

Table S1. Chemical composition of fruit decoction.

No .	Name	Formula	Rt	[M + H] ⁺	[M - H] ⁻	Frag-ment 1	Frag-ment 2	Frag-ment 3	Frag-ment 4	Frag-ment 5
1	Quinic acid	C7H12O6	1,21		191,055 57	173,044 6	127,038 9	111,043 7	93,0332	85,0280
2	Citric acid	C6H8O7	1,56		191,019 18	173,008 4	129,018 3	111,007 5	87,0073	85,0281
3	Brugierol	C3H6O2S2	1,64	138,988 75		120,977 9	102,967 5		92,9832	86,9904
4	Gallocatechin (Casuarin, Gallocatechol)	C15H14O7	4,58		305,066 13	261,076 9	219,066 1	179,034 3	137,023 4	125,023 2
5	Protocatechuic acid (3,4-Dihydroxybenzoic acid)	C7H6O4	4,65		153,018 79	109,028 2	108,020 4		91,0177	81,0329
6	Neochlorogenic acid (5-O-Caffeoylquinic acid)	C16H18O9	8,64	355,102 91		163,039 0	145,028 6	135,044 3	117,033 8	89,0390
7	Procyanidin B	C30H26O12	12,05		577,134 60	425,088 9	407,078 2	289,072 6	161,023 6	125,023 1
8	3-O-(4-Coumaroyl)quinic acid	C16H18O8	12,45		337,092 35	191,055 6	173,044 8	163,039 1	119,048 9	93,0331
9 ¹	Catechin	C15H14O6	13,32		289,071 21	245,082 0	205,050 4	203,070 9	125,023 2	109,028 2
10 ¹	Epigallocatechin (Epigallocatechol)	C15H14O7	13,62		305,066 13	261,076 9	219,065 9	179,034 2	137,023 4	125,023 2
11 ¹	Chlorogenic acid (3-O-Caffeoylquinic acid)	C16H18O9	14,23	355,102 91		163,039 0	145,028 6	135,044 3	117,033 8	89,0389
12	3-O-Feruloylquinic acid	C17H20O9	14,50		367,102 91	193,050 3	191,056 0	173,044 0	134,036 3	93,0330
13	Ampelopsin (Ampeloptin, Dihydromyricetin)	C15H12O8	14,71		319,045 40	301,036 4	193,013 8	178,997 4	153,018 2	125,023 2
14 ¹	Vanillin	C8H8O3	15,51	153,055 17		125,060 0	111,044 5	110,036 5	93,0340	65,0393

15	Chryptochlorogenic acid (4-O-Caffeoylquinic acid)	C16H18O9	15,57	355,102 91	163,039	145,028	135,044	117,033	89,0390
16 ¹	Epicatechin	C15H14O6	17,08		289,071 21	245,082 2	205,050 1	203,070 7	125,023 2
17	4-O-(4-Coumaroyl)quinic acid	C16H18O8	17,55		337,092 35	191,055 8	173,044 6	163,039 1	119,049 0
18 ¹	4-Coumaric acid	C9H8O3	17,75		163,039 52	119,049 0	93,0332		
19	Loliolide or Isololiolide	C11H16O3	18,24	197,117 77	179,106 8	161,096 3	135,116 9	133,101 6	107,086 0
20	4-O-Feruloylquinic acid	C17H20O9	18,52		367,102 91	193,050 1	191,056 7	173,044 7	134,036 1
21	Ferulic acid	C10H10O4	19,31		193,050 09	178,026 5	149,059 6	137,023 3	134,036 1
22	Loliolide or Isololiolide	C11H16O3	19,50	197,117 77	179,106 8	161,096 2	135,117 1	133,101 4	107,085 9
23 ¹	Sinapic acid (Sinapinic acid)	C11H12O5	19,86	225,076 30	207,065 4	192,042 1	175,039 3	147,044 2	119,049 5
24	Myricetin-3-O-rutinoside	C27H30O17	21,04		625,140 48	317,030 5	316,022 9	287,020 3	271,025 3
25 ¹	Rutin (Quercetin-3-O-rutinoside)	C27H30O16	23,03	611,161 22	465,096 3	303,050 3	129,055 4	85,0290	71,0499
26	Azelaic acid	C9H16O4	24,49		187,097 04	169,086 6	143,106 5	125,095 9	123,080 3
27	Kaempferol-3-O-rutinoside (Nicotiflorin)	C27H30O15	24,86		593,150 65	327,052 9	285,043 0	284,034 2	255,030 3
28	Gramrione (5,5'-Dimethoxy-3',4',7-trihydroxyflavone)	C17H14O7	25,04		329,066 13	314,044 0	299,019 4	271,024 9	
29 ¹	Naringenin (4',5,7-Trihydroxyflavanone)	C15H12O5	27,23		271,060 65	177,018 6	151,003 1	119,048 8	107,012 3
30	Sebacic acid	C10H18O4	28,00		201,112 68	183,102 3	157,121 9	139,111 8	111,080 1
31	Bruguierol A	C12H14O2	36,08	191,107 21	173,096 8	161,096 0	147,080 6	135,080 7	107,049 6

Table S2. Chemical composition of fruit maceration.

N o.	Name	Formula	Rt	[M + H] ⁺	[M - H] ⁻	Frag- ment 1	Frag- ment 2	Frag- ment 3	Frag- ment 4	Frag- ment 5
1	Quinic acid	C7H12O6	1,26		191,05 557	173,044 6	127,038 8	111,043 6	93,0330	85,0279
2	Citric acid	C6H8O7	1,30		191,01 918	173,008 2	129,018 1	111,007 4	87,0072	85,0280
3	Brugierol	C3H6O2S 2	1,66	138,98 875		120,977 9	102,967 5	92,9832	86,9904	
4	Gallocatechin (Casuarin, Gallocatechol)	C15H14O 7	4,54		305,06 613	261,077 1	219,065 3	179,034 2	137,023 2	125,023 0
5	Protocatechuic acid (3,4-Dihydroxybenzoic acid)	C7H6O4	4,65		153,01 879	109,028 1	108,020 3	91,0173	81,0331	
6	Neochlorogenic acid (5-O-Caffeoylquinic acid)	C16H18O 9	8,68	355,10 291		163,039 0	145,028 5	135,044 2	117,033 7	89,0390
7	Procyanidin B	C30H26O 12	12,0 5		577,13 460	425,088 0	407,077 4	289,072 2	161,023 3	125,023 0
8	3-O-(4-Coumaroyl)quinic acid	C16H18O 8	12,4 4		337,09 235	191,055 5	173,044 4	163,039 0	119,048 9	93,0331
9 ¹	Catechin	C15H14O 6	13,3 0		289,07 121	245,082 1	205,049 9	203,070 8	125,023 0	109,028 0
10 ¹	Epigallocatechin (Epigallocatechol)	C15H14O 7	13,6 0		305,06 613	261,075 5	219,065 8	179,032 8	137,023 5	125,022 9
11	3-O-Feruloylquinic acid	C17H20O 9	14,4 6		367,10 291	193,050 0	191,055 5	173,044 4	134,036 1	93,0329
12	Ampelopsin (Ampeloptin, Dihydromyricetin)	C15H12O 8	14,7 0		319,04 540	301,034 8	193,013 5	178,997 7	153,018 1	125,022 9
13	Chryptochlorogenic acid (4-O-Caffeoylquinic acid)	C16H18O 9	15,5 5	355,10 291		163,038 9	145,028 5	135,044 3	117,034 0	89,0390
14 ¹	Epicatechin	C15H14O 6	17,0 7		289,07 121	245,081 8	205,050 4	203,070 5	125,023 1	109,028 0
15	3-(Benzoyloxy)-2-hydroxypropylglucuronic acid	C16H20O 10	17,5 9		371,09 783	249,061 4	231,050 7	175,023 5	121,028 1	113,023 0

