

Supplementary Materials: Bio-Guided Isolation of Methanol Soluble Metabolites of Common Spruce (*Picea abies*) Bark by-Products and Investigation of Their Dermo-Cosmetic Properties

Apostolis Angelis, Jane Hubert, Nektarios Aligiannis, Rozalia Michalea, Amin Abedini, Jean-Marc Nuzillard, Sophie C. Gangloff, Alexios-Leandros Skaltsounis and Jean-Hugues Renault

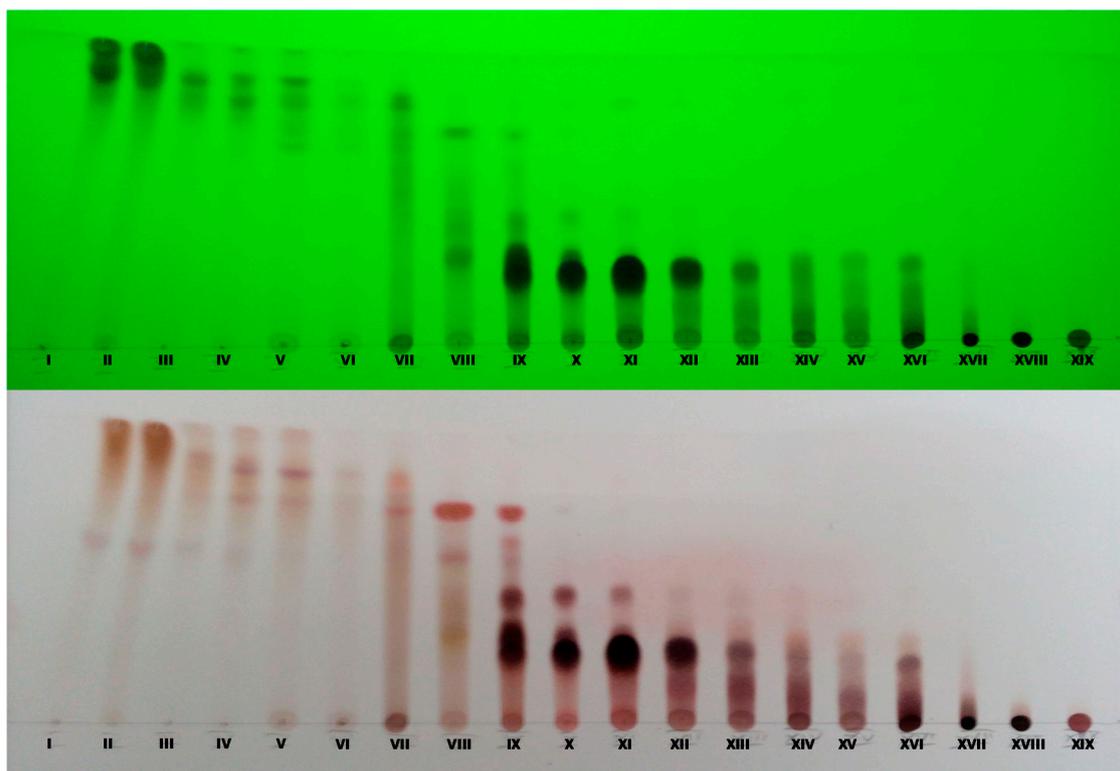


Figure S1. TLC chromatogram of the compared CPC fractions under UV lamb (254 nm **top**) and after spray with vanillin/H₂SO₄/MeOH solution and heating (**below**).

Table S1. The weights and chemical composition of CPC fractions of *P. abies* bark extract.

Fractions	Weight (mg)	Chemical Composition	Fractions	Weight (mg)	Chemical Composition
I	65	Comp1/FC	XI	420	Comp8(M)/Comp9
II	210	Comp1/FC	XII	90	Comp8(M)/Comp9
III	10	Comp2/AD/FC	XIII	75	Comp8/Comp 9/Comp 10
IV	10	Comp2/Comp3/UFA	XIV	45	Comp10/Comp 11/Comp 12
V	13	Comp3/ UFA	XV	40	Comp10/Comp 11/Comp 12/Comp 13
VI	18	UFA	XVI	120	Comp 12/Comp13/Comp14/Tannins
VII	80	Comp4 (M)/ Comp5/MC	XVII	900	Comp14/Tannins(M)
VIII	90	Comp4/Comp5 (M)/MC	XVIII	300	Comp14 + Tannins(M)
IX	225	Comp6/ Comp7/ Comp8	XIX	30	Tannins
X	425	Comp7/Comp8(M) /Comp9			

FC = Fatty compounds, AD = Abietane diterpenes, UFA = Unsaturated Fatty Acid, MC = Minor Compounds, (M) = major compound.

