



Natural Computation Group



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XDSD User Manual

XDSD

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DSDui is a graphical user interface for [DSDPy](#) package.

TUTORIAL

1.1 Prerequisites

- To create the Anaconda environment:

```
conda env create -f environment.yml  
(dsdui) > dot -c
```

- Manual installation:

```
conda install -c alubbock pysb  
conda install -c conda-forge networkx  
conda install -c conda-forge matplotlib  
conda install -c anaconda pyqt  
conda install -c conda-forge bidict  
conda install -c alubbock graphviz pygraphviz
```

1.2 Run program

```
python main.py
```

1.3 Usage

Upon running the program a standalone application appears:

1.3.1 Input

1. **DSD model** tab accepts the text input in the form described in [DSDPy manual](#).
 - choose if the parsing algorithm should be able to: permute the strands, flip the strands, flip the domains
 - choose if the dots, denoting the destination of the pair, should be displayed

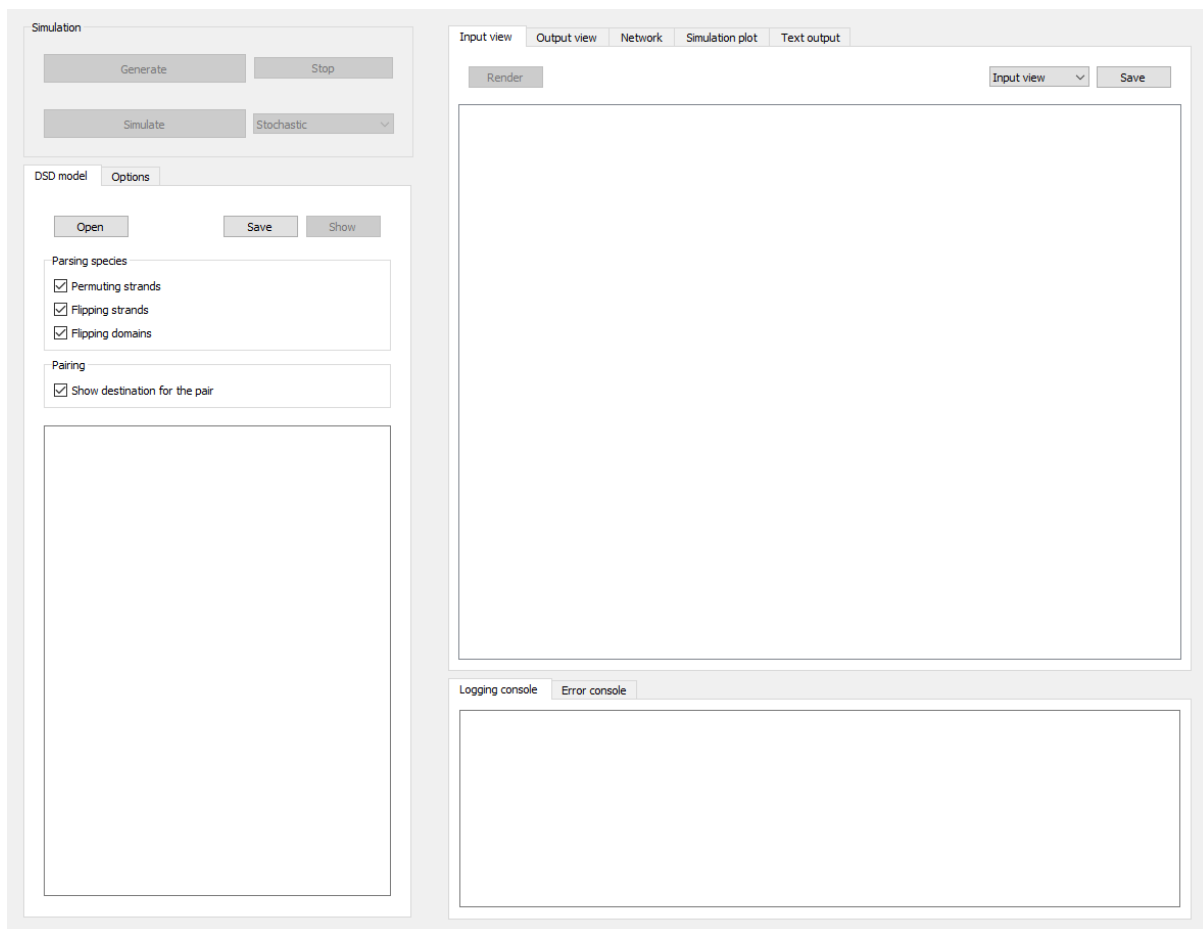


Fig. 1.1: DSDPy user interface

