Title:	Metabolomic studies of plant response to environmental cues and phytochemical analysis of medicinal plants using NMR spectroscopy
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Abstract: Metabolomics is the large-scale study of small molecules in cells, biofluids, tissues, or organisms. These small molecules are called metabolites. The most prevalent ap- proaches in the field of metabolomics are nuclear magnetic resonance (NMR) spec- troscopy and mass spectrometry (MS). These approaches are used to investigate the metabolic profile of a living organism. NMR spectroscopy is primarily used in thera- peutics, traditional medicine, environmental monitoring, the diagnosis of human dis- ease, and food quality management. This thesis discusses the applications of NMR-based metabolomics analysis to pro- vide a metabolic profile of phytomedicinal compounds in Momordica Charantia (Bitter melon), Phyllanthus emblica (Amla), and Tinospora cordifolia (Giloy). Various por- tions of the medicinal fruits have their own unique metabolic profile of beneficial min- erals, proteins, and vitamins, in addition to a wide variety of vital bioactive chemicals. The later part of the thesis focuses on the applications of NMR-based metabolomics to study the plant metabolome. These studies include several elements of plant physiol- ogy, such as circadian rhythm, stress metabolism, and plants signaling. The last part of the thesis highlights the importance of NMR-based metabolomics in understanding several facets of insect physiology, including the evolution of insect immune response. The main objective is to obtain an understanding of the metabolic pathway that ulti- mately result in a series of chemical reactions occurring within a cell. The contents of the chapters of the thesis are briefly described below. Chapter 1 The introductory chapter briefly introduces the basics of NMR spectroscopy, the var- ious analytical techniques used for metabolomics and the role of metabolomics in i0. Abstract system biology. The chapter also provides details about NMR pulse sequences, pre- processing of raw spectral data, univariate and multivariate statistical methods used in metabolomics. Chapter 2 This chapter discusses the use of NMR in the analysis of phytomedicinal compounds identified in the pericarp, skin, and seeds of Momordica charantia (bitter melon). The Momordica charantia plant has a long history of usage as a medicinal plant, and has been included in a variety of different traditional medical systems. A multivari- ate statistical analysis revealed that the metabolic profiles of the seeds and pericarp were grouped together, and that these two groups were clearly differentiated from the metabolic profile of the skin part of Momordica charantia. A few phytosterols such as charantin and momordicine were identified which are known to correlate with antidia- betic action. Chapter 3 This chapter details the metabolomic profiles of phytomedicinal compounds in Phyllanthus emblica and Tinospora cordifolia using one- and two-dimensional NMR spectroscopy. Phyllanthus emblica is an Ayurvedic herb which is used as a medication and tonic to restore vitality. Tinospora cordifolia has long been recognized as an important herb in traditional Ayurvedic medicine, where it has been utilized for the treatment of a wide range of conditions, including fever, diarrhoea, cancer and eye disorders. In this study, 1 H NMR spectroscopy coupled with multivariate statistical data analysis such as principal component analysis (PCA) was applied to investigate metabolomic variations among Phyllanthus emblica raw fruits and juice ((procured from Patanjali Ayurveda). The assignments of primary and secondary metabolites in Phyllanthus emblica fruit and Tinospora cordifolia stem have been carried out making use of 1 H and 2D NMR (1 H- 1 H COSY, 1 H- 1 H TOCSY, 1 H- 13 C HSQC) spectroscopy. Chapter 4 This chapter focuses on the utility of NMR-based metabolomics for metabolite profil- ing. The in vivo metabolic profile was constructed from the stems of young Helianthus iiannuus L. (sunflower) during the circadian cycle. This metabolic profile reveals metabo- lites and the functional periodicity of the circadian rhythm that they exhibit. One- and two-dimensional NMR spectroscopy methods were used to profile various metabo- lites, including sugars, amino acids, and tri-carboxylic acid (TCA) intermediates, of the immature sunflower stems. Chapter 5 This chapter highlights the utility of NMR-based methods in studying plant metabolite response to air pollution stress. We used one- and two-dimensional NMR spectroscopy to perform metabolite fingerprinting on the leaves of Bougainvillea spectabilis, which is a plant that is known to be tolerant to different types of abiotic stresses. It was observed a few metabolites exhibit a consistent rhythmic pattern throughout the circa- dian cycle, which is evidence that circadian rhythms have a significant impact on the metabolic processes that occur in plants. Chapter 6 This chapter emphasizes the utility of NMR-based metabolomics to study plant re- sponse against wounding stress. NMR metabolomic methods were used to study the metabolic alterations that occurred in the leaves of the Bougainvillea spectabilis plant following a wounding treatment that was designed to simulate a herbivore attack. It was observed that the content of amino acids, carbohydrates, and a few secondary metabolites varied in wounded plants. Chapter 7 This chapter describes the application of NMR-based metabolomics approaches to the study of evolution in the fruit fly Drosophila melanogaster at different ages. Metabolic variations between a fly population chosen for increased immunity and the control pop- ulation, reveal that populations develop diverse metabolomes in response to selection at three different ages namely young (5 days old), middle (20 days old) and old (35 days old) aged flies. Also, the metabolic response to prick injury/infection was exam- ined between immune-selected and control populations. It was noted that the immune iii0. Abstract selected population continues to be able to mount a stronger immune response to prick injury/infection even after it matures in age. Chapter 8 In the last chapter, a summary of all the studies that were carried out and the conclu- sions that were made from those

	research is presented. In addition to this, the chapter contains some observations about the role that NMR-based metabolomics will play in different disciplines.
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