

Leaves and Spiny Burs of *Castanea Sativa* from an Experimental Chestnut Grove: Metabolomic Analysis and Anti-neuroinflammatory Activity

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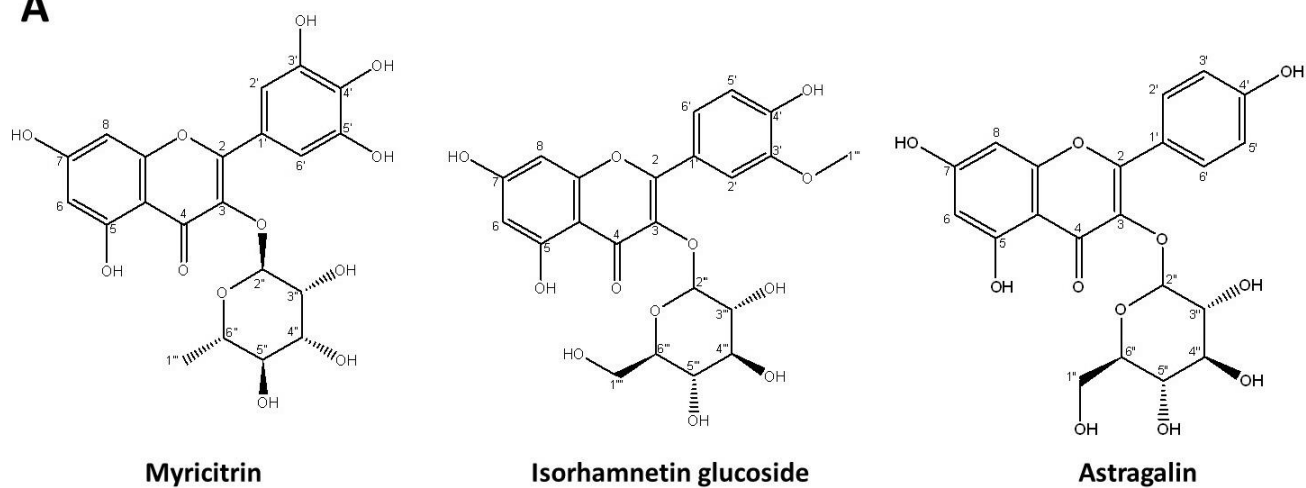
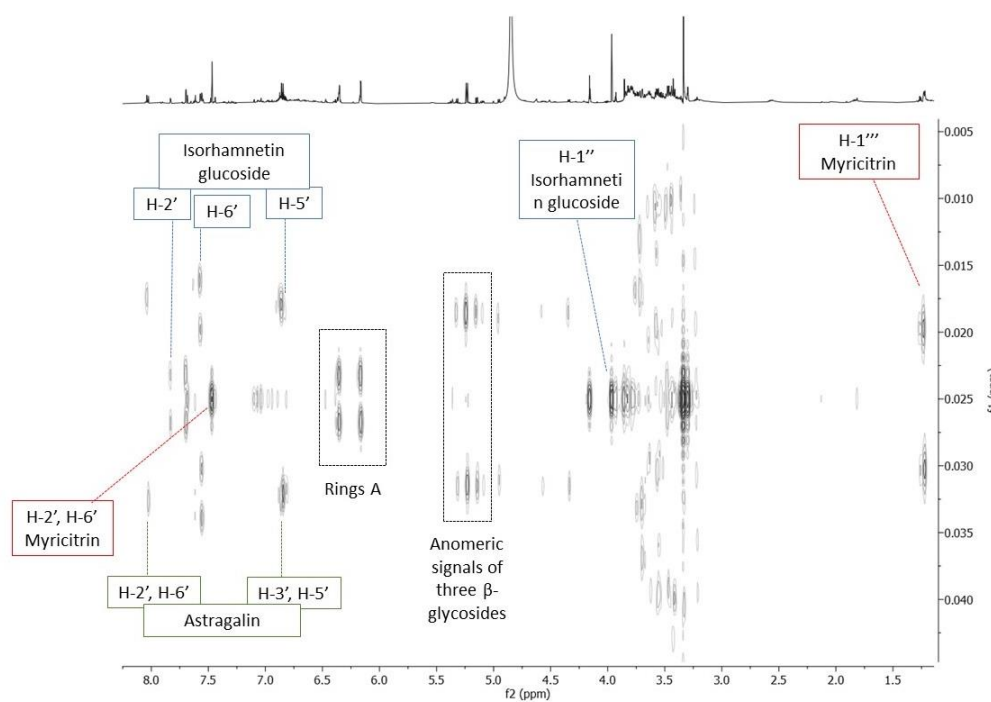
A**B**

Figure 1. Structure of the main flavonoids identified in *Castanea* extracts (A) and assigned J-res spectrum of the fraction in which they were contained (B).

