Rapid Species-level Identification of *Salvias* by Chemometric Processing of Ambient Ionization Mass Spectrometry-derived Chemical Profiles

SUPPORTING MATERIAL

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This document contains thirty-six additional figures and five tables of supporting information associated with the entitled article. The figures show DART-HRMS in-source CID spectral data and GC-MS spectral data of *Salvia* plant material compared to authentic chemical standards used for confirmation of the presence or absence of biomarkers. The tables contain information on plant spectra including accurate masses and relative abundances of various peaks, as well as relevant biomarker peak information.

Figures

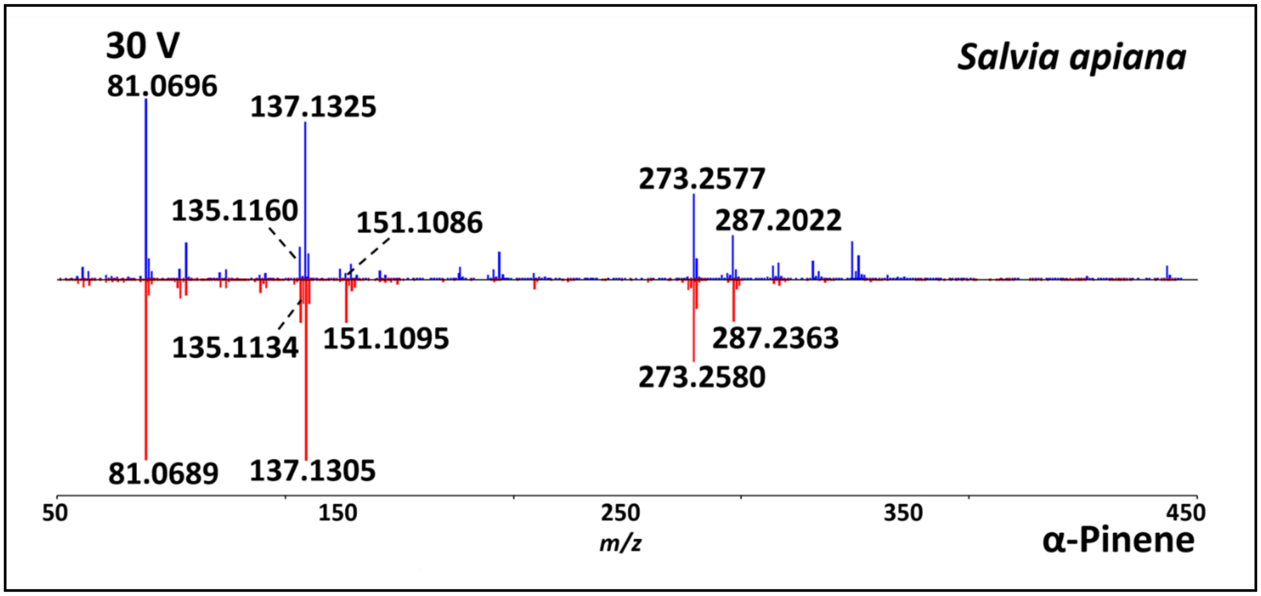

Figure S-1. Head-to-tail plot depicting positive-ion mode in-source CID DART-HRMS spectra of plant material for the purpose of identifying biomarkers. The top spectrum depicts *S. apiana* fresh plant material analyzed at 30 V and the spectrum on the bottom of the panel is the chemical standard α-pinene tested at the same voltage. The presence of the peaks from the standard in the plant material indicates that the biomarker is found in the plant. The top spectrum (plant material) represent an average of 5 individual leaf spectra. The bottom spectra (chemical standard) represent an average of 3 individual analyses.

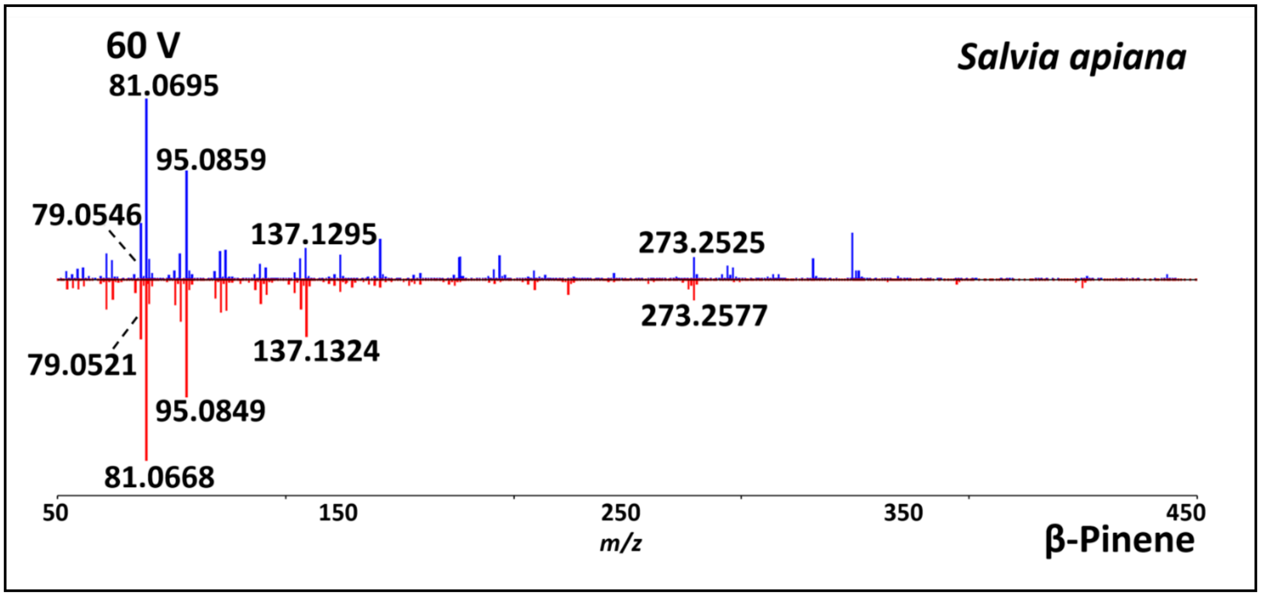

Figure S-2. Head-to-tail plot depicting positive-ion mode in-source CID DART-HRMS spectra of plant material for the purpose of identifying biomarkers. The top spectrum depicts *S. apiana* fresh plant material analyzed at 60 V and the spectrum on the bottom of the panel is the chemical standard β-pinene tested at the same voltage. The presence of the peaks from the standard in the plant material indicates that the biomarker is found in the plant. The top spectrum (plant material) represent an average of 5 individual leaf spectra. The bottom spectra (chemical standard) represent an average of 3 individual analyses.

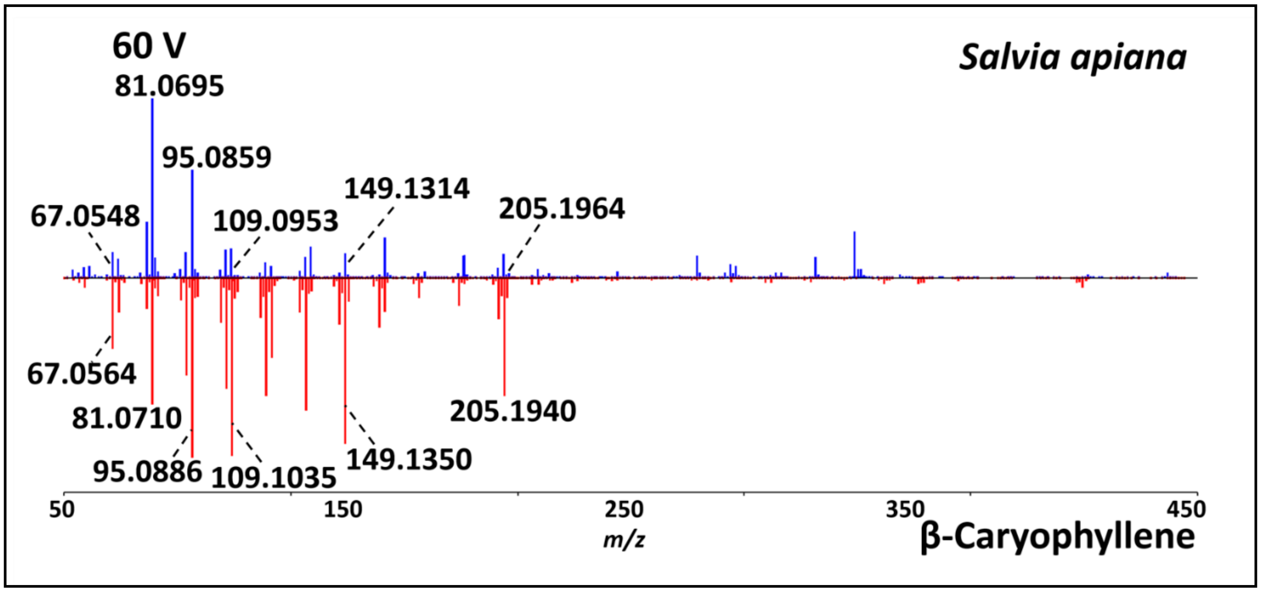

Figure S-3. Head-to-tail plot depicting positive-ion mode in-source CID DART-HRMS spectra of plant material for the purpose of identifying biomarkers. The top spectrum depicts *S. apiana* fresh plant material analyzed at 60 V and the spectrum on the bottom of the panel is the chemical standard β-caryophyllene tested at the same voltage. The presence of the peaks from the standard in the plant material indicates that the biomarker is found in the plant. The top spectrum (plant material) represent an average of 5 individual leaf spectra. The bottom spectra (chemical standard) represent an average of 3 individual analyses.

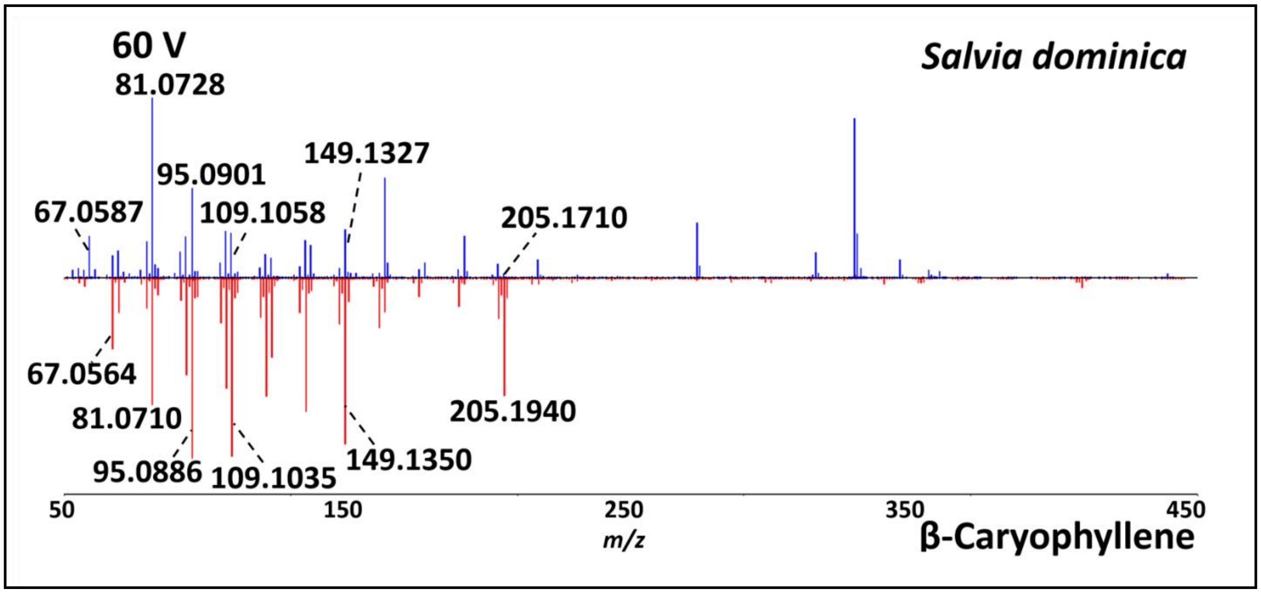

Figure S-4. Head-to-tail plot depicting positive-ion mode in-source CID DART-HRMS spectra of plant material for the purpose of identifying biomarkers. The top spectrum depicts *S. dominica* fresh plant material analyzed at 60 V and the spectrum on the bottom of the panel is the chemical standard β-caryophyllene tested at the same voltage. The presence of the peaks from the standard in the plant material indicates that the biomarker is found in the plant. The top spectrum (plant material) represent an average of 5 individual leaf spectra. The bottom spectra (chemical standard) represent an average of 3 individual analyses.

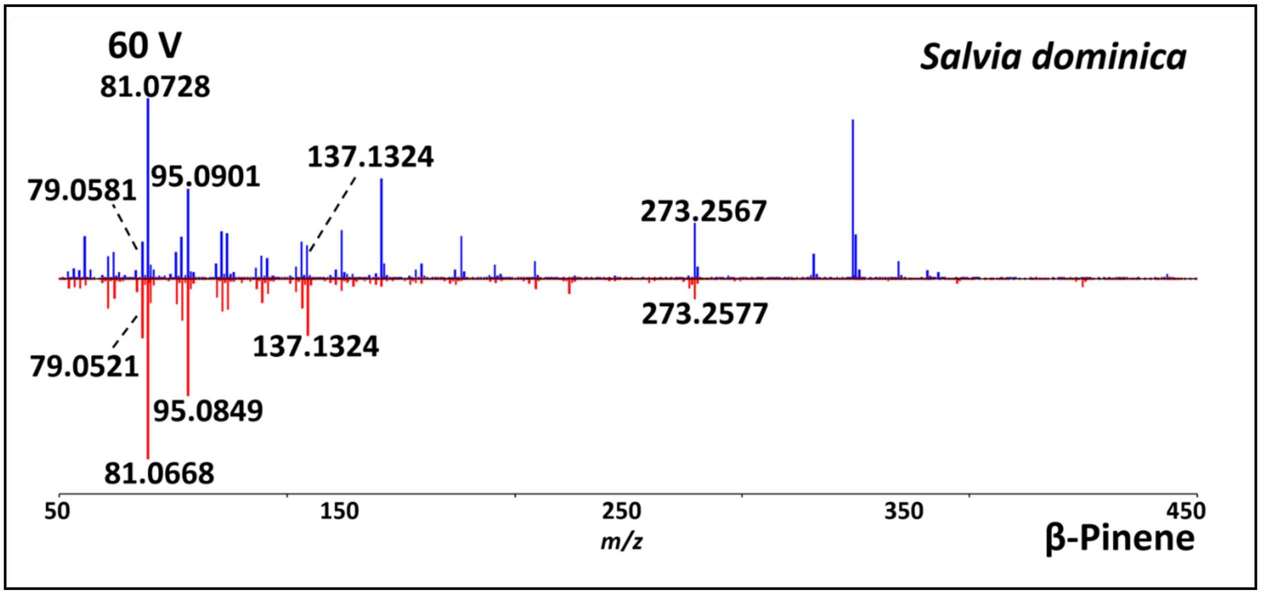

Figure S-5. Head-to-tail plot depicting positive-ion mode in-source CID DART-HRMS spectra of plant material for the purpose of identifying biomarkers. The top spectrum depicts *S. dominica* fresh plant material analyzed at 60 V and the spectrum on the bottom of the panel is the chemical standard β-pinene tested at the same voltage. The presence of the peaks from the standard in the plant material indicates that the biomarker is found in the plant. The top spectrum (plant material) represent an average of 5 individual leaf spectra. The bottom spectra (chemical standard) represent an average of 3 individual analyses.

