

Metabolomic differences between invasive alien plants from native and invaded habitats

Short title: Metabolomic profiling of invasive alien species

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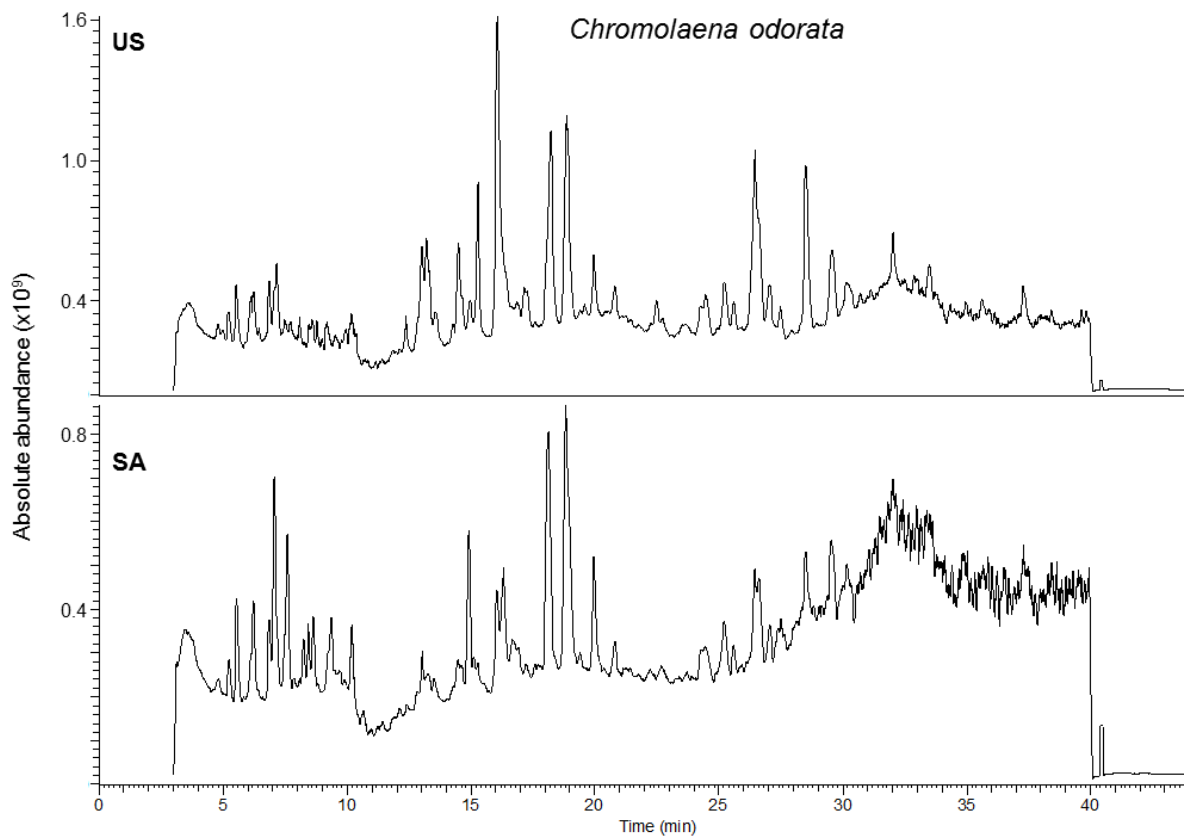
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Supplementary Information

