

Supplementary Information

Chemotaxonomy of the Amazonian *Unonopsis* Species Based on Leaf Alkaloid Fingerprint Direct Infusion ESI-MS and Chemometric Analysis

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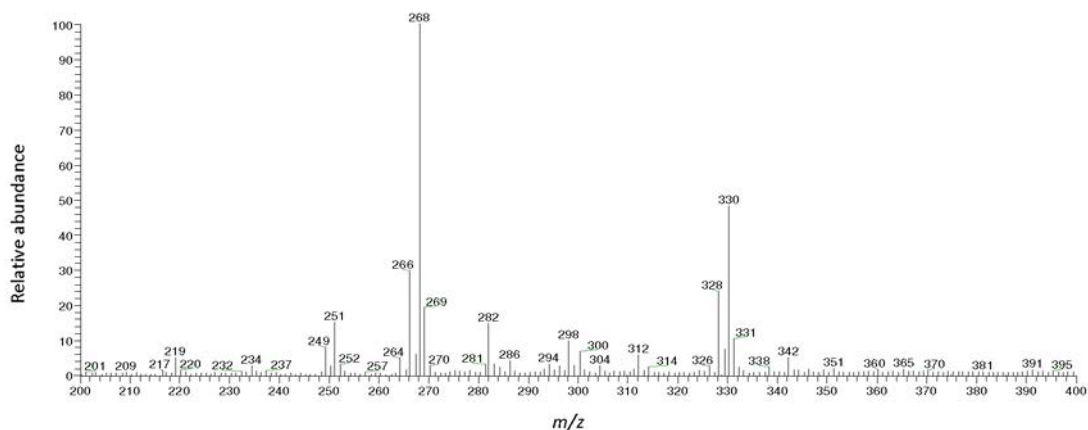


Figure S1. ESI-MS spectrum (positive mode) of the alkaloidal fraction from *U. guatterioides* (GU).

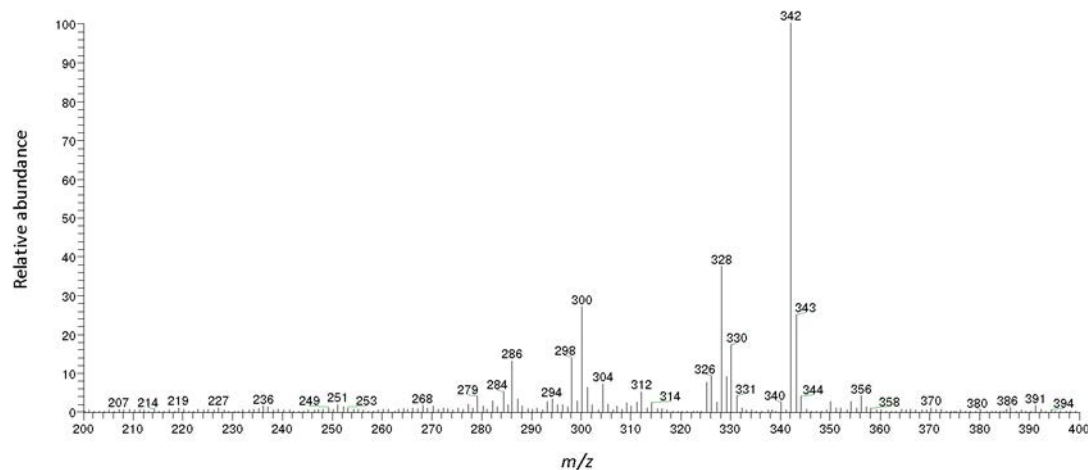


Figure S2. ESI-MS spectrum (positive mode) of the alkaloidal fraction from *U. stipitata* (SUA).