16 ¹	4-Coumaric acid	C9H8O3	17,7 4	163,03 952	119,048 8	93,0332			
17	Antiarol (3,4,5-Trimethoxyphenol)	C9H12O4	17,9 3	185,08 139	170,057 2	154,062 4	153,054 6	139,039 0	125,059 9
18	Loliolide or Isololiolide	C11H16O	18,2 3	197,11 777	179,106 8	161,096 4	135,117 1	133,101 4	107,085 9
19	4-O-Feruloylquinic acid	C17H20O	18,4 9	367,10 291	193,049 5	191,056 7	173,044 5	134,036 2	93,0330
20	Riboflavin	C17H20N 4O6	18,6 3	377,14 611	359,135 1	243,087 7	200,082 5	172,087 1	99,0444
21	Indole-3-lactic acid	C11H11N O3	18,7 8	204,06 607	186,055 5	158,060 0	142,065 1	128,049 4	72,9916
22	Ferulic acid	C10H10O	19,2 4	193,05 009	178,026 1	149,059 3	137,023 3	134,036 1	121,028 1
23	Loliolide or Isololiolide	C11H16O	19,4 3	197,11 777	179,106 8	161,096 1	135,117 0	133,101 3	107,085 9
24 ¹	Sinapic acid (Sinapinic acid)	C11H12O	19,8 5	225,07 630	207,065 3	192,042 0	175,039 1	147,044 2	119,049 4
25	Myricetin-3-O-rutinoside	C27H30O	21,0 17	625,14 048	317,030 4	316,022 6	287,020 1	271,025 1	178,997 8
26	Theaflavin	C29H24O	21,6 12	565,13 461	427,102 8	271,060 5	259,059 5	139,039 1	
27	Dihydrokaempferol (Aromadendrin, Katuranin)	C15H12O	21,8 6	287,05 557	259,061 4	243,065 4	177,054 7	151,002 6	125,023 1
28	Cinchonain I	C24H20O	22,2 9	451,10 291	341,067 2	217,013 4	189,018 7		
29 ¹	Rutin (Quercetin-3-O-rutinoside)	C27H30O	23,0 16	611,16 122	465,101 4	303,050 0	129,054 9	85,0290	71,0498
30 ¹	Myricetin (Cannabiscetin, Myricetol, 3,3',4',5,5',7-Hexahydroxyflavone)	C15H10O	24,1 8	317,02 974	271,026 9	178,997 7	151,002 5	137,023 2	109,028 1
31	Azelaic acid	C9H16O4	24,4 7	187,09 704	169,086 0	143,106 5	125,095 8	123,080 2	97,0645
32	Kaempferol-3-O-rutinoside (Nicotiflorin)	C27H30O	24,8 15	593,15 065	327,052 6	285,041 0	284,033 1	255,030 3	227,033 9

33	Gramrione (5,5'-Dimethoxy-3',4',7-trihydroxyflavone)	C17H14O 25,0 7 1	329,06 314,043 299,019 271,025 613 6 9 6
34	Dihydroxy-trimethoxy(iso)flavone	C18H16O 26,8 7 9	343,08 328,058 327,050 313,034 299,056 285,041 178 8 4 2 0 0
35 ¹	Quercetin (3,3',4',5,7-Pentahydroxyflavone)	C15H10O 26,9 7 8	301,03 273,041 229,050 178,997 151,002 121,028 483 4 5 8 5 1
36 ¹	Naringenin (4',5,7-Trihydroxyflavanone)	C15H12O 27,1 5 9	271,06 177,018 151,002 119,048 107,012 93,0332 065 8 7 8 4
37	Sebacic acid	C10H18O 27,9 4 6	201,11 183,101 157,122 139,111 111,080 268 9 2 7 2
38	Undecanedioic acid	C11H20O 30,8 4 5	215,12 197,117 153,127 125,095 834 8 3 5
39	Bruguierol A	C12H14O 36,0 191,10 2 5 721	173,096 161,096 147,080 135,080 107,049 0 0 5 6 5

Table S3. Chemical composition of leaf decoction.

No.	Name	Formula	Rt	[M + H] ⁺	[M - H] ⁻	Frag- ment 1	Frag- ment 2	Frag- ment 3	Frag- ment 4	Frag- ment 5
1	Quinic acid	C7H12O6	1,24		191,05557	173,0444	127,0389	111,0439	93,0331	185,0281
2	Brugierol	C3H6O2S2	1,67	138,98875		120,9779	102,9677		92,9833	386,9905
3	Gallocatechin	C15H14O7	4,54		305,06613	261,0768	219,0658	167,0339	137,0232	125,0232
4	Protocatechuic acid (3,4-Dihydroxybenzoic acid)	C7H6O4	4,71		153,01879	109,0282	108,0205		91,0174	481,0332
5	Neochlorogenic acid (5-O-Caffeoylquinic acid)	C16H18O9	8,66	355,10291		163,0391	145,0286	135,0444	117,0338	89,0390
6	Procyanidin B isomer 1	C30H26O12	12,07		577,13460	425,0888	407,0739	289,0729	161,0232	125,0230
7	3-O-(4-Coumaroyl)quinic acid	C16H18O8	12,46		337,09235	191,0561	173,0456	163,0393	119,0490	93,0329

8 ¹	Catechin	C15H14O6	13,31	289,07 121	245,081 9	205,050 5	203,071 2	125,023 2	109,028 2
9 ¹	Epigallocatechin	C15H14O7	13,62	305,06 613	261,076 9	219,065 8	167,034 1	137,023 5	125,023 2
10 ¹	Chlorogenic acid (3-O-Caffeoylquinic acid)	C16H18O9	14,24	355,10 291	163,039 1	145,028 6	135,044 3	117,033 9	89,0391
11	Caffeic acid	C9H8O4	14,34	179,03 444	135,044 1	107,048 9			
12	3-O-Feruloylquinic acid	C17H20O9	14,48	367,10 291	193,050 4	191,055 5	173,043 7	134,036 3	93,0330
13	Procyanidin B isomer 2	C30H26O12	15,22	577,13 460	425,089 3	407,077 3	289,072 6	161,023 2	125,023 2
14 ¹	Vanillin	C8H8O3	15,49	153,05 517	125,060 0	111,044 5	110,036 7	93,0341	165,0393
15	Chryptochlorogenic acid (4-O-Caffeoylquinic acid)	C16H18O9	15,57	355,10 291	163,039 2	145,028 7	135,044 4	117,033 9	89,0391
16 ¹	Epicatechin	C15H14O6	17,08	289,07 121	245,082 0	205,050 2	203,071 1	125,023 1	109,028 2
17	4-O-(4-Coumaroyl)quinic acid	C16H18O8	17,52	337,09 235	191,055 1	173,044 7	163,039 0	119,048 9	93,0332
18	3-(Benzoyloxy)-2-hydroxypropylglucuronic acid	C16H20O10	17,60	371,09 783	249,061 7	123,050 6	175,023 6	121,028 2	113,023 1
19 ¹	4-Coumaric acid	C9H8O3	17,73	163,03 952	119,049 0	93,0332			
20	Antiarol (3,4,5-Trimethoxyphenol)	C9H12O4	17,92	185,08 139	170,057 7	154,062 5	153,054 8	139,039 3	125,060 0
21	Loliolide or Isololiolide	C11H16O3	18,23	197,11 777	179,107 0	161,096 3	135,117 3	133,101 4	107,086 0
22	4-O-Feruloylquinic acid	C17H20O9	18,49	367,10 291	193,050 3	191,056 7	173,044 6	134,036 3	93,0331
23	Riboflavin	C17H20N4O 6	18,64	377,14 611	359,134 3	243,087 6	200,081 7	172,086 5	99,0444
24	Cinchonain I isomer 1	C24H20O9	18,90	451,10 291	341,066 4	217,014 3	189,018 9		

