

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)
 $r = \text{getPossibleReactions}(S, c_i)$
 2. Choose a random possible reaction (r_{choice}) to perform
 $r_{choice} = \text{chooseRandomReaction}(r)$
 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 Muñoz-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.