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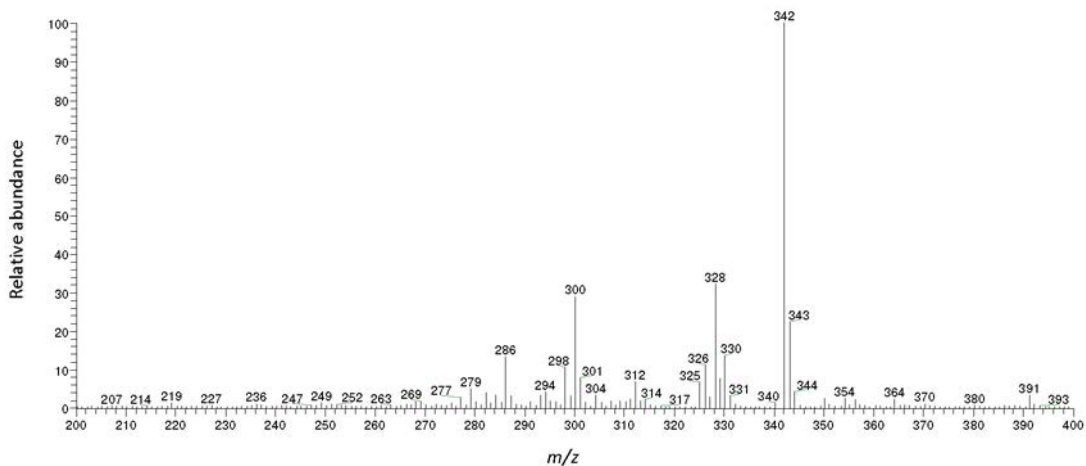


Figure S3. ESI-MS spectrum (positive mode) of the alkaloidal fraction from *U. stipitata* (SUB).

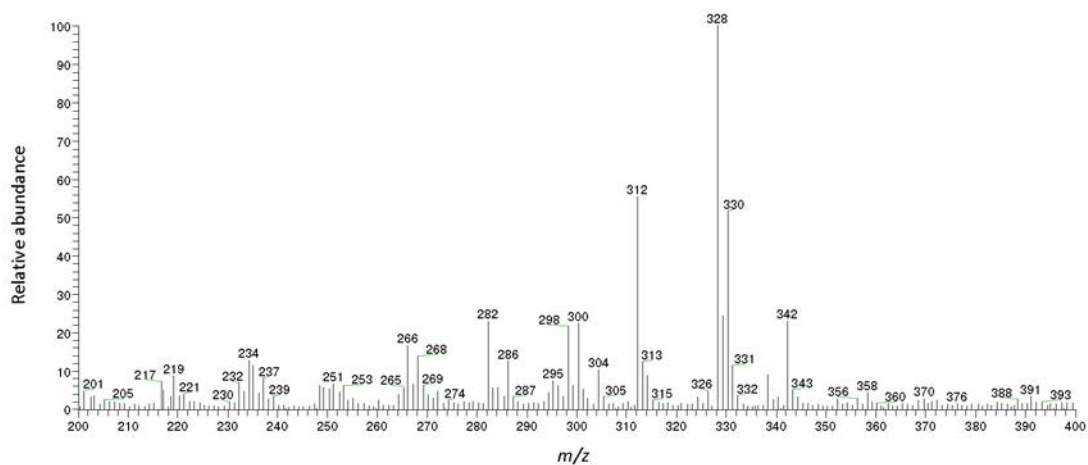


Figure S4. ESI-MS spectrum (positive mode) of the alkaloidal fraction from *U. floribunda* (FDA).

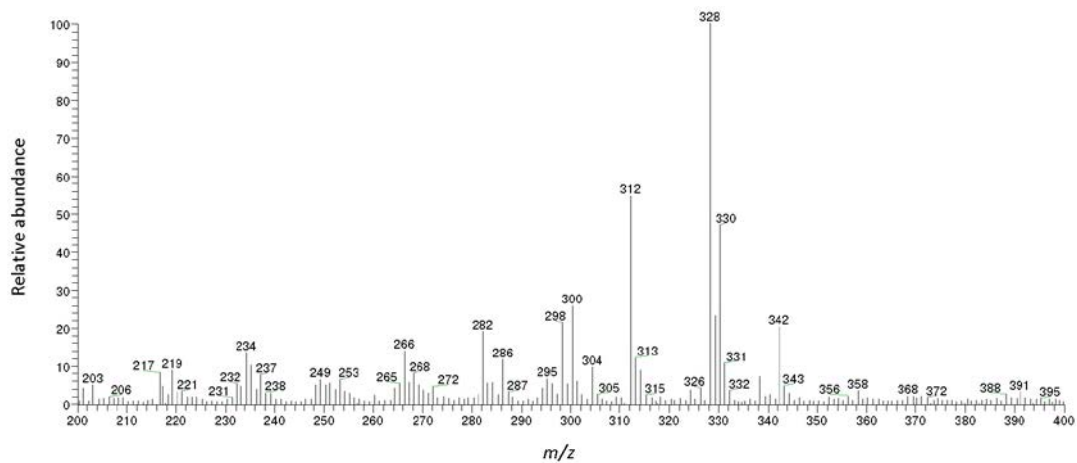


Figure S5. ESI-MS spectrum (positive mode) of the alkaloidal fraction from *U. floribunda* (FDB).

