

Title: Structural elucidation of tannins of spent coffee grounds by CP-MAS C-13 NMR and MALDI-TOF MS

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Abstract: In this study, carbon-13 nuclear magnetic resonance in the solid state using cross-polarization and magic angle spinning (CP-MAS ¹³C NMR) spectroscopic and matrix-assisted laser desorption ionization-time of flight (MALDI-TOF) mass spectrometric methods were applied to characterize the composition, constituent monomer and oligomeric structure of tannins of spent coffee grounds (SCG). The findings elucidated that the monomeric constituents of tannins of SCG primarily composed of catechin, gallic acid, chebulic acid, gallic acid-3-O-gallate and accompanied by minor amount of fisetinidin concurrently. Appreciable amount of catechin was found among the observed components. Hence, this simply implied that catechin was the main substructure of the tannins of SCG. It is expected that the present findings will serve as a platform towards a structural understanding of tannins of SCG in filling up the gaps in the field of study of SCG, and simultaneously promoting the use of SCG as a renewable resource for tannins.