## Complexation

**Model implementation.** This process models the formation of all macromolecular complexes except for the formation of 70S ribosomes from 30S and 50S subunits, which is performed by `Translation`. Macromolecular complexation is done by identifying complexation reactions that are possible (which are reactions that have sufficient counts of all sub-components), performing one randomly chosen possible reaction, and re-identifying all possible complexation reactions. This process assumes that macromolecular complexes form spontaneously, and that complexation reactions are fast and complete within the time step of the simulation. This approach is very similar to the *M. genitalium* model of complexation with the exception that the selection of a complexation reaction was weighted by a multinomial distribution parameterized by substrate availability rather than a uniform distribution. We found that the choice of distribution had no major effect on behavior of the process. Additionally, the *M. genitalium* simulations describe 201 macromolecular complexes, whereas over 5 times as many are implemented in the *E. coli* model.

**Algorithm 1:** Macromolecular complexation

**Input :** $c_i$ counts of molecules where $i = 1$ **to** $n_{molecules}$

**Input :** $S$ matrix describing reaction stoichiometries where $S_{i,j}$ describes the coefficient for the $i^{th}$ molecule in the $j^{th}$ reaction

**Input :** `getPossibleReactions` function that takes $c_i$ and $S$ and returns all reactions that are possible

**Input :** `chooseRandomReaction` function that takes all possible reactions and returns one randomly chosen reaction

**while** *possible reactions remaining* **do**

**1.** Get all possible reactions ($r$)

$r =$ `getPossibleReactions`$(S, c_i)$

**2.** Choose a random possible reaction ($r_{choice}$) to perform

$r_{choice} =$ `chooseRandomReaction`$(r)$

**3.** Perform $r_{choice}$ by incrementing product counts and decrementing reactant counts

**Result:** Macromolecule complexes are formed from their subunits according to their known stoichiometries.

### Associated data

Stoichiometric coefficients that define 1,023 complexation reactions from EcoCyc [1].

### Associated files

| `wcEcoli` Path | File | Type |
|---|---|---|
| `wcEcoli/models/ecoli/processes` | `complexation.py` | process |
| `wcEcoli/reconstruction/ecoli/dataclasses/process` | `complexation.py` | data |
| `wcEcoli/reconstruction/ecoli/flat` | `complexationReactions.tsv` | raw data |

Table 1: Table of files for complexation.

# References

[1] Ingrid M Keseler, Amanda Mackie, Martin Peralta-Gil, Alberto Santos-Zavaleta, Socorro Gama-Castro, César Bonavides-Martínez, Carol Fulcher, Araceli M Huerta, Anamika Kothari, Markus Krummenacker, Mario Latendresse, Luis Muñiz-Rascado, Quang Ong, Suzanne Paley, Imke Schröder, Alexander G Shearer, Pallavi Subhraveti, Mike Travers, Deepika Weerasinghe, Verena Weiss, Julio Collado-Vides, Robert P Gunsalus, Ian Paulsen, and Peter D Karp. EcoCyc: fusing model organism databases with systems biology. *Nucleic acids research*, 41(Database issue):D605–12, January 2013.