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Published in:
Nature Protocols (Online)

Link to article, DOI:
[10.1038/nprot.2007.99](https://doi.org/10.1038/nprot.2007.99)

Publication date:
2007

Document Version
Publisher's PDF, also known as Version of record

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Citation (APA):
Beck, S. A., Feist, A., Mo, M. L., Hannum, G., Palsson, B. O., & Herrgard, M. (2007). Quantitative prediction of cellular metabolism with constraint-based models: the COBRA Toolbox. *Nature Protocols (Online)*, 2(3), 727-738. <https://doi.org/10.1038/nprot.2007.99>

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Protocol

Nature Protocols **2**, 727 - 738 (2007)

Published online: 29 March 2007 | doi:10.1038/nprot.2007.99

Subject Categories: [Genomics and proteomics](#) | [Computational and theoretical biology](#) | [Biochemistry and protein analysis](#)

Quantitative prediction of cellular metabolism with constraint-based models: the COBRA Toolbox

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The manner in which microorganisms utilize their metabolic processes can be predicted using constraint-based analysis of genome-scale metabolic networks. Herein, we present the constraint-based reconstruction and analysis toolbox, a software package running in the Matlab environment, which allows for quantitative prediction of cellular behavior using a constraint-based approach. Specifically, this software allows predictive computations of both steady-state and dynamic optimal growth behavior, the effects of gene deletions, comprehensive robustness analyses, sampling the range of possible cellular metabolic states and the determination of network modules. Functions enabling these calculations are included in the toolbox, allowing a user to input a genome-scale metabolic model distributed in Systems Biology Markup Language format and perform these calculations with just a few lines of code. The results are predictions of cellular behavior that have been verified as accurate in a growing body of research. After software installation,

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calculation time is minimal, allowing the user to focus on the interpretation of the computational results.

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Nature Protocols ISSN 1754-2189 EISSN 1750-2799

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