

Supplementary Information

Open Access

Elmira Bekbolatova, Wirginia Kukula-Koch*, Tomasz Baj, Natalia Stasiak, Galiya Ibadullayeva, Wojciech Koch, Kazimierz Głowniak, Saken Tulemissov, Zuriyadda Sakipova, Fabio Boylan

Phenolic composition and antioxidant potential of different organs of Kazakh *Crataegus almaatensis* Pojark: A comparison with the European *Crataegus oxyacantha* L. flowers

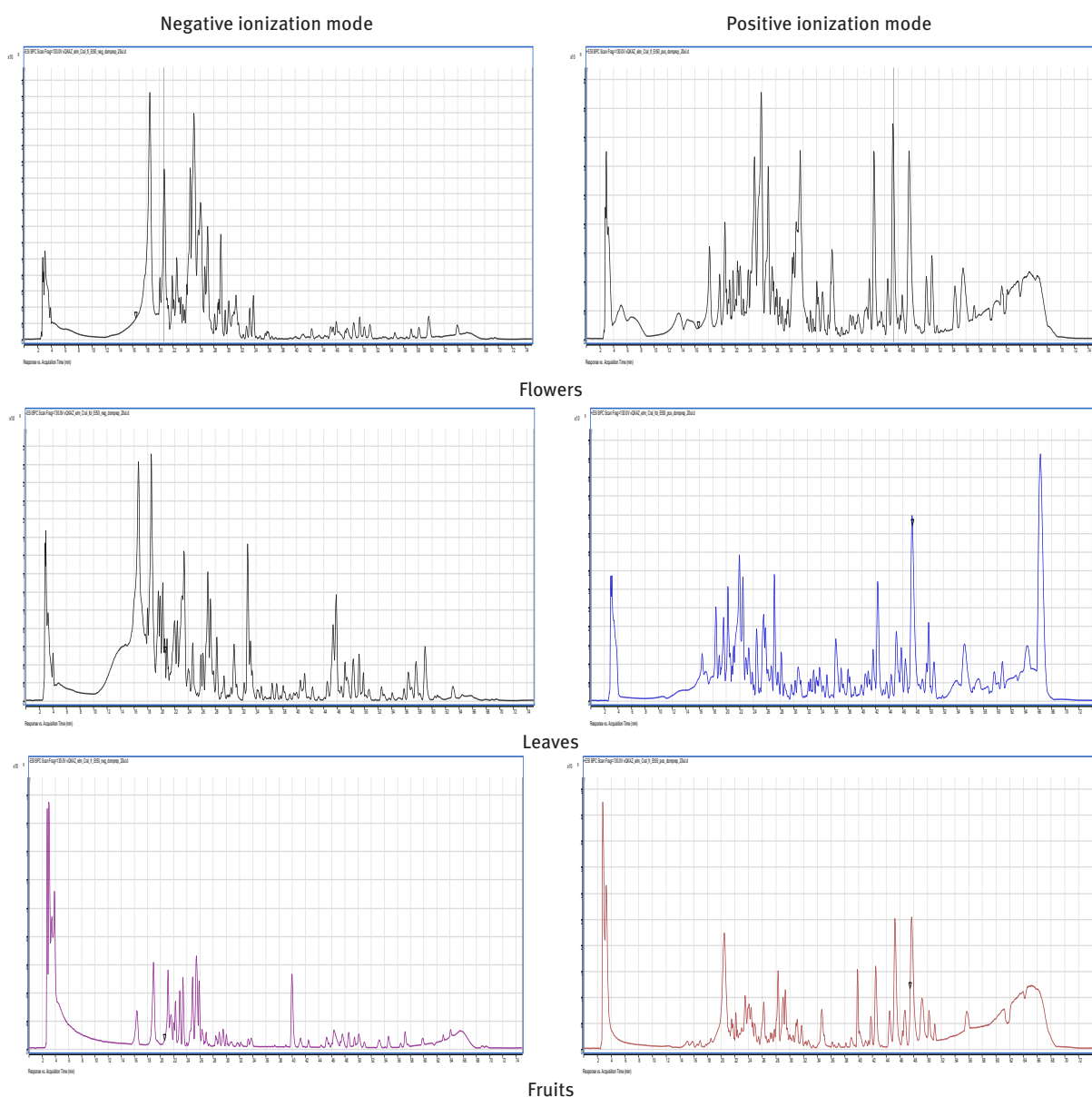


Figure S1. The TIC chromatograms obtained for *Crataegus almaatensis* 50% ethanol extracts

