name = 'lacY', type = 'cds', loc = 'cyt', prot = None),
            Parameter ('fwd_fr_lacY_cds', 1.000000))
493
   Rule('fr lacA cds',
494
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
495
            rna(name = 'lacA', type = 'cds', loc = 'cyt', prot = 1) >>
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
            rna(name = 'lacA', type = 'cds', loc = 'cyt', prot = None),
498
            Parameter('fwd_fr_lacA_cds', 1.000000))
499
   Initial(prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = ...)
500
    →None, up = None, dw = None),
            Parameter('t0_prot_lacZ_cyt', 0))
501
502
   Observable('obs_prot_lacZ_cyt',
            prot (name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
    →None, up = None, dw = None))
   Initial(prot(name = 'lacY', loc = 'cyt', dna = None, met = None, prot = None, rna = ...)
504
    →None, up = None, dw = None),
            Parameter('t0_prot_lacY_cyt', 0))
505
   Observable('obs_prot_lacY_cyt',
            prot(name = 'lacY', loc = 'cyt', dna = None, met = None, prot = None, rna =
                                                                                (continues on next page)
    \rightarrowNone, up = None, dw = None))
```

```
Initial(prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = _
508
    →None, up = None, dw = None),
            Parameter('t0_prot_lacA_cyt', 0))
509
    Observable ('obs_prot_lacA_cyt',
            prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = __
511
    →None, up = None, dw = None))
    Initial(dna(name = 'lacZ', type = 'pro4', loc = 'cyt', dna = None, met = None, prot = _
512
    →None, rna = None, up = None, dw = 1) %
            dna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot = _
513
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            dna (name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
515
    ⇒prot = None, rna = None, up = 3, dw = 4) %
            dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, _
516
    \rightarrowprot = None, rna = None, up = 4, dw = 5) %
            dna(name = 'lacZ', type = 'prol', loc = 'cyt', dna = None, met = None, prot = _
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            dna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
518
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            dna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
519
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
520
    \rightarrowprot = None, rna = None, up = 8, dw = 9) %
            dna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
521
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            dna (name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
522
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            dna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
523
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            dna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
524
    →None, rna = None, up = 12, dw = 13) %
            dna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
525
    \rightarrowNone, rna = None, up = 13, dw = 14) %
            dna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
526
    \rightarrowNone, rna = None, up = 14, dw = 15) %
            dna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = _
527
    →None, rna = None, up = 15, dw = None),
            Parameter('t0_dna_lacZlacYlacA', 0))
528
    Observable ('obs_dna_lacZlacYlacA',
529
            dna(name = 'lacZ', type = 'pro4', loc = 'cyt', dna = None, met = None, prot = __
530
    \rightarrowNone, rna = None, up = None, dw = 1) %
            dna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot = _
531
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            dna(name = 'lacz', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = _
532
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,...
533
    \rightarrowprot = None, rna = None, up = 3, dw = 4) %
            dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, _
534
    \rightarrowprot = None, rna = None, up = 4, dw = 5) %
            dna(name = 'lacZ', type = 'prol', loc = 'cyt', dna = None, met = None, prot = _
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            dna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
536
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            dna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
537
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
                                                                                    (continues on next page)
     \rightarrowprot = None, rna = None, up = 8, dw = 9) %
```

42

```
dna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = _
539
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            dna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
540
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            dna(name = 'lacy', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
541
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            dna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
542
    \rightarrowNone, rna = None, up = 12, dw = 13) %
            dna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
543
    \rightarrowNone, rna = None, up = 13, dw = 14) %
            dna (name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 14, dw = 15) %
            dna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = ...
545
    \rightarrowNone, rna = None, up = 15, dw = None))
    Initial(rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot = _
546
    \rightarrowNone, rna = None, up = None, dw = 1) %
            rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = _
547
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None, __
548
    ⇒prot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, __
549
    →prot = None, rna = None, up = 3, dw = 4) %
            rna(name = 'lacZ', type = 'prol', loc = 'cyt', dna = None, met = None, prot = _
550
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
551
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
552
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
553
    →prot = None, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = ...
554
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
555
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
556
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
557
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
558
    \rightarrowNone, rna = None, up = 12, dw = 13) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
559
    →None, rna = None, up = 13, dw = None),
560
            Parameter('t0_rna_lacZlacYlacA_form1', 0))
561
    Observable('obs_rna_lacZlacYlacA_form1',
            rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot = _
562
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacz', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = ...
563
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
564
    \rightarrowprot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
    \rightarrowprot = None, rna = None, up = 3, dw = 4) %
            rna (name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = ...
566
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
567
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
                                                                                    (continues on next page)
    \rightarrowNone, rna = None, up = 6, dw = 7) %
```

```
rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
569
    →prot = None, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
570
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
571
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
572
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
573
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
574
    \rightarrowNone, rna = None, up = 12, dw = 13) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = ...
575
    \rightarrowNone, rna = None, up = 13, dw = None))
    Initial(rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot = _
576
    \rightarrowNone, rna = None, up = None, dw = 1) %
            rna(name = 'lacz', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = _
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None, __
578
    ⇒prot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, __
579
    →prot = None, rna = None, up = 3, dw = 4) %
            rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
580
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
581
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
582
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
583
    →prot = None, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = ...
584
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
585
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
586
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
587
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
588
    \rightarrowNone, rna = None, up = 12, dw = 13) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
589
    →None, rna = None, up = 13, dw = 14) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = _
    →None, rna = None, up = 14, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form2', 0))
591
    Observable('obs_rna_lacZlacYlacA_form2',
592
            rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot = __
593
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacz', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = __
594
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
    →prot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,...
596
    ⇒prot = None, rna = None, up = 3, dw = 4) %
            rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =_
597
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
                                                                                   (continues on next page)
    \rightarrowNone, rna = None, up = 5, dw = 6) %
```

```
rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
599
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None, ...
600
    →prot = None, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
601
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =_
602
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
603
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
605
    \rightarrowNone, rna = None, up = 12, dw = 13) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
606
    \rightarrowNone, rna = None, up = 13, dw = 14) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = _
607
    \rightarrowNone, rna = None, up = 14, dw = None))
    Initial(rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = __
608
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None, __
609
    →prot = None, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
610
    →prot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
611
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
612
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
613
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,...
614
    \rightarrowprot = None, rna = None, up = 6, dw = 7) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = ...
615
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
616
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
617
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
618
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
619
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =_
620
    →None, rna = None, up = 12, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form3', 0))
621
622
    Observable('obs_rna_lacZlacYlacA_form3',
            rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = __
623
    \rightarrowNone, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
624
    \rightarrowprot = None, rna = None, up = 1, dw = 2) %
625
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
    →prot = None, rna = None, up = 2, dw = 3) %
            rna (name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = ...
626
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
627
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
                                                                                    (continues on next page)
    \rightarrowNone, rna = None, up = 5, dw = 6) %
```

