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SCHOOL OF MATHEMATICAL AND NATURAL SCIENCES

DEPARTMENT OF CHEMISTRY

A study of the chemical components of extracts from *Kirkia wilmsii* and an investigation into their properties.

MSc Research Project Dissertation

By

K. Chigayo Student No. 11592848

Handwritten signature of K. Chigayo.

Supervisor: Mr Paul E. L. Mojapelo (University of Venda)

Handwritten signature of Mr Paul E. L. Mojapelo.

Co-supervisor: Prof. Luke Chimuka (Wits University)

Handwritten signature of Prof. Luke Chimuka.

Co-supervisor: Prof. Pascal O. Bessong (University of Venda)

Handwritten signature of Prof. Pascal O. Bessong.

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Abstract

Aqueous extraction was performed on the plant *Kirkia wilmsii* roots at room temperature. The extracts were filtered and stored at 4 °C. An analytical high performance liquid chromatographic (HPLC) method was developed for determination of the components of *Kirkia wilmsii* roots. A gradient elution programme was developed that employed two mobile phases. Mobile phase A water while the pH was adjusted with trifluoroacetic acid (TFA). Mobile phase B was organic, made up of acetonitrile, where the pH was also adjusted with TFA. A C18 column and a photo diode array (PDA) detector were used. Flow rate was changed continuously during the run, to ensure the best resolution of the peaks. The resolved peaks were then collected into different containers using the fraction collector on the HPLC. The peaks that were chosen for this research were those at 16.7, 20.3, 28.2, 31.5, 40.4, 50.1, 56.5 and 64.2 mins. Collected components were then freeze dried as opposed to using a rotary evaporator, to avoid heating samples whose chemical properties were not yet known. The net dry weight of each component was determined.

The purity of the components was checked by gas chromatography (GC), where each component was dissolved in acetone and then run on the GC.

Electrochemical properties of the components were investigated using cyclic voltammetry and anti-oxidant properties were exhibited by four components. All four components showed that they could undergo reversible reactions. The I_{pc} , E_{pc} , I_{pa} , E_{pa} , E , ΔE_p , I_{pc}/I_{pa} and the number of electrons involved in the process for each component were calculated.

Possible structures of bioactive compounds were identified using Gas Chromatography – Mass Spectrometry (GC-MS). These results indicated the possible structure of the isolated compounds. Compound 1 contained triphenylphosphine oxide, (carbethoxymethyl)-triphenylphosphonium bromide or formaldehyde, triphenylphosphoranylidene) hydrazone. Compound 5 was made up of diisooctyl phthalate, phthalic acid, di(2-propylpentyl) ester or phthalic acid octyl 2-propylpentyl ester. Compound 7 contained 1,2,3-benzenetriol, 1,2,4-benzenetriol or 3-methyl-pyrazole-5-carboxylic acid, while compound 8 contained catechol, resorcinol or hydroquinone.

All the components analysed by GC-MS showed possible structures that have functional groups that can undergo reversible reactions. This was confirmed by the cyclic voltammetric results.