atlas Documentation

Release 1.4

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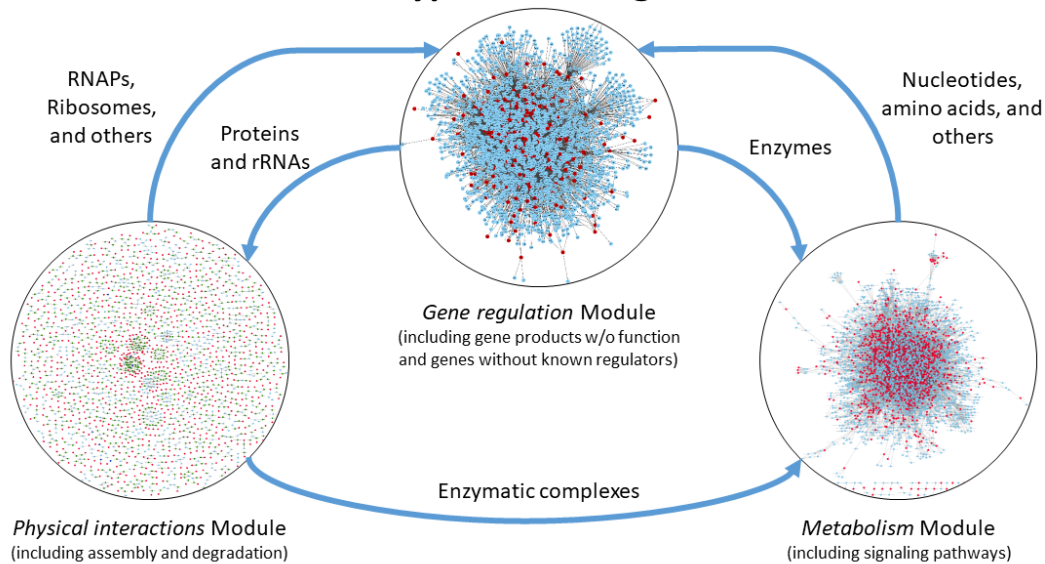**Alberto J.M. Martín**

Nov 19, 2020

CONTENTS

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

RNAPs, Ribosomes, and others

Proteins and rRNAs

Enzymes

Nucleotides, amino acids, and others

Gene regulation Module
(including gene products w/o function and genes without known regulators)

Enzymatic complexes

Physical interactions Module
(including assembly and degradation)

Metabolism Module
(including signaling pathways)

ONE

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 invoque. You could install pip3 with `sudo apt-get install python3-pip` if you have system rights, or install python3 from source, and adding `<python3 path>/bin/pip3` to the path, or linking it in a directory like `$HOME/bin` which is commonly added to the path at 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

FOUR
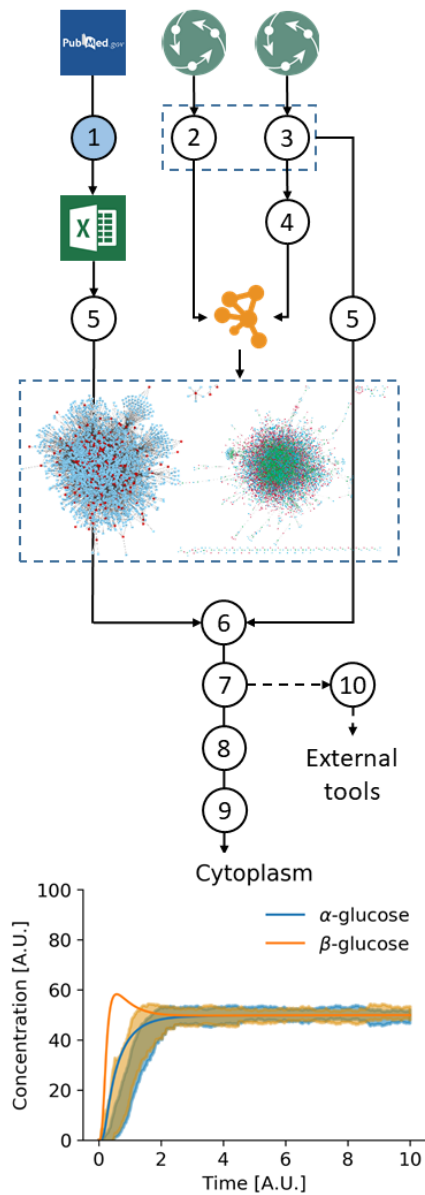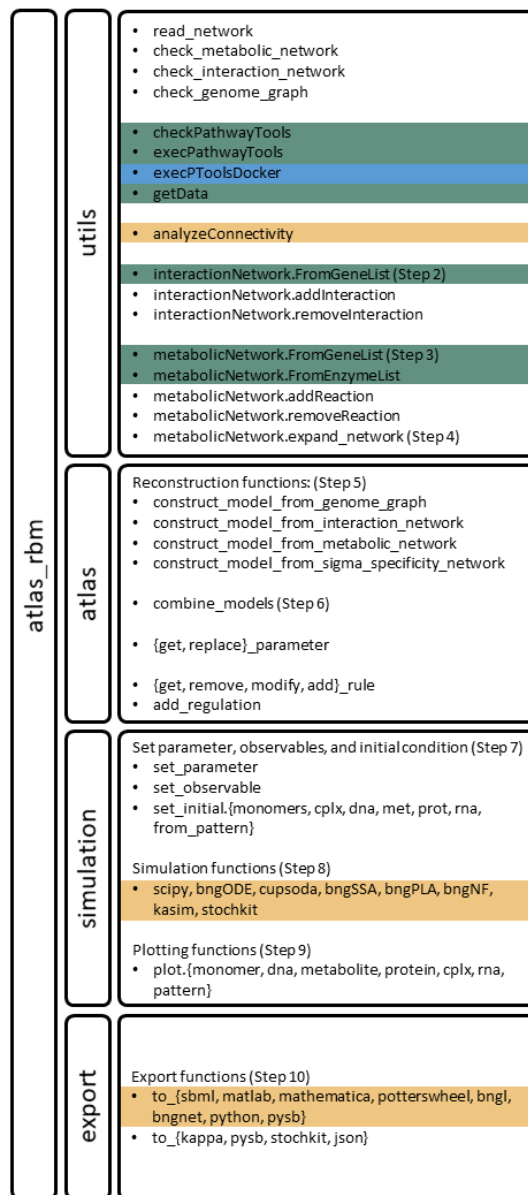
RULE BASED MODELING BASICS

