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Title: Evolutionary algorithm for metabolic pathways

synthesis

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## Abstract

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- 6 Metabolic pathway building is an active field of research, necessary to
- 7 understand and manipulate the metabolism of organisms. There are dif-
- 8 ferent approaches, mainly based on classical search methods, to find linear
- 9 sequences of reactions linking two compounds. However, an important lim-
- 10 itation of these methods is the exponential increase of search trees when
- a large number of compounds and reactions is considered. Besides, such
- search, leading to solutions that lack biological feasibility in many cases.

models do not take into account all substrates for each reaction during the

- 14 This work proposes a new evolutionary algorithm that allows searching not
- only linear, but also branched metabolic pathways, formed by feasible reac-
- tions that relate multiple compounds simultaneously. Tests performed using
- 17 several sets of reactions show that this algorithm is able to find feasible linear
- and branched metabolic pathways.
- 19 Keywords: Evolutionary algorithms, search strategies, de novo pathway
- 20 building, reactions network, sets of compounds.

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