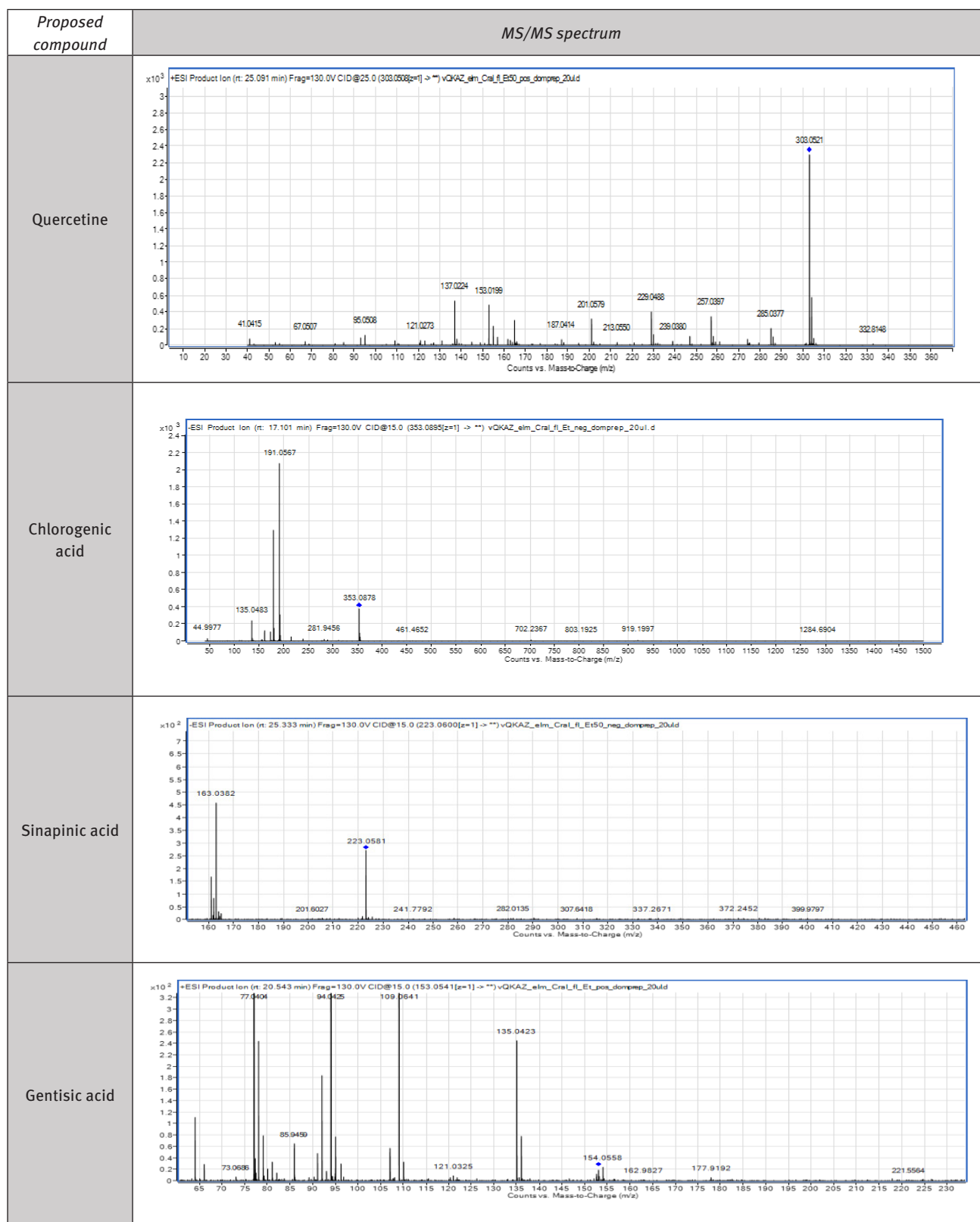
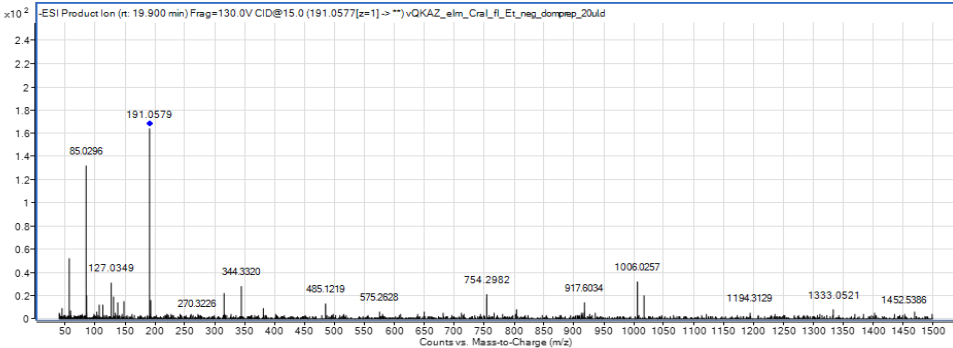
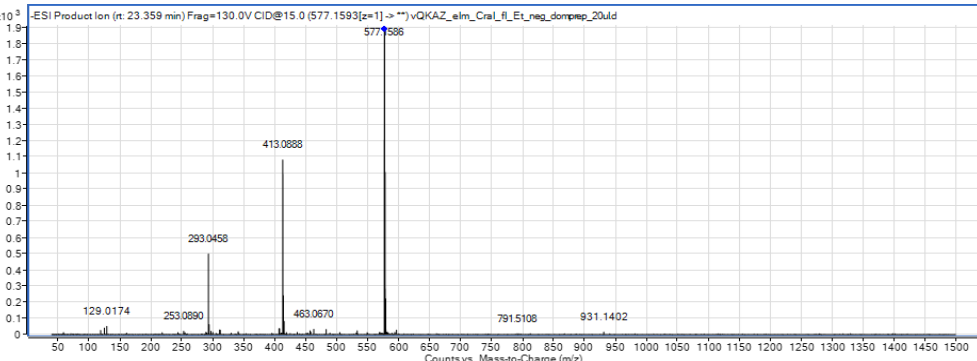