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 optionals, 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 italized 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']})
```

(continues on next page)

```
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 be able 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 purporsely created interaction sites, complex of *agents* are defined by unique numbered bonds that are shared by the interactions sites:

> For instance, the dimer [lacZ,lacZ,lacZ,lacZ] (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=2) %
3  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None, up=2,
   →dw=3) %
4  prot(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None, up=3,
   →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. Not bonded agents are 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)
```

Next, the rules are defined by a name, the substrates, the products, and rate(s):

Unidireccional 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 bidireccional 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))
```

Finally, a model is complete with necessary initials and observables:

```
1  # Parameter is a name and a value
2  Parameter('t0_prot_lacZ_cyt', 1.0)
3
4  # Initial is a complete description of an agent or complex of agents and a
   ↪parameter
5  Initial(name='lacZ', loc='cyt', dna=None, met=None, prot=None, rna=None,
   ↪up=None, dw=None), t0_prot_lacZ_cyt)
6
7  # Observable is an alias and a complete or partial description of an agent
   ↪or complex of agents
8  Observable('obs_prot_lacZ_cyt', name='lacZ', loc='cyt', dna=None, met=None,
   ↪prot=None, rna=None, up=None, dw=None))
```

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:

```
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-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
```

(continues on next page)

```
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
```

<div align="right">(continued from previous page)</div>

```
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 enconding the reactions. Click on `Style`, then on `Node` and bypass the `Fill Color`. In the new window, you could set-up the color, e.g. #00AA50

   2. Write `GENE_PROD` that will select nodes encoding the gene name, protein name, or the enzyme name. Click on `Style`, then on `Node` and bypass the `Fill Color`. In the new window, you could set-up the color, e.g. #CC0033

   3. Write `MET` that will select nodes encoding substrate metabolites. Click on `Style`, then on `Node` and bypass the `Fill Color`. In the new window, you could set-up the color, e.g. #00ABDD. Also, set a shape for nodes, to differentiate substrates from products.

3. On the selector, click on `Node:   TARGET_NODE_ATTRIBUTE:`

   1. Write `MET` that will select nodes encoding product metabolites. Click on `Style`, then on `Node` and bypass the `Fill Color`. In the new window, you could set-up the color, e.g. #00ABDD
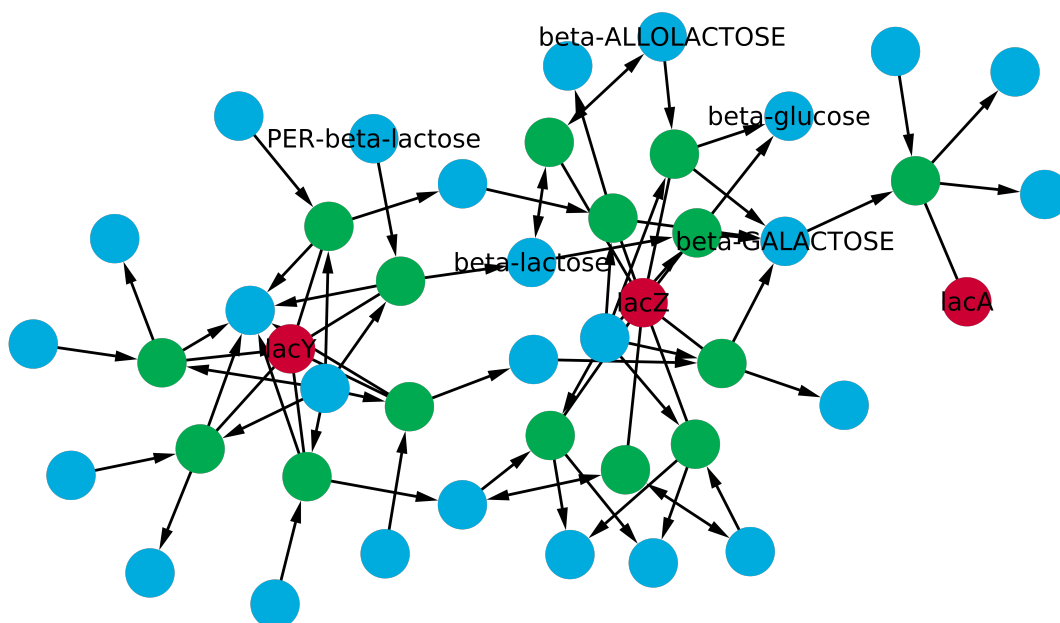
Finally, execute `atlas_rbm.construct_model_from_metabolic_network(network, verbose = False)` to obtain the model.

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

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

- `atlas_rbm.simulation.set_initial.cplx(model, complex_name, location, positive_number)`

- `atlas_rbm.simulation.set_initial.dna(model, dna_name, positive_number)`

- `atlas_rbm.simulation.set_initial.met(model, metabolite, location, positive_number)`

- `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`):