```
rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
629
    →prot = None, rna = None, up = 6, dw = 7) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = __
630
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacy', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
631
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
632
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
633
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = ...
635
    \rightarrowNone, rna = None, up = 12, dw = None))
    Initial(rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = _
636
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None, __
    →prot = None, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, _
638
    ⇒prot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacz', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
639
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
640
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
641
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None, _
642
    \rightarrowprot = None, rna = None, up = 6, dw = 7) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
643
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
645
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
646
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'terl', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 12, dw = 13) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = __
649
    \rightarrowNone, rna = None, up = 13, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form4', 0))
651
    Observable('obs_rna_lacZlacYlacA_form4',
            rna(name = 'lacz', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = _
652
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
653
    \rightarrowprot = None, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, _
654
    \rightarrowprot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
656
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
657
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
                                                                                   (continues on next page)
     →prot = None, rna = None, up = 6, dw =
```

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```
rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = _
659
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
660
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
661
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
662
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
663
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 12, dw = 13) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 13, dw = None))
    Initial(rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None, _
666
    →prot = None, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, __
667
    →prot = None, rna = None, up = 1, dw = 2) %
            rna(name = 'lacZ', type = 'prol', loc = 'cyt', dna = None, met = None, prot = __
668
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
669
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
670
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
671
    →prot = None, rna = None, up = 5, dw = 6) %
            rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = _
672
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
673
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
674
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
675
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
676
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
677
    →None, rna = None, up = 11, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form5', 0))
678
    Observable ('obs_rna_lacZlacYlacA_form5',
679
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
680
    →prot = None, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, __
681
    →prot = None, rna = None, up = 1, dw = 2) %
682
            rna(name = 'lacZ', type = 'prol', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
683
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
684
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
    →prot = None, rna = None, up = 5, dw = 6) %
            rna (name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = ...
686
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
687
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
                                                                                   (continues on next page)
    \rightarrowNone, rna = None, up = 8, dw = 9) %
```

```
rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
689
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
690
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
691
    →None, rna = None, up = 11, dw = None))
    Initial(rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,...)
692
    →prot = None, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, __
693
    →prot = None, rna = None, up = 1, dw = 2) %
            rna(name = 'lacZ', type = 'prol', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
695
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
696
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
    →prot = None, rna = None, up = 5, dw = 6) %
            rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = __
698
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
699
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
700
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
701
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
702
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = __
703
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = ...
    →None, rna = None, up = 12, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form6', 0))
705
    Observable('obs_rna_lacZlacYlacA_form6',
706
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None, _
707
    →prot = None, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
    \rightarrowprot = None, rna = None, up = 1, dw = 2) %
            rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
710
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
711
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
712
    \rightarrowprot = None, rna = None, up = 5, dw = 6) %
            rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = __
713
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
714
    \rightarrowNone, rna = None, up = 7, dw = 8) %
715
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
716
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
717
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
                                                                                    (continues on next page)
    \rightarrowNone, rna = None, up = 11, dw = 12) %
```

48

```
rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = _
719
    \rightarrowNone, rna = None, up = 12, dw = None))
    Initial(rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
720
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
721
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None, _
722
    ⇒prot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
723
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
725
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
726
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = __
728
    →None, rna = None, up = 8, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form7', 0))
729
    Observable('obs_rna_lacZlacYlacA_form7',
730
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
731
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
732
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None, _
733
    →prot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
734
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
735
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
736
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
737
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
738
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacA', type = 'terl', loc = 'cyt', dna = None, met = None, prot = ...
739
    \rightarrowNone, rna = None, up = 8, dw = None))
    Initial(rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =_
740
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
741
    \rightarrowNone, rna = None, up = 1, dw = 2) %
742
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
    \rightarrowprot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = __
743
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
744
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
746
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
747
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
                                                                                    (continues on next page)
    \rightarrowNone, rna = None, up = 8, dw = 9) %
```

50

```
rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = _
749
    \rightarrowNone, rna = None, up = 9, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form8', 0))
750
   Observable('obs_rna_lacZlacYlacA_form8',
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
752
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
753
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None, _
754
    →prot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = __
755
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
756
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
757
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
759
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = ...
760
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = _
761
    →None, rna = None, up = 9, dw = None))
    Initial(rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
762
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
763
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
764
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
765
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
766
    →None, rna = None, up = 4, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form9', 0))
767
    Observable ('obs_rna_lacZlacYlacA_form9',
768
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
771
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
772
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
773
    →None, rna = None, up = 4, dw = None))
    Initial(rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
774
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
775
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
777
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = __
778
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
                                                                                   (continues on next page)
    →None, rna = None, up = 5, dw = None),
```

```
Parameter('t0_rna_lacZlacYlacA_form10', 0))
780
    Observable ('obs_rna_lacZlacYlacA_form10',
781
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
782
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
783
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
784
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
785
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = __
786
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 5, dw = None))
```

3.6 Genome Graphs

The Genome Graphs have ten columns:

1. The 1st declares the UPSTREAM and the 2nd declares the DOWNSTREAM DNA feature.

The DNA features are five: pro followed by a number, rbs, cds, ter followed by a number, and BS- to define DNA binding sites.

- 2. The next columns declare rates:
 - RNAP_FWD_DOCK_RATE and RNAP_RVS_DOCK_RATE are valid values only for the description of the reversible interaction of the RNA Polymerase to the promoters.
 - RNAP_FWD_SLIDE_RATE are valid values for the transition of the RNA Polymerase from the UPSTREAM to the DOWNSTREAM DNA parts. We describe rules where the RNA Polymerase could not move back.
 - RNAP_FWD_FALL_RATE are valid values only for the description of the unbinding of the RNA Polymerase and the UPSTREAM identifiying a DNA terminator.
 - RIB_FWD_DOCK_RATE and RIB_RVS_DOCK_RATE are valid values only for the description of the reversible interaction of the bacterial Ribosome to the RBS.
 - RIB_FWD_SLIDE_RATE are valid values for the transition of the Ribosome from the UPSTREAM to the DOWNSTREAM RNA parts. We describe rules where the Ribosome could not move back.
 - RIB_FWD_FALL_RATE are valid values only for the description of the unbinding of the Ribosome and the UPSTREAM identifying a CDS.