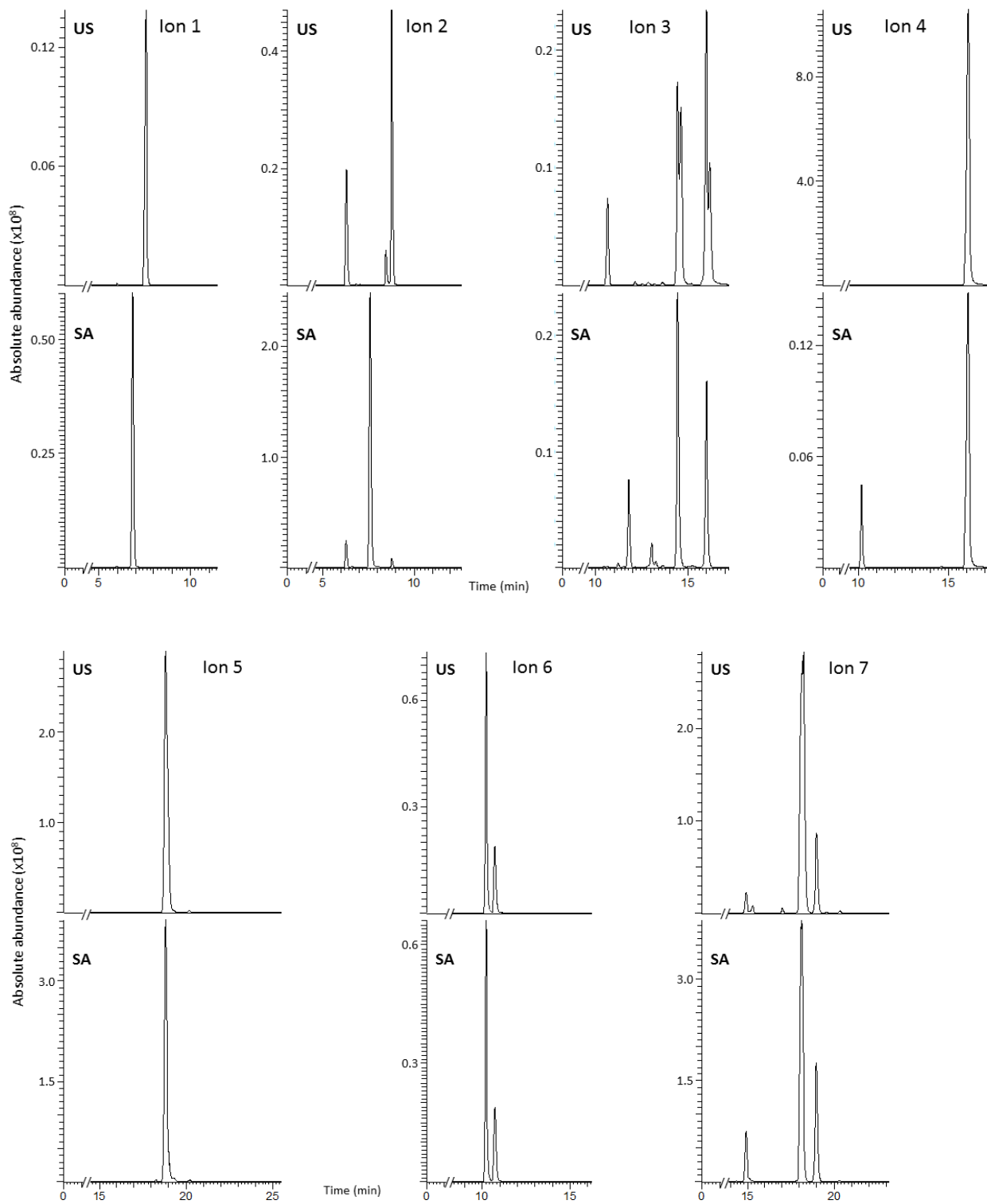
S1 Table. Collection details on samples collected for the purpose of this study including country of origin, common and Latin names, date, GPS coordinates and collector initials (SS: Skubel, Sarah; RI: Raskin, Ilya, PhD). Identifier numbers shown are continued from samples previously collected but unrelated to this study.