```python
from pysb import *
Model()

Monomer('met',
        ['name', 'loc', 'dna', 'met', 'prot', 'rna'],
        { 'name' : [ 'ACETYL_COA', 'CO_A', 'CPD_3561', 'CPD_3785', 'CPD_3801', 'D_
ARABINOSE', 'Fructofuranose', 'MELIBIOSE', 'PROTON', 'WATER', '_6_Acetyl_beta_D_
Galactose', 'alpha_ALLOLACTOSE', 'alpha_GALACTOSE', 'alpha_glucose', 'alpha_lactose
', 'beta_ALLOLACTOSE', 'beta_GALACTOSE', 'beta_glucose', 'beta_lactose' ],
        'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
 'omem']})
Monomer('prot',
        ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
        { 'name' : [ 'LACY_MONOMER', 'spontaneous' ],
        'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
 'omem']})
Monomer('cplx',
        ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
        { 'name' : [ 'BETAGALACTOSID_CPLX', 'GALACTOACETYLTRAN_CPLX' ],
        'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
 'omem']})
Observable('obs_met_ACETYL_COA_cyt', met(name = 'ACETYL_COA', loc = 'cyt'))
Observable('obs_met_CO_A_cyt', met(name = 'CO_A', loc = 'cyt'))
Observable('obs_met_CPD_3561_cyt', met(name = 'CPD_3561', loc = 'cyt'))
Observable('obs_met_CPD_3785_cyt', met(name = 'CPD_3785', loc = 'cyt'))
Observable('obs_met_CPD_3801_cyt', met(name = 'CPD_3801', loc = 'cyt'))
Observable('obs_met_D_ARABINOSE_cyt', met(name = 'D_ARABINOSE', loc = 'cyt'))
Observable('obs_met_Fructofuranose_cyt', met(name = 'Fructofuranose', loc = 'cyt'))
Observable('obs_met_MELIBIOSE_cyt', met(name = 'MELIBIOSE', loc = 'cyt'))
Observable('obs_met_PROTON_cyt', met(name = 'PROTON', loc = 'cyt'))
Observable('obs_met_WATER_cyt', met(name = 'WATER', loc = 'cyt'))
Observable('obs_met__6_Acetyl_beta_D_Galactose_cyt', met(name = '_6_Acetyl_beta_D_
Galactose', loc = 'cyt'))
Observable('obs_met_alpha_ALLOLACTOSE_cyt', met(name = 'alpha_ALLOLACTOSE', loc = 'cyt
'))
Observable('obs_met_alpha_GALACTOSE_cyt', met(name = 'alpha_GALACTOSE', loc = 'cyt'))
Observable('obs_met_alpha_glucose_cyt', met(name = 'alpha_glucose', loc = 'cyt'))
Observable('obs_met_alpha_lactose_cyt', met(name = 'alpha_lactose', loc = 'cyt'))
Observable('obs_met_beta_ALLOLACTOSE_cyt', met(name = 'beta_ALLOLACTOSE', loc = 'cyt
'))
Observable('obs_met_beta_GALACTOSE_cyt', met(name = 'beta_GALACTOSE', loc = 'cyt'))
Observable('obs_met_beta_glucose_cyt', met(name = 'beta_glucose', loc = 'cyt'))
Observable('obs_met_beta_lactose_cyt', met(name = 'beta_lactose', loc = 'cyt'))
Initial(met(name = 'ACETYL_COA', loc = 'cyt', dna = None, met = None, prot = None,
rna = None), Parameter('t0_met_ACETYL_COA_cyt', 0))
```

```
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),
```

```
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) +
```

```
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))
```

```
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 |
```

```
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:
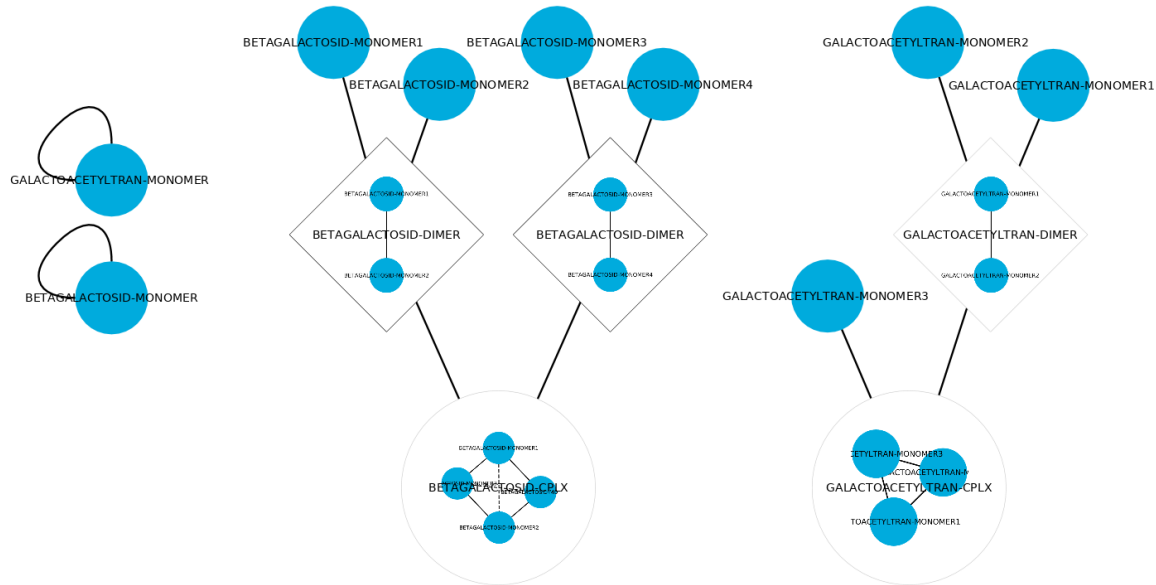
   1. If the number of locations match the number of components of the complex, each location is mapped in the same order to each component.