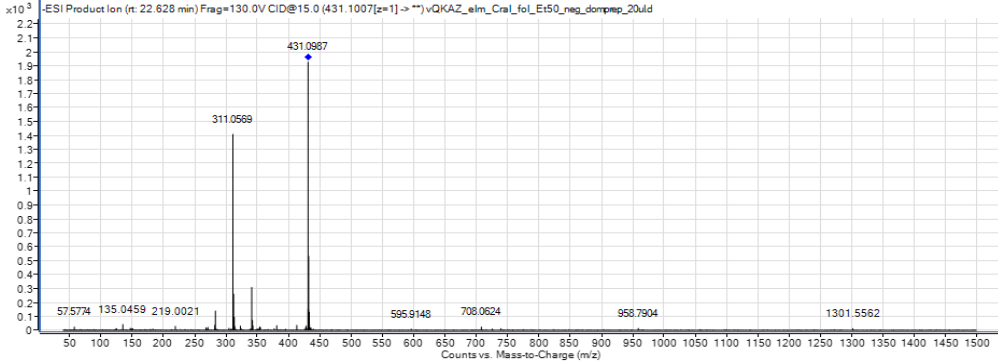
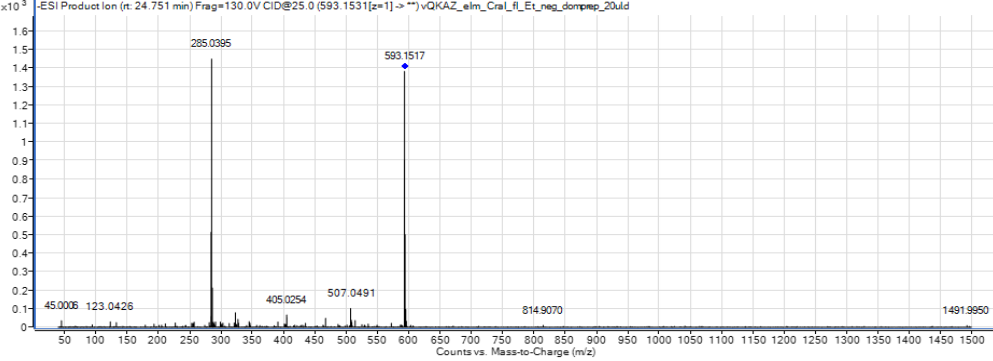


