### Complexation

**Model implementation.** This process models the formation of all macromolecular complexes except for 70S ribosome formation, which is handled 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.

**Algorithm 1:** Algorithm for 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 ($r$)

$r = \texttt{getPossibleReactions}(S, c_i)$

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

$r_{choice} = \texttt{chooseRandomReaction}(r)$

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

**Result:** Macromolecule complexes are formed from their subunits.

**Associated files**

| wcEcoli Path | File | Type |
|---|---|---|
| wcEcoli/models/ecoli/processes | complexation.py | process |
| wcEcoli/reconstruction/ecoli/dataclasses/process | complexation.py | data |

Table 1: Table of files for complexation.

**Associated data.** Stoichiometric coefficients that define 1,023 reactions to form protein complexes from EcoCyc [1].

**Difference from *M. genitalium* model.** This sub-model is implemented very similarly to the *M. genitalium* model of complexation. In the *M. genitalium* simulations, however, 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.

# 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.