Supplementary Material

for

Metabolomic Profiling of *Guadua* Species and its Correlation with Antioxidant and Cytotoxic Activities

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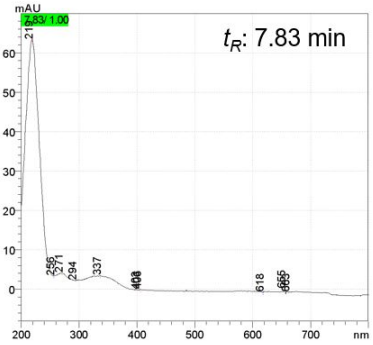
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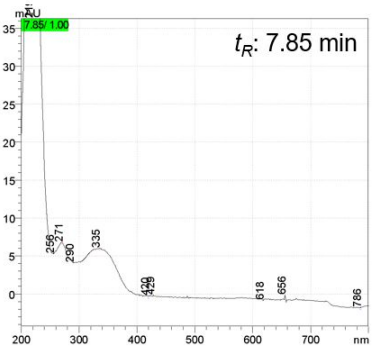
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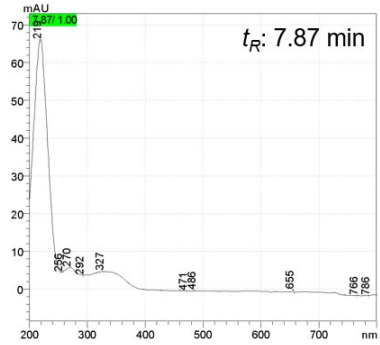
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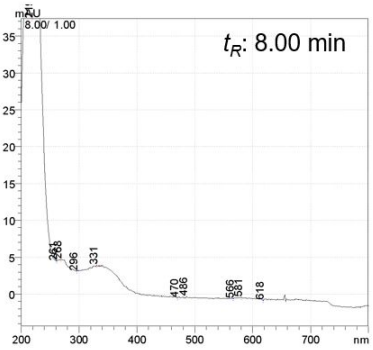
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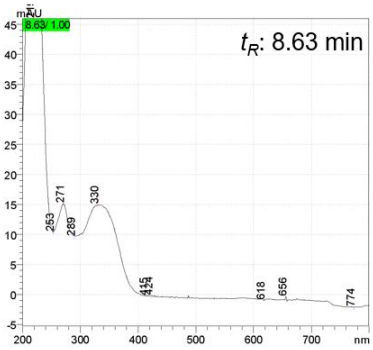
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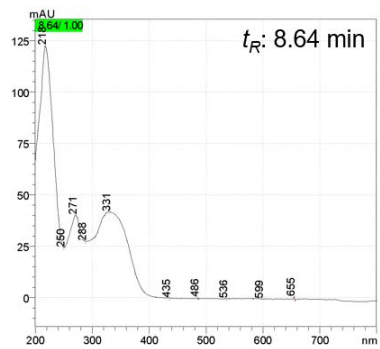
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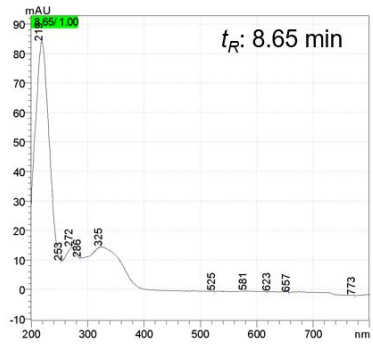
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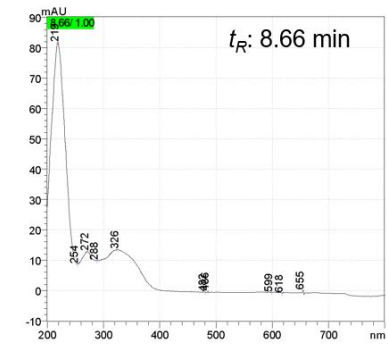
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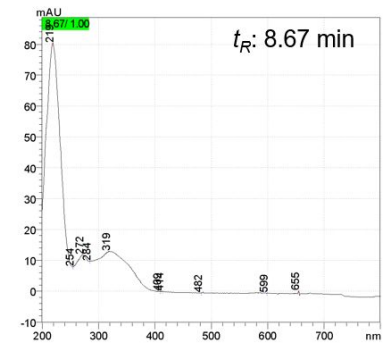
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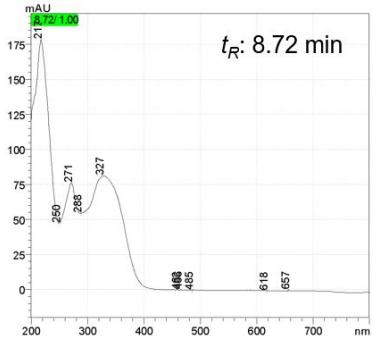
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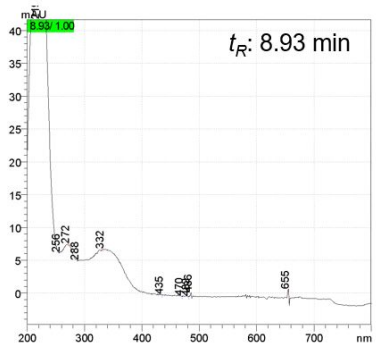
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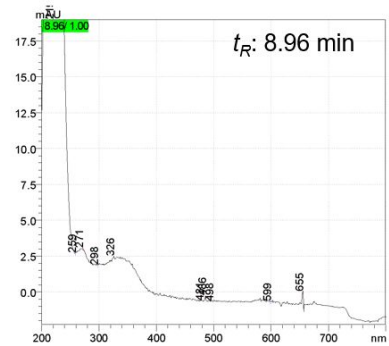
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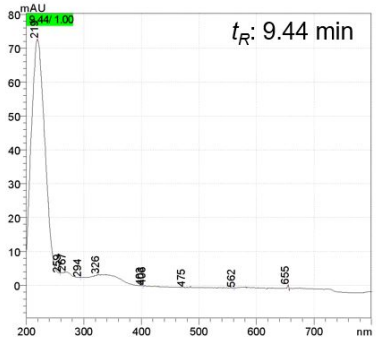
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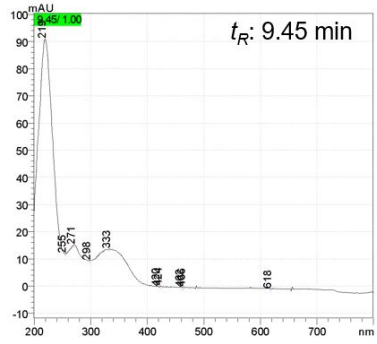
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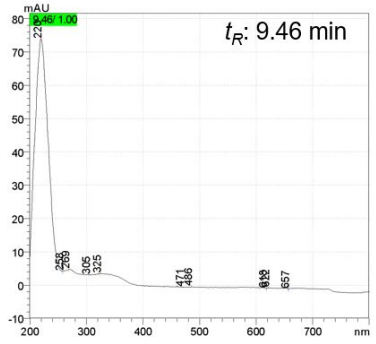
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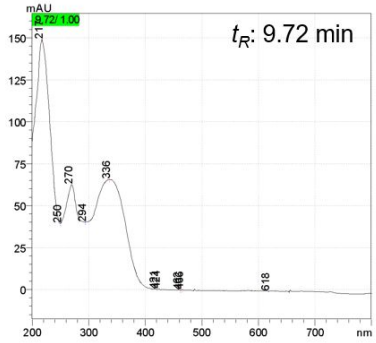
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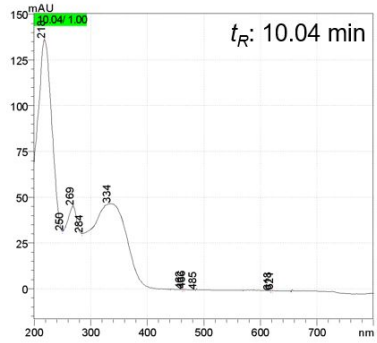
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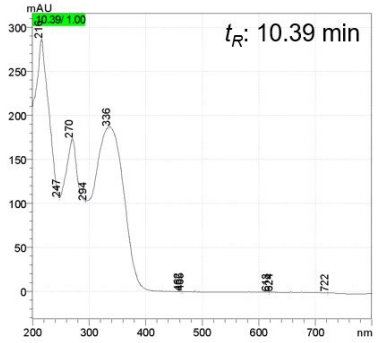
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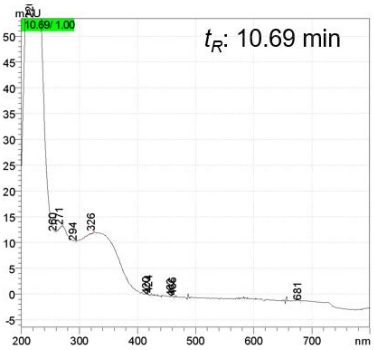
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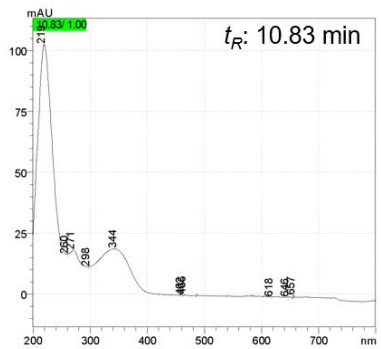
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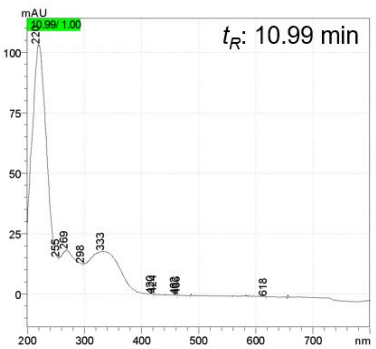
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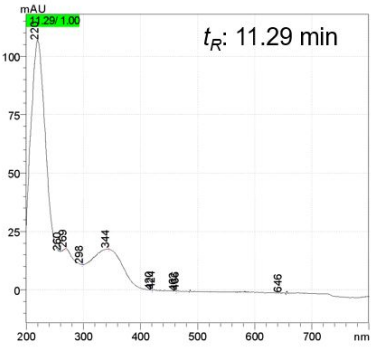
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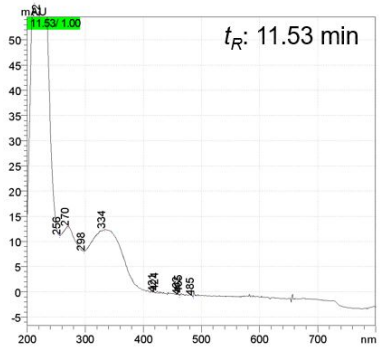
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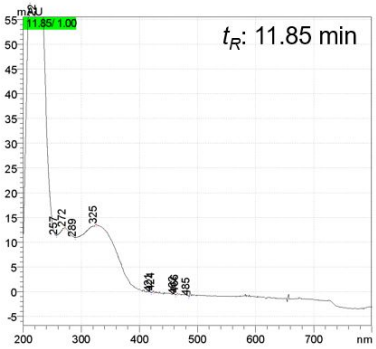
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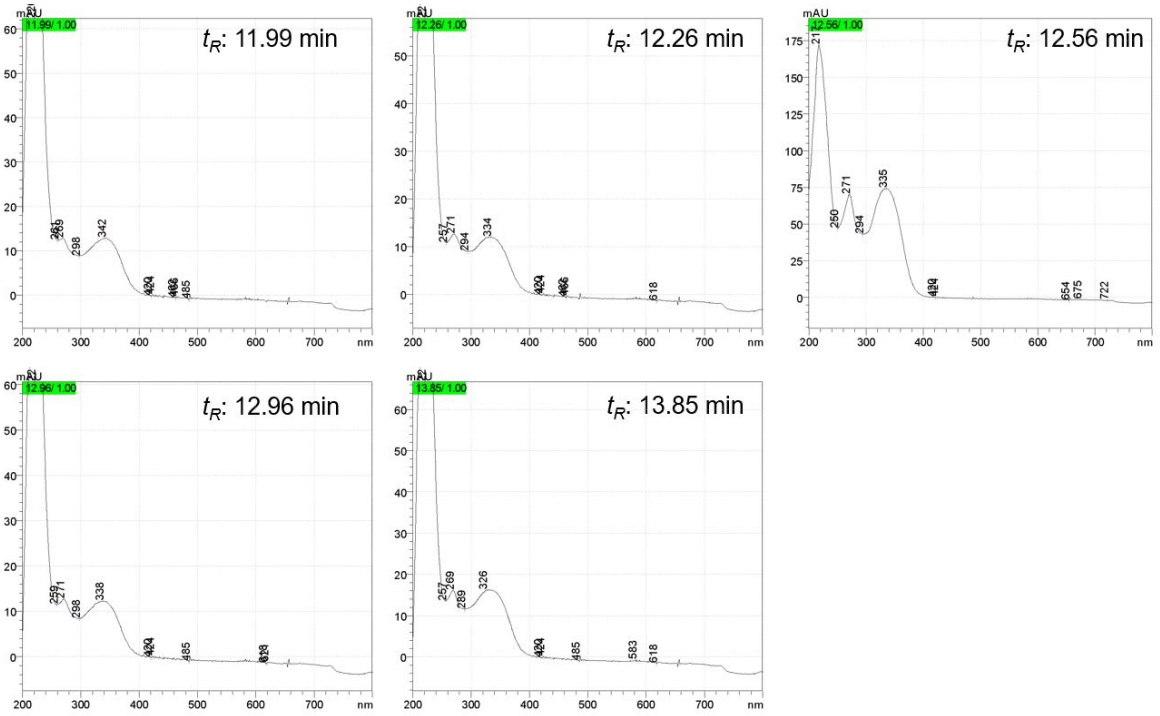