25	Ferulic acid	C10H10O4	19,29	193,05	178,02	149,05	137,02	134,03	121,02	8
				009	5	3	4	4	1	
26	Loliolide or Isololiolide	C11H16O3	19,50	197,11	179,10	161,09	135,11	133,10	110,08	6
				777	0	3	1	5	0	
27	Dimethoxy-trihydroxy(iso)flavone-O-hexoside isomer 1	C23H24O12	20,14	491,11	329,06	7328,05	9314,04	4313,03	7285,04	1
				896	1	2	6	5	7	
28	Dihydroxy-methoxy(iso)flavone-O-hexoside	C22H22O10	20,72	445,11	283,06	2282,05	3268,03	8240,04	2	
				348	0	7	4	3		
29	Quercetin-O-dirhamnosylhexoside	C33H40O20	20,81	755,20	300,02	8271,02	4255,03	0		
				347	4	4	7			
30	Myricetin-3-O-rutinoside	C27H30O17	21,03	625,14	317,03	0316,02	3287,02	1271,02	5178,99	7
				048	5	0	0	4	8	
31	Cinchonain I isomer 2	C24H20O9	21,30	451,10	341,06	7217,01	4189,01	8		
				291	1	1	8			
32	Kaempferol-O-dirhamnosylhexoside	C33H40O19	22,11	739,20	327,05	1285,04	0284,03	3255,03	0227,03	4
				856	4	5	2	1	8	
33	Cinchonain I isomer 3	C24H20O9	22,30	451,10	341,06	5217,01	3189,01	8		
				291	2	4	5			
34	Methoxy-tetrahydroxy(iso)flavone isomer 1	C16H12O7	22,67	315,05	300,02	8299,02	0272,03	3256,03	7	
				048	1	7	4	8		
35 ¹	Isoquercitrin (Hirsutrin, Quercetin-3-O-glucoside)	C21H20O12	22,93	463,08	301,03	5300,02	7271,02	4255,02	9178,99	7
				765	6	8	3	0	9	
36	Dimethoxy-trihydroxy(iso)flavone-O-hexoside isomer 2	C23H24O12	23,01	491,11	329,06	7314,04	4313,03	6299,02	0271,02	4
				896	4	0	9	3	7	
37 ¹	Rutin (Quercetin-3-O-rutinoside)	C27H30O16	23,05	611,16	465,10	4303,05	0129,05	5	85,02	9071,04
				122	1	1	1			98
38	Apigenin-O-rhamnosylhexoside	C27H30O14	24,48	577,15	269,04	6268,03	8			
				573	4	9				
39	Azelaic acid	C9H16O4	24,48	187,09	169,08	6143,10	7125,09	6123,08	0	97,06
				704	3	1	0	2	46	
40	Methoxy-trihydroxy(iso)flavone	C16H12O6	24,70	299,05	284,03	3283,02	5256,03	8133,02	8	
				556	4	5	0	4		
41	Kaempferol-3-O-rutinoside (Nicotiflorin)	C27H30O15	24,85	593,15	327,05	1285,04	1284,03	3255,03	0227,03	4
				065	4	1	3	2	7	

42	Cinchonain I isomer 4	C24H20O9	24,95	451,10	341,06	721,01	3189,018				
				291	1	3	6				
43	Gramrione (5,5'-Dimethoxy-3',4',7-trihydroxyflavone)	C17H14O7	25,03	329,06	314,04	3299,02	271,025				
				613	9	5	5				
44	Dimethoxy-trihydroxy(iso)flavone-O-hexoside isomer 3	C23H24O12	26,00	491,11	329,06	6328,06	0314,04	4313,03	6285,041		
				896	8	0	0	2	6		
45	Dihydroxy-methoxy(iso)flavone	C16H12O5	26,51	283,06	268,03	8267,03	0240,04	2239,03	4211,039		
				065	3	4	7	2	5		
46	Dihydroxy-dimethoxy(iso)flavone	C17H14O6	26,85	315,08	300,06	3299,05	5285,04	0272,06	8257,044		
				686	2	4	7	6	4		
47	Dihydroxy-trimethoxy(iso)flavone	C18H16O7	26,89	343,08	328,05	9327,05	1313,03	6299,05	6285,041		
				178	5	3	1	7	1		
48	Methoxy-tetrahydroxy(iso)flavone isomer 2	C16H12O7	28,08	315,05	300,02	8272,03	2256,036				
				048	1	8	8				
49	Dimethoxy-trihydroxy(iso)flavone-O-rhamnoside	C23H24O11	29,16	475,12	328,05	9327,05	1314,04	4313,03	6285,041		
				404	5	5	2	1	0		
50	Bruguierol A	C12H14O2	36,06	191,10	173,09	6161,09	6147,08	0135,08	0107,049		
				721	4	1	8	7	6		

Table S4. Chemical composition of leaf maceration.

N o.	Name	Formula	Rt	[M + H] ⁺	[M - H] ⁻	Frag-ment 1	Frag-ment 2	Frag-ment 3	Frag-ment 4	Frag-ment 5
1	Brugierol	C3H6O2S	1,67	138,98		120,977	102,967	92,983	286,990	4
		2		875		8	2			
2	Methoxy-trihydroxybenzene	C7H8O4	3,25	155,03	140,010	139,002				
				443	2	4				
3	Protocatechuic acid (3,4-Dihydroxybenzoic acid)	C7H6O4	4,67	153,01	109,028	108,020		91,017	581,033	2
				879	1	3				
4	Catechol	C6H6O2	5,12	109,02	108,020		91,017	381,033		
				896	3					
5	Gentisic acid (2,5-Dihydroxybenzoic acid)	C7H6O4	8,97	153,01	123,007	109,028	108,020		95,012	485,028
				879	4	1	3			

6	Dihydroxybenzoic acid isomer	C7H6O4	12,4 8	153,01 879	123,007 3	109,028 0	108,020 2	95,0123 81,0331
7	Caffeic acid	C9H8O4	14,3 3	179,03 444	135,043 9	107,048 8		
8	3-O-Feruloylquinic acid	C17H20O	14,4 9 8	367,10 291	193,049 9	191,055 2	173,044 5	134,036 1 93,0330
9	Chryptochlorogenic acid (4-O-Caffeoylquinic acid)	C16H18O	15,5 355,10 9 9 291		163,038 9	145,028 5	135,044 1	117,033 9 89,0391
10	Antiarol (3,4,5-Trimethoxyphenol)	C9H12O4	17,9 185,08 5 139		170,057 1	154,062 3	153,054 5	139,039 0 125,059
11	Lolilide or Isololilide	C11H16O	18,2 197,11 3 5 777		179,106 7	161,096 0	135,117 0	133,101 4 107,085
12	4-O-Feruloylquinic acid	C17H20O	18,4 9 9	367,10 291	193,049 9	191,056 7	173,044 5	134,035 8 93,0329
13	Lolilide or Isololilide	C11H16O	19,5 197,11 3 2 777		179,106 7	161,096 2	135,117 0	133,101 3 107,085
14	Isoferulic acid	C10H10O	20,3 4 0	193,05 009	178,026 6	149,059 8	137,023 7	134,036 1
15	Methoxy-tetrahydroxy(iso)flavone isomer 1	C16H12O	22,6 7 7	315,05 048	300,027 8	299,019 9	272,032 8	256,037 1
16	Azelaic acid	C9H16O4	24,4 7	187,09 704	169,085 6	143,106 7	125,095 8	123,080 2 97,0645
17	Methoxy-trihydroxy(iso)flavone	C16H12O	24,7 6 0	299,05 556	284,032 8	283,025 1	256,037 6	133,028 2
18	Gramrione (5,5'-Dimethoxy-3',4',7-trihydroxyflavone)	C17H14O	25,0 7 1	329,06 613	314,043 4	299,019 8	271,024 9	
19	Dihydroxy-methoxy(iso)flavone	C16H12O	26,5 5 0	283,06 065	268,037 9	267,029 9	240,042 3	239,035 5 211,039
20	Dihydroxy-dimethoxy(iso)flavone	C17H14O	26,8 315,08 6 5 686		300,062 5	299,054 6	285,039 3	272,067 4 257,044
21	Dihydroxy-trimethoxy(iso)flavone	C18H16O	26,8 7 8	343,08 178	328,058 9	327,052 2	313,035 7	299,056 3 285,041
22 ¹	Luteolin (3',4',5,7-Tetrahydroxyflavone)	C15H10O	27,8 6 4	285,03 991	217,050 0	199,039 4	175,037 9	151,002 3 133,028