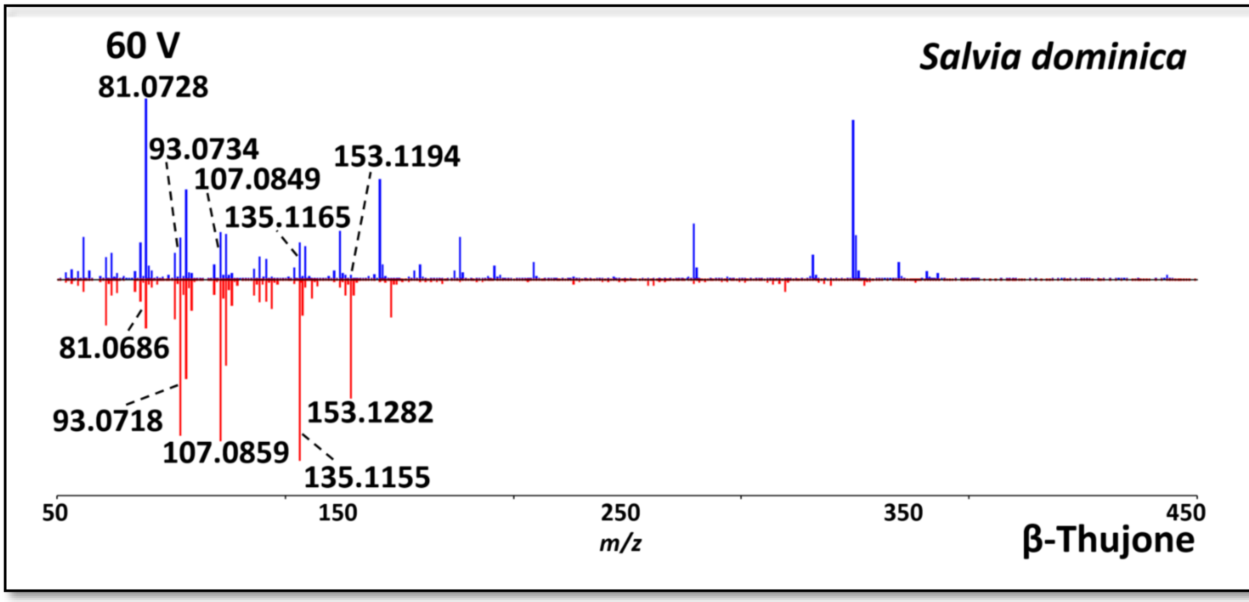

Figure S-6. Head-to-tail plot depicting positive-ion mode in-source CID DART-HRMS spectra of plant material for the purpose of identifying biomarkers. The top spectrum depicts *S. dominica* fresh plant material analyzed at 60 V and the spectrum on the bottom of the panel is the chemical standard β-thujone tested at the same voltage. The presence of the peaks from the standard in the plant material indicates that the biomarker is found in the plant. The top spectrum (plant material) represent an average of 5 individual leaf spectra. The bottom spectra (chemical standard) represent an average of 3 individual analyses.

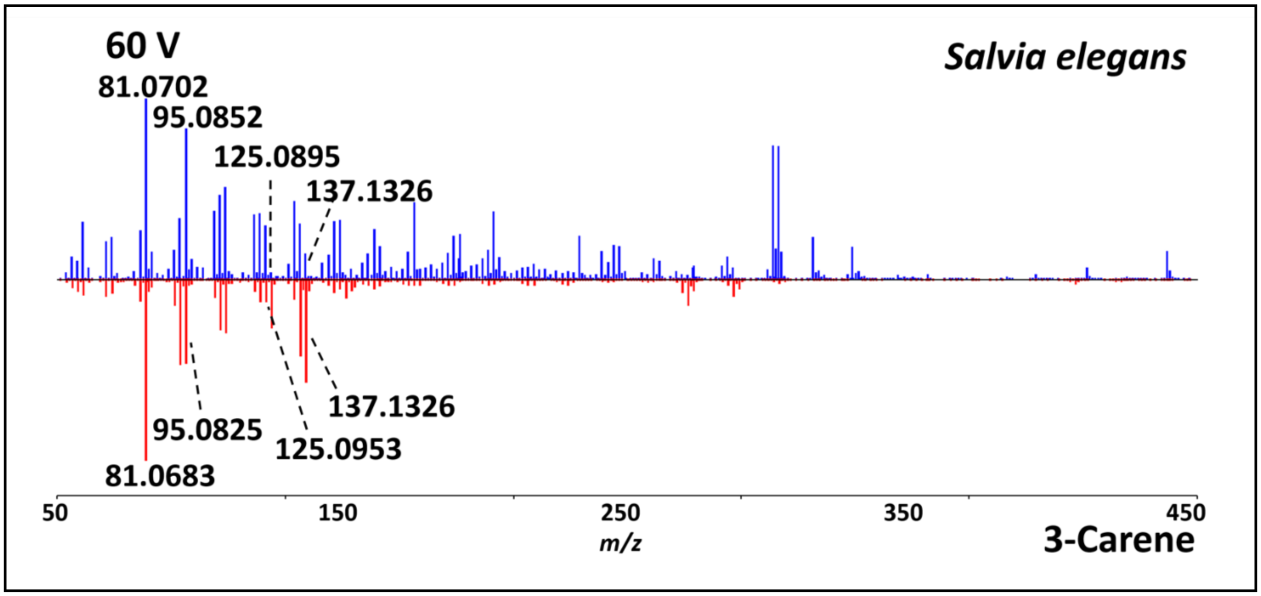

Figure S-7. Head-to-tail plot depicting positive-ion mode in-source CID DART-HRMS spectra of plant material for the purpose of identifying biomarkers. The top spectrum depicts *S. elegans* fresh plant material analyzed at 60 V and the spectrum on the bottom of the panel is the chemical standard 3-carene tested at the same voltage. The presence of the peaks from the standard in the plant material indicates that the biomarker is found in the plant. The top spectrum (plant material) represent an average of 5 individual leaf spectra. The bottom spectra (chemical standard) represent an average of 3 individual analyses.

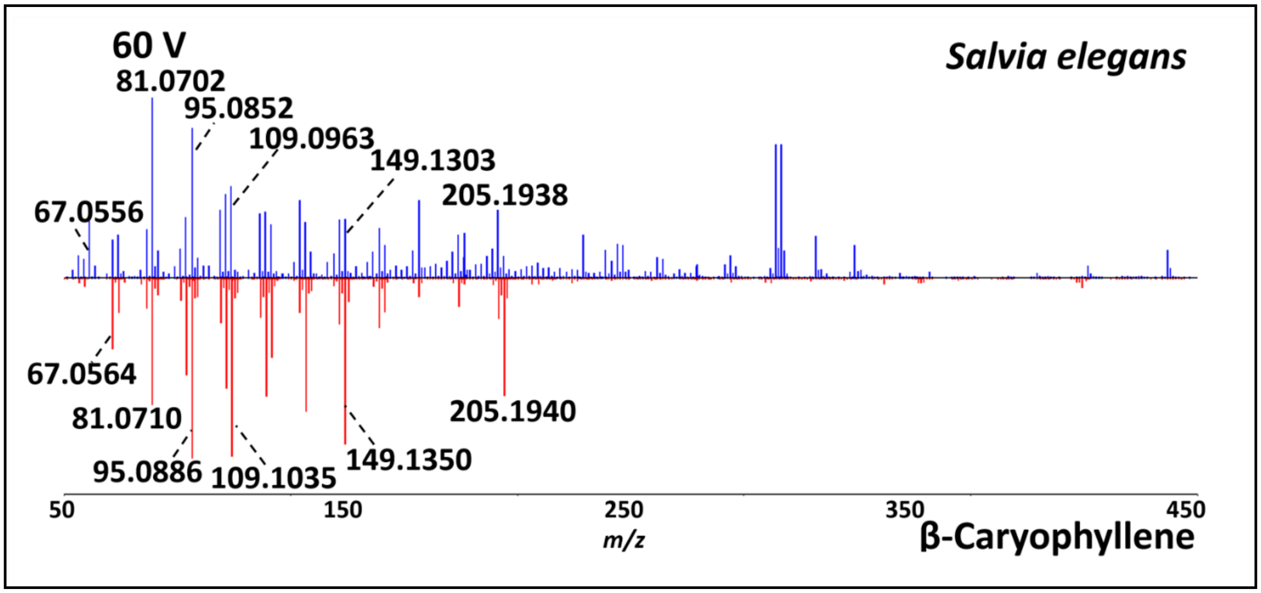

Figure S-8. Head-to-tail plot depicting positive-ion mode in-source CID DART-HRMS spectra of plant material for the purpose of identifying biomarkers. The top spectrum depicts *S. elegans* fresh plant material analyzed at 60 V and the spectrum on the bottom of the panel is the chemical standard β-caryophyllene tested at the same voltage. The presence of the peaks from the standard in the plant material indicates that the biomarker is found in the plant. The top spectrum (plant material) represent an average of 5 individual leaf spectra. The bottom spectra (chemical standard) represent an average of 3 individual analyses.

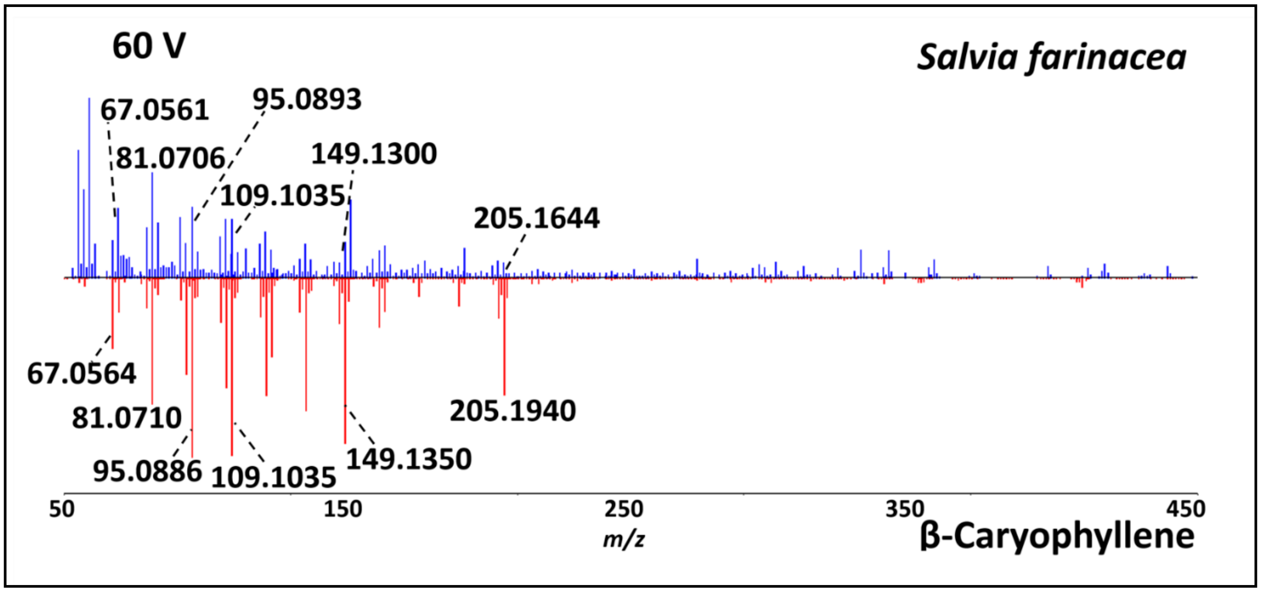

Figure S-9. Head-to-tail plot depicting positive-ion mode in-source CID DART-HRMS spectra of plant material for the purpose of identifying biomarkers. The top spectrum depicts *S. farinacea* fresh plant material analyzed at 60 V and the spectrum on the bottom of the panel is the chemical standard β-caryophyllene tested at the same voltage. The presence of the peaks from the standard in the plant material indicates that the biomarker is found in the plant. The top spectrum (plant material) represent an average of 5 individual leaf spectra. The bottom spectra (chemical standard) represent an average of 3 individual analyses.

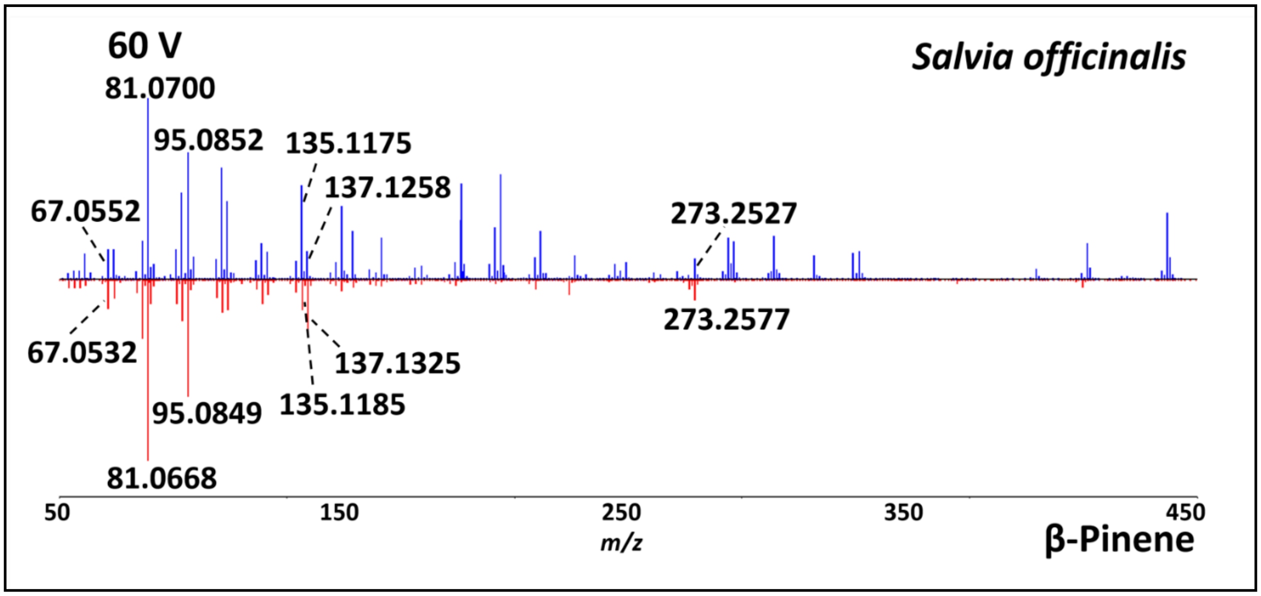

Figure S-10. Head-to-tail plot depicting positive-ion mode in-source CID DART-HRMS spectra of plant material for the purpose of identifying biomarkers. The top spectrum depicts *S. officinalis* fresh plant material analyzed at 60 V and the spectrum on the bottom of the panel is the chemical standard β-pinene tested at the same voltage. The presence of the peaks from the standard in the plant material indicates that the biomarker is found in the plant. The top spectrum (plant material) represent an average of 5 individual leaf spectra. The bottom spectra (chemical standard) represent an average of 3 individual analyses.

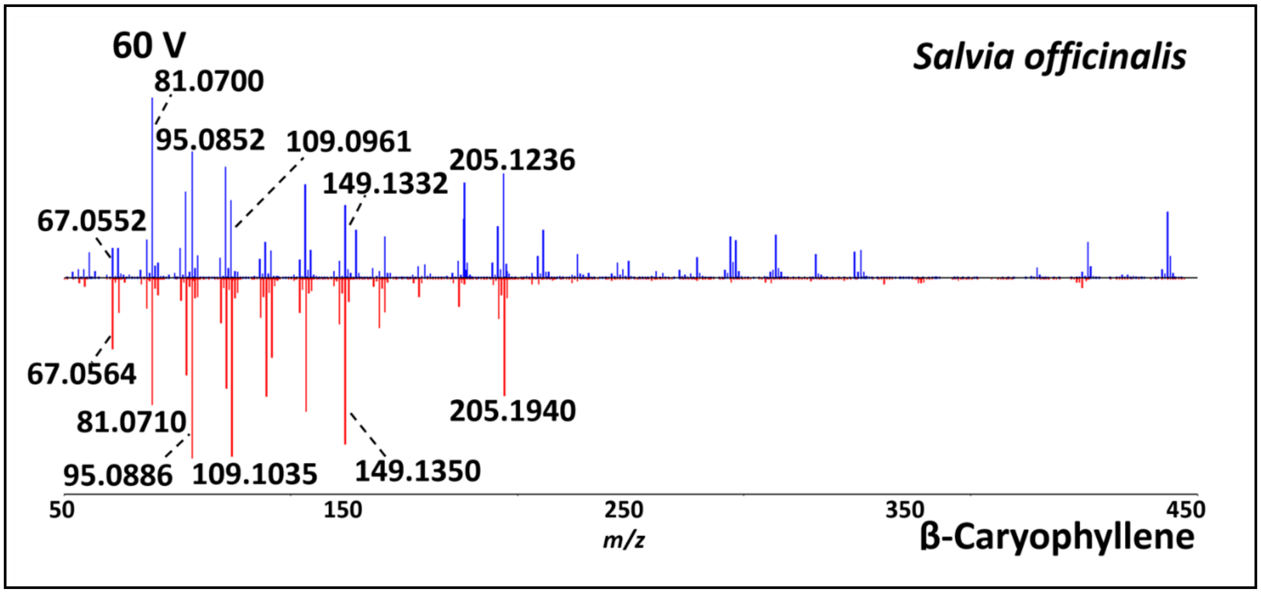

Figure S-11. Head-to-tail plot depicting positive-ion mode in-source CID DART-HRMS spectra of plant material for the purpose of identifying biomarkers. The top spectrum depicts *S. officinalis* fresh plant material analyzed at 60 V and the spectrum on the bottom of the panel is the chemical standard β-caryophyllene tested at the same voltage. The presence of the peaks from the standard in the plant material indicates that the biomarker is found in the plant. The top spectrum (plant material) represent an average of 5 individual leaf spectra. The bottom spectra (chemical standard) represent an average of 3 individual analyses.