DSD model
Options

Open
Save
Show

Parsing species
☒ Permuting strands
☒ Flipping strands
☒ Flipping domains

Pairing
☒ Show destination for the pair

```

<d1 b!1 a!2 2^!3>
<2^*!3 a*!2 c*!4 1^*>
<c!4 b*!1>
//
<1^!1 c!2 a!3>
<2^* a*!3 b*!4 d2 3^>
<b!4 c*!2 1^*!1>
//
<d1!1 d2!2>
<3^* d2*!2 d1*!1>
//
<1^ c a>
--
ss1 1000
ss2 1000
ss3 1400
ss4 500
--
RB 0.0003
RU 0.1126
R3 20
R4 2

```

Fig. 1.2: DSD model tab

2. **Options** tab provides settings for:

- threshold of iterations in reaction network generation
- rendering speed - the greater the speed, the quicker and less accurate the output rendering (default settings: exponentially increasing for simple species, linearly increasing for pseudoknots)
- render button starts the rendering of the current view

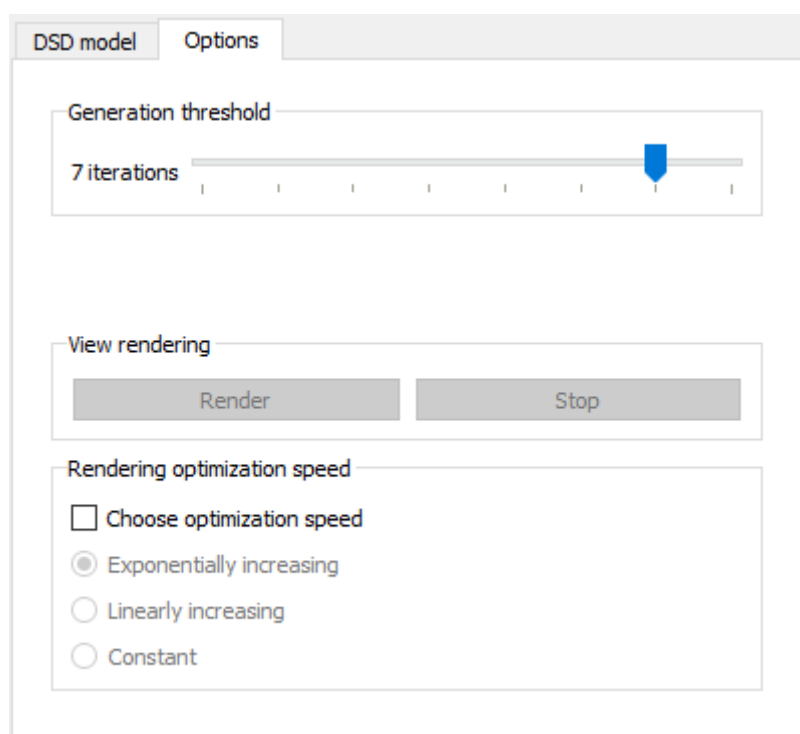


Fig. 1.3: Options tab

1.3.2 Simulation

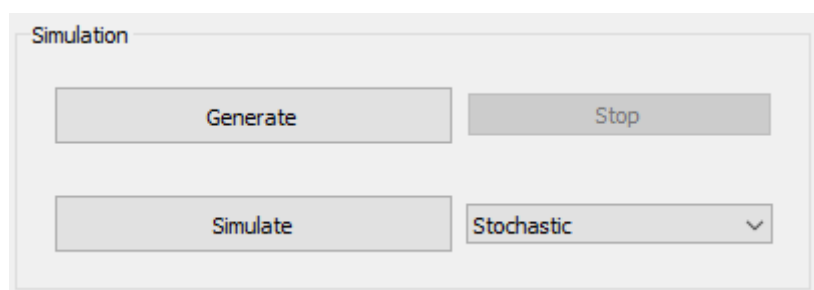


Fig. 1.4: Simulation buttons group

1. **Generate** button starts the reaction network generation
2. **Simulate** button starts the simulation - choose the mode from the combo box (stochastic / deterministic)