23	Methoxy-tetrahydroxy(iso)flavone isomer 2	C16H12O	28,0	315,05	300,027	272,032	256,036		
		7	7	048	7	1	8		
24 ¹	Apigenin (4',5,7-Trihydroxyflavone)	C15H10O	29,6	269,04	225,056	151,002	149,023	117,033	107,012
		5	6	500	5	6	0	1	3
25	Bruguierol A	C12H14O	36,0	191,10	173,095	161,096	147,079	135,080	107,049
		2	5	721	9	4	9	5	5

Table S5. Chemical composition of root decoction.

No.	Name	Formula	Rt	[M + H] ⁺	[M - H] ⁻	Frag-ment 1	Frag-ment 2	Frag-ment 3	Frag-ment 4	Frag-ment 5
1	Quinic acid	C7H12O6	1,20		191,05 557	173,04 48	127,03 90	111,04 38	93,033 3	85,028 1
2	Citric acid	C6H8O7	1,56		191,01 918	173,00 87	129,01 82	111,00 74	87,007 3	85,028 0
3	Brugierol	C3H6O2S2	1,63	138,98 875		120,97 80	102,96 77	92,983 3	86,990 5	
4	Gallocatechin	C15H14O7	4,37		305,06 613	261,07 72	219,06 62	167,03 40	137,02 33	125,02 31
5	Unidentified compound	C9H19NO6S 2	4,64	302,07 320		285,04 64	180,08 68	163,06 03	145,04 98	122,99 36
6	Protocatechuic acid (3,4-Dihydroxybenzoic acid)	C7H6O4	4,67		153,01 879	109,02 82	108,02 04	91,017 4	81,033 4	
7	Neochlorogenic acid (5-O-Caffeoylquinic acid)	C16H18O9	8,61	355,10 291		163,03 92	145,02 87	135,04 44	117,03 39	89,039 0
8	Syringic acid-O-hexoside	C15H20O10	10,60		359,09 783	197,04 51	182,02 14	166,99 78	153,05 47	138,03 12
9	Prodelphinidin C	C30H26O13	10,78		593,12 952	425,08 85	407,07 79	289,07 24	177,01 85	125,02 32
10 ¹	Catechin	C15H14O6	13,31		289,07 121	245,08 22	205,05 05	203,07 09	125,02 31	109,02 82
11 ¹	Epigallocatechin	C15H14O7	13,61		305,06 613	261,07 71	219,06 61	167,03 41	137,02 34	125,02 32

12 ¹	Chlorogenic acid (3-O-Caffeoylquinic acid)	C16H18O9	14,24	355,10 291	163,03 92	145,02 88	135,04 45	117,03 39	89,039 3
13	Procyanidin B	C30H26O12	15,22	577,13 460	425,08 88	407,07 78	289,07 25	161,02 34	125,02 32
14 ¹	Vanillin	C8H8O3	15,54	153,05 517	125,06 00	111,04 45	110,03 65	93,034 0	65,039 3
15	Chryptochlorogenic acid (4-O-Caffeoylquinic acid)	C16H18O9	15,57	355,10 291	163,03 92	145,02 87	135,04 44	117,03 39	89,039 0
16	Procyanidin C	C45H38O18	16,98	865,19 799	577,13 61	407,07 77	289,07 25	161,02 34	125,02 32
17 ¹	Epicatechin	C15H14O6	17,09	289,07 121	245,08 21	205,05 03	203,07 10	125,02 32	109,02 82
18	3-(Benzoyloxy)-2-hydroxypropylglucuronic acid	C16H20O10	17,60	371,09 783	249,06 18	231,05 11	175,02 42	121,02 83	113,02 31
19	Antiarol (3,4,5-Trimethoxyphenol)	C9H12O4	17,95	185,08 139	170,05 75	154,06 26	153,05 48	139,03 92	125,06 00
20	Cinchonain I isomer 1	C24H20O9	18,91	451,10 291	341,06 72	217,01 41	189,01 89		
21	Epiafzelechin	C15H14O5	19,05	273,07 630	255,06 71	229,08 60	189,05 46	137,02 31	97,028 3
22	Ferulic acid	C10H10O4	19,29	193,05 009	178,02 61	149,05 99	137,02 27	134,03 62	121,02 80
23	4-Hydroxy-3-methoxycinnamaldehyde (Coniferyl aldehyde)	C10H10O3	20,02	179,07 082	161,06 00	147,04 43	133,06 53	119,04 95	55,018 6
24	Myricetin-3-O-rutinoside	C27H30O17	21,03	625,14 048	317,03 11	316,02 30	287,02 07	271,02 43	178,99 75
25	Cinchonain I isomer 2	C24H20O9	21,27	451,10 291	341,06 71	217,01 37	189,01 88		
26	Cinchonain I isomer 3	C24H20O9	22,30	451,10 291	341,06 72	217,01 36	189,01 88		
27 ¹	Rutin (Quercetin-3-O-rutinoside)	C27H30O16	23,02	611,16 122	465,10 30	303,05 01	129,05 49	85,029 0	71,049 8
28	Azelaic acid	C9H16O4	24,49	187,09 704	169,08 62	143,10 69	125,09 59	123,08 05	97,064 6

29	Methoxy-trihydroxy(iso)flavone	C16H12O6	24,73	299,05 556	284,03 21	283,02 64	256,03 81	133,02 86	
30	Cinchonain I isomer 4	C24H20O9	24,97	451,10 291	341,06 73	217,01 36	189,01 88		
31	Gramrione (5,5'-Dimethoxy-3',4',7-trihydroxyflavone)	C17H14O7	25,04	329,06 613	314,04 37	299,01 95	271,02 48		
32	Sebacic acid	C10H18O4	28,00	201,11 268	183,10 21	157,12 28	139,11 18	111,08 06	
33	16,17-Dihydroxy-9(11)-kauren-19-al or Steviol	C20H30O3	33,80	319,22 732	301,21 66	283,20 57	273,22 10	255,21 14	241,19 51
34	1-Hydroxy-8(14)-isopimaren-1,15,16-triol or isomer	C20H34O3	33,88	323,25 862	305,24 75	287,23 72	269,22 67	245,22 69	81,070 5
35	13-Hydroxy-16-kauren-19-al or isomer	C20H30O2	35,52	303,23 241	285,22 16	275,23 71	267,21 12	257,22 67	95,086 2
36	Bruguierol A	C12H14O2	36,08	191,10 721	173,09 63	161,09 57	147,08 03	135,08 08	107,04 97
37	1-Hydroxy-8(14)-isopimaren-1,15,16-triol or isomer	C20H34O3	36,41	323,25 862	305,24 75	287,23 70	269,22 64	257,22 64	95,086 0
38	1-Hydroxy-8(14)-isopimaren-1,15,16-triol or isomer	C20H34O3	38,10	323,25 862	305,24 74	287,23 70	269,22 67	257,22 61	95,086 1
39	13-Hydroxy-16-kauren-19-al or isomer	C20H30O2	39,41	303,23 241	285,22 16	275,23 68	267,21 08	257,22 66	109,10 16
40	Unidentified xanthone isomer 1	C18H16O7	41,84	343,08 178	328,05 92	313,03 64	259,06 14	231,06 60	83,012 4
41	Unidentified xanthone isomer 2	C18H16O7	43,33	343,08 178	328,05 98	313,03 64	259,06 15	231,06 62	83,012 3
42	Isopimar-7-en-15,16-diol or isomer	C20H34O2	43,75	307,26 371	289,25 31	271,24 25	247,24 31	231,21 12	81,070 5
43	Isopimar-7-en-15,16-diol or isomer	C20H34O2	43,99	307,26 371	289,25 30	271,24 22	247,24 31	231,21 05	81,070 5