   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:

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

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`):

```python
from pysb import *
Model()

Monomer('prot',
        ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
        { 'name' : [ 'lacA', 'lacI', 'lacZ' ],
        'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
↪ 'omem']})
```

(continues on next page)

```
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) %
```

```
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))
```

```
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:

```
1  SOURCE           TARGET           FWD_RATE        RVS_RATE        LOCATION
2  [lacI,lacI]        SMALL-alpha-ALLOLACTOSE          10.0        0.0001        cytosol
3  [lacI,lacI,SMALL-alpha-ALLOLACTOSE]        SMALL-alpha-ALLOLACTOSE        10.
   →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`):

```python
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',
   → 'omem']})
8  Monomer('prot',
9         ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
10         { 'name' : [ 'lacI' ],
11         'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
   → 'omem']})
12  Observable('obs_met_alpha_ALLOLACTOSE_cyt', met(name = 'alpha_ALLOLACTOSE', loc = 'cyt
   →'))
13  Initial(met(name = 'alpha_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot =
   →None, rna = None), Parameter('t0_met_alpha_ALLOLACTOSE_cyt', 0))
14  Observable('obs_met_beta_ALLOLACTOSE_cyt', met(name = 'beta_ALLOLACTOSE', loc = 'cyt
   →'))
15  Initial(met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, met = None, prot =
   →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) %
```

```
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),
```

5.3. Protein-Small compounds Interaction Networks

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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,
   → up = None, dw = 1) %
85          prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =␣
   →None, up = 1, dw = None) %
86          met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 2, met = None,␣
   →rna = None) +
87          met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = None, met =␣
   →None, rna = None) |
88          prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 2, rna = None,
   → up = None, dw = 1) %
89          prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = 3, rna = None,
   → up = 1, dw = None) %
90          met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 3, met = None,␣
   →rna = None) %
91          met(name = 'beta_ALLOLACTOSE', loc = 'cyt', dna = None, prot = 2, met = None,␣
   →rna = None),
92          Parameter('fwd_PhysicalInteractionRule_4', 10.000000),
93          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 bewteen proteins and DNA. The network have five columns:

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

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

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

```
1 SOURCE           TARGET          FWD_RATE         RVS_RATE         LOCATION
2 # lacZYA
3 [lacI,lacI]         BS-lacI-422-402     1.0          0.01           cytosol
4 [lacI,lacI]         BS-lacI-21-1      1.0       0.01        cytosol
5 [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`):

```python
from pysb import *
Model()

Monomer('prot',
        ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
        { 'name' : [ 'lacI' ],
        'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
→ 'omem']})
Monomer('dna',
        ['name', 'type', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
        { 'name' : [ 'lacI_21_1', 'lacI_422_402', 'lacI_72_92' ],
        'type' : ['BS'],
        'loc' : ['cyt']})
Observable('obs_prot_lacI_cyt', prot(name = 'lacI', loc = 'cyt', dna = None, met =
→None, prot = None, rna = None, up = None, dw = None))
Initial(prot(name = 'lacI', loc = 'cyt', dna = None, met = None, prot = None, rna =
→None, up = None, dw = None), Parameter('t0_prot_lacI_cyt', 0))
Rule('PhysicalInteractionRule_1',
        prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
→None, up = None, dw = 1) %
        prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
→None, up = 1, dw = None) +
        dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, prot = None,
→met = None, rna = None, up = WILD, dw = WILD) |
        prot(name = 'lacI', loc = 'cyt', dna = None, prot = None, met = None, rna =
→None, up = None, dw = 1) %
        prot(name = 'lacI', loc = 'cyt', dna = 2, prot = None, met = None, rna = None,
→ up = 1, dw = None) %
        dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, prot = 2,
→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:

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

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

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

- `atlas_rbm.simulation.set_initial.cplx(model, complex_name, location, positive_number)`

- `atlas_rbm.simulation.set_initial.dna(model, dna_name, positive_number)`

- `atlas_rbm.simulation.set_initial.met(model, metabolite, location, positive_number)`

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

- `atlas_rbm.simulation.set_initial.rna(model, rna_name, positive_number)`

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

```python
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           'type' : ['BS', 'cds', 'pro1', 'pro2', 'pro3', 'pro4', 'rbs', 'ter1', 'ter2'],
8           'loc' : ['cyt']})
9   Monomer('rna',
10          ['name', 'type', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
11          { 'name' : ['lacA', 'lacI_21_1', 'lacI_422_402', 'lacI_72_92', 'lacY', 'lacZ
    ↪'],
12          'type' : ['BS', 'cds', 'pro1', 'pro2', 'pro3', 'pro4', 'rbs', 'ter1', 'ter2'],
13          'loc' : ['cyt']})
14  Monomer('prot',
15          ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
16          { 'name' : ['lacA', 'lacI_21_1', 'lacI_422_402', 'lacI_72_92', 'lacY', 'lacZ
    ↪'],
17          'loc' : ['cyt', 'mem']})
18  Monomer('cplx',
19          ['name', 'loc', 'dna', 'met', 'prot', 'rna'],
20          { 'name' : ['RIBOSOME_CPLX'],
21          'loc' : ['cyt']})
22  Rule('docking_1_lacZ_pro4',
23          prot(name = 'rpoA', loc = 'cyt', dna = None, met = None, up = None, dw = 1) %
24          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) %
```

```
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) +
```