ID	Country	Common Name	Latin Name	Date Collected	Coordinates	Collected By
10-13	US	Blue Mistflower	<i>Chromolaena odorata</i>	5/30/2018	27°56'7"N, 81°34'29"W	SS
14-16				5/30/2018	27°56'4"N, 81°34'42"W	SS
17-19				5/30/2018	27°56'21"N, 81°34'42"W	SS
20-23				5/30/2018	27°56'21"N, 81°34'42"W	SS
24-27		Rough Cocklebur	<i>Xanthium strumarium</i>	6/27/2018	40°47'57"N, 73°55'11"W	SS
28-31				6/27/2018	40°48'23"N, 73°55'33"W	SS
32-35				6/27/2018	40°47'57"N, 73°55'10"W	SS
36-38		Jimsonweed	<i>Datura stramonium</i>	6/27/2018	40°47'7"N, 73°56'7"W	SS
39-42				6/27/2018	40°46'59"N, 73°56'41"W	SS
43-46				7/02/2018	40°27'27"N, 74°24'35"W	SS
50-53	SA	Blue Mistflower	<i>Chromolaena odorata</i>	7/24/2018	24°58'9"S, 31°35'38"E	SS & RI
54-58		Jimsonweed	<i>Datura stramonium</i>	7/24/2018	24°58'9"S 31°35'38"E	SS & RI
59-61				7/25/2018	24°59'1"S, 31°38'33"E	SS & RI
62-67		Rough Cocklebur	<i>Xanthium strumarium</i>	7/26/2018	24°57'26"S, 31°42'56"E	SS & RI
68-74				7/28/2018	23°73"S, 31°27'22"E	SS & RI
75-81				7/28/2018	23°8'41"S, 31°27'44"E	SS & RI
82-88				7/28/2018	23°6'30"S, 31°26'16"E	SS & RI

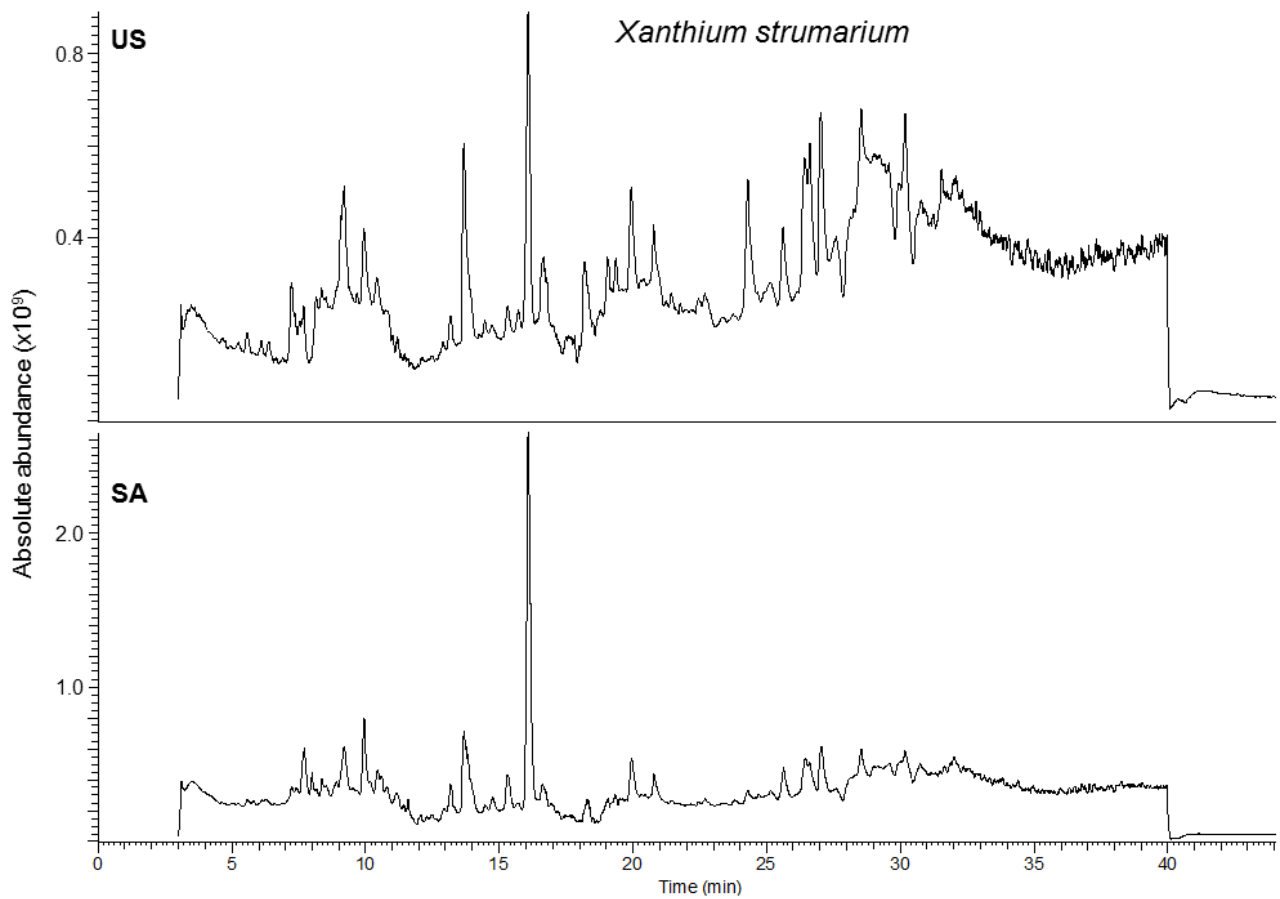
89-99	SA	Blue Mistflower	<i>Chromolaena odorata</i>	7/30/2018	22°25'31"S, 31°15'17"E	SS & RI
100-107				7/31/2018	22°25'21S, 31°14'0"E	SS & RI
108-115				7/31/2018	22°25'19"S, 31°14'59"E	SS & RI
116-123				7/31/2018	22°25'20"S, 31°14'46"E	SS & RI
124-130		Rough Cocklebur	<i>Xanthium strumarium</i>	7/31/2018	22°25'21"S, 31°14'40"E	SS & RI
131-138				8/3/2018	23°45'27"S, 31°22'17"E	SS & RI