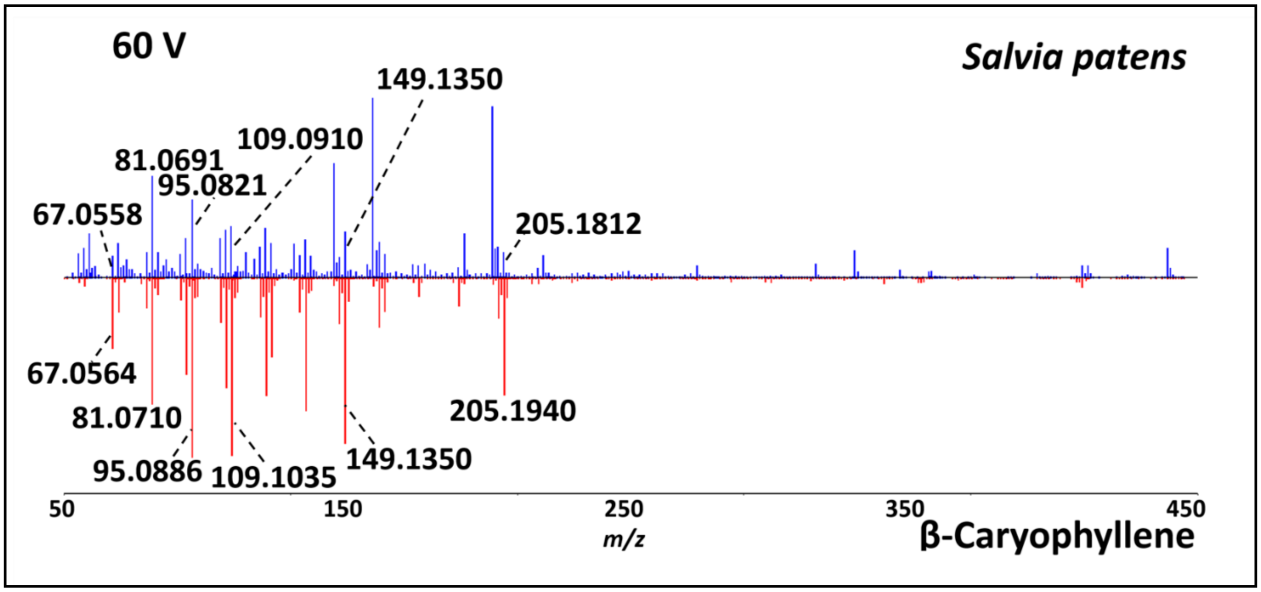

Figure S-12. Head-to-tail plot depicting positive-ion mode in-source CID DART-HRMS spectra of plant material for the purpose of identifying biomarkers. The top spectrum depicts *S. patens* fresh plant material analyzed at 60 V and the spectrum on the bottom of the panel is the chemical standard β-caryophyllene tested at the same voltage. The presence of the peaks from the standard in the plant material indicates that the biomarker is found in the plant. The top spectrum (plant material) represent an average of 10 individual leaf spectra. The bottom spectra (chemical standard) represent an average of 3 individual analyses.

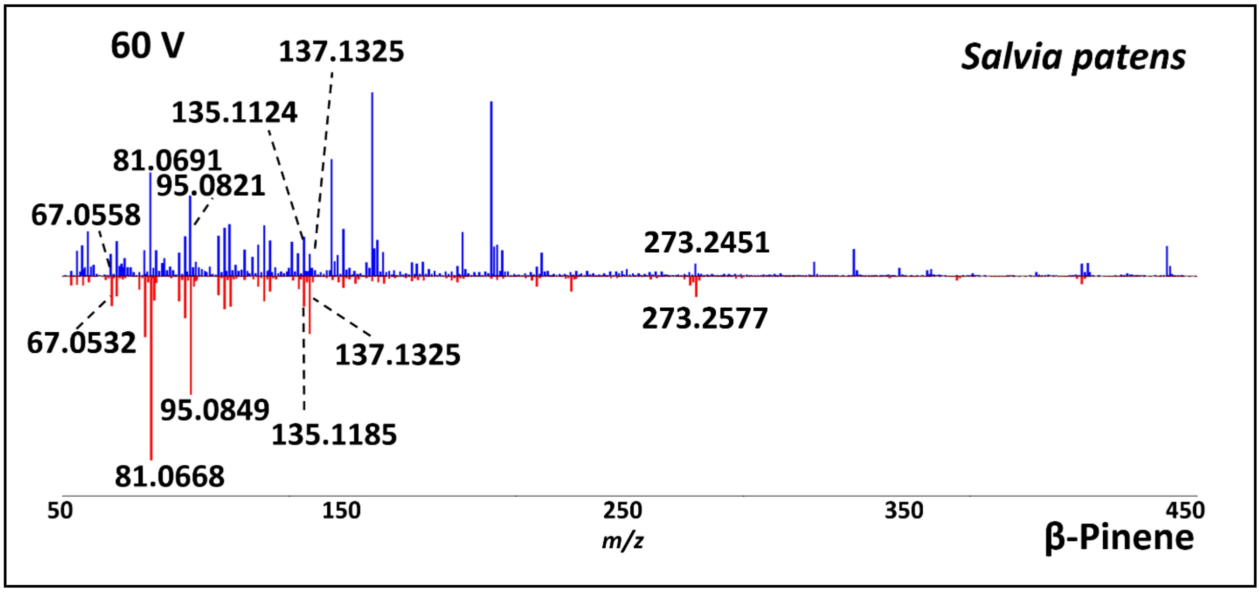

Figure S-13. Head-to-tail plot depicting positive-ion mode in-source CID DART-HRMS spectra of plant material for the purpose of identifying biomarkers. The top spectrum depicts *S. patens* fresh plant material analyzed at 60 V and the spectrum on the bottom of the panel is the chemical standard β-pinene tested at the same voltage. The presence of the peaks from the standard in the plant material indicates that the biomarker is found in the plant. The top spectrum (plant material) represent an average of 10 individual leaf spectra. The bottom spectra (chemical standard) represent an average of 3 individual analyses.

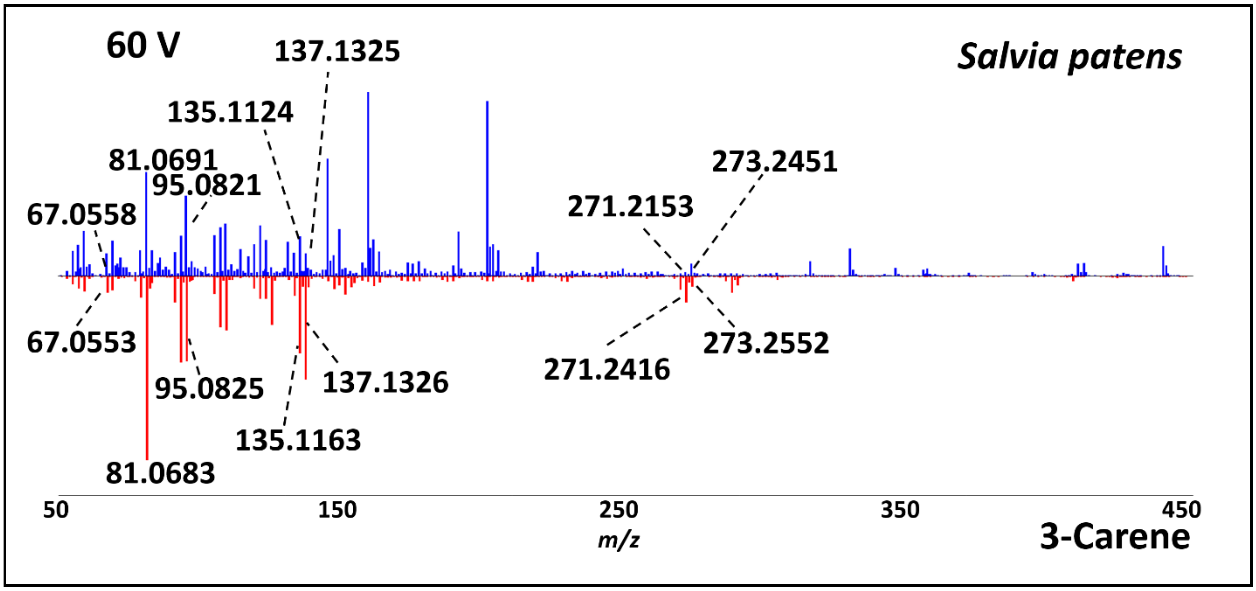

Figure S-14. Head-to-tail plot depicting positive-ion mode in-source CID DART-HRMS spectra of plant material for the purpose of identifying biomarkers. The top spectrum depicts *S. patens* fresh plant material analyzed at 60 V and the spectrum on the bottom of the panel is the chemical standard 3-carene tested at the same voltage. The presence of the peaks from the standard in the plant material indicates that the biomarker is found in the plant. The top spectrum (plant material) represent an average of 10 individual leaf spectra. The bottom spectra (chemical standard) represent an average of 3 individual analyses.

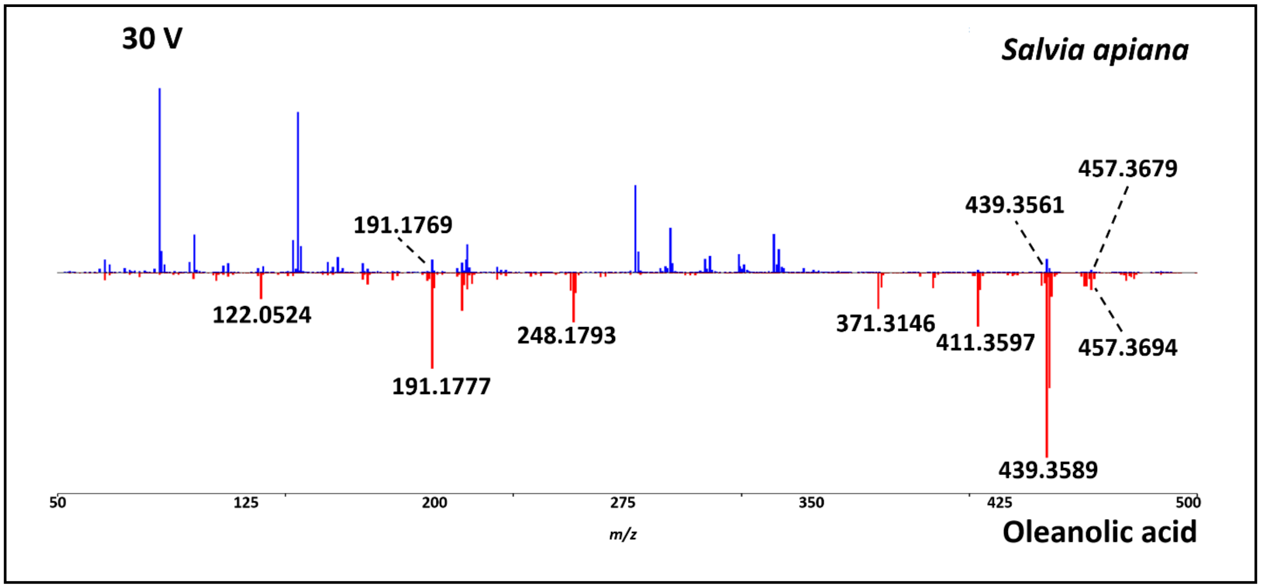

Figure S-15. Head-to-tail plot showing positive-ion mode in-source CID DART-HRMS spectra of *S. apiana* fresh leaf material (top spectrum) compared to that of an oleanolic acid standard (bottom spectrum), both analyzed at 30 V. The absence in the *S. apiana* spectrum of diagnostic oleanolic acid fragment peaks, indicates that oleanolic acid was not detected in the plant material. The top panel represents an average of 5 individual leaf analyses and the bottom panel depicts an average of 3 analyses of the standard.

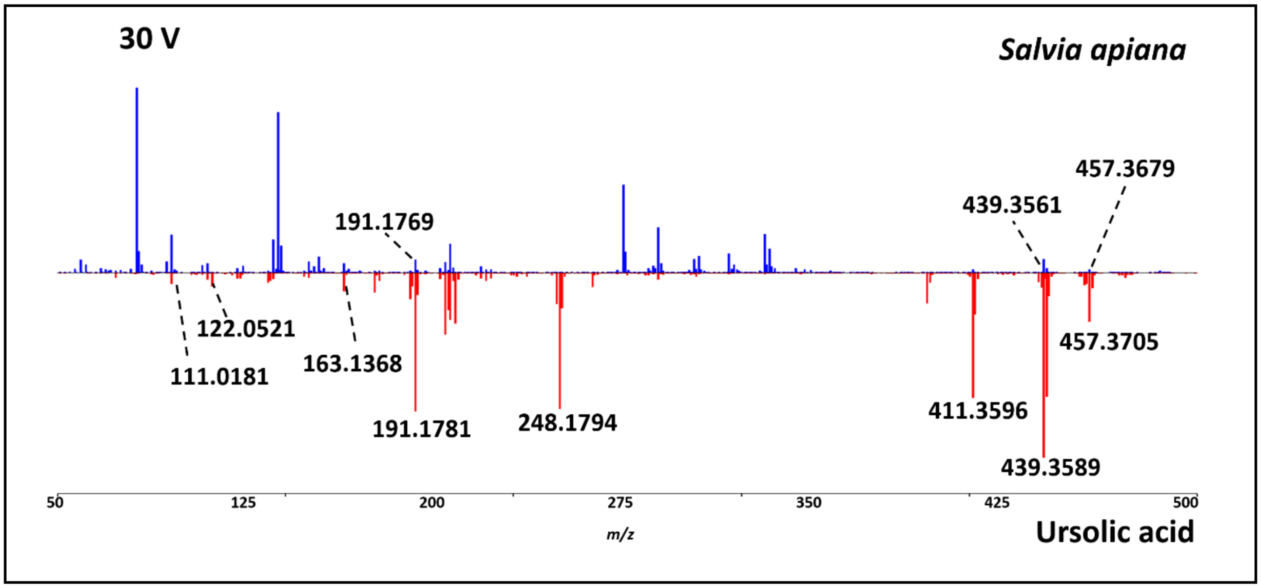

Figure S-16. Head-to-tail plot showing positive-ion mode in-source CID DART-HRMS spectra of *S. apiana* fresh leaf material (top spectrum) compared to that of an ursolic acid standard (bottom spectrum), both analyzed at 30 V. The absence in the *S. apiana* spectrum of diagnostic ursolic acid fragment peaks, indicates that ursolic acid was not detected in the plant material. The top panel represents an average of 5 individual leaf analyses and the bottom panel depicts an average of 3 analyses of the standard.

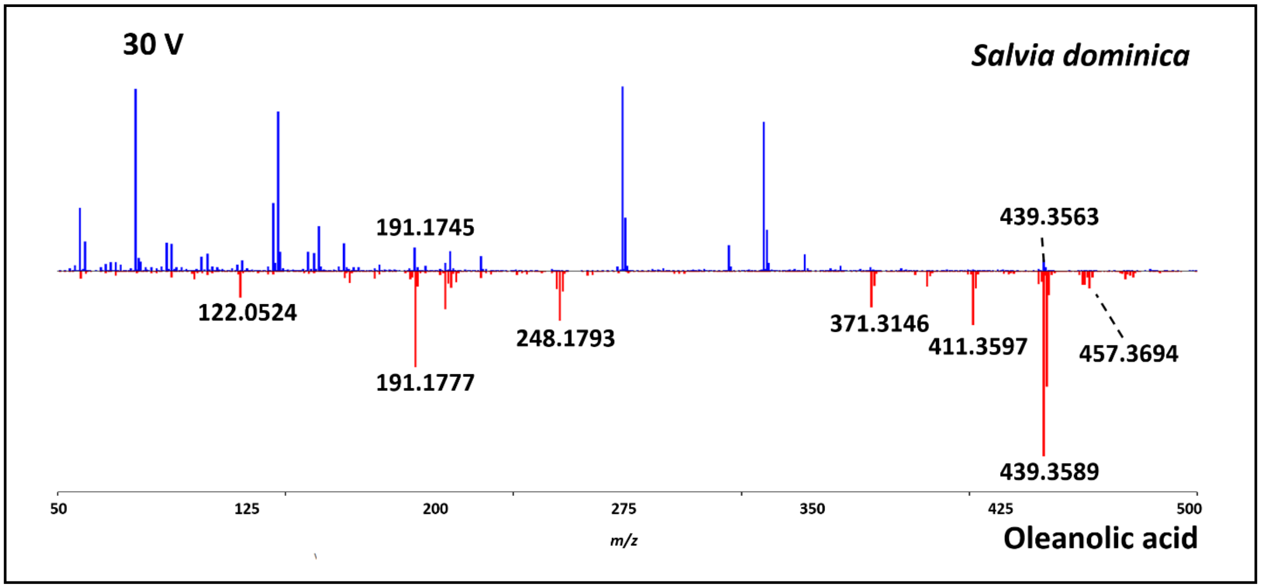

Figure S-17. Head-to-tail plot showing positive-ion mode in-source CID DART-HRMS spectra of *S. dominica* fresh leaf material (top spectrum) compared to that of an oleanolic acid standard (bottom spectrum), both analyzed at 30 V. The absence in the *S. dominica* spectrum of diagnostic oleanolic acid fragment peaks, indicates that oleanolic acid was not detected in the plant material. The top panel represents an average of 5 individual leaf analyses and the bottom panel depicts an average of 3 analyses of the standard.