5.5. Sigma Factor-Promoter Interaction Networks

```
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) %
```

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

```
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),
```

```
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) %
```

```
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 =
    →None, up = None, dw = None),
501         Parameter('t0_prot_lacZ_cyt', 0))
502 Observable('obs_prot_lacZ_cyt',
503         prot(name = 'lacZ', loc = 'cyt', dna = None, met = None, prot = None, rna =
    →None, up = None, dw = None))
504 Initial(prot(name = 'lacY', loc = 'cyt', dna = None, met = None, prot = None, rna =
    →None, up = None, dw = None),
505         Parameter('t0_prot_lacY_cyt', 0))
506 Observable('obs_prot_lacY_cyt',
507         prot(name = 'lacY', loc = 'cyt', dna = None, met = None, prot = None, rna =
    →None, up = None, dw = None))
508 Initial(prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
    →None, up = None, dw = None),
509         Parameter('t0_prot_lacA_cyt', 0))
510 Observable('obs_prot_lacA_cyt',
511         prot(name = 'lacA', loc = 'cyt', dna = None, met = None, prot = None, rna =
    →None, up = None, dw = None))
512 Initial(dna(name = 'lacZ', type = 'pro4', loc = 'cyt', dna = None, met = None, prot =
    →None, rna = None, up = None, dw = 1) %
513         dna(name = 'lacZ', type = 'pro3', loc = 'cyt', dna = None, met = None, prot =
    →None, rna = None, up = 1, dw = 2) %
514         dna(name = 'lacZ', type = 'pro2', loc = 'cyt', dna = None, met = None, prot =
    →None, rna = None, up = 2, dw = 3) %
515         dna(name = 'lacI_72_92', type = 'BS', loc = 'cyt', dna = None, met = None,
    →prot = None, rna = None, up = 3, dw = 4) %
516         dna(name = 'lacI_21_1', type = 'BS', loc = 'cyt', dna = None, met = None,
    →prot = None, rna = None, up = 4, dw = 5) %
517         dna(name = 'lacZ', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
    →None, rna = None, up = 5, dw = 6) %
518         dna(name = 'lacZ', type = 'rbs', loc = 'cyt', dna = None, met = None, prot =
    →None, rna = None, up = 6, dw = 7) %
519         dna(name = 'lacZ', type = 'cds', loc = 'cyt', dna = None, met = None, prot =
    →None, rna = None, up = 7, dw = 8) %
520         dna(name = 'lacI_422_402', type = 'BS', loc = 'cyt', dna = None, met = None,
    →prot = None, rna = None, up = 8, dw = 9) %
521         dna(name = 'lacY', type = 'pro1', loc = 'cyt', dna = None, met = None, prot =
    →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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5.5. Sigma Factor-Promoter Interaction Networks

```
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) %
```

5.5. Sigma Factor-Promoter Interaction Networks

```
672          rna(name = 'lacY', type = 'pro1', 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 = 'pro1', 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 = 'pro1', 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 = 'pro1', 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 = 'pro1', 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) %
```

```
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) %
```

```
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) %
```

(continued from previous page)

```
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))
```

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 identifiying a DNA terminator.

   - RIB_FWD_DOCK_RATE and RIB_RVS_DOCK_RATE are valid values only for the description of the reversible interaction of the bacterial Ribosome to the RBS.

   - RIB_FWD_SLIDE_RATE are valid values for the transition of the Ribosome from the UPSTREAM to the DOWNSTREAM RNA parts. We describe rules where the Ribosome could not move back.

   - RIB_FWD_FALL_RATE are valid values only for the description of the unbinding of the Ribosome and the UPSTREAM identifiying 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:

```
1   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         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         1
13  lacY-cds          lacA-rbs                           1
14  lacA-rbs          lacA-
    →cds                       1                 1         1         1         1
15  lacA-cds          lacA-ter1                         1         1
16  lacA-ter1          lacA-ter2]                         1         1
```

OR