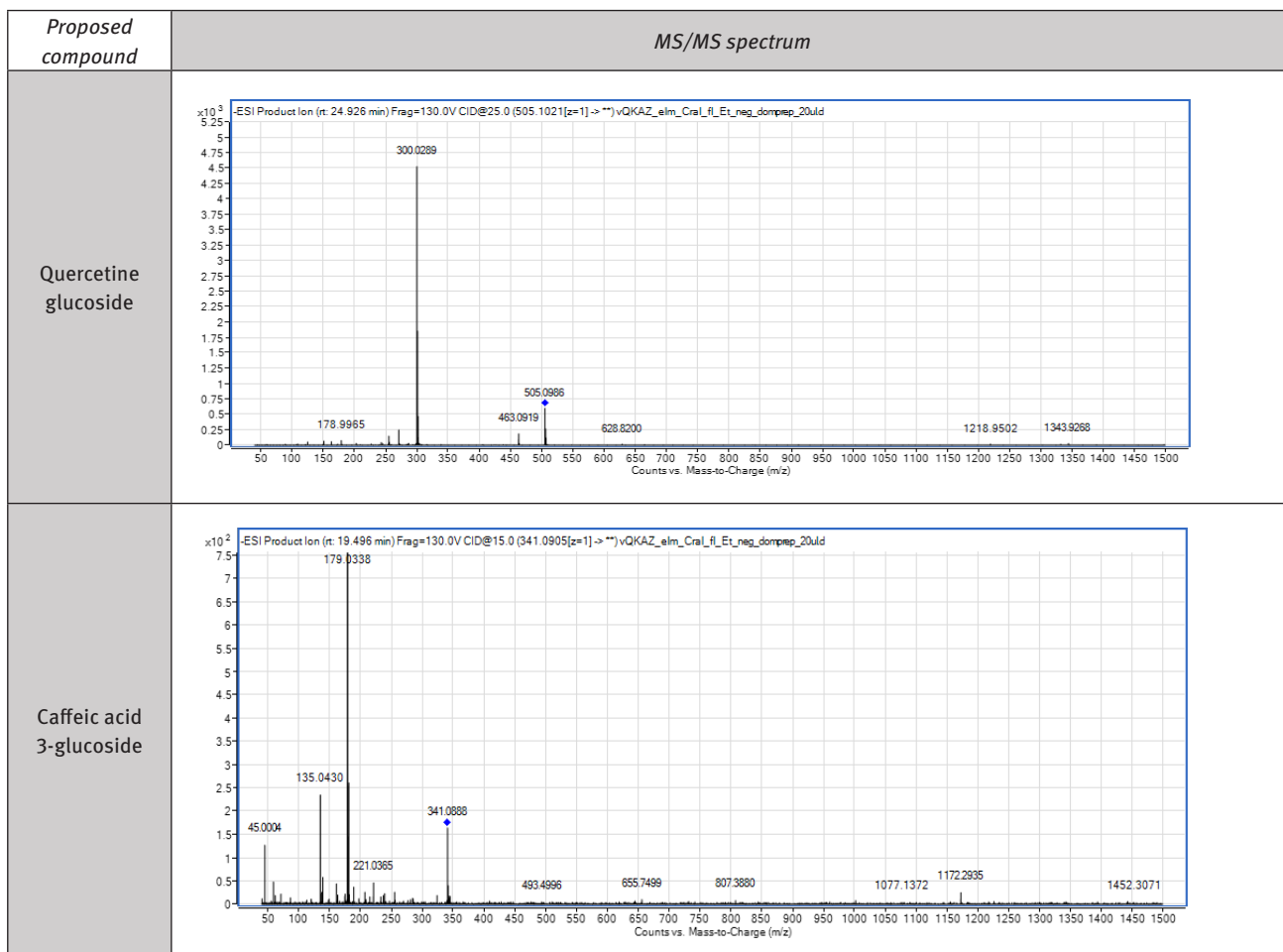
Figure S2: The fragmentation patterns obtained for all identified compounds.

