

SUPPLEMENTARY FILE

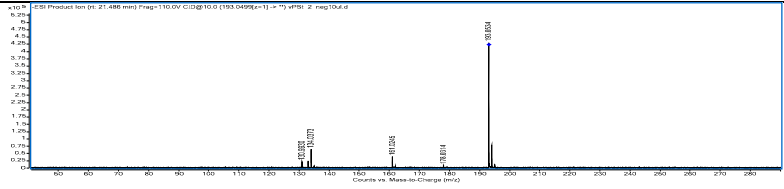
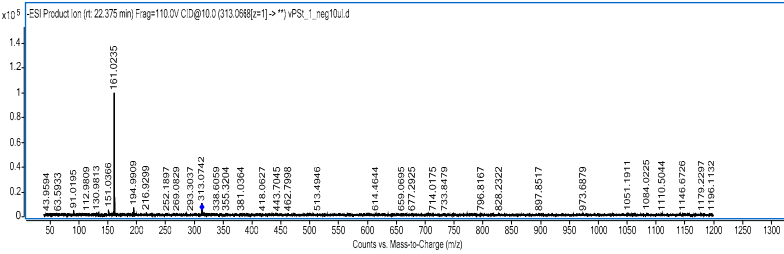
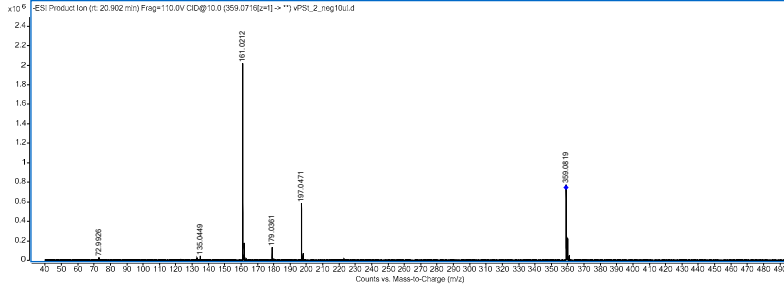
Table S1. Mass chromatograms of the tested samples recorded in negative and positive ionization modes

Type of mass chromatogram	Chromatogram
Mass chromatogram from the aerial parts in the negative ionization mode	
Mass chromatogram from the aerial parts in the positive ionization mode	
Mass chromatogram from the roots in the negative ionization mode	
Mass chromatogram from the root in the positive ionization mode	

Table S2. The list of MS/MS spectra of the tentatively identified compounds

No	MS/MS spectrum	Proposed compound
1		Propylglutaric acid

2	<p>ESI Product Ion (rt: 12.167 min) Frag=110.0V CID@20.0 (167.0356)*[$^{-}$]* vPSL_1_neg10uL.d</p>	Vanillic acid
3	<p>ESI Product Ion (rt: 12.167 min) Frag=110.0V CID@20.0 (167.0356)*[$^{-}$]* vPSL_1_neg10uL.d</p>	Syringic acid
4	<p>ESI Product Ion (rt: 12.167 min) Frag=110.0V CID@20.0 (167.0356)*[$^{-}$]* vPSL_1_neg10uL.d</p>	Dihydroxybenzoic acid
5	<p>ESI Product Ion (rt: 15.219 min) Frag=110.0V CID@20.0 (137.0227)*[$^{-}$]* vPSL_1_neg10uL.d</p>	Hydroxybenzoic acid
6	<p>ESI Scan (rt: 17.183 min) Frag=110.0V vPSL_2_neg10uL.d</p>	Rosmarinic acid isomer
7	<p>ESI Product Ion (rt: 17.154 min) Frag=110.0V CID@10.0 (176.0341)*[$^{-}$]* vPSL_1_neg10uL.d</p>	Caffeic acid
8	<p>ESI Product Ion (rt: 19.401 min) Frag=110.0V CID@10.0 (193.0381)*[$^{-}$]* vPSL_2_neg10uL.d</p>	Coumaric acid
9		Ferulic acid

	 <p>ESI Product Ion (t: 21.486 min) Frag=110.0V CID@10.0 (193.0496<+1>-*) vPSt_2_neg10u.d</p>	
10	 <p>ESI Product Ion (t: 22.375 min) Frag=110.0V CID@10.0 (313.0688<+1>-*) vPSt_1_neg10u.d</p> <p>Counts vs. Mass-to-Charge (m/z)</p>	Crisimaritin
11	 <p>ESI Product Ion (t: 20.902 min) Frag=110.0V CID@10.0 (359.0716<+1>-*) vPSt_2_neg10u.d</p> <p>Counts vs. Mass-to-Charge (m/z)</p>	Rosmarinic acid