139-144				8/3/2018	23°45'14"S, 31°22'0"E	SS & RI
145-152		Jimsonweed	<i>Datura stramonium</i>	8/3/2018	23°45'14"S, 31°22'0"E	SS & RI
153-160				8/6/2018	23°40'55"S, 30°59'44"E	SS & RI
161-168				8/6/2018	23°40'18"S, 30°59'20"E	SS & RI



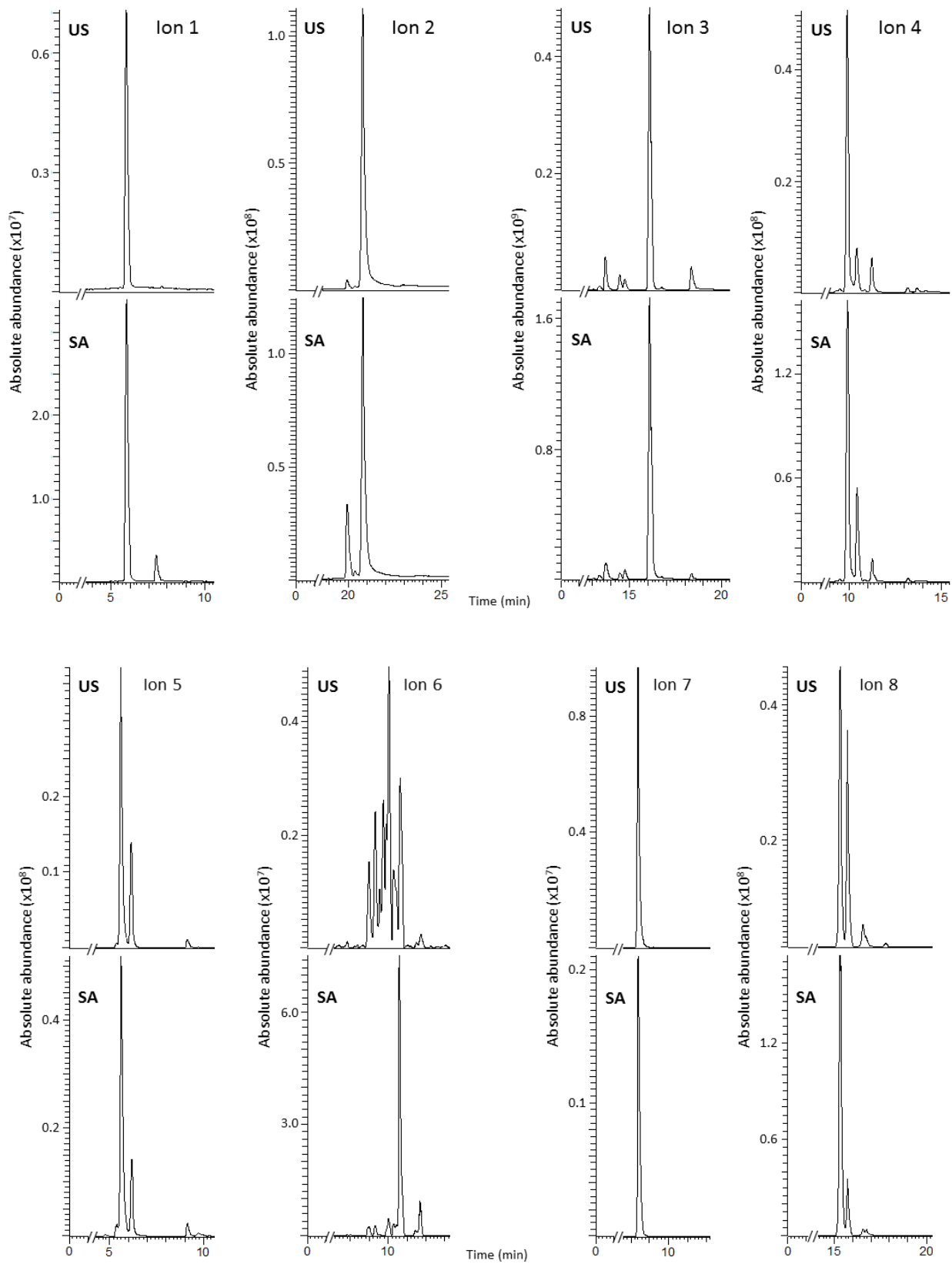
S2 Fig. 1. (-)ESI MS total ion current chromatograms [m/z 100 – m/z 1000] of disk eluates from *Chromolaena odorata* extracts from plants originating in the United States (US), and South Africa (SA).



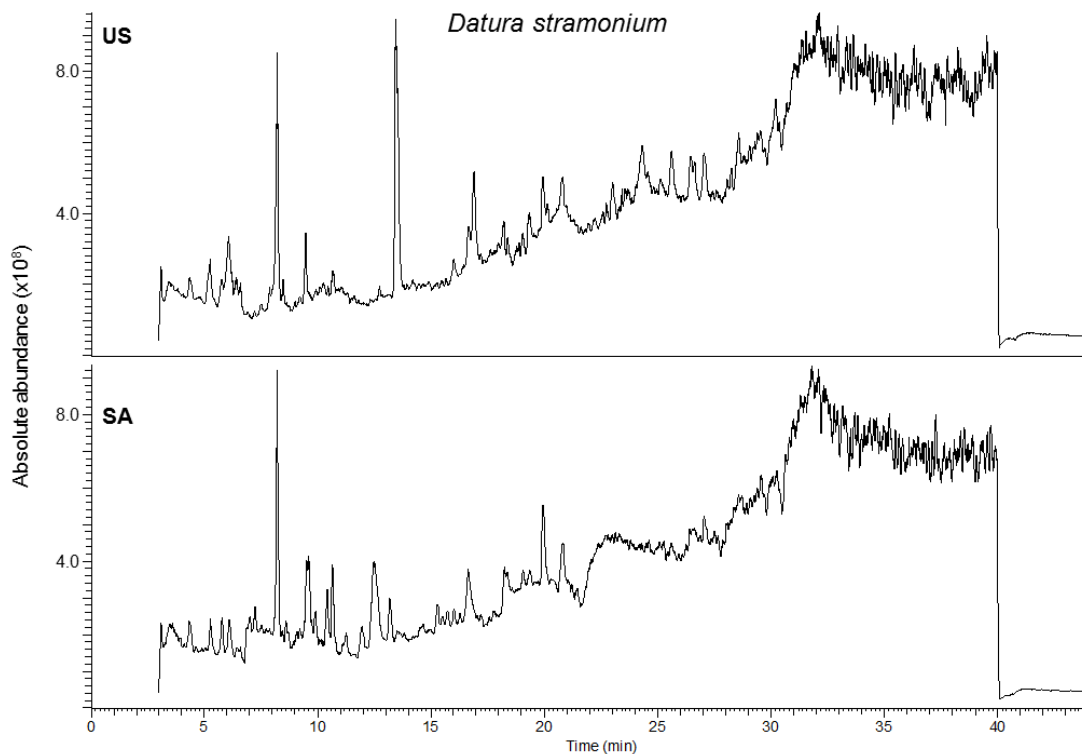
S2 Fig. 2. (-)ESI MS extracted ion current chromatograms of disk eluates from *Chromolaena odorata* extracts from plants originating in the United States (US), and South Africa (SA). Ion number details – see Table 1.