```
1   UPSTREAM        DOWNSTREAM        RNAP_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   [rpoA-pro1        rpoA-rbs        1        1        1
3   rpoA-rbs        rpoA-
    →cds                                1              1        1        1        1
4   rpoA-cds        rpoA-ter1]                                1        1
5
6   [rpoB-pro1        rpoB-rbs        1        1        1
7   rpoB-rbs        rpoB-
    →cds                                1              1        1        1        1
8   rpoB-cds        rpoC-rbs                        1
9   rpoC-rbs        rpoC-
    →cds                                1              1        1        1        1
10  rpoC-cds        rpoC-ter1]                                1        1
11
12  [rpoD-pro1        rpoD-rbs        1        1        1
13  rpoD-rbs        rpoD-
    →cds                                1              1        1        1        1
14  rpoD-cds        rpoD-ter1]                                1        1
15
16  [rpoE-pro1        rpoE-rbs        1        1        1
17  rpoE-rbs        rpoE-
    →cds                                1              1        1        1        1
18  rpoE-cds        rpoE-ter1]                                1        1
19
20  [rpoH-pro1        rpoH-rbs        1        1        1
21  rpoH-rbs        rpoH-
    →cds                                1              1        1        1        1
22  rpoH-cds        rpoH-ter1]                                1        1
23
24  [rpoN-pro1        rpoN-rbs        1        1        1
25  rpoN-rbs        rpoN-
    →cds                                1              1        1        1        1
26  rpoN-cds        rpoN-ter1]                                1        1
27
28  [rpoS-pro1        rpoS-rbs        1        1        1
29  rpoS-rbs        rpoS-
    →cds                                1              1        1        1        1
30  rpoS-cds        rpoS-ter1]                                1        1
31
32  [fliA-pro1        fliA-rbs        1        1        1
33  fliA-rbs        fliA-
    →cds                                1              1        1        1        1
34  fliA-cds        fliA-ter1]                                1        1
35
36  [fecI-pro1        fecI-rbs        1        1        1
37  fecI-rbs        fecI-
    →cds                                1              1        1        1        1
38  fecI-cds        fecI-ter1]                                1        1
```

Note: Visualization in Cytoscape. Colors and arrows remains to the user for customization. The genome graph (outer nodes) could be complemented with a description of sigma factor specifity for promoter (inner nodes), as in the following network:
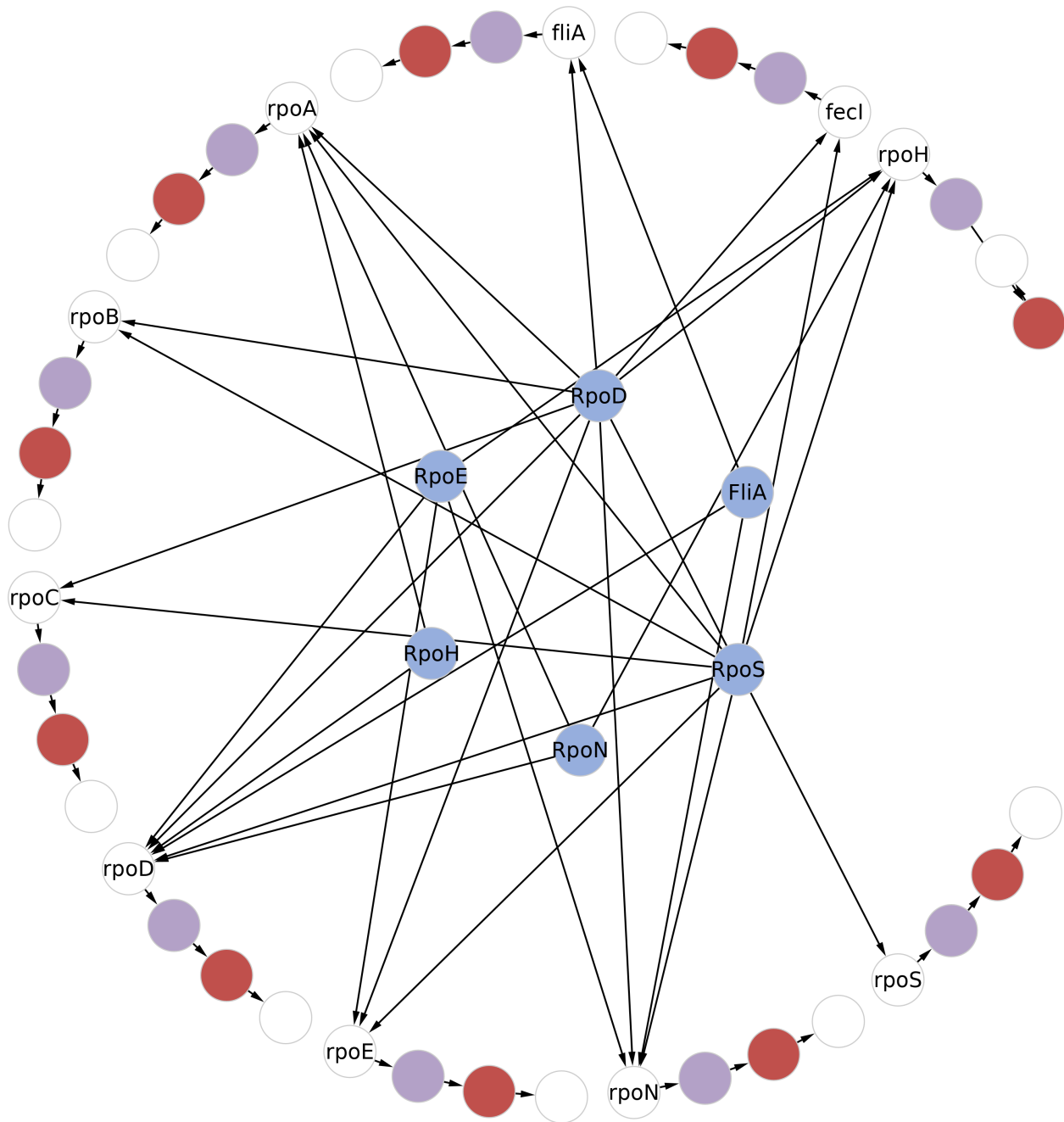
Finally, execute `atlas_rbm.construct_model_from_genome_graph(network, verbose = False)` to obtain the model.

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

```python
from pysb import *
Model()

Monomer('dna',
        ['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']})
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']})
Monomer('prot',
        ['name', 'loc', 'dna', 'met', 'prot', 'rna', 'up', 'dw'],
        { 'name' : ['lacA', 'lacY', 'lacZ'],
        'loc' : ['cyt', 'cytosk', 'ex', 'mem', 'per', 'wall', 'bnuc', 'cproj', 'imem',
↪ 'omem']})
Monomer('cplx',
        ['name', 'loc', 'dna', 'met', 'prot', 'rna'],
        { 'name' : ['RNAP_CPLX', 'RIBOSOME_CPLX'],
        'loc' : ['cyt']})
Rule('docking_lacZ_pro4',
        cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = None) +
        dna(name = 'lacZ', type = 'pro4', loc = 'cyt', prot = None) |
        cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
        dna(name = 'lacZ', type = 'pro4', loc = 'cyt', prot = 1),
        Parameter('fwd_docking_lacZ_pro4', 1.000000),
        Parameter('rvs_docking_lacZ_pro4', 1.000000))
Rule('docking_lacZ_pro3',
        cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = None) +
        dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = None) |
        cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
        dna(name = 'lacZ', type = 'pro3', loc = 'cyt', prot = 1),
        Parameter('fwd_docking_lacZ_pro3', 1.000000),
        Parameter('rvs_docking_lacZ_pro3', 1.000000))
Rule('docking_lacZ_pro2',
        cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = None) +
        dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = None) |
        cplx(name = 'RNAP_CPLX', loc = 'cyt', dna = 1) %
        dna(name = 'lacZ', type = 'pro2', loc = 'cyt', prot = 1),
        Parameter('fwd_docking_lacZ_pro2', 1.000000),
        Parameter('rvs_docking_lacZ_pro2', 1.000000))
Rule('docking_lacZ_pro1',
```

(continues on next page)