Figure S1. UV spectra of the major peaks found in the BLEs obtained by HPLC-DAD. The retention time of each peak and its corresponding spectrum are described in highlighted green (t_R/1.00).

Table S1. Phytochemicals tentatively identified in BLEs using UHPLC-QTOF-MS.

Peak	t_R (min)	UV λ_{max} (nm)	Molecular formula	Adduct ion	Calculated mass (*m/z*)	Experimental mass (*m/z*)	Mass error (ppm)	Main fragment ions (MS/MS)	Identification confidence level	Tentative identification	Chemical class	Plant species	Reference or Database[a]
15	0.57	-	$C_7H_{12}O_6$	$[M-H]^-$	191.0551	191.0543	-4.2	175, 147, 129, 111	2	Quinic acid	Organic acid	*G. aculeata* *G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*	[1–3]
16	1.20	Low intensity	$C_{16}H_{18}O_9$	$[M-H]^-$	353.0878	353.0861	-4.8	191, 179, 155, 135	3	Not identified	Cinnamic acid and derivatives	*G. superba* *G. weberbaueri*	
17	1.94	Low intensity	$C_{15}H_{16}O_{10}$	$[M-H]^-$	355.0670	355.0669	-0.3	209, 191, 163, 147, 129	3	Not identified	Cinnamic acid and derivatives	*G. aculeata* *G. amplexifolia* *G. angustifolia* *G. incana*	
18	1.98	Low intensity	$C_{17}H_{20}O_9$	$[M-H]^-$	367.1034	367.1024	-2.7	207, 193, 134	2	*O*-Feruloylquinic acid	Cinnamic acid and derivatives	*G. angustifolia* *G. superba* *G. uncinata*	[3–7] and GNPS
19	2.04	290^{sh}, 310	$C_{25}H_{24}O_{12}$	$[M-H]^-$	515.1195	515.1193	-0.4	353, 191, 179, 137	2	Dicaffeoylquinic acid	Cinnamic acid and derivatives	*G. aculeata* *G. superba* *G. venezuelae* *G. weberbaueri*	[3] and GNPS

20	2.33	Low intensity	$C_{16}H_{18}O_8$	$[M-H]^-$	337.0928	337.0945	5.0	191, 173, 164, 119	2	*O*-Coumaroylquinic acid	Cinnamic acid and derivatives	*G. aculeata* *G. superba* *G. venezuelae* *G. weberbaueri*	[1,3,8,9] and GNPS
21	2.36	270, 327	$C_{27}H_{30}O_{16}$	$[M-H]^-$	609.1461	609.1466	0.8	547, 519, 489, 429, 399	3	Luteolin 6-*C*-hexoside 8-*C*-pentoside	Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. uncinata*	
2	2.46	292[sh], 326	$C_{16}H_{18}O_9$	$[M-H]^-$	353.0878	353.0864	-4.0	191, 179, 135	1	Chlorogenic acid[st]	Cinnamic acid and derivatives	*G. aculeata* *G. superba* *G. venezuelae* *G. weberbaueri*	[10–13] and GNPS
22	2.51	274, 336	$C_{21}H_{20}O_{10}$	$[M-H]^-$	431.0983	431.0981	-0.5	387, 341, 311, 179	3	Not identified	Flavone glycosides	*G. aculeata* *G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata*	

23	2.68	272, 325	$C_{27}H_{30}O_{15}$	$[M-H]^-$	593.1511	593.1513	0.3	503, 473, 383, 353, 297	2	Vicenin 2	Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. incana* *G. superba* *G. uncinata* *G. venezuelae*	[1,14] and GNPS
24	2.70	269, 325	$C_{21}H_{20}O_{11}$	$[M-H]^-$	447.0932	447.0931	-0.2	327, 299, 285, 133, 109	3	Not identified	Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* var. *bicolor* *G. incana* *G. uncinata*	
25	2.71	268, 337	$C_{27}H_{30}O_{15}$	$[M-H]^-$	593.1511	593.1517	1.0	457, 383, 353, 297	2	Apigenin 6,8-digalactoside	Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. incana* *G. superba* *G. uncinata* *G. venezuelae*	[8] and GNPS
				$[M+H]^+$	595.1668	595.1660	-1.3	541, 481, 457, 379, 325, 295					
26	2.71	267, 326	$C_{26}H_{28}O_{14}$	$[M-H]^-$	563.1406	563.1411	0.9	473, 443, 383, 353, 325, 2.97	3	Not identified	Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*	

3	2.74	311	$C_9H_8O_4$	$[M-H]^-$	179.0349	179.0352	1.7	135, 119	1	Caffeic acid[st]	Cinnamic acid and derivatives	*G. aculeata* *G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. incana* *G. superba* *G. uncinata* *G. venezuelae*	[10,11,15]
27	2.77	271, 333	$C_{26}H_{28}O_{14}$	$[M-H]^-$	563.1406	563.1410	0.7	445, 355, 325, 297	3	Not identified	Flavone glycosides	*G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata*	
28	2.80	269, 334	$C_{26}H_{28}O_{14}$	$[M-H]^-$	563.1416	563.1415	-0.2	473, 443, 401, 383, 353, 311	3	Not identified	Flavone glycosides	*G. aculeata* *G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. incana* *G. superba* *G. uncinata* *G. venezuelae*	
29	2.87	265, 341	$C_{27}H_{30}O_{14}$	$[M-H]^-$	577.1562	577.1565	0.5	413, 341, 293, 175	2	Vitexin 2"-*O*-rhamnoside	Flavone glycosides	*G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor*	[1] and GNPS
				$[M+H]^+$	579.1719	579.171	-1.6	433, 415, 367, 313, 283					

												G. incana *G. superba* *G. uncinata*	
30	2.88	269, 342	$C_{27}H_{30}O_{15}$	$[M-H]^-$	593.1511	593.1519	1.3	473, 431, 353, 311, 297, 282	2	Saponarin or Isosaponarin	Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*	[1,8] and GNPS
31	2.91	271, 335	$C_{26}H_{28}O_{14}$	$[M-H]^-$	563.1406	563.1401	-0.9	473, 443, 383, 353, 325, 297	2	Schaftoside or Isoschaftoside	Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. uncinata* *G. venezuelae* *G. weberbaueri*	[1,3,4,8,9,16] and GNPS
				$[M+H]^+$	565.1562	565.1563	0.2	547, 529, 499, 457, 427, 379					
32	3.13	273, 339	$C_{26}H_{28}O_{14}$	$[M+H]^+$	565.1562	565.1564	0.4	525, 481, 405, 337, 295	3	Vicenin 1 or Vicenin 3	Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*	

33	3.16	270, 344	$C_{28}H_{32}O_{16}$	$[M-H]^-$	623.1617	623.1617	0.0	504, 443, 353, 323	3	Isoscoparin 2"-*O*-hexoside	Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. uncinata*	
34	3.18	271, 342	$C_{28}H_{32}O_{15}$	$[M+H]^+$	609.1824	609.1824	0.0	430, 393, 327, 297, 267	3	Spinosin or Isospinosin	Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*	
8	3.20	Low intensity	$C_9H_8O_3$	$[M-H]^-$	163.0400	163.0400	0.0	119	1	*p*-Coumaric acid[st]	Cinnamic acid and derivatives	*G. aculeata* *G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. incana* *G. superba* *G. uncinata* *G. venezuelae*	[17] and GNPS

35	3.23	270, 341	$C_{27}H_{30}O_{14}$	$[M-H]^-$	577.1562	577.1569	1.2	533, 472, 413, 353, 293	2	Violanthin or Isoviolanthin	Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*	[18]
36	3.24	269, 332	$C_{27}H_{30}O_{15}$	$[M-H]^-$	593.1511	593.1512	0.2	285, 218, 151	2	Kaempferol 7-*O*-neohesperidoside	Flavonol glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. uncinata*	[18] and GNPS
37	3.28	270, 325	$C_{33}H_{40}O_{19}$	$[M-H]^-$	739.2091	739.209	-0.1	593, 431, 281	3	Kaempferol 3-*O*-disaccharoside-7-*O*-pentoside	Flavonol glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. uncinata*	