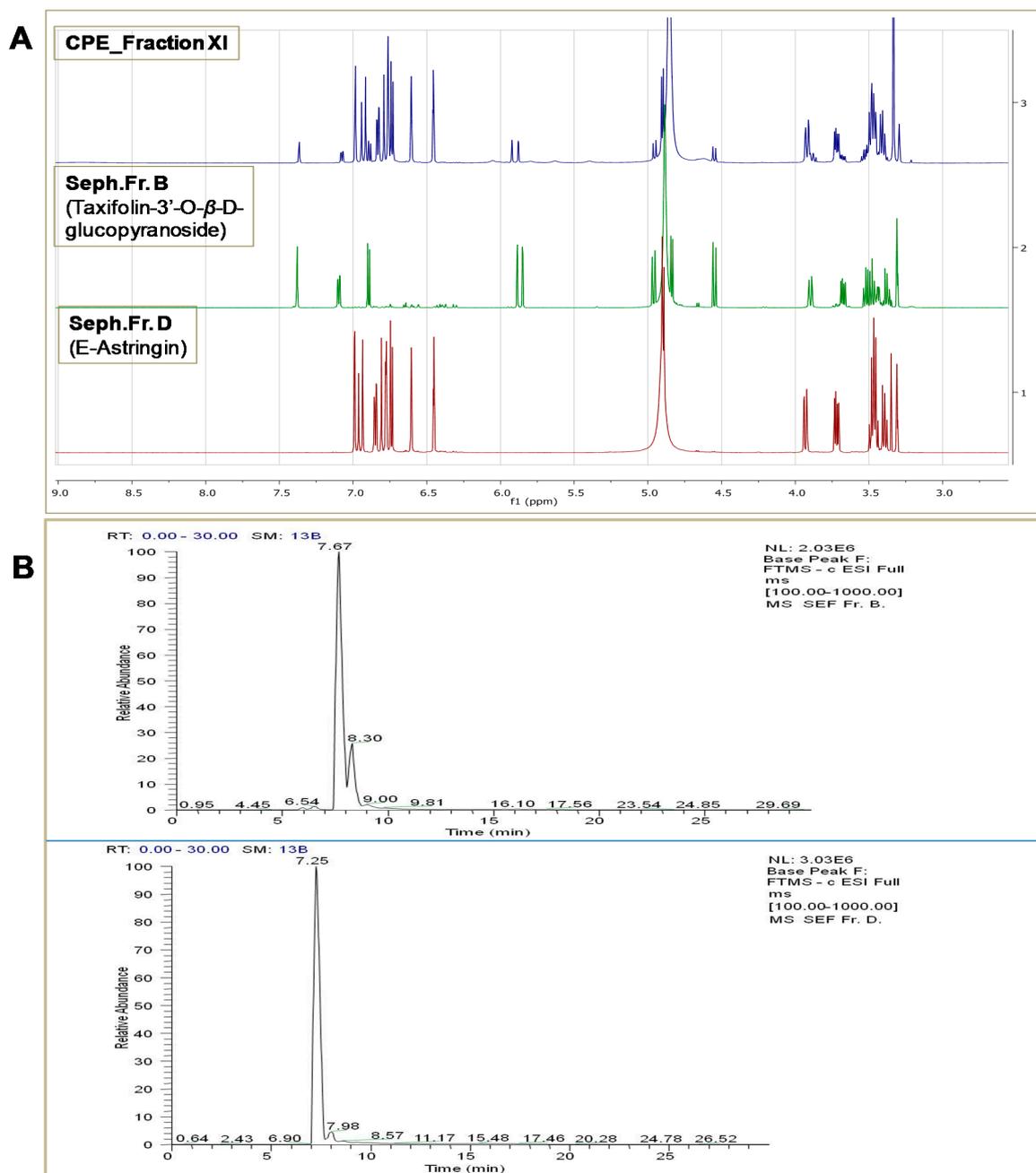


Figure S2. ^1H -NMR spectra (**A**) and LC-ESI(-)-HRMS spectra (**B**) of *E*-astringin and taxifolin-3'-O- β -D-glucopyranoside obtained from the analysis of CPC_Fr. XI by Sephadex LH-20 Column Chromatography

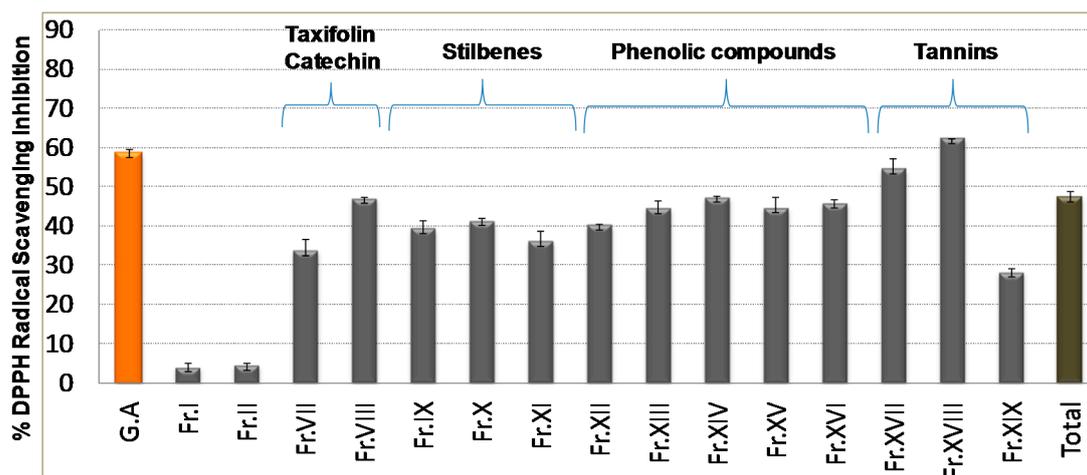


Figure S3. % DPPH Inhibition of CPC fractions at 25 $\mu\text{g/mL}$. GA: Gallic Acid (at 5.0 $\mu\text{g/mL}$), Total: Crude Methanolic Extract from bark of *P. abies* (at 25 $\mu\text{g/mL}$).