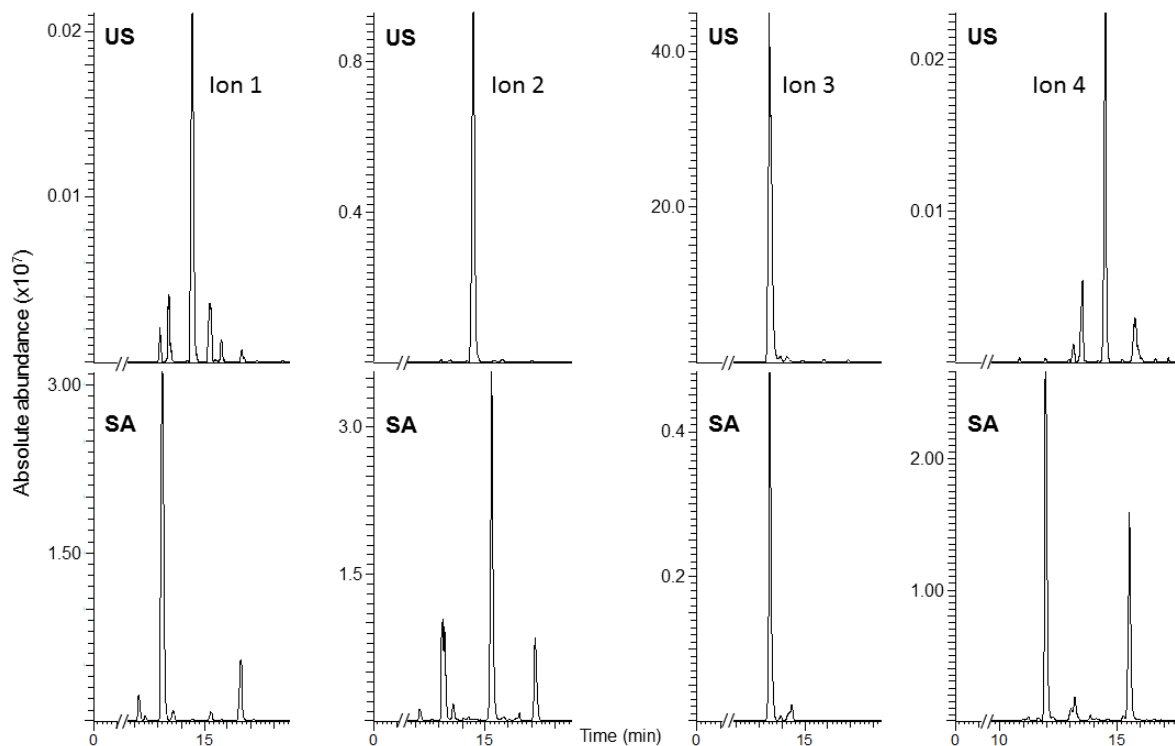
S2 Fig. 3. (-)ESI MS total ion current chromatograms [m/z 100 – m/z 1000] of disk eluates from *Xanthium strumarium* extracts from plants originating in the United States (US), and South Africa (SA).