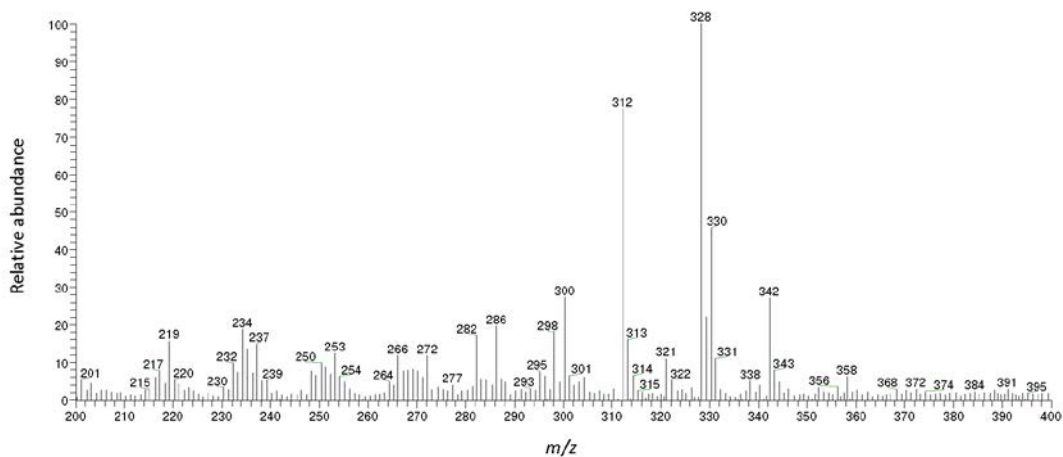


Figure S6. ESI-MS spectrum (positive mode) of the alkaloidal fraction from *U. rufescens* (RD).

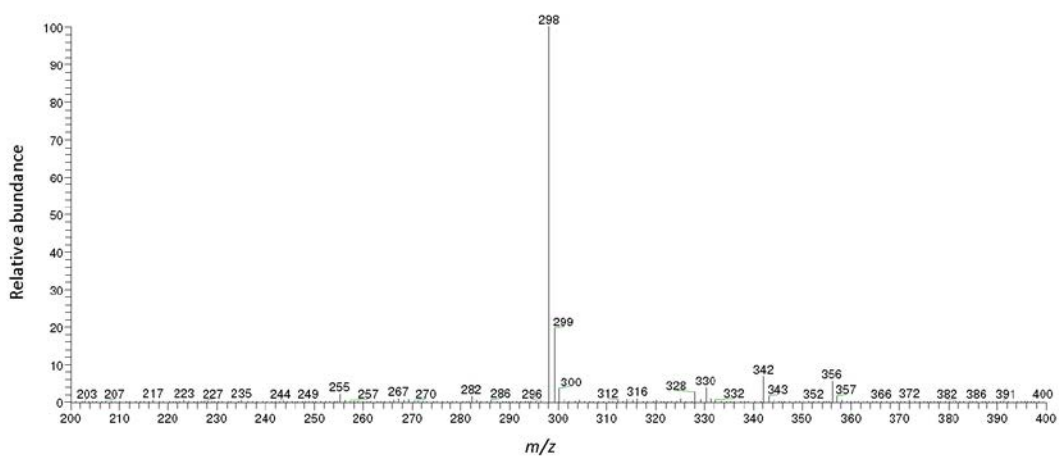


Figure S7. ESI-MS spectrum (positive mode) of the alkaloidal fraction from *U. duckei* (DRA).

