

S1 Table. Retention time, mass, molecular formula, chemical class of compounds of figure 2 that were also positively correlated to EC₉₀ but with a relative intensity of masses lower than 20000.

Peak	Ret (min.)	[M-H] ⁻	Molecular formula	Class	Compounds
Unknown 11	1.23	173.0414	---	---	Unknown
Unknown 12	1.50	290.0878	---	---	Unknown
Unknown 13	2.34	345.1222	C ₁₅ H ₂₂ O ₉	---	Unknown
Unknown 14	2.49	423.1480	C ₁₇ H ₂₈ O ₁₂	---	Unknown
Unknown 16	3.93	353.0878	C ₁₆ H ₁₈ O ₉	Phenylpropanoid	Caffeoylquinic acid
Unknown 18	10.01	389.1042	C ₁₆ H ₂₂ O ₁₁	---	Unknown
Unknown 19	10.50	473.1292	C ₂₀ H ₂₆ O ₁₃	---	Unknown
Unknown 20	11.27	381.0933	C ₁₅ H ₂₃ ClO ₉	---	Unknown
Unknown 25	16.49	596.1331	C ₂₆ H ₂₈ O ₁₆	Flavonol	Unknown
Unknown 26	16.62	475.0306*	C ₄₁ H ₂₈ O ₂₇	---	Unknown
Unknown 30	17.86	453.0379*	C ₄₀ H ₂₈ O ₂₅	---	Unknown
Unknown 32	18.63	515.1163	C ₂₅ H ₂₄ O ₁₂	Phenylpropanoid	Dicaffeoylquinic acid
Unknown 34	18.80	591.1653	C ₃₅ H ₂₈ O ₉	---	Unknown
Unknown 35	19.00	607.1591	C ₃₅ H ₂₈ O ₁₀	---	Unknown
Unknown 36	19.16	433.0755	C ₂₀ H ₁₈ O ₁₁	---	Unknown
Unknown 42	21.13	507.1467	C ₂₄ H ₂₈ O ₁₂	Phenylpropanoid	Unknown
Unknown 43	23.20	677.1498	C ₃₄ H ₃₀ O ₁₅	---	Unknown
Unknown 44	23.79	677.1491	C ₃₄ H ₃₀ O ₁₅	---	Unknown
Unknown 45	23.95	421.2035	C ₁₉ H ₃₄ O ₁₀	---	Unknown
Unknown 47	30.27	793.9424	C ₄₂ H ₆₆ O ₁₄	---	Unknown
Unknown 53	31.36	558.2535*	C ₅₇ H ₈₂ O ₂₂	---	Unknown
Unknown 55	32.16	939.4924	C ₄₈ H ₇₆ O ₁₈	---	Unknown
Unknown 57	32.85	399.1429	C ₂₂ H ₂₄ O ₇	---	Unknown

*[M-2H]⁻²