EXTRACTION, ISOLATION AND STRUCTURAL DETERMINATION OF ORGANIC COMPOUNDS FROM *SCAEVOLA SPINESCENS* R.Br.

A thesis submitted towards a

Doctor of Philosophy

by

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ABSTRACT

The aim of this project was to extract, isolate and determine the structure of organic compounds from *Scaevola spinescens*, which is found widely in the arid to semi-arid regions of South Australia and through into most other states of Australia.

Scaevola spinescens is an Australian native plant that the Aboriginal people of Hawker in South Australia have traditionally used as a natural medicine to treat a variety of symptoms. There is much anecdotal evidence that indicates that *Scaevola spinescens* is a useful plant in traditional medicine.

Seventeen organic compounds were isolated and their structures elucidated by spectroscopic methods. Four further compounds were isolated but have not been completely identified.

The compounds isolated include triterpenes, iridoids, coumarins, flavonoids and other compounds.

Four novel compounds were isolated. They were:

- judarrylol, a triterpene
- emmarin, a coumarin
- alilydijosioside, an iridoid, which may be an artefact of the extraction process
- katecateroside, an iridoid

Of the seventeen organic compounds isolated, four were novel, fifteen were new to *Scaevola spinescens* and thirteen had not been reported from any plant from any species of *Scaevola*.

A table of the compounds (**Table A.1**) isolated and their structures are illustrated below.

All crude extracts were first tested with Meyers reagent (a test for alkaloids) with no positive results recorded.

The structures were deduced from MS data as well as routine and 2D NMR experiments, apart from (**95**) which was derived solely from GC/MS data.

Table A.1 : Compounds isolated from *Scaevola spinescens*

Compound	Novel	New to *Scaevola spinescens*	New to *Scaevola* genera
Hexadecanoic acid, methyl ester (**95**)		*	*
Taraxerol acetate (**92**)			
Taraxerol (**73**)			
Judarrylol (**96**)	*	*	*
Ursolic acid (**97**)		*	*
Emmarin (**98**)	*	*	*
Vanillic acid(**99**)		*	*
Daucesterol (**100**)		*	*
Alidyjosioside (**108**)	*	*	*
Scaevoloside (**6**)		*	
Katecateroside (**109**)	*	*	*
Loganin (**5**)		*	
Luteolin-7-*O*-glucuronide methyl ester (**110**)		*	*
2-C-(Hydroxymethyl)-D-ribonic acid-γ-lactone (**111**)		*	*
L-*threo*-Guaiacyl glycerol (112)		*	*
Luteolin-7-*O*- glycoside (**113**)		*	*
2-Deoxy-D-*chiro*-inositol(**114**)		*	*

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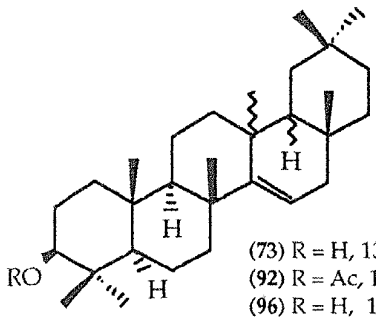
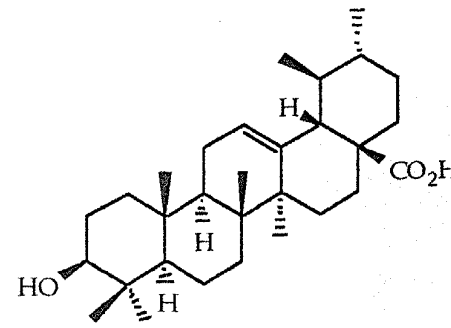


(**73**) R = H, 13α-CH_3, 18β-H
(**92**) R = Ac, 13α-CH_3, 18β-H
(**96**) R = H, 13β-CH_3, 18α-H



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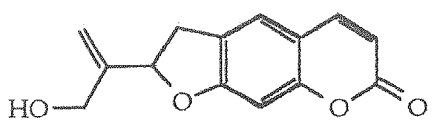

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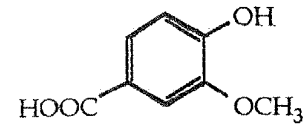

