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TOWARDS SEPARATION OF TEN THOUSAND COMPOUNDS WITH COMPREHENSIVE MULTIDIMENSIONAL GAS

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Multidimensional gas chromatography (MDGC) is a high-performance separation technique with enhanced peak capacity for analysis of multi-component samples such as petroleum, essential oils, food, beverages, pharmaceutical and environmental. Hyphenation with mass spectrometry (MS) provides high confidence identification of several hundred volatiles within a single analysis. In this presentation, experimental design, instrumental and data analysis approaches in MDGC-MS comprising a range of comprehensive multiple heart-cut (H/C) and comprehensive two-dimensional GC (GCXGC) techniques will be demonstrated. A special focus is on the system employing a micro fluidic device called Deans Switch to perform comprehensive H/C MDGC with different H/C windows and number of injections. Data analysis approaches will be presented so that the experimental results can be represented as contour plots and evaluated according to peak capacity and the number of separated peaks. To this end, the 'continuum in MDGC' technology can be established via plots of analysis time vs separation performance. It will also be illustrated that this simple system can offer up to 10,000 analyte peak capacity which is ~10 times compared with that provided by conventional GC×GC. This work describes a proof of theoretical concept with simple configuration for effective practical application, making valuable contribution to high resolution chromatography research.

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LC-MS/MS BASED PHYTOCHEMICAL FINGERPRINTING OF MALAYSIAN HERBS

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Majority of Malaysians apply herbs or herbal products in their daily life, solely based on the traditional knowledge and practices. Many herbal products have recently been developed and promoted in the market for the convenience of consumers to enhance their overall well-being. This includes *Eurycoma longifolia* (King of herb), *Labisia pumila* (Queen of herb) and other popular herbs such as *Orthosiphon aristatus*, *Andrographis paniculata* and *Ficus deltoidea*. The functionality of the herbal products is strongly related to their phytochemicals which are very complex in nature. Therefore, it is important to have an unbiased and reliable technique to identify or authenticate the products, especially those products with functional claims. Phytochemical fingerprinting using the hyphenated technique of LC-MS/MS is suggested to be a comprehensive analytical platform because it is sensitive enough even for trace quantity of phytochemicals. Phytochemicals are secondary metabolites which usually possess certain biological functions in the defense mechanism of plants. This explains the ethnopharmacological properties of herbal plants. The complex mixture of plant samples is separated by liquid chromatography, and individually flowed into mass spectrometer for ionization and detection. Huge dataset that are generated during fingerprinting could be statistically analyzed using chemometric tools for sample classification and identification. High performance and unsupervised multivariate data analysis techniques such as principal component analysis, hierarchical clustering analysis and heat mapping are the common pattern recognition tools for quality control and standardization of herbal samples. Therefore, phytochemical fingerprinting coupled with chemometrics is a reliable technique to describe the entirety of phenotypes for quality control and quality assurance of herbal samples.

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QSAR AND MOLECULAR MODELING STUDIES ON CALCIUM CHANNEL BLOCKERS: A COMPREHENSIVE NOTE

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Calcium channel blockers (CCBs) have got potential therapeutic uses against several cardiovascular and non-cardiovascular diseases, such as angina, hypertension, arrhythmias, asthma, dysmenorrhea, premature labor, cancer, epilepsy, glaucoma etc. The three principal structural classes of compounds have been found to act as potent calcium channel blockers and they are phenylalkylamines, 1, 4-dihydropyridines (DHPs) and benzodiazepines. Recently, a few more classes of CCBs have been studied. All these classes of CCBs have been found to be the most effective drugs against vasospastic angina. These drugs selectively inhibit Ca^{2+} influx into heart muscles by blocking slow inward channels for Ca^{2+} or inhibit Ca^{2+} influx into vascular smooth muscles. The result is negative inotropism of smooth muscle relaxation, which is translated into hypotension. Author intend to present a comprehensive review, including the most recent studies, on quantitative structure-activity relationship (QSAR) and molecular modeling studies on all kinds of CCBs. These studies lead to highlight the essential structural features and physicochemical properties that the compounds should possess to act as potential CCBs. These studies also describe vividly the mechanism of interaction of CCBs with the calcium channel. These studies provide the ways to find new more potent calcium channel blockers to be therapeutically more useful.