

IDENTIFICATION AND QUANTIFICATION OF GLUCOSINOLATES IN PLANT MATERIAL BY ESI (-) VE ION LC-ION TRAP MASS SPECTROMETRY-A NOVEL FRAGMENTATION

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Glucosinolates, a class of phytochemical found in the Brassica and Cruciferae plant families, have a diverse range of properties. For example, glucoraphanin, which is present in broccoli, breaks down to produce sulforaphane which exhibits anti-cancer properties, and sinigrin breaks down to produce the characteristic taste in mustard seed. Other glucosinolates, eg progoitrin, are toxic when ingested in high levels. Therefore it is important to be able to identify and accurately measure the levels of these compounds in plant products. Methodologies used to determine the glucosinolate content of plants and seeds include measuring the glucosinolates' enzyme breakdown products and the desulphated glucosinolates and intact glucosinolates by LC-UV detection. However, these methods are either non-specific or time consuming. LC-mass spectrometry offers the advantages speed, simplicity, sensitivity and accuracy for the analysis of bioactive compounds in complex matrices. Plant and seed extracts containing a number of commonly occurring glucosinolates were assayed by ESI (-) ve ion LC-ion trap ms. All glucosinolates gave a strong molecular ion and ms^{2/3} fragmentation of this ion produced a common ion at m/z 259, irrespective of the parent compound. These two ions can then be used to screen for and quantify the levels of the glucosinolates present in sample extracts. Examples will be given for the identification and determination of glucoraphanin in broccoli florets and sinigrin in mustard seeds.