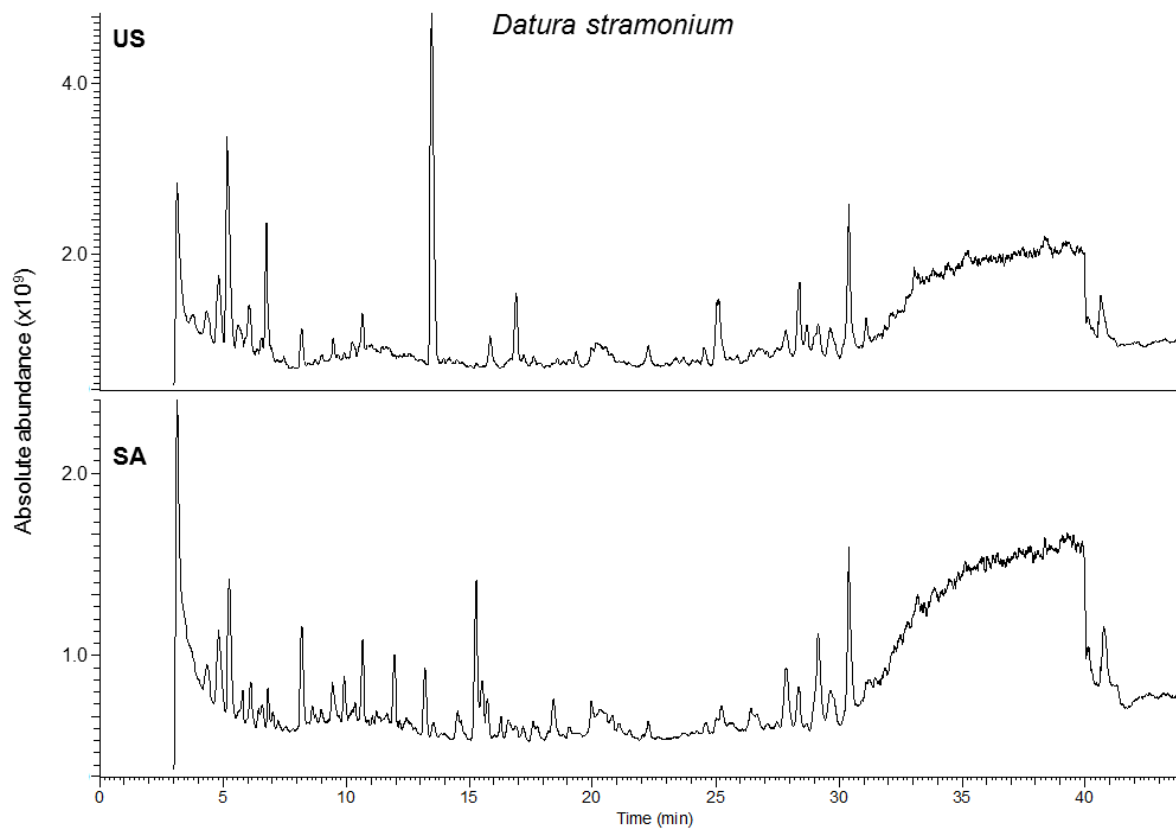
S2 Fig. 4. (-)ESI MS extracted ion current chromatograms of disk eluates from *Xanthium strumarium* extracts from plants originating in the United States (US), and South Africa (SA). Ion number details – see Table 2.