Example, and note the use of the prefix BS- to tell *Atlas* the component is a DNA binding site followed by a name and two coordinates:

```
UPSTREAM
                  DOWNSTREAM
                                    RNAP_FWD_DOCK_RATE
                                                              RNAP_RVS_DOCK_
   →RATE
                RNAP_FWD_SLIDE_RATE
                                          RNAP_FWD_FALL_RATE
                                                                    RIB_FWD_DOCK_
   →RATE
                RIB_RVS_DOCK_RATE
                                         RIB_FWD_SLIDE_RATE
                                                                   RIB_FWD_FALL_RATE
                                             1
                                                      1
  [lacZ-pro4
                    lacZ-pro3
                                     1
2
  lacZ-pro3
                   lacZ-pro2
                                    1
                                             1
  lacZ-pro2
                   BS-lacI-72-92
                                        1
                                                 1
                                                          1
  BS-lacI-72-92
                      BS-lacI-21-1
                                                           1
  BS-lacI-21-1
                      lacZ-pro1
                                                       1
```

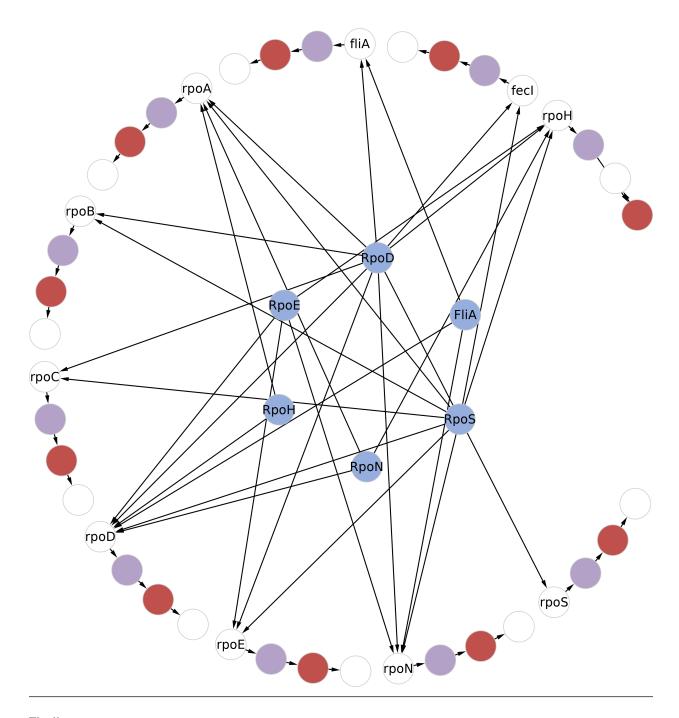
								,	1 10/
7	lacZ-pro1	lacZ-rbs	1	1		1			
8	lacZ-rbs	lacZ-							
	-cds	1			1		1	1	1
9	lacZ-cds	BS-lacI-422-402					1		
10	BS-lacI-422-402	lacY-pro	1				1		
11	lacY-pro1	lacY-rbs	0	0		1			
12	lacY-rbs	lacY-							
	-cds	1			1		1	1	1
13	lacY-cds	lacA-rbs			1				
14	lacA-rbs	lacA-							
	-cds	1			1		1	1	1
15	lacA-cds	lacA-ter1			1		1		
16	lacA-ter1	lacA-ter2]				1	1		

OR

,													
1	UPSTREAM	DOWNSTREAM		RNAP_	_FWDD	OCI	K_R.	ATE			RNAP	_RVS_I	DOCK_
	⇔RATE	RNAP_FWD_SLIDE_F	RATE		RNA	.P_1	FWD.	_FAI	LL_I	RATE		RII	B_FWD_DOCK_
	→RATE	RIB_RVS_DOCK_RAT	ΓE		RIB_F	'WD_	_SL	IDE_	_RA'	ΓE		RIB_l	FWD_FALL_RATE
2	[rpoA-pro1	rpoA-rbs		1	1				1				
3	rpoA-rbs	rpoA-											
	⇔cds		1				1			1		1	1
4	rpoA-cds	rpoA-ter1]						1			1		
5													
6	[rpoB-pro1	rpoB-rbs		1	1				1				
7	rpoB-rbs	rpoB-											
	→ cds		1				1			1		1	1
8	rpoB-cds	rpoC-rbs					1						
9	rpoC-rbs	rpoC-											
	->cds		1				1			1		1	1
10	rpoC-cds	rpoC-ter1]						1			1		
11													
12	[rpoD-pro1	rpoD-rbs		1	1				1				
13	rpoD-rbs	rpoD-											
	->cds		1				1			1		1	1
14	rpoD-cds	rpoD-ter1]						1			1		
15													
16	[rpoE-pro1	rpoE-rbs		1	1				1				
17	rpoE-rbs	rpoE-											
	⇔cds	-	1				1			1		1	1
18	rpoE-cds	rpoE-ter1]						1			1		
19													
20	[rpoH-pro1	rpoH-rbs		1	1				1				
21	rpoH-rbs	rpoH-											
	⇔cds		1				1			1		1	1
22	rpoH-cds	rpoH-ter1]						1			1		
23													
24	[rpoN-pro1	rpoN-rbs		1	1				1				
25	rpoN-rbs	rpoN-											
	→ cds	-	1				1			1		1	1
26	rpoN-cds	rpoN-ter1]						1			1		
27													
28	[rpoS-pro1	rpoS-rbs		1	1				1				
29	rpoS-rbs	rpoS-											
	⇔cds		1				1			1		1	1
30	rpoS-cds	rpoS-ter1]						1			1		
31													
													(continues on next page

32 33	[fliA-pro1 fliA-rbs	fliA-rbs fliA-		1	1		1				
	⇔cds		1			1		1		1	1
34	fliA-cds	fliA-ter1]					1		1		
35											
36	[fecI-pro1	fecI-rbs		1	1		1				
37	fecI-rbs	fecI-									
	⇔cds		1			1		1		1	1
38	fecI-cds	fecI-ter1]					1		1		

Note: Visualization in Cytoscape. Colors and arrows remains to the user for customization. The network could be complemented with a description of sigma factor specifity for promoter, as the following network



 $\label{eq:finally} Finally, \qquad execute \qquad \verb|atlas_rbm.construct_model_from_genome_graph(network, verbose = False) to obtain the model. \\$

Note: Simulation. The model can be simulated only with the instantiation of Initials:

- atlas_rbm.simulation.set_initial.cplx(model, complex_name, location, positive_number)
- atlas_rbm.simulation.set_initial.dna(model, dna_name, positive_number)
- atlas_rbm.simulation.set_initial.met(model, metabolite, location, positive_number)

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- atlas_rbm.simulation.set_initial.prot(model, prot_name, location, positive_number)
- atlas_rbm.simulation.set_initial.rna(model, rna_name, positive_number)