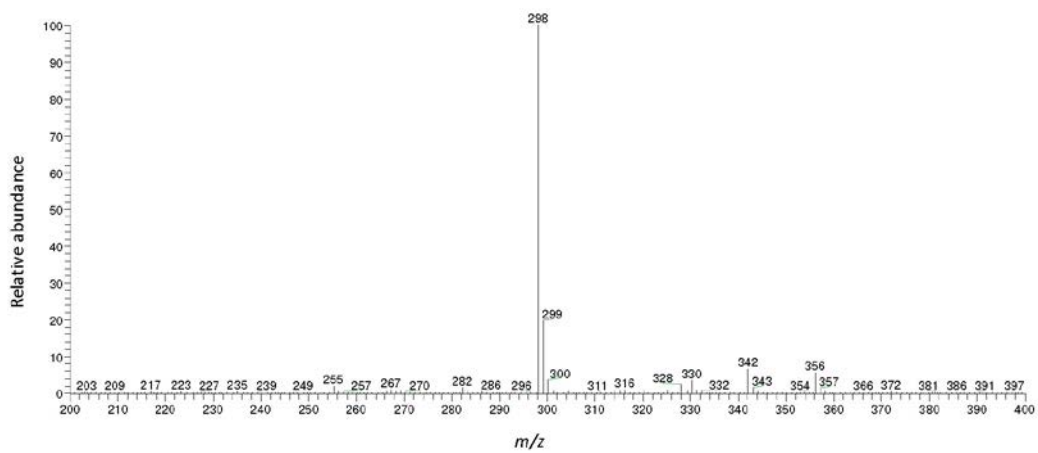


Figure S8. ESI-MS spectrum (positive mode) of the alkaloidal fraction from *U. duckei* (DRB).

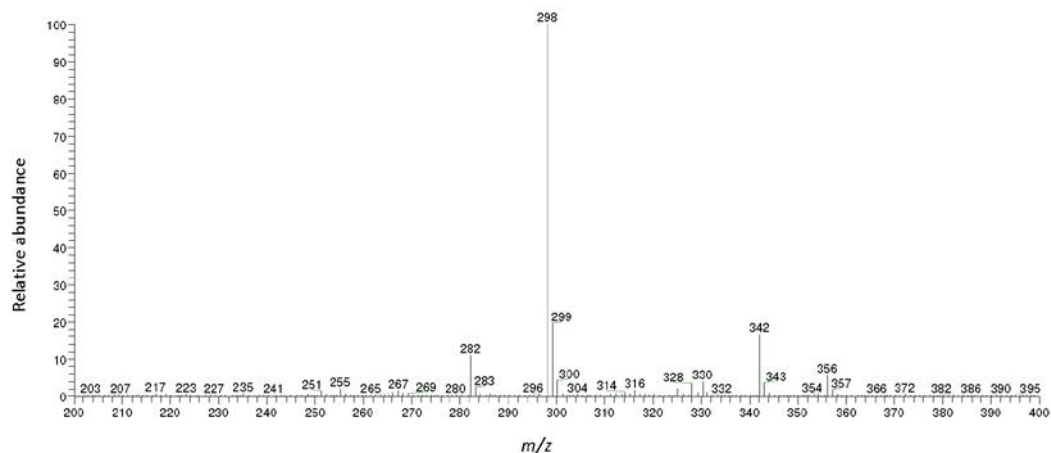


Figure S9. ESI-MS spectrum (positive mode) of the alkaloidal fraction from *U. duckei* (DDA).

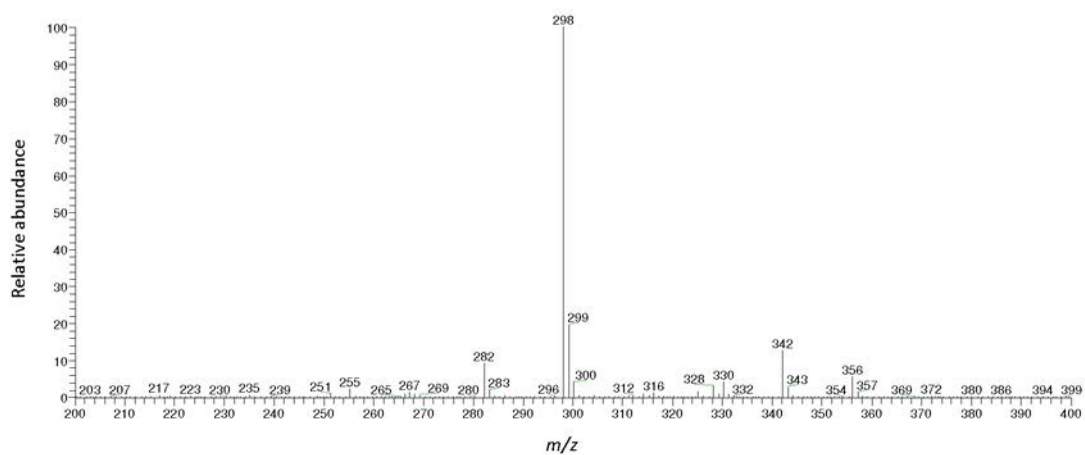


Figure S10. ESI-MS spectrum (positive mode) of the alkaloidal fraction from *U. duckei* (DDB).