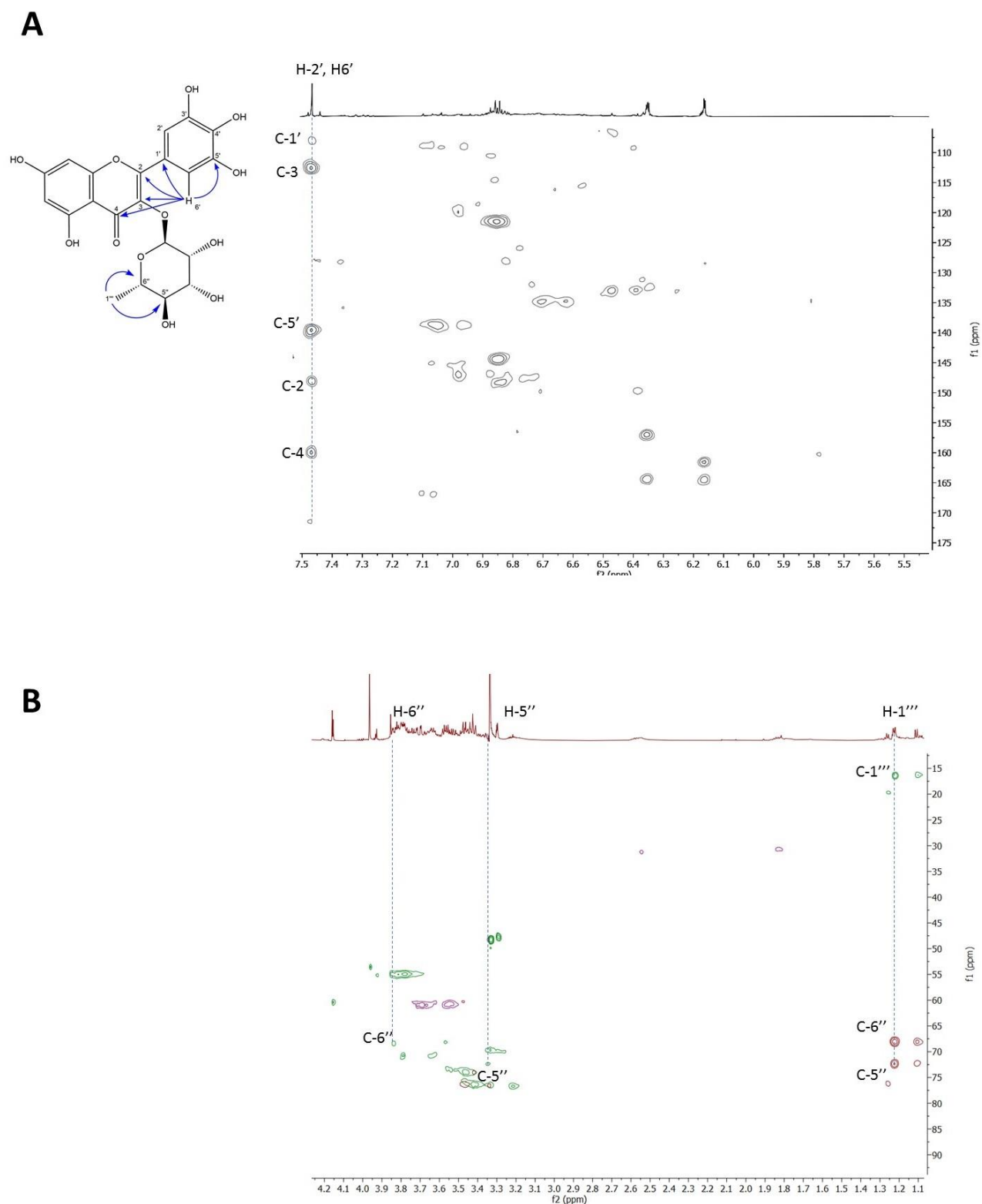


Figure 2. HMBC spectrum highlighting diagnostic ^{13}C - ^{13}C correlations of myricitrin (A). Superimposed spectra HSQC (green and purple dots) and HMBC (red dots) highlighting other important correlations to detect myricitrin in the analyzed fraction.