Proposed compound	MS/MS spectrum																						
Quercetrin	<p>ES-ESI Product Ion (rt: 25.764 min) Frag=130.0V CID@15.0 (447.0958[z=1]->**) vQKAZ_elm_CraL_fI_Et_neg_dompreg_20uld</p> <table border="1"> <caption>Peak Data for Quercetrin</caption> <thead> <tr> <th>m/z</th> <th>Relative Intensity (approx. x10³)</th> </tr> </thead> <tbody> <tr><td>57.0341</td><td>0.1</td></tr> <tr><td>151.0040</td><td>0.2</td></tr> <tr><td>301.0336</td><td>0.4</td></tr> <tr><td>341.0669</td><td>0.8</td></tr> <tr><td>401.1446</td><td>0.3</td></tr> <tr><td>447.0885</td><td>1.3</td></tr> <tr><td>563.9572</td><td>0.1</td></tr> <tr><td>778.6714</td><td>0.1</td></tr> <tr><td>953.5625</td><td>0.1</td></tr> <tr><td>1399.8529</td><td>0.1</td></tr> </tbody> </table>	m/z	Relative Intensity (approx. x10 ³)	57.0341	0.1	151.0040	0.2	301.0336	0.4	341.0669	0.8	401.1446	0.3	447.0885	1.3	563.9572	0.1	778.6714	0.1	953.5625	0.1	1399.8529	0.1
m/z	Relative Intensity (approx. x10 ³)																						
57.0341	0.1																						
151.0040	0.2																						
301.0336	0.4																						
341.0669	0.8																						
401.1446	0.3																						
447.0885	1.3																						
563.9572	0.1																						
778.6714	0.1																						
953.5625	0.1																						
1399.8529	0.1																						
Cyanidin 3-glucoside	<p>ESI Scan (rt: 20.725 min) Frag=130.0V vQKAZ_elm_CraL_fI_Et50_pos_dompreg_20uld</p> <table border="1"> <caption>Peak Data for Cyanidin 3-glucoside</caption> <thead> <tr> <th>m/z</th> <th>Relative Intensity (approx. x10⁶)</th> </tr> </thead> <tbody> <tr><td>195.0884</td><td>0.4</td></tr> <tr><td>355.1025</td><td>0.1</td></tr> <tr><td>449.1083</td><td>1.3</td></tr> <tr><td>541.2257</td><td>0.1</td></tr> <tr><td>648.1978</td><td>0.1</td></tr> <tr><td>741.2043</td><td>0.1</td></tr> <tr><td>867.2086</td><td>0.1</td></tr> </tbody> </table>	m/z	Relative Intensity (approx. x10 ⁶)	195.0884	0.4	355.1025	0.1	449.1083	1.3	541.2257	0.1	648.1978	0.1	741.2043	0.1	867.2086	0.1						
m/z	Relative Intensity (approx. x10 ⁶)																						
195.0884	0.4																						
355.1025	0.1																						
449.1083	1.3																						
541.2257	0.1																						
648.1978	0.1																						
741.2043	0.1																						
867.2086	0.1																						
Epigallo-catechin	<p>ES-ESI Product Ion (rt: 19.577 min) Frag=130.0V CID@15.0 (307.0785[z=1]->**) vQKAZ_elm_CraL_fI_Et_pos_dompreg_20uld</p> <table border="1"> <caption>Peak Data for Epigallo-catechin</caption> <thead> <tr> <th>m/z</th> <th>Relative Intensity (approx. x10³)</th> </tr> </thead> <tbody> <tr><td>139.0389</td><td>0.1</td></tr> <tr><td>185.0409</td><td>0.8</td></tr> <tr><td>261.0373</td><td>0.1</td></tr> <tr><td>307.0817</td><td>0.7</td></tr> <tr><td>548.9961</td><td>0.1</td></tr> <tr><td>665.6743</td><td>0.1</td></tr> <tr><td>913.8466</td><td>0.1</td></tr> <tr><td>1086.0335</td><td>0.1</td></tr> <tr><td>1196.0883</td><td>0.1</td></tr> <tr><td>1396.8704</td><td>0.1</td></tr> </tbody> </table>	m/z	Relative Intensity (approx. x10 ³)	139.0389	0.1	185.0409	0.8	261.0373	0.1	307.0817	0.7	548.9961	0.1	665.6743	0.1	913.8466	0.1	1086.0335	0.1	1196.0883	0.1	1396.8704	0.1
m/z	Relative Intensity (approx. x10 ³)																						
139.0389	0.1																						
185.0409	0.8																						
261.0373	0.1																						
307.0817	0.7																						
548.9961	0.1																						
665.6743	0.1																						
913.8466	0.1																						
1086.0335	0.1																						
1196.0883	0.1																						
1396.8704	0.1																						
Rutin	<p>ES-ESI Product Ion (rt: 23.930 min) Frag=130.0V CID@15.0 (609.1498[z=1]->**) vQKAZ_elm_CraL_fI_Et_neg_dompreg_20uld</p> <table border="1"> <caption>Peak Data for Rutin</caption> <thead> <tr> <th>m/z</th> <th>Relative Intensity (approx. x10³)</th> </tr> </thead> <tbody> <tr><td>145.0185</td><td>0.1</td></tr> <tr><td>300.0272</td><td>0.2</td></tr> <tr><td>483.0795</td><td>0.1</td></tr> <tr><td>609.1457</td><td>3.3</td></tr> <tr><td>718.9011</td><td>0.1</td></tr> <tr><td>906.7010</td><td>0.1</td></tr> <tr><td>1327.0126</td><td>0.1</td></tr> </tbody> </table>	m/z	Relative Intensity (approx. x10 ³)	145.0185	0.1	300.0272	0.2	483.0795	0.1	609.1457	3.3	718.9011	0.1	906.7010	0.1	1327.0126	0.1						
m/z	Relative Intensity (approx. x10 ³)																						
145.0185	0.1																						
300.0272	0.2																						
483.0795	0.1																						
609.1457	3.3																						
718.9011	0.1																						
906.7010	0.1																						
1327.0126	0.1																						