Note: Kappa BioBrick Framework. The *Rules* for transcription and translation come from the work of Stewart and Wilson-Kanamori (See more here). A "pure" genome graph uses the originally defined rules, while a genome graph + sigma factor specifity uses a modified *rules* to model the release of the sigma factor from the RNA Polymerase at the transcription initiation.

```
from pysb import *
   Model()
2
   Monomer ('dna',
            ['name', 'type', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
            { 'name' : ['lacI_21_1', 'lacI_422_402', 'lacI_72_92', 'lacA', 'lacY', 'lacZ
6
   'type': ['BS', 'cds', 'pro1', 'pro2', 'pro3', 'pro4', 'rbs', 'ter1', 'ter2'],
           'loc' : ['cyt']})
9
   Monomer ('rna',
            ['name', 'type', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
10
            { 'name' : ['lacI_21_1', 'lacI_422_402', 'lacI_72_92', 'lacA', 'lacY', 'lacZ
11
   ' ],
            'type': ['BS', 'cds', 'pro1', 'pro2', 'pro3', 'pro4', 'rbs', 'ter1', 'ter2'],
12
           'loc' : ['cyt']})
13
   Monomer ('prot',
            ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
            { 'name' : ['lacA', 'lacY', 'lacZ'],
16
           'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
17
   → 'omem']})
   Monomer ('cplx',
18
            ['name', 'loc', 'dna', 'met', 'prot', 'rna'],
19
            { 'name' : ['RNAP_CPLX', 'RIBOSOME_CPLX'],
20
            'loc' : ['cyt']})
21
   Rule ('docking_lacZ_pro4',
22
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = None) +
23
           dna(name = 'lacZ', type = 'pro4', loc = 'cyt', prot = None) |
24
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
25
           dna(name = 'lacZ', type = 'pro4', loc = 'cyt', prot = 1),
           Parameter ('fwd_docking_lacZ_pro4', 1.000000),
27
           Parameter ('rvs_docking_lacZ_pro4', 1.000000))
28
   Rule ('docking lacZ pro3',
29
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = None) +
30
           dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = None) |
31
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
32
           dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = 1),
33
           Parameter ('fwd_docking_lacZ_pro3', 1.000000),
34
           Parameter('rvs_docking_lacZ_pro3', 1.000000))
35
   Rule ('docking_lacZ_pro2',
36
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = None) +
37
           dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = None) |
38
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
           dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = 1),
           Parameter ('fwd_docking_lacZ_pro2', 1.000000),
41
           Parameter('rvs_docking_lacZ_pro2', 1.000000))
42
   Rule ('docking_lacZ_pro1',
```

```
cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = None) +
44
           dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = None) |
45
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
46
           dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = 1),
47
           Parameter ('fwd_docking_lacZ_pro1', 1.000000),
48
           Parameter('rvs_docking_lacZ_pro1', 1.000000))
49
   Rule ('docking_lacY_pro1',
50
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = None) +
51
           dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = None) |
52
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
53
           dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = 1),
           Parameter ('fwd_docking_lacY_pro1', 0.000000),
55
           Parameter('rvs_docking_lacY_pro1', 0.000000))
   Rule ('sliding_lacZ_pro4',
57
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
58
           dna(name = 'lacZ', type = 'pro4', loc = 'cyt', prot = 1) +
59
           dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = None) +
60
           None >>
61
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
62
           dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = 1) +
63
           dna(name = 'lacZ', type = 'pro4', loc = 'cyt', prot = None) +
64
           rna(name = 'lacz', type = 'pro3', loc = 'cyt', dna = None, met = None, prot = _
65
   →None, rna = None, up = None, dw = None),
           Parameter('fwd_sliding_lacZ_pro4', 1.000000))
   Rule('sliding_lacZ_pro3',
68
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
           dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = 1) +
69
           dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = None) +
70
71
           None >>
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
72
           dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = 1) +
73
           dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = None) +
74
           rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = _
75
   →None, rna = None, up = None, dw = None),
           Parameter('fwd_sliding_lacZ_pro3', 1.000000))
76
   Rule('sliding_lacZ_pro2',
77
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
78
           dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = 1) +
           dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = None) +
81
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
82
           dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = 1) +
83
           dna(name = 'lacz', type = 'pro2', loc = 'cyt', prot = None) +
84
           rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,...
   →prot = None, rna = None, up = None, dw = None),
           Parameter ('fwd_sliding_lacZ_pro2', 1.000000))
86
   Rule ('sliding_BS_lacI_72_92',
87
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
88
           dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = 1) +
89
           dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', prot = None) +
           None >>
           cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
           dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', prot = 1) +
93
           dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = None) +
94
           rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, __
95
   →prot = None, rna = None, up = None, dw = None),
           Parameter('fwd_sliding_BS_lacI_72_92', 1.000000))
```

```
Rule('sliding_BS_lacI_21_1',
97
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
98
            dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', prot = 1) +
gg
            dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = None) +
100
            None >>
101
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
102
            dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = 1) +
103
            dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', prot = None) +
104
            rna(name = 'lacz', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
105
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_BS_lacI_21_1', 1.000000))
   Rule ('sliding_lacZ_pro1',
107
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
108
            dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = 1) +
109
            dna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = None) +
110
111
            None >>
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
112
            dna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = 1) +
113
            dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = None) +
114
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
115
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_lacZ_pro1', 1.000000))
116
   Rule('sliding_lacZ_rbs',
117
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
118
            dna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = 1) +
119
            dna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = None) +
120
            None >>
121
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
122
            dna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = 1) +
123
            dna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = None) +
124
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
125
    →None, rna = None, up = None, dw = None),
            Parameter ('fwd_sliding_lacZ_rbs', 1.000000))
126
   Rule('sliding_lacZ_cds',
127
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
128
            dna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = 1) +
129
            dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', prot = None) +
130
131
            None >>
132
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
            dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', prot = 1) +
133
            dna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = None) +
134
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
135
    →prot = None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_lacZ_cds', 1.000000))
136
137
   Rule('sliding_BS_lacI_422_402',
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
138
            dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', prot = 1) +
139
            dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = None) +
140
141
            None >>
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
142
143
            dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = 1) +
            dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', prot = None) +
144
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = ...
145
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_BS_lacI_422_402', 1.000000))
146
147
   Rule('sliding_lacY_pro1',
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
148
```

```
dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = 1) +
149
            dna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = None) +
150
151
            None >>
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
152
            dna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = 1) +
153
            dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = None) +
154
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
155
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_lacY_pro1', 1.000000))
156
   Rule('sliding_lacY_rbs',
157
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
158
            dna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = 1) +
159
            dna(name = 'lacY', type = 'cds', loc = 'cyt', prot = None) +
160
            None >>
161
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
162
            dna(name = 'lacY', type = 'cds', loc = 'cyt', prot = 1) +
163
            dna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = None) +
164
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
165
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_lacY_rbs', 1.000000))
166
   Rule('sliding_lacY_cds',
167
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
168
            dna(name = 'lacY', type = 'cds', loc = 'cyt', prot = 1) +
169
            dna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = None) +
170
171
            None >>
172
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
            dna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = 1) +
173
            dna(name = 'lacY', type = 'cds', loc = 'cyt', prot = None) +
174
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
175
    →None, rna = None, up = None, dw = None),
            Parameter('fwd_sliding_lacY_cds', 1.000000))
176
   Rule('sliding_lacA_rbs',
177
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
178
            dna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = 1) +
179
            dna(name = 'lacA', type = 'cds', loc = 'cyt', prot = None) +
180
            None >>
181
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
            dna(name = 'lacA', type = 'cds', loc = 'cyt', prot = 1) +
            dna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = None) +
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
185
    →None, rna = None, up = None, dw = None),
186
            Parameter('fwd_sliding_lacA_rbs', 1.000000))
187
   Rule('sliding_lacA_cds',
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
188
            dna(name = 'lacA', type = 'cds', loc = 'cyt', prot = 1) +
189
            dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = None) +
190
            None >>
191
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
192
            dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = 1) +
193
            dna(name = 'lacA', type = 'cds', loc = 'cyt', prot = None) +
194
195
            rna(name = 'lacA', type = 'terl', loc = 'cyt', dna = None, met = None, prot = _
    →None, rna = None, up = None, dw = None),
            Parameter ('fwd_sliding_lacA_cds', 1.000000))
196
   Rule('sliding_lacA_ter1',
197
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
198
            dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = 1) +
199
            dna(name = 'lacA', type = 'ter2', loc = 'cyt', prot = None) +
```

```
None >>
201
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
202
            dna(name = 'lacA', type = 'ter2', loc = 'cyt', prot = 1) +
203
            dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = None) +
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = _
205
    →None, rna = None, up = None, dw = None),
            Parameter ('fwd_sliding_lacA_ter1', 1.000000))
206
    Rule('falloff_lacA_ter1',
207
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
208
            dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = 1) >>
209
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = None) +
            dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = None),
211
            Parameter('fwd_falloff_lacA_ter1', 1.000000))
212
    Rule ('falloff_lacA_ter2',
213
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
214
            dna(name = 'lacA', type = 'ter2', loc = 'cyt', prot = 1) >>
215
            cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = None) +
216
            dna(name = 'lacA', type = 'ter2', loc = 'cyt', prot = None),
217
            Parameter('fwd_falloff_lacA_ter2', 1.000000))
218
    Rule('dr_lacZ_rbs',
219
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
220
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = None) |
221
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
222
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = 1),
223
            Parameter('fwd_dr_lacZ_rbs', 1.000000),
224
225
            Parameter('rvs_dr_lacZ_rbs', 1.000000))
   Rule ('dr_lacY_rbs',
226
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
227
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = None) |
228
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
229
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = 1),
230
            Parameter('fwd_dr_lacY_rbs', 1.000000),
231
            Parameter('rvs_dr_lacY_rbs', 1.000000))
232
    Rule('dr_lacA_rbs',
233
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
234
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = None) |
235
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
236
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = 1),
238
            Parameter ('fwd_dr_lacA_rbs', 1.000000),
            Parameter ('rvs_dr_lacA_rbs', 1.000000))
239
    Rule('sr lacZ rbs',
240
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
241
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = 1) +
242
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = None) +
243
244
            None >>
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
245
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = 1) +
246
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = None) +
247
            prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = _
248
    →None, up = None, dw = None),
249
            Parameter('fwd_sr_lacZ_rbs', 1.000000))
250
   Rule('sr lacY rbs',
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
251
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = 1) +
252
            rna(name = 'lacY', type = 'cds', loc = 'cyt', prot = None) +
253
254
            None >>
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
```