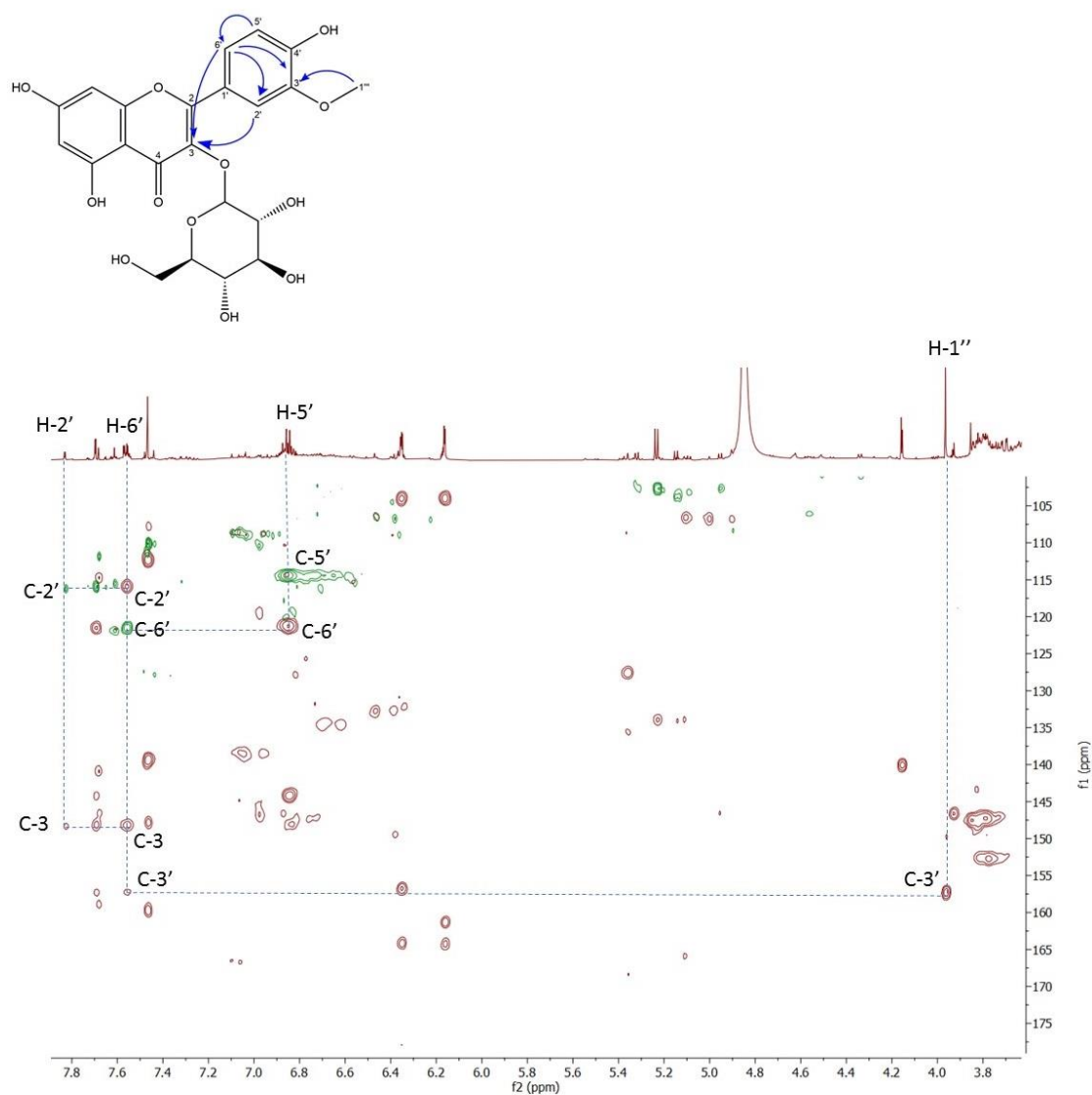


Figure 3. Superimposed HMBC (red dots) and HSQC (green dots) spectra highlighting diagnostic correlations of isorhamnetin glucoside.