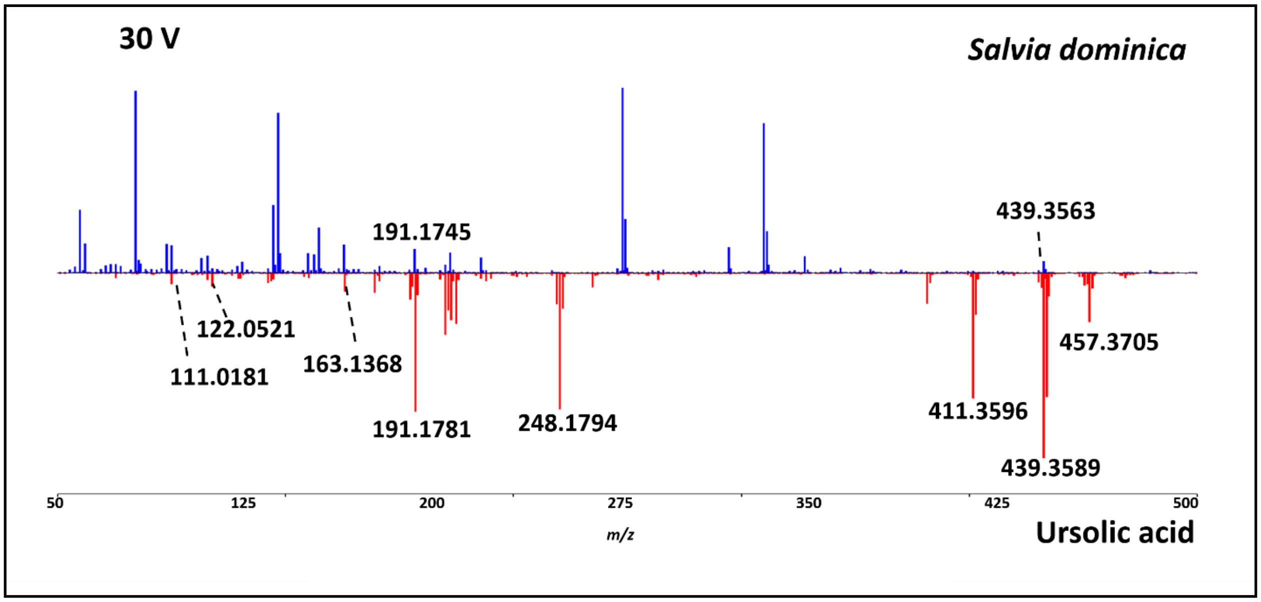

Figure S-18. Head-to-tail plot showing positive-ion mode in-source CID DART-HRMS spectra of *S. dominica* fresh leaf material (top spectrum) compared to that of an ursolic acid standard (bottom spectrum), both analyzed at 30 V. The absence in the *S. dominica* spectrum of diagnostic ursolic acid fragment peaks, indicates that ursolic acid was not detected in the plant material. The top panel represents an average of 5 individual leaf analyses and the bottom panel depicts an average of 3 analyses of the standard.

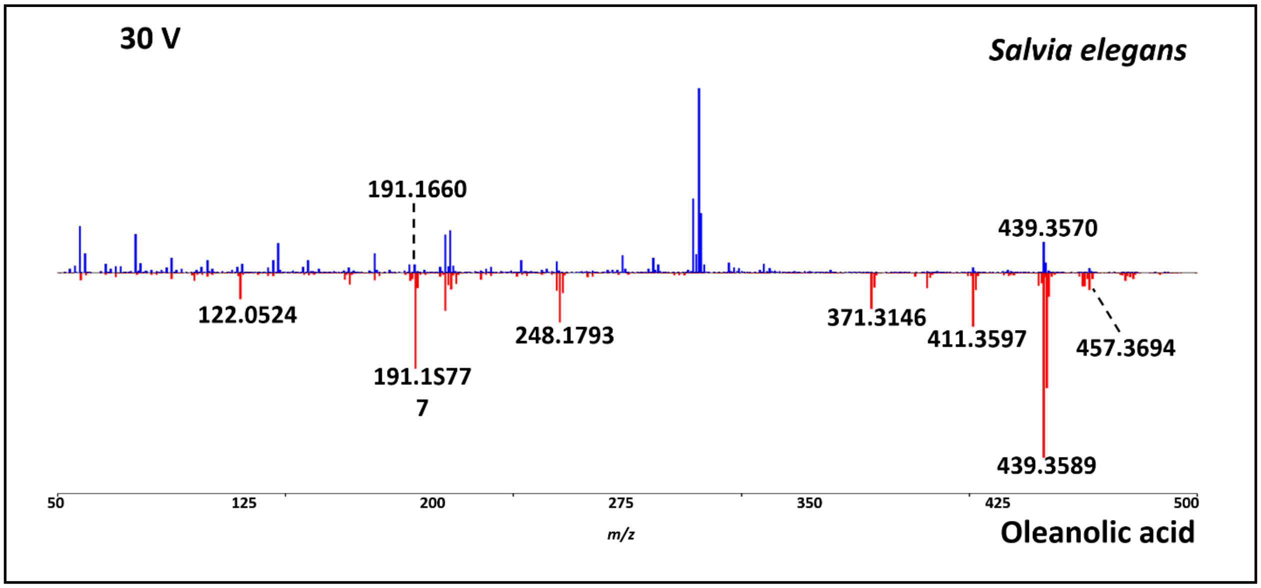

Figure S-19. Head-to-tail plot showing positive-ion mode in-source CID DART-HRMS spectra of *S. elegans* fresh leaf material (top spectrum) compared to that of an oleanolic acid standard (bottom spectrum), both analyzed at 30 V. The absence in the *S. elegans* spectrum of diagnostic oleanolic acid fragment peaks, indicates that oleanolic acid was not detected in the plant material. The top panel represents an average of 5 individual leaf analyses and the bottom panel depicts an average of 3 analyses of the standard.

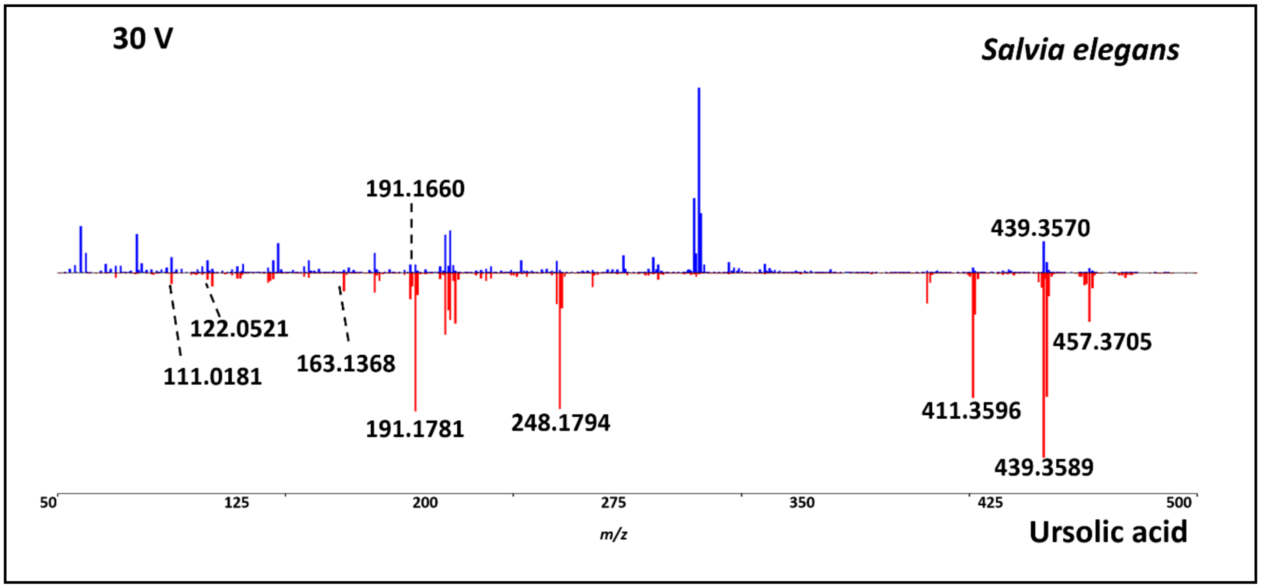

Figure S-20. Head-to-tail plot showing positive-ion mode in-source CID DART-HRMS spectra of *S. elegans* fresh leaf material (top spectrum) compared to that of an ursolic acid standard (bottom spectrum), both analyzed at 30 V. The absence in the *S. elegans* spectrum of diagnostic ursolic acid fragment peaks, indicates that oleanolic acid was not detected in the plant material. The top panel represents an average of 5 individual leaf analyses and the bottom panel depicts an average of 3 analyses of the standard.

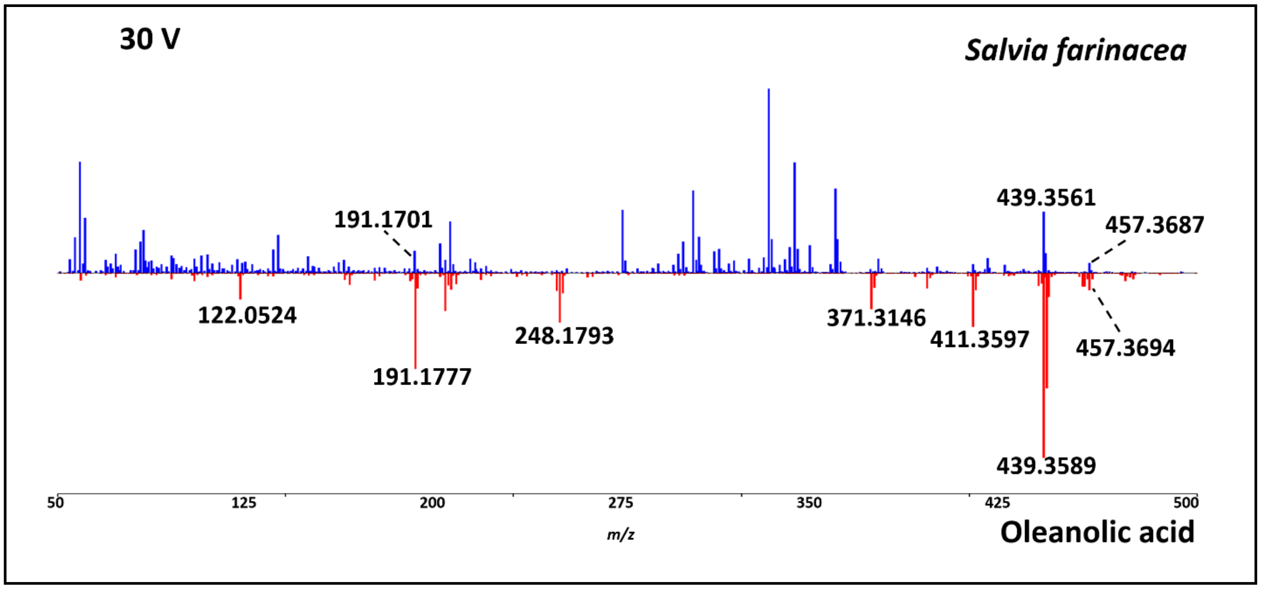

Figure S-21. Head-to-tail plot showing positive-ion mode in-source CID DART-HRMS spectra of *S. farinacea* fresh leaf material (top spectrum) compared to that of an oleanolic acid standard (bottom spectrum), both analyzed at 30 V. The absence in the *S. farinacea* spectrum of diagnostic oleanolic acid fragment peaks, indicates that oleanolic acid was not detected in the plant material. The top panel represents an average of 5 individual leaf analyses and the bottom panel depicts an average of 3 analyses of the standard.

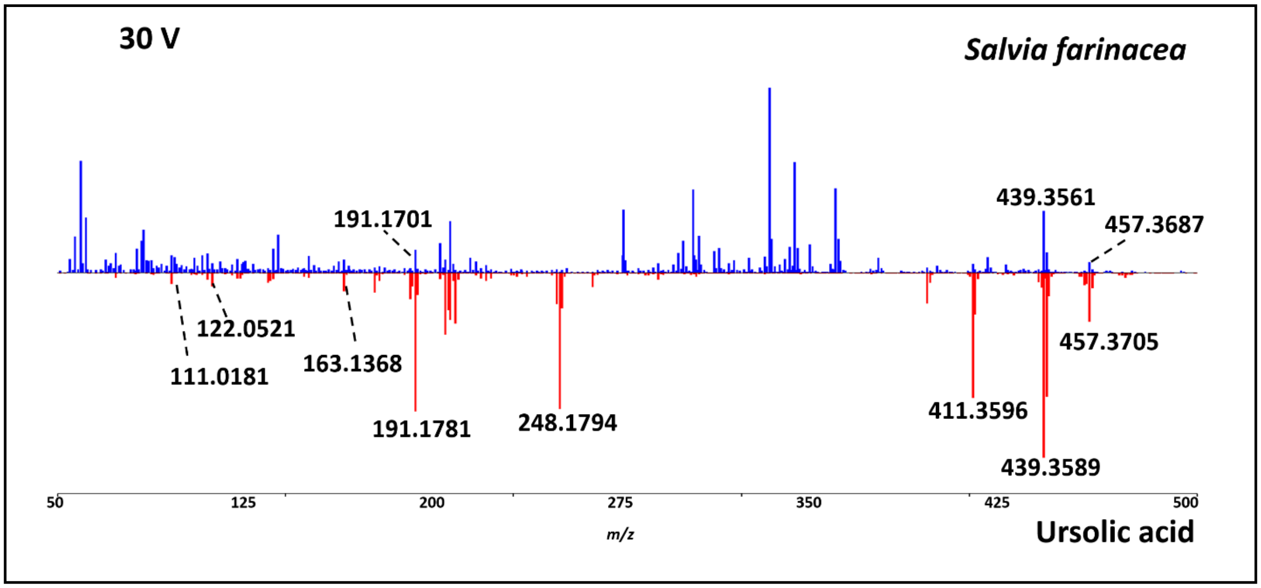

Figure S-22. Head-to-tail plot showing positive-ion mode in-source CID DART-HRMS spectra of *S. farinacea* fresh leaf material (top spectrum) compared to that of an ursolic acid standard (bottom spectrum), both analyzed at 30 V. The absence in the *S. farinacea* spectrum of diagnostic ursolic acid fragment peaks, indicates that ursolic acid was not detected in the plant material. The top panel represents an average of 5 individual leaf analyses and the bottom panel depicts an average of 3 analyses of the standard.

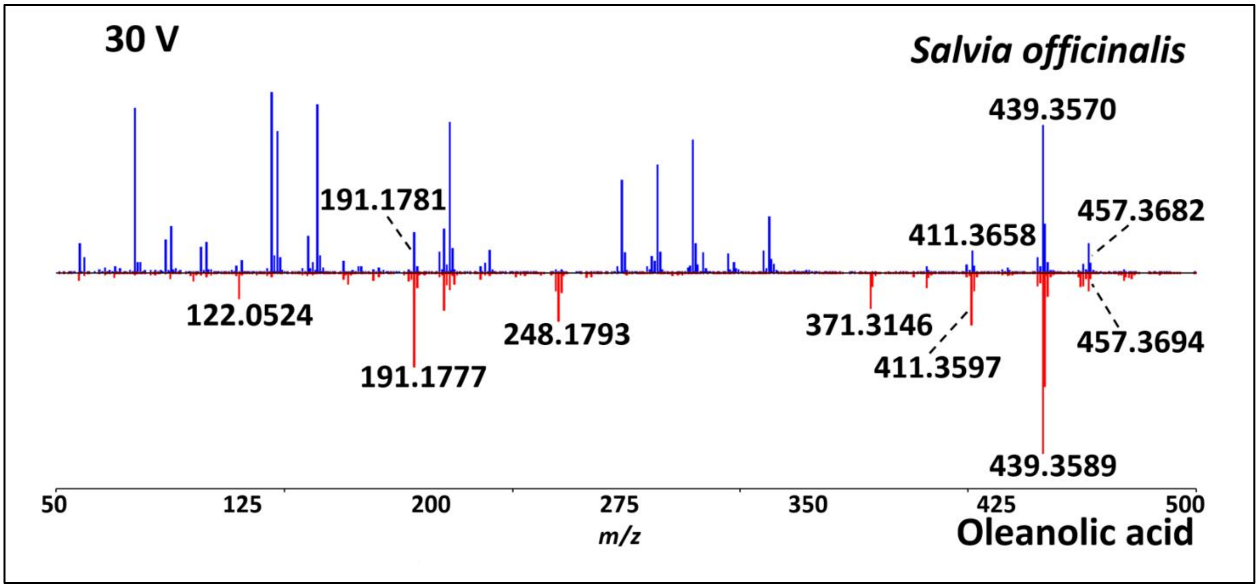

Figure S-23. Head-to-tail plot showing positive-ion mode in-source CID DART-HRMS spectra of *S. officinalis* fresh leaf material (top spectrum) compared to that of an oleanolic acid standard (bottom spectrum), both analyzed at 30 V. The absence in the *S. officinalis* spectrum of diagnostic oleanolic acid fragment peaks, indicates that oleanolic acid was not detected in the plant material. The top panel represents an average of 5 individual leaf analyses and the bottom panel depicts an average of 3 analyses of the standard.