38	3.28	270, 326	$C_{27}H_{30}O_{15}$	$[M+H]^+$	595.1668	595.1667	-0.2	449, 287	3	Kaempferol 3-*O*-disaccharoside		Flavonol glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. uncinata*	
39	3.35	272, 326	$C_{21}H_{18}O_{13}$	$[M-H]^-$	477.0674	477.0675	0.2	431, 301, 179	3	Quercetin 3-*O*-hexoside		Flavonol glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*	
40	3.37	270, 325	$C_{21}H_{20}O_{12}$	$[M-H]^-$	463.0882	463.0880	-0.4	372, 300, 271, 255, 243, 151	2	Hyperoside		Flavonol glycosides	*G. aculeata* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae*	[17]

41	3.41	271, 329	$C_{28}H_{32}O_{17}$	$[M-H]^-$	639.1566	639.1570	0.6	403, 328, 313, 285, 270, 242	3	Isorhamnetin 3,4'-hexoside		Flavonol glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*
42	3.54	271, 344	$C_{27}H_{30}O_{14}$	$[M-H]^-$	577.1562	577.1561	-0.2	269, 117	3	Apigenin 7-*O*-disaccharoside		Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. uncinata* *G. venezuelae*
43	3.56	269, 342	$C_{27}H_{30}O_{14}$	$[M+H]^+$	579.1719	579.1718	-0.2	433, 363, 271, 153	3	Apigenin 7-*O*-disaccharoside		Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*

44	3.58	268, 331	$C_{22}H_{22}O_{11}$	$[M-H]^-$	461.1089	461.1087	-0.4	415, 341, 313, 298	3	Not identified	Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. uncinata* *G. venezuelae*
45	3.59	270, 325	$C_{28}H_{34}O_{15}$	$[M-H]^-$	609.1824	609.1843	3.1	325, 301, 286, 151	3	Hesperidin	Flavanone glycoside	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. uncinata*
46	3.61	271, 344	$C_{28}H_{32}O_{15}$	$[M+H]^+$	609.1826	609.1810	-2.6	463, 301, 286, 258	3	Diosmetin 7-*O*-disaccharoside	Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae*

47	3.64	269, 326	$C_{28}H_{32}O_{16}$	$[M-H]^-$	623.1617	623.1620	0.5	329, 314, 299, 271, 243, 187	3	Isorhamnetin 3-*O*-hexoside-6"-disaccharoside		Flavonol glycosides	*G. aculeata* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae*	
48	3.73	265, 341	$C_{27}H_{30}O_{15}$	$[M-H]^-$	593.1511	593.1512	0.2	473, 431, 353, 341, 311, 283	3	Apigenin hexoside-7-*O*-hexoside	6-*C*-	Flavone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. uncinata* *G. venezuelae*	
				$[M+H]^+$	595.1668	595.1667	-0.2	415, 379, 337, 313, 283, 165						
49	4.47	264, 356	$C_{15}H_{10}O_6$	$[M-H]^-$	285.0404	285.0403	-0.4	199, 169, 151, 133	2	Luteolin		Flavone aglycones	*G. aculeata* *G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*	[12,19,20]
50	4.57	270, 319	$C_{15}H_{12}O_3$	$[M-H]^-$	239.0713	239.0699	-5.9	211, 195, 179, 135	3	6-Hidroxyflavanone		Flavone aglycones	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var.	

											bicolor *G. incana*	
51	4.88	264, 329	$C_{23}H_{24}O_{12}$	$[M-H]^-$	491.1195	491.1198	0.6	461, 328, 313, 285, 226	2	Tricin 7-*O*-glucoside	Flavone glycosides	*G. aculeata* *G. amplexifolia* *G. angustifolia* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae*	[8]
52	4.92	264, 335	$C_{27}H_{32}O_{14}$	$[M-H]^-$	579.1719	579.1720	0.2	271, 177, 151, 119	3	Naringenin-7-*O*-disaccharoside	Flavanone glycosides	*G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. uncinata*	

53	4.95	263, 334	$C_{21}H_{22}O_{10}$	$[M-H]^-$	433.1140	433.1145	1.2	271, 151, 119	3	Naringenin-7-*O*-hexoside	Flavanone glycosides	*G. aculeata* *G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*	
54	4.97	271, 358	$C_{15}H_{10}O_5$	$[M-H]^-$	269.0455	269.0460	1.9	227, 181, 151, 117	2	Apigenin	Flavone aglycones	*G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*	[19]
55	5.01	244, 315	$C_{15}H_{10}O_6$	$[M-H]^-$	285.0404	285.0405	0.4	211, 183, 149, 121	3	3,6,2',3'-Tetrahydroxyflavone	Flavone aglycones	*G. aculeata* *G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*	

56	5.03	245, 319	$C_{15}H_{10}O_5$	$[M-H]^-$	269.0455	269.0461	2.2	239, 211, 187, 143, 117	3	6,7,4'-Trihydroxyisoflavone	Flavone aglycones	*G. aculeata* *G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*	
57	5.04	269, 354	$C_{15}H_{10}O_6$	$[M-H]^-$	285.0404	285.0420	5.6	255, 227, 187, 159, 143, 117	2	Kaempferol	Flavonol aglycones	*G. aculeata* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*	[18,19]
58	5.09	245, 319	$C_{17}H_{14}O_7$	$[M-H]^-$	329.0666	329.0671	1.5	271, 243, 227, 161, 133	3	4',5,7-Trihydroxy-3,6-dimethoxyflavone	Flavone aglycones	*G. aculeata* *G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata*	

											G. venezuelae *G. weberbaueri*	
59	5.12	244, 325	$C_{16}H_{12}O_6$	$[M-H]^-$	299.0561	299.0561	0.0	256, 227, 212, 183, 151	3	3,5,7-Trihydroxy-4'-methoxyflavone	Flavone aglycones	*G. aculeata* *G. amplexifolia* *G. angustifolia* *G. angustifolia* biotype *San calixto* *G. angustifolia* var. *bicolor* *G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*	
60	5.15	244, 354	$C_{17}H_{14}O_7$	$[M-H]^-$	329.0666	329.0669	0.9	229, 271, 227, 215, 161	2	Tricin	Flavone aglycones	*G. incana* *G. superba* *G. uncinata* *G. venezuelae* *G. weberbaueri*	[19]
				$[M+H]^+$	331.0823	331.0820	-0.9	313, 285, 270, 258, 203, 153					

[a] The references described compounds found in the literature for leaves, culms, and shoots of several bamboos' plants and database sources such as PubChem, METLIN, KEGG, GNPS; [st] The identification of compounds has been verified by using authentic standards; [sh] shoulder peak; *m/z* data were obtained by UHPLC-QTOF-MS based on time and peak areas. λ_{max}: UV maximum absorbance wavelength. Phytochemicals were annotated with identification confidence levels as recommended by the Metabolomics Standards Initiative (MSI) according to: Level 0: *Unambiguous 3D Structure: isolated, pure compound, including full stereochemistry*; Level 1: *Confident 2D structure: uses reference standard match or full 2D structure elucidation;* Level 2: *Probable structure: matched to literature data or databases by diagnostic evidence*, Level 3: *Possible structure or class: most likely structure, isomers possible, substance class or substructure match*; Level 4: *Unknown feature of interest*.[21]