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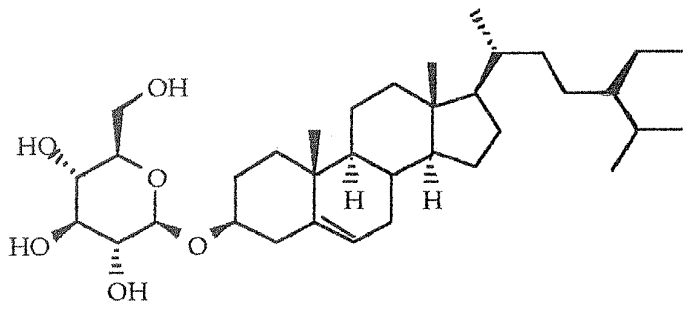

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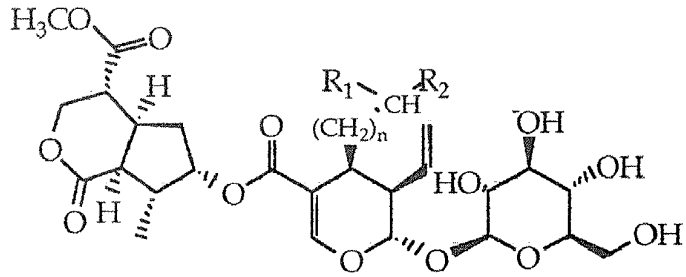
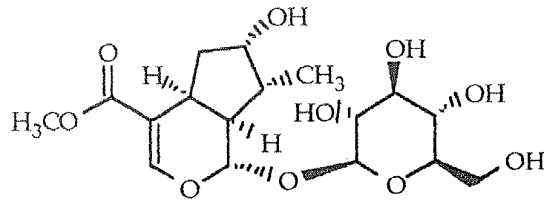


(6) R_1, R_2 = O, n = 1
(108) $R_1 = R_2 = OCH_3$
(109) R_1, R_2 = O, n = 2



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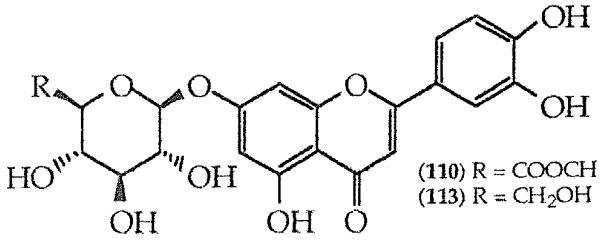
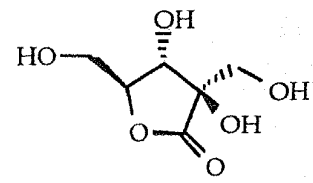


(110) R = $COOCH_3$
(113) R = CH_2OH



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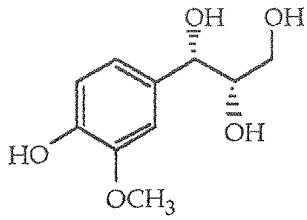

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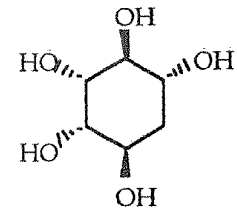

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A range of biological tests were carried out on both crude extracts, semi - purified fractions and certain isolated and purified compounds, as outlined in Chapter 11.

Crude Fractions 4, 8 and 9 showed moderate anti bacterial activity.

One novel coumarin - emmarin (**98**) - and vanillic acid (**99**) were isolated from Fraction 4.

The four iridoids - loganin (**5**), scaevoloside (**6**) alidyjosioside (**108**) and katecateroside (**109**) - were isolated from Fraction 8.

Luteolin-7-*O*-glucuronic acid methyl ester (**110**), 2-C-(hydroxymethyl)-D-ribonic acid-γ-lactone (**111**) and L-*threo*-guaiacyl glycerol (**112**) were isolated from Fraction 9.

These compounds need to be tested to determine whether they have anti bacterial activity.

The initial cytotoxicity test used - Procedure A - indicated a massive stimulatory effect at high concentrations of the more polar extracts on three cancer cell lines, while at lower concentrations there was some inhibition of growth. However these results could not be reproduced. Other cytotoxicity tests were inconclusive.

The anti viral tests showed no activity.