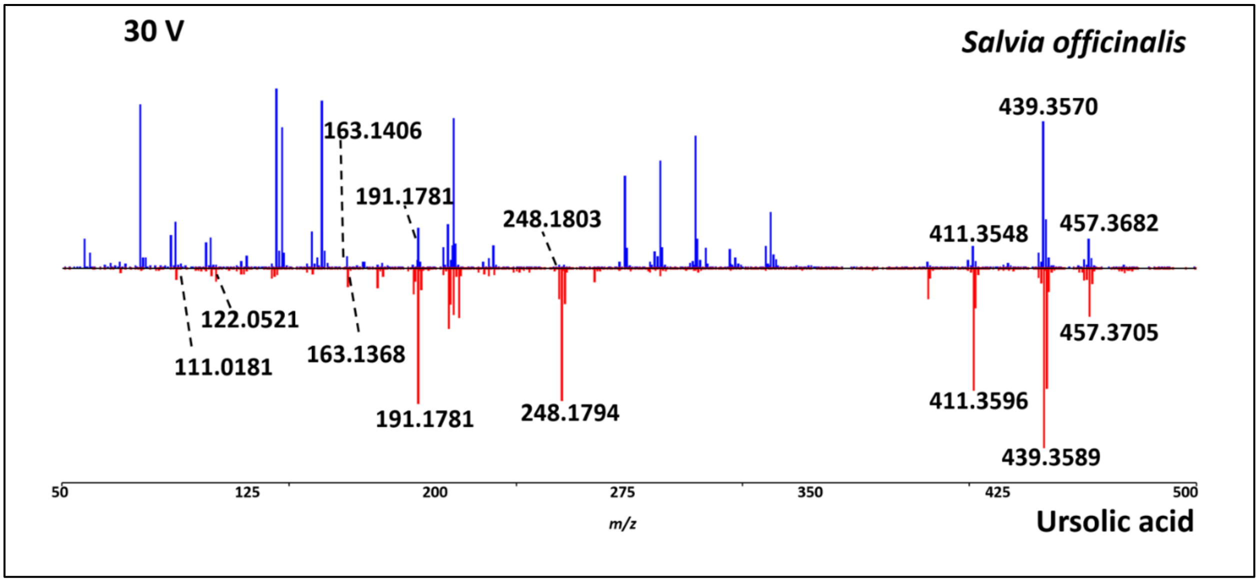

Figure S-24. Head-to-tail plot showing positive-ion mode in-source CID DART-HRMS spectra of *S. officinalis* fresh leaf material (top spectrum) compared to that of an ursolic acid standard (bottom spectrum), both analyzed at 30 V. The absence in the *S. officinalis* spectrum of diagnostic ursolic acid fragment peaks, indicates that ursolic acid was not detected in the plant material. The top panel represents an average of 5 individual leaf analyses and the bottom panel depicts an average of 3 analyses of the standard.

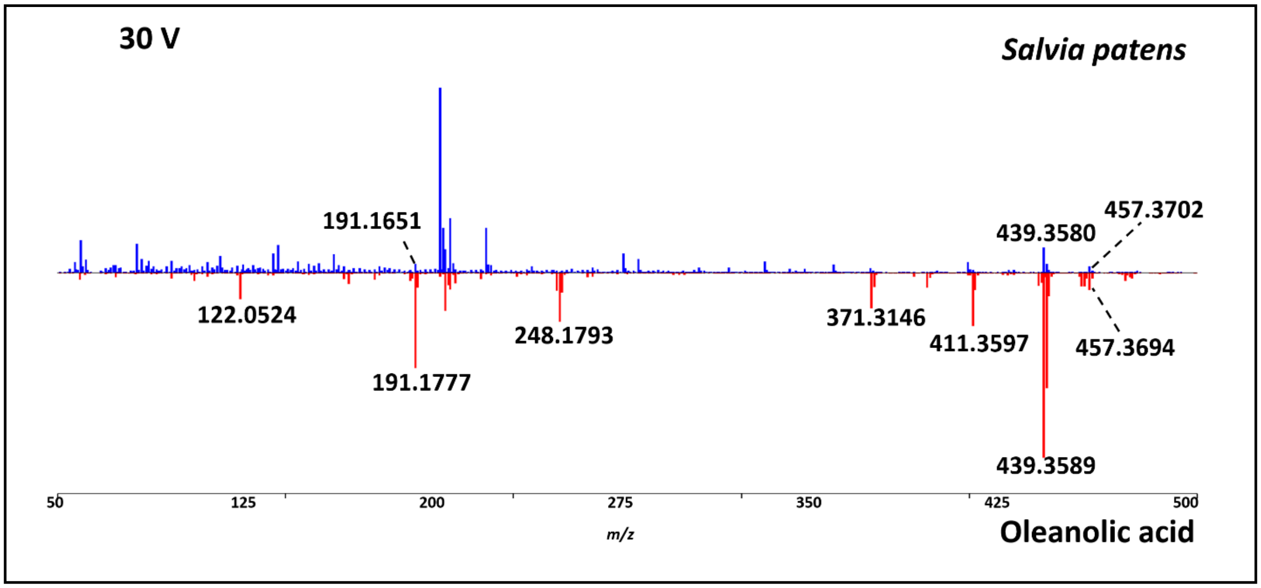

Figure S-25. Head-to-tail plot showing positive-ion mode in-source CID DART-HRMS spectra of *S. patens* fresh leaf material (top spectrum) compared to that of an oleanolic acid standard (bottom spectrum), both analyzed at 30 V. The absence in the *S. patens* spectrum of diagnostic oleanolic acid fragment peaks, indicates that oleanolic acid was not detected in the plant material. The top panel represents an average of 10 individual leaf analyses and the bottom panel depicts an average of 3 analyses of the standard.

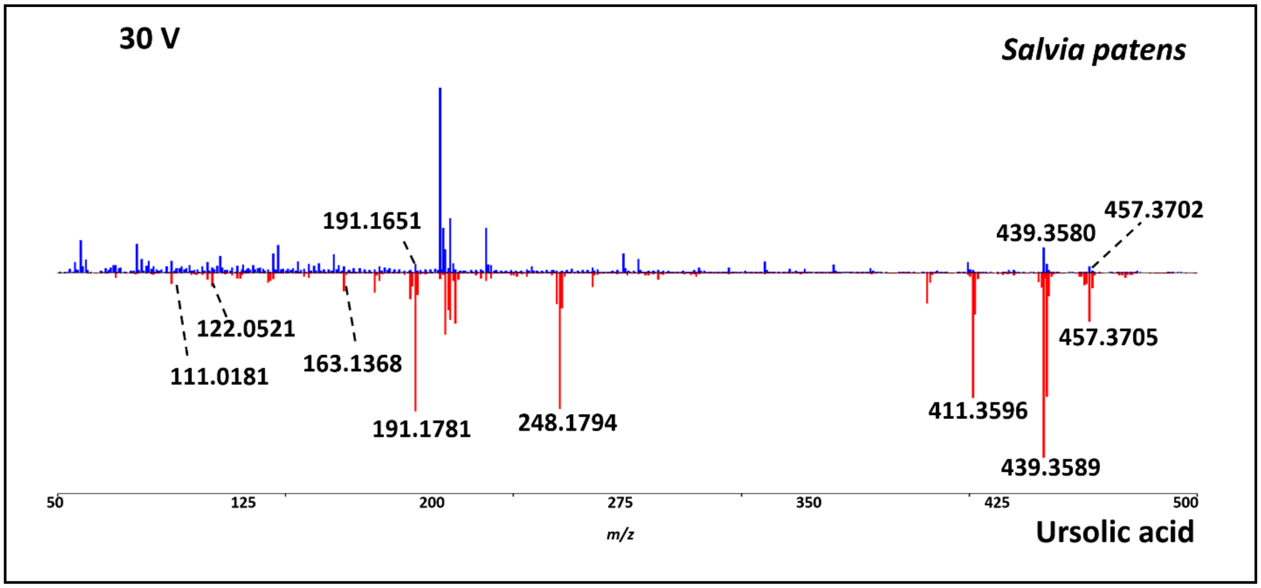

Figure S-26. Head-to-tail plot showing positive-ion mode in-source CID DART-HRMS spectra of *S. patens* fresh leaf material (top spectrum) compared to that of an ursolic acid standard (bottom spectrum), both analyzed at 30 V. The absence in the *S. patens* spectrum of diagnostic ursolic acid fragment peaks, indicates that ursolic acid was not detected in the plant material. The top panel represents an average of 10 individual leaf analyses and the bottom panel depicts an average of 3 analyses of the standard.

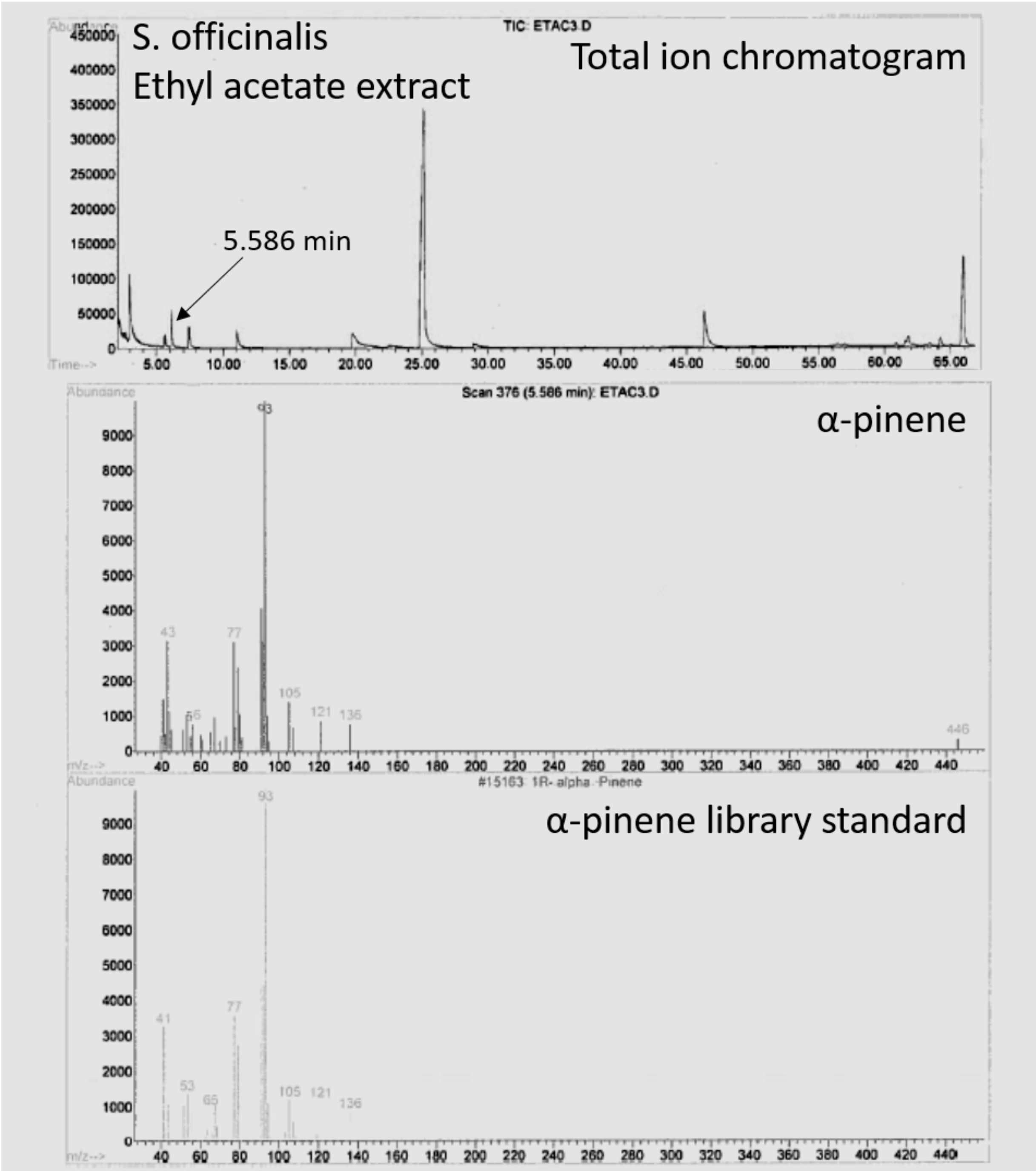

Figure S-27. Results of GC-MS experiments performed to further confirm the presence of diagnostic *Salvia* biomarkers. The top panel shows the total ion chromatogram of an ethyl acetate extraction of *S. officinalis*. The middle panel shows the mass spectrum for α-pinene, retention time 5.586 min. The bottom panel depicts the NIST EI-MS library entry for α-pinene as a comparison.

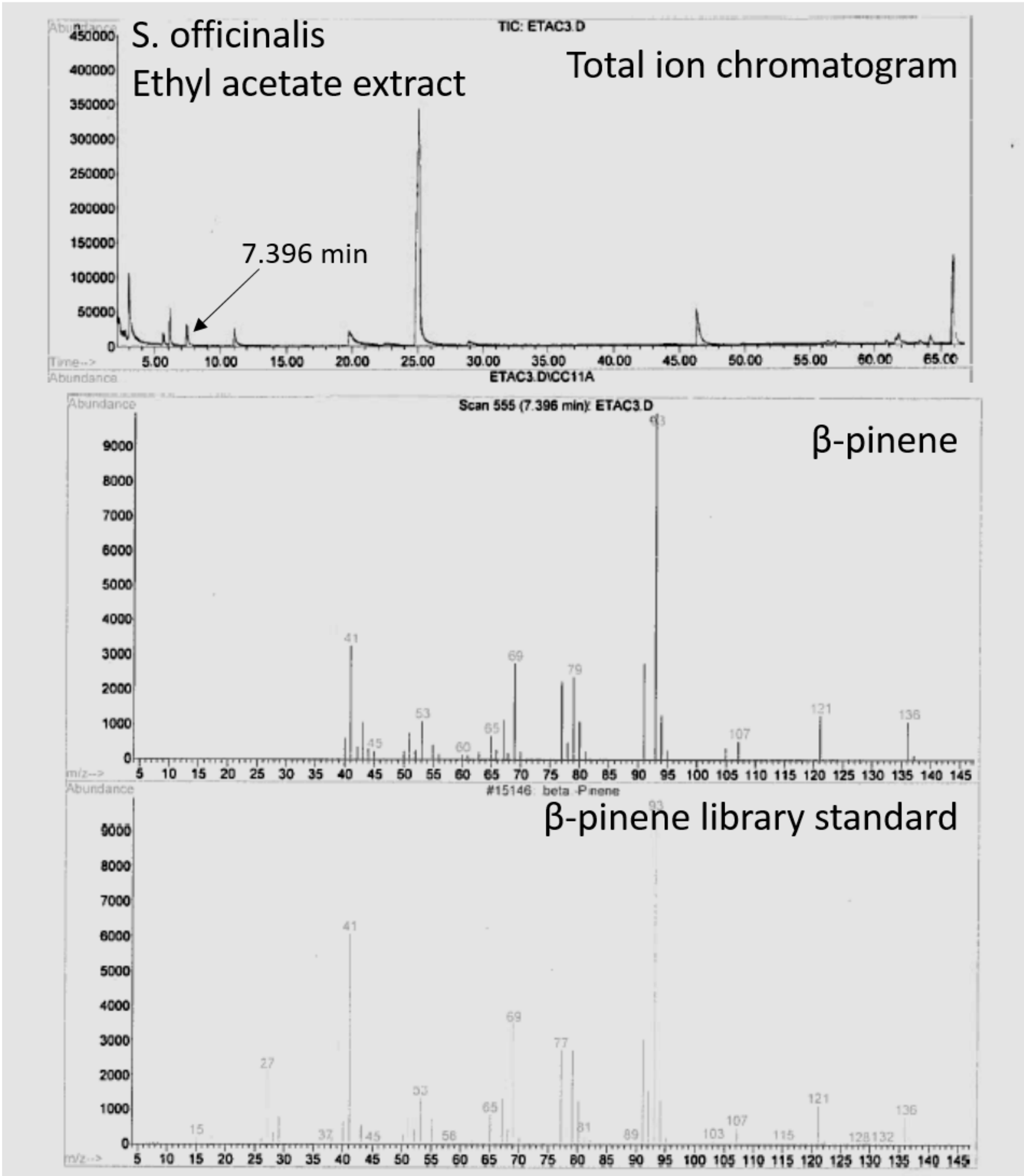

Figure S-28. Results of GC-MS experiments performed to further confirm the presence of diagnostic *Salvia* biomarkers. The top panel shows the total ion chromatogram of an ethyl acetate extraction of *S. officinalis*. The middle panel shows the mass spectrum for β-pinene, retention time 7.396 min. The bottom panel depicts the NIST EI-MS library entry for β-pinene as a comparison.