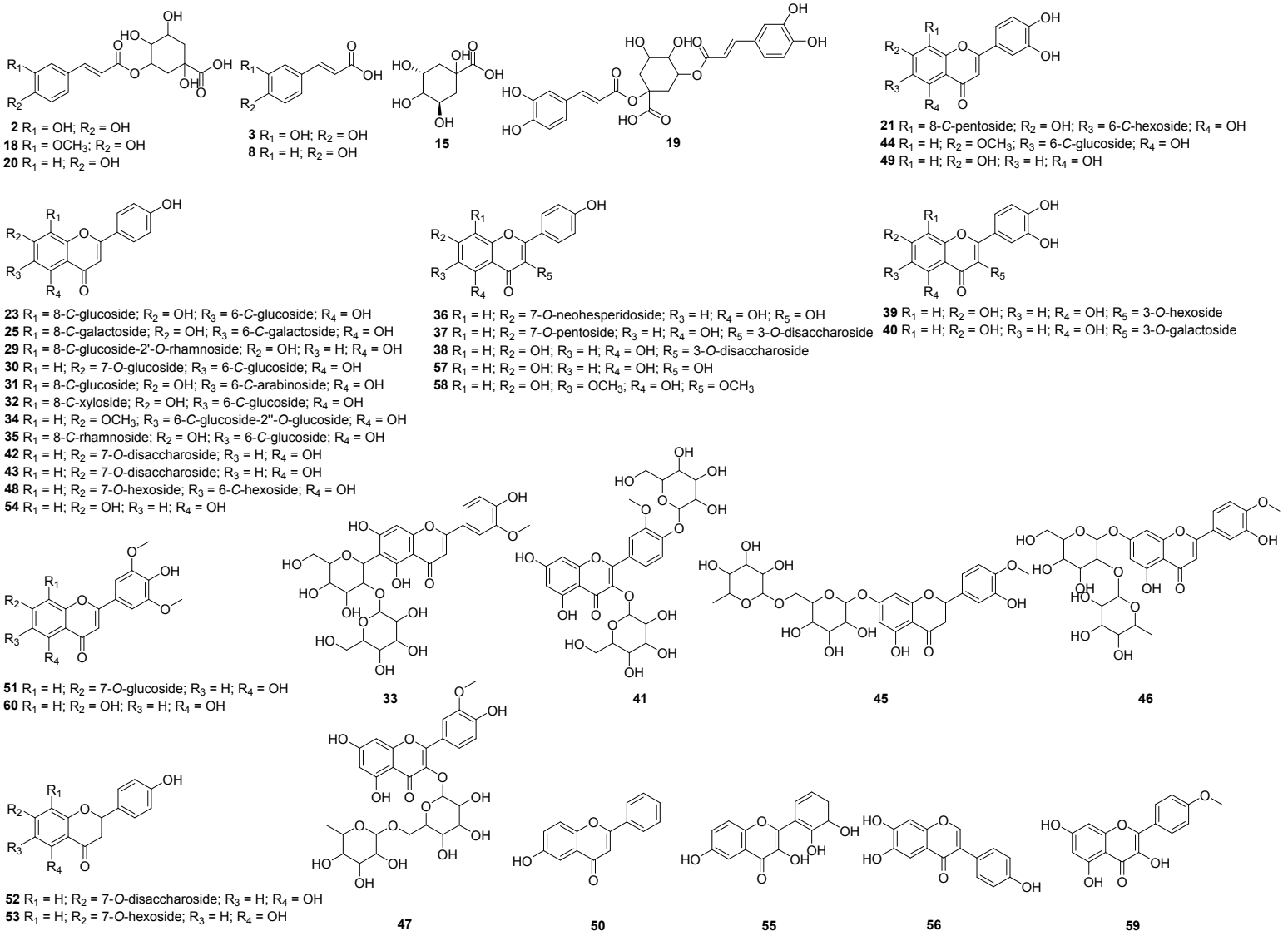
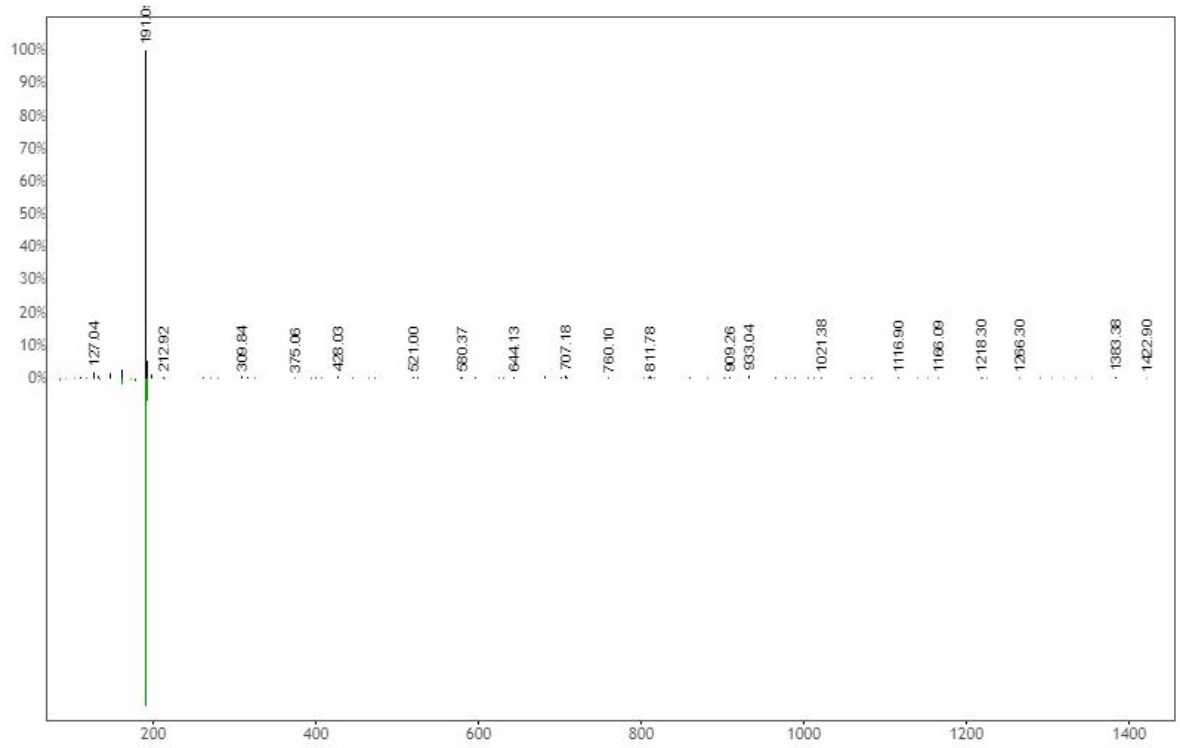
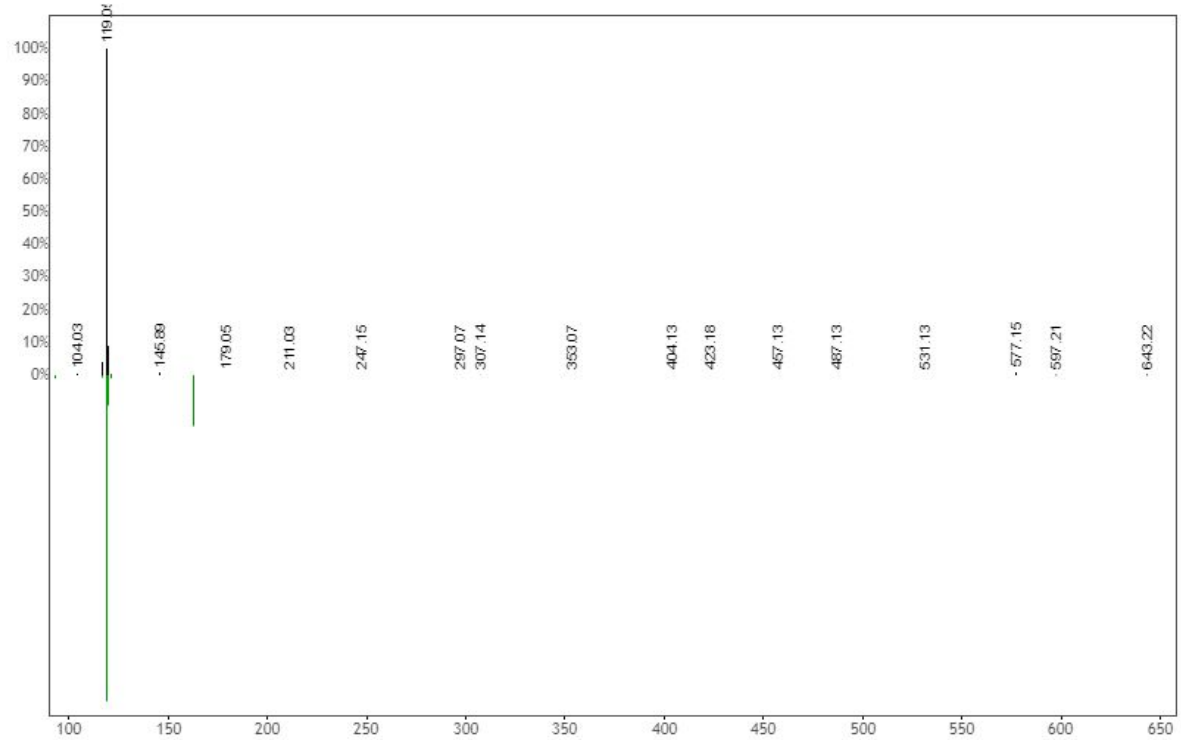


Figure S2. Chemical structures of the metabolites were found in BLEs.