60

```
rna(name = 'lacY', type = 'cds', loc = 'cyt', prot = 1) +
256
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = None) +
257
            prot(name = 'lacY', loc = 'cyt', dna = None, met = None, prot = None, rna = __
258
    →None, up = None, dw = None),
            Parameter('fwd_sr_lacY_rbs', 1.000000))
259
    Rule('sr_lacA_rbs',
260
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
261
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = 1) +
262
            rna(name = 'lacA', type = 'cds', loc = 'cyt', prot = None) +
263
            None >>
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', prot = 1) +
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = None) +
            prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = _
268
    →None, up = None, dw = None),
            Parameter('fwd_sr_lacA_rbs', 1.000000))
269
    Rule('fr_lacZ_cds',
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
271
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = 1) >>
272
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
273
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = None),
274
            Parameter('fwd_fr_lacZ_cds', 1.000000))
275
    Rule('fr_lacY_cds',
276
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
277
            rna(name = 'lacY', type = 'cds', loc = 'cyt', prot = 1) >>
278
279
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
            rna(name = 'lacY', type = 'cds', loc = 'cyt', prot = None),
280
            Parameter('fwd_fr_lacY_cds', 1.000000))
281
    Rule('fr_lacA_cds',
282
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
283
            rna(name = 'lacA', type = 'cds', loc = 'cyt', prot = 1) >>
            cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
285
            rna(name = 'lacA', type = 'cds', loc = 'cyt', prot = None),
286
            Parameter ('fwd_fr_lacA_cds', 1.000000))
287
    Initial(prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
288
    →None, up = None, dw = None),
            Parameter('t0_prot_lacZ_cyt', 0))
289
    Observable('obs_prot_lacZ_cyt',
            prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna = __
    \rightarrowNone, up = None, dw = None))
    Initial(prot(name = 'lacY', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
292
    \rightarrowNone, up = None, dw = None),
            Parameter('t0_prot_lacY_cyt', 0))
293
294
    Observable('obs_prot_lacY_cyt',
            prot(name = 'lacY', loc = 'cyt', dna = None, met = None, prot = None, rna = _
295
    \rightarrowNone, up = None, dw = None))
    Initial(prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =...
296
    →None, up = None, dw = None),
            Parameter('t0_prot_lacA_cyt', 0))
297
298
    Observable('obs_prot_lacA_cyt',
            prot (name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna = ...
    →None, up = None, dw = None))
    Initial(dna(name = 'lacZ', type = 'pro4', loc = 'cyt', dna = None, met = None, prot = ...
300
    →None, rna = None, up = None, dw = 1) %
            dna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot = _
301
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            dna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
302
    \rightarrowNone, rna = None, up = 2, dw = 3)
                                                                                 (continues on next page)
```

```
dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
303
    →prot = None, rna = None, up = 3, dw = 4) %
            dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, __
304
    \rightarrowprot = None, rna = None, up = 4, dw = 5) %
            dna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
305
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            dna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
306
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            dna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =_
307
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
    →prot = None, rna = None, up = 8, dw = 9) %
            dna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            dna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
310
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            dna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
311
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            dna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
312
    \rightarrowNone, rna = None, up = 12, dw = 13) %
            dna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
313
    \rightarrowNone, rna = None, up = 13, dw = 14) %
            dna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
314
    \rightarrowNone, rna = None, up = 14, dw = 15) %
            dna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = __
315
    →None, rna = None, up = 15, dw = None),
            Parameter('t0_dna_lacZlacYlacA', 0))
316
    Observable('obs_dna_lacZlacYlacA',
317
            dna(name = 'lacZ', type = 'pro4', loc = 'cyt', dna = None, met = None, prot = __
318
    →None, rna = None, up = None, dw = 1) %
            dna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot = ...
319
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            dna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = ...
320
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
321
    \rightarrowprot = None, rna = None, up = 3, dw = 4) %
            dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
322
    \rightarrowprot = None, rna = None, up = 4, dw = 5) %
323
            dna(name = 'lacZ', type = 'prol', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            dna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
324
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            dna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =_
325
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
326
    \rightarrowprot = None, rna = None, up = 8, dw = 9) %
            dna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = __
327
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            dna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
328
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            dna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            dna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
330
    \rightarrowNone, rna = None, up = 12, dw = 13) %
            dna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
331
    \rightarrowNone, rna = None, up = 13, dw = 14) %
            dna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
                                                                                    (continues on next page)
     \rightarrowNone, rna = None, up = 14, dw = 15) %
```