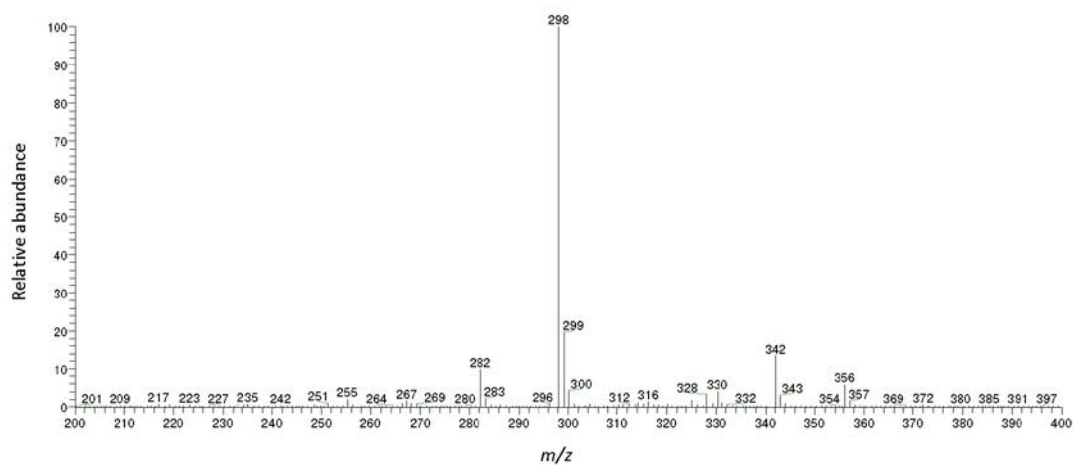


Figure S11. ESI-MS spectrum (positive mode) of the alkaloidal fraction from *U. duckei* (DDC).

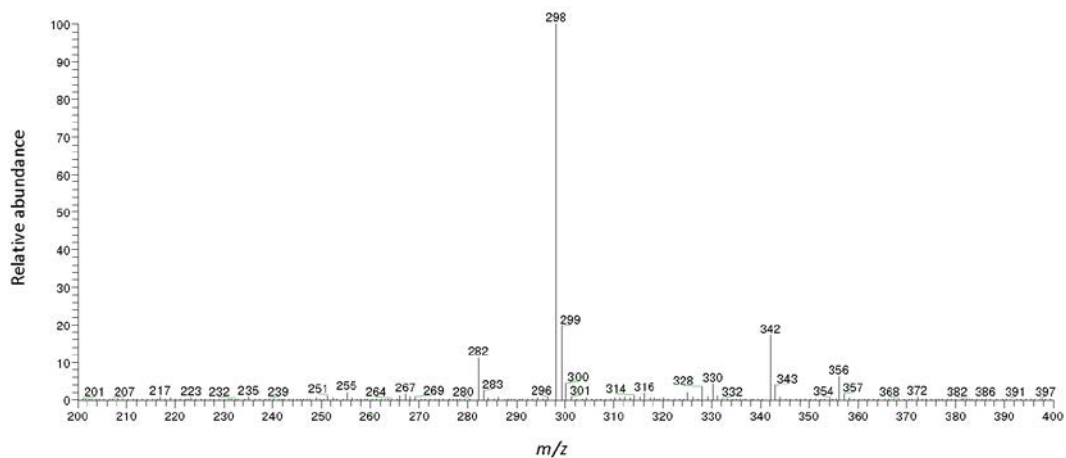


Figure S12. ESI-MS spectrum (positive mode) of the alkaloidal fraction from *U. duckei* (DDD).

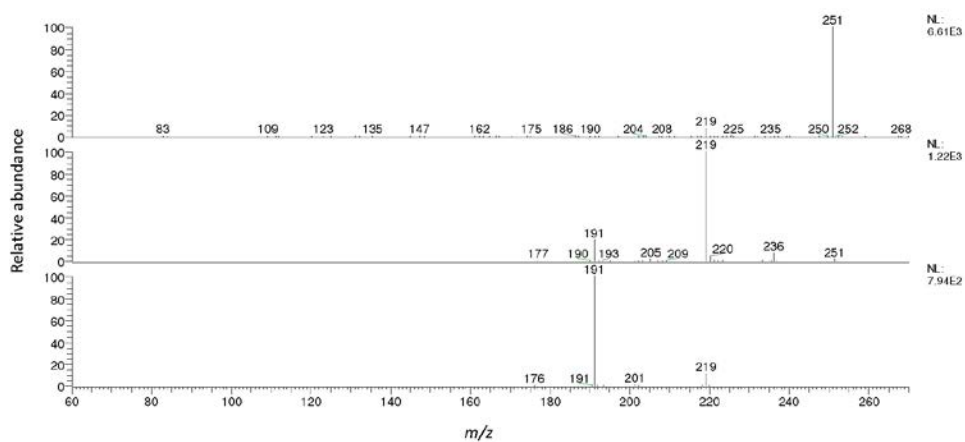


Figure S13. ESI-MSⁿ spectra (positive mode) of the ion at m/z 268 present in the leaves of *U. guatterioides*.