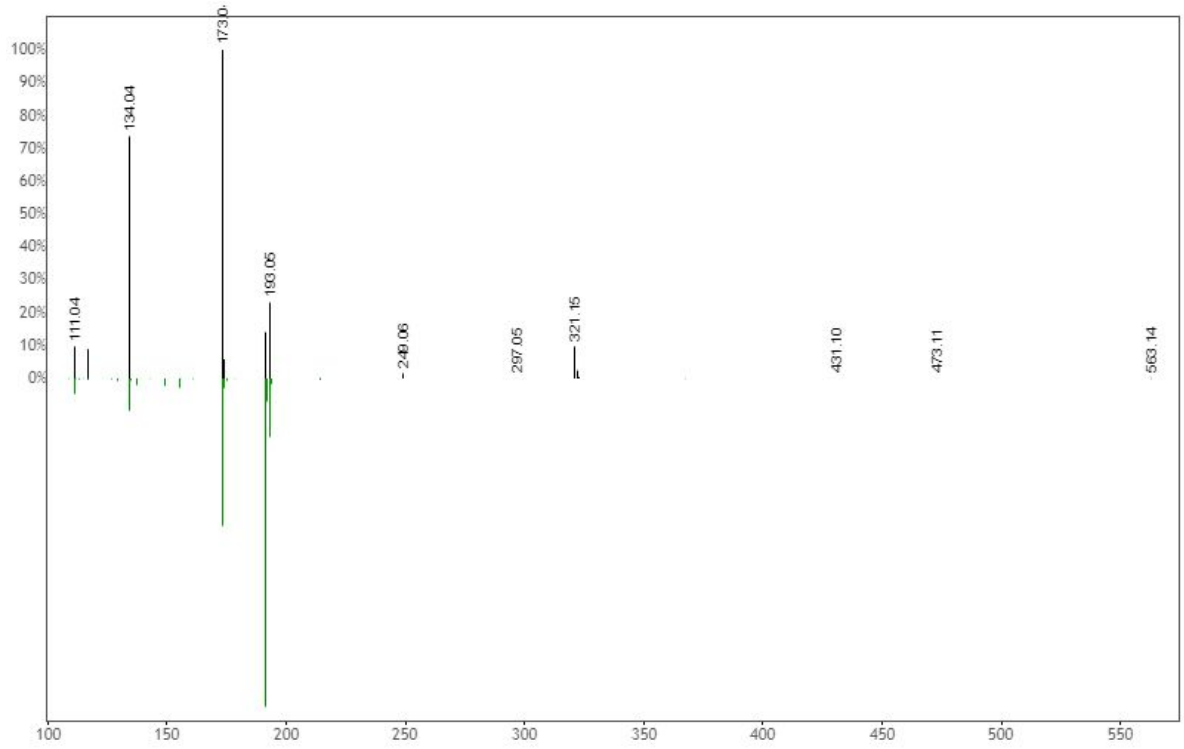
Compound 2



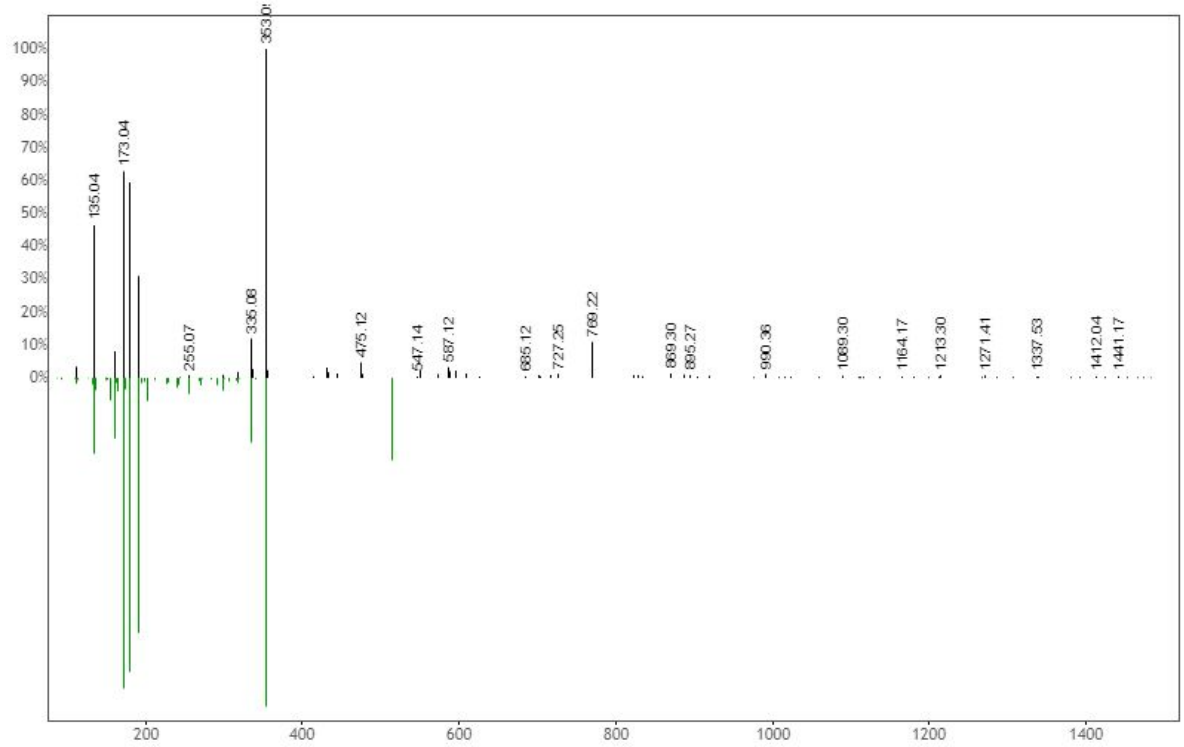
Compound 8



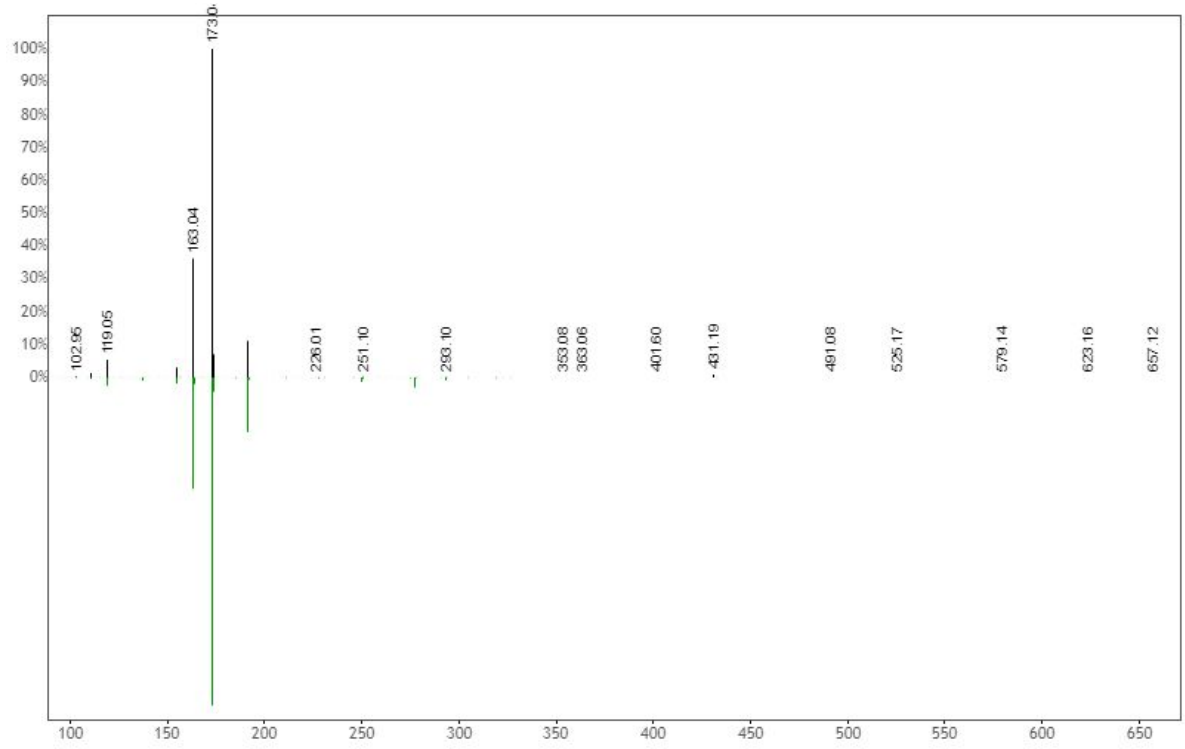
Compound 18



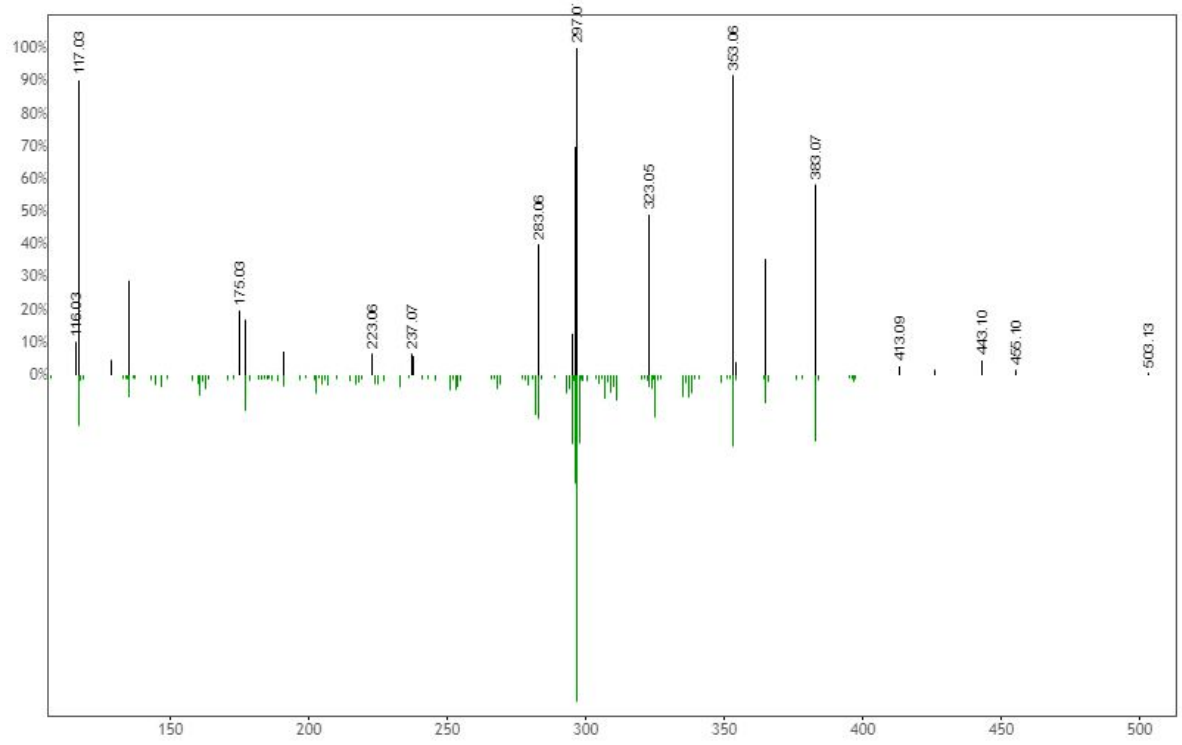
Compound 19



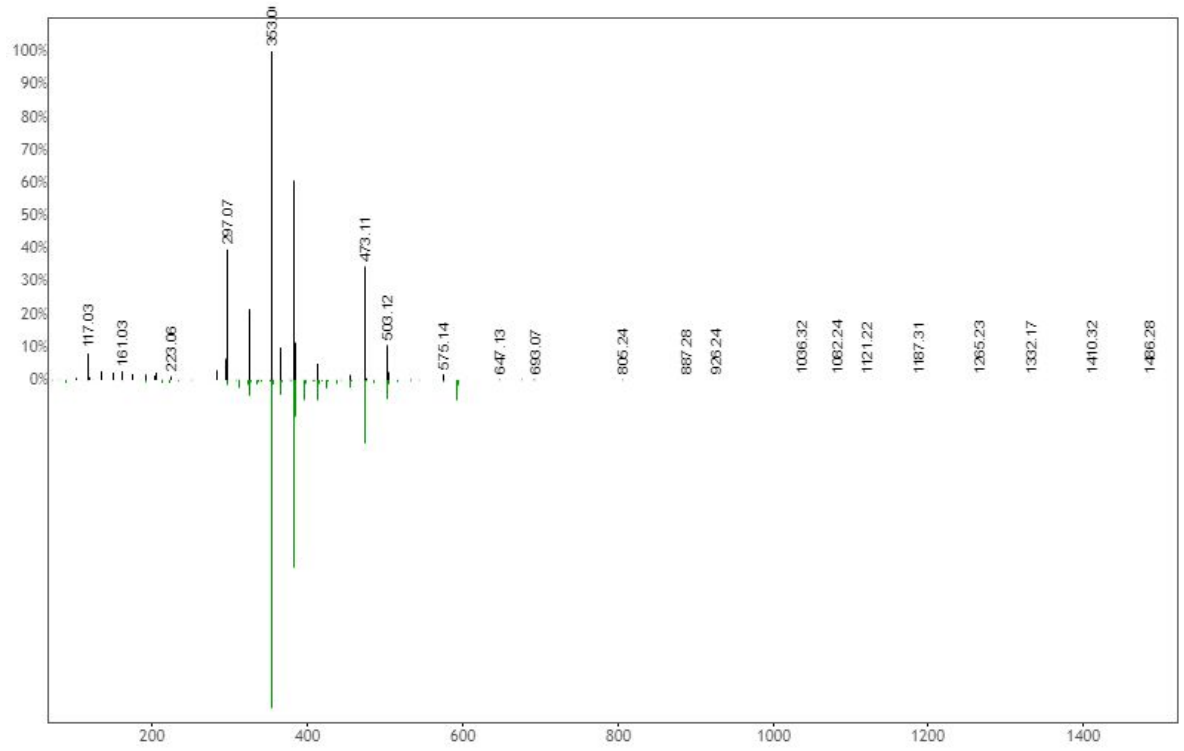
Compound 20



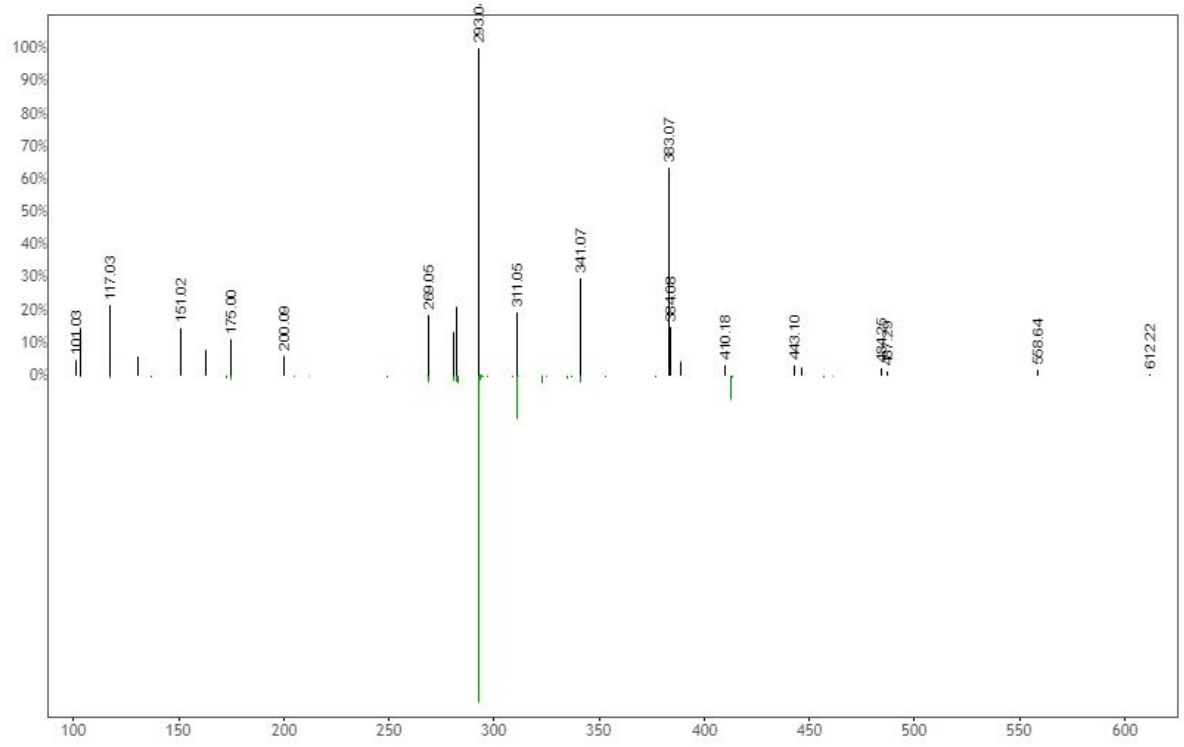
Compound 23



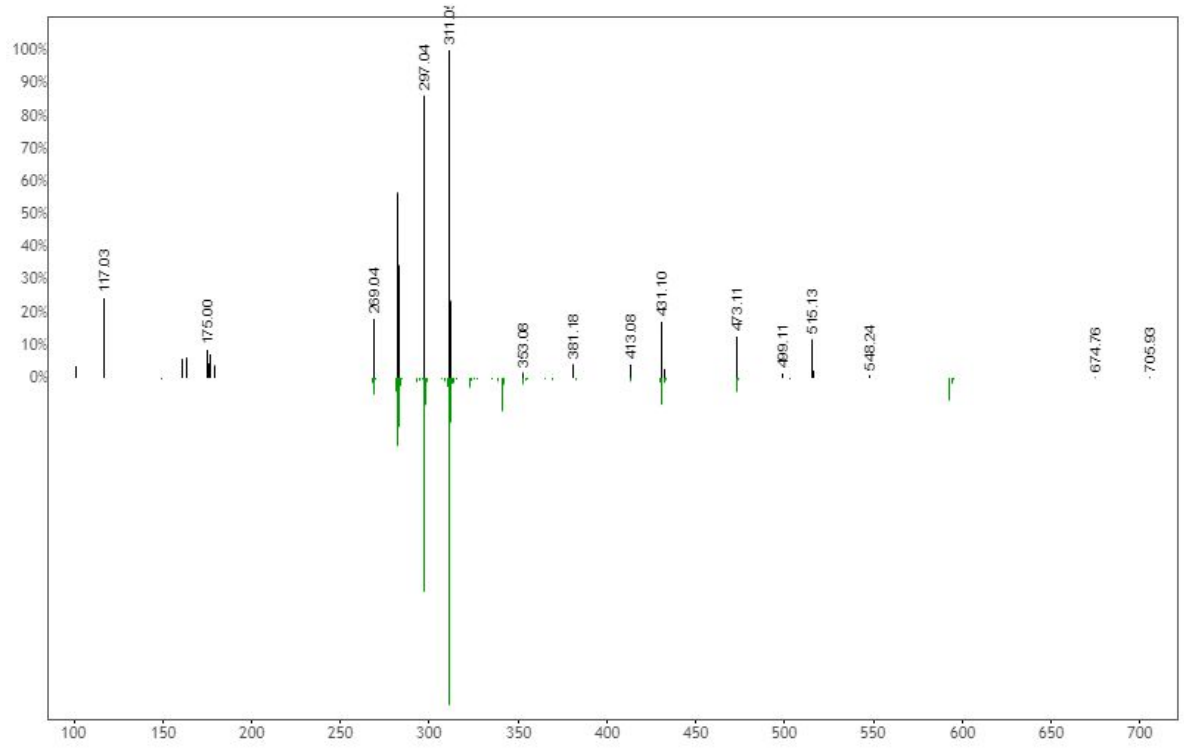
Compound 25



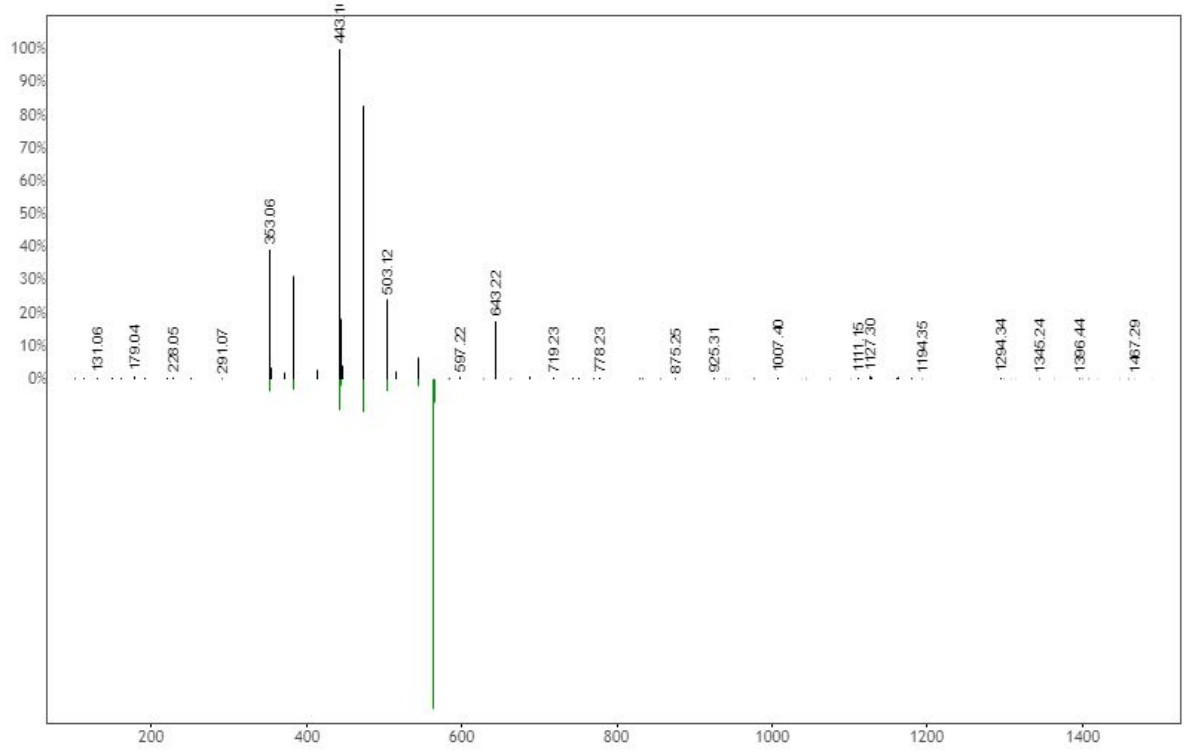