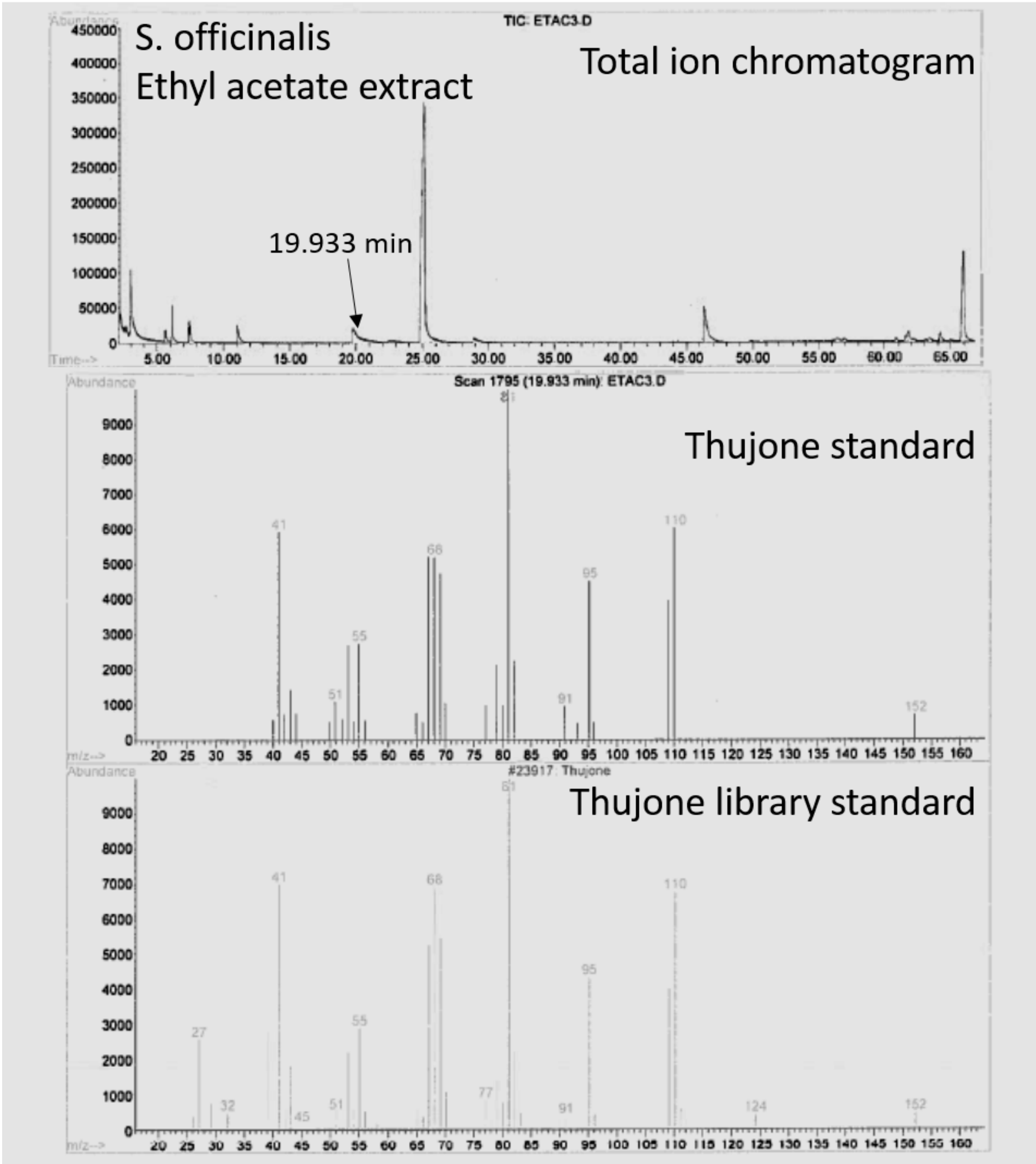

Figure S-29. Results of GC-MS experiments performed to further confirm the presence of diagnostic *Salvia* biomarkers. The top panel shows the total ion chromatogram of an ethyl acetate extraction of *S. officinalis*. The middle panel shows the mass spectrum for thujone, retention time 19.933 min. The bottom panel depicts the NIST EI-MS library entry for thujone as a comparison.

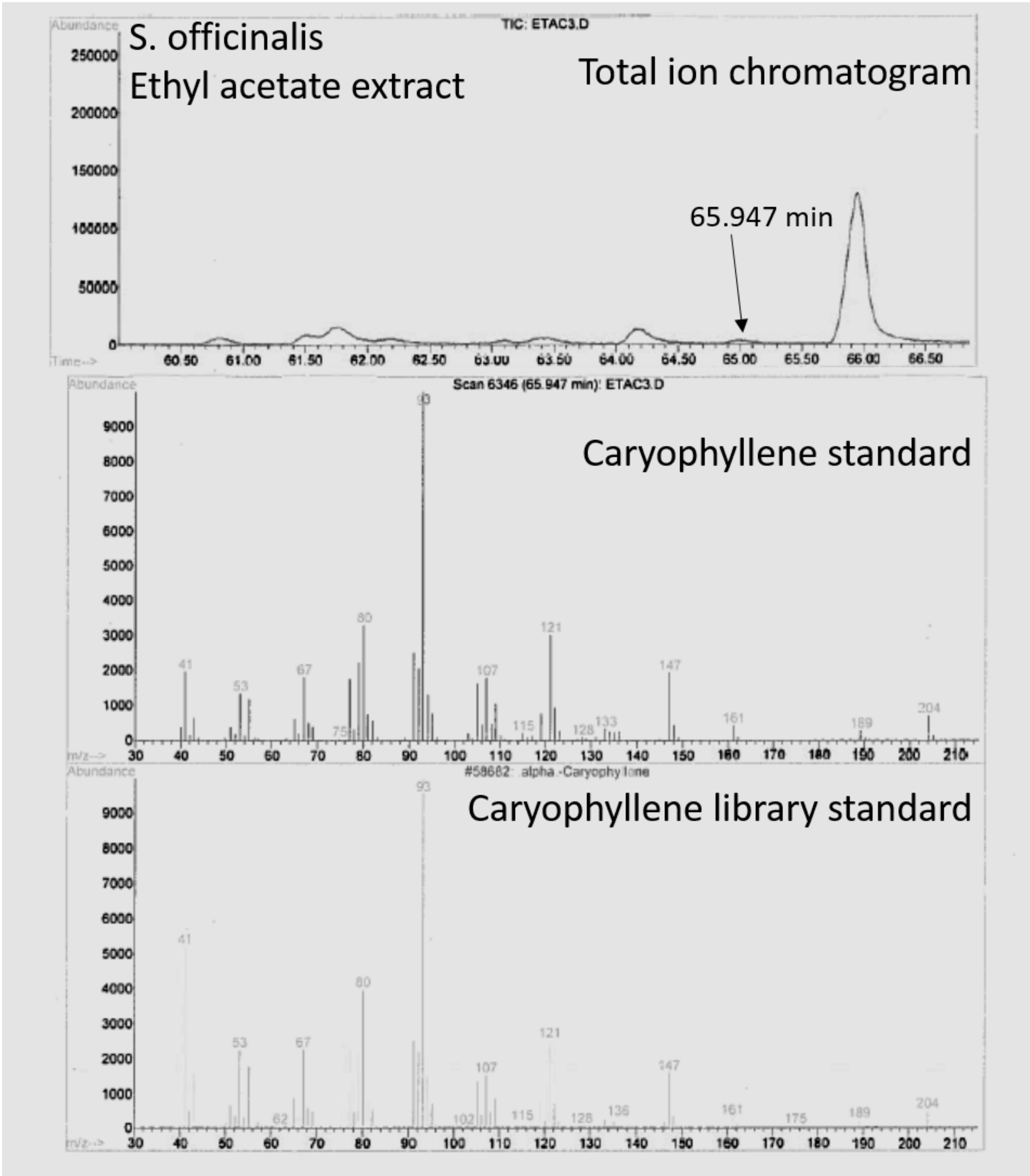

Figure S-30. Results of GC-MS experiments performed to further confirm the presence of diagnostic *Salvia* biomarkers. The top panel shows the total ion chromatogram of an ethyl acetate extraction of *S. officinalis*. The middle panel shows the mass spectrum for caryophyllene, retention time 65.947 min. The bottom panel depicts the NIST EI-MS library entry for caryophyllene as a comparison.

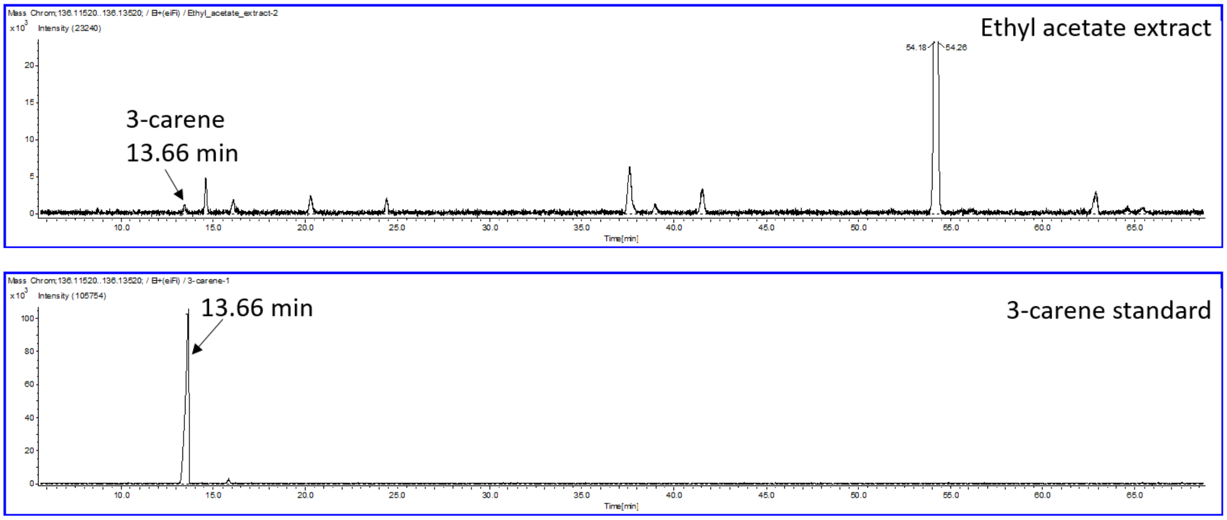

Figure S-31. Results of GC-MS experiments performed to further confirm the presence of diagnostic *Salvia* biomarkers. The first panel shows the total ion chromatogram of a 3-carene standard. The bottom panel depicts the total ion chromatogram of the *S. officinalis* ethyl acetate extract showing the peak for 3-carene.

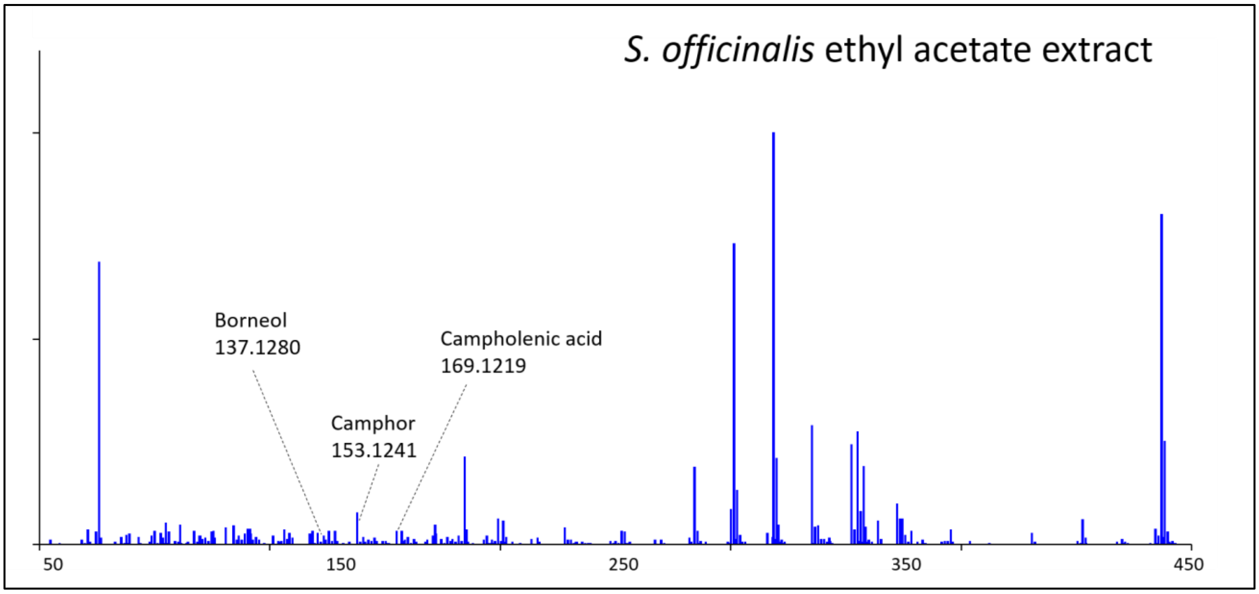

Figure S-32. Results for ethyl acetate extract of *S. officinalis* analyzed by DART-HRMS (20 V). Borneol, camphor and campholenic acid were detected, as confirmed by the GC-MS results (see Figure S-34).

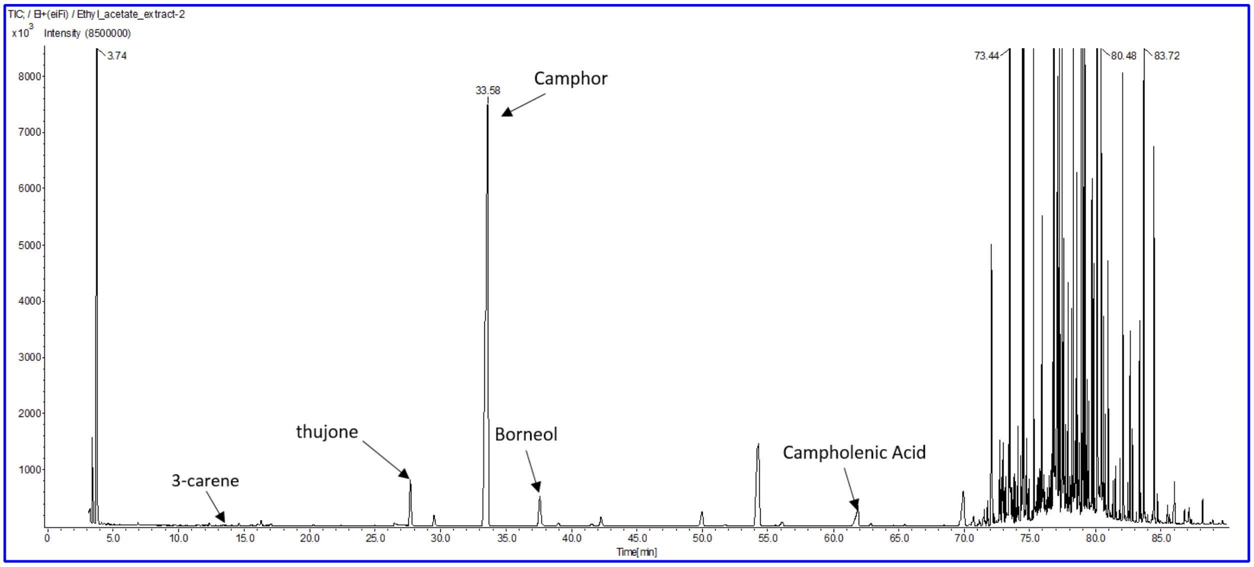

Figure S-33. Results of GC-MS experiment performed on the ethyl acetate extract of *S. officinalis* leaves. 3-Carene, β-thujone, camphor, borneol and campholenic acid were identified. Compounds were also detected by: (1) DART-HRMS; and (2) NIST EI-MS database matching.

