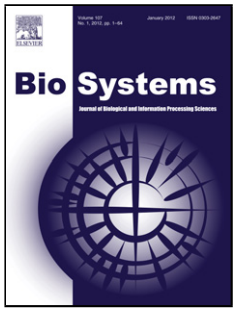

Title: Evolutionary algorithm for metabolic pathways synthesis

Author: Matias F. Gerard Georgina Stegmayer Diego H. Milone

PII: S0303-2647(16)30035-1
DOI: http://dx.doi.org/doi:10.1016/j.biosystems.2016.04.002
Reference: BIO 3650

To appear in: *BioSystems*

Received date: 16-11-2015
Revised date: 1-3-2016
Accepted date: 1-4-2016

Please cite this article as: Matias F. Gerard, Georgina Stegmayer, Diego H. Milone, Evolutionary algorithm for metabolic pathways synthesis, <*![CDATA[BioSystems]]*> (2016), http://dx.doi.org/10.1016/j.biosystems.2016.04.002

Evolutionary algorithm for metabolic pathways synthesis

Matias F. Gerard*, Georgina Stegmayer, Diego H. Milone

Research Institute for Signals, Systems and Computational Intelligence (sinc(i)), FICH–UNL/CONICET, Argentina.

Abstract

Metabolic pathway building is an active field of research, necessary to understand and manipulate the metabolism of organisms. There are different approaches, mainly based on classical search methods, to find linear sequences of reactions linking two compounds. However, an important limitation of these methods is the exponential increase of search trees when a large number of compounds and reactions is considered. Besides, such models do not take into account all substrates for each reaction during the search, leading to solutions that lack biological feasibility in many cases. This work proposes a new evolutionary algorithm that allows searching not only linear, but also branched metabolic pathways, formed by feasible reactions that relate multiple compounds simultaneously. Tests performed using several sets of reactions show that this algorithm is able to find feasible linear and branched metabolic pathways.

Keywords: Evolutionary algorithms, search strategies, *de novo* pathway building, reactions network, sets of compounds.

*Corresponding author. Tel: +54 (0342) 457 5234 int 118.
Email addresses: mgerard@sinc.unl.edu.ar (Matias F. Gerard), gstegmayer@sinc.unl.edu.ar (Georgina Stegmayer), dmilone@sinc.unl.edu.ar (Diego H. Milone)