Compound 29



Compound 30



Compound 31



Compound 36

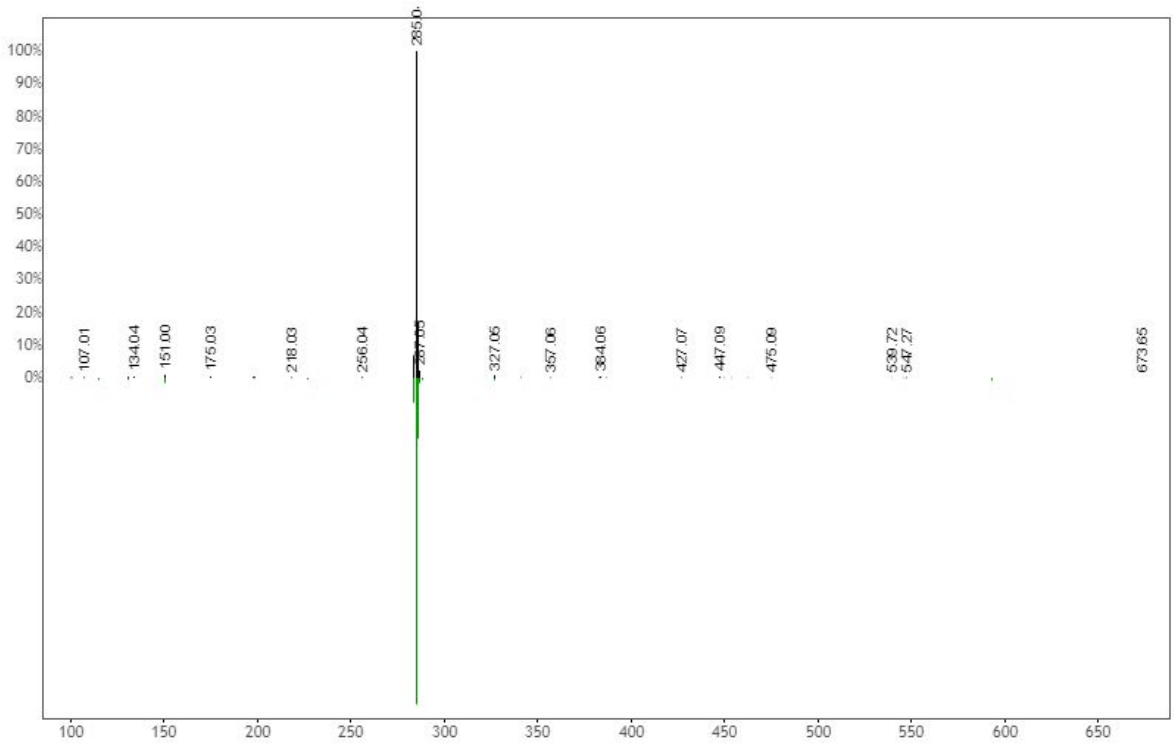


Figure S3. MS^2 spectrum match feature of GNPS showing the similarity of fragments patterns of the experimental and library data.

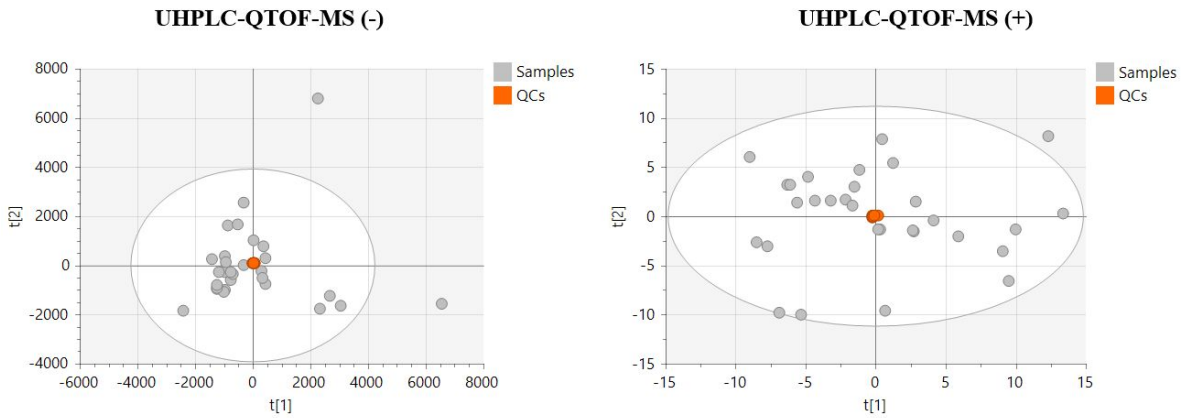


Figure S4. PCA score plot including Quality Controls (QCs) and all samples from UHPLC-QTOF-MS analysis in both negative and positive ion mode.