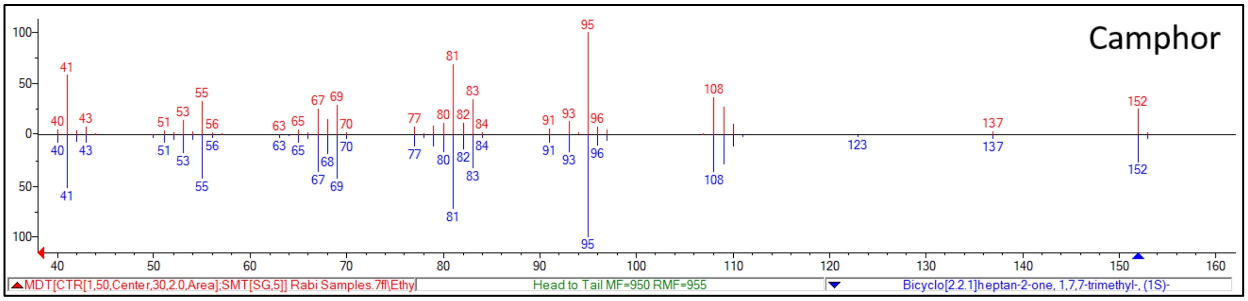

Figure S-34. Head-to-tail plot depicting the results of GC-MS experiments performed on the ethyl acetate extract of *S. officinalis* leaves. The top panel displays the mass spectrum for camphor detected in the plant material, and the bottom panel shows the NIST library spectrum for camphor.

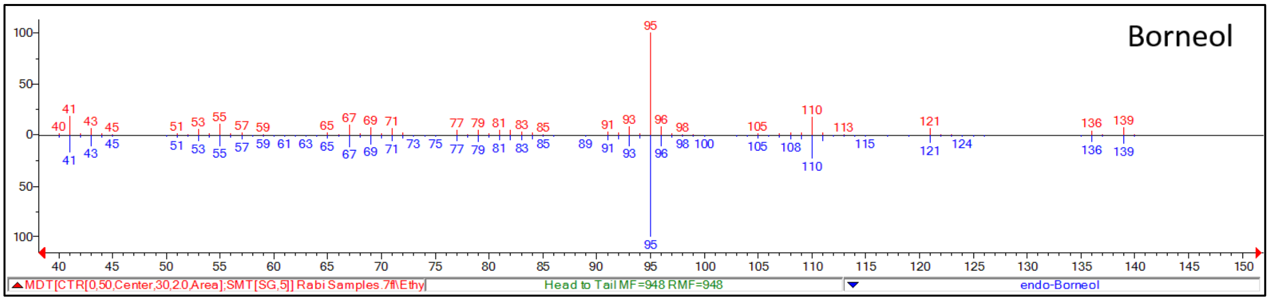

Figure S-35. Head-to-tail plot depicting the results of GC-MS experiments performed on the ethyl acetate extract of *S. officinalis* leaves. The top panel displays the mass spectrum for borneol detected in the plant material, and the bottom panel shows the NIST library spectrum for camphor.

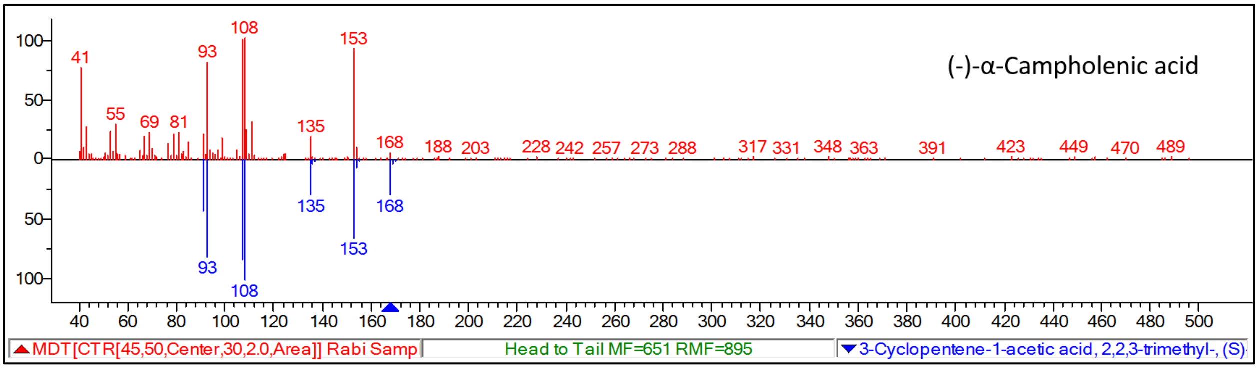

Figure S-36. Head-to-tail plot depicting the results of GC-MS experiments performed on the ethyl acetate extract of *S. officinalis* leaves. The top panel displays the mass spectrum for α-campholenic acid detected in the plant material, and the bottom panel shows the Wiley library standard spectrum for α-campholenic acid.

Tables

Table S-1. Positive-ion mode DART-HRMS of the *Salvia* spp. featured in Figure 2.											
S. apiana		***S. dominica***		***S. elegans***		***S. farinacea***		***S. officinalis***		***S. patens***	
m/z	Rel. Int.	*m/z*	Rel. Int.	*m/z*	Rel. Int.	*m/z*	Rel. Int.	*m/z*	Rel. Int.	*m/z*	Rel. Int.
59.0510	7.0	59.0551	22.4	57.0723	3.0	45.0356	10.4	47.0498	2.6	55.0412	22.5
61.0292	3.9	61.0332	11.1	59.0516	21.0	47.0497	64.4	59.0511	10.6	57.0722	4.0
81.0690	83.8	73.0673	2.9	61.0298	8.3	51.0469	8.9	61.0313	5.0	59.0519	13.7
82.0738	7.7	75.0483	2.7	69.0699	2.8	55.0420	57.7	81.0703	58.7	61.0306	5.6
83.0853	3.2	81.0733	59.9	71.0865	2.5	57.0712	30.5	82.0748	3.6	73.0635	2.9
93.0694	3.8	82.0773	3.7	73.0644	3.6	58.0693	2.2	83.0859	4.0	75.0459	2.2
95.0875	7.4	83.0892	2.7	75.0455	3.5	59.0509	100.0	93.0695	9.2	81.0705	10.3
135.1156	17.4	93.0730	7.9	81.0705	18.1	60.0483	6.4	95.0879	13.0	83.0863	5.1
136.1230	2.1	95.0900	4.2	83.0862	3.7	61.0307	46.0	107.0779	4.7	95.0882	2.4
137.1327	100.0	107.0784	2.2	95.0883	3.8	62.0610	2.1	109.1052	8.4	109.1036	2.2
138.1377	16.7	109.1069	2.3	109.1035	2.0	63.0440	3.9	123.1125	3.3	127.0416	2.7
149.1246	2.8	123.1111	2.9	111.1107	2.3	65.0616	15.3	135.1180	99.3	135.1160	9.5
151.1091	3.7	135.1182	28.8	135.1122	3.1	69.0710	6.0	136.1213	10.3	137.1332	18.7
153.1264	11.1	136.1224	3.4	137.1336	23.2	70.0677	2.7	137.1338	89.2	149.1237	2.1
191.1768	3.5	137.1338	93.6	138.1280	2.3	71.0509	2.5	138.1383	9.9	151.1110	3.0
203.1763	4.6	138.1389	11.4	149.1260	3.3	71.0851	8.0	149.1298	8.8	153.1259	5.1
205.1940	17.6	149.1262	3.5	165.1216	2.8	72.0825	2.3	151.1093	6.0	159.1185	2.5
206.1972	2.9	151.1116	8.6	175.1437	5.7	73.0649	17.3	153.1295	89.7	163.1371	2.0
217.1895	2.0	153.1285	25.6	191.1660	2.5	74.0606	4.3	154.1316	9.4	191.1742	4.4
273.2582	48.8	154.1322	2.5	203.1780	18.2	75.0450	8.3	155.1328	2.9	201.1641	100.0
274.2617	11.8	163.1448	3.3	204.1861	3.0	81.0701	15.3	163.1406	2.9	202.1681	21.7
287.2031	24.3	169.1182	2.4	205.1922	28.2	82.0747	2.2	169.1209	3.5	203.1775	11.4
288.2095	5.0	191.1732	5.7	206.1956	4.5	83.0860	23.2	170.1540	8.1	204.1858	2.2
301.2122	7.4	195.1338	3.9	221.1818	3.3	84.0455	22.4	191.1784	16.8	205.1933	36.0
303.2030	8.2	205.1908	11.6	233.1550	2.8	85.0306	5.5	192.1753	2.4	206.1960	5.9
315.0906	7.0	217.1920	5.5	247.1700	3.2	85.0657	4.1	201.1627	6.6	219.1745	22.8
315.2261	3.4	271.2389	2.2	273.2536	8.1	85.1016	6.0	203.1787	20.0	220.1781	3.9
317.2136	4.4	273.2574	100.0	285.2206	5.8	86.0604	5.4	204.1864	4.0	221.1844	4.5
329.1052	18.1	273.4120	2.1	287.2044	5.6	87.0478	7.7	205.1234	2.3	237.1812	3.4
330.1072	3.5	274.2613	30.4	301.2176	38.6	87.0818	4.0	205.1947	100.0	261.1892	4.1
331.1872	9.4	275.2330	3.0	302.2189	9.8	88.0789	3.4	206.1988	16.5	273.2575	14.9
332.1964	2.4	315.0884	9.4	303.2320	100.0	89.0575	4.9	217.1895	2.5	274.2581	3.2
333.2075	3.0	329.1033	73.6	304.2372	33.1	90.0592	3.0	219.1688	3.3	279.1962	11.3
341.3254	2.4	330.1017	16.8	305.2389	4.6	91.0544	5.5	221.1865	11.6	303.2332	3.2
439.3591	7.0	331.1015	3.2	315.0906	4.1	93.0665	2.3	271.2404	3.2	315.0902	4.6
440.3648	2.3	345.0987	6.4	317.2145	2.6	95.0534	4.6	273.2581	63.2	329.1055	6.0
		359.1160	2.2	319.2306	2.2	95.0889	4.6	274.2604	13.7	339.2190	3.4
		439.3572	4.6	329.1066	3.0	96.0469	8.0	283.1751	2.5	356.2455	4.8
				331.1919	2.6	97.0312	3.8	285.1929	5.2	409.3811	10.6
				411.2686	2.1	97.1031	5.7	286.1947	4.5	410.3829	3.4
				439.3572	15.5	98.0605	2.8	287.2028	62.7	425.3806	2.3
				440.3633	5.1	98.0988	2.4	288.2060	12.7	427.3919	2.5
				457.3692	2.5	99.0463	2.1	289.2369	2.4	439.3577	21.0
				637.4474	4.6	99.0817	14.6	300.2017	2.4	440.2622	6.9
						100.1147	3.2	301.2154	69.4	457.3693	5.0

						101.0598	5.0	302.2199	15.2	694.4551	4.0
						101.0969	5.0	303.2199	3.6		
						102.0960	2.4	305.2506	19.9		
						103.0429	2.6	306.2554	4.0		
						104.0733	5.5	315.0901	8.4		
						105.0658	2.8	315.2024	2.4		
						107.0760	9.4	317.2142	5.2		
						109.0676	7.3	329.1063	8.7		
						109.1029	5.8	331.1909	29.7		
						111.1186	7.0	332.1947	7.6		
						113.0956	2.1	333.2069	8.0		
						114.0903	7.7	393.3530	3.0		
						115.0805	3.1	409.3750	3.8		
						115.1085	3.9	411.3670	10.4		
						116.0752	2.6	412.3676	3.0		
						117.0869	2.9	425.3766	2.9		
						119.0850	4.9	437.3395	8.0		
						121.0687	3.1	438.3506	3.3		
						121.1056	4.2	439.3571	81.8		
						123.0544	3.8	440.3611	27.0		
						123.1169	3.4	441.3673	6.0		
						124.0428	4.2	455.3545	4.8		
						125.1377	3.0	457.3682	17.7		
						127.0429	4.6	458.3715	5.5		
						127.1182	3.0				
						129.1206	3.3				
						133.0882	2.0				
						135.1076	12.6				
						137.0626	24.9				
						137.1370	7.6				
						138.0682	2.3				
						141.1181	2.3				
						142.0733	3.0				
						143.1031	3.5				
						145.0558	3.9				
						145.1289	2.6				
						147.0738	2.4				
						147.1230	2.6				
						149.1176	2.8				
						151.1028	3.3				
						152.1248	2.3				
						153.1090	3.0				
						155.1494	2.1				
						157.1086	2.3				
						157.1637	2.0				
						159.1258	3.8				
						161.0980	7.5				
						163.0770	4.2				
						163.1359	5.4				
						165.0950	2.2				

						167.1046	2.8				
						169.1180	2.5				
						171.1436	3.0				
						177.1238	3.2				
						179.1032	3.7				
						191.1664	5.3				
						201.1615	6.7				
						203.1707	3.4				
						205.1924	14.9				
						206.1943	2.8				
						219.1747	2.3				
						273.0787	6.0				
						273.2568	18.8				
						274.2576	2.8				
						295.1382	6.3				
						297.1527	11.3				
						301.0742	42.6				
						301.2126	5.6				
						302.0778	6.7				
						303.2301	7.6				
						309.1170	10.1				
						310.1228	2.1				
						311.1313	9.4				
						315.0931	3.7				
						317.0706	4.4				
						323.1338	3.7				
						327.1287	3.0				
						329.1111	6.1				
						330.0848	2.6				
						331.0841	89.8				
						332.0881	15.6				
						332.1885	3.5				
						333.0875	2.5				
						335.0966	3.4				
						337.1121	4.3				
						339.1257	9.8				
						340.1330	2.6				
						341.1394	60.6				
						342.1452	12.6				
						343.1548	2.0				
						347.0775	11.7				
						348.0847	2.4				
						355.1173	4.0				
						357.1340	50.7				
						358.1575	31.5				
						359.1590	9.1				
						371.1103	3.5				
						373.1312	2.1				
						374.1595	18.1				
						375.1623	5.1				

						397.3899	4.9					
						411.3846	3.8					
						416.3681	3.9					
						417.3774	13.2					
						418.3739	4.4					
						424.1752	6.7					
						431.3714	3.0					
						433.3739	2.4					
						439.3583	25.1					
						440.1780	2.6					
						440.3620	8.1					
						457.3716	4.4					
						681.2776	6.5					
						682.2853	2.3					
						697.2817	3.2					
						698.3014	5.1					
						699.3148	2.1					
						714.2905	3.5					

Table S-2. Positive-ion mode DART-HRMS of the *Salvia* spp. featured in Figure 3, and sampled in the day and at night.

Species	*m/z*	Rel. Abundance		Species	*m/z*	Rel. Abundance	
		Day	Night			Day	Night
S. apiana	81.0690	83.8	84.9	***S. dominica***	61.0332	11.1	3.4
	82.0738	7.7	7.7		81.0733	59.9	64.8
	95.0875	7.4	7.0		82.0773	3.7	4.1
	135.1156	17.4	4.1		93.0730	7.9	4.2
	137.1327	100.0	100.0		95.0900	4.2	4.0
	138.1377	16.7	20.1		123.1111	2.9	2.2
	149.1246	2.8	2.9		135.1182	28.8	29.5
	153.1264	11.1	3.0		136.1224	3.4	3.6
	191.1768	3.5	5.3		137.1338	93.6	100.0
	203.1763	4.6	5.9		138.1389	11.4	11.5
	205.1940	17.6	38.0		149.1262	3.5	3.6
	206.1972	2.9	6.1		151.1116	8.6	10.7
	273.2582	48.8	3.0		153.1285	25.6	20.7
	288.2095	5.0	10.2		163.1448	3.3	3.0
	301.2122	7.4	10.5		191.1732	5.7	5.1
	303.2030	8.2	19.6		195.1338	3.9	2.9
	315.0906	7.0	15.6		205.1908	11.6	11.5
	315.2261	3.4	4.3		217.1920	5.5	5.0
	317.2136	4.4	4.2		273.2574	100.0	80.1
	329.1052	18.1	20.3		274.2613	30.4	29.7
	330.1072	3.5	4.0		275.2330	3.0	3.0
	331.1872	9.4	12.8		315.0884	9.4	7.1
	332.1964	2.4	3.4		329.1033	73.6	40.6
	333.2075	3.0	8.8		330.1017	16.8	8.4
	341.3254	2.4	3.2		345.0987	6.4	2.7
	439.3591	7.0	21.2		439.3572	4.6	2.6
	440.3648	2.3	7.1				
S. elegans	81.0705	18.1	3.3	***S. farinacea***	45.0360	7.4	10.0
	137.1336	23.2	5.2		47.0502	33.8	52.0
	165.1216	2.8	2.4		51.0474	3.6	5.0
	175.1437	5.7	5.3		55.0421	61.0	100.0
	203.1780	18.2	15.8		57.0717	18.5	29.2
	204.1861	3.0	2.6		59.0510	56.1	87.9
	205.1922	28.2	15.3		60.0486	3.1	5.5
	206.1956	4.5	2.3		61.0309	25.8	27.6
	221.1818	3.3	3.3		63.0424	2.5	3.9
	233.1550	2.8	2.9		65.0617	8.2	14.9
	247.1700	3.2	3.1		69.0709	6.2	7.4
	285.2206	5.8	5.4		70.0658	6.1	3.0
	301.2176	38.6	33.7		71.0849	2.6	9.0
	302.2189	9.8	9.1		72.0826	2.3	2.4
	303.2320	100.0	100.0		73.0648	11.1	15.7
	304.2372	33.1	43.2		74.0596	5.9	3.3
	305.2389	4.6	5.5		75.0449	5.9	5.5
	319.2306	2.2	2.2		81.0701	13.5	39.5