1.3.3 Output

1. **Input view** tab displays the parsed input species to the DSDPy. **Output view** tab displays the parsed output species from the DSDPy.
 - **Render** button starts the rendering of the current view
 - choose the input and output of the render from the combo box
 - save the views as a PNG with save button
2. **Network** tab displays the chemical reaction network
 - choose the network layout from the options in the combo box
 - zoom and pan to navigate through the network
 - click on the species' name to view the species
 - click on the reaction name to view the reactants, products and reaction rate of the reaction
3. **Simulation plot** tab displays BNG simulation plot
4. **Text output** tab displays the text output from the DSDPy

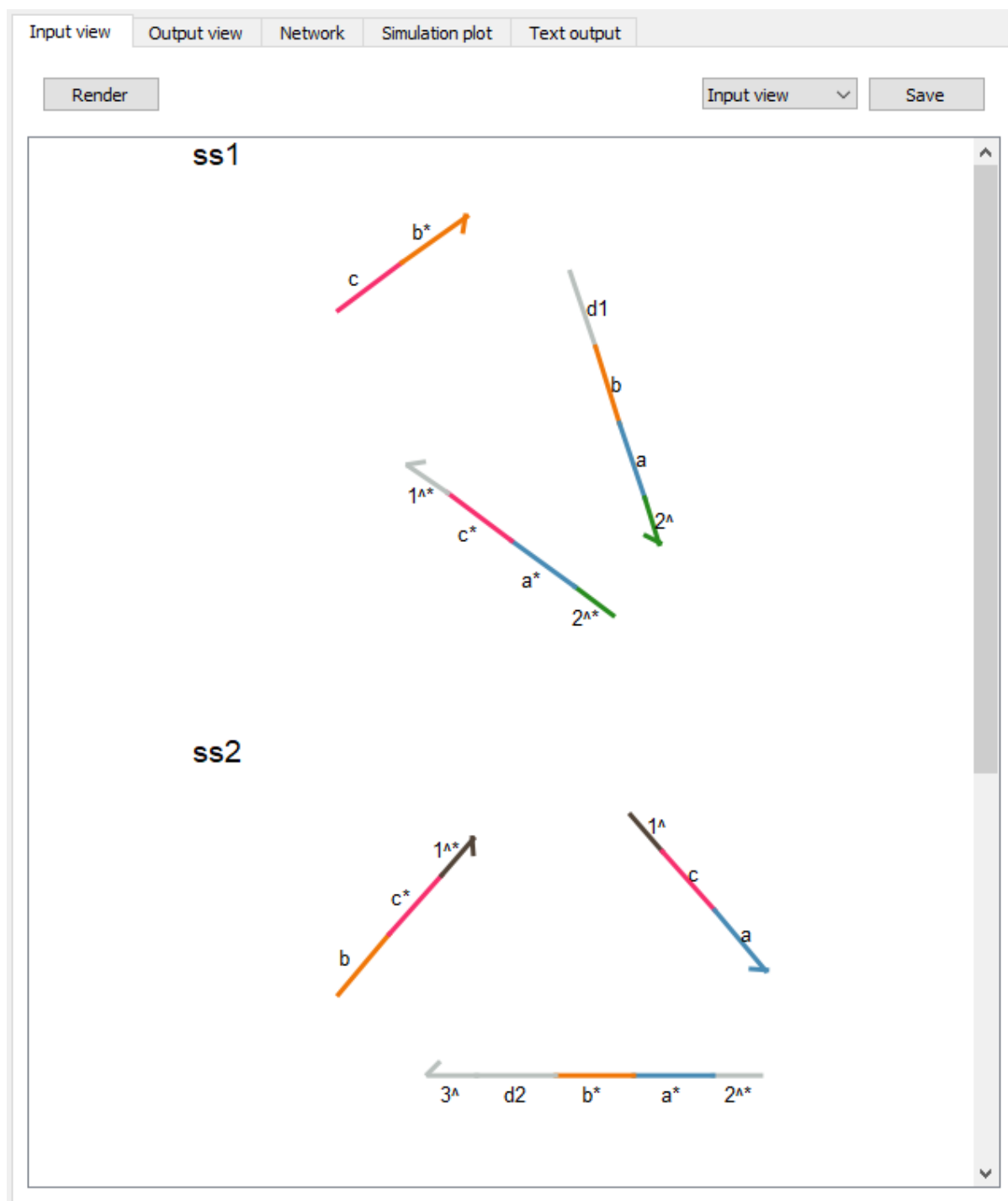


Fig. 1.5: DSD species before rendering

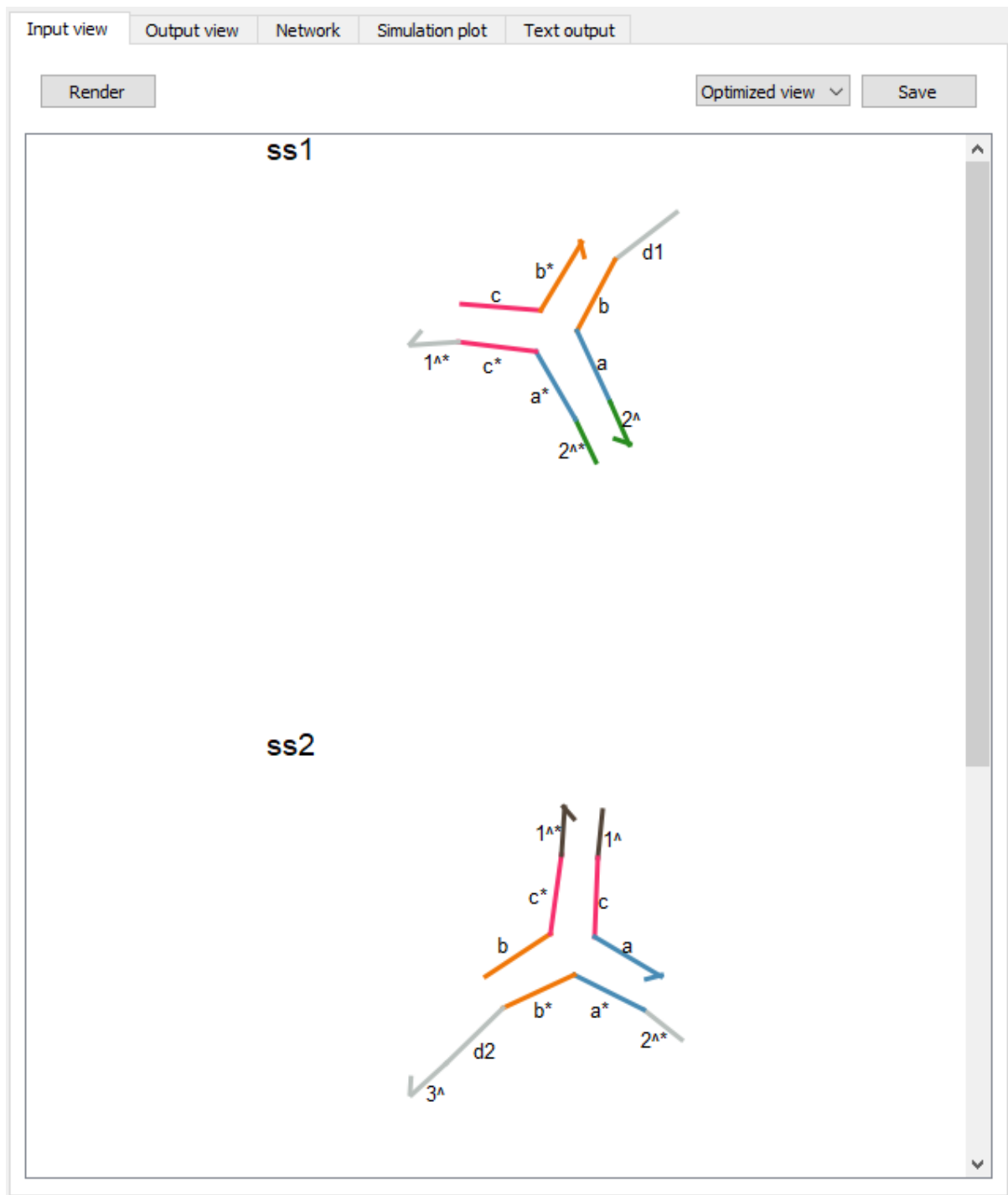


Fig. 1.6: DSD species after rendering

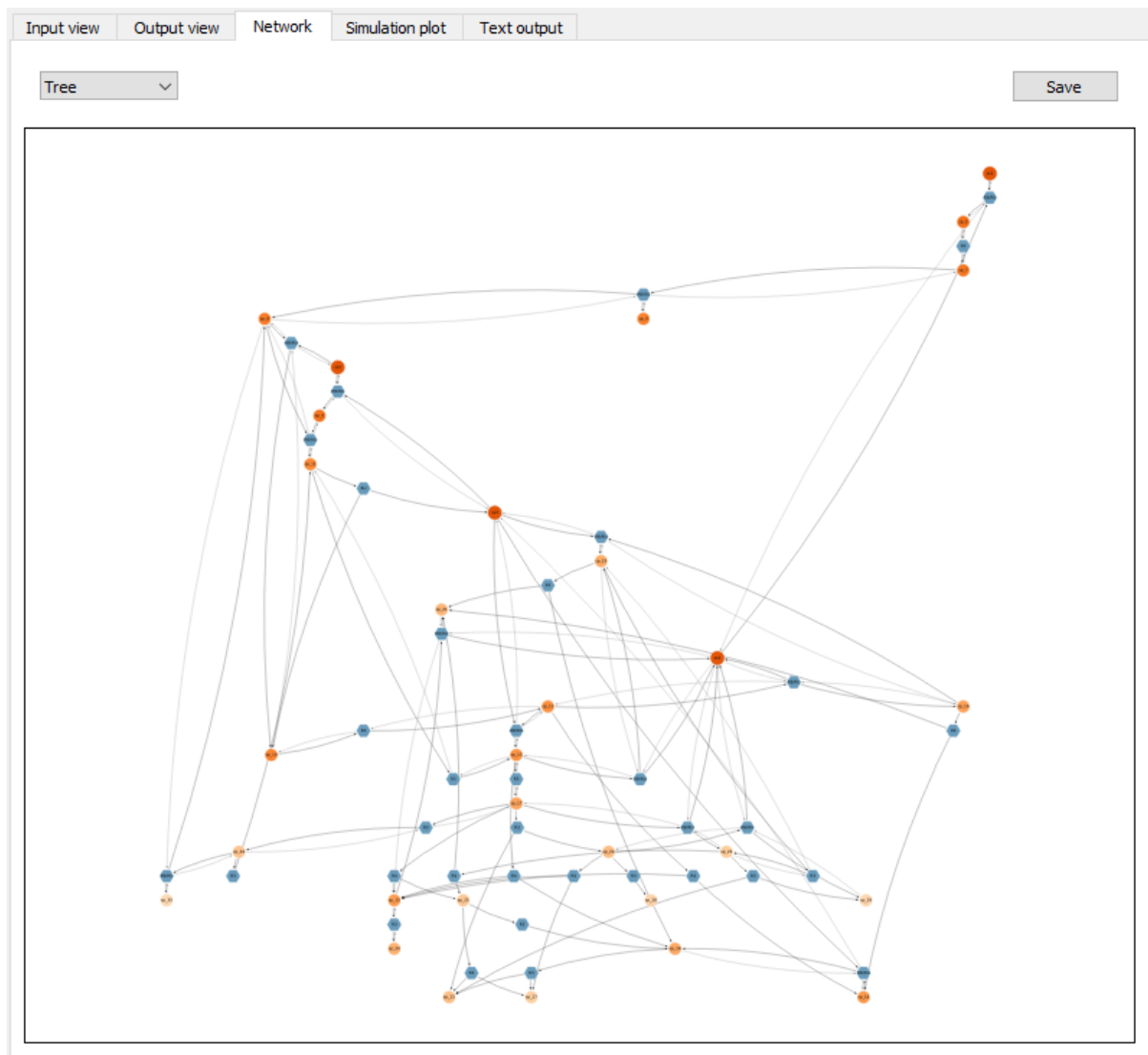