Table S2. List and information on the environmental variables of collection of the *Guadua* species used for the study.

Species	Sample code	Location	Collection date	Latitude	Longitude	Altitude	AMAT (°C)	AMET (°C)	AMIT (°C)	MP (mm)	RH (%)
G. aculeata Rupr. ex E. Fourn.	*Gac-Q1*	Quindío	12/2021	4.52086	-75.80102	1256	28.0	24.0	21.0	200-300	82.0
G. amplexifolia J.Presl	*Gam-Q1*	Quindío	03/2021	4.52083	-75.80108	1256	28.0	24.0	21.0	200-300	82.0
	Gam-Q2	Quindío	12/2021	4.52083	-75.80108	1256	28.0	24.0	21.0	200-300	82.0
	Gam-Q3	Quindío	12/2021	4.52083	-75.80108	1256	28.0	24.0	21.0	200-300	82.0
G. angustifolia Kunth	*Gan-C1*	Cundinamarca	09/2020	5.18127	-74.19519	1343	31.5	25.5	23.5	100-200	82.5
	Gan-C2	Cundinamarca	09/2020	5.18127	-74.19519	1343	31.5	25.5	23.5	100-200	82.5
	Gan-C3	Cundinamarca	09/2020	5.18127	-74.19519	1343	31.5	25.5	23.5	100-200	82.5
	Gan-C4	Cundinamarca	10/2022	5.18127	-74.19519	1343	31.5	25.5	23.5	100-200	82.5
	Gan-C5	Cundinamarca	09/2020	5.18127	-74.19519	1343	31.5	25.5	23.5	100-200	82.5
	Gan-C6	Cundinamarca	09/2020	5.18127	-74.19519	1343	31.5	25.5	23.5	100-200	82.5
	Gan-C7	Cundinamarca	10/2021	5.18127	-74.19519	1343	31.5	25.5	23.5	100-200	82.5
	Gan-N1	Nariño	06/2021	1.37383	-77.27988	1857	20.6	17.5	12.3	100-200	60.0
	Gan-N2	Nariño	12/2021	1.32755	-77.48088	1720	21.8	16.8	13.6	100-200	65.0
	Gan-N3	Nariño	12/2021	1.32755	-77.48088	1720	21.8	16.8	13.6	100-200	65.0
	Gan-N4	Nariño	01/2022	1.32755	-77.48088	1720	21.8	16.8	13.6	100-200	65.0
	Gan-N5	Nariño	01/2022	1.54900	-78.67738	21	28.0	26.0	24.0	200-300	85.0
	Gan-N6	Nariño	01/2022	1.54900	-78.67738	21	28.0	26.0	24.0	200-300	85.0
	Gan-Q1	Quindío	12/2021	4.52053	-75.79973	1256	28.0	24.0	21.0	200-300	82.0
	Gan-Q2	Quindío	04/2022	4.52053	-75.79973	1256	28.0	24.0	21.0	200-300	82.0
G. angustifolia Kunth biotype San Calixto	*Ganc-Q1*	Quindío	04/2022	4.52063	-75.80041	1256	29.0	23.0	18.0	200-300	80.0

G. angustifolia var. *bicolor* Londoño	*Ganb-Q1*	Quindío	04/2022	4.52018	-75.80056	1256	29.0	23.0	18.0	200-300	80.0
G. incana Londoño	*Gin-P1*	Putumayo	12/2021	1.17730	-76.66477	604	26.0	22.5	20.0	100-200	85.0
	Gin-Q1	Quindío	03/2021	4.52102	-75.80013	1256	28.0	24.0	21.0	200-300	82.0
	Gin-Q2	Quindío	12/2021	4.52102	-75.80013	1256	28.0	24.0	21.0	200-300	82.0
G. superba Huber	*Gsu-Q1*	Quindío	04/2022	4.52100	-75.80036	1256	29.0	23.0	18.0	200-300	80.0
G. uncinata Londoño & L.G.Clark	*Gun-Q1*	Quindío	03/2021	4.51816	-75.80033	1256	28.0	24.0	21.0	200-300	82.0
	Gun-Q2	Quindío	12/2021	4.51816	-75.80033	1256	28.0	24.0	21.0	200-300	82.0
	Gun-Q3	Quindío	12/2021	4.51816	-75.80033	1256	28.0	24.0	21.0	200-300	82.0
G. venezuelae Munro	*Gve-Q1*	Quindío	04/2022	4.52057	-75.80005	1256	29.0	23.0	18.0	200-300	80.0
G. weberbaueri Pilg.	*Gwe-Q1*	Quindío	04/2022	4.52043	-75.80057	1256	29.0	23.0	18.0	200-300	80.0

Annual Maximum Temperature (AMAT), Annual Mean Temperature (AMET), Annual Minimum Temperature (AMIT), Monthly Precipitation (MP), and Relative Humidity (RH).

Table S3. Comparison of retention times of reference standards between HPLC-DAD and UHPLC-QTOF-MS analyses.

No	Chemical standard	Chemical class	UV λ_{max} (nm)	Molecular formula	t_R (min) HPLC[a]	t_R (min) UHPLC[b]	Exact mass	$[M-H]^-$	$[M+H]^+$
1	Gallic acid	Organic acid	275	$C_7H_6O_5$	4.36	1.09	170.0215	169.0132	-
2	Chlorogenic acid (CGA)	Cinnamic acid and derivatives	275sh, 325	$C_{16}H_{18}O_9$	7.72	2.42	354.3095	353.0863	-
3	Caffeic acid	Cinnamic acid and derivatives	275	$C_9H_8O_4$	9.08	2.55	180.0422	179.0344	-
4	Isoorientin	Flavone glycosides	274, 355	$C_{21}H_{20}O_{11}$	9.39	2.96	448.3775	447.0954	449.1094
5	Ampelopsin	Flavanonol aglycones	300	$C_{15}H_{12}O_8$	9.88	2.88	320.0532	319.0458	-
6	Rutin	Flavonol glycosides	274, 355	$C_{27}H_{30}O_{16}$	10.42	3.20	610.1533	609.1531	611.1603
7	Vitexin	Flavone glycosides	273, 335	$C_{21}H_{20}O_{10}$	10.56	3.26	432.1056	431.0923	433.1123
8	*p*-Coumaric acid	Cinnamic acid and derivatives	295sh, 310	$C_9H_8O_3$	11.15	3.36	164.0473	163.0390	-
9	Sinapinic acid	Cinnamic acid and derivatives	325	$C_{11}H_{12}O_5$	11.55	3.78	224.2101	223.0684	-
10	Morin	Flavonol aglycones	264, 354	$C_{15}H_{10}O_7$	14.79	4.19	302.0426	301.0351	303.0512
11	Coumarin	Coumarins	275, 325	$C_9H_6O_2$	15.19	4.35	146.1432	-	147.0377
12	Quercetin	Flavonol aglycones	275, 358	$C_{15}H_{10}O_7$	15.86	4.49	302.0426	301.0344	303.0494
13	Cinnamic acid	Cinnamic acid and derivatives	275	$C_9H_8O_2$	16.84	4.63	148.1597	147.0524	-
14	Naringenin	Flavanone aglycones	275, 325	$C_{15}H_{12}O_5$	17.75	4.93	272.0684	271.0611	273.0764

[a] Column: Luna C18 column (150 x 4.6 mm, 5 µm, 100 Å)
[b] Column: ACQUITY UPLC HSS T3 C18 column (2.1 × 100 mm, 1.8 µm)

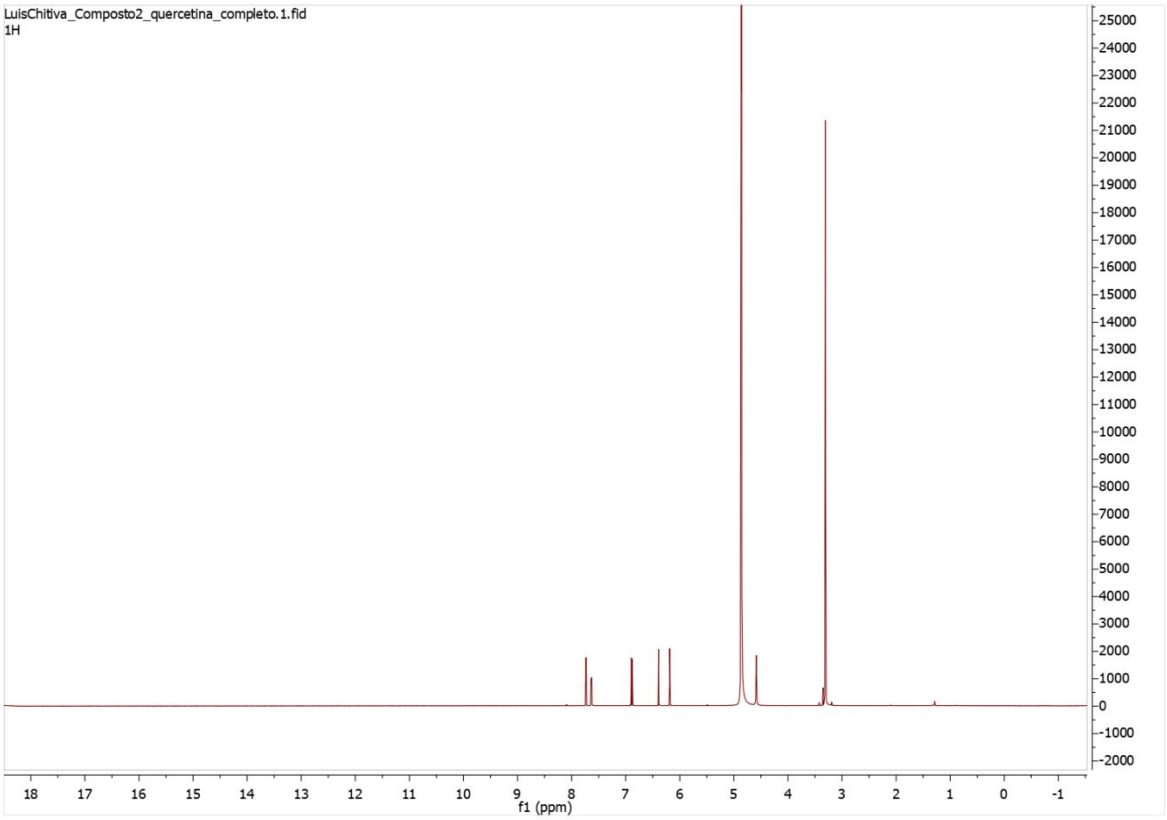


Figure S5. ^{1}H-NMR spectra obtained for quercetin.