62

```
dna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = _
333
    \rightarrowNone, rna = None, up = 15, dw = None))
    Initial(rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot = _
334
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacz', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = _
335
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None, __
336
    \rightarrowprot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, __
337
    \rightarrowprot = None, rna = None, up = 3, dw = 4) %
            rna(name = 'lacZ', type = 'prol', loc = 'cyt', dna = None, met = None, prot = _
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
339
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
340
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
341
    →prot = None, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = _
342
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
343
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
344
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
345
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
346
    \rightarrowNone, rna = None, up = 12, dw = 13) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
347
    →None, rna = None, up = 13, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form1', 0))
    Observable('obs_rna_lacZlacYlacA_form1',
349
            rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot = _
350
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = _
351
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
352
    →prot = None, rna = None, up = 2, dw = 3) %
353
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
    →prot = None, rna = None, up = 3, dw = 4) %
            rna(name = 'lacZ', type = 'prol', loc = 'cyt', dna = None, met = None, prot = __
354
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
356
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
357
    \rightarrowprot = None, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = _
358
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
360
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
361
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
                                                                                   (continues on next page)
    \rightarrowNone, rna = None, up = 12, dw = 13)
```

```
rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
363
    \rightarrowNone, rna = None, up = 13, dw = None))
    Initial(rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot = _
364
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacz', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = _
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None, __
366
    ⇒prot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, __
367
    \rightarrowprot = None, rna = None, up = 3, dw = 4) %
            rna(name = 'lacZ', type = 'prol', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
370
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
371
    →prot = None, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = __
372
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
373
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
374
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
375
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
376
    \rightarrowNone, rna = None, up = 12, dw = 13) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = __
377
    \rightarrowNone, rna = None, up = 13, dw = 14) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = ...
378
    →None, rna = None, up = 14, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form2', 0))
379
    Observable ('obs_rna_lacZlacYlacA_form2',
380
            rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot = _
381
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = __
382
    \rightarrowNone, rna = None, up = 1, dw = 2) %
383
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
    \rightarrowprot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
384
    →prot = None, rna = None, up = 3, dw = 4) %
            rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
385
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
386
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
387
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
388
    \rightarrowprot = None, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = _
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
390
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
391
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
                                                                                   (continues on next page)
    \rightarrowNone, rna = None, up = 11, dw = 12) %
```

```
rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
393
    \rightarrowNone, rna = None, up = 12, dw = 13) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
394
    \rightarrowNone, rna = None, up = 13, dw = 14) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = _
395
    \rightarrowNone, rna = None, up = 14, dw = None))
    Initial(rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = _
396
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None, __
397
    →prot = None, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
    →prot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
400
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
401
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
    →prot = None, rna = None, up = 6, dw = 7) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
403
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
404
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
406
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
407
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = ...
    →None, rna = None, up = 12, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form3', 0))
409
    Observable ('obs_rna_lacZlacYlacA_form3',
410
            rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =_
411
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None, __
412
    ⇒prot = None, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
413
    \rightarrowprot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
414
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
415
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
416
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
417
    \rightarrowprot = None, rna = None, up = 6, dw = 7) %
            rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = _
418
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
420
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
421
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
                                                                                   (continues on next page)
    \rightarrowNone, rna = None, up = 11, dw = 12)
```

```
rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
423
    \rightarrowNone, rna = None, up = 12, dw = None))
    Initial(rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = _
424
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None, __
425
    →prot = None, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
426
    \rightarrowprot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
427
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
429
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None, __
430
    \rightarrowprot = None, rna = None, up = 6, dw = 7) %
            rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = _
431
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
432
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
433
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
434
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
435
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
436
    \rightarrowNone, rna = None, up = 12, dw = 13) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = _
437
    →None, rna = None, up = 13, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form4', 0))
438
    Observable('obs_rna_lacZlacYlacA_form4',
439
            rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot = _
440
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None, __
441
    \rightarrowprot = None, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
442
    →prot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
444
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
445
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
    \rightarrowprot = None, rna = None, up = 6, dw = 7) %
            rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = __
447
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
448
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
450
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
451
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
452
                                                                                    (continues on next page)
    \rightarrowNone, rna = None, up = 12, dw = 13) %
```

```
rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = _
453
    \rightarrowNone, rna = None, up = 13, dw = None))
    Initial(rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None, __
454
     →prot = None, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, _
455
    \rightarrowprot = None, rna = None, up = 1, dw = 2) %
            rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
456
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
457
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
458
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
459
    →prot = None, rna = None, up = 5, dw = 6) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
460
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
463
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
464
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
    →None, rna = None, up = 11, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form5', 0))
466
    Observable('obs_rna_lacZlacYlacA_form5',
467
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
468
    →prot = None, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None, _
    \rightarrowprot = None, rna = None, up = 1, dw = 2) %
            rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
470
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
471
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
472
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
    \rightarrowprot = None, rna = None, up = 5, dw = 6) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
474
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
475
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
477
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
478
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'terl', loc = 'cyt', dna = None, met = None, prot = _
    \rightarrowNone, rna = None, up = 11, dw = None))
    Initial(rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,...)
480
    ⇒prot = None, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
481
    \rightarrowprot = None, rna = None, up = 1, dw = 2) %
            rna(name = 'lacZ', type = 'prol', loc = 'cyt', dna = None, met = None, prot =
                                                                                   (continues on next page)
    \rightarrowNone, rna = None, up = 2, dw = 3) %
```

```
rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
483
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
484
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None, __
485
    →prot = None, rna = None, up = 5, dw = 6) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
486
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
487
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
489
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
490
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
491
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = __
492
    →None, rna = None, up = 12, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form6', 0))
493
    Observable ('obs_rna_lacZlacYlacA_form6',
494
            rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
495
    →prot = None, rna = None, up = None, dw = 1) %
            rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
    \rightarrowprot = None, rna = None, up = 1, dw = 2) %
            rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
497
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
498
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None, ...
500
    →prot = None, rna = None, up = 5, dw = 6) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
501
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
502
    \rightarrowNone, rna = None, up = 7, dw = 8) %
503
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
504
    \rightarrowNone, rna = None, up = 9, dw = 10) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
505
    \rightarrowNone, rna = None, up = 10, dw = 11) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
    \rightarrowNone, rna = None, up = 11, dw = 12) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = _
507
    \rightarrowNone, rna = None, up = 12, dw = None))
    Initial(rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
508
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,...
510
    ⇒prot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
511
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
                                                                                   (continues on next page)
    \rightarrowNone, rna = None, up = 4, dw = 5) %
```

```
rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
513
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
514
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
515
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
516
    \rightarrowNone, rna = None, up = 8, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form7', 0))
517
    Observable('obs_rna_lacZlacYlacA_form7',
518
            rna(name = 'lacz', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
520
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None, __
521
    \rightarrowprot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot = _
     \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
523
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
524
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
525
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
526
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
527
    \rightarrowNone, rna = None, up = 8, dw = None))
    Initial(rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
528
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacz', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
529
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None, ...
530
    →prot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot = _
531
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
532
    \rightarrowNone, rna = None, up = 4, dw = 5) %
533
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
534
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
535
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
536
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = __
537
    →None, rna = None, up = 9, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form8', 0))
538
539
    Observable('obs_rna_lacZlacYlacA_form8',
            rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
541
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
542
    \rightarrowprot = None, rna = None, up = 2, dw = 3) %
            rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
                                                                                    (continues on next page)
    \rightarrowNone, rna = None, up = 3, dw = 4) %
```

```
rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
544
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
545
    \rightarrowNone, rna = None, up = 5, dw = 6) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
546
    \rightarrowNone, rna = None, up = 6, dw = 7) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
547
    \rightarrowNone, rna = None, up = 7, dw = 8) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
548
    \rightarrowNone, rna = None, up = 8, dw = 9) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 9, dw = None))
    Initial(rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
550
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
551
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
552
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
553
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
554
    \rightarrowNone, rna = None, up = 4, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form9', 0))
555
    Observable('obs_rna_lacZlacYlacA_form9',
556
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = __
557
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = _
558
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
559
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = ...
560
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = ...
561
    →None, rna = None, up = 4, dw = None))
    Initial(rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
562
    →None, rna = None, up = None, dw = 1) %
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
565
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot = _
566
    \rightarrowNone, rna = None, up = 4, dw = 5) %
            rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = __
    →None, rna = None, up = 5, dw = None),
            Parameter('t0_rna_lacZlacYlacA_form10', 0))
568
    Observable('obs_rna_lacZlacYlacA_form10',
569
            rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = _
570
    →None, rna = None, up = None, dw = 1) %
571
            rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
    \rightarrowNone, rna = None, up = 1, dw = 2) %
            rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot = ...
572
    \rightarrowNone, rna = None, up = 2, dw = 3) %
            rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot = __
573
    \rightarrowNone, rna = None, up = 3, dw = 4) %
            rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
                                                                                    (continues on next page)
    \rightarrowNone, rna = None, up = 4, dw = 5) %
```

```
rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot = None, rna = None, up = 5, dw = None))
```