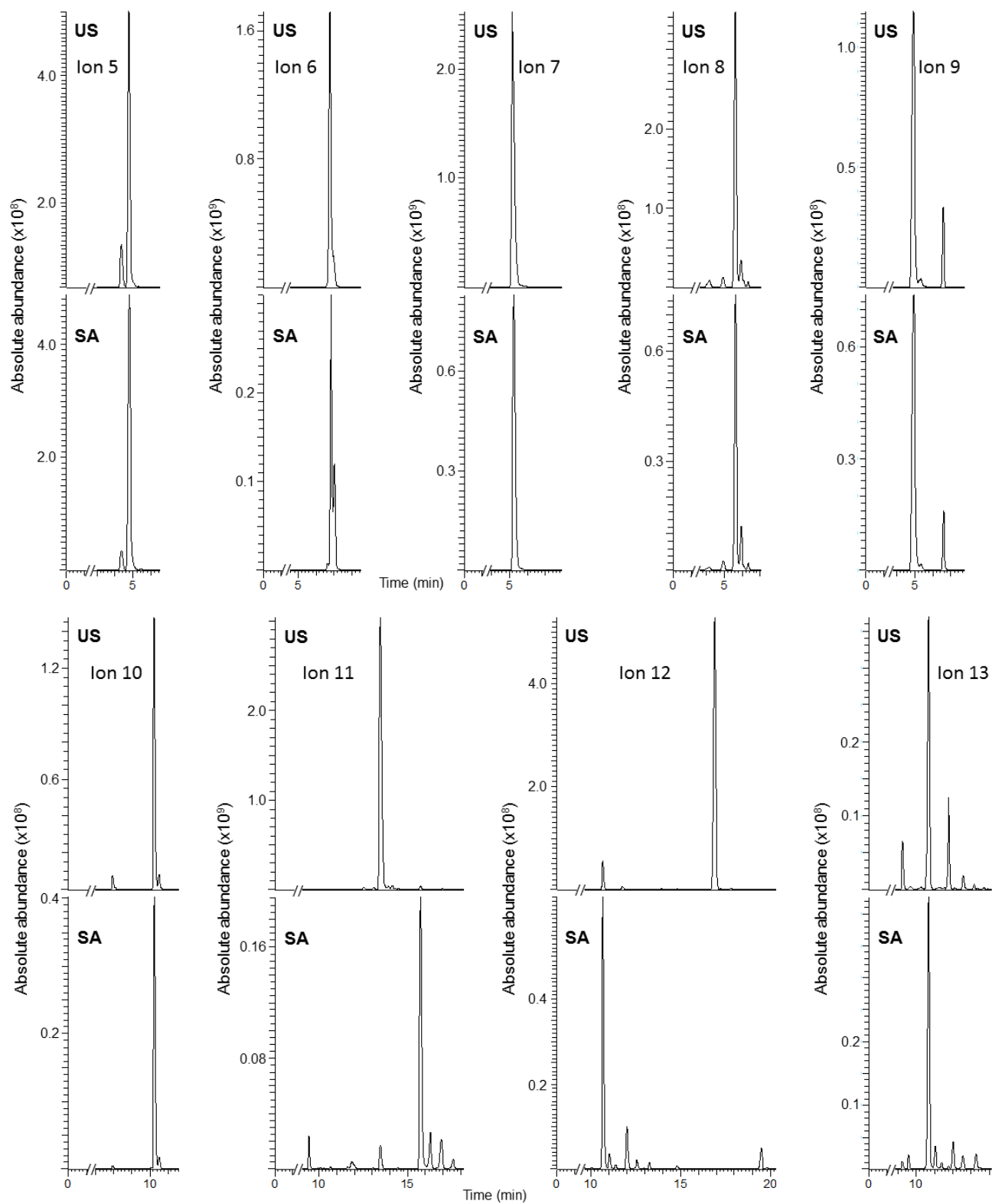
S2 Fig. 5. (-)ESI MS total ion current chromatograms [m/z 100 – m/z 1000] of disk eluates from *Datura stramonium* extracts of plants from the United States (US), and South Africa (SA).



S2 Fig. 6. (-)ESI MS extracted ion current chromatograms of disk eluates from *Datura stramonium* extracts from plants originating in the United States (US), and South Africa (SA). Ion number details – see Table 3.



S2 Fig. 7. (+)ESI MS total ion current chromatograms [m/z 100 – m/z 1000] of disk eluates from *Datura stramonium* extracts of plants from the United States (US), and South Africa (SA).



S2 Fig. 8. (+)ESI MS extracted ion current chromatograms of disk eluates from *Datura stramonium* extracts from plants originating in the United States (US), and South Africa (SA). Ion number details – see Table 3.