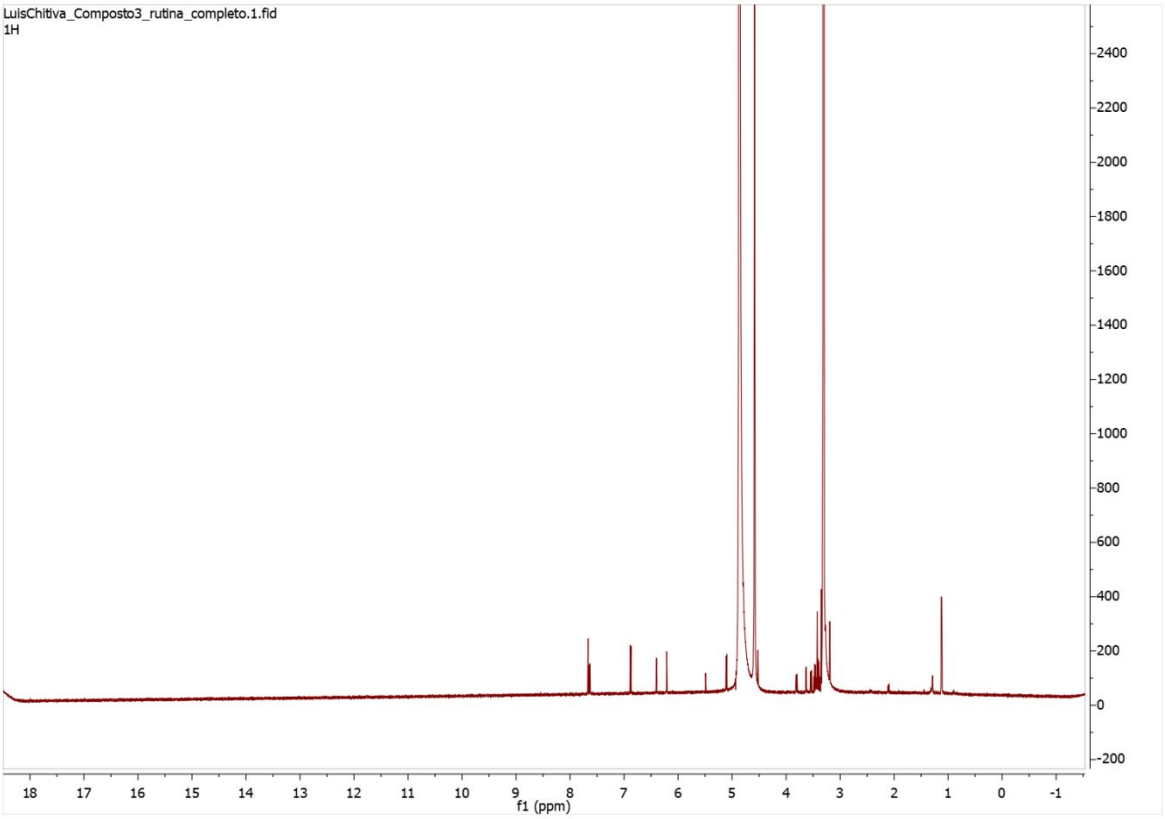


Figure S6. ^{1}H-NMR spectra obtained for rutin.

Table S4. Parameters used in the GNPS Classical Molecular Networking.

GNPS Classical Molecular Networking	
Processing step	**Parameters**
Basic options	Classical Molecular Networking Precursor Ion Mass Tolerance: 0.02 Da Fragment Ion Mass Tolerance: 0.02 Da
Advance Network Options	Min Pair Cos: 0.6 Network TopK: 10 Maximum Connected Component Size: 100 Minimun Matched Fragment Ions: 4 Minimum Cluster Size: 2 Maximum shift: 1999 Da Run MSCluster: yes
Advance Library Search Options	Library Search Min Matched Peaks: 4 Search Analogs: Do Search Score Threshold: 0.6 Maximum Analog Search Mass Difference: 100 Da

Table S5. Parameters used in the MZmine 2.53 software for processing the data obtained by UHPLC-QTOF-MS.

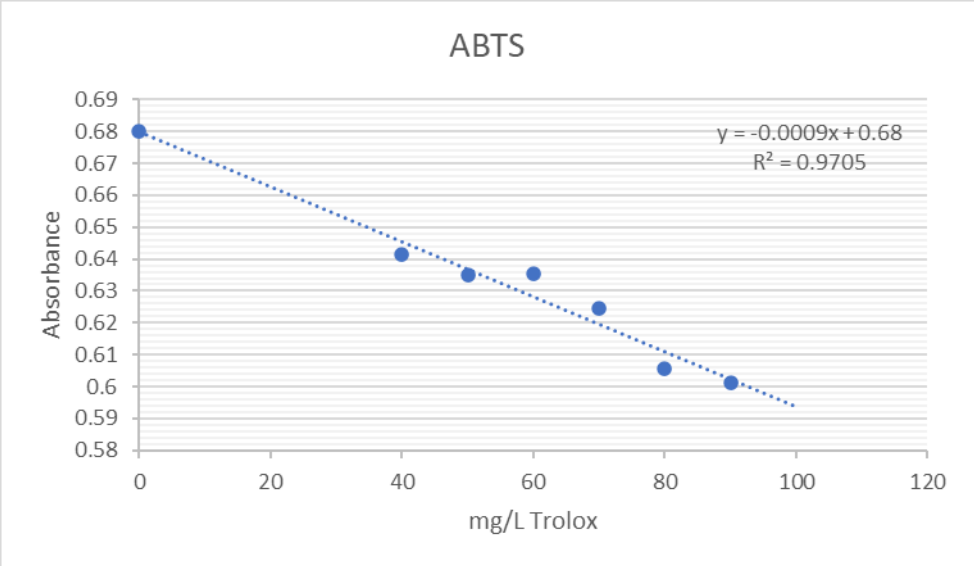
MZmine version 2.53 software	
Preprocessing step	**Parameters**
Feature detection	*Mass Detection* MS level: 1 Set filters Retention time: 0.2 - 10 min Mass detector: Centroid Noise level: 1E3 MS level: 2 Set filters Retention time: 0.2 - 10 min Mass detector: Centroid Noise level: 1E2
Chromatogram builder	*ADAP Chromatogram Builder* MS level: 1 Min group size in # of scans: 5 Group intensity threshold: 1E3 Min highest intensity: 3E3 *m/z* tolerance: 0 *m/z* or 20 ppm
Deconvolution	*Chromatogram deconvolution* Algorithm: Baseline cut-off Min peak height: 1E3 Peak duration range (min): 0 to 3 min Baseline level: 1E3 *m/z* range for MS2 scan pairing (Da): 0.01 RT range for MS2 scan pairing (min): 0.02
Isotopes	*Isotopic peaks grouper* *m/z* tolerance: 0 *m/z* or 20 ppm Retention time tolerance: 0.02 min Max charge: 2 Representative isotope: Most intense
Alignment	*Join aligner* *m/z* tolerance: 0 *m/z* or 20 ppm Weight for *m/z*: 75 Retention time tolerance: 0.25 absolute (min) Weight for RT: 25
Filtering	*Feature list rows filter* Minimum peaks in a row (X): 1 Minimum peaks in an isotope pattern (X): 1 *m/z* range: 75 to 2000 Reset peak number ID: True Keep only peaks with MS2 scan (GNPS): (X)
Gap Filling	*Peak finder* Intensity tolerance: 10% *m/z* tolerance: 0 *m/z* or 10 ppm RT tolerance: 0.05 min

Export	*Export to CSV file* (X) Export row (X) Export row *m/z* (X) Export row retention time (X) Peak area
Formula prediction	Charge: 2 Ionization type: M-H *m/z* tolerance: 0.01 *m/z* or 10 ppm Max best formulas per peak: 3 O 50 H 100 C 100

Table S6. Parameters used in the NMRProcFlow software for processing the data obtained by ^{1}H-NMR.

NMRProcFlow	
Preprocessing step	**Parameters**
PPM Calibration	*Range of the PPM reference:* Not applicable *PPM value of the center of resonance:* 0 *noisy PPM range:* 10.5 10.2
Normalization	*Normalization Method:* Constant Sum Normalization *Reference PPM ranges:* Not applicable
Baseline correction	*Type of Correction:* Local Correction *noisy PPM range:* 10.5 10.2 *Restricted PPM range:* Not applicable *Level of Correction:* 1 *Order:* 1
Alignment	*Align. Method:* Least Square *Relative max. shift:* 0.05 *Reference spectrum:* Auto reference *PPM Ranges to align:* Not applicable
PPM shift	*PPM shift value:* 0 *PPM Ranges to shift:* Not applicable
Zeroing	*PPM Ranges to clean:* 4.99 4.75
Bucketing	

Bucketing Method *Intelligent Bucketing*	*Resolution Factor:* 0.5 *SNR threshold:* 3 *noisy PPM range:* 10.5 10.2 *PPM Ranges:* 10.0 0.0
Data export	
Data matrix	*Export Format:* Comma Separator Value (CSV) *SNR threshold:* 3 *noisy PPM range:* 10.5 10.2 *Normalization Method:* Constant Sum Normalization *PPM range of the Reference:* Not applicable
Buckets table	*Export Format:* Comma Separator Value (CSV)



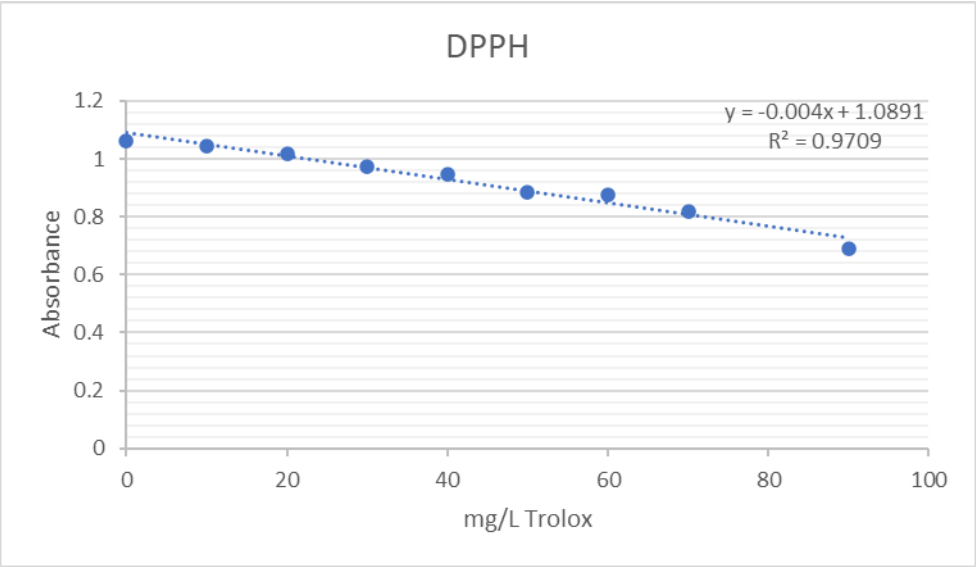


Figure S7. Calibration curves obtained for the determination of antioxidant capacity by ABTS and DPPH.

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