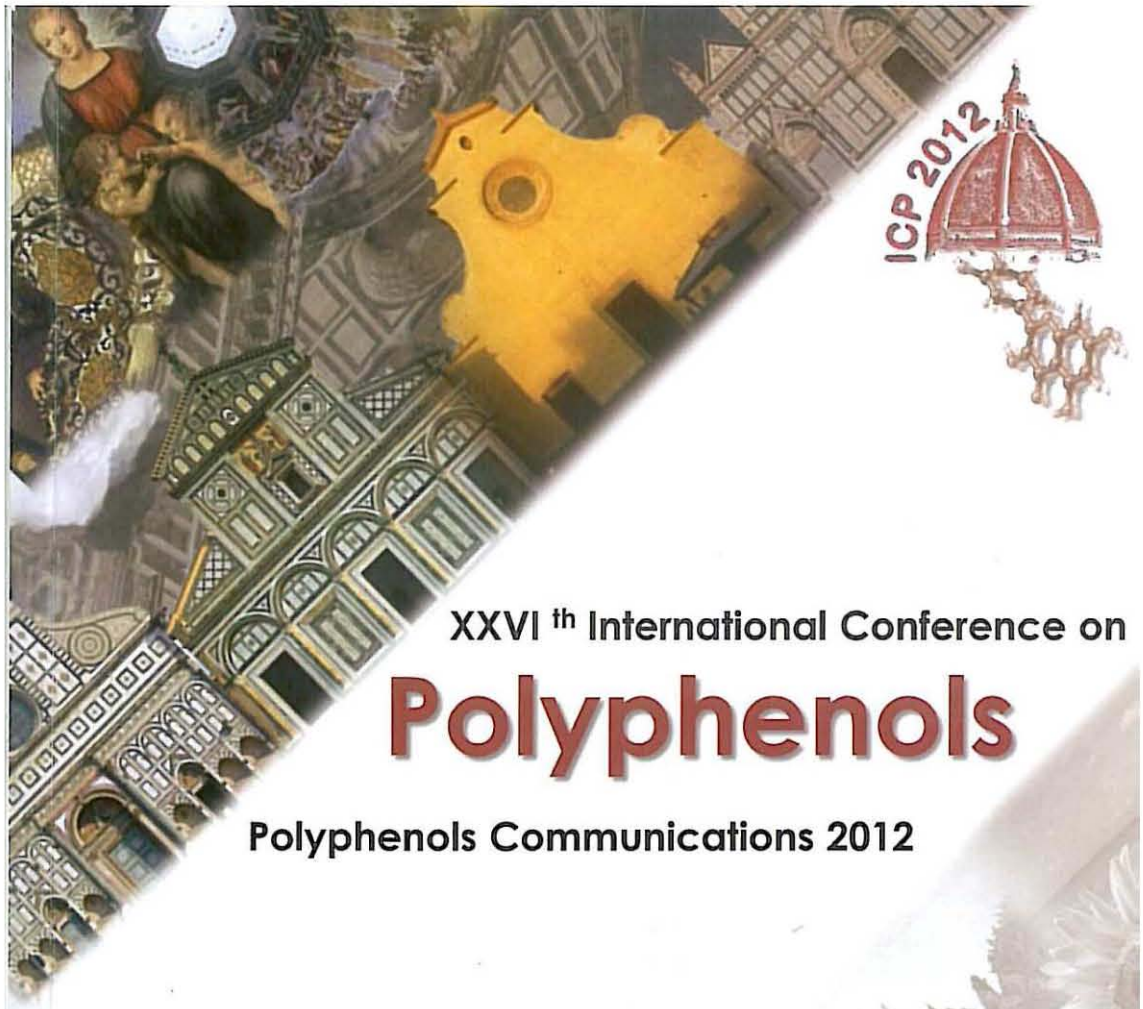

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Phenylethanoids and isoscutellarein derivatives from *Lamium album* L.

Olívia R. Pereira[1,2], Maria R.M. Domingues[3], Artur M. S. Silva[3], Susana M. Cardoso[1,4]*

[1]CERNAS - Escola Superior Agrária, Instituto Politécnico de Coimbra, Bencanta, 3040-316 Coimbra, Portugal; [2]Departamento de Tecnologias de Diagnóstico e Terapêutica, Escola Superior de Saúde, Instituto Politécnico de Bragança, Av. D. Afonso V, 5300-121 Bragança, Portugal; [3]Departamento de Química & QOPNA, Universidade de Aveiro, 3810-193 Aveiro, Portugal; [4]CIMO - Escola Superior Agrária, Instituto Politécnico de Bragança, Campus de Santa Apolónia - Apartado 1038 - 5301-854, Bragança, Portugal
*corresponding author: scardoso@esac.pt

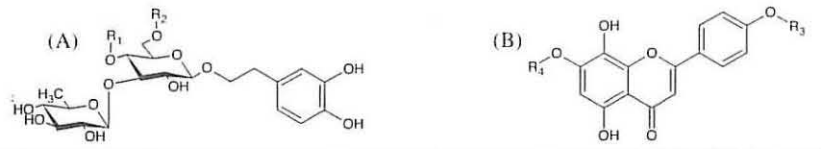
Abstract. *Lamium album* L., a plant commonly known as white dead nettle, has been used in folk medicine in the treatment of several ailments. Some of their benefitial properties are closely related to its phenolic content, however the exact polyphenolic composition is far from being understood. In this context, the present work aims to determine the phenolic composition of an ethanolic extract of *L. album* using high performance liquid chromatography with diode array detection, electrospray mass spectrometry and nuclear magnetic resonance techniques.
The phenolic extract of *L. album* was mainly composed by the phenylethanoid verbascoside and its isomer isoverbascoside. Still, it also contained significant amounts of isoscutellarein derivatives, which were herein detected for the first time in the genus *Lamium*. As isoscutellarein derivatives appear as major components of *Lamium Album* L., it is feasible that they can be correlated to the beneficial human health properties of this plant.

