
atlas Documentation

Release 1.4

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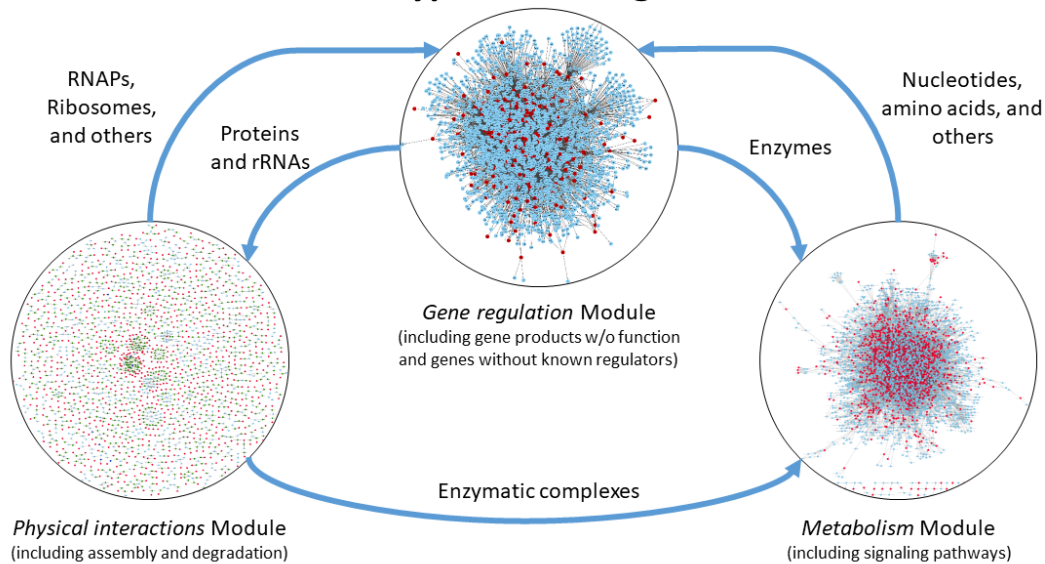
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Atlas is a small software developed to use simple text files that encode biological networks and write Rule-Based Models (RBMs). Atlas writes rules and others model components for the PySB python package [PySB](#), PMID 23423320. The RBMs could be simulated within PySB with [NFsim](#), PMID 26556387 (within the [BioNetGen2](#) software, PMID 27402907), [KaSim](#) (PMID 29950016), and other software. Models could be exported to text files in [BioNetGen Language](#) or [Kappa](#) language for further simulation, calibration (e.g., [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



REQUIREMENTS

1. PathwayTools must be installed and running to obtain data from the BioCyc databases. Please, execute in a terminal ``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 here <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 following the instruction from <https://anaconda.org/alubbock>.
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 other networks.
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 could be done with libRoadRunner (<http://libroadrunner.org/>), Tellurium (<http://tellurium.analogmachine.org/>), COPASI (<http://copasi.org/>), etc.

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.

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, the stochastic simulators BNG2, NFsim, KaSim, and Stochkit, and the Jupyter server. After building of 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 execute 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:

```
wget https://files.pythonhosted.org/packages/ec/ed/
↳ 8b94e0a29f69a24ddb18ba4a4e6463d3ecede308576774e86baf6a84b998/atlas_rbm-1.0.2-
↳ py3-none-any.whl
pip3 install atlas_rbm-1.0.2-py3-none-any.whl --user
```

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 invoke. 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 user 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 pip or 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 Atlas repository

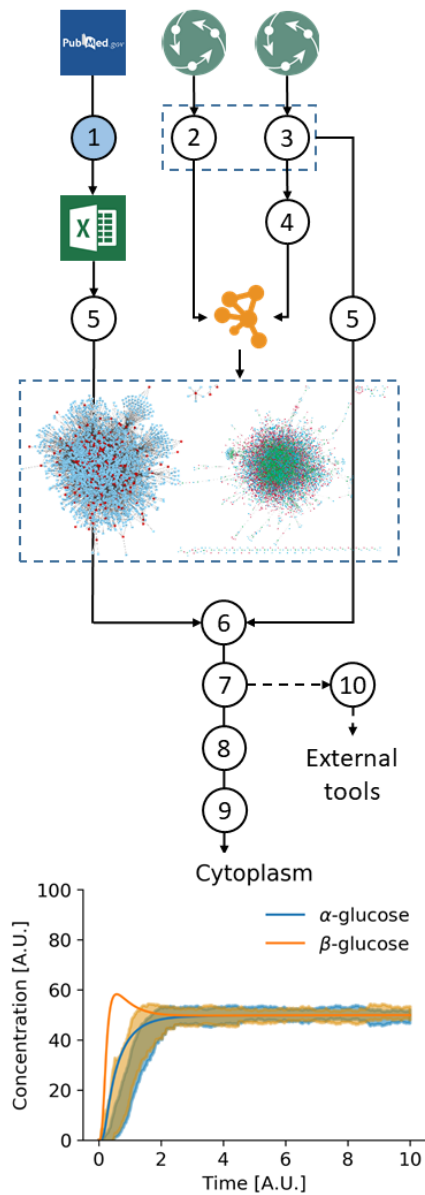
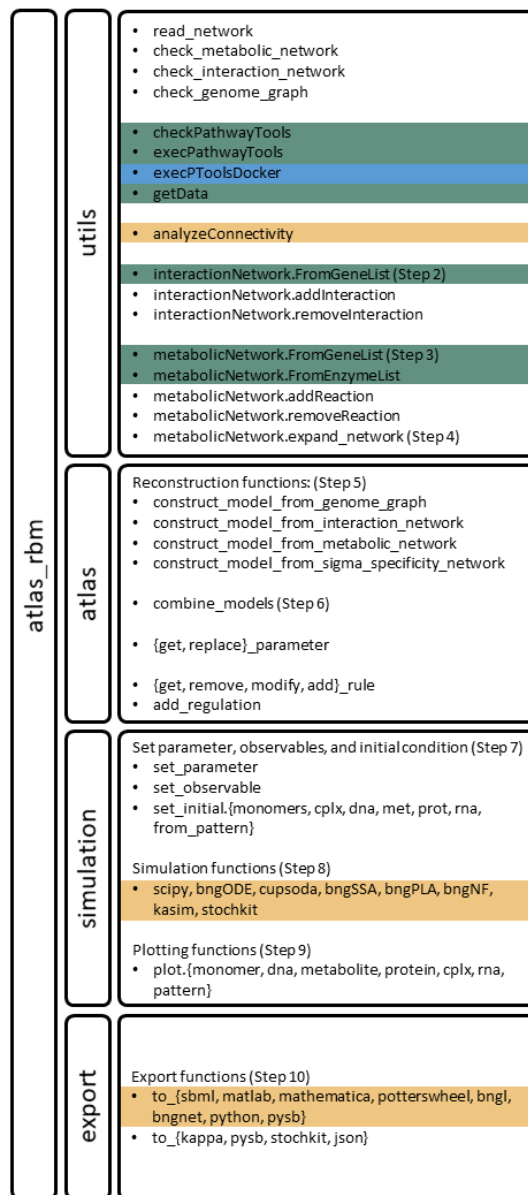
1. Clone with git

The source code is uploaded and maintained through Github at <https://github.com/networkbiolab/atlas>. Therefore, you could download or clone the repository locally, and then add the directory to the PYTHONPATH. Beware that you should install the *pysb* package (*pysb*) and others packages by any mean, specially the Jupyter Notebook project (<https://jupyter.org>) that aid the modeling process and visualize models.

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

Note: Adding the path to `$HOME/.profile` allows python to find the package installation directory after each user login. Similarly, adding the path to `$HOME/.bashrc` allows python to find the package after each bash 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 if it would be downloaded from the PyPI server.

OVERVIEW



RULE BASED MODELING BASICS

Rule-based models (RBM) are characterized by the utilization of a formal language. The language defines basic transformations:

- Addition: two *agents* join together;
- Separation: a complex of *agents* split into components;
- Creation: An *agent* or a complex of *agents* appears in the system;
- Deletion: An *agent* or a complex of *agents* is removed from the system; and
- State change: A property of the *agent* is modified.

However, a rule-based model requires additional elements that shape the final form of rules and this note is intended as an introduction to modeling with pySB. For more information, please visit <https://pysb.readthedocs.io/en/stable/tutorial.html>. Rule-based models are defined by:

- Monomers (*agents*): The complete definition of the possible characteristics of *agents*;
- Parameters: The name and value of model parameters. Parameters are used as rule rates and *agent* initial quantities;
- Rules: The formalized description of transformations involving *agents*;
- Initials: The complete (*concrete* in terms of pySB) definition of an *agent* and its initial quantity; and
- Observables: The complete or partial definition of *agents* that will be quantified throughout a simulation and an alias.

Note: Observables are optional, but its no inclusion will result in a simulation without trackable entities.

Rationale behind monomers definition in Atlas:

We defined five types of *agents*: metabolites, proteins, DNA, RNA, and Complex. The four first types of agents refer to the components of cells while the *Complex* was defined to be aliases of complex of *agents*, e.g., the *RNAP_CPLX agent* is an alias of the real protein complex that otherwise would be modeled by four interacting proteins. Next, because genes, RNA, and proteins share the same name (and normally are written capitalized or italicized to differentiate them), we decided to create a name site that define the name:

```
1 Monomer('rna', ['name'], {'name': ['lacI_21_1', 'lacI_422_402', 'lacI_72_92', 'lacA',  
  ↪ 'lacY', 'lacZ']})  
2 Monomer('cplx', ['name'], {'name': ['RNAP_CPLX', 'RIBOSOME_CPLX']})  
3 Monomer('prot', ['name'], {'name': ['lacA', 'lacI', 'lacY', 'lacZ']})
```

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```

4 Monomer('met', ['name'], {'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']})
5 Monomer('dna', ['name'], {'name': ['lacA', 'lacI_21_1', 'lacI_422_402', 'lacI_72_92',
  ↳'lacY', 'lacZ']})

```

Note: Monomers define the complete set of sites and site states that *agents* could adopt in the system. If a component of a rule, initial or observable do not match the monomer definition, pySB will raise an error. In addition, an initial must be concrete, meaning that all sites must be included and defined with a value.

Next, we created a `loc` site that define the location of the monomer. Bacterial cells has many compartments (see [Metabolic Networks](#) for a complete list of valid names) and monomers could exist on them:

```

1 Monomer('rna', ['name', 'loc'], {'name': ['lacI_21_1', 'lacI_422_402', 'lacI_72_92',
  ↳'lacA', 'lacY', 'lacZ'], 'loc': ['cyt']})
2 Monomer('cplx', ['name', 'loc'], {'name': ['RNAP_CPLX', 'RIBOSOME_CPLX'], 'loc': ['cyt
  ↳']})
3 Monomer('prot', ['name', 'loc'], {'name': ['lacA', 'lacI', 'lacY', 'lacZ'], 'loc': [
  ↳'bnuc', 'cproj', 'cyt', 'cytosk', 'ex', 'imem', 'mem', 'omem', 'per', 'wall']})
4 Monomer('met', ['name', 'loc'], {'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': ['bnuc', 'cproj', 'cyt', 'cytosk', 'ex', 'imem', 'mem', 'omem', 'per',
  ↳'wall']})
5 Monomer('dna', ['name', 'loc'], {'name': ['lacA', 'lacI_21_1', 'lacI_422_402', 'lacI_
  ↳72_92', 'lacY', 'lacZ'], 'loc': ['cyt']})

```

Moreover, we created a `type` site for DNAs and RNAs. Both molecules normally has features that interact specifically with proteins. For instance, promoters interact with the RNA Polymerase and Ribosome Binding Sites interact (obviously) with the ribosome. We defined five types: promoter (PRO), ribosome binding site (RBS), coding DNA sequence (CDS), terminator (TER), and binding site (BS). The DNA binding sites interact with Transcription Factors and other proteins, while RNA binding sites interact with RNA-binding proteins (e.g., RNase E):

```

1 Monomer('rna', ['name', 'type', 'loc'], {'name': ['lacI_21_1', 'lacI_422_402', 'lacI_
  ↳72_92', 'lacA', 'lacY', 'lacZ'], 'type': ['BS', 'cds', 'pro1', 'pro2', 'pro3', 'pro4
  ↳', 'rbs', 'ter1', 'ter2'], 'loc': ['cyt']})
2 Monomer('cplx', ['name', 'loc'], {'name': ['RNAP_CPLX', 'RIBOSOME_CPLX'], 'loc': ['cyt
  ↳']})
3 Monomer('prot', ['name', 'loc'], {'name': ['lacA', 'lacI', 'lacY', 'lacZ'], 'loc': [
  ↳'bnuc', 'cproj', 'cyt', 'cytosk', 'ex', 'imem', 'mem', 'omem', 'per', 'wall']})
4 Monomer('met', ['name', 'loc'], {'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': ['bnuc', 'cproj', 'cyt', 'cytosk', 'ex', 'imem', 'mem', 'omem', 'per',
  ↳'wall']})
5 Monomer('dna', ['name', 'type', 'loc'], {'name': ['lacA', 'lacI_21_1', 'lacI_422_402',
  ↳', 'lacI_72_92', 'lacY', 'lacZ'], 'loc': ['cyt'], 'type': ['BS', 'cds', 'pro1', 'pro2
  ↳', 'pro3', 'pro4', 'rbs', 'ter1', 'ter2']})

```

After we solved how to describe concisely *agents* without creating single monomers for each one, we defined interaction sites. All five types of monomers has four interactions sites to interact with another *agent* of the type of the site: `met` to interact with a Metabolite, `prot` to interact with a protein, `dna` to interact with a DNA feature or part,

and rna to interact with a RNA feature or part. However and as anticipated, a single site constraints the number of partners to one (of the type of the interaction site). To overcome the limit, we used the up and dw sites that Stewart & Wilson-Kanamori used for the description of DNA and RNA features in [Kappa BioBrick Framework](#) to make polymers of proteins:

```

1 Monomer('cplx', ['name', 'loc', 'dna', 'met', 'prot', 'rna'], {'name': ['RNAP_CPLX',
  ↪ 'RIBOSOME_CPLX'], 'loc': ['cyt']})
2 Monomer('rna', ['name', 'type', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'], {
  ↪ 'name': ['lacI_21_1', 'lacI_422_402', 'lacI_72_92', 'lacA', 'lacY', 'lacZ'], 'type'
  ↪ ': ['BS', 'cds', 'pro1', 'pro2', 'pro3', 'pro4', 'rbs', 'ter1', 'ter2'], 'loc': [
  ↪ 'cyt']})
3 Monomer('dna', ['dna', 'dw', 'loc', 'met', 'name', 'prot', 'rna', 'type', 'up'], {
  ↪ 'name': ['lacA', 'lacI_21_1', 'lacI_422_402', 'lacI_72_92', 'lacY', 'lacZ'], 'loc':
  ↪ ['cyt'], 'type': ['BS', 'cds', 'pro1', 'pro2', 'pro3', 'pro4', 'rbs', 'ter1', 'ter2'
  ↪ '']})
4 Monomer('met', ['dna', 'loc', 'met', 'name', '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': ['bnuc', 'cproj', 'cyt', 'cytosk
  ↪ ', 'ex', 'imem', 'mem', 'omem', 'per', 'wall']})
5 Monomer('prot', ['dna', 'dw', 'loc', 'met', 'name', 'prot', 'rna', 'up'], {'name': [
  ↪ 'lacA', 'lacI', 'lacY', 'lacZ', 'spontaneous'], 'loc': ['bnuc', 'cproj', 'cyt',
  ↪ 'cytosk', 'ex', 'imem', 'mem', 'omem', 'per', 'wall']})

```

Now that we have a suitable definition of *agents* with purposely created interaction sites, complex of *agents* are defined by unique numbered bonds that are shared by the interactions sites:

For instance, the dimer [lacI, lacI] (see [Protein-Protein Interaction Networks](#) for details of the notation) is converted to:

