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IDENTIFICATION OF CATALYTIC OR METABOLIC PATHWAYS: A GRAPH-THEORETIC APPROACH*

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ABSTRACT

A mathematically exact algorithmic approach is presented for carrying out the synthesis of the networks of plausible elementary or metabolic reactions constituting stoichiometrically exact and potentially feasible catalytic or metabolic pathways; this synthesis is profoundly complex combinatorially. The approach is based on the unique graph-representation in terms of P-graphs (process graphs), a set of axioms, and a group of combinatorial algorithms. The inclusion or exclusion of a step of each elementary or metabolic reaction in the pathway of interest hinges on the general combinatorial properties of feasible reaction networks. The methodology, on which the approach is based, is outlined at the outset. The methodology is then illustrated by implementing it to three examples comprising two catalytic reactions, i.e., catalytic combustion of hydrogen and reduction of nitrogen oxide, and one metabolic reaction, involved in the production of ethanol by yeast. The efficacy of the approach is discussed in light of the results obtained from these examples.

Key Words: pathway, catalytic reaction, metabolic reaction, algorithmic identification, graph-theoretic.

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