Introduction. Plants have been studied as a source of natural antioxidants because of their association to beneficial activities for human health. *Lamium album* L. is a perennial herb which is famous due to its antioxidant, antispasmodic and mucolytic, diuretic, astringent and anti-septic activities. Additionally, its aerial parts are often used in the treatment of menorrhagia, uterine hemorrhage, vaginal and cervical inflammation, leucorrhoea, wound healing and skin problems because of its haemostatic and anti-inflammatory activities. The effects of *Lamium Album* L. have been associated to its phenolic portion [1]. The phenolic compounds already described in this *Lamium* species include flavonols (quercetin, quercetin-3-*O*-glucoside, rutin, isoquercitrin, kaempferol-3-*O*-glucoside and tiliroside), phenolic acids (protocatechuic, chlorogenic, vanillic and caffeic acids) and phenylpropanoid glycosides ester derivatives (lamalboside, acteoside and isoacteoside) [1,2].

Materials and Methods. An enrich phenolic extract of *L. album* was obtained by extraction with an aqueous ethanolic mixture (80:20) (v/v) and further purification on C18 cartridges. In order to determine the exact phenolic profile of the plant, this extract was fractionated by reversed-phase high performance liquid chromatography (HPLC) and the phenolic compounds of each fraction were further identified with HPLC-DAD, combined with data obtained from off line HPLC electrospray mass spectrometry (ESI-MS) and MS^n according the method described by Pereira *et al* [3]. The HPLC analysis was performed on a RP-C18 column 250 mm× 4 mm id, 5μm bead diameter (temperature of 30ºC, flow rate of 1 mL/min). The mobile phase comprised (A) 0.1% formic acid in water and (B) acetonitrile. HPLC- collected fractions were directly injected into the ESI source by means of a syringe pump, at a flow rate of 8 μL min^{-1}. Studies were performed in the negative mode using a Linear Ion trap LXQ (ThermoFinnigan, San Jose, CA, USA) [4]. The structure of the main fraction was confirmed by ^1H and ^{13}C nuclear magnetic resonance (NMR) spectroscopy. The quantification of the main phenolic compounds of the ethanolic extract was achieved by the external standard method.

Results and Discussion. The quantified phenolic compounds in the purified ethanolic extract of aerial parts of *L. album* accounted for 550.7±50.0 mg/g of extract. These mainly includes the two phenylethanoids verbascoside (233.7±13.6 mg/g of extract) and isobervascoside (39.2±5.6 mg/g of extract). Also, derivatives of the unusual flavone isoscutellarein represented

approximately one third of the total phenolics quantified (27%). The isoscutellarein derivatives (Fig.1) included isoscutellarein-7-*O*-allosyl(1→2)glucoside, its *O*-methyl derivative, three acetyl derivatives of isoscutellarein-*O*-allosyl glucoside and one acetylated form of *O*-methylisoscutellarein-7-*O*-allosyl(1→2)glucoside. Additionally, the main isoscutellarein derivative (37.4±4.4 mg/g of extract) was assigned to isoscutellarein-7-*O*-(6-*O*-acetyl-β-allosyl)(1→2)-β-glucoside and its structure was corroborated by NMR data. Besides these compounds, the ethanolic extract of *L. album* contained glycosyl derivatives of common flavones apigenin and luteolin and the flavanone naringenin. Overall, this work is an important contribution for the chemical characterization of *L. album*, also reporting new compounds in the genus *Lamium*. Attending that verbascoside and isoscutellarein derivatives are the main components of *L. album* ethanolic extract, and also that these compounds have been demonstrated to possess important biological activities [5,6], it is possible that they are associated to the health benefits of this plant.



	R_1	R_2	R_3	R_4	
Verbascoside	Caff	H			
Isoverbascoside	H	Caff			
			H	Allo-Glc	Isoscutellarein-7-*O*-allosyl(1→2)glucoside
			H	Allo-Glc	Isoscutellarein-7-*O*-allosyl(1→2)glucoside
			H	Ac-Allo-Glc	Isoscutellarein-7-*O*-(6-*O*-acetyl allosyl)(1→2)glucoside
			Me	Allo-Glc	4'-*O*-Methylisoscutellarein-7-*O*-allosyl(1→2)glucoside
			Me	Ac-Allo-Glc	4'-*O*-Methylisoscutellarein-7-*O*-(6-*O*-acetylallosyl)(1→2)glucoside

Fig. 1. Structures of verbascoside and isoverbascoside (A) and isoscutellarein derivatives (B) found in purified extract of *Lamium album* L..

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