```
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))
```

```
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) %
```

```
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) +
```

```
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) %
```

```
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) %
```

```
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) %
```

```
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) %
```

5.6. Genome Graphs

```
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) %
```

```
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) %
```

```
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.

```
# simulation
bng = '/opt/git-repositories/bionetgen.RuleWorld/bng2/'
kasim = '/opt/git-repositories/KaSim4.Kappa-Dev/'
cupsoda = '/opt/git-repositories/cupSODA.aresio/'
stochkit = '/opt/git-repositories/StochKit.StochSS' # not the bin folder

data0 = simulation.scipy(model, start = 0, finish = 10, points = 2000)
data1 = simulation.cupsoda(model, start = 0, finish = 10, points = 2000, path =
↪cupsoda) # only if you have a GPU NVIDIA; comment if not.
data2 = simulation.bngODE(model, start = 0, finish = 10, points = 2000, path = bng)
data3 = simulation.bngSSA(model, start = 0, finish = 10, points = 2000, n_runs = 20,
↪path = bng)
data4 = simulation.bngPLA(model, start = 0, finish = 10, points = 2000, n_runs = 20,
↪path = bng)
data5 = simulation.bngNF(model, start = 0, finish = 10, points = 2000, n_runs = 20,
↪path = bng)
data6 = simulation.kasim(model, start = 0, finish = 10, points = 2000, n_runs = 20,
↪path = kasim)
data7 = simulation.stochkit(model, start = 0, finish = 10, points = 2000, n_runs = 20,
↪ path = stochkit)
```

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

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

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

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

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

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

- rna: `atlas_rbm.simulation.plot.rna(data, rna_name, plt_kws, **kwargs)`

- complexes: `atlas_rbm.simulation.plot.cplx(data, complex_name, location, plt_kws, **kwargs)`

- metabolites: `atlas_rbm.simulation.plot.metabolite(data, metabolite, location, plt_kws, **kwargs)`

- proteins: `atlas_rbm.simulation.plot.protein(data, protein_name, location, plt_kws, **kwargs)`

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

- observable: `atlas_rbm.simulation.plot.monomer(data, observable_name, plt_kws, **kwargs)`

```python
import seaborn
import matplotlib.pyplot as plt

palette = seaborn.color_palette('colorblind')

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

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

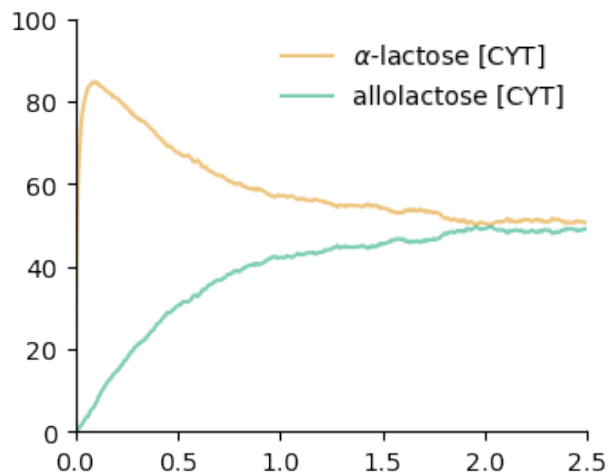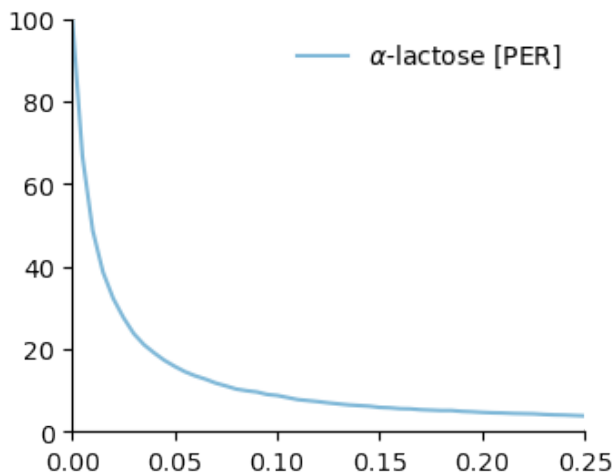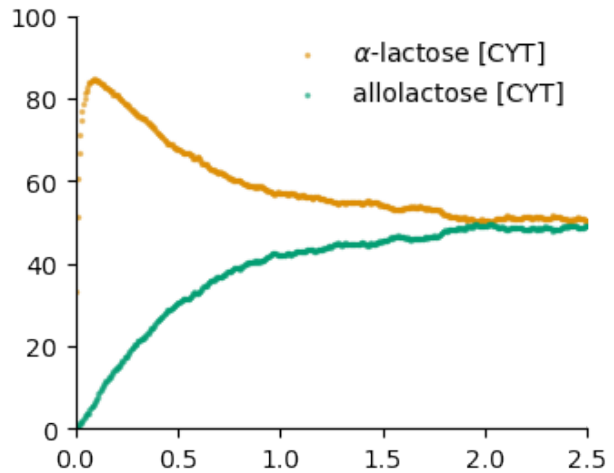```
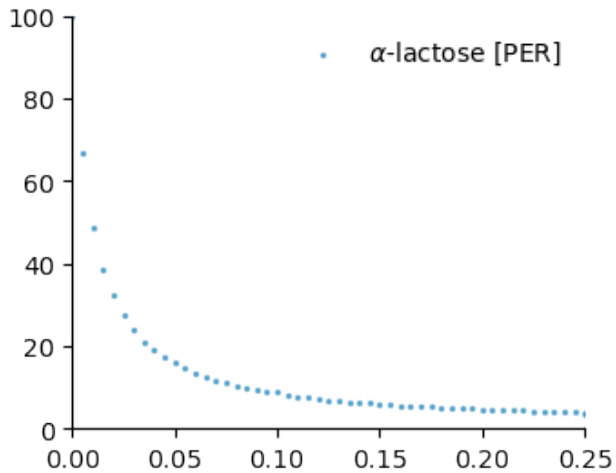
(continues on next page)

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



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