Continued **Figure S2:** The fragmentation patterns obtained for all identified compounds.

Proposed compound	MS/MS spectrum
Quinic acid	 <p>ES-ESI Production (rt: 19.900 min) Frag=130.0V CID@15.0 (191.0577[z=1]->**) vQKAZ_elm_Cra_fI_Et_neg_domprep_20uld</p> <p>Major peaks (m/z): 85.0296, 127.0349, 191.0579, 270.3226, 344.3320, 485.1219, 575.2628, 754.2982, 917.6034, 1006.0257, 1194.3129, 1333.0521, 1452.5386</p>
Vitexin 2'' -O-rhamnoside	 <p>ES-ESI Production (rt: 23.359 min) Frag=130.0V CID@15.0 (577.1593[z=1]->**) vQKAZ_elm_Cra_fI_Et_neg_domprep_20uld</p> <p>Major peaks (m/z): 129.0174, 253.0890, 293.0458, 413.0688, 463.0670, 577.5586, 791.5108, 931.1402</p>
Vitexin	 <p>ES-ESI Production (rt: 22.628 min) Frag=130.0V CID@15.0 (431.1007[z=1]->**) vQKAZ_elm_Cra_foL_Et50_neg_domprep_20uld</p> <p>Major peaks (m/z): 57.5774, 135.0459, 219.0021, 311.0569, 431.0987, 595.9148, 708.0624, 958.7904, 1301.5562</p>
Vitexin 4'' -O-glucoside	 <p>ES-ESI Production (rt: 24.751 min) Frag=130.0V CID@25.0 (593.1531[z=1]->**) vQKAZ_elm_Cra_fI_Et_neg_domprep_20uld</p> <p>Major peaks (m/z): 45.0006, 123.0426, 285.0395, 405.0254, 507.0491, 593.1517, 814.9070, 1491.9950</p>

Continued **Figure S2:** The fragmentation patterns obtained for all identified compounds.



Continued **Figure S2:** The fragmentation patterns obtained for all identified compounds.

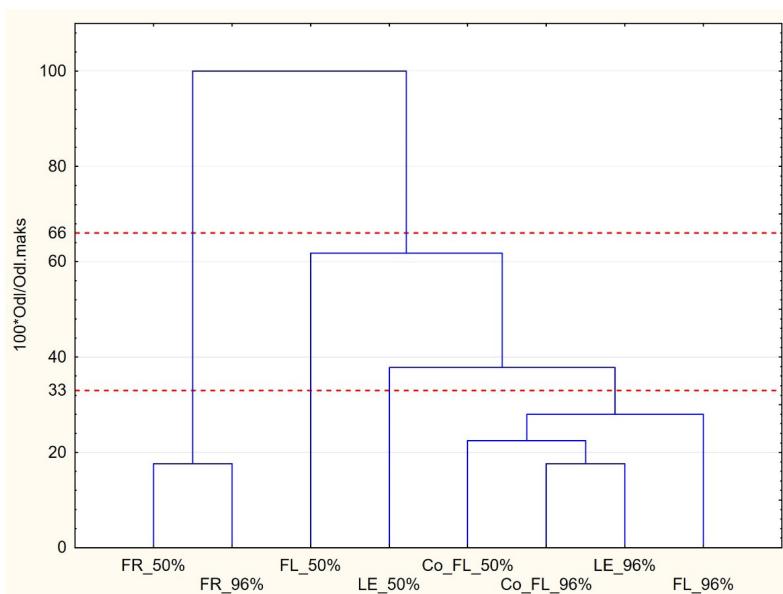


Figure S3: A dendrogram depicting the similarities between the obtained extracts (*C. almatensis*: FR – fruit extract, FL – flower extract, LE – leaf extract; *C. oxyacantha* – Co_FL – flower extract).