

Title Green pigment in crushed garlic (*Allium sativum* L.) cloves: purification and partial characterization

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Abstract

Unknown green pigments, responsible for greening in crushed garlic, were purified using column chromatography in series, and identified using liquid chromatography - electrospray ionization (LC-ESI), matrix assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectrometry (MS), and magnetic nuclear resonance (NMR) spectroscopy (C^{13} , H^1 , DEPT 135, COSY, TOCSY, HMBC, HMQC). Green pigment extracted from crushed garlic showed two maxima of absorbance at 440 and 590 nm. LC-ESI and MALDI-TOF MS suggested that the green pigment had a molecular weight (MW.) A molecular ion with a peak at m/z 412 was the compound that resulted in greening. Complete isolation of the compound was not achieved under the chromatographic conditions examined and hence the proper structure was not elucidated. However this compound consisted of one sulfur atom and one or three nitrogen atoms, and 25 to 30 carbon atoms. The presence of methyl and carbonyl groups, alcoholic carbons, and an aromatic ring in the compound could be inferred from the C^{13} spectrum of NMR spectroscopy. The observed values for an aromatic ring were 137.6, 130.0, 126.2, and 128.2 ppm, which indicate that these substituents are related to aromatic ring in the meta position. The carbonyl carbon does not appear in the DEPT spectrum indicating that it has no attached hydrogen atoms.