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FOUR

SIMULATION

Simulation could be done within the PySB python package (See more at PySB documentation). Here is the relevant code that able the simulation of any PySB model, albeit PySB exports the model, calls the simulator, and imports the results under the hood. See *Plotting* for a simple example on how to plot simulation results.

```
# simulation
   bng = '/opt/git-repositories/bionetgen.RuleWorld/bng2/'
2
   kasim = '/opt/git-repositories/KaSim4.Kappa-Dev/'
3
   cupsoda = '/opt/git-repositories/cupSODA.aresio/'
   stochkit = '/opt/git-repositories/StochKit.StochSS' # not the bin folder
   data0 = simulation.scipy(model, start = 0, finish = 10, points = 2000)
7
   data1 = simulation.cupsoda(model, start = 0, finish = 10, points = 2000, path = __
   →cupsoda) # only if you have a GPU NVIDIA; comment if not.
   data2 = simulation.bngODE(model, start = 0, finish = 10, points = 2000, path = bng)
   data3 = simulation.bngSSA(model, start = 0, finish = 10, points = 2000, n_runs = 20,
   →path = bng)
   data4 = simulation.bngPLA(model, start = 0, finish = 10, points = 2000, n_runs = 20,...
11
   →path = bng)
   data5 = simulation.bnqNF(model, start = 0, finish = 10, points = 2000, n_runs = 20,...
   →path = bnq)
   data6 = simulation.kasim(model, start = 0, finish = 10, points = 2000, n_runs = 20,...
   \rightarrowpath = kasim)
   data7 = simulation.stochkit(model, start = 0, finish = 10, points = 2000, n_runs = 20,
   → path = stochkit)
```

Note: Please follow the instructions at BioNetGen and at KaSim documentations to install the stochactic simulators. Also, you could install the simulators from here if you have anaconda or conda installed on your system.

In the case of the cupSODA, modify the compile.sh file to match the compute architecture of your NVIDIA GPU and compile the executable as cupSODA.

For network-based simulations (Ordinary Differential Equations and Gillespie's algorithm), BioNetGen is required to perform the network generation. Change the corresponding paths (lines 2-5) to match the parent folder for the BNG2.pl or KaSim executable.

PLOTTING

The simulation functions returns a dataframe in the case of deterministic simulations and a dictionary in the case of stochastic simulations:

- The sims key of the dictionary is a list of dataframes, one for each simulation.
- The avrg key is a dataframe with the average of all simulations.
- The stdv key is a dataframe with the standard deviation of all simulations.

We provide three kind of plots: plot (continuous line), scatter, and fill_between (avrg \pm weight * stdv).

The plt_kws is a dictionary that aids to pass arguments to the matplotlib functions used to plot the results.

To plot an observable, please execute one of the following functions:

```
• dna: atlas_rbm.simulation.plot.dna(data, dna_name, plt_kws, **kwargs)
```

- rna: atlas_rbm.simulation.plot.rna(data, rna_name, plt_kws, **kwargs)
- complexes: atlas_rbm.simulation.plot.cplx(data, complex_name, location, plt_kws, **kwargs)
- metabolites: atlas_rbm.simulation.plot.metabolite(data, metabolite, location, plt_kws, **kwargs)
- proteins: atlas_rbm.simulation.plot.protein(data, protein_name, location, plt_kws, **kwargs)

You could explore the available observables with model.observable.observables._map.keys() and use the name of the observable:

 observable: atlas_rbm.simulation.plot.monomer(data, observable_name, plt_kws, **kwarqs)

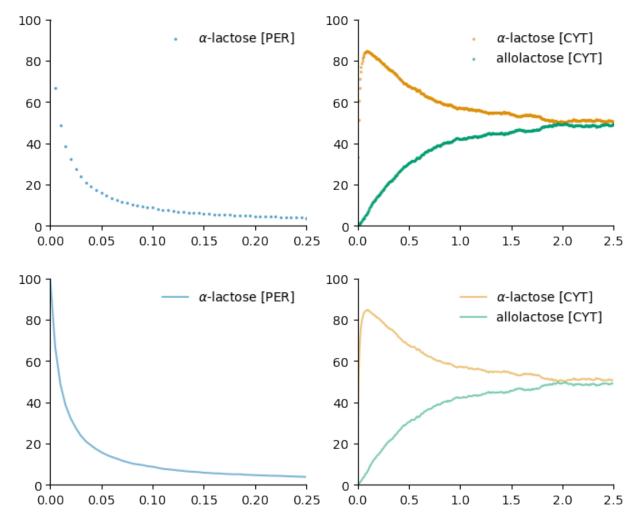
```
import seaborn
import matplotlib.pyplot as plt

palette = seaborn.color_palette('colorblind')

for kind in ['scatter', 'plot']:
    # first plot, periplasmic concentration
    fig, ax = plt.subplots(1, 2, figsize = (4*2, 3*1), dpi = 100)

simulation.plot.metabolite(data3['avrg'], 'Alpha_lactose', 'per', ax = ax[0], **{
    'kind' : kind},
    plt_kws = {'s' : 2, 'color' : palette[0], 'label' : r'$\alpha$-lactose [PER]',
    'alpha' : .5})
```

```
simulation.plot.metabolite(data3['avrg'], 'Alpha_lactose', 'cyt', ax = ax[1], **{
13
    \rightarrow 'kind' : kind},
           plt_kws = {'s' : 2, 'color' : palette[1], 'label' : r'$\alpha$-lactose [CYT]',
14
      'alpha' : .5})
15
       simulation.plot.metabolite(data3['avrg'], 'ALLOLACTOSE', 'cyt', ax = ax[1], **{
16
    \rightarrow 'kind' : kind},
           plt_kws = {'s' : 2, 'color' : palette[2], 'label' : r'allolactose [CYT]',
17
    →'alpha' : .5})
18
       ax[0].set_xlim((0,.25))
       ax[1].set_xlim((0,2.5))
21
       ax[0].set_ylim((0,100))
       ax[1].set_ylim((0,100))
22
23
       seaborn.despine()
```



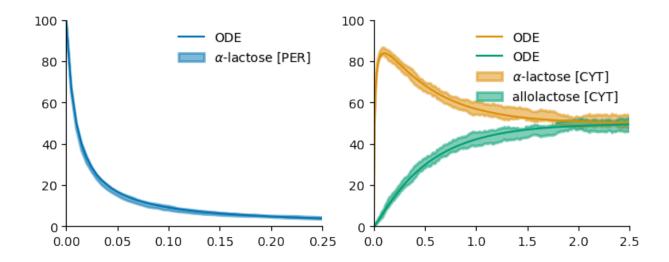
```
import seaborn
import matplotlib.pyplot as plt

palette = seaborn.color_palette('colorblind')

(continues on next page)
```

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```
# first plot, periplasmic concentration
6
   fig, ax = plt.subplots(1, 2, figsize = (4*2, 3*1), dpi = 100)
7
   simulation.plot.metabolite(data3, 'Alpha_lactose', 'per', ax = ax[0], **{'kind':
    →'fill_between', 'weight' : .5},
      plt_kws = {'s' : 2, 'color' : palette[0], 'label' : r'$\alpha$-lactose [PER]',
    \hookrightarrow 'alpha' : .5})
10
   # second plot, cytoplasmic concentration
11
   simulation.plot.metabolite(data3, 'Alpha_lactose', 'cyt', ax = ax[1], **{'kind' :
12
   →'fill_between', 'weight' : .5},
     plt_kws = {'s' : 2, 'color' : palette[1], 'label' : r'$\alpha$-lactose [CYT]',
    \rightarrow 'alpha' : .5})
14
   # second plot, cytoplasmic concentration
15
   simulation.plot.metabolite(data3, 'ALLOLACTOSE', 'cyt', ax = ax[1], **{'kind' : 'fill_
16
    →between', 'weight' : .5},
      plt_kws = {'s' : 2, 'color' : palette[2], 'label' : r'allolactose [CYT]', 'alpha'_
    \hookrightarrow: .5})
18
   # first plot, periplasmic concentration
19
   simulation.plot.metabolite(data0, 'Alpha_lactose', 'per', ax = ax[0], **{'kind':
20
   → 'plot'},
      plt_kws = {'s' : 2, 'color' : palette[0], 'label' : r'ODE'})
21
22
   # second plot, cytoplasmic concentration
24
   simulation.plot.metabolite(data0, 'Alpha_lactose', 'cyt', ax = ax[1], **{'kind':
    → 'plot'},
      plt_kws = {'s' : 2, 'color' : palette[1], 'label' : r'ODE'})
25
26
   # second plot, cytoplasmic concentration
27
   simulation.plot.metabolite(data0, 'ALLOLACTOSE', 'cyt', ax = ax[1], **{'kind' : 'plot
    \hookrightarrow '},
      plt_kws = {'s' : 2, 'color' : palette[2], 'label' : r'ODE'})
29
30
   ax[0].set_xlim((0,.25))
31
   ax[1].set_xlim((0,2.5))
32
   ax[0].set_ylim((0,100))
   ax[1].set_ylim((0,100))
35
   seaborn.despine()
```



Note: Atlas produces automatically Observables for metabolites and other components. However, Atlas do not produce Observables for every possible component and the user could add observables with atlas_rbm.simulation.set_observable(model, pattern, alias).

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EXPORT TO

The PySB python package could export to different languages (See more here). Use the following code to export to the supported formats:

```
# export to
export.to_sbml(model, 'export-to-sbml.sbml')
export.to_matlab(model, 'export-to-matlab.m')
export.to_mathematica(model, 'export-to-mathematica.wl')
export.to_potterswheel(model, 'export-to-potterswheel.m')
export.to_bngl(model, 'export-to-bngl.bngl')
export.to_bngnet(model, 'export-to-bngnet.net')
export.to_kappa(model, 'export-to-kappa.kappa')
export.to_python(model, 'export-to-python.py')
export.to_pysb(model, 'export-to-pysb.py')
export.to_stochkit(model, 'export-to-stochkit.xml')
export.to_json(model, 'export-to-json.json')
```

Note: In the case of matlab, mathematica, potterswheel, python, and stochkit, PySB requires to expand the rules to determine all mass-balances to write ODE-based models, a process call network generation and could take excessive time to finish.

CHAPTER

SEVEN

INDICES AND TABLES

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