```

1 prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None,
  ↪ up=None, dw=1) %
2 prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None, up=1,
  ↪ dw=None)

```

And a more complicated complex [lacI, lacI, SMALL-beta-ALLOLACTOSE] (see [Protein-Small compounds Interaction Networks](#) for details of the notation) is converted to:

```

1 prot(name='lacI', loc='cyt', dna=None, met=2, prot=None, rna=None, up=None,
  ↪ dw=1) %
2 prot(name='lacI', loc='cyt', dna=None, met=3, prot=None, rna=None, up=1,
  ↪ dw=None) %
3 met(name='beta_ALLOLACTOSE', loc='cyt', dna=None, met=None, prot=3,
  ↪ rna=None) %
4 met(name='beta_ALLOLACTOSE', loc='cyt', dna=None, met=None, prot=2, rna=None)

```

Note: Valid site values are: None defines the site is empty, not bonded to any other agent; ANY defines the site is linked to an agent without explicitly write which it is; WILD defines the site could be linked or not, again without explicit mention to which agent; and a string that defines the state of the site (in the case of Atlas: name, location or type).

PySB requires agents that are components of a complex must be separated by the % symbol.

The same number must be repeated only twice. If a bond appears one time means that an *agent* has a dangling bond while three or more times mean the bond is ambiguous.

In the case of *kappa* language, the bond number must be unique in the rule, even if it describes a link that appear in

different complexes:

```

1  # This is wrong when exported to kappa
2  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None,
    ↪up=None, dw=1) %
3  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None, up=1,
    ↪dw=None) +
4  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None,
    ↪up=None, dw=1) %
5  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None, up=1,
    ↪dw=None)
6
7  # This is correct when exported to kappa
8  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None,
    ↪up=None, dw=1) %
9  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None, up=1,
    ↪dw=None) +
10 prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None,
    ↪up=None, dw=2) %
11 prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None, up=2,
    ↪dw=None)

```

Finally, the notation of rules:

Unidirectional rules employ the >> symbols to separate substrates (Left-hand side) and products (Right-hand side):

```

1  Rule('name_of_the_rule',
2  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None,
    ↪up=None, dw=None) +
3  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None,
    ↪up=None, dw=None) >>
4  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None,
    ↪up=None, dw=1) %
5  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None, up=1,
    ↪dw=None),
6  Parameter('name_of_the_forward_rate_parameter', a_positive_value))

```

While bidirectional rules employ the | symbol:

```

1  Rule('name_of_the_rule',
2  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None,
    ↪up=None, dw=None) +
3  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None,
    ↪up=None, dw=None) |
4  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None,
    ↪up=None, dw=1) %
5  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None, up=1,
    ↪dw=None),
6  Parameter('name_of_the_forward_rate_parameter', a_positive_value),
7  Parameter('name_of_the_reverse_rate_parameter', another_positive_value))

```

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*

5.1 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 in the same order to each component.
2. If the number of locations unmatch the number of components, the first location is used for every component. The remaining locations are disregarded.
3. If the number of locations is one, the location is used for every component.

Valid location 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 value; and finally

7. The 7th declares the reverse reaction rate value.

Examples:

	GENE OR COMPLEX	ENZYME			
1	↪LOCATION	REACTION	SUBSTRATES	PRODUCTS	FWD_
	↪RATE	RVS_RATE			
2	spontaneous	cytosol	LACTOSE-MUTAROTATION		alpha-
	↪lactose	beta-lactose	1 1		
3	spontaneous	cytosol	GALACTOSE-MUTAROTATION		alpha-
	↪GALACTOSE	beta-GALACTOSE	1 1		
4	spontaneous	cytosol	GLUCOSE-MUTAROTATION		alpha-
	↪glucose	beta-glucose	1 1		
5	LACY-MONOMER	inner membrane	TRANS-RXN-24		PER-PROTON, PER-alpha-
	↪lactose	PROTON, alpha-lactose	1 0		
6	LACY-MONOMER	inner membrane	TRANS-RXN-24-beta		PER-PROTON, PER-
	↪beta-lactose	PROTON, beta-lactose	1 0		
7	LACY-MONOMER	inner membrane	TRANS-RXN-94		PER-PROTON, PER-
	↪MELIBIOSE	PROTON, MELIBIOSE	1 0		
8	LACY-MONOMER	inner membrane	RXN0-7215		PER-PROTON, PER-CPD-
	↪3561	PROTON, CPD-3561	1 0		
9	LACY-MONOMER	inner membrane	RXN0-7217		PER-PROTON, PER-CPD-
	↪3785	PROTON, CPD-3785	1 0		
10	LACY-MONOMER	inner membrane	RXN-17755		PER-PROTON, PER-CPD-
	↪3801	PROTON, CPD-3801	1 0		
11	BETAGALACTOSID-CPLX	cytosol	BETAGALACTOSID-RXN		beta-lactose,
	↪WATER	beta-GALACTOSE, beta-glucose	1 0		
12	BETAGALACTOSID-CPLX	cytosol	BETAGALACTOSID-RXN-alpha		alpha-
	↪lactose, WATER	alpha-GALACTOSE, alpha-glucose	1 0		
13	BETAGALACTOSID-CPLX	cytosol	RXN0-5363		alpha-lactose alpha-
	↪ALLOLACTOSE	1 1			
14	BETAGALACTOSID-CPLX	cytosol	RXN0-5363-beta		beta-
	↪lactose	beta-ALLOLACTOSE	1 1		
15	BETAGALACTOSID-CPLX	cytosol	ALLOLACTOSE-DEG-alpha		alpha-
	↪ALLOLACTOSE	alpha-GALACTOSE, alpha-glucose	1 0		
16	BETAGALACTOSID-CPLX	cytosol	ALLOLACTOSE-DEG-beta		beta-
	↪ALLOLACTOSE	beta-GALACTOSE, beta-glucose	1 0		
17	BETAGALACTOSID-CPLX	cytosol	RXN-17726		CPD-3561, WATER beta-
	↪GALACTOSE, Fructofuranose	1 0			
18	BETAGALACTOSID-CPLX	cytosol	RXN0-7219		CPD-3785, WATER beta-
	↪GALACTOSE, D-ARABINOSE	1 0			

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19	GALACTOACETYLTRAN-CPLX	cytosol	GALACTOACETYLTRAN-RXN-
	↪galactose	beta-GALACTOSE, ACETYL-COA	6-Acetyl-beta-D-Galactose, CO-
	↪A	1	0

OR

1	GENE OR COMPLEX	ENZYME_			
	↪LOCATION	REACTION	SUBSTRATES	PRODUCTS	FWD_
	↪RATE	RVS_RATE			
2	spontaneous	cytosol	LACTOSE-MUTAROTATION	alpha-	
	↪lactose	beta-lactose	1	1	
3	spontaneous	cytosol	GALACTOSE-MUTAROTATION	alpha-	
	↪GALACTOSE	beta-GALACTOSE	1	1	
4	spontaneous	cytosol	GLUCOSE-MUTAROTATION	alpha-	
	↪glucose	beta-glucose	1	1	
5	lacY	inner membrane	TRANS-RXN-24	PER-PROTON, PER-alpha-	
	↪lactose	PROTON, alpha-lactose	1	0	
6	lacY	inner membrane	TRANS-RXN-24-beta	PER-PROTON, PER-beta-	
	↪lactose	PROTON, beta-lactose	1	0	
7	lacY	inner membrane	TRANS-RXN-94	PER-PROTON, PER-	
	↪MELIBIOSE	PROTON, MELIBIOSE	1	0	
8	lacY	inner membrane	RXN0-7215	PER-PROTON, PER-CPD-	
	↪3561	PROTON, CPD-3561	1	0	
9	lacY	inner membrane	RXN0-7217	PER-PROTON, PER-CPD-	
	↪3785	PROTON, CPD-3785	1	0	
10	lacY	inner membrane	RXN-17755	PER-PROTON, PER-CPD-	
	↪3801	PROTON, CPD-3801	1	0	
11	lacZ	cytosol	BETAGALACTOSID-RXN	beta-lactose, WATER	beta-
	↪GALACTOSE, beta-glucose	1	0		
12	lacZ	cytosol	BETAGALACTOSID-RXN-alpha	alpha-lactose,	
	↪WATER	alpha-GALACTOSE, alpha-glucose	1	0	
13	lacZ	cytosol	RXN0-5363	alpha-lactose	alpha-
	↪ALLOLACTOSE	1	1		
14	lacZ	cytosol	RXN0-5363-beta	beta-lactose	beta-
	↪ALLOLACTOSE	1	1		
15	lacZ	cytosol	ALLOLACTOSE-DEG-alpha	alpha-ALLOLACTOSE,	
	↪WATER	alpha-GALACTOSE, alpha-glucose	1	0	
16	lacZ	cytosol	ALLOLACTOSE-DEG-beta	beta-ALLOLACTOSE,	
	↪WATER	beta-GALACTOSE, beta-glucose	1	0	
17	lacZ	cytosol	RXN-17726	CPD-3561, WATER	beta-GALACTOSE,
	↪Fructofuranose	1	0		
18	lacZ	cytosol	RXN0-7219	CPD-3785, WATER	beta-GALACTOSE, D-
	↪ARABINOSE	1	0		
19	lacA	cytosol	GALACTOACETYLTRAN-RXN-galactose	beta-GALACTOSE,	
	↪ACETYL-COA	6-Acetyl-beta-D-Galactose, CO-A	1	0	

OR

1	GENE OR COMPLEX	ENZYME_			
	↪LOCATION	REACTION	SUBSTRATES	PRODUCTS	FWD_
	↪RATE	RVS_RATE			
2	spontaneous	cytosol	LACTOSE-MUTAROTATION	alpha-	
	↪lactose	beta-lactose	1	1	
3	spontaneous	cytosol	GALACTOSE-MUTAROTATION	alpha-	
	↪GALACTOSE	beta-GALACTOSE	1	1	
4	spontaneous	cytosol	GLUCOSE-MUTAROTATION	alpha-	
	↪glucose	beta-glucose	1	1	

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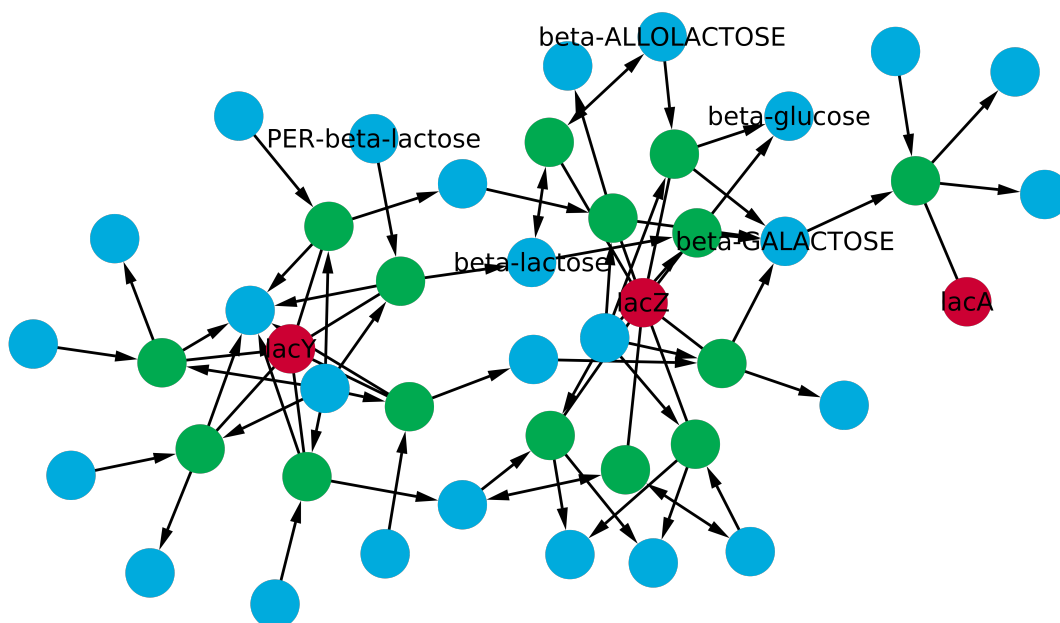
5	lacY	inner membrane	TRANS-RXN-24	PER-PROTON, PER-alpha-	
	↪ lactose	PROTON, alpha-lactose	1	0	
6	lacY	inner membrane	TRANS-RXN-24-beta	PER-PROTON, PER-beta-	
	↪ lactose	PROTON, beta-lactose	1	0	
7	lacY	inner membrane	TRANS-RXN-94	PER-PROTON, PER-	
	↪ MELIBIOSE	PROTON, MELIBIOSE	1	0	
8	lacY	inner membrane	RXN0-7215	PER-PROTON, PER-CPD-	
	↪ 3561	PROTON, CPD-3561	1	0	
9	lacY	inner membrane	RXN0-7217	PER-PROTON, PER-CPD-	
	↪ 3785	PROTON, CPD-3785	1	0	
10	lacY	inner membrane	RXN-17755	PER-PROTON, PER-CPD-	
	↪ 3801	PROTON, CPD-3801	1	0	
11	[lacZ, lacZ, lacZ, lacZ]	[cytosol, cytosol, cytosol, cytosol]	BETAGALACTOSID-		
	↪ RXN	beta-lactose, WATER	beta-GALACTOSE, beta-glucose	1	0
12	[lacZ, lacZ, lacZ, lacZ]	[cytosol, cytosol, cytosol, cytosol]	BETAGALACTOSID-		
	↪ RXN-alpha	alpha-lactose, WATER	alpha-GALACTOSE, alpha-		
	↪ glucose	1	0		
13	[lacZ, lacZ, lacZ, lacZ]	[cytosol, cytosol, cytosol, cytosol]	RXN0-		
	↪ 5363	alpha-lactose	alpha-ALLOLACTOSE	1	1
14	[lacZ, lacZ, lacZ, lacZ]	[cytosol, cytosol, cytosol, cytosol]	RXN0-5363-		
	↪ beta	beta-lactose	beta-ALLOLACTOSE	1	1
15	[lacZ, lacZ, lacZ, lacZ]	[cytosol, cytosol, cytosol, cytosol]	ALLOLACTOSE-DEG-		
	↪ alpha	alpha-ALLOLACTOSE, WATER	alpha-GALACTOSE, alpha-		
	↪ glucose	1	0		
16	[lacZ, lacZ, lacZ, lacZ]	[cytosol, cytosol, cytosol, cytosol]	ALLOLACTOSE-DEG-		
	↪ beta	beta-ALLOLACTOSE, WATER	beta-GALACTOSE, beta-		
	↪ glucose	1	0		
17	[lacZ, lacZ, lacZ, lacZ]	[cytosol, cytosol, cytosol, cytosol]	RXN-		
	↪ 17726	CPD-3561, WATER	beta-GALACTOSE, Fructofuranose	1	0
18	[lacZ, lacZ, lacZ, lacZ]	[cytosol, cytosol, cytosol, cytosol]	RXN0-		
	↪ 7219	CPD-3785, WATER	beta-GALACTOSE, D-ARABINOSE	1	0
19	[lacA, lacA, lacA]	[cytosol, cytosol, cytosol]	GALACTOACETYLTRAN-RXN-		
	↪ galactose	beta-GALACTOSE, ACETYL-COA	6-Acetyl-beta-D-Galactose, CO-		
	↪ A	1	0		

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 encoding 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)`
- `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 = True` and the `noInitials = True` arguments will make a faster compilation, while later you could add specific 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`):