Table S6. Chemical composition of root maceration.

N o.	Name	Formula	Rt	[M + H] ⁺	[M - H] ⁻	Frag- ment 1	Frag- ment 2	Frag- ment 3	Frag- ment 4	Frag- ment 5
1	Quinic acid	C7H12O6	1,27		191,05 557	173,044 5	127,038 4	111,043 7	93,0329	85,0279
2	Citric acid	C6H8O7	1,58		191,01 918	173,008 0	129,018 1	111,007 3	87,0071	85,0279
3	Brugierol	C3H6O2S 2	1,64	138,99		120,977 8	102,967 4	92,9832	86,9904	
4	Gallocatechin	C15H14O 7	4,55		305,06 613	261,076 0	219,065 6	167,033 8	137,023 1	125,023 0
5	Unidentified compound	C9H19N O6S2	4,64	302,07 32		285,046 6	180,085 9	163,060 2	145,049 6	122,993 4
6	Protocatechuic acid (3,4-Dihydroxybenzoic acid)	C7H6O4	4,67		153,01 879	109,028 0	108,020 3	91,0173	81,0331	
7	Neochlorogenic acid (5-O-Caffeoylquinic acid)	C16H18O 9	8,59	355,10 291		163,038 9	145,028 4	135,044 1	117,033 4	89,0391
8	Syringic acid-O-hexoside	C15H20O 10	10,6		359,10	197,044 7	182,021 2	166,996 0	153,054 4	138,030 8
9	Prodelphinidin C	C30H26O 13	10,8		593,13	425,089 1	407,077 1	289,071 8	177,018 2	125,023 0
10	Unidentified compound	C11H14O 5	13,1		225,08	207,065 6	163,075 3	123,043 7	101,022 9	
11 ¹	Catechin	C15H14O 6	13,3		289,07	245,081 5	205,050 0	203,070 8	125,023 0	109,028 0
12 ¹	Epigallocatechin	C15H14O 7	13,6		305,07	261,077 2	219,065 7	167,033 8	137,023 2	125,023 0
13 ¹	Chlorogenic acid (3-O-Caffeoylquinic acid)	C16H18O 9	14,2	355,10		163,039 0	145,028 2	135,044 2	117,033 9	89,0392
14	Caffeic acid	C9H8O4	14,3		179,03	135,043 8	107,048 8			
15	Unidentified compound	C11H12O 4	15		207,07	163,075 2	122,035 9	109,028 0		

16	Procyanidin B	C30H26O ₁₂	15,2	577,13	425,088	407,077	289,072	161,023	125,023
17	Chryptochlorogenic acid (4-O-Caffeoylquinic acid)	C16H18O ₉	15,6	355,10	163,038	145,028	135,044	117,033	89,0389
18	Procyanidin C	C45H38O ₁₈	17	865,20	577,134	407,077	289,072	161,023	125,023
19 ¹	Epicatechin	C15H14O ₆	17,1	289,07	245,081	205,050	203,070	125,023	109,028
20	3-(Benzoyloxy)-2-hydroxypropylglucuronic acid	C16H20O ₁₀	17,6	371,10	249,061	231,050	175,023	121,028	113,022
21	Antiarol (3,4,5-Trimethoxyphenol)	C9H12O ₄	17,9	185,08	170,057	154,062	153,054	139,039	125,059
22	3,4-Dihydro-3-hydroxy-7-methoxy-2H-1,5-benzodithiepine-6,9-dione	C10H10O ₄ S ₂	18,2	259,01	240,998	225,021	208,019	207,011	73,0112
23	Cinchonain I isomer 1	C24H20O ₉	18,9	451,10	341,066	217,013	189,018		
24	Epiarazelechin	C15H14O ₅	19	273,08	255,065	229,086	189,054	137,023	97,0281
25 ¹	Taxifolin (Dihydroquercetin)	C15H12O ₇	19,3	303,05	285,041	217,051	175,038	153,018	125,022
26	Ferulic acid	C10H10O ₄	19,3	193,05	178,026	149,059	137,023	134,036	121,027
27	Myricetin-3-O-rutinoside	C27H30O ₁₇	21	625,14	317,028	316,022	287,020	271,024	178,998
28	Cinchonain I isomer 2	C24H20O ₉	21,3	451,10	341,067	217,013	189,018		
29	Cinchonain I isomer 3	C24H20O ₉	22,3	451,10	341,067	217,013	189,018		
30 ¹	Rutin (Quercetin-3-O-rutinoside)	C27H30O ₁₆	23	611,16	465,103	303,049	129,054	85,0289	71,0497
31	Azelaic acid	C9H16O ₄	24,5	187,10	169,085	143,106	125,095	123,080	97,0644
32	Cinchonain I isomer 4	C24H20O ₉	25	451,10	341,066	217,013	189,018		

33	Sebacic acid	C10H18O 4	28	201,11	183,101 8	157,121 4	139,111 6	111,079 8	
34 ¹	Phloretin	C15H14O 5	28,1	273,08	229,086 7	179,034 0	167,033 8	123,043 8	119,048 9
35	Norstictic acid	C18H12O 9	32,5	371,04	327,050 8	283,060 5	255,065 2	243,029 1	227,034 6
36	16,17-Dihydroxy-9(11)-kauren-19-al or Steviol	C20H30O 3	33,8	319,23	301,215 9	283,205 2	273,220 8	255,210 3	241,195 0
37	1-Hydroxy-8(14)-isopimaren-1,15,16-triol or isomer	C20H34O 3	33,9	323,26	305,247 2	287,236 7	269,225 9	245,226 4	81,0704
38	13-Hydroxy-16-kauren-19-al or isomer	C20H30O 2	35,5	303,23	285,221 3	275,236 7	267,210 6	257,225 9	95,0860
39	Bruguierol A	C12H14O 2	36,1	191,11	173,095 8	161,095 5	147,080 1	135,080 6	107,049 5
40	1-Hydroxy-8(14)-isopimaren-1,15,16-triol or isomer	C20H34O 3	36,4	323,26	305,247 3	287,236 8	269,226 1	257,226 0	95,0859
41	Dihydroxy-methoxy-methylxanthone	C15H12O 5	37,8	271,06	256,037 5	228,042 8	227,034 7		
42	1-Hydroxy-8(14)-isopimaren-1,15,16-triol or isomer	C20H34O 3	38,1	323,26	305,247 4	287,236 8	269,226 2	257,226 2	95,0859
43	13-Hydroxy-16-kauren-19-al or isomer	C20H30O 2	39,4	303,23	285,221 1	275,237 6	267,210 9	257,226 4	109,101 4
44	Unidentified xanthone	C18H16O 7	43,3	343,08	328,058 9	313,036 2	259,061 3	231,065 6	83,0123
45	Isopimar-7-en-15,16-diol or isomer	C20H34O 2	43,7	307,26	289,252 4	271,242 2	247,241 3	231,210 5	81,0704
46	Isopimar-7-en-15,16-diol or isomer	C20H34O 2	44	307,26	289,252 7	271,242 1	247,242 2	231,210 6	81,0704

Table S7. Chemical composition of twigs decoction.