Fig. 1.7: Network tab after clicking Generate button

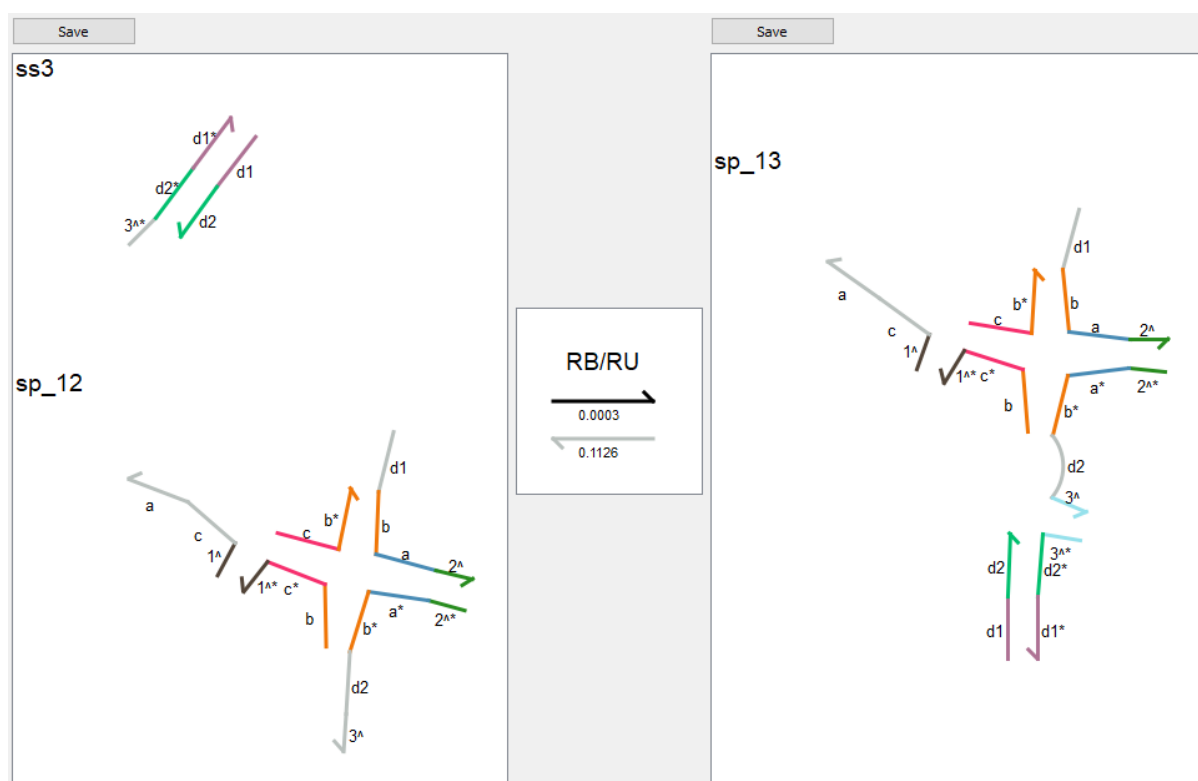


Fig. 1.8: Reaction window after clicking on a reaction node

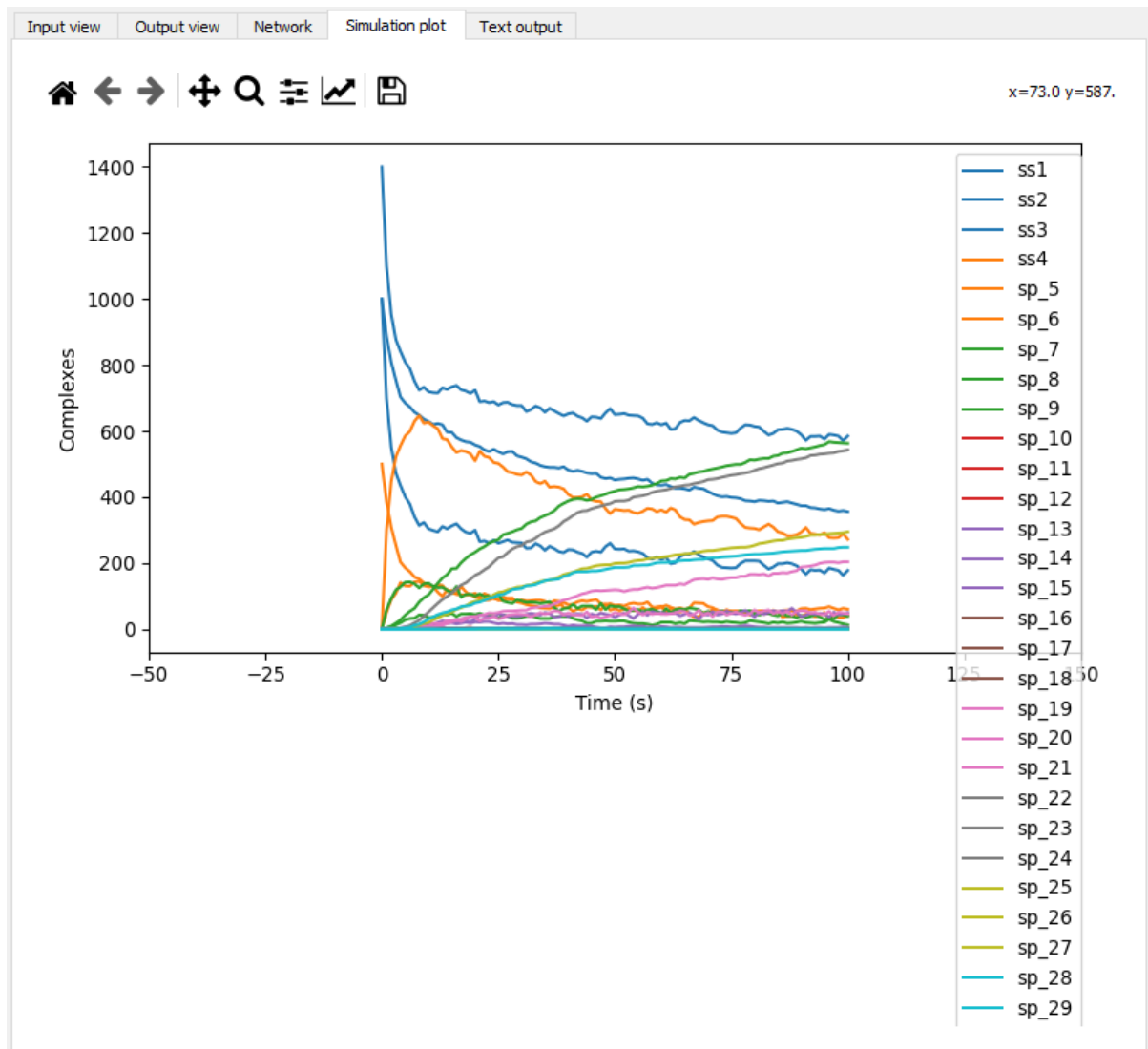


Fig. 1.9: Simulation tab after clicking Simulate button

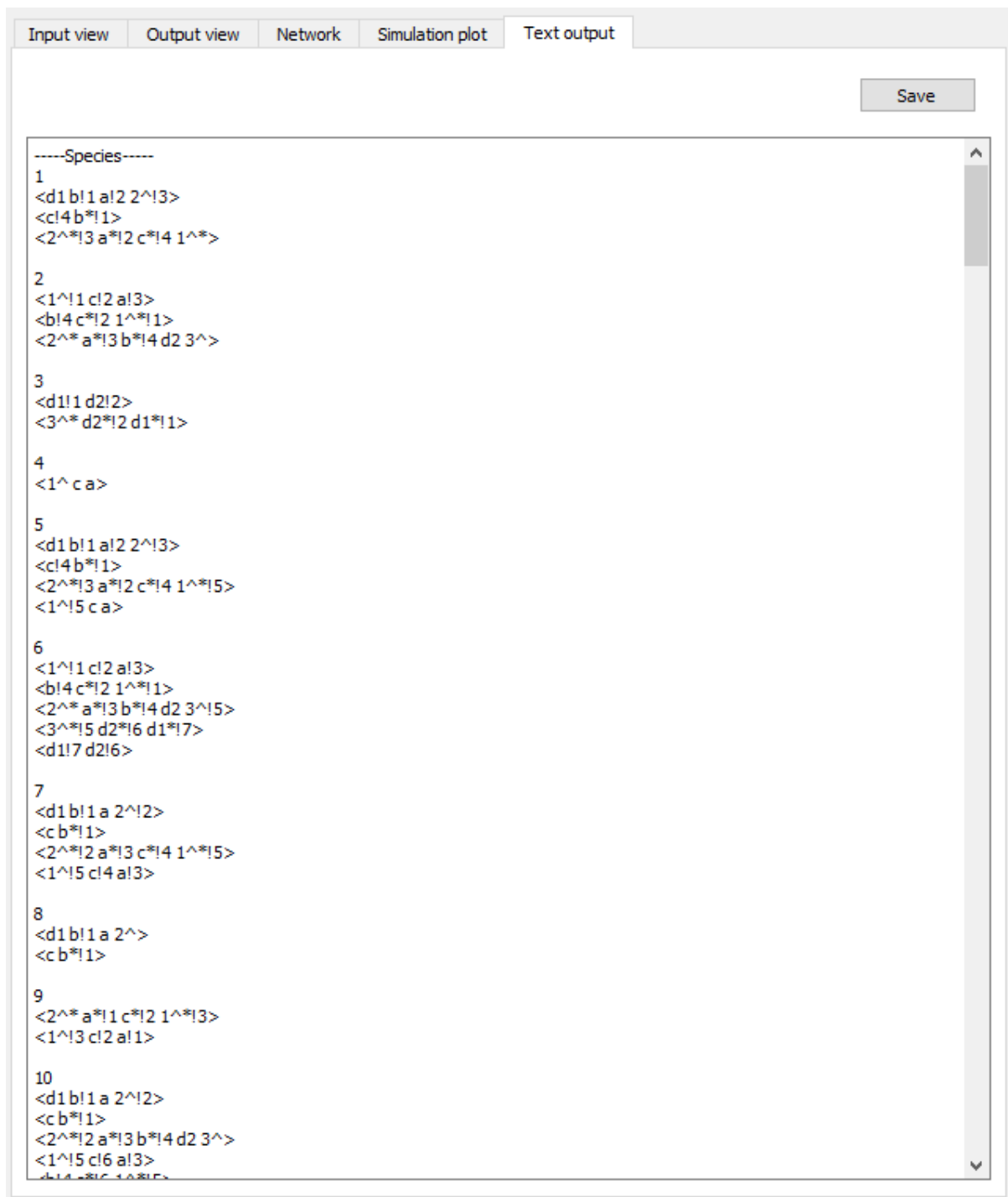


Fig. 1.10: Text output tab after clicking Generate button

MAIN MODULES

2.1 elements

Contains wrapper classes for the main concepts of the DSDPy package like Domain, Strand and Species.

2.2 interface

Contains the Ui and UiControl and other classes responsible for the view and control of the user interface.

2.3 model

Contains the UiModel class, holding the data and current state of the user interface.

2.4 optimization

Contains the logic of the rendering optimization - simulated annealing.

2.5 parsing

Contains the input and output files parsers.

2.6 utils

Contains the utility functions and the configuration files.

INDICES AND TABLES:

- genindex
- modindex
- search