

# Metabolomic analysis of isonitrosoacetophenone-induced perturbations in phenolic metabolism of *Nicotiana tabacum* cells

Ntakadzeni E. Madalaa, Paul A. Steenkampa,b, Lizelle A. Piater a, Ian A. Duberya,†

*a*Department of Biochemistry, University of Johannesburg, Auckland Park 2006, South Africa

*b*Discovery Chemistry, CSIR Biosciences, Pretoria 0001, South Africa

## Abstract

Plants have developed biochemical and molecular responses to adapt to different stress environments. One of the characteristics of the multi-component defence response is the production of defence-related metabolites. Plant defences can be triggered by various stimuli, including synthetic or naturally occurring molecules, especially those derived from pathogens. In the current study, *Nicotiana tabacum* cell suspensions were treated with isonitrosoacetophenone (INAP), a subcomponent of a plant-derived stress metabolite with anti-fungal and anti-oxidant properties, in order to investigate the effect thereof on cellular metabolism. Subsequent metabolomic-based analyses were employed to evaluate changes in the metabolome. UPLC-MS in conjunction with multivariate data analyses was found to be an appropriate approach to study the effect of chemical inducers like INAP on plant metabolism in this model system. Principal component analysis (PCA) indicated that INAP is capable of inducing time-dependent metabolic perturbations in the cultured cells. Orthogonal projection to latent structures discriminant analysis (OPLS-DA) revealed metabolites of which the levels are affected by INAP, and eight of these were tentatively annotated from the mass spectral data and online databases. These metabolites are known in the context of plant stress- and defence responses and include benzoic- or cinnamic acid derivatives that are either glycosylated or quinilated as well as flavonoid derivatives. The results indicate that INAP affects the shikimate-, phenylpropanoid- and flavonoid pathways, the products of which may subsequently lead to an anti-oxidant environment *in vivo*.