No.	Name	Formula	Rt	[M + H] ⁺	[M - H] ⁻	Frag-ment 1	Frag-ment 2	Frag-ment 3	Frag-ment 4	Frag-ment 5
1	Quinic acid	C7H12O6	1,19		191,05557	173,044127	127,038111	111,0438	93,033185	185,0280
2	Citric acid	C6H8O7	1,57		191,01918	173,008129	129,018111	111,0074	87,007385	185,0280
3	Brugierol	C3H6O2S2	1,66	138,98875		120,978102	102,9676	92,983286	99,9905	
4	Gallocatechin	C15H14O7	4,53		305,06613	261,077219	219,066167	167,034137	137,023125	125,023
5	Protocatechuic acid (3,4-Dihydroxybenzoic acid)	C7H6O4	4,69		153,01879	109,028108	108,0204	91,017581	103,033	
6	Neochlorogenic acid (5-O-Caffeoylquinic acid)	C16H18O9	8,67	355,10291		163,039145	145,028135	135,044117	117,0339	89,0389
7	Syringic acid-O-hexoside	C15H20O10	10,61		359,09783	197,045182	182,021166	166,997153	153,054138	138,0312
8	Procyanidin B isomer 1	C30H26O12	12,06		577,13460	425,089407	407,077289	389,072161	231,023125	125,023
9 ¹	Catechin	C15H14O6	13,32		289,07121	245,082205	205,050203	203,071125	125,023109	109,028
10	Procyanidin B isomer 2	C30H26O12	13,47		577,13460	425,088407	407,078289	389,072161	231,023125	125,023
11 ¹	Epigallocatechin	C15H14O7	13,62		305,06613	261,077219	219,066167	167,034137	137,023125	125,023
12 ¹	Chlorogenic acid (3-O-Caffeoylquinic acid)	C16H18O9	14,23	355,10291		163,039145	145,028135	135,044117	117,0338	89,0391
13	Caffeic acid	C9H8O4	14,36		179,03444	135,044107	107,0489			
14	Procyanidin B isomer 3	C30H26O12	15,23		577,13460	425,088407	407,077289	389,072161	231,023125	125,023
15	Chryptochlorogenic acid (4-O-Caffeoylquinic acid)	C16H18O9	15,58	355,10291		163,039145	145,028135	135,044117	117,0340	89,0392

16	Syringic acid	C ₉ H ₁₀ O ₅	15,83	197,04 500	182,02 5	1166,99 6	7153,05 7	4138,03 1	1123,00 5	7
17	Procyanidin C	C ₄₅ H ₃₈ O ₁₈	16,95	865,19 799	577,13 1	4407,07 1	8289,07 1	3161,02 5	23125,02 1	3
18 ¹	Epicatechin	C ₁₅ H ₁₄ O ₆	17,09	289,07 121	245,08 0	2205,05 3	203,07 1	1125,02 1	23109,02 2	8
19	3-(Benzoyloxy)-2-hydroxypropylglucuronic acid	C ₁₆ H ₂₀ O ₁₀	17,60	371,09 783	249,06 7	1231,05 8	0175,02 4	4121,02 2	8113,02 1	3
20 ¹	4-Coumaric acid	C ₉ H ₈ O ₃	17,75	163,03 952	119,04 0	93,03 31				
21	Antiarol (3,4,5-Trimethoxyphenol)	C ₉ H ₁₂ O ₄	17,94	185,08 139	170,05 6	7154,06 6	2153,05 8	4139,03 2	9125,06 0	6
22	3,4-Dihydro-3-hydroxy-7-methoxy-2H-1,5-benzodithiepine-6,9-dione	C ₁₀ H ₁₀ O ₄ S ₂	18,25	259,00 988	240,99 0	99225,02 1	2208,01 8	18207,01 6	1173,01 73,01	13
23	Cinchonain I isomer 1	C ₂₄ H ₂₀ O ₉	18,90	451,10 291	341,06 1	7217,01 6	3189,01 6			
24	Ferulic acid	C ₁₀ H ₁₀ O ₄	19,29	193,05 009	178,02 4	26149,05 6	9137,02 3	3134,03 3	6121,02 1	8
25	Loliolide or Isololiolide	C ₁₁ H ₁₆ O ₃	19,52	197,11 777	179,10 9	6161,09 1	6135,11 2	7133,10 5	1107,08 0	6
26 ¹	Rutin (Quercetin-3-O-rutinoside)	C ₂₇ H ₃₀ O ₁₆	23,04	611,16 122	465,10 0	3303,05 3	0129,05 1	5585,02 85,02	9171,04 98	
27	Azelaic acid	C ₉ H ₁₆ O ₄	24,49	187,09 704	169,08 2	6143,10 7	6125,09 9	5123,08 0	97,06 45	
28	Methoxy-trihydroxy(iso)flavone	C ₁₆ H ₁₂ O ₆	24,72	299,05 556	284,03 7	3283,02 6	5256,03 7	7133,02 4		
29	Kaempferol-3-O-rutinoside (Nicotiflorin)	C ₂₇ H ₃₀ O ₁₅	24,86	593,15 065	327,05 9	2285,04 0	41284,03 9	3255,02 3	2227,03 2	4
30	Cinchonain I isomer 2	C ₂₄ H ₂₀ O ₉	24,95	451,10 291	341,06 9	6217,01 7	3189,01 9			
31	Gramrione (5,5'-Dimethoxy-3',4',7-trihydroxyflavone)	C ₁₇ H ₁₄ O ₇	25,04	329,06 613	314,04 0	4299,02 5	20271,02 4			
32	Dihydroxy-trimethoxy(iso)flavone	C ₁₈ H ₁₆ O ₇	26,91	343,08 178	328,05 6	8327,04 8	9313,03 7	5299,05 5	6285,04 2	1

33	16,17-Dihydroxy-9(11)-kauran-19-al	C20H32O3	32,40	321,24 297	303,231285,221273,220267,210255,210
34	16,17-Dihydroxy-9(11)-kauren-19-al or Steviol	C20H30O3	33,78	319,22 732	301,217283,206273,221255,210241,195
35	Methyl 16 α ,17-dihydroxy-9(11)-kauren-19-oate or isomer	C21H32O4	34,79	349,23 788	331,226299,200271,206253,195121,101
36	13-Hydroxy-16-kauren-19-al or isomer	C20H30O2	35,51	303,23 241	285,221275,236267,210257,226 95,0861
37	16,17-Dihydroxy-9(11)-kauran-19-al isomer	C20H32O3	35,67	321,24 297	303,232285,221273,221267,210255,211
38	Bruguierol A	C12H14O2	36,08	191,10 721	173,096161,096147,080135,080107,049
39	Methyl 16 α ,17-dihydroxy-9(11)-kauren-19-oate or isomer	C21H32O4	36,14	349,23 788	331,226299,200271,206253,195121,101

Table S8. Chemical composition of twigs maceration.