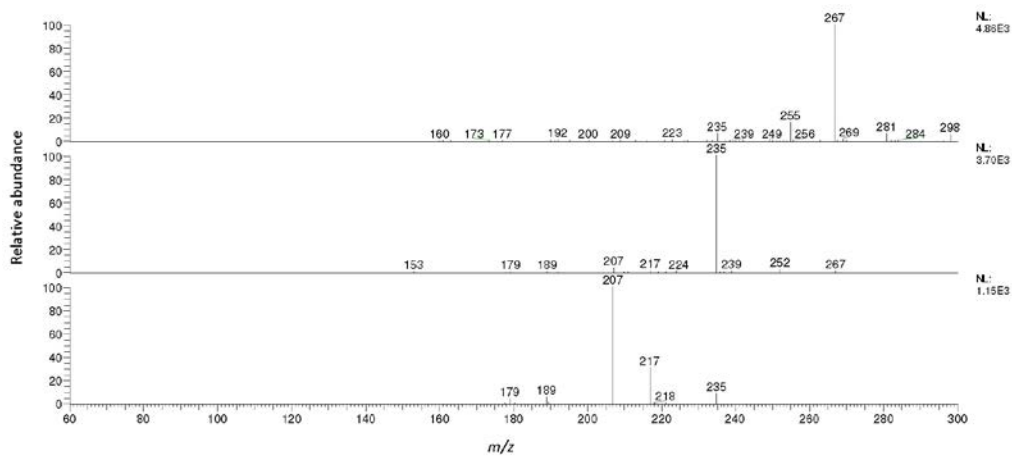


Figure S14. ESI-MSⁿ spectra (positive mode) of the ion at m/z 298 present in the leaves of *U. duckei*.

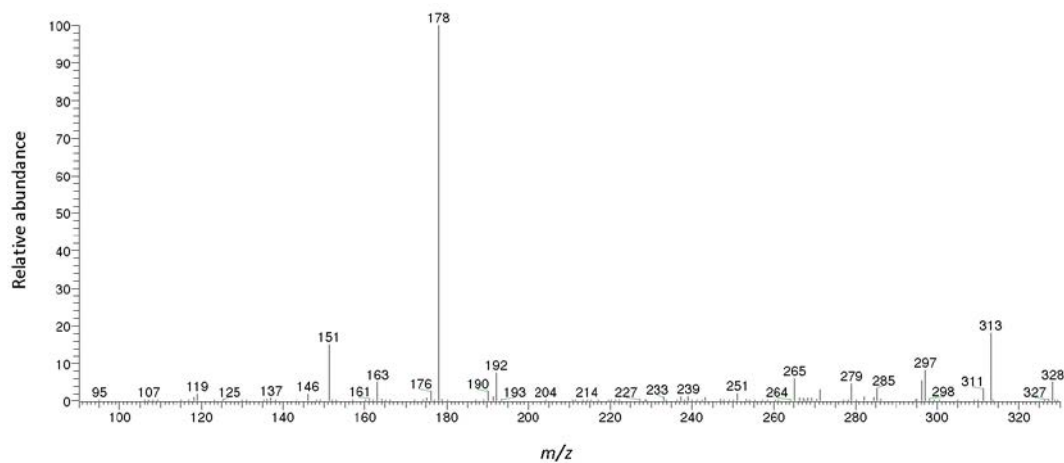


Figure S15. ESI-MS³ spectrum (positive mode) of the ion at m/z 328 present in the leaves of *U. floribunda*.

