Creation and analysis of biochemical constraint-based models using the COBRA Toolbox v.3.0 - DTU Orbit (04/08/2019)

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Constraint-based reconstruction and analysis (COBRA) provides a molecular mechanistic framework for integrative analysis of experimental molecular systems biology data and quantitative prediction of physicochemically and biochemically feasible phenotypic states. The COBRA Toolbox is a comprehensive desktop software suite of interoperable COBRA methods. It has found widespread application in biology, biomedicine, and biotechnology because its functions can be flexibly combined to implement tailored COBRA protocols for any biochemical network. This protocol is an update to the COBRA Toolbox v.1.0 and v.2.0. Version 3.0 includes new methods for quality-controlled reconstruction, modeling, topological analysis, strain and experimental design, and network visualization, as well as network integration of chemoinformatic, metabolomic, transcriptomic, proteomic, and thermochemical data. New multi-lingual code integration also enables an expansion in COBRA application scope via high-precision, high-performance, and nonlinear numerical optimization solvers for multi-scale, multi-cellular, and reaction kinetic modeling, respectively. This protocol provides an overview of all these new features and can be adapted to generate and analyze constraint-based models in a wide variety of scenarios. The COBRA Toolbox v.3.0 provides an unparalleled depth of COBRA methods.

General information
Publication status: Published
Organisations: Novo Nordisk Foundation Center for Biosustainability, Big Data 2 Knowledge, Network Reconstruction in Silico Biology, University of Luxembourg, University of Chile, University of California at San Diego, European Bioinformatics Institute, Pennsylvania State University, Sinopia Biosciences, Georgia Institute of Technology, University of Navarra, University of Utah, Institut National de la Santé et de la Recherche Médicale, Stanford University, Michigan State University, University of Utah, Imperial College London, University of Alicante, California Institute of Technology
Corresponding author: Fleming, R. M. T.
Number of pages: 64
Pages: 639-702
Publication date: 2019
Peer-reviewed: Yes

Publication information
Journal: Nature Protocols
Volume: 14
Issue number: 3
ISSN (Print): 1750-2799
Ratings:
Web of Science (2019): Indexed yes
Original language: English
DOIs:
10.1038/s41596-018-0098-2
Source: FindIt
Source-ID: 2444118580
Research output: Contribution to journal › Journal article – Annual report year: 2019 › Research › peer-review