```

1 from pysb import *
2 Model()
3
4 Monomer('met',
5         ['name', 'loc', 'dna', 'met', 'prot', 'rna'],
6         { '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' ],
7         'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
→ 'omem'] })
8 Monomer('prot',
9         ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
10        { 'name' : [ 'LACY_MONOMER', 'spontaneous' ],
11        'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
→ 'omem'] })
12 Monomer('cplx',
13        ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
14        { 'name' : [ 'BETAGALACTOSID_CPLX', 'GALACTOACETYLTRAN_CPLX' ],
15        'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
→ 'omem'] })
16 Observable('obs_met_ACETYL_COA_cyt', met(name = 'ACETYL_COA', loc = 'cyt'))
17 Observable('obs_met_CO_A_cyt', met(name = 'CO_A', loc = 'cyt'))
18 Observable('obs_met_CPD_3561_cyt', met(name = 'CPD_3561', loc = 'cyt'))
19 Observable('obs_met_CPD_3785_cyt', met(name = 'CPD_3785', loc = 'cyt'))
20 Observable('obs_met_CPD_3801_cyt', met(name = 'CPD_3801', loc = 'cyt'))
21 Observable('obs_met_D_ARABINOSE_cyt', met(name = 'D_ARABINOSE', loc = 'cyt'))
22 Observable('obs_met_Fructofuranose_cyt', met(name = 'Fructofuranose', loc = 'cyt'))
23 Observable('obs_met_MELIBIOSE_cyt', met(name = 'MELIBIOSE', loc = 'cyt'))
24 Observable('obs_met_PROTON_cyt', met(name = 'PROTON', loc = 'cyt'))
25 Observable('obs_met_WATER_cyt', met(name = 'WATER', loc = 'cyt'))
26 Observable('obs_met__6_Acetyl_beta_D_Galactose_cyt', met(name = '_6_Acetyl_beta_D_
→ Galactose', loc = 'cyt'))
27 Observable('obs_met_alpha_ALLOLACTOSE_cyt', met(name = 'alpha_ALLOLACTOSE', loc = 'cyt
→ '))
28 Observable('obs_met_alpha_GALACTOSE_cyt', met(name = 'alpha_GALACTOSE', loc = 'cyt'))
29 Observable('obs_met_alpha_glucose_cyt', met(name = 'alpha_glucose', loc = 'cyt'))
30 Observable('obs_met_alpha_lactose_cyt', met(name = 'alpha_lactose', loc = 'cyt'))
31 Observable('obs_met_beta_ALLOLACTOSE_cyt', met(name = 'beta_ALLOLACTOSE', loc = 'cyt
→ '))
32 Observable('obs_met_beta_GALACTOSE_cyt', met(name = 'beta_GALACTOSE', loc = 'cyt'))
33 Observable('obs_met_beta_glucose_cyt', met(name = 'beta_glucose', loc = 'cyt'))
34 Observable('obs_met_beta_lactose_cyt', met(name = 'beta_lactose', loc = 'cyt'))
35 Initial(met(name = 'ACETYL_COA', loc = 'cyt', dna = None, met = None, prot = None,
→ rna = None), Parameter('t0_met_ACETYL_COA_cyt', 0))

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```

36 Initial(met(name = 'CO_A', loc = 'cyt', dna = None, met = None, prot = None, rna =
    ↪None), Parameter('t0_met_CO_A_cyt', 0))
37 Initial(met(name = 'CPD_3561', loc = 'cyt', dna = None, met = None, prot = None, rna
    ↪= None), Parameter('t0_met_CPD_3561_cyt', 0))
38 Initial(met(name = 'CPD_3785', loc = 'cyt', dna = None, met = None, prot = None, rna
    ↪= None), Parameter('t0_met_CPD_3785_cyt', 0))
39 Initial(met(name = 'CPD_3801', loc = 'cyt', dna = None, met = None, prot = None, rna
    ↪= None), Parameter('t0_met_CPD_3801_cyt', 0))
40 Initial(met(name = 'D_ARABINOSE', loc = 'cyt', dna = None, met = None, prot = None,
    ↪rna = None), Parameter('t0_met_D_ARABINOSE_cyt', 0))
41 Initial(met(name = 'Fructofuranose', loc = 'cyt', dna = None, met = None, prot = None,
    ↪ rna = None), Parameter('t0_met_Fructofuranose_cyt', 0))
42 Initial(met(name = 'MELIBIOSE', loc = 'cyt', dna = None, met = None, prot = None, rna
    ↪= None), Parameter('t0_met_MELIBIOSE_cyt', 0))
43 Initial(met(name = 'PROTON', loc = 'cyt', dna = None, met = None, prot = None, rna =
    ↪None), Parameter('t0_met_PROTON_cyt', 0))
44 Initial(met(name = 'WATER', loc = 'cyt', dna = None, met = None, prot = None, rna =
    ↪None), Parameter('t0_met_WATER_cyt', 0))
45 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))
46 Initial(met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot =
    ↪None, rna = None), Parameter('t0_met_alpha_ALLOLACTOSE_cyt', 0))
47 Initial(met(name = 'alpha_GALACTOSE', loc = 'cyt', dna = None, met = None, prot =
    ↪None, rna = None), Parameter('t0_met_alpha_GALACTOSE_cyt', 0))
48 Initial(met(name = 'alpha_glucose', loc = 'cyt', dna = None, met = None, prot = None,
    ↪rna = None), Parameter('t0_met_alpha_glucose_cyt', 0))
49 Initial(met(name = 'alpha_lactose', loc = 'cyt', dna = None, met = None, prot = None,
    ↪rna = None), Parameter('t0_met_alpha_lactose_cyt', 0))
50 Initial(met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot =
    ↪None, rna = None), Parameter('t0_met_beta_ALLOLACTOSE_cyt', 0))
51 Initial(met(name = 'beta_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = None,
    ↪ rna = None), Parameter('t0_met_beta_GALACTOSE_cyt', 0))
52 Initial(met(name = 'beta_glucose', loc = 'cyt', dna = None, met = None, prot = None,
    ↪rna = None), Parameter('t0_met_beta_glucose_cyt', 0))
53 Initial(met(name = 'beta_lactose', loc = 'cyt', dna = None, met = None, prot = None,
    ↪rna = None), Parameter('t0_met_beta_lactose_cyt', 0))
54 Initial(prot(name = 'LACY_MONOMER', loc = 'cyt', dna = None, met = None, prot = None,
    ↪rna = None, up = None, dw = None), Parameter('t0_prot_LACY_MONOMER_cyt', 0))
55 Initial(prot(name = 'spontaneous', loc = 'cyt', dna = None, met = None, prot = None,
    ↪rna = None, up = None, dw = None), Parameter('t0_prot_spontaneous_cyt', 0))
56 Initial(cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot
    ↪= None, rna = None, up = None, dw = None), Parameter('t0_cplx_BETAGALACTOSID_CPLX_
    ↪cyt', 0))
57 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))
58 Rule('LACTOSE_MUTAROTATION_CYT',
59     met(name = 'alpha_lactose', loc = 'cyt', dna = None, met = None, prot = None,
    ↪rna = None) |
60     met(name = 'beta_lactose', loc = 'cyt', dna = None, met = None, prot = None,
    ↪rna = None),
61     Parameter('fwd_LACTOSE_MUTAROTATION_CYT', 1.000000),
62     Parameter('rvs_LACTOSE_MUTAROTATION_CYT', 1.000000))
63 Rule('GALACTOSE_MUTAROTATION_CYT',
64     met(name = 'alpha_GALACTOSE', loc = 'cyt', dna = None, met = None, prot =
    ↪None, rna = None) |
65     met(name = 'beta_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = None,
    ↪ rna = None),

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```

66     Parameter('fwd_GALACTOSE_MUTAROTATION_CYT', 1.000000),
67     Parameter('rvs_GALACTOSE_MUTAROTATION_CYT', 1.000000))
68 Rule('GLUCOSE_MUTAROTATION_CYT',
69     met(name = 'alpha_glucose', loc = 'cyt', dna = None, met = None, prot = None,
↪ rna = None) |
70     met(name = 'beta_glucose', loc = 'cyt', dna = None, met = None, prot = None,
↪ rna = None),
71     Parameter('fwd_GLUCOSE_MUTAROTATION_CYT', 1.000000),
72     Parameter('rvs_GLUCOSE_MUTAROTATION_CYT', 1.000000))
73 Rule('TRANS_RXN_24',
74     prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
↪ rna = None, up = None, dw = None) +
75     met(name = 'PROTON', loc = 'per', dna = None, met = None, prot = None, rna =
↪ None) +
76     met(name = 'alpha_lactose', loc = 'per', dna = None, met = None, prot = None,
↪ rna = None) |
77     prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
↪ rna = None, up = None, dw = None) +
78     met(name = 'PROTON', loc = 'cyt', dna = None, met = None, prot = None, rna =
↪ None) +
79     met(name = 'alpha_lactose', loc = 'cyt', dna = None, met = None, prot = None,
↪ rna = None),
80     Parameter('fwd_TRANS_RXN_24', 1.000000),
81     Parameter('rvs_TRANS_RXN_24', 0.000000))
82 Rule('TRANS_RXN_24_beta',
83     prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
↪ rna = None, up = None, dw = None) +
84     met(name = 'PROTON', loc = 'per', dna = None, met = None, prot = None, rna =
↪ None) +
85     met(name = 'beta_lactose', loc = 'per', dna = None, met = None, prot = None,
↪ rna = None) |
86     prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
↪ rna = None, up = None, dw = None) +
87     met(name = 'PROTON', loc = 'cyt', dna = None, met = None, prot = None, rna =
↪ None) +
88     met(name = 'beta_lactose', loc = 'cyt', dna = None, met = None, prot = None,
↪ rna = None),
89     Parameter('fwd_TRANS_RXN_24_beta', 1.000000),
90     Parameter('rvs_TRANS_RXN_24_beta', 0.000000))
91 Rule('TRANS_RXN_94',
92     prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
↪ rna = None, up = None, dw = None) +
93     met(name = 'PROTON', loc = 'per', dna = None, met = None, prot = None, rna =
↪ None) +
94     met(name = 'MELIBIOSE', loc = 'per', dna = None, met = None, prot = None, rna
↪ = None) |
95     prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
↪ rna = None, up = None, dw = None) +
96     met(name = 'PROTON', loc = 'cyt', dna = None, met = None, prot = None, rna =
↪ None) +
97     met(name = 'MELIBIOSE', loc = 'cyt', dna = None, met = None, prot = None, rna
↪ = None),
98     Parameter('fwd_TRANS_RXN_94', 1.000000),
99     Parameter('rvs_TRANS_RXN_94', 0.000000))
100 Rule('RXN0_7215',
101     prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
↪ rna = None, up = None, dw = None) +

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102     met(name = 'PROTON', loc = 'per', dna = None, met = None, prot = None, rna =
↪ None) +
103     met(name = 'CPD_3561', loc = 'per', dna = None, met = None, prot = None, rna
↪ = None) |
104     prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
↪ rna = None, up = None, dw = None) +
105     met(name = 'PROTON', loc = 'cyt', dna = None, met = None, prot = None, rna =
↪ None) +
106     met(name = 'CPD_3561', loc = 'cyt', dna = None, met = None, prot = None, rna
↪ = None),
107     Parameter('fwd_RXN0_7215', 1.000000),
108     Parameter('rvs_RXN0_7215', 0.000000))
109 Rule('RXN0_7217',
110     prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
↪ rna = None, up = None, dw = None) +
111     met(name = 'PROTON', loc = 'per', dna = None, met = None, prot = None, rna =
↪ None) +
112     met(name = 'CPD_3785', loc = 'per', dna = None, met = None, prot = None, rna
↪ = None) |
113     prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
↪ rna = None, up = None, dw = None) +
114     met(name = 'PROTON', loc = 'cyt', dna = None, met = None, prot = None, rna =
↪ None) +
115     met(name = 'CPD_3785', loc = 'cyt', dna = None, met = None, prot = None, rna
↪ = None),
116     Parameter('fwd_RXN0_7217', 1.000000),
117     Parameter('rvs_RXN0_7217', 0.000000))
118 Rule('RXN_17755',
119     prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
↪ rna = None, up = None, dw = None) +
120     met(name = 'PROTON', loc = 'per', dna = None, met = None, prot = None, rna =
↪ None) +
121     met(name = 'CPD_3801', loc = 'per', dna = None, met = None, prot = None, rna
↪ = None) |
122     prot(name = 'LACY_MONOMER', loc = 'imem', dna = None, met = None, prot = None,
↪ rna = None, up = None, dw = None) +
123     met(name = 'PROTON', loc = 'cyt', dna = None, met = None, prot = None, rna =
↪ None) +
124     met(name = 'CPD_3801', loc = 'cyt', dna = None, met = None, prot = None, rna
↪ = None),
125     Parameter('fwd_RXN_17755', 1.000000),
126     Parameter('rvs_RXN_17755', 0.000000))
127 Rule('BETAGALACTOSID_RXN',
128     cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot
↪ = None, rna = None) +
129     met(name = 'beta_lactose', loc = 'cyt', dna = None, met = None, prot = None,
↪ rna = None) +
130     met(name = 'WATER', loc = 'cyt', dna = None, met = None, prot = None, rna =
↪ None) |
131     cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot
↪ = None, rna = None) +
132     met(name = 'beta_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = None,
↪ rna = None) +
133     met(name = 'beta_glucose', loc = 'cyt', dna = None, met = None, prot = None,
↪ rna = None),
134     Parameter('fwd_BETAGALACTOSID_RXN', 1.000000),
135     Parameter('rvs_BETAGALACTOSID_RXN', 0.000000))

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```

136 Rule('BETAGALACTOSID_RXN_alpha',
137     cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
↪= None, rna = None) +
138     met(name = 'alpha_lactose', loc = 'cyt', dna = None, met = None, prot = None, _
↪rna = None) +
139     met(name = 'WATER', loc = 'cyt', dna = None, met = None, prot = None, rna = _
↪None) |
140     cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
↪= None, rna = None) +
141     met(name = 'alpha_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = _
↪None, rna = None) +
142     met(name = 'alpha_glucose', loc = 'cyt', dna = None, met = None, prot = None, _
↪rna = None),
143     Parameter('fwd_BETAGALACTOSID_RXN_alpha', 1.000000),
144     Parameter('rvs_BETAGALACTOSID_RXN_alpha', 0.000000))
145 Rule('RXN0_5363',
146     cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
↪= None, rna = None) +
147     met(name = 'alpha_lactose', loc = 'cyt', dna = None, met = None, prot = None, _
↪rna = None) |
148     cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
↪= None, rna = None) +
149     met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = _
↪None, rna = None),
150     Parameter('fwd_RXN0_5363', 1.000000),
151     Parameter('rvs_RXN0_5363', 1.000000))
152 Rule('RXN0_5363_beta',
153     cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
↪= None, rna = None) +
154     met(name = 'beta_lactose', loc = 'cyt', dna = None, met = None, prot = None, _
↪rna = None) |
155     cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
↪= None, rna = None) +
156     met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = _
↪None, rna = None),
157     Parameter('fwd_RXN0_5363_beta', 1.000000),
158     Parameter('rvs_RXN0_5363_beta', 1.000000))
159 Rule('ALLOLACTOSE_DEG_alpha',
160     cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
↪= None, rna = None) +
161     met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = _
↪None, rna = None) +
162     None |
163     cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
↪= None, rna = None) +
164     met(name = 'alpha_GALACTOSE', loc = 'cyt', dna = None, met = None, prot = _
↪None, rna = None) +
165     met(name = 'alpha_glucose', loc = 'cyt', dna = None, met = None, prot = None, _
↪rna = None),
166     Parameter('fwd_ALLOLACTOSE_DEG_alpha', 1.000000),
167     Parameter('rvs_ALLOLACTOSE_DEG_alpha', 0.000000))
168 Rule('ALLOLACTOSE_DEG_beta',
169     cplx(name = 'BETAGALACTOSID_CPLX', loc = 'cyt', dna = None, met = None, prot_
↪= None, rna = None) +
170     met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = _
↪None, rna = None) +
171     None |

```

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```

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

```

5.2 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. For non-symmetrical complexes (e.g., `[araF, araH, araH, araG, araG]`), the user must be aware that the order in `SOURCE` and `TARGET` defines the order in the product: `[SOURCE, TARGET]`.