```python
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' :
    →'fill_between', 'weight' : .5},
9       plt_kws = {'s' : 2, 'color' : palette[0], 'label' : r'$\alpha$-lactose [PER]',
    →'alpha' : .5})
10
11  # second plot, cytoplasmic concentration
12  simulation.plot.metabolite(data3, 'Alpha_lactose', 'cyt', ax = ax[1], **{'kind' :
    →'fill_between', 'weight' : .5},
13      plt_kws = {'s' : 2, 'color' : palette[1], 'label' : r'$\alpha$-lactose [CYT]',
    →'alpha' : .5})
14
15  # second plot, cytoplasmic concentration
16  simulation.plot.metabolite(data3, 'ALLOLACTOSE', 'cyt', ax = ax[1], **{'kind' : 'fill_
    →between', 'weight' : .5},
17      plt_kws = {'s' : 2, 'color' : palette[2], 'label' : r'allolactose [CYT]', 'alpha'
    →: .5})
18
19  # first plot, periplasmic concentration
20  simulation.plot.metabolite(data0, 'Alpha_lactose', 'per', ax = ax[0], **{'kind' :
    →'plot'},
21      plt_kws = {'s' : 2, 'color' : palette[0], 'label' : r'ODE'})
22
23  # second plot, cytoplasmic concentration
24  simulation.plot.metabolite(data0, 'Alpha_lactose', 'cyt', ax = ax[1], **{'kind' :
    →'plot'},
25      plt_kws = {'s' : 2, 'color' : palette[1], 'label' : r'ODE'})
26
27  # second plot, cytoplasmic concentration
28  simulation.plot.metabolite(data0, 'ALLOLACTOSE', 'cyt', ax = ax[1], **{'kind' : 'plot
    →'},
29      plt_kws = {'s' : 2, 'color' : palette[2], 'label' : r'ODE'})
30
31  ax[0].set_xlim((0,.25))
32  ax[1].set_xlim((0,2.5))
33  ax[0].set_ylim((0,100))
34  ax[1].set_ylim((0,100))
35
36  seaborn.despine()
```
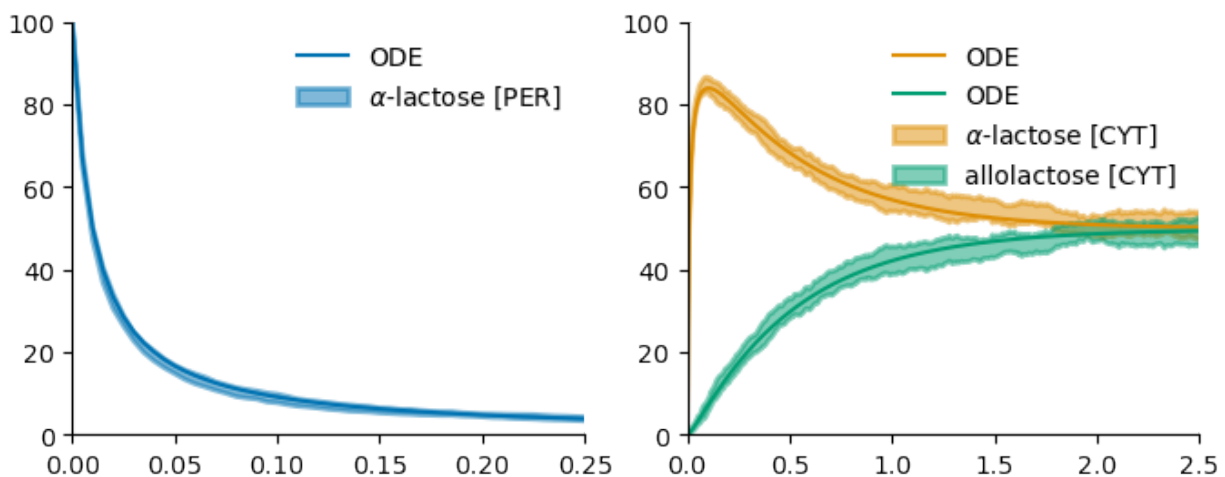
Note: *Atlas* produces automatically `Observables` for metabolites and other components. However, *Atlas* do not produce `Observables` for every possible component and the user could add observables with `atlas_rbm.simulation.set_observable(model, pattern, alias)`.

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 proccess call network generation and could take excessive time to finish.

INDICES AND TABLES

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- modindex
- search