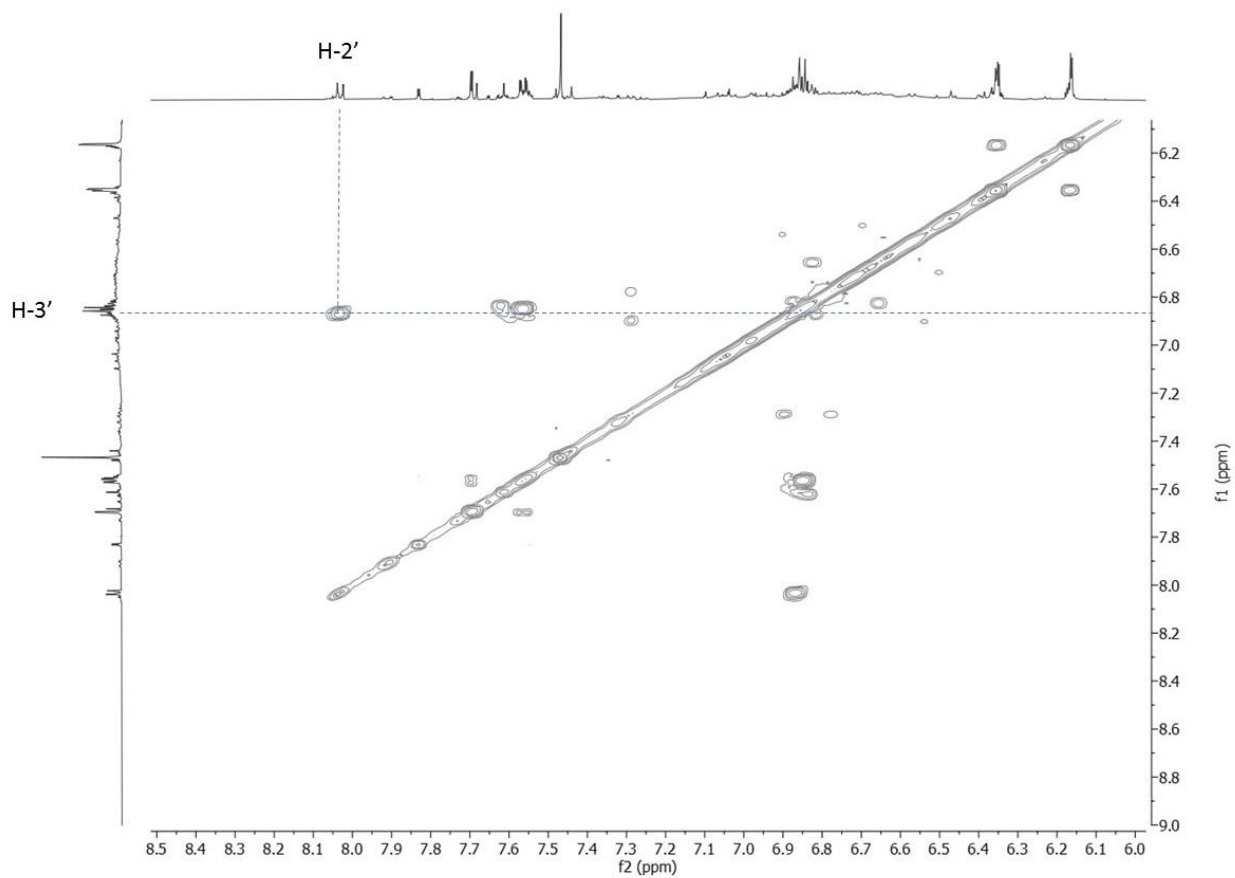


Figure 4. COSY spectrum of the flavonoids containing fraction in which it is highlighted the characteristic correlation between the protons of the B ring.

Compound	Position	¹ H (δ)	¹³ C (δ)
Astragalin	1'		121.14
	2', 6'	8.03 (d, J=8.95 Hz)	130.76
	3', 5'	6.87 (d, J=8.95 Hz)	114.13
	4'		159.95
Isorhamnetin glucoside	2'	7.69 (d, J=2.17 Hz)	115.96
	3'		157.44
	4'		148.12
	5'	6.85 (d, J=8.48 Hz)	114.39
	6'	7.56 (dd, J=2.17, 8.48 Hz)	121.51
	OCH ₃	3.91 (s)	53.58
Myricitrin	1'		112.4
	2', 6'	7.46 (s)	110.29
	3', 5'		147.73
	4'		139.36

Table 1. NMR references for flavonoids identified in *Castanea sativa* leaves extract.