2. The 3rd and 4th columns declare the forward and the reverse reaction rate values, respectively.

3. The 5th column declares the location of the complex components:

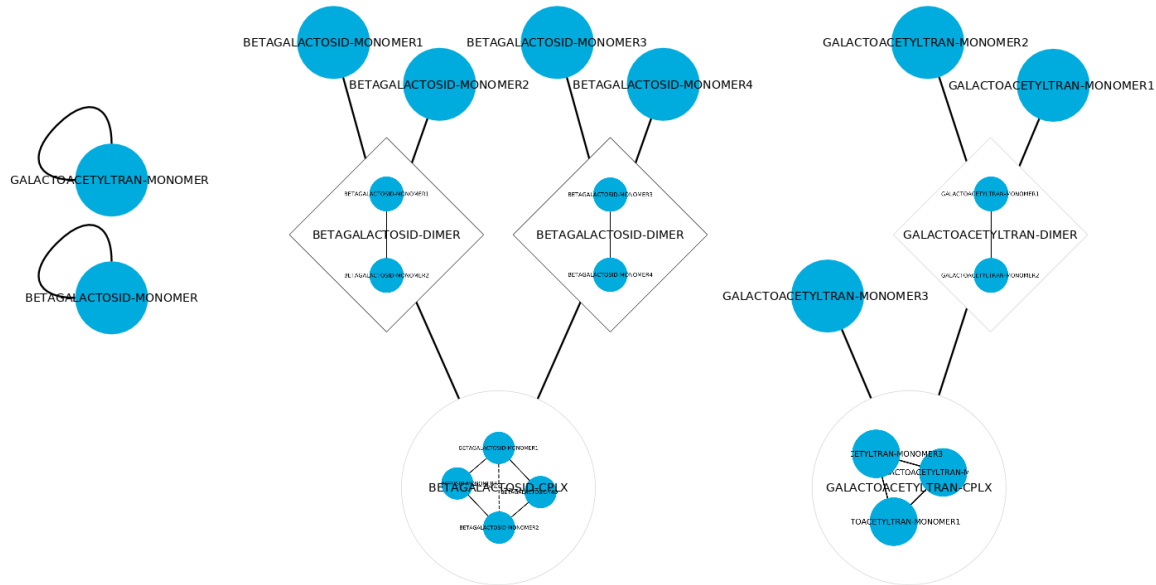
1. If the number of locations match the number of components of the complex, each location is mapped in the same order to each component.
2. If the number of locations unmatch the number of components, the first location is used for every component. The remaining locations are disregarded.
3. If the number of locations is one, the location is used for every component.

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

Examples:

	SOURCE	TARGET	FWD_RATE	RVS_RATE	LOCATION
1	lacZ	lacZ	1.0	0.0	cytosol
2	[lacZ, lacZ]	[lacZ, lacZ]	1.0	0.0	cytosol
3	lacA	lacA	1.0	0.0	cytosol
4	lacA	[lacA, lacA]	1.0	0.0	cytosol
5	lacI	lacI	1.0	0.0	cytosol
6					

Note: Visualization in Cytoscape. Currently, *Atlas* do not export networks into graphml that could be imported into Cytoscape. To construct visual representations, please create simple networks and right-click to embed a subnetwork in the corresponding node.



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 DataFrame the networks (employing `pandas.concat(list)`) or concatenate externally and employ 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`):

```
1 from pysb import *
2 Model()
3
4 Monomer('prot',
5         ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
6         {'name' : [ 'lacA', 'lacI', 'lacZ' ],
7          'loc' : [ 'cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
8                  'omem' ]})
```

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```

8 Observable('obs_prot_lacA_cyt', prot(name = 'lacA', loc = 'cyt', dna = None, met =
  ↳None, prot = None, rna = None, up = None, dw = None))
9 Initial(prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = None, dw = None), Parameter('t0_prot_lacA_cyt', 0))
10 Observable('obs_prot_lacI_cyt', prot(name = 'lacI', loc = 'cyt', dna = None, met =
  ↳None, prot = None, rna = None, up = None, dw = None))
11 Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = None, dw = None), Parameter('t0_prot_lacI_cyt', 0))
12 Observable('obs_prot_lacZ_cyt', prot(name = 'lacZ', loc = 'cyt', dna = None, met =
  ↳None, prot = None, rna = None, up = None, dw = None))
13 Initial(prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = None, dw = None), Parameter('t0_prot_lacZ_cyt', 0))
14 Initial(prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = None, dw = 1) %
15     prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = 1, dw = 2) %
16     prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = 2, dw = None),
17     Parameter('t0_cplx_lacAx3_cyt', 0))
18 Observable('obs_cplx_lacAx3_cyt',
19     prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = None, dw = 1) %
20     prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = 1, dw = 2) %
21     prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = 2, dw = None))
22 Initial(prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = None, dw = 1) %
23     prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = 1, dw = None),
24     Parameter('t0_cplx_lacAx2_cyt', 0))
25 Observable('obs_cplx_lacAx2_cyt',
26     prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = None, dw = 1) %
27     prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = 1, dw = None))
28 Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = None, dw = 1) %
29     prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = 1, dw = None),
30     Parameter('t0_cplx_lacIx2_cyt', 0))
31 Observable('obs_cplx_lacIx2_cyt',
32     prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = None, dw = 1) %
33     prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = 1, dw = None))
34 Initial(prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = None, dw = 1) %
35     prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = 1, dw = 2) %
36     prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = 2, dw = 3) %
37     prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = 3, dw = None),
38     Parameter('t0_cplx_lacZx4_cyt', 0))
39 Observable('obs_cplx_lacZx4_cyt',
40     prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
  ↳None, up = None, dw = 1) %
  ↳None, up = None, dw = 1) %

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```

41     prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
↪None, up = 1, dw = 2) %
42     prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
↪None, up = 2, dw = 3) %
43     prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
↪None, up = 3, dw = None))
44 Initial(prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
↪None, up = None, dw = 1) %
45     prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
↪None, up = 1, dw = None),
46     Parameter('t0_cplx_lacZx2_cyt', 0))
47 Observable('obs_cplx_lacZx2_cyt',
48     prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
↪None, up = None, dw = 1) %
49     prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
↪None, up = 1, dw = None))
50 Rule('PhysicalInteractionRule_1',
51     prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = None) +
52     prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = None) |
53     prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = 1) %
54     prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = 1, dw = None),
55     Parameter('fwd_PhysicalInteractionRule_1', 1.000000),
56     Parameter('rvs_PhysicalInteractionRule_1', 0.000000))
57 Rule('PhysicalInteractionRule_2',
58     prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = 1) %
59     prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = 1, dw = None) +
60     prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = 2) %
61     prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = 2, dw = None) |
62     prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = 1) %
63     prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = 1, dw = 2) %
64     prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = 2, dw = 3) %
65     prot(name = 'lacZ', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = 3, dw = None),
66     Parameter('fwd_PhysicalInteractionRule_2', 1.000000),
67     Parameter('rvs_PhysicalInteractionRule_2', 0.000000))
68 Rule('PhysicalInteractionRule_3',
69     prot(name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = None) +
70     prot(name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = None) |
71     prot(name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = 1) %
72     prot(name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = 1, dw = None),
73     Parameter('fwd_PhysicalInteractionRule_3', 1.000000),
74     Parameter('rvs_PhysicalInteractionRule_3', 0.000000))

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```

75 Rule('PhysicalInteractionRule_4',
76     prot(name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = None) +
77     prot(name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = 1) %
78     prot(name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = 1, dw = None) |
79     prot(name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = 1) %
80     prot(name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = 1, dw = 2) %
81     prot(name = 'lacA', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = 2, dw = None),
82     Parameter('fwd_PhysicalInteractionRule_4', 1.000000),
83     Parameter('rvs_PhysicalInteractionRule_4', 0.000000))
84 Rule('PhysicalInteractionRule_5',
85     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = None) +
86     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = None) |
87     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = 1) %
88     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = 1, dw = None),
89     Parameter('fwd_PhysicalInteractionRule_5', 1.000000),
90     Parameter('rvs_PhysicalInteractionRule_5', 0.000000))

```

5.3 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., [lacZ, SMALL-alpha-ALLOLACTOSE]) as a complex, therefore, the components are internally linked.

2. The 3rd and 4th columns declare the forward and the reverse reaction rate values, respectively.
3. The 5th column 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. The remaining locations are disregarded.
 3. If the number of locations is one, the location is used for every component.

Valid location 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	
1	[lacI, lacI]	SMALL-alpha-ALLOLACTOSE	10.0	0.0001	cytosol	
2	[lacI, lacI, SMALL-alpha-ALLOLACTOSE]	SMALL-alpha-ALLOLACTOSE	10.			
3	↪ 0	0.0001	cytosol			
4	[lacI, lacI]	SMALL-beta-ALLOLACTOSE	10.0	0.0001	cytosol	
5	[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 DataFrame the networks (employing `pandas.concat(list)`) or concatenate externally and employ 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):

```

1 from pysb import *
2 Model()
3
4 Monomer('met',
5         ['name', 'loc', 'dna', 'met', 'prot', 'rna'],
6         { 'name' : [ 'alpha_ALLOLACTOSE', 'beta_ALLOLACTOSE' ],
7           'loc' : [ 'cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
8             ↪ 'omem' ] })
9 Monomer('prot',
10         ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
11         { 'name' : [ 'lacI' ],
12           'loc' : [ 'cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
13             ↪ 'omem' ] })
14 Observable('obs_met_alpha_ALLOLACTOSE_cyt', met(name = 'alpha_ALLOLACTOSE', loc = 'cyt
15             ↪'))
16 Initial(met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot =
17             ↪None, rna = None), Parameter('t0_met_alpha_ALLOLACTOSE_cyt', 0))
18 Observable('obs_met_beta_ALLOLACTOSE_cyt', met(name = 'beta_ALLOLACTOSE', loc = 'cyt
19             ↪'))
20 Initial(met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot =
21             ↪None, rna = None), Parameter('t0_met_beta_ALLOLACTOSE_cyt', 0))

```

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```

16 Observable('obs_prot_lacI_cyt', prot(name = 'lacI', loc = 'cyt', dna = None, met =
    ↪ None, prot = None, rna = None, up = None, dw = None))
17 Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna =
    ↪ None, up = None, dw = None), Parameter('t0_prot_lacI_cyt', 0))
18 Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
    ↪ up = None, dw = 1) %
19     prot(name = 'lacI', loc = 'cyt', dna = None, met = 3, prot = None, rna = None,
    ↪ up = 1, dw = None) %
20     met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 3,
    ↪ rna = None) %
21     met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2,
    ↪ rna = None),
22     Parameter('t0_cplx_lacIx2_alpha_ALLOLACTOSEx2_cyt', 0))
23 Observable('obs_cplx_lacIx2_alpha_ALLOLACTOSEx2_cyt',
24     prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
    ↪ up = None, dw = 1) %
25     prot(name = 'lacI', loc = 'cyt', dna = None, met = 3, prot = None, rna = None,
    ↪ up = 1, dw = None) %
26     met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 3,
    ↪ rna = None) %
27     met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2,
    ↪ rna = None))
28 Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
    ↪ up = None, dw = 1) %
29     prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna =
    ↪ None, up = 1, dw = None) %
30     met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2,
    ↪ rna = None),
31     Parameter('t0_cplx_lacIx2_alpha_ALLOLACTOSEx1_cyt', 0))
32 Observable('obs_cplx_lacIx2_alpha_ALLOLACTOSEx1_cyt',
33     prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
    ↪ up = None, dw = 1) %
34     prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna =
    ↪ None, up = 1, dw = None) %
35     met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2,
    ↪ rna = None))
36 Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
    ↪ up = None, dw = 1) %
37     prot(name = 'lacI', loc = 'cyt', dna = None, met = 3, prot = None, rna = None,
    ↪ up = 1, dw = None) %
38     met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 3,
    ↪ rna = None) %
39     met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2,
    ↪ rna = None),
40     Parameter('t0_cplx_lacIx2_beta_ALLOLACTOSEx2_cyt', 0))
41 Observable('obs_cplx_lacIx2_beta_ALLOLACTOSEx2_cyt',
42     prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
    ↪ up = None, dw = 1) %
43     prot(name = 'lacI', loc = 'cyt', dna = None, met = 3, prot = None, rna = None,
    ↪ up = 1, dw = None) %
44     met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 3,
    ↪ rna = None) %
45     met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2,
    ↪ rna = None))
46 Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
    ↪ up = None, dw = 1) %
47     prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna =
    ↪ None, up = 1, dw = None) %