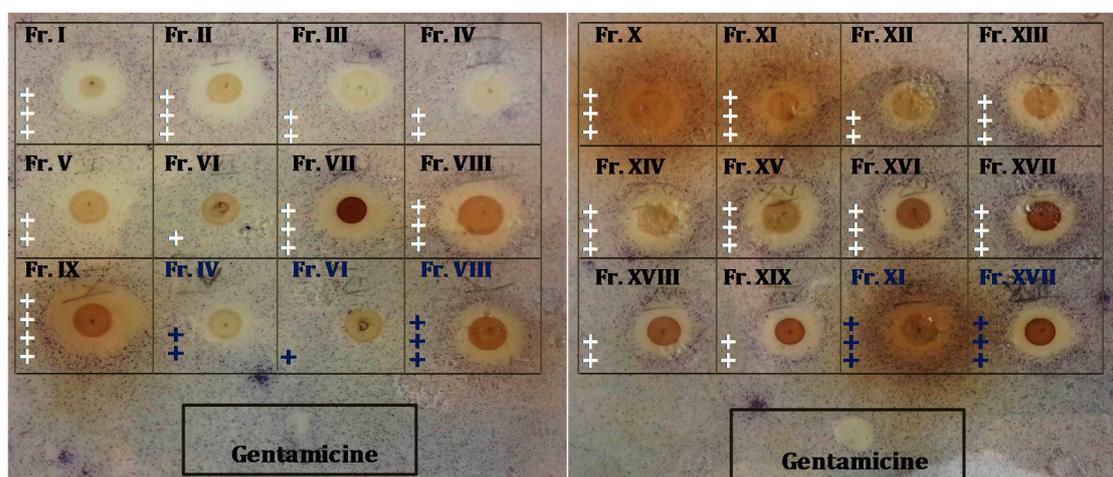


Figure S4. Antimicrobial activity of CPC fractions against *Staphylococcus aureus* by using bioautographic method. (+): low activity, (++): middle activity, (+++): high activity, (++++): very high activity). Fractions IV, VI, VIII, XI and XVII were spotted twice in the TLC plate (blue color) in order to verify the accuracy of the method

ESI(-)-HRMS Spectra of Identified Compounds

CPC_fr_II # 1665 RT: 17.92 AV: 1 NL: 1.61E5
F: FTMS - c ESI Full ms [100.00-1000.00]

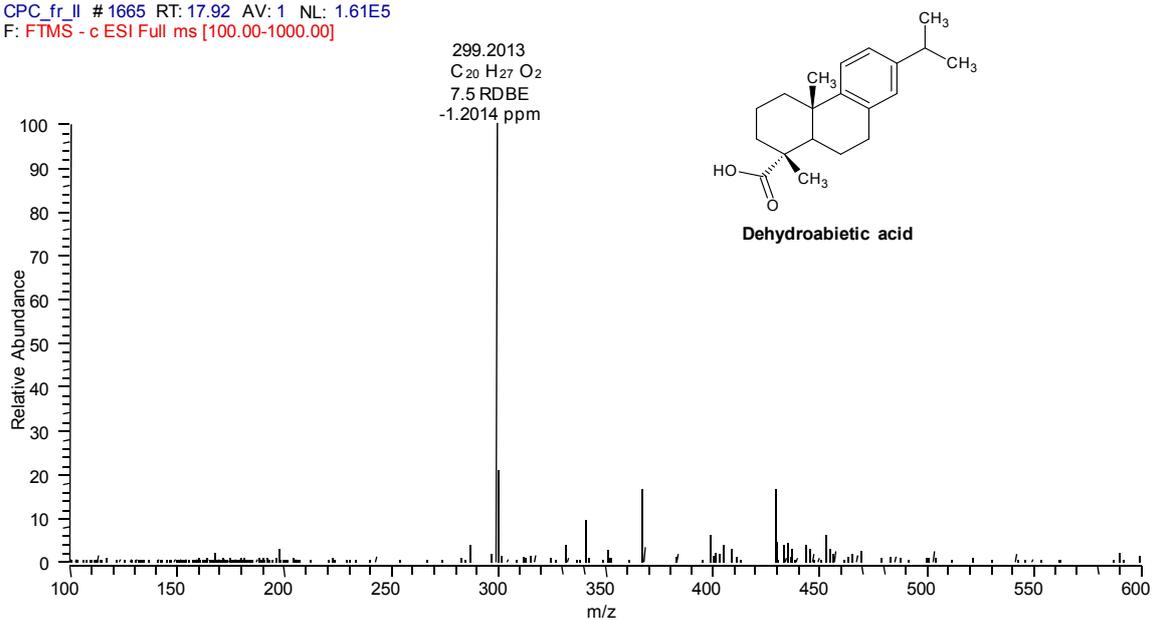


Figure S5. ESI(-)-HRMS spectrum of dehydroabietic acid.