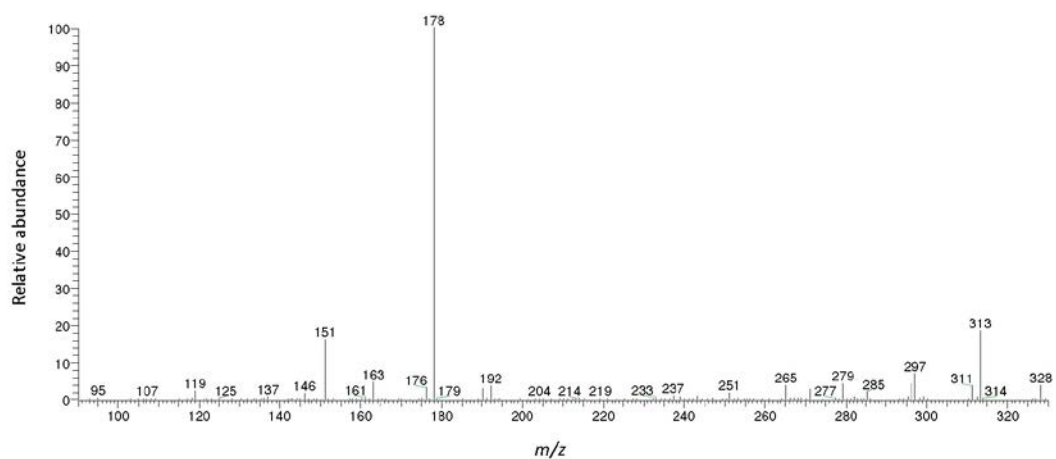


Figure S16. ESI-MS³ spectrum (positive mode) of the ion at m/z 328 present in the leaves of *U. rufescens*.

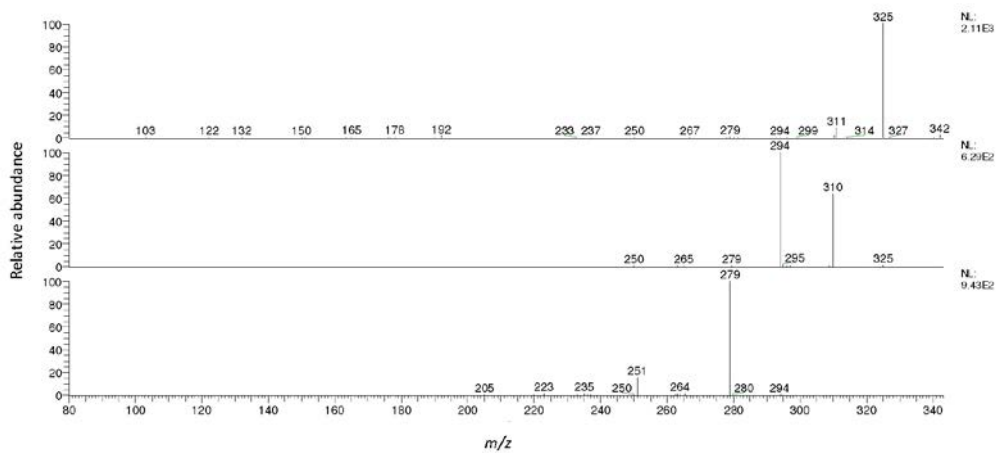


Figure S17. ESI-MSⁿ spectra (positive mode) of the ion at m/z 342 present in the leaves of *U. stipitata*.



Figure S18. Collection sites near the metropolitan area of Manaus.

Table S1. Data used in the PCA analysis based in the peak intensities obtained between 200 to 400 m/z , after elimination of those signals which had intensities below to 5% than the intensity of the base peak