```

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```

48     met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2,
↳ rna = None),
49     Parameter('t0_cplx_lacIx2_beta_ALLOLACTOSEx1_cyt', 0))
50 Observable('obs_cplx_lacIx2_beta_ALLOLACTOSEx1_cyt',
51     prot(name = 'lacI', loc = 'cyt', dna = None, met = 2, prot = None, rna = None,
↳ up = None, dw = 1) %
52     prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna =
↳ None, up = 1, dw = None) %
53     met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot = 2,
↳ rna = None))
54 Rule('PhysicalInteractionRule_1',
55     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↳ None, up = None, dw = 1) %
56     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↳ None, up = 1, dw = None) +
57     met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, prot = None, met =
↳ None, rna = None) |
58     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 2, rna = None,
↳ up = None, dw = 1) %
59     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↳ None, up = 1, dw = None) %
60     met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 2, met = None,
↳ rna = None),
61     Parameter('fwd_PhysicalInteractionRule_1', 10.000000),
62     Parameter('rvs_PhysicalInteractionRule_1', 0.000100))
63 Rule('PhysicalInteractionRule_2',
64     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 2, rna = None,
↳ up = None, dw = 1) %
65     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↳ None, up = 1, dw = None) %
66     met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 2, met = None,
↳ rna = None) +
67     met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, prot = None, met =
↳ None, rna = None) |
68     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 2, rna = None,
↳ up = None, dw = 1) %
69     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 3, rna = None,
↳ up = 1, dw = None) %
70     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),
72     Parameter('fwd_PhysicalInteractionRule_2', 10.000000),
73     Parameter('rvs_PhysicalInteractionRule_2', 0.000100))
74 Rule('PhysicalInteractionRule_3',
75     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↳ None, up = None, dw = 1) %
76     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↳ None, up = 1, dw = None) +
77     met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = None, met =
↳ None, rna = None) |
78     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 2, rna = None,
↳ up = None, dw = 1) %
79     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↳ None, up = 1, dw = None) %
80     met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 2, met = None,
↳ rna = None),

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```

81     Parameter('fwd_PhysicalInteractionRule_3', 10.000000),
82     Parameter('rvs_PhysicalInteractionRule_3', 0.000100))
83 Rule('PhysicalInteractionRule_4',
84     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 2, rna = None,
85     ↪ up = None, dw = 1) %
86     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
87     ↪ None, up = 1, dw = None) %
88     met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 2, met = None,
89     ↪ rna = None) +
90     met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = None, met =
91     ↪ None, rna = None) |
92     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 2, rna = None,
93     ↪ up = None, dw = 1) %
94     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 3, rna = None,
95     ↪ up = 1, dw = None) %
96     met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 3, met = None,
97     ↪ rna = None) %
98     met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 2, met = None,
99     ↪ rna = None),
100     Parameter('fwd_PhysicalInteractionRule_4', 10.000000),
101     Parameter('rvs_PhysicalInteractionRule_4', 0.000100))

```

5.4 Transcription Factor-DNA Binding Site Interaction Networks

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

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

It does not matter the order, as the two columns define a bimolecular reaction whose product is the merge of all components into one complex. *Atlas* understands components inside brackets (e.g., [lacI, lacI, BS-lacI-422-402]) as a complex, therefore, the components are internally linked.

2. The 3rd and 4th columns declare the forward and the reverse reaction rate values, respectively.

3. The 5th column declares the location of the complex components:

1. If the number of locations matches the number of components of the complex, each location is mapped to the component.
2. If the number of locations mismatches the number of components, the first location is used for every component. The remaining locations are disregarded.
3. If the number of locations is one, the location is used for every component.

Valid location 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:

	SOURCE	TARGET	FWD_RATE	RVS_RATE	LOCATION
1	# lacZYA				
2	[lacI, lacI]	BS-lacI-422-402	1.0	0.01	cytosol
3	[lacI, lacI]	BS-lacI-21-1	1.0	0.01	cytosol
4	[lacI, lacI]	BS-lacI-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 `DataFrame` the networks (employing `pandas.concat(list)`) or concatenate externally and employ 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`):

```

1 from pysb import *
2 Model()
3
4 Monomer('prot',
5         ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
6         { 'name' : [ 'lacI' ],
7           'loc' : [ 'cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
8             ↪ 'omem' ] })
9 Monomer('dna',
10         ['name', 'type', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
11         { 'name' : [ 'lacI_21_1', 'lacI_422_402', 'lacI_72_92' ],
12           'type' : [ 'BS' ],
13           'loc' : [ 'cyt' ] })
14 Observable('obs_prot_lacI_cyt', prot(name = 'lacI', loc = 'cyt', dna = None, met = ↪
15   ↪ None, prot = None, rna = None, up = None, dw = None))
16 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))
18 Rule('PhysicalInteractionRule_1',
19     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = ↪
20   ↪ None, up = None, dw = 1) %
21     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = ↪
22   ↪ None, up = 1, dw = None) +
23     dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, prot = None, ↪
24   ↪ met = None, rna = None, up = WILD, dw = WILD) |
25     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna = ↪
26   ↪ None, up = None, dw = 1) %
27     prot(name = 'lacI', loc = 'cyt', dna = 2, prot = None, met = None, rna = None, ↪
28   ↪ up = 1, dw = None) %
29     dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, prot = 2, ↪
30   ↪ met = None, rna = None, up = WILD, dw = WILD),

```

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```

22     Parameter('fwd_PhysicalInteractionRule_1', 1.000000),
23     Parameter('rvs_PhysicalInteractionRule_1', 0.010000))
24 Rule('PhysicalInteractionRule_2',
25     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = 1) %
26     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = 1, dw = None) +
27     dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, prot = None,
↪met = None, rna = None, up = WILD, dw = WILD) |
28     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = 1) %
29     prot(name = 'lacI', loc = 'cyt', dna = 2, prot = None, met = None, rna = None,
↪ up = 1, dw = None) %
30     dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, prot = 2, met =
↪None, rna = None, up = WILD, dw = WILD),
31     Parameter('fwd_PhysicalInteractionRule_2', 1.000000),
32     Parameter('rvs_PhysicalInteractionRule_2', 0.010000))
33 Rule('PhysicalInteractionRule_3',
34     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = 1) %
35     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = 1, dw = None) +
36     dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, prot = None,
↪met = None, rna = None, up = WILD, dw = WILD) |
37     prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
↪None, up = None, dw = 1) %
38     prot(name = 'lacI', loc = 'cyt', dna = 2, prot = None, met = None, rna = None,
↪ up = 1, dw = None) %
39     dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, prot = 2, met =
↪None, rna = None, up = WILD, dw = WILD),
40     Parameter('fwd_PhysicalInteractionRule_3', 1.000000),
41     Parameter('rvs_PhysicalInteractionRule_3', 0.010000))

```

5.5 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 rate values:

- 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 (see *Genome Graphs*).

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

Examples:

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

```

1 from pysb import *
2 Model()
3
4 Monomer('dna',
5     ['name', 'type', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
6     { 'name' : ['lacA', 'lacI_21_1', 'lacI_422_402', 'lacI_72_92', 'lacY', 'lacZ
7     ↪'],
8     'type' : ['BS', 'cds', 'pro1', 'pro2', 'pro3', 'pro4', 'rbs', 'ter1', 'ter2'],
9     'loc' : ['cyt']})
10 Monomer('rna',
11     ['name', 'type', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
12     { 'name' : ['lacA', 'lacI_21_1', 'lacI_422_402', 'lacI_72_92', 'lacY', 'lacZ
13     ↪'],
14     'type' : ['BS', 'cds', 'pro1', 'pro2', 'pro3', 'pro4', 'rbs', 'ter1', 'ter2'],
15     'loc' : ['cyt']})
16 Monomer('prot',
17     ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
18     { 'name' : ['lacA', 'lacI_21_1', 'lacI_422_402', 'lacI_72_92', 'lacY', 'lacZ
19     ↪'],
20     'loc' : ['cyt', 'mem']})
21 Monomer('cplx',
22     ['name', 'loc', 'dna', 'met', 'prot', 'rna'],
23     { 'name' : ['RIBOSOME_CPLX'],
24     'loc' : ['cyt']})
25 Rule('docking_1_lacZ_pro4',
26     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
27     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %

```

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```

25     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
26     prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
27     prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = 4, dw = None) +
28     dna(name = 'lacZ', type = 'pro4', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) |
29     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
30     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
31     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
32     prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
33     prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
34     dna(name = 'lacZ', type = 'pro4', loc = 'cyt', prot = 5, up = WILD, dw =
↪WILD),
35     Parameter('fwd_docking_1_lacZ_pro4', 1.000000),
36     Parameter('rvs_docking_1_lacZ_pro4', 1.000000))
37 Rule('docking_2_lacZ_pro3',
38     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
39     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
40     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
41     prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
42     prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = 4, dw = None) +
43     dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) |
44     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
45     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
46     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
47     prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
48     prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
49     dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = 5, up = WILD, dw =
↪WILD),
50     Parameter('fwd_docking_2_lacZ_pro3', 1.000000),
51     Parameter('rvs_docking_2_lacZ_pro3', 1.000000))
52 Rule('docking_3_lacZ_pro2',
53     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
54     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
55     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
56     prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
57     prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = 4, dw = None) +
58     dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) |
59     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
60     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
61     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) %
63     prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
64     dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = 5, up = WILD, dw =
↪WILD),
65     Parameter('fwd_docking_3_lacZ_pro2', 1.000000),
66     Parameter('rvs_docking_3_lacZ_pro2', 1.000000))
67 Rule('docking_4_lacZ_pro1',
68     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
69     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
70     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
71     prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
72     prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = 4, dw = None) +
73     dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) |
74     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %

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75     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
76     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
77     prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
78     prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
79     dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = 5, up = WILD, dw =
↪WILD),
80     Parameter('fwd_docking_4_lacZ_pro1', 1.000000),
81     Parameter('rvs_docking_4_lacZ_pro1', 1.000000))
82 Rule('docking_5_lacY_pro1',
83     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
84     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
85     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
86     prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
87     prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = 4, dw = None) +
88     dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) |
89     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
90     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
91     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
92     prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
93     prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
94     dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = 5, up = WILD, dw =
↪WILD),
95     Parameter('fwd_docking_5_lacY_pro1', 1.000000),
96     Parameter('rvs_docking_5_lacY_pro1', 1.000000))
97 Rule('sliding_1_lacZ_pro4_pro3_holoenzyme',
98     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
99     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
100    prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
101    prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
102    prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
103    dna(name = 'lacZ', type = 'pro4', loc = 'cyt', prot = 5, up = WILD, dw =
↪WILD) +
104    dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) +
105    None >>
106    prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
107    prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
108    prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
109    prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
110    prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = None, dw =
↪None) %
111    dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = 4, up = WILD, dw =
↪WILD) +
112    dna(name = 'lacZ', type = 'pro4', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) +
113    rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = None),
114    Parameter('fwd_sliding_1_lacZ_pro4_pro3_holoenzyme', 1.000000))
115 Rule('sliding_2_lacZ_pro3_pro2_holoenzyme',
116     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
117     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
118     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
119     prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
120     prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
121     dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = 5, up = WILD, dw =
↪WILD) +

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122     dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) +
123     None >>
124     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
125     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
126     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
127     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
128     prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = None, dw =
↪None) %
129     dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = 4, up = WILD, dw =
↪WILD) +
130     dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) +
131     rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = None),
132     Parameter('fwd_sliding_2_lacZ_pro3_pro2_holoenzyme', 1.000000))
133 Rule('sliding_3_lacZ_pro2_92_holoenzyme',
134     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
135     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
136     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
137     prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
138     prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
139     dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = 5, up = WILD, dw =
↪WILD) +
140     dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) +
141     None >>
142     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
143     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
144     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
145     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
146     prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = None, dw =
↪None) %
147     dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = 4, up = WILD, dw =
↪WILD) +
148     dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) +
149     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = None, dw = None),
150     Parameter('fwd_sliding_3_lacZ_pro2_92_holoenzyme', 1.000000))
151 Rule('sliding_4_lacZ_pro1_rbs_holoenzyme',
152     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
153     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
154     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
155     prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
156     prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
157     dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = 5, up = WILD, dw =
↪WILD) +
158     dna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) +
159     None >>
160     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
161     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
162     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
163     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
164     prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = None, dw =
↪None) %

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165     dna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
166     ↪+
167     dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = None, up = WILD, dw =
168     ↪WILD) +
169     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
170     ↪None, rna = None, up = None, dw = None),
171     Parameter('fwd_sliding_4_lacZ_pro1_rbs_holoenzyme', 1.000000))
172 Rule('sliding_5_lacY_pro1_rbs_holoenzyme',
173     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
174     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
175     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
176     prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = 4) %
177     prot(name = 'rpoD', loc = 'cyt', dna = 5, met = None, up = 4, dw = None) %
178     dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = 5, up = WILD, dw =
179     ↪WILD) +
180     dna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw =
181     ↪WILD) +
182     None >>
183     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
184     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
185     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
186     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
187     prot(name = 'rpoD', loc = 'cyt', dna = None, met = None, up = None, dw =
188     ↪None) %
189     dna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
190     ↪+
191     dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = None, up = WILD, dw =
192     ↪WILD) +
193     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
194     ↪None, rna = None, up = None, dw = None),
195     Parameter('fwd_sliding_5_lacY_pro1_rbs_holoenzyme', 1.000000))
196 Rule('sliding_1_lacZ_pro3_to_lacZ_pro2',
197     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
198     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
199     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
200     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
201     dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = 4, up = WILD, dw =
202     ↪WILD) +
203     dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = None, up = WILD, dw =
204     ↪WILD) +
205     None >>
206     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
207     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
208     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
209     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
210     dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = 4, up = WILD, dw =
211     ↪WILD) +
212     dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = None, up = WILD, dw =
213     ↪WILD) +
214     rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
215     ↪None, rna = None, up = None, dw = None),
216     Parameter('fwd_sliding_1_lacZ_pro3_to_lacZ_pro2', 1.000000))
217 Rule('sliding_2_lacZ_pro2_to_BS_lacI_72_92',
218     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
219     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
220     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
221     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %

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208     dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = 4, up = WILD, dw =
↳WILD) +
209     dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = None, up = WILD, dw
↳= WILD) +
210     None >>
211     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
212     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
213     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
214     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
215     dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = 4, up = WILD, dw =
↳WILD) +
216     dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = None, up = WILD, dw =
↳WILD) +
217     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = None, dw = None),
218     Parameter('fwd_sliding_2_lacZ_pro2_to_BS_lacI_72_92', 1.000000))
219 Rule('sliding_3_BS_lacI_72_92_to_BS_lacI_21_1',
220     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
221     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
222     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
223     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
224     dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = 4, up = WILD, dw =
↳WILD) +
225     dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', prot = None, up = WILD, dw
↳= WILD) +
226     None >>
227     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
228     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
229     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
230     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
231     dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', prot = 4, up = WILD, dw =
↳WILD) +
232     dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', prot = None, up = WILD, dw
↳= WILD) +
233     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = None, dw = None),
234     Parameter('fwd_sliding_3_BS_lacI_72_92_to_BS_lacI_21_1', 1.000000))
235 Rule('sliding_4_BS_lacI_21_1_to_lacZ_pro1',
236     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
237     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
238     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
239     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
240     dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', prot = 4, up = WILD, dw =
↳WILD) +
241     dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = None, up = WILD, dw =
↳WILD) +
242     None >>
243     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
244     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
245     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
246     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
247     dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = 4, up = WILD, dw =
↳WILD) +
248     dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', prot = None, up = WILD, dw
↳= WILD) +
249     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = None, dw = None),

