

**Supplementary Table S2** Identification of phenolic compounds in American pokeweed in negative ionization with HPLC-MS and MS<sup>2</sup>/MS<sup>3</sup>

Phenolic group	$\lambda$ (nm)	[M-H] <sup>-</sup> ( <i>m/z</i> )	MS <sup>2</sup> ( <i>m/z</i> )	MS <sup>3</sup> ( <i>m/z</i> )
<b>Hydroxycinnamic acid derivatives</b>				
3- <i>p</i> -Coumaroylquinic acid	312	337	163	
3-Feruloylquinic acid	320	367	193,134	149
3-Caffeoylquinic acid	234, 326	353	191, 179, 135	173, 127, 85
4-Caffeoylquinic acid	234, 328	353	173, 179	
4- <i>p</i> -Coumaroylquinic acid	312	337	173, 163, 155, 137, 191	
5-Caffeoylquinic acid 1	234,328	353	191,179,135	173,127,85
5-Caffeoylquinic acid 2	234,328	353	191,179,135	
5- <i>p</i> -Coumaroylquinic acid 1	312	337	191,173,163	
5- <i>p</i> -Coumaroylquinic acid 2	311	337	191,163,173	
Dicaffeoylquinic acid 1	246,316	515	353	179,173
Dicaffeoylquinic acid 2	246, 316	515	353	179,173
<i>p</i> -Coumaric acid hexoside	322,275	325	163,119	
<i>p</i> -Coumaric acid	310	163	119	
<b>Flavanols</b>				
Epicatechin	234,279	289	245	
Catechin	234,279	289	245	
Catechin gallate	235,280	441	289,169,135	
Catechin hexoside	235,280	451	289	
<b>Flavones</b>				
Apigenin dihexoside	268,331	431	269	
<b>Flavonols</b>				
Kaempferol glucuronyl dihexoside	348, 265	785	609	285
Kaempferol glucuronyl pentoside hexoside	347, 266	755	579	285
Kaempferol hexoside	266,346	447	285	
Kaempferol-3-rutinoside	264,345	593	285	
Kaempferol pentosyl hexoside	266, 347	579	447	285
Kaempferol rhamnosyl dihexoside	265, 346	755	609	285
Quercetin-3-xyloside	356,255	433	301	
Quercetin-3-arabinofuranoside	355,255	433	301	
Quercetin dihexoside	255,356	625	301	
Quercetin pentosyl hexoside 1	256,355	595	463	301
Quercetin pentosyl hexoside 2	256,356	595	463	301
Quercetin rhamnosyl hexoside	255,355	609	463	301
Quercetin-3-glucoside	255,355	463	301	
<b>Stilbenes</b>				
Piceatannol hexoside 1	324	405	243	
Piceatannol hexoside 2	324	405	243	
Piceatannol hexoside 3	324	405	243	