	<i>U. guatterioides</i> (GU)	<i>U. stipitata</i> (SUA)	<i>U. stipitata</i> (SUB)	<i>U. floribunda</i> (FDA)	<i>U. floribunda</i> (FDB)	<i>U. rufescens</i> (RD)	<i>U. duckei</i> (DRA)	<i>U. duckei</i> (DRB)	<i>U. duckei</i> (DDA)	<i>U. duckei</i> (DDB)	<i>U. duckei</i> (DDC)	<i>U. duckei</i> (DDD)
201	0	0	0	0	0	5.12	0	0	0	0	0	0
216	0	0	0	0	0	5.93	0	0	0	0	0	0
217	0	0	0	7.05	8.08	7.49	0	0	0	0	0	0
219	5.1	0	0	8.57	8.7	15.45	0	0	0	0	0	0
220	0	0	0	0	0	5.21	0	0	0	0	0	0
232	0	0	0	6.73	5.13	9.5	0	0	0	0	0	0
233	0	0	0	0	0	7.18	0	0	0	0	0	0
234	0	0	0	12.54	13.33	18.62	0	0	0	0	0	0
235	0	0	0	11.07	10.13	13.37	0	0	0	0	0	0
236	0	0	0	0	0	7.12	0	0	0	0	0	0
237	0	0	0	7.92	7.48	14.72	0	0	0	0	0	0
239	0	0	0	0	0	5.02	0	0	0	0	0	0
248	0	0	0	6.09	0	7.49	0	0	0	0	0	0
249	7.8	0	0	5.59	6.34	6.38	0	0	0	0	0	0
250	0	0	0	5.2	0	9.56	0	0	0	0	0	0
251	15.05	0	0	6.43	5.44	8.49	0	0	0	0	0	0
252	0	0	0	0	0	6.56	0	0	0	0	0	0
253	0	0	0	5.83	6.3	12.29	0	0	0	0	0	0
254	0	0	0	0	0	5.95	0	0	0	0	0	0
265	0	0	0	5.67	5.27	0	0	0	0	0	0	0
266	29.61	0	0	16.5	13.76	11.42	0	0	0	0	0	0
267	5.91	0	0	6.55	5.63	7.47	0	0	0	0	0	0
268	100	0	0	13.68	7.88	7.75	0	0	0	0	0	0
269	19.24	0	0	6.06	0	8.15	0	0	0	0	0	0
270	0	0	0	0	0	7.41	0	0	0	0	0	0
271	0	0	0	0	0	5.91	0	0	0	0	0	0
272	0	0	0	0	0	11.52	0	0	0	0	0	0
282	14.75	0	0	22.86	18.96	16.83	0	0	9.22	9.44	10.85	10.92
283	0	0	0	5.5	5.48	5.48	0	0	0	0	0	0
284	0	5.05	0	5.67	5.65	5.03	0	0	0	0	0	0
286	0	12.94	13.27	12.47	11.55	19.45	0	0	0	0	0	0
287	0	0	0	0	0	5.42	0	0	0	0	0	0
295	0	0	0	7.21	6.52	7.34	0	0	0	0	0	0
296	0	0	0	6.06	5.27	6.2517.74	0	0	0	0	0	0
298	9.72	13.89	10.39	21.37	21.13	0	100	100	100	100	100	100

Table S1. Data used in the PCA analysis based in the peak intensities obtained between 200 to 400 *m/z*, after elimination of those signals which had intensities below to 5% than the intensity of the base peak (cont.)

	<i>U. guatterioides</i> (GU)	<i>U. stipitata</i> (SUA)	<i>U. stipitata</i> (SUB)	<i>U. floribunda</i> (FDA)	<i>U. floribunda</i> (FDB)	<i>U. rufescens</i> (RD)	<i>U. duckei</i> (DRA)	<i>U. duckei</i> (DRB)	<i>U. duckei</i> (DDA)	<i>U. duckei</i> (DDB)	<i>U. duckei</i> (DDC)	<i>U. duckei</i> (DDD)
299	0	0	0	6.14	5.18	27.23	19.35	19.47	19.66	19.29	19.36	19.37
300	6.63	26.87	28.78	22.3	25.71	6.23	0	0	0	0	0	0
301	0	6.15	7.7	0	5.8	5.78	0	0	0	0	0	0
304	0	7.08	0	10.09	9.43	77.43	0	0	0	0	0	0
312	5.57	0	6.71	55.47	54.65	15.81	0	0	0	0	0	0
313	0	0	0	12.2	11.91	6.31	0	0	0	0	0	0
314	0	0	0	8.65	8.8	10.72	0	0	0	0	0	0
321	0	0	0	0	0	0	0	0	0	0	0	0
325	0	7.4	6.48	0	0	0	0	0	0	0	0	0
326	0	9.16	10.97	0	0	100	0	0	0	0	0	0
328	23.92	37.35	32.01	100	100	21.94	0	0	0	0	0	0
329	7.23	8.83	7.52	24.36	23.15	45.65	0	0	0	0	0	0
330	48.27	17.21	13.41	51.46	47.1	10.81	0	0	0	0	0	0
331	10.43	0	0	11.11	10.59	0	0	0	0	0	0	0
338	0	0	0	8.92	7.1	0	0	0	0	0	0	0
342	5.12	100	100	22.82	20.22	26.96	6.64	6.37	12.56	13.12	16.49	16.92
343	0	24.83	22.26	0	2	7.65	0	0	0	0	0	0
356	0	0	0	0	0	0	5.35	5.36	5.49	5.62	5.46	5.94
358	0	0	0	0	0	6.1	0	0	0	0	0	0