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250     Parameter('fwd_sliding_4_BS_lacI_21_1_to_lacZ_pro1', 1.000000))
251 Rule('sliding_5_lacZ_pro1_to_lacZ_rbs',
252     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
253     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
254     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
255     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
256     dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = 4, up = WILD, dw =
↳ WILD) +
257     dna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw =
↳ WILD) +
258     None >>
259     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
260     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
261     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
262     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
263     dna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
↳ +
264     dna(name = 'lacZ', type = 'pro1', loc = 'cyt', prot = None, up = WILD, dw =
↳ WILD) +
265     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳ None, rna = None, up = None, dw = None),
266     Parameter('fwd_sliding_5_lacZ_pro1_to_lacZ_rbs', 1.000000))
267 Rule('sliding_6_lacZ_rbs_to_lacZ_cds',
268     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
269     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
270     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
271     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
272     dna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
↳ +
273     dna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = None, up = WILD, dw =
↳ WILD) +
274     None >>
275     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
276     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
277     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
278     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
279     dna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
↳ +
280     dna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw =
↳ WILD) +
281     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳ None, rna = None, up = None, dw = None),
282     Parameter('fwd_sliding_6_lacZ_rbs_to_lacZ_cds', 1.000000))
283 Rule('sliding_7_lacZ_cds_to_BS_lacI_422_402',
284     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
285     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
286     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
287     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
288     dna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
↳ +
289     dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', prot = None, up = WILD,
↳ dw = WILD) +
290     None >>
291     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
292     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
293     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
294     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %

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295     dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', prot = 4, up = WILD, dw =
↳= WILD) +
296     dna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = None, up = WILD, dw =
↳WILD) +
297     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = None, dw = None),
298     Parameter('fwd_sliding_7_lacZ_cds_to_BS_lacI_422_402', 1.000000))
299 Rule('sliding_8_BS_lacI_422_402_to_lacY_pro1',
300     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
301     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
302     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
303     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
304     dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', prot = 4, up = WILD, dw =
↳= WILD) +
305     dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = None, up = WILD, dw =
↳WILD) +
306     None >>
307     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
308     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
309     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
310     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
311     dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = 4, up = WILD, dw =
↳WILD) +
312     dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', prot = None, up = WILD,
↳dw = WILD) +
313     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = None, dw = None),
314     Parameter('fwd_sliding_8_BS_lacI_422_402_to_lacY_pro1', 1.000000))
315 Rule('sliding_9_lacY_pro1_to_lacY_rbs',
316     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
317     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
318     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
319     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
320     dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = 4, up = WILD, dw =
↳WILD) +
321     dna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw =
↳WILD) +
322     None >>
323     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
324     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
325     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
326     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
327     dna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
↳+
328     dna(name = 'lacY', type = 'pro1', loc = 'cyt', prot = None, up = WILD, dw =
↳WILD) +
329     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = None, dw = None),
330     Parameter('fwd_sliding_9_lacY_pro1_to_lacY_rbs', 1.000000))
331 Rule('sliding_10_lacY_rbs_to_lacY_cds',
332     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
333     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
334     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
335     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
336     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) +

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338     None >>
339     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
340     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
341     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
342     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
343     dna(name = 'lacY', type = 'cds', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
↪+
344     dna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) +
345     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = None),
346     Parameter('fwd_sliding_10_lacY_rbs_to_lacY_cds', 1.000000))
347 Rule('sliding_11_lacY_cds_to_lacA_rbs',
348     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
349     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
350     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
351     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
352     dna(name = 'lacY', type = 'cds', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
↪+
353     dna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) +
354     None >>
355     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
356     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
357     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
358     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
359     dna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
↪+
360     dna(name = 'lacY', type = 'cds', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) +
361     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = None),
362     Parameter('fwd_sliding_11_lacY_cds_to_lacA_rbs', 1.000000))
363 Rule('sliding_12_lacA_rbs_to_lacA_cds',
364     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
365     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
366     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
367     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
368     dna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
↪+
369     dna(name = 'lacA', type = 'cds', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) +
370     None >>
371     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
372     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
373     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
374     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
375     dna(name = 'lacA', type = 'cds', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
↪+
376     dna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) +
377     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = None),
378     Parameter('fwd_sliding_12_lacA_rbs_to_lacA_cds', 1.000000))
379 Rule('sliding_13_lacA_cds_to_lacA_ter1',
380     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
381     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %

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382     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
383     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
384     dna(name = 'lacA', type = 'cds', loc = 'cyt', prot = 4, up = WILD, dw = WILD)
↪+
385     dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) >>
386     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
387     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
388     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
389     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
390     dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = 4, up = WILD, dw =
↪WILD) +
391     dna(name = 'lacA', type = 'cds', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD),
392     Parameter('fwd_sliding_13_lacA_cds_to_lacA_ter1', 1.000000))
393 Rule('sliding_14_lacA_ter1_to_lacA_ter2',
394     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
395     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
396     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
397     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
398     dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = 4, up = WILD, dw =
↪WILD) +
399     dna(name = 'lacA', type = 'ter2', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD) >>
400     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
401     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
402     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
403     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
404     dna(name = 'lacA', type = 'ter2', loc = 'cyt', prot = 4, up = WILD, dw =
↪WILD) +
405     dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD),
406     Parameter('fwd_sliding_14_lacA_ter1_to_lacA_ter2', 1.000000))
407 Rule('falloff_from_lacA_ter1',
408     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
409     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
410     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
411     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
412     dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = 4, up = WILD, dw =
↪WILD) >>
413     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
414     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
415     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
416     prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = None) +
417     dna(name = 'lacA', type = 'ter1', loc = 'cyt', prot = None, up = WILD, dw =
↪WILD),
418     Parameter('fwd_falloff_from_lacA_ter1', 1.000000))
419 Rule('falloff_from_lacA_ter2',
420     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
421     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
422     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %
423     prot(name = 'rpoC', loc = 'cyt', dna = 4, met = None, up = 3, dw = None) %
424     dna(name = 'lacA', type = 'ter2', loc = 'cyt', prot = 4, up = WILD, dw =
↪WILD) >>
425     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
426     prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = 1, dw = 2) %
427     prot(name = 'rpoB', loc = 'cyt', dna = None, met = None, up = 2, dw = 3) %

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428     prot(name = 'rpoC', loc = 'cyt', dna = None, met = None, up = 3, dw = None) +
429     dna(name = 'lacA', type = 'ter2', loc = 'cyt', prot = None, up = WILD, dw =
↳WILD),
430     Parameter('fwd_falloff_from_lacA_ter2', 1.000000))
431 Rule('dr_lacZ_rbs',
432     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
433     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = None) |
434     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
435     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = 1),
436     Parameter('fwd_dr_lacZ_rbs', 1.000000),
437     Parameter('rvs_dr_lacZ_rbs', 1.000000))
438 Rule('dr_lacY_rbs',
439     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
440     rna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = None) |
441     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
442     rna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = 1),
443     Parameter('fwd_dr_lacY_rbs', 1.000000),
444     Parameter('rvs_dr_lacY_rbs', 1.000000))
445 Rule('dr_lacA_rbs',
446     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
447     rna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = None) |
448     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
449     rna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = 1),
450     Parameter('fwd_dr_lacA_rbs', 1.000000),
451     Parameter('rvs_dr_lacA_rbs', 1.000000))
452 Rule('sr_lacZ_rbs',
453     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
454     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = 1) +
455     rna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = None) +
456     None >>
457     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
458     rna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = 1) +
459     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', prot = None) +
460     prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
↳None, up = None, dw = None),
461     Parameter('fwd_sr_lacZ_rbs', 1.000000))
462 Rule('sr_lacY_rbs',
463     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
464     rna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = 1) +
465     rna(name = 'lacY', type = 'cds', loc = 'cyt', prot = None) +
466     None >>
467     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
468     rna(name = 'lacY', type = 'cds', loc = 'cyt', prot = 1) +
469     rna(name = 'lacY', type = 'rbs', loc = 'cyt', prot = None) +
470     prot(name = 'lacY', loc = 'cyt', dna = None, met = None, prot = None, rna =
↳None, up = None, dw = None),
471     Parameter('fwd_sr_lacY_rbs', 1.000000))
472 Rule('sr_lacA_rbs',
473     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
474     rna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = 1) +
475     rna(name = 'lacA', type = 'cds', loc = 'cyt', prot = None) +
476     None >>
477     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
478     rna(name = 'lacA', type = 'cds', loc = 'cyt', prot = 1) +
479     rna(name = 'lacA', type = 'rbs', loc = 'cyt', prot = None) +
480     prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
↳None, up = None, dw = None),

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481     Parameter('fwd_sr_lacA_rbs', 1.000000))
482 Rule('fr_lacZ_cds',
483     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
484     rna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = 1) >>
485     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
486     rna(name = 'lacZ', type = 'cds', loc = 'cyt', prot = None),
487     Parameter('fwd_fr_lacZ_cds', 1.000000))
488 Rule('fr_lacY_cds',
489     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
490     rna(name = 'lacY', type = 'cds', loc = 'cyt', prot = 1) >>
491     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
492     rna(name = 'lacY', type = 'cds', loc = 'cyt', prot = None),
493     Parameter('fwd_fr_lacY_cds', 1.000000))
494 Rule('fr_lacA_cds',
495     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = 1) %
496     rna(name = 'lacA', type = 'cds', loc = 'cyt', prot = 1) >>
497     cplx(name = 'RIBOSOME_CPLX', loc = 'cyt', rna = None) +
498     rna(name = 'lacA', type = 'cds', loc = 'cyt', prot = None),
499     Parameter('fwd_fr_lacA_cds', 1.000000))
500 Initial(prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
501     ↪None, up = None, dw = None),
502     Parameter('t0_prot_lacZ_cyt', 0))
503 Observable('obs_prot_lacZ_cyt',
504     prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
505     ↪None, up = None, dw = None))
506 Initial(prot(name = 'lacY', loc = 'cyt', dna = None, met = None, prot = None, rna =
507     ↪None, up = None, dw = None),
508     Parameter('t0_prot_lacY_cyt', 0))
509 Observable('obs_prot_lacY_cyt',
510     prot(name = 'lacY', loc = 'cyt', dna = None, met = None, prot = None, rna =
511     ↪None, up = None, dw = None))
512 Initial(prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
513     ↪None, up = None, dw = None),
514     Parameter('t0_prot_lacA_cyt', 0))
515 Observable('obs_prot_lacA_cyt',
516     prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
517     ↪None, up = None, dw = None))
518 Initial(dna(name = 'lacZ', type = 'pro4', loc = 'cyt', dna = None, met = None, prot =
519     ↪None, rna = None, up = None, dw = 1) %
520     dna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot =
521     ↪None, rna = None, up = 1, dw = 2) %
522     dna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
523     ↪None, rna = None, up = 2, dw = 3) %
524     dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
525     ↪prot = None, rna = None, up = 3, dw = 4) %
526     dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
527     ↪prot = None, rna = None, up = 4, dw = 5) %
528     dna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
529     ↪None, rna = None, up = 5, dw = 6) %
530     dna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
531     ↪None, rna = None, up = 6, dw = 7) %
532     dna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
533     ↪None, rna = None, up = 7, dw = 8) %
534     dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
535     ↪prot = None, rna = None, up = 8, dw = 9) %
536     dna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
537     ↪None, rna = None, up = 9, dw = 10) %

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522     dna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
523     dna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
524     dna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = 13) %
525     dna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 13, dw = 14) %
526     dna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 14, dw = 15) %
527     dna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 15, dw = None),
528     Parameter('t0_dna_lacZlacYlacA', 0))
529 Observable('obs_dna_lacZlacYlacA',
530     dna(name = 'lacZ', type = 'pro4', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
531     dna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
532     dna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 2, dw = 3) %
533     dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 3, dw = 4) %
534     dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 4, dw = 5) %
535     dna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
536     dna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
537     dna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
538     dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 8, dw = 9) %
539     dna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
540     dna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
541     dna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
542     dna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = 13) %
543     dna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 13, dw = 14) %
544     dna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 14, dw = 15) %
545     dna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 15, dw = None))
546 Initial(rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
547     rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
548     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
549     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 3, dw = 4) %
550     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
551     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %

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552     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
553     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 7, dw = 8) %
554     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
555     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
556     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
557     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
558     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = 13) %
559     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 13, dw = None),
560     Parameter('t0_rna_lacZlacYlacA_form1', 0))
561 Observable('obs_rna_lacZlacYlacA_form1',
562     rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
563     rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
564     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
565     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 3, dw = 4) %
566     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
567     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
568     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
569     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 7, dw = 8) %
570     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
571     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
572     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
573     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
574     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = 13) %
575     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 13, dw = None))
576 Initial(rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
577     rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
578     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
579     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 3, dw = 4) %
580     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
581     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %

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582     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
583     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 7, dw = 8) %
584     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
585     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
586     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
587     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
588     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = 13) %
589     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 13, dw = 14) %
590     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 14, dw = None),
591     Parameter('t0_rna_lacZlacYlacA_form2', 0))
592 Observable('obs_rna_lacZlacYlacA_form2',
593     rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
594     rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
595     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
596     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 3, dw = 4) %
597     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
598     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
599     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
600     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 7, dw = 8) %
601     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
602     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
603     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
604     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
605     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = 13) %
606     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 13, dw = 14) %
607     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 14, dw = None))
608 Initial(rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
609     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 1, dw = 2) %
610     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
611     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %

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612     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
613     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
614     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 6, dw = 7) %
615     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
616     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
617     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
618     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
619     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
620     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = None),
621     Parameter('t0_rna_lacZlacYlacA_form3', 0))
622 Observable('obs_rna_lacZlacYlacA_form3',
623     rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
624     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = 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) %
626     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
627     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
628     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
629     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 6, dw = 7) %
630     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
631     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
632     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
633     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
634     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
635     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = None))
636 Initial(rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
637     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 1, dw = 2) %
638     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
639     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
640     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
641     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %

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642     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 6, dw = 7) %
643     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
644     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
645     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
646     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
647     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
648     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = 13) %
649     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 13, dw = None),
650     Parameter('t0_rna_lacZlacYlacA_form4', 0))
651 Observable('obs_rna_lacZlacYlacA_form4',
652     rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
653     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 1, dw = 2) %
654     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
655     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
656     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
657     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
658     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 6, dw = 7) %
659     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
660     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
661     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
662     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
663     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
664     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = 13) %
665     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 13, dw = None))
666 Initial(rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = None, dw = 1) %
667     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 1, dw = 2) %
668     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 2, dw = 3) %
669     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
670     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
671     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 5, dw = 6) %

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672     rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
673     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
674     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
675     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
676     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
677     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = None),
678     Parameter('t0_rna_lacZlacYlacA_form5', 0))
679 Observable('obs_rna_lacZlacYlacA_form5',
680     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = None, dw = 1) %
681     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 1, dw = 2) %
682     rna(name = 'lacZ', type = 'prol', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 2, dw = 3) %
683     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
684     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
685     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 5, dw = 6) %
686     rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
687     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
688     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
689     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
690     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
691     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = None))
692 Initial(rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = None, dw = 1) %
693     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 1, dw = 2) %
694     rna(name = 'lacZ', type = 'prol', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 2, dw = 3) %
695     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
696     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
697     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 5, dw = 6) %
698     rna(name = 'lacY', type = 'prol', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
699     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
700     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
701     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %

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702     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
703     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
704     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = None),
705     Parameter('t0_rna_lacZlacYlacA_form6', 0))
706 Observable('obs_rna_lacZlacYlacA_form6',
707     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = None, dw = 1) %
708     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 1, dw = 2) %
709     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 2, dw = 3) %
710     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
711     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
712     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 5, dw = 6) %
713     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
714     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
715     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
716     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
717     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
718     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
719     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = None))
720 Initial(rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
721     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
722     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
723     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
724     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
725     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
726     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
727     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
728     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = None),
729     Parameter('t0_rna_lacZlacYlacA_form7', 0))
730 Observable('obs_rna_lacZlacYlacA_form7',
731     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
732     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %

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733     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
734     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
735     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
736     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
737     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
738     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
739     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = None))
740 Initial(rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
741     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
742     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
743     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
744     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
745     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
746     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
747     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
748     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
749     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = None),
750     Parameter('t0_rna_lacZlacYlacA_form8', 0))
751 Observable('obs_rna_lacZlacYlacA_form8',
752     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
753     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
754     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
755     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
756     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
757     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
758     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
759     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
760     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
761     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = None))
762 Initial(rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %

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763     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
764     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 2, dw = 3) %
765     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
766     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = None),
767     Parameter('t0_rna_lacZlacYlacA_form9', 0))
768 Observable('obs_rna_lacZlacYlacA_form9',
769     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
770     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
771     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 2, dw = 3) %
772     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
773     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = None))
774 Initial(rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
775     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
776     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 2, dw = 3) %
777     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
778     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
779     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = None),
780     Parameter('t0_rna_lacZlacYlacA_form10', 0))
781 Observable('obs_rna_lacZlacYlacA_form10',
782     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
783     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
784     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 2, dw = 3) %
785     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
786     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
787     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = None))

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5.6 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 rate values:

- 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 identifying 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.

