

Metabolomics: A Novel Tool to Bridge Phenome to Genome under Changing Climate to Ensure Food Security

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Global Climate Change Affecting Plant Fitness and Reproductive Success

Anthropogenic activities that contribute to global climate change, thereby affecting plant growth and survival are carbon dioxide (CO₂), ozone (O₃), and temperature. There has been unprecedented increase in atmospheric CO₂ concentration (present atmospheric CO₂ concentration is 387 ppm), 40% more than the levels before industrial revolution [1] and is expected to increase to 500-900 ppm by the end of the twenty first century [2]. The concentration of O₃ in lower troposphere has increased to 20-50% at an average of 38% since pre-industrial era [3]. The Intergovernmental Panel on Climate Change (IPCC), forecasts a temperature rise of 2.5 to 10 degrees Fahrenheit over the next century (<http://climate.nasa.gov/effects>). Plant photosynthetic rates are influenced by these factors which in turn affect subsequent allocation of carbohydrates, cellulose, lignins, tannins pool, which in long term affect CO₂ sequestration [4]. Global climate change may directly alter plant fitness, as well as alter the reproductive success of plants and their interactions through impacts on flowering phenology [5-8].

Chemical Ecology and Plant Secondary Metabolites

Plants produce an array of secondary metabolites, which are not directly involved in primary metabolism of plant growth and development. These plant secondary metabolites (PSMs) belong to different chemical groups such as phenylpropanoids, flavonoids, terpenoids, and alkaloids. Chemical ecology is an area that deals with studies of interactions between organisms and their biotic and abiotic environment that are mediated by chemicals. Stahl (1888) is known as an early pioneer of chemical ecology who proposed that the various chemical protective means of plants were shaped and optimized under the selection pressure of the animal kingdom that surrounds the plants [9]. Fifty four years ago, PSMs were placed in an ecological context by Fraenkel [10]. The ability of plants to synthesize secondary compounds has been selected throughout the course of evolution in different plant lineages when such compounds addressed specific needs [11]. For example, floral scent volatiles and pigments were evolved to attract insect pollinators and thus enhanced fertilization rates. The ability to synthesize toxic chemicals was evolved to ward off pathogens and herbivores or to suppress the growth of neighboring plants which involve deterrence/anti-feedant activity, toxicity or acting as precursors to physical defense systems [11-13].

PSMs vis-à-vis Global Climate Change

Stressful environments including adverse climatic effects (e.g. high temperature, elevated CO₂ concentration, high doses of UV radiations etc.) may lead to altered production of PSMs due to allocation of fixed carbon to secondary metabolism instead of channelizing it for primary metabolic functions required for growth and survival [14]. The role of PSM among a multitude of anthropogenic forces that influence ecosystems in a global scale is still less recognized. Interactions among organisms and their environment are mediated by PSM at different

levels of ecological organization. Therefore, genes encoding for PSM biosynthetic enzymes can have effects from individual organisms to all the way to global environmental processes. Lindroth (2010) has extensively detailed on the effect of global climate change on PSMs [4]. Elevated O₃ significantly increased concentrations of phenolic acids and flavonoids in different tree species [15]. Studies have been undertaken to understand the role of either increasing CO₂ or temperature on secondary compounds including isoprene, terpenes, tannin, flavonol and/or phenolic production [16-20]. Lignin and tannin concentrations in trees have been shown to be increased by high CO₂ levels [4,21].

Studies on the effects of high temperature and enriched CO₂ on phenolic composition of three deciduous tree species revealed that the level of total phenolic compounds decreased under high temperature but increased under enriched CO₂ [22]. Interestingly, there was no effect on phenolic compounds when high temperature and enriched CO₂ were combined [23]. Moreover, it has been reported that high temperature resulted in a significant decrease of apple peel anthocyanin concentration through modulation of the anthocyanin regulatory complex [24]. Albert et al. showed that increased phenolic composition of *Arnica montana* is associated with lower temperature [25]. Ultraviolet radiation (UV) is also influencing the production of different secondary metabolites such as phenolics, flavonoids, alkaloids, terpenoids, and glucosinolates [26]. UV-B radiation enhanced the rosmarinic and carnosic acids concentrations in rosemary plants [27]. Contents of peppermint flavonoids; eriocitrin, hesperidin, and kaempferol 7-O-rutinoside have been reported to be increased by UV-B induction [28]. UV-A and UV-B radiation induction exhibited increased content of caffeoylquinic acids and iridoids in *Lonicera japonica* Thunb [29]. However, the effect of global climate change on PSM does not show any definitive trend and appear to be specific to plant species and environmental stress under study [30]. Detailed studies with focus on individual and combination of stresses will provide a clearer picture.

Importance of Metabolomics in Ensuring Food Security

Feeding the world by next 50-100 years is a great challenge for scientists and people involved in food and agriculture industry, and particularly the challenge is even more difficult keeping in mind the ever-increasing population and limited availability of agricultural land. Scientist from various fields, which include but are not limited

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to agriculture, breeding and biotechnology are putting their hands together to meet the challenge. Biotechnological interventions that utilize various OMICs approaches (e.g. genomics, transcriptomics, proteomics, metabolomics etc.) have an important role to play along with classical agricultural approaches. Next generation sequencing and other OMICs technologies has enabled to sequence large and complex genomes in very less time in a very precise manner. However, assigning function to such a large pool of genes is yet another challenging task. Post-genomic era depends heavily on many related technologies to bridge the information gap however, none delivers an effective route to assign exact function of genes. A number of post-transcriptional and post-translational modifications at gene and enzyme level are involved and therefore, none of the approach leads to the identification of genes with final outcome with regard to phenotypic traits. Metabolomics is the study of complete set of metabolites in a cell, organ or an individual and serves as an excellent tool to bridge the information gap [31]. It is accomplished by analytic tools such as gas-chromatography or liquid-chromatography and is comparatively cheaper, rapid and has wide range of applications than other OMICS approaches. Since metabolites are close to phenotype and are the actual representatives of any visible change, metabolomic profiling of crops, in response to climate change will provide useful insights into genetic mechanisms of plants adaptation. The information obtained from the systematic metabolomic studies on response of plants to climate change can be exploited to identify candidate genes responsible for conferring specific traits of stress tolerance. The identified stress induced metabolites can be mapped on the metabolic pathways to pinpoint their rate limiting catalytic enzymes. Further, the publically available genome databases are searched to identify respective genes of the rate limiting enzymes. These genes can be further exploited to alter or divert the metabolic flux of plants for increasing the production, nutrition versatility and/or the adaptive plasticity of the plants by means of either cis- or transgenic technologies. Different parameters of climate change studied alone and/or in combination, will provide significant information on metabolomic adjustments in response to environmental variables that can be used to prepare predictive models and interaction networks. This will help the scientific community and policy makers to design strategies to mitigate the adverse climatic effects. Especially it will be of great value for application in crop plants, wherein genes can be mapped in the quantitative trait loci (QTLs) [32], which further can be used for breeding programmes to mitigate the adverse effects of climate change. Since metabolites affect the complex organizations of ecosystems, it will help us predict the ecosystem organization in response to global climate change. Hence, there is a need to conduct systematic studies in order to get deeper insights and to develop a wholistic and rationale approach wherein, metabolomics can play a pivotal role.

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