CPC_fr_III # 1065 RT: 11.99 AV: 1 NL: 2.34E5
F: FTMS - c ESI Full ms [100.00-1000.00]

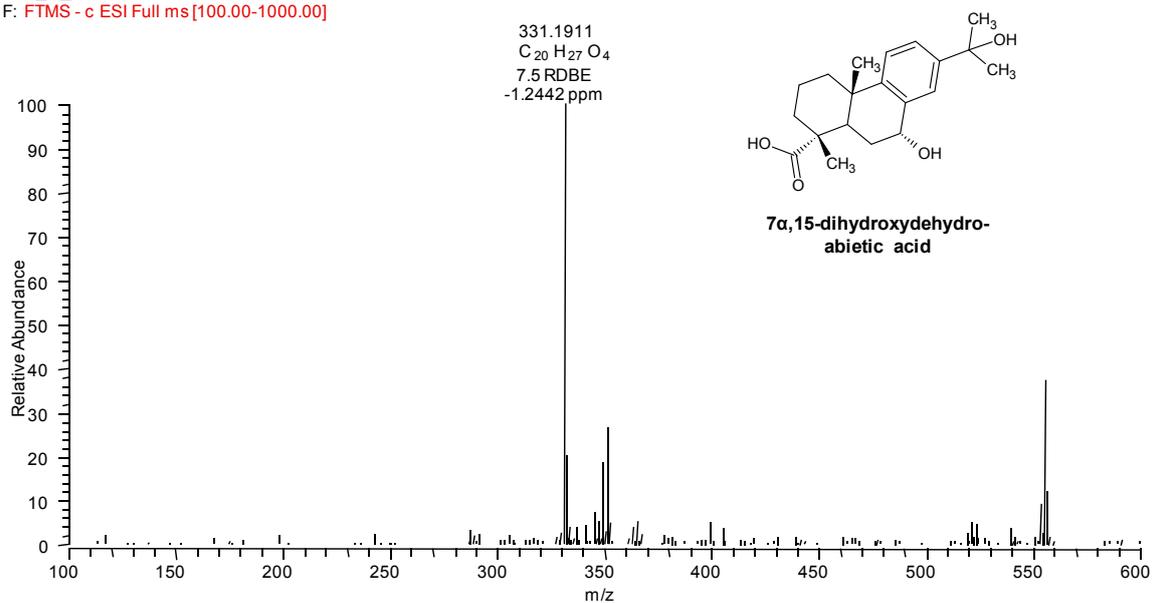


Figure S6. ESI(-)-HRMS spectrum of 7a,15-dihydroxydehydroabietic acid.

CPC_fr_VII # 673 RT: 8.14 AV: 1 NL: 5.59E5
F: FTMS - c ESI Full ms [100.00-1000.00]

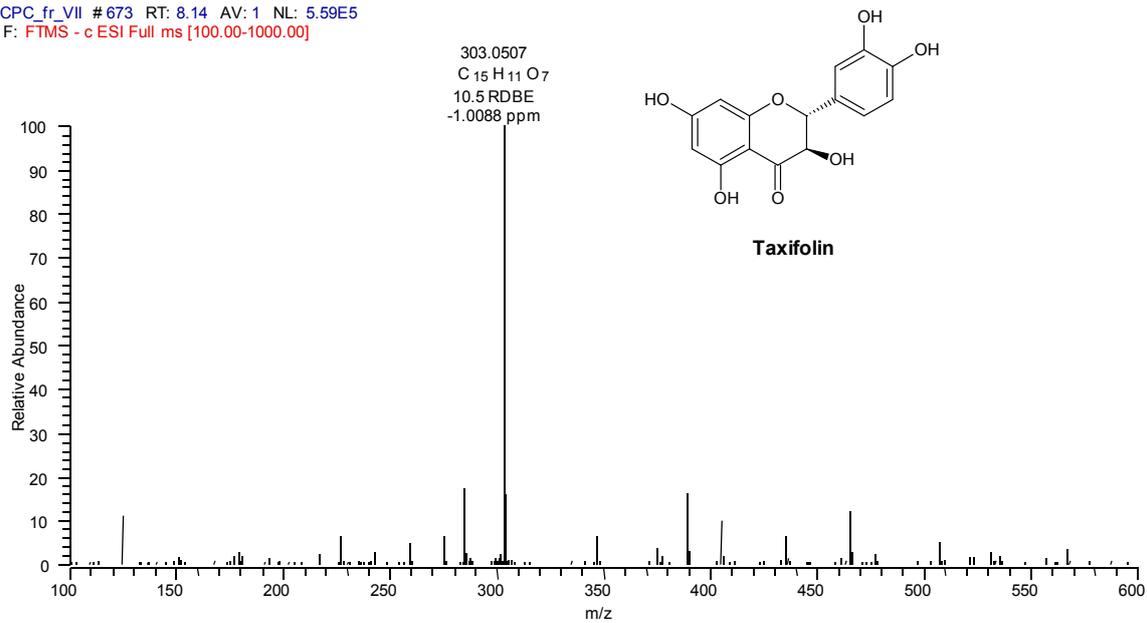


Figure S7. ESI(-)-HRMS spectrum of taxifoline.

CPC_fr_VIII # 451 RT: 5.95 AV: 1 NL: 1.08E6
F: FTMS - c ESI Full ms [100.00-1000.00]

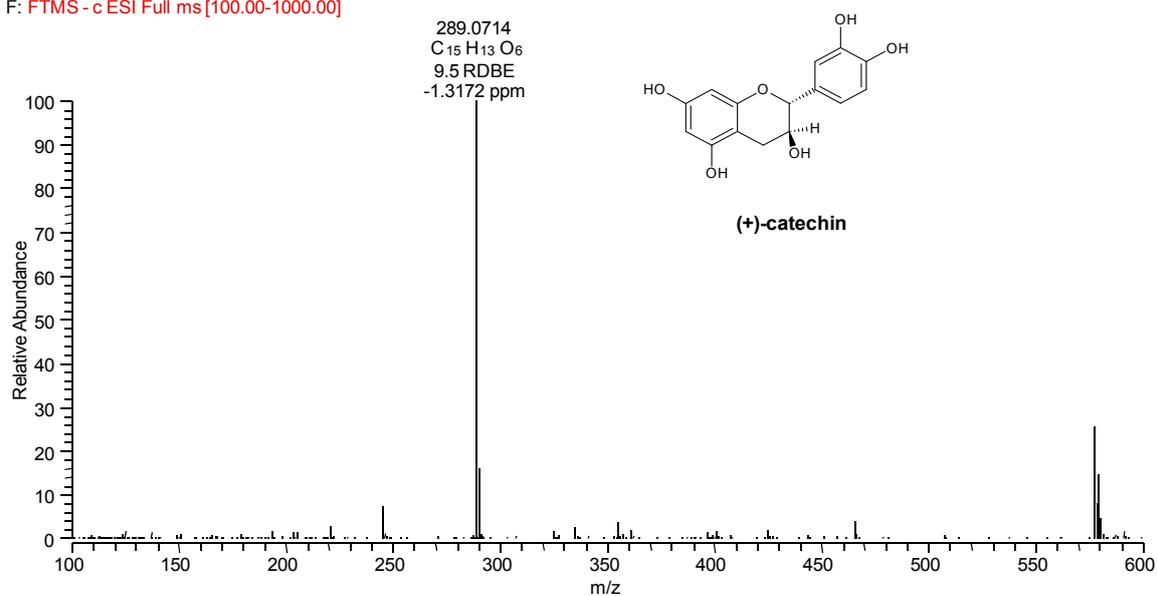


Figure S8. ESI(-)-HRMS spectrum of (+)-catechin.

CPC_fr_IX # 653 RT: 7.94 AV: 1 NL: 1.15E6
F: FTMS - c ESI Full ms [100.00-1000.00]

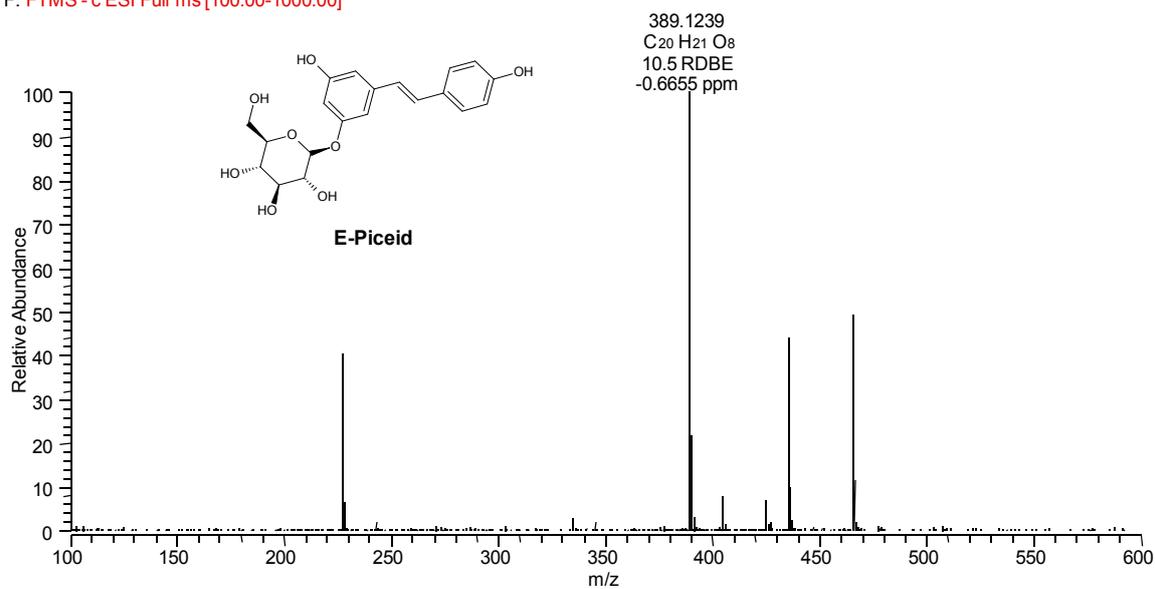


Figure S9. ESI(-)-HRMS spectrum of *E*-piceid.

CPC_fr_IX # 687 RT: 8.28 AV: 1 NL: 1.10E6
F: FTMS - c ESI Full ms [100.00-1000.00]

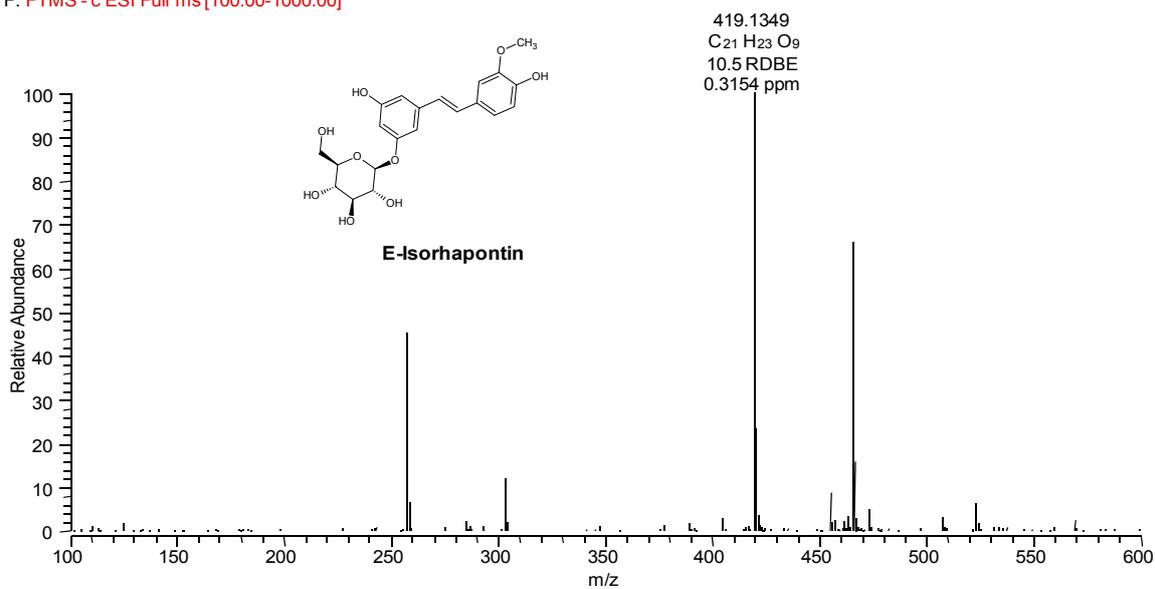


Figure S10. ESI(-)-HRMS spectrum of *E*-isorhapontin.

CPC_fr_X # 573 RT: 7.16 AV: 1 NL: 3.77E6
F: FTMS - c ESI Full ms [100.00-1000.00]

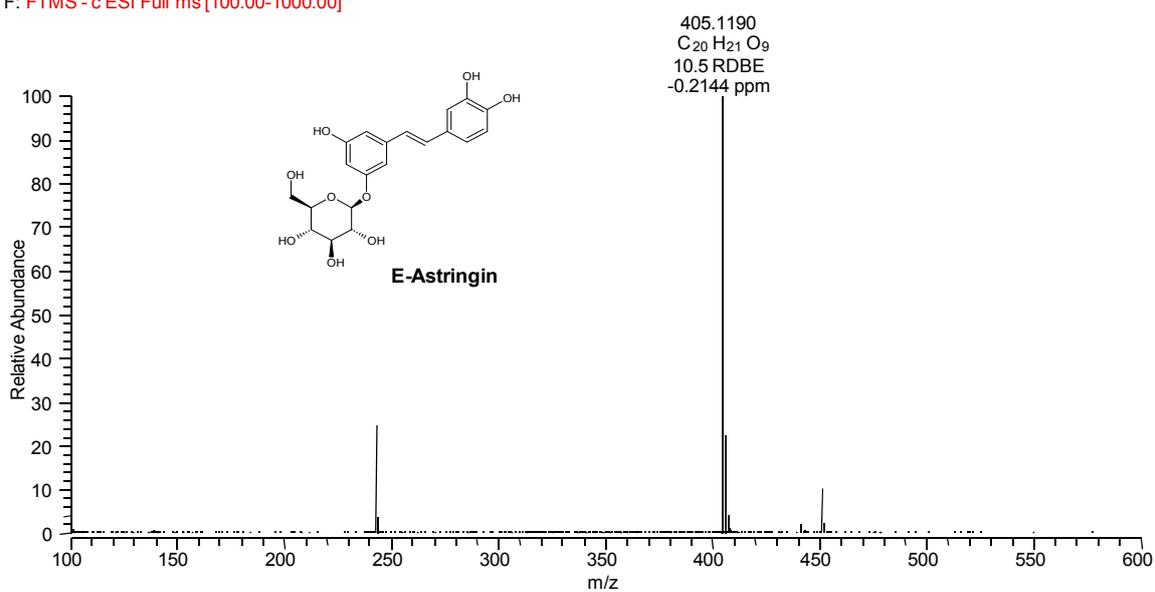


Figure S11. ESI(-)-HRMS spectrum of E-astringin.

CPC_fr_XI # 615 RT: 7.57 AV: 1 NL: 3.22E6
F: FTMS - c ESI Full ms [100.00-1000.00]

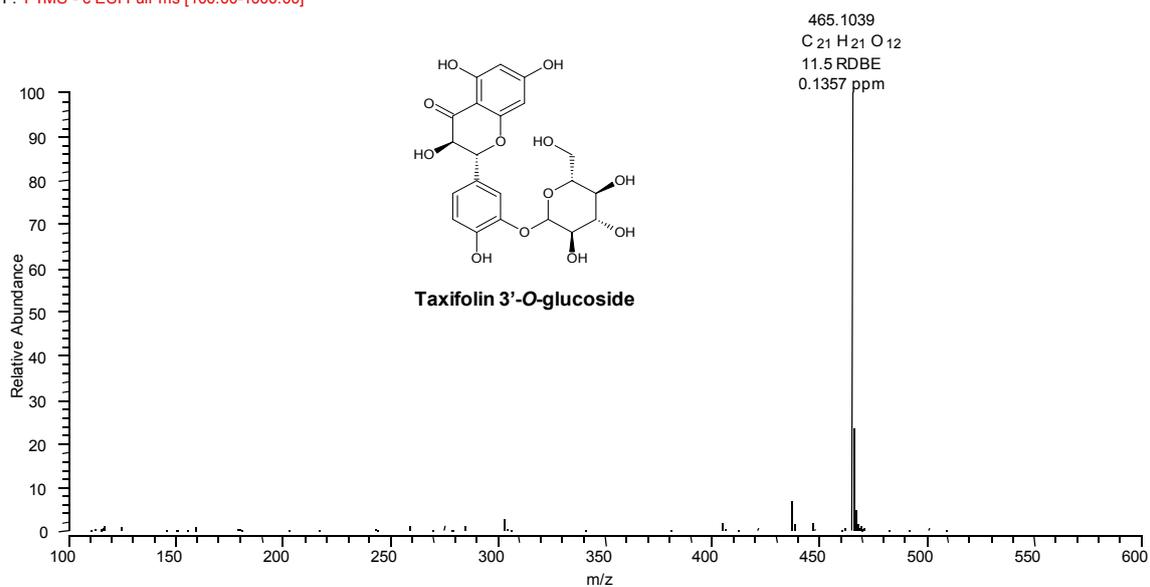


Figure S12. ESI(-)-HRMS spectrum of taxifoline-3'-O-β-D-glucopyranoside.

CPC_fr_XV # 375 RT: 5.16 AV:1 NL: 3.97E4
F: FTMS - c ESI Full ms [100.00-1000.00]

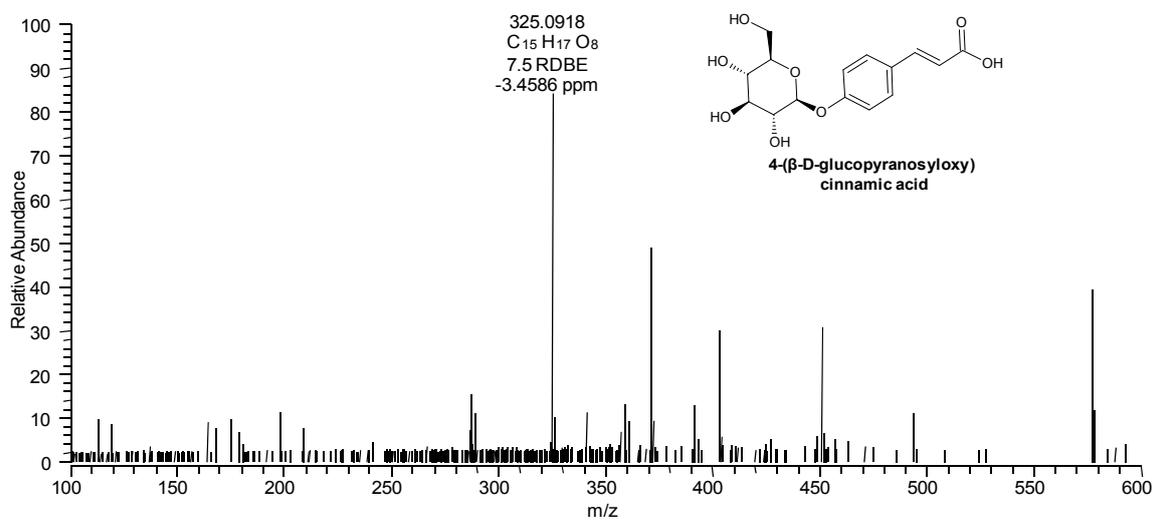


Figure S13. ESI(-)-HRMS spectrum of 4-(β-D-glucopyranosyloxy)cinnamic acid.

CPC_fr_X_V # 459 RT: 6.03 AV:1 NL: 7.33E4
F: FTMS - c ESI Full ms [100.00-1000.00]

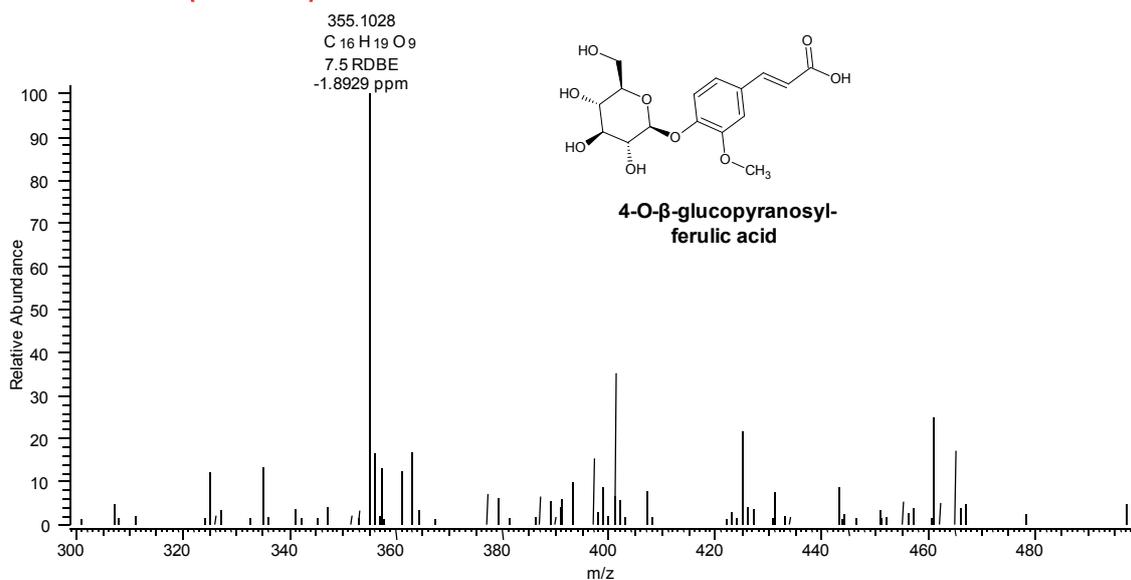


Figure S14. ESI(-)-HRMS spectrum of 4-O-β-glucopyranosyl-ferulic acid.

CPC_fr_XV # 149 RT: 1.87 AV:1 NL: 4.29E4
F: FTMS - c ESI Full ms [100.00-1000.00]

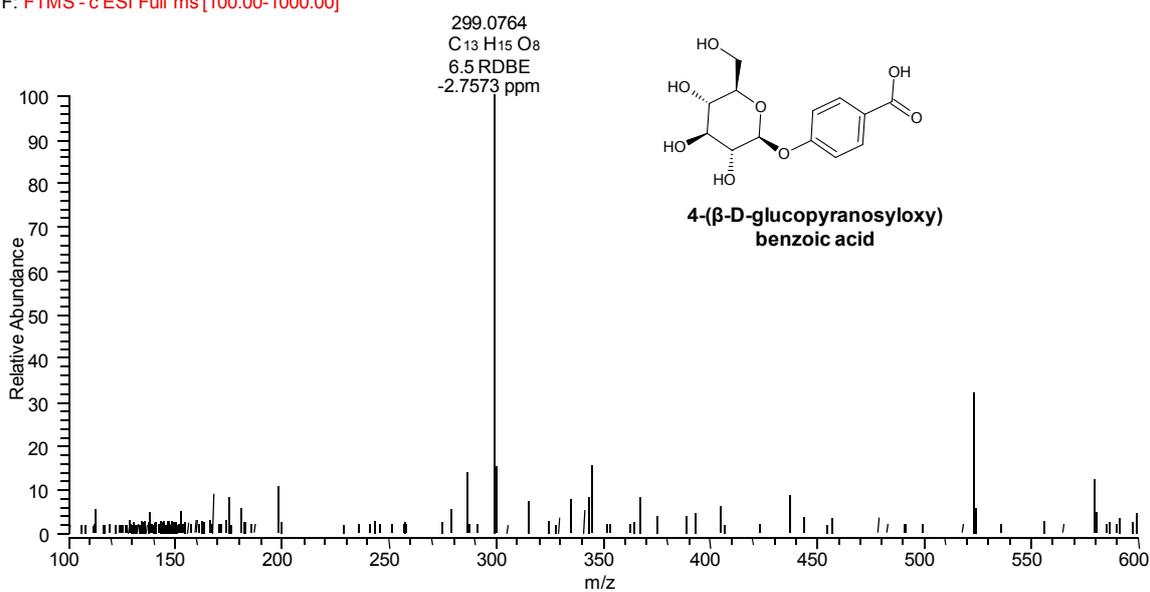


Figure S15. ESI(-)-HRMS spectrum of 4-(β-D-glucopyranosyloxy)benzoic acid.

CPC_fr_XVII # 42 RT: 0.62 AV:1 NL:1.27E6
F: FTMS - c ESI Full ms [100.00-1000.00]

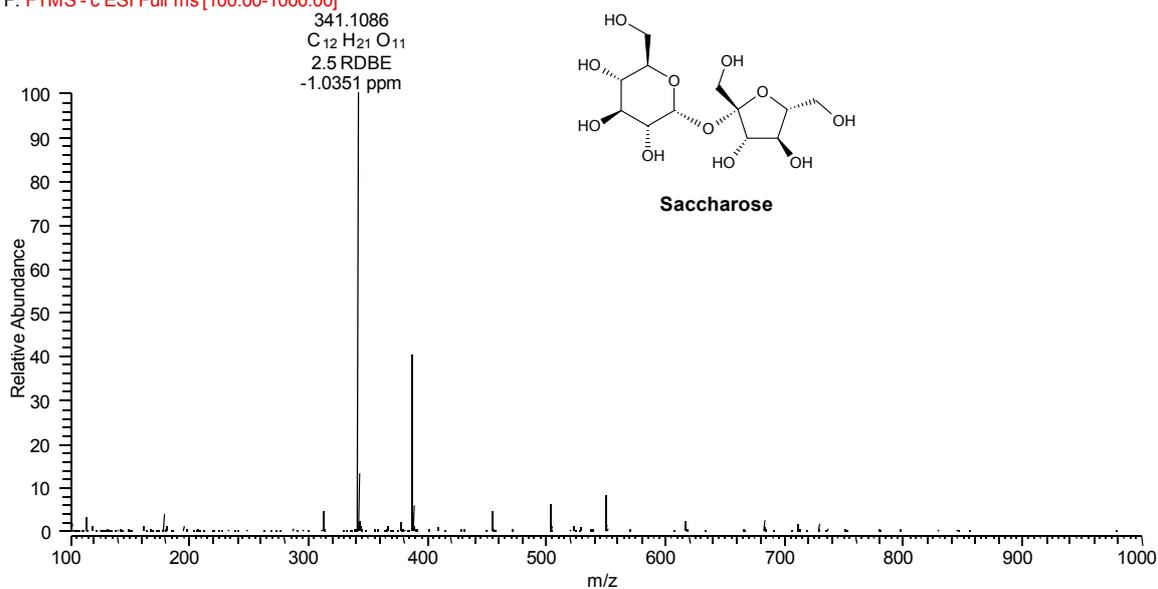


Figure S16. ESI(-)-HRMS spectrum of saccharose.