N o.	Name	Formula	Rt	[M + H] ⁺	[M - H] ⁻	Frag-ment 1	Frag-ment 2	Frag-ment 3	Frag-ment 4	Frag-ment 5
1	Brugierol	C3H6O2S	1,6 2	138,98 7	875	120,977 8	102,967 0	92,9831	86,9903	
2	Protocatechuic acid (3,4-Dihydroxybenzoic acid)	C7H6O4	4,7		153,01 879	109,028 1	108,020 2	91,0175	81,0331	
3	Caffeic acid	C9H8O4	14, 4		179,03 444	135,043 9	107,048 7			
4	Antiarol (3,4,5-Trimethoxyphenol)	C9H12O4	17, 9	185,08 139		170,057 1	154,062 4	153,054 6	139,039 1	125,059 9
5	Riboflavin	C17H20N 4O6	18, 7	377,14 611		359,133 5	243,087 7	200,082 4	172,086 7	99,0444
6	Azelaic acid	C9H16O4	24, 5		187,09 704	169,086 0	143,106 2	125,095 8	123,079 8	97,0643
7	16,17-Dihydroxy-9(11)-kauran-19-al	C20H32O	32, 3	321,24 4	297	303,231 2	285,221 1	273,221 9	267,210 8	255,210 4

8	16,17-Dihydroxy-9(11)-kauren-19-al or Steviol	C ₂₀ H ₃₀ O	33,	319,22	301,215	283,206	273,221	255,209	241,195
			3	8	732	8	4	7	3
9	Bruguierol A	C ₁₂ H ₁₄ O	36,	191,10	173,096	161,095	147,080	135,080	107,049
			2	1	721	3	9	5	6

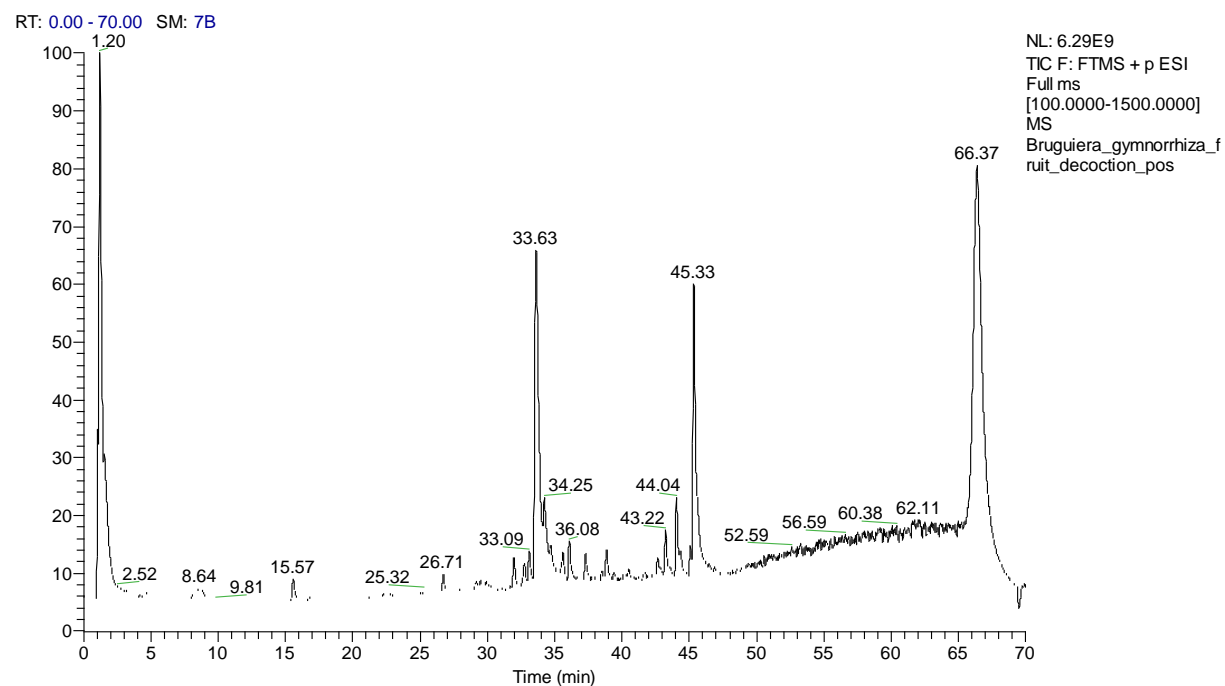


Figure S1. *Bruguiera gymnorrhiza* fruit decoction TIC positive.

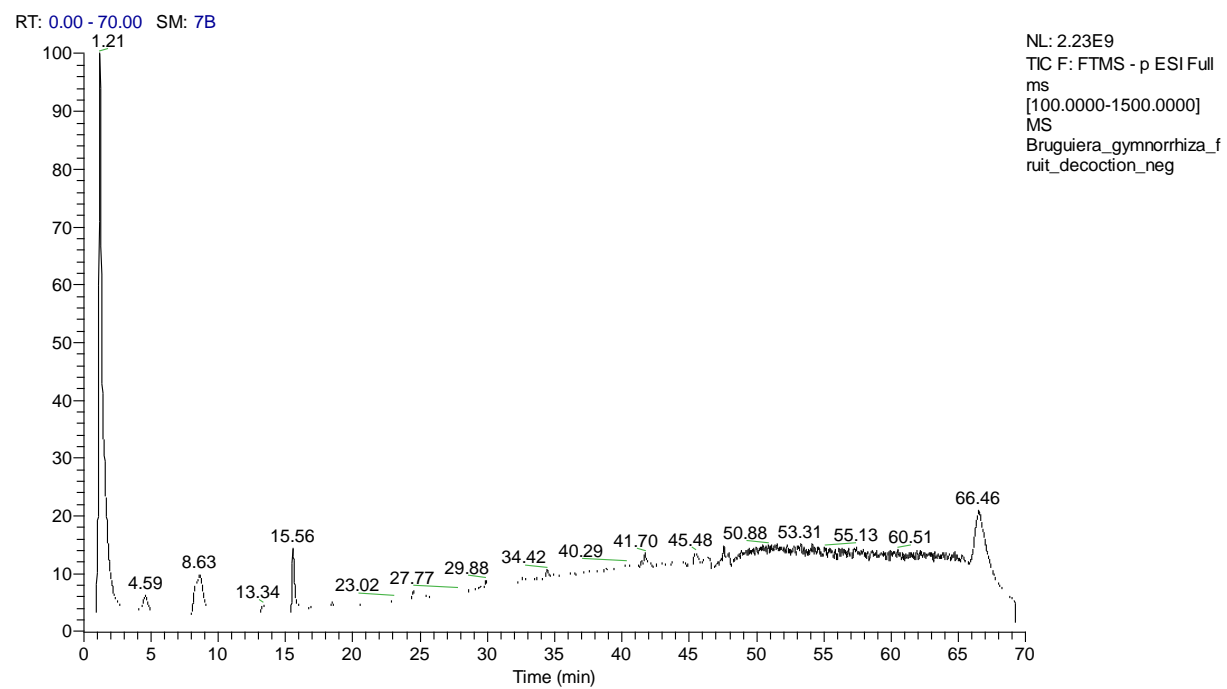


Figure S2. *Bruguiera gymnorhiza* fruit decoction TIC negative.

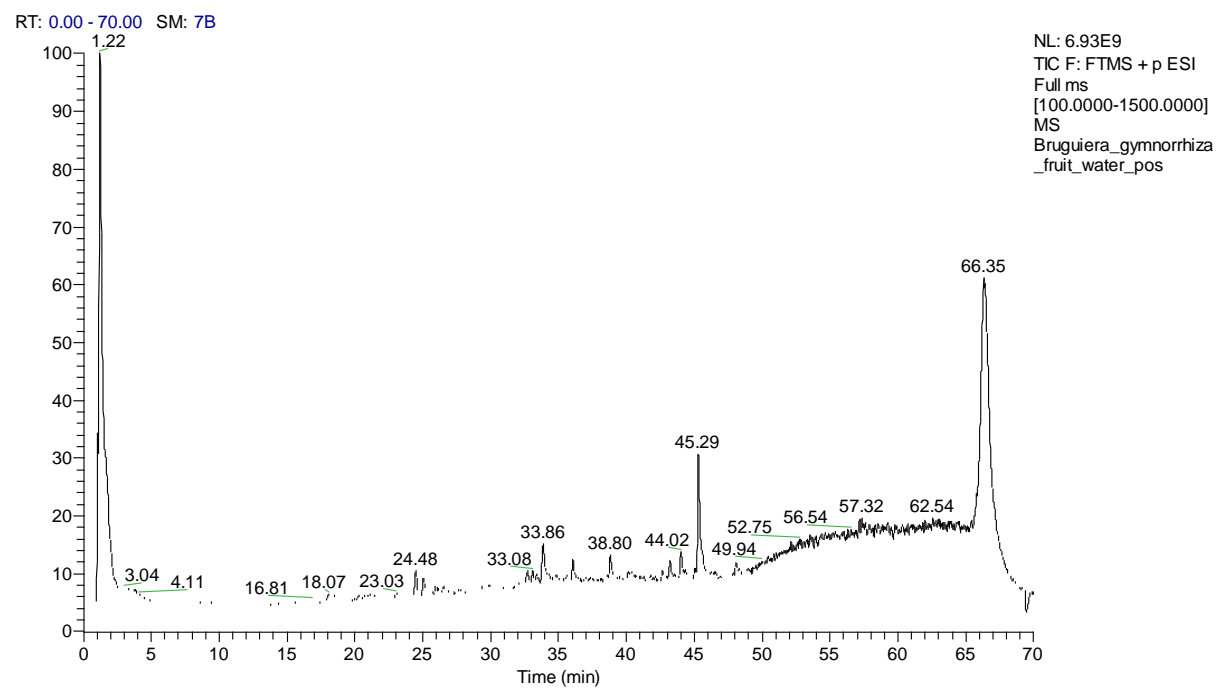


Figure S3. *Bruguiera gymnorrhiza* fruit water TIC positive.

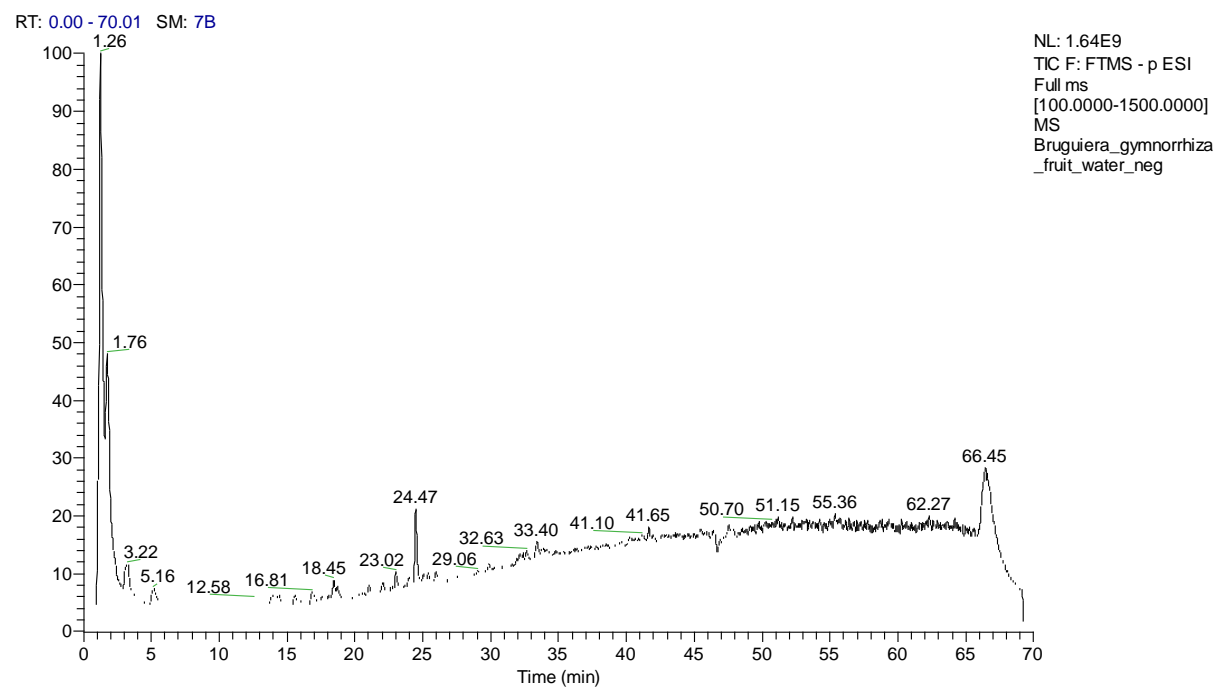


Figure S4. *Bruguiera gymnorrhiza* fruit water TIC negative.

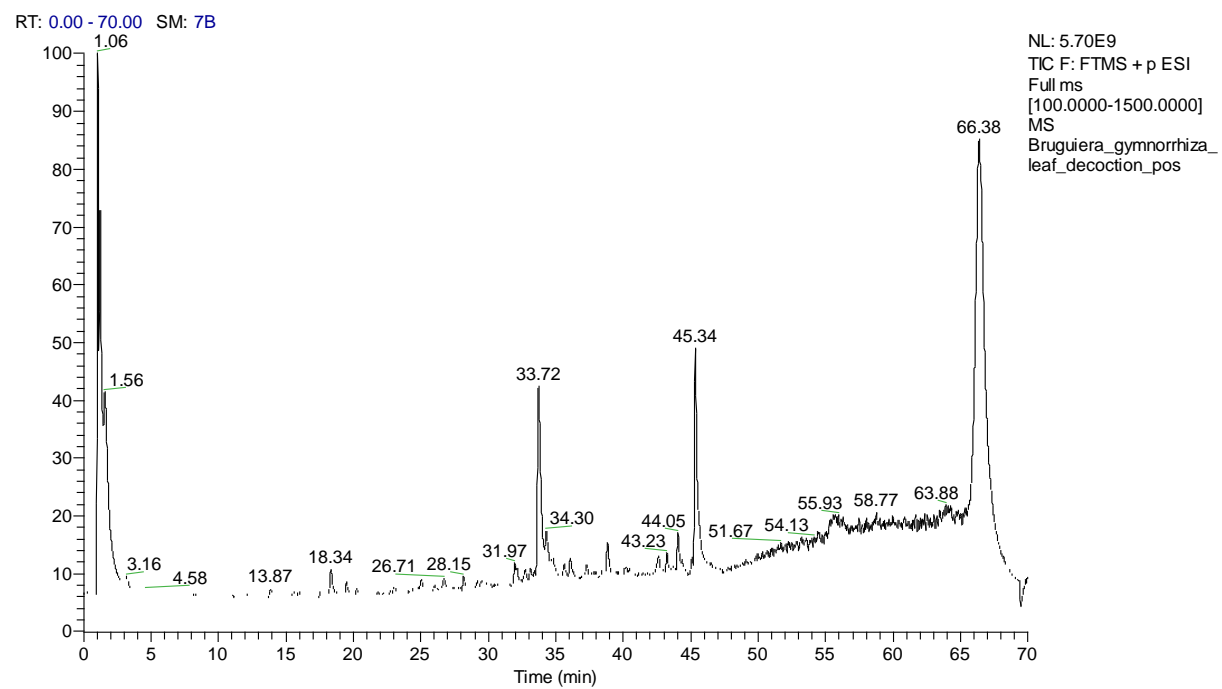


Figure S5. *Bruguiera gymnorhiza* leaf decoction TIC positive.