	439.3572	15.5	10.7		83.0841	49.3	58.9
	440.3633	5.1	3.5		84.0864	5.6	4.7
	457.3692	2.5	2.4		85.0297	17.2	5.7
	637.4474	4.6	3.1		86.0572	3.9	2.9
					87.0816	3.0	3.9
S. officinalis	81.0703	58.7	32.7		89.0568	3.3	4.4
	82.0748	3.6	2.0		90.0588	2.7	3.0
	93.0695	9.2	7.9		91.0526	3.8	5.2
	95.0879	13.0	10.4		93.0675	2.9	4.2
	107.0779	4.7	4.3		95.0886	3.8	5.2
	109.1052	8.4	5.7		97.1024	3.6	5.1
	135.1180	99.3	100.0		99.0814	16.9	44.6
	136.1213	10.3	11.7		100.1142	2.7	5.1
	137.1338	89.2	54.7		101.0989	15.3	19.9
	138.1383	9.9	5.7		102.0936	2.5	3.6
	149.1298	8.8	4.5		104.0716	8.4	3.7
	151.1093	6.0	3.9		105.0657	3.2	3.1
	153.1295	89.7	66.8		107.0754	6.0	7.4
	154.1316	9.4	6.8		109.0616	5.0	7.3
	169.1209	3.5	3.3		109.1026	5.1	7.0
	170.1540	8.1	4.2		111.1181	4.9	6.4
	191.1784	16.8	8.7		114.0893	5.9	9.7
	203.1787	20.0	15.3		115.0796	2.6	5.7
	204.1864	4.0	2.8		116.0733	3.1	4.9
	205.1234	2.3	2.1		117.0809	2.9	4.2
	205.1947	100.0	57.8		119.0879	2.0	5.3
	206.1988	16.5	9.0		121.1052	3.2	4.4
	221.1865	11.6	10.7		123.1165	4.2	4.9
	273.2581	63.2	29.7		125.1370	2.4	3.6
	274.2604	13.7	6.1		127.1177	2.8	3.3
	285.1929	5.2	4.4		129.1312	2.3	3.5
	286.1947	4.5	4.1		130.0775	2.6	2.7
	287.2028	62.7	70.3		133.0870	2.2	2.4
	288.2060	12.7	14.8		135.1103	18.2	17.8
	301.2154	69.4	62.9		137.1365	6.4	9.5
	302.2199	15.2	14.1		143.1035	4.2	6.2
	303.2199	3.6	10.8		145.1251	3.5	2.7
	305.2506	19.9	19.7		147.0724	2.1	2.0
	306.2554	4.0	4.0		149.1130	3.6	4.4
	315.0901	8.4	6.9		151.1057	5.9	6.1
	317.2142	5.2	3.8		152.1220	3.6	2.8
	329.1063	8.7	2.6		153.1222	4.5	6.2
	331.1909	29.7	20.4		159.1227	3.0	4.7
	332.1947	7.6	5.6		161.0963	4.3	8.3
	333.2069	8.0	10.6		163.0647	7.2	3.9
	411.3670	10.4	4.7		165.0926	7.7	4.4
	437.3395	8.0	3.3		167.1064	2.8	3.1
	439.3571	81.8	36.3		169.1179	3.7	3.0
	440.3611	27.0	11.8		171.1382	2.4	3.2
	441.3673	6.0	2.4		175.1539	2.3	2.3

	455.3545	4.8	2.1		177.1378	2.9	4.7
	457.3682	17.7	7.7		179.1018	2.8	4.7
	458.3715	5.5	2.4		191.1718	12.4	6.1
					195.1219	2.7	3.2
S. patens	55.0412	22.5	7.3		198.0976	6.2	3.6
	57.0722	4.0	2.6		199.1530	2.3	3.8
	59.0519	13.7	10.0		201.1589	12.2	11.8
	61.0306	5.6	5.9		202.1598	2.3	2.3
	73.0635	2.9	2.4		203.1716	5.5	6.7
	81.0705	10.3	14.1		205.1908	13.7	39.6
	83.0863	5.1	2.6		206.1915	2.6	6.7
	95.0882	2.4	3.1		217.1871	3.0	3.7
	109.1036	2.2	2.4		219.1679	4.1	4.9
	127.0416	2.7	7.3		221.1742	2.2	3.9
	135.1160	9.5	9.4		229.1987	2.1	3.7
	137.1332	18.7	21.9		237.1807	2.6	4.7
	149.1237	2.1	2.6		251.1616	2.1	2.6
	151.1110	3.0	2.2		273.0845	55.3	54.9
	153.1259	5.1	4.2		274.2608	10.5	10.7
	159.1185	2.5	3.8		279.2001	3.6	2.7
	191.1742	4.4	8.2		287.2230	2.6	3.0
	201.1641	100.0	100.0		295.1391	4.6	3.5
	202.1681	21.7	29.9		297.1526	8.2	6.7
	203.1775	11.4	12.7		301.0709	64.2	5.6
	204.1858	2.2	2.3		301.2129	7.3	5.4
	205.1933	36.0	34.3		303.2311	14.8	14.9
	206.1960	5.9	5.3		304.2374	3.9	3.7
	219.1745	22.8	34.4		309.1179	6.6	7.4
	220.1781	3.9	5.5		311.1323	6.1	5.5
	221.1844	4.5	4.0		329.1054	6.7	4.1
	237.1812	3.4	2.2		331.0810	100.0	13.3
	261.1892	4.1	3.9		332.0874	18.3	2.1
					339.1285	6.6	5.0
					341.1394	49.6	51.0
					342.1447	10.7	10.7
					357.1341	35.1	38.2
					358.1589	27.8	23.2
					359.1588	8.1	8.5
					371.1102	3.2	4.0
					373.1479	2.6	2.0
					374.1598	16.5	15.2
					375.1624	4.6	4.4
					411.3676	6.1	5.7
					417.3726	9.1	31.5
					418.3753	3.2	9.8
					431.3810	4.0	3.0

Table S-3. Positive-ion mode DART-HRMS data of the *Salvia* spp. featured in Figure 4. Spectra were measured in July 2014 and May 2015.

Species	*m/z*	Rel. Abundance		Species	*m/z*	Rel. Abundance	
		July 2014	May 2015			July 2014	May 2015
S. apiana	81.0690	49.2	83.8	***S. dominica***	81.0733	6.6	59.9
	82.0738	2.4	7.7		93.0730	3.4	7.9
	95.0875	2.7	7.4		135.1182	3.2	28.8
	137.1327	100.0	100.0		137.1338	13.7	93.6
	138.1377	12.2	16.7		149.1262	3.8	3.5
	155.0000	10.3	4.4		151.1116	3.6	8.6
	203.1763	2.3	4.6		153.1285	12.1	25.6
	205.1940	11.0	17.6		163.1448	3.5	3.3
	273.2582	4.5	48.8		191.1732	5.3	5.7
	287.2031	16.8	24.3		205.1908	6.1	11.6
	288.2095	3.6	5.0		217.1920	4.8	5.5
	301.2122	7.0	7.4		273.2574	100.0	100.0
	303.2030	16.9	8.2		274.2613	29.8	30.4
	315.0906	4.3	7.0		275.2330	3.4	3.0
	329.1052	8.0	18.1		315.0884	3.5	9.4
	331.1872	5.0	9.4		329.1033	30.1	73.6
	333.2075	5.0	3.0		330.1017	8.1	16.8
	341.3254	3.8	2.4		345.0987	3.2	6.4
	439.3591	4.5	7.0		439.3572	7.5	4.6
S. elegans	81.0705	31.6	18.1	***S. farinacea***	73.0648	15.0	11.1
	95.0883	3.0	3.8		74.0596	9.6	5.9
	137.1336	60.3	23.2		75.0449	4.1	5.9
	138.1280	5.6	2.3		81.0701	8.4	13.5
	149.1260	2.5	3.3		83.0841	15.4	49.3
	203.1780	21.3	18.2		85.0654	2.4	17.2
	204.1861	3.7	3.0		87.0475	2.8	3.0
	205.1922	100.0	28.2		89.0568	4.1	3.3
	206.1956	16.8	4.5		90.0588	2.7	2.7
	221.1818	5.8	3.3		91.0526	2.4	3.8
	247.1700	14.3	3.2		95.0886	2.6	3.8
	301.2176	19.3	38.6		99.0814	14.2	16.9
	302.2189	4.4	9.8		101.0597	7.6	15.3
	303.2320	38.6	100.0		104.0716	6.9	8.4
	304.2372	7.7	33.1		109.1026	2.7	5.1
	319.2306	18.0	2.2		111.1181	4.7	4.9
	329.1066	17.7	3.0		114.0893	7.6	5.9
	439.3572	24.5	15.5		115.0796	4.1	2.6
	440.3633	7.9	5.1		116.1051	4.6	3.1
	457.3692	5.2	2.5		117.0809	100.0	2.9
					119.0879	6.1	2.0
S. officinalis	81.0703	23.3	58.7		123.0561	2.1	4.2
	93.0695	9.4	9.2		127.1177	5.7	2.8
	95.0879	9.0	13.0		129.1312	4.1	2.3
	107.0779	3.2	4.7		130.0775	3.0	2.6
	109.1052	6.4	8.4		133.0870	8.5	2.2

	123.1125	2.6	3.3		137.1365	10.0	6.4
	135.1180	66.4	99.3		143.1035	2.9	4.2
	136.1213	8.8	10.3		151.1057	2.1	5.9
	137.1338	57.1	89.2		152.1220	11.5	3.6
	138.1383	5.9	9.9		153.1222	5.7	4.5
	149.1298	5.2	8.8		159.1227	2.3	3.0
	151.1093	6.1	6.0		165.0926	9.7	7.7
	153.1295	100.0	89.7		198.0976	4.2	6.2
	154.1316	11.8	9.4		199.1530	5.2	2.3
	169.1209	3.3	3.5		203.1716	4.0	5.5
	170.1540	3.9	8.1		205.1908	33.3	13.7
	191.1784	12.1	16.8		206.1915	5.3	2.6
	203.1787	15.0	20.0		273.0845	5.7	55.3
	204.1864	2.6	4.0		303.2311	2.5	14.8
	205.1947	78.8	100.0		311.1323	3.8	6.1
	206.1988	13.1	16.5		339.1285	7.3	6.6
	221.1865	7.7	11.6		341.1394	33.5	49.6
	271.2404	2.4	3.2		342.1447	7.2	10.7
	273.2581	87.4	63.2		357.1341	25.4	35.1
	274.2604	19.1	13.7		358.1589	13.1	27.8
	283.1751	2.0	2.5		359.1588	4.6	8.1
	285.1929	4.3	5.2		371.1102	6.3	3.2
	286.1947	2.3	4.5		374.1598	7.8	16.5
	287.2028	66.9	62.7		375.1624	2.0	4.6
	288.2060	14.1	12.7		411.3676	4.1	6.1
	289.2369	2.5	2.4		417.3726	11.9	9.1
	301.2154	70.9	69.4		418.3753	3.3	3.2
	302.2199	16.0	15.2		431.3810	6.5	4.0
	303.2199	3.7	3.6		439.3557	18.6	53.5
	305.2506	33.7	19.9		440.3603	5.6	17.1
	306.2554	7.1	4.0		457.3667	3.7	9.7
	315.0901	19.9	8.4		681.2594	2.9	4.4
	315.2024	2.9	2.4				
	317.2142	4.1	5.2		81.0705	7.8	10.3
	329.1063	25.5	8.7		137.1332	17.2	18.7
	331.1909	23.9	29.7		191.1742	3.6	4.4
	332.1947	5.6	7.6		201.1641	100.0	100.0
	333.2069	14.1	8.0		202.1681	23.6	21.7
	393.3530	4.0	3.0		203.1775	9.3	11.4
	409.3750	3.5	3.8		205.1933	27.0	36.0
	411.3670	8.3	10.4		206.1960	4.2	5.9
	412.3676	2.6	3.0	***S. patens***	219.1745	30.5	22.8
	425.3766	4.0	2.9		220.1781	4.8	3.9
	437.3395	9.8	8.0		221.1844	2.4	4.5
	438.3506	3.3	3.3		237.1812	2.6	3.4
	439.3571	97.2	81.8		261.1892	4.0	4.1
	440.3611	32.4	27.0		273.2575	1.4	14.9
	441.3673	7.5	6.0		279.1962	11.5	11.3
	455.3545	4.8	4.8		315.0902	3.0	4.6
	457.3682	21.6	17.7		329.1055	5.2	6.0

	458.3715	7.1	5.5		339.2190	2.8	3.4
					356.2455	7.8	4.8
					409.3811	8.7	10.6
					410.3829	8.7	3.4
					425.3806	2.6	2.3
					427.3919	2.4	2.5
					439.3577	34.6	21.0
					440.2622	12.0	6.9
					457.3693	7.8	5.0
					694.4551	2.4	4.0

Table S-4. Positive-ion DART-HRMS data of the *Salvia* spp. highlighting biomarkers confirmed to be present. The data correspond to the spectra shown in Figure 5 and Supporting Information Figures S-1 – S-19.

Species	Compound	Formula	Adduct	Measured Mass	Calculated Mass	Difference (mmu)	Rel. Int.
S. apiana	α-Pinene	$C_{10}H_{16}$	$+H^+$	137.1327	137.1330	0.32	100.00
	β-Caryophyllene	$C_{15}H_{24}$	$+H^+$	205.1940	205.1956	1.63	17.64
	β-Pinene	$C_{10}H_{16}$	$+H^+$	137.1327	137.1330	0.32	100.00
S. dominica	β-Pinene	$C_{10}H_{16}$	$+H^+$	137.1338	137.1330	-0.78	93.61
	β-Thujone	$C_{10}H_{16}O$	$+H^+$	153.1285	153.1280	-0.55	25.61
	β-Caryophyllene	$C_{15}H_{24}$	$+H^+$	205.1908	205.1956	4.83	11.63
S. elegans	3-Carene	$C_{10}H_{16}$	$+H^+$	137.1336	137.1330	-0.58	23.18
	β-Caryophyllene	$C_{15}H_{24}$	$+H^+$	205.1922	205.1956	3.34	28.17
S. farinacea	β-Caryophyllene	$C_{15}H_{24}$	$+H^+$	205.1924	205.1956	3.23	14.94
S. officinalis	β-Pinene	$C_{10}H_{16}$	$+H^+$	137.1338	137.1330	-0.78	89.19
	β-Caryophyllene	$C_{15}H_{24}$	$+H^+$	205.1947	205.1956	0.93	100.00
S. patens	3-Carene	$C_{10}H_{16}$	$+H^+$	137.1326	137.1330	0.42	19.43
	β-Caryophyllene	$C_{15}H_{24}$	$+H^+$	205.1960	205.1956	4.03	36.18
	β-Pinene	$C_{10}H_{16}$	$+H^+$	137.1326	137.1330	0.42	19.43

Table S-5. Positive-ion mode in-source CID DART-HRMS data showing diagnostic fragment peaks for oleanolic and ursolic acids.

Oleanolic acid		Ursolic acid	
m/z	**Rel. Int.**	***m/z***	**Rel. Int.**
54.9477	2.4	46.9457	4.5
58.9612	2.3	111.0181	7.4
122.0525	11.8	122.0521	9.8
190.1673	2.4	163.1368	5.2
191.1776	34.9	175.1380	4.4
192.1801	5.2	177.1468	2.4
203.1796	9.0	189.1614	5.6
204.1857	4.4	190.1680	4.9
205.1943	6.4	191.1774	51.1
207.1721	5.4	192.1789	7.9
247.1737	6.6	203.1798	15.1
248.1793	25.3	204.1859	17.2
249.1831	9.6	205.1917	19.3
372.3085	2.9	206.1839	3.4
393.3488	5.8	207.1756	24.9
411.3597	24.4	208.1758	3.7
412.3647	7.8	221.1833	2.6
437.3418	5.8	247.1731	15.0
438.3479	4.6	248.1795	63.9
439.3592	100.0	249.1821	16.1
439.5877	2.3	261.1924	4.9
439.6485	2.1	287.2068	3.2
440.3597	56.3	393.3483	11.8
441.3618	11.0	394.3534	3.8
454.3493	5.7	411.3596	52.5
455.3533	6.3	412.3642	17.1
456.3599	2.6	413.3631	2.8
457.3708	9.3	437.3418	4.1
458.3715	3.0	438.3484	6.5
471.3530	3.4	439.3592	100.0
473.3706	2.3	439.5588	3.7
474.3977	3.0	440.3594	55.4
		441.3609	10.5
		455.3541	6.1
		456.3615	5.6
		457.3710	25.0
		458.3725	8.1
		471.3561	2.2
		474.3975	2.1