

Targeted and Untargeted Metabolomics to Explore the Bioavailability of the Secoiridoids from a Seed/Fruit Extract (*Fraxinus angustifolia* Vahl) in Human Healthy Volunteers: A Preliminary Study

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Table S1. Targeted metabolomics analysis: potential compounds specifically derived from the metabolic transformation of the secoiridoid glucosides identified in the *Fraxinus angustifolia* Vahl extract.

Parent Compounds			Aglycone Fragments		
Potential Metabolite	Molecular formula	Exact Mass	Potential Metabolite	Molecular formula	Exact Mass
Nuzhenide/ Excelside B/1-O-β-D-glucosylformoside *	C ₃₁ H ₄₂ O ₁₇	685.2349	Tyrosol	C ₈ H ₁₀ O ₂	137.0608
+ glucuronide	C ₃₇ H ₅₀ O ₂₃	861.2670	+ glucuronide	C ₁₄ H ₁₈ O ₈	313.0929
+ sulfate	C ₃₁ H ₄₂ O ₂₀ S	765.1917	+ sulfate	C ₈ H ₁₀ O ₅ S	217.0176
+ sulfoglucuronide	C ₃₇ H ₅₀ O ₂₆ S	941.2238	+ sulfoglucuronide	C ₁₄ H ₁₈ O ₁₁ S	393.0497
+ methyl	C ₃₈ H ₅₂ O ₂₆ S	955.2395	+ methyl	C ₉ H ₁₂ O ₂	151.0765
GL3/nuzhenide 11-methyl oleoside *	C ₄₈ H ₆₄ O ₂₇	1071.3562	Hydroxytyrosol (Tyrosol+OH)	C ₈ H ₁₀ O ₃	153.0557
+ glucuronide	C ₅₄ H ₇₂ O ₃₃	1247.3883	+ glucuronide	C ₁₄ H ₁₈ O ₉	329.0878
+ sulfate	C ₄₈ H ₆₄ O ₃₀ S	1151.3130	+ sulfate	C ₈ H ₁₀ O ₆ S	233.0125
+ sulfoglucuronide	C ₅₄ H ₇₂ O ₃₆ S	1327.3451	+ sulfoglucuronide	C ₁₄ H ₁₈ O ₁₂ S	409.0446
+ methyl	C ₄₉ H ₆₆ O ₂₇	1085.3719	+ methyl	C ₉ H ₁₂ O ₃	167.0714
GL5	C ₄₂ H ₅₄ O ₂₂	909.3034	Ligstroside-aglycone	C ₁₉ H ₂₂ O ₇	361.1293
+ glucuronide	C ₄₈ H ₆₂ O ₂₈	1085.3355	+ glucuronide	C ₂₅ H ₃₀ O ₁₃	537.1614
+ sulfate	C ₄₂ H ₅₄ O ₂₅ S	989.3602	+ sulfate	C ₁₉ H ₂₂ O ₁₀ S	441.0861
+ sulfoglucuronide	C ₄₈ H ₆₂ O ₃₁ S	1165.2923	+ sulfoglucuronide	C ₂₅ H ₃₀ O ₁₆ S	617.1182
+ methyl	C ₄₃ H ₅₆ O ₂₂	923.319	+ methyl	C ₂₀ H ₂₄ O ₇	375.1449
Salidroside (Tyrosol glucose)	C ₁₄ H ₂₀ O ₇	299.1136	Oleuropein aglycone (Ligstroside-aglycone + OH)	C ₁₉ H ₂₂ O ₈	377.1242
+ glucuronide	C ₂₀ H ₂₈ O ₁₃	475.1457	+ glucuronide	C ₂₅ H ₃₀ O ₁₄	553.1563
+ sulfate	C ₁₄ H ₂₀ O ₁₀ S	379.0704	+ sulfate	C ₁₉ H ₂₂ O ₁₁ S	457.0810
+ sulfoglucuronide	C ₂₀ H ₂₈ O ₁₆ S	555.1025	+ sulfoglucuronide	C ₂₅ H ₃₀ O ₁₇ S	633.1131
+ methyl	C ₁₅ H ₂₂ O ₇	313.1293	+ methyl	C ₂₀ H ₂₄ O ₈	391.1398
Oleoside	C ₁₆ H ₂₂ O ₁₁	389.1089	Elenolic acid	C ₁₁ H ₁₄ O ₆	241.0718
+ glucuronide	C ₂₂ H ₃₀ O ₁₇	565.1410	+ glucuronide	C ₁₇ H ₂₂ O ₁₂	417.1038
+ sulfate	C ₁₆ H ₂₂ O ₁₄ S	469.0657	+ sulfate	C ₁₁ H ₁₄ O ₉ S	321.0286

Table S1. *Cont.*

Parent Compounds			Aglycone Fragments		
+ sulfoglucuronide	C ₂₂ H ₃₀ O ₂₀ S	645.0978	+ sulfoglucuronide	C ₁₇ H ₂₂ O ₁₅ S	497.0607
+ methyl	C ₁₇ H ₂₄ O ₁₁	403.1246	+ methyl	C ₁₂ H ₁₆ O ₆	255.0874
Elenolic acid glucose (Oleoside-11 methyl ester)	C ₁₇ H ₂₄ O ₁₁	403.1246	Demethyl-elenuolic acid	C ₁₀ H ₁₂ O ₆	227.0561
+glucuronide	C ₂₃ H ₃₂ O ₁₇	579.1567	+ glucuronide	C ₁₆ H ₂₀ O ₁₂	403.0882
+sulfate	C ₁₇ H ₂₄ O ₁₄ S	483.0814	+ sulfate	C ₁₀ H ₁₂ O ₉ S	307.0129
+sulfoglucuronide	C ₂₃ H ₃₂ O ₂₀ S	659.1135	+ sulfoglucuronide	C ₁₆ H ₂₀ O ₁₅ S	483.045
+ methyl	C ₁₈ H ₂₆ O ₁₁	417.1402			
Ligstroside	C ₂₅ H ₃₂ O ₁₂	523.1821	Elenolic-Tyrosol-Elenolic	C ₃₀ H ₃₄ O ₁₂	585.1978
+ glucuronide	C ₃₁ H ₄₀ O ₁₈	699.2142	+ glucuronide	C ₃₆ H ₄₂ O ₁₈	761.2298
+ sulfate	C ₂₅ H ₃₂ O ₁₅ S	603.2142	+ sulfate	C ₃₀ H ₃₄ O ₁₅ S	665.1546
+ sulfoglucuronide	C ₃₁ H ₄₀ O ₂₁ S	779.1710	+ sulfoglucuronide	C ₃₆ H ₄₂ O ₂₁ S	841.1867
+ methyl	C ₂₆ H ₃₄ O ₁₂	537.1978	+ methyl	C ₃₁ H ₃₆ O ₁₂	599.2134

*: isomers with the same molecular formulae.