MODELLING LIPID BIOSYNTHESIS PATHWAYS OF OIL PALM BY BOOLEAN AND GRAPHICAL APPROACHES^{*}

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ABSTRACT

The mathematical modelling provides an alternative way for the interpretation and prediction of cellular metabolisms. This study delves into the modelling of lipid biosynthesis pathway and the primary metabolism in the fruit of the oil palm (Elaeis guineensis). Two different data are used for the analysis. In the first dataset, the distribution of carbon flux into the major classes of lipids, i.e., triacylglycerols, diacylglycerols, monoacylglycerols, phospholipids, and free fatty acids, is investigated using radioactive isotope. Then, the model of carbon flux is constructed based on the Boolean approach. On the other hand in the second dataset, the graphical methods are implemented to construct a model for the lipid contents of the developing oil palm mesocarp based on the major lipid metabolites of this system as listed previously. Moreover, the generated models are analysed for the control structure depending on the relative ranking of degree for each lipid class in the pathway. The results demonstrate the ability of the models to predict the site of control in this biosynthetic system. Furthermore, the analyses of the networks of lipids do not only reveal underlying interactions between the major classes of lipids but also the response of these networks towards changing environments.

1 INTRODUCTION

With the rapid accumulation of experimental data in biology, mathematical models have been developed to describe either individual or overall functions of cellular processes. Various ways to develop mathematical models are available such as linear ones [28, 30], differential equations [3, 9, 10, 11, 12], Boolean [17], graphical models [31], Bayesian ones [8, 21, 22], and neural networks [29]. These approaches represent different levels of abstraction of the cellular metabolism. These features may be exploited within biotechnology for the production of compounds which may serve as pharmaceuticals, food additives, and so on.

The modelling of the primary metabolism in plants

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provides a powerful tool for the interpretation and prediction of experimental models and cellular phenomena. A *mathematical model* implies an abstraction of the actual phenomena or processes. These phenomena and processes constitute a complex network of interconnecting pathways, comprising hundreds of biochemical reactions, and metabolites associated with the respective systems. Moreover, the metabolism of a living cell is subject to control and regulatory mechanisms [5]. Thus, the modelling of a cellular process depends on the types of measurement which have influence on it in interpreting and predicting the cellular and physiological functions.



Figure 1: The lipid biosynthesis pathway via the *Kennedy pathway* for formation of triacylglycerols, storage oils.

The study of the lipid biosynthesis in plants has been intensive in recent years [15, 18, 27, 29]. Various attempts have