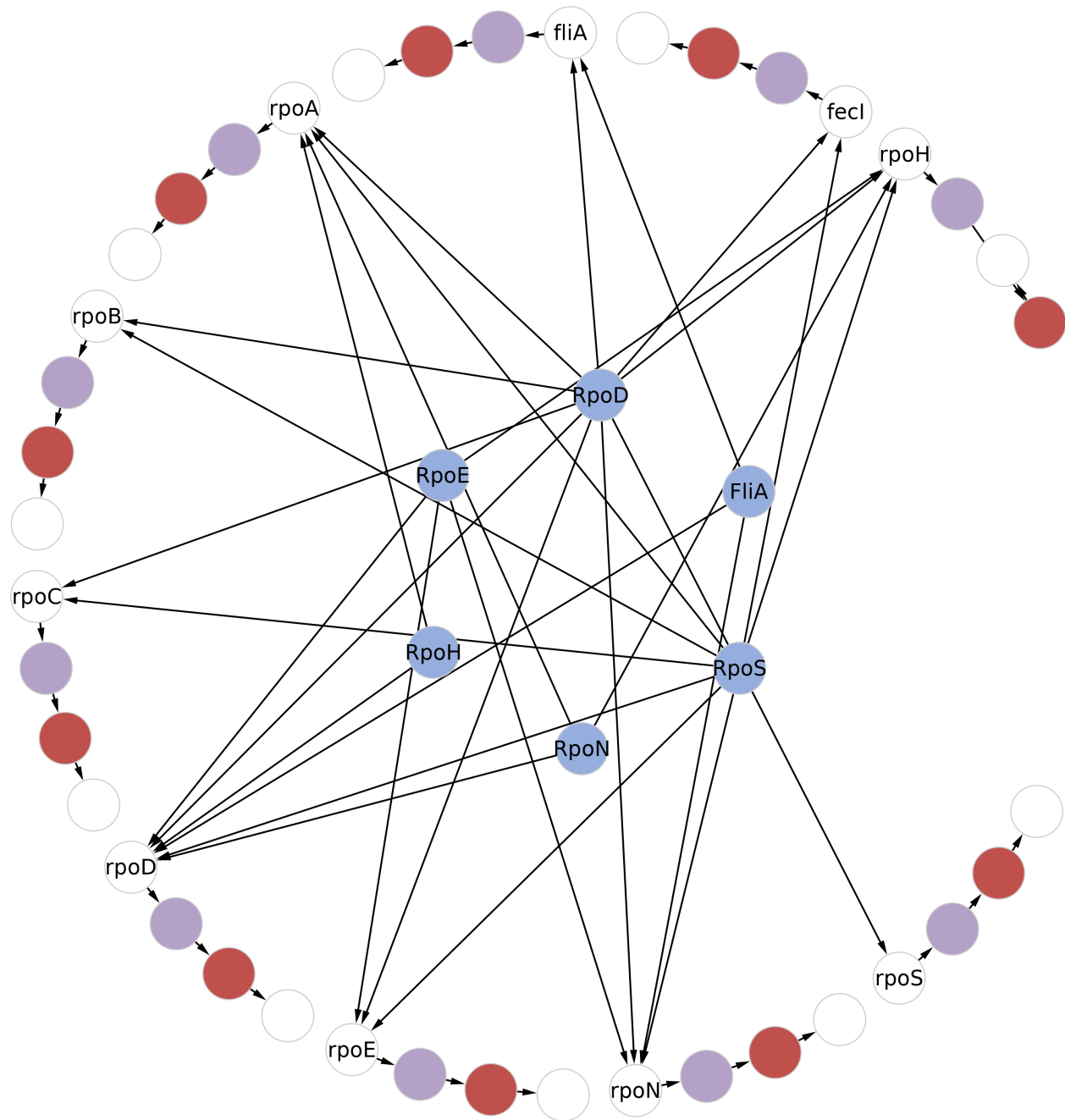
Example, and note the use of the prefix BS- to tell *Atlas* the component is a DNA binding site followed by a name and two coordinates:

	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	
2	[lacZ-pro4	lacZ-pro3	1	1	1	
3	lacZ-pro3	lacZ-pro2	1	1	1	
4	lacZ-pro2	BS-lacI-72-92	1	1	1	
5	BS-lacI-72-92	BS-lacI-21-1				1
6	BS-lacI-21-1	lacZ-pro1			1	
7	lacZ-pro1	lacZ-rbs	1	1	1	
8	lacZ-rbs	lacZ-				
	↪cds			1	1	1
9	lacZ-cds	BS-lacI-422-402			1	
10	BS-lacI-422-402	lacY-pro1			1	
11	lacY-pro1	lacY-rbs	0	0	1	
12	lacY-rbs	lacY-				
	↪cds		1	1	1	1
13	lacY-cds	lacA-rbs		1		
14	lacA-rbs	lacA-				
	↪cds		1	1	1	1
15	lacA-cds	lacA-ter1		1	1	
16	lacA-ter1	lacA-ter2]		1	1	

OR

	UPSTREAM	DOWNSTREAM	RNAP_FWD_DOCK_RATE		RNAP_FWD_FALL_RATE		RNAP_RVS_DOCK_		RIB_FWD_DOCK_
	↪RATE	RNAP_FWD_SLIDE_RATE							RIB_FWD_FALL_RATE
	↪RATE	RIB_RVS_DOCK_RATE							
1	[rpoA-pro1	rpoA-rbs	1	1	1				
2	rpoA-rbs	rpoA-							
3	↪cgs		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-							
8	↪cgs		1	1	1		1		1
9	rpoB-cds	rpoC-rbs			1				
10	rpoC-rbs	rpoC-							
11	↪cgs		1	1	1		1		1
12	rpoC-cds	rpoC-ter1]			1		1		
13									
14	[rpoD-pro1	rpoD-rbs	1	1	1				
15	rpoD-rbs	rpoD-							
16	↪cgs		1	1	1		1		1
17	rpoD-cds	rpoD-ter1]			1		1		
18									
19	[rpoE-pro1	rpoE-rbs	1	1	1				
20	rpoE-rbs	rpoE-							
21	↪cgs		1	1	1		1		1
22	rpoE-cds	rpoE-ter1]			1		1		
23									
24	[rpoH-pro1	rpoH-rbs	1	1	1				
25	rpoH-rbs	rpoH-							
26	↪cgs		1	1	1		1		1
27	rpoH-cds	rpoH-ter1]			1		1		
28									
29	[rpoN-pro1	rpoN-rbs	1	1	1				
30	rpoN-rbs	rpoN-							
31	↪cgs		1	1	1		1		1
32	rpoN-cds	rpoN-ter1]			1		1		
33									
34	[rpoS-pro1	rpoS-rbs	1	1	1				
35	rpoS-rbs	rpoS-							
36	↪cgs		1	1	1		1		1
37	rpoS-cds	rpoS-ter1]			1		1		
38									
39	[fliA-pro1	fliA-rbs	1	1	1				
40	fliA-rbs	fliA-							
41	↪cgs		1	1	1		1		1
42	fliA-cds	fliA-ter1]			1		1		
43									
44	[fecI-pro1	fecI-rbs	1	1	1				
45	fecI-rbs	fecI-							
46	↪cgs		1	1	1		1		1
47	fecI-cds	fecI-ter1]			1		1		

Note: Visualization in Cytoscape. Colors and arrows remains to the user for customization. The genome graph (outer nodes) could be complemented with a description of sigma factor specificity for promoter (inner nodes), as in the following network:



Finally, execute `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)`

- `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 specificity uses a modified *rules* to model the release of the sigma factor from the RNA Polymerase at the transcription initiation.

```

1 from pysb import *
2 Model()
3
4 Monomer('dna',
5         ['name', 'type', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
6         { 'name' : ['lacI_21_1', 'lacI_422_402', 'lacI_72_92', 'lacA', 'lacY', 'lacZ
7         ↪'],
8         'type' : ['BS', 'cds', 'pro1', 'pro2', 'pro3', 'pro4', 'rbs', 'ter1', 'ter2'],
9         'loc' : ['cyt']})
10 Monomer('rna',
11         ['name', 'type', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
12         { 'name' : ['lacI_21_1', 'lacI_422_402', 'lacI_72_92', 'lacA', 'lacY', 'lacZ
13         ↪'],
14         'type' : ['BS', 'cds', 'pro1', 'pro2', 'pro3', 'pro4', 'rbs', 'ter1', 'ter2'],
15         'loc' : ['cyt']})
16 Monomer('prot',
17         ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
18         { 'name' : ['lacA', 'lacY', 'lacZ'],
19         'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
20         ↪ 'omem']})
21 Monomer('cplx',
22         ['name', 'loc', 'dna', 'met', 'prot', 'rna'],
23         { 'name' : ['RNAP_CPLX', 'RIBOSOME_CPLX'],
24         'loc' : ['cyt']})
25 Rule('docking_lacZ_pro4',
26     cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = None) +
27     dna(name = 'lacZ', type = 'pro4', loc = 'cyt', prot = None) |
28     cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
29     dna(name = 'lacZ', type = 'pro4', loc = 'cyt', prot = 1),
30     Parameter('fwd_docking_lacZ_pro4', 1.000000),
31     Parameter('rvs_docking_lacZ_pro4', 1.000000))
32 Rule('docking_lacZ_pro3',
33     cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = None) +
34     dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = None) |
35     cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
36     dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = 1),
37     Parameter('fwd_docking_lacZ_pro3', 1.000000),
38     Parameter('rvs_docking_lacZ_pro3', 1.000000))
39 Rule('docking_lacZ_pro2',
40     cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = None) +
41     dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = None) |
42     cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
43     dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = 1),
44     Parameter('fwd_docking_lacZ_pro2', 1.000000),
45     Parameter('rvs_docking_lacZ_pro2', 1.000000))
46 Rule('docking_lacZ_pro1',

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

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

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

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

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

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

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333     dna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 15, dw = None))
334 Initial(rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
335     rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
336     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
337     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 3, dw = 4) %
338     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
339     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
340     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
341     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 7, dw = 8) %
342     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
343     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
344     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
345     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
346     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = 13) %
347     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 13, dw = None),
348     Parameter('t0_rna_lacZlacYlacA_form1', 0))
349 Observable('obs_rna_lacZlacYlacA_form1',
350     rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
351     rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
352     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪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) %
354     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
355     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
356     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
357     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 7, dw = 8) %
358     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
359     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
360     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
361     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
362     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = 13) %

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363     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 13, dw = None))
364 Initial(rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
365     rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
366     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
367     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 3, dw = 4) %
368     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
369     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
370     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
371     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 7, dw = 8) %
372     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
373     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
374     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
375     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
376     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = 13) %
377     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 13, dw = 14) %
378     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 14, dw = None),
379     Parameter('t0_rna_lacZlacYlacA_form2', 0))
380 Observable('obs_rna_lacZlacYlacA_form2',
381     rna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
382     rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
383     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
384     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 3, dw = 4) %
385     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
386     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
387     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
388     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 7, dw = 8) %
389     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
390     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
391     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
392     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %

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393     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = 13) %
394     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 13, dw = 14) %
395     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 14, dw = None))
396 Initial(rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
397     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 1, dw = 2) %
398     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
399     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
400     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
401     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
402     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 6, dw = 7) %
403     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
404     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
405     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
406     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
407     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %
408     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 12, dw = None),
409     Parameter('t0_rna_lacZlacYlacA_form3', 0))
410 Observable('obs_rna_lacZlacYlacA_form3',
411     rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
412     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 1, dw = 2) %
413     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
414     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
415     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
416     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
417     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 6, dw = 7) %
418     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
419     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
420     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = 10) %
421     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 10, dw = 11) %
422     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 11, dw = 12) %

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423     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 12, dw = None))
424 Initial(rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = None, dw = 1) %
425     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = 1, dw = 2) %
426     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = 2, dw = 3) %
427     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 3, dw = 4) %
428     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 4, dw = 5) %
429     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 5, dw = 6) %
430     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = 6, dw = 7) %
431     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 7, dw = 8) %
432     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 8, dw = 9) %
433     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 9, dw = 10) %
434     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 10, dw = 11) %
435     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 11, dw = 12) %
436     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 12, dw = 13) %
437     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 13, dw = None),
438     Parameter('t0_rna_lacZlacYlacA_form4', 0))
439 Observable('obs_rna_lacZlacYlacA_form4',
440     rna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = None, dw = 1) %
441     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = 1, dw = 2) %
442     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = 2, dw = 3) %
443     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 3, dw = 4) %
444     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 4, dw = 5) %
445     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 5, dw = 6) %
446     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = 6, dw = 7) %
447     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 7, dw = 8) %
448     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 8, dw = 9) %
449     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 9, dw = 10) %
450     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 10, dw = 11) %
451     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 11, dw = 12) %
452     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 12, dw = 13) %

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453     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 13, dw = None))
454 Initial(rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = None, dw = 1) %
455     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = 1, dw = 2) %
456     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 2, dw = 3) %
457     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 3, dw = 4) %
458     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 4, dw = 5) %
459     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = 5, dw = 6) %
460     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 6, dw = 7) %
461     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 7, dw = 8) %
462     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 8, dw = 9) %
463     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 9, dw = 10) %
464     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 10, dw = 11) %
465     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 11, dw = None),
466     Parameter('t0_rna_lacZlacYlacA_form5', 0))
467 Observable('obs_rna_lacZlacYlacA_form5',
468     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = None, dw = 1) %
469     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = 1, dw = 2) %
470     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 2, dw = 3) %
471     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 3, dw = 4) %
472     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 4, dw = 5) %
473     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = 5, dw = 6) %
474     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 6, dw = 7) %
475     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 7, dw = 8) %
476     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 8, dw = 9) %
477     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 9, dw = 10) %
478     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 10, dw = 11) %
479     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 11, dw = None))
480 Initial(rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = None, dw = 1) %
481     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = 1, dw = 2) %
482     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 2, dw = 3) %

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483     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 3, dw = 4) %
484     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 4, dw = 5) %
485     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = 5, dw = 6) %
486     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 6, dw = 7) %
487     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 7, dw = 8) %
488     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 8, dw = 9) %
489     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 9, dw = 10) %
490     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 10, dw = 11) %
491     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 11, dw = 12) %
492     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 12, dw = None),
493     Parameter('t0_rna_lacZlacYlacA_form6', 0))
494 Observable('obs_rna_lacZlacYlacA_form6',
495     rna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = None, dw = 1) %
496     rna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = 1, dw = 2) %
497     rna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 2, dw = 3) %
498     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 3, dw = 4) %
499     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 4, dw = 5) %
500     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = 5, dw = 6) %
501     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 6, dw = 7) %
502     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 7, dw = 8) %
503     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 8, dw = 9) %
504     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 9, dw = 10) %
505     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 10, dw = 11) %
506     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 11, dw = 12) %
507     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 12, dw = None))
508 Initial(rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = None, dw = 1) %
509     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 1, dw = 2) %
510     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↳prot = None, rna = None, up = 2, dw = 3) %
511     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 3, dw = 4) %
512     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↳None, rna = None, up = 4, dw = 5) %

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513     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
514     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
515     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
516     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = None),
517     Parameter('t0_rna_lacZlacYlacA_form7', 0))
518 Observable('obs_rna_lacZlacYlacA_form7',
519     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
520     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
521     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
522     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
523     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
524     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
525     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
526     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
527     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = None))
528 Initial(rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
529     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
530     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
531     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
532     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
533     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
534     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
535     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
536     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
537     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = None),
538     Parameter('t0_rna_lacZlacYlacA_form8', 0))
539 Observable('obs_rna_lacZlacYlacA_form8',
540     rna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
541     rna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
542     rna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
↪prot = None, rna = None, up = 2, dw = 3) %
543     rna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %

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544     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
545     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = 6) %
546     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 6, dw = 7) %
547     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 7, dw = 8) %
548     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 8, dw = 9) %
549     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 9, dw = None))
550 Initial(rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
551     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
552     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 2, dw = 3) %
553     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
554     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = None),
555     Parameter('t0_rna_lacZlacYlacA_form9', 0))
556 Observable('obs_rna_lacZlacYlacA_form9',
557     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
558     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
559     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 2, dw = 3) %
560     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
561     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = None))
562 Initial(rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
563     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
564     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 2, dw = 3) %
565     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
566     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %
567     rna(name = 'lacA', type = 'ter2', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 5, dw = None),
568     Parameter('t0_rna_lacZlacYlacA_form10', 0))
569 Observable('obs_rna_lacZlacYlacA_form10',
570     rna(name = 'lacY', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = None, dw = 1) %
571     rna(name = 'lacY', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 1, dw = 2) %
572     rna(name = 'lacA', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 2, dw = 3) %
573     rna(name = 'lacA', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 3, dw = 4) %
574     rna(name = 'lacA', type = 'ter1', loc = 'cyt', dna = None, met = None, prot =
↪None, rna = None, up = 4, dw = 5) %

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

SIMULATION

Simulation could be done within the PySB python package (See more at [PySB documentation](#)). Here is the relevant code that enable the simulation of any PySB model. Step are done internally by PySB: export of the model, call to the simulator, and import of the results.

Note: See [Plotting](#) for a simple example on how to plot simulation results.

```

1 # simulation
2 bng = '/opt/git-repositories/bionetgen.RuleWorld/bng2/'
3 kasim = '/opt/git-repositories/KaSim4.Kappa-Dev/'
4 cupsoda = '/opt/git-repositories/cupSODA.aresio/'
5 stochkit = '/opt/git-repositories/StochKit.StochSS' # not the bin folder
6
7 data0 = simulation.scipy(model, start = 0, finish = 10, points = 2000)
8 data1 = simulation.cupsoda(model, start = 0, finish = 10, points = 2000, path = ↵
↵ cupsoda) # only if you have a GPU NVIDIA; comment if not.
9 data2 = simulation.bngODE(model, start = 0, finish = 10, points = 2000, path = bng)
10 data3 = simulation.bngSSA(model, start = 0, finish = 10, points = 2000, n_runs = 20, ↵
↵ path = bng)
11 data4 = simulation.bngPLA(model, start = 0, finish = 10, points = 2000, n_runs = 20, ↵
↵ path = bng)
12 data5 = simulation.bngNF(model, start = 0, finish = 10, points = 2000, n_runs = 20, ↵
↵ path = bng)
13 data6 = simulation.kasim(model, start = 0, finish = 10, points = 2000, n_runs = 20, ↵
↵ path = kasim)
14 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 stochastic 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. If using the pleiades docker instance, there is no necessity to set the path.

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` ($\text{avrg} \pm \text{weight} * \text{stdv}$).

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, **kwargs)`

```
1 import seaborn
2 import matplotlib.pyplot as plt
3
4 palette = seaborn.color_palette('colorblind')
5
6 for kind in ['scatter', 'plot']:
7     # first plot, periplasmic concentration
8     fig, ax = plt.subplots(1, 2, figsize = (4*2, 3*1), dpi = 100)
9
10    simulation.plot.metabolite(data3['avrg'], 'Alpha_lactose', 'per', ax = ax[0], **{
11    ↪ 'kind' : kind},
12    ↪ plt_kws = {'s' : 2, 'color' : palette[0], 'label' : r'$\alpha$-lactose [PER]',
13    ↪ 'alpha' : .5})
```

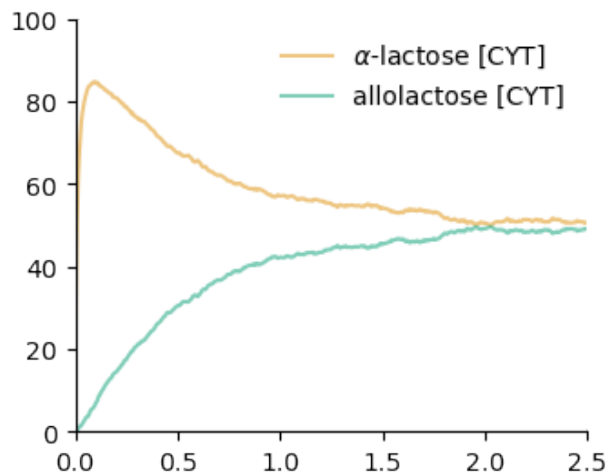
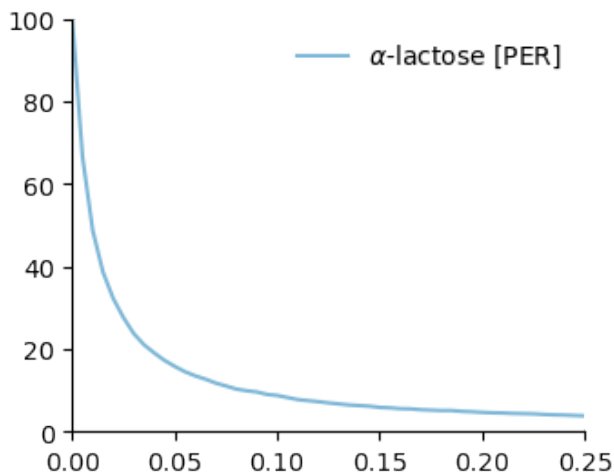
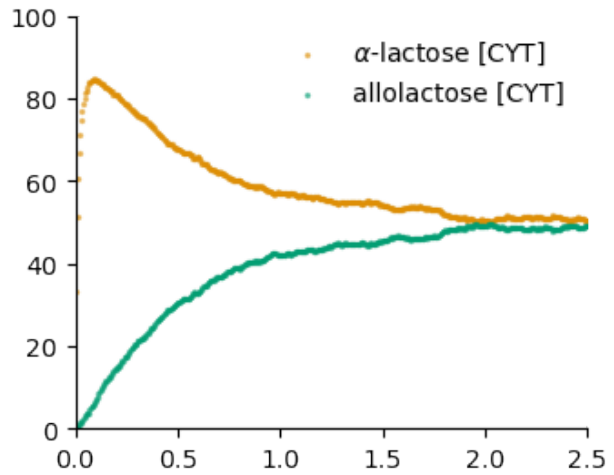
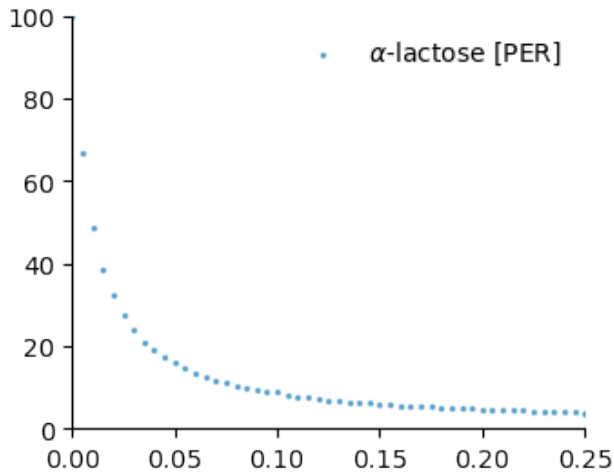
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```

13     simulation.plot.metabolite(data3['avrg'], 'Alpha_lactose', 'cyt', ax = ax[1], **{
14 ↪ 'kind' : kind},
15     plt_kws = {'s' : 2, 'color' : palette[1], 'label' : r'$\alpha$-lactose [CYT]',
16 ↪ 'alpha' : .5})
17
18     simulation.plot.metabolite(data3['avrg'], 'ALLOLACTOSE', 'cyt', ax = ax[1], **{
19 ↪ 'kind' : kind},
20     plt_kws = {'s' : 2, 'color' : palette[2], 'label' : r'allolactose [CYT]',
21 ↪ 'alpha' : .5})
22
23     ax[0].set_xlim((0, .25))
24     ax[1].set_xlim((0, 2.5))
25     ax[0].set_ylim((0, 100))
26     ax[1].set_ylim((0, 100))
27
28     seaborn.despine()

```



```

1 import seaborn
2 import matplotlib.pyplot as plt
3
4 palette = seaborn.color_palette('colorblind')

```

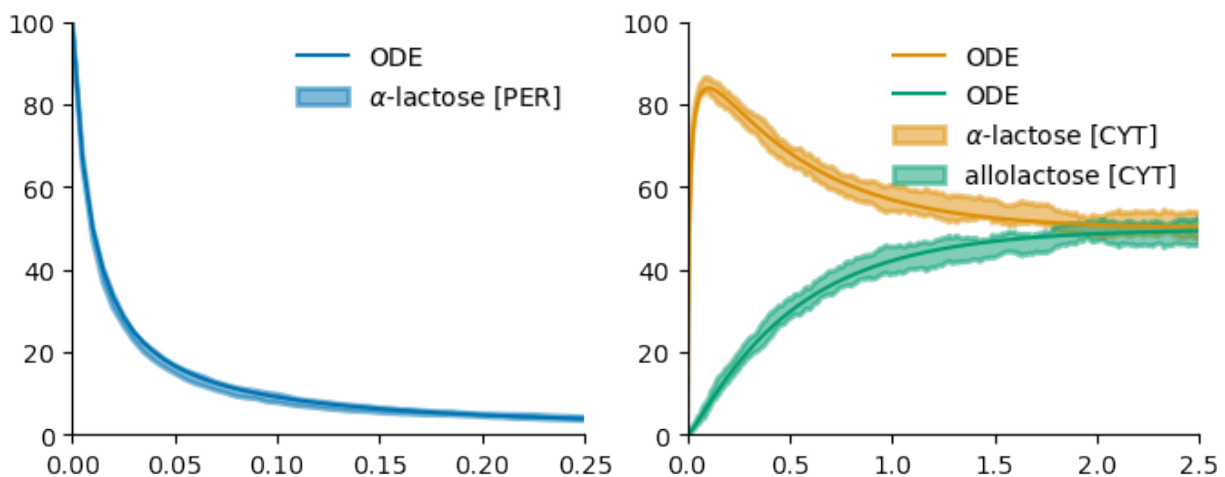
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```

5
6 # first plot, periplasmic concentration
7 fig, ax = plt.subplots(1, 2, figsize = (4*2, 3*1), dpi = 100)
8 simulation.plot.metabolite(data3, 'Alpha_lactose', 'per', ax = ax[0], **{'kind' :
9     ↪ 'fill_between', 'weight' : .5},
10     plt_kws = {'s' : 2, 'color' : palette[0], 'label' : r'$\alpha$-lactose [PER]',
11     ↪ 'alpha' : .5})
12
13 # second plot, cytoplasmic concentration
14 simulation.plot.metabolite(data3, 'Alpha_lactose', 'cyt', ax = ax[1], **{'kind' :
15     ↪ 'fill_between', 'weight' : .5},
16     plt_kws = {'s' : 2, 'color' : palette[1], 'label' : r'$\alpha$-lactose [CYT]',
17     ↪ 'alpha' : .5})
18
19 # second plot, cytoplasmic concentration
20 simulation.plot.metabolite(data3, 'ALLOLACTOSE', 'cyt', ax = ax[1], **{'kind' : 'fill_
21     ↪ between', 'weight' : .5},
22     plt_kws = {'s' : 2, 'color' : palette[2], 'label' : r'allolactose [CYT]', 'alpha' :
23     ↪ .5})
24
25 # first plot, periplasmic concentration
26 simulation.plot.metabolite(data0, 'Alpha_lactose', 'per', ax = ax[0], **{'kind' :
27     ↪ 'plot'},
28     plt_kws = {'s' : 2, 'color' : palette[0], 'label' : r'ODE'})
29
30 # second plot, cytoplasmic concentration
31 simulation.plot.metabolite(data0, 'Alpha_lactose', 'cyt', ax = ax[1], **{'kind' :
32     ↪ 'plot'},
33     plt_kws = {'s' : 2, 'color' : palette[1], 'label' : r'ODE'})
34
35 # second plot, cytoplasmic concentration
36 simulation.plot.metabolite(data0, 'ALLOLACTOSE', 'cyt', ax = ax[1], **{'kind' : 'plot
37     ↪ '},
38     plt_kws = {'s' : 2, 'color' : palette[2], 'label' : r'ODE'})
39
40 ax[0].set_xlim((0, .25))
41 ax[1].set_xlim((0, 2.5))
42 ax[0].set_ylim((0, 100))
43 ax[1].set_ylim((0, 100))
44
45 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)`.

EXPORT TO

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

```
1 # export to
2 export.to_sbml(model, 'export-to-sbml.sbml')
3 export.to_matlab(model, 'export-to-matlab.m')
4 export.to_mathematica(model, 'export-to-mathematica.wl')
5 export.to_potterswheel(model, 'export-to-potterswheel.m')
6 export.to_bngl(model, 'export-to-bngl.bngl')
7 export.to_bngnet(model, 'export-to-bngnet.net')
8 export.to_kappa(model, 'export-to-kappa.kappa')
9 export.to_python(model, 'export-to-python.py')
10 export.to_pysb(model, 'export-to-pysb.py')
11 export.to_stochkit(model, 'export-to-stochkit.xml')
12 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.

INDICES AND TABLES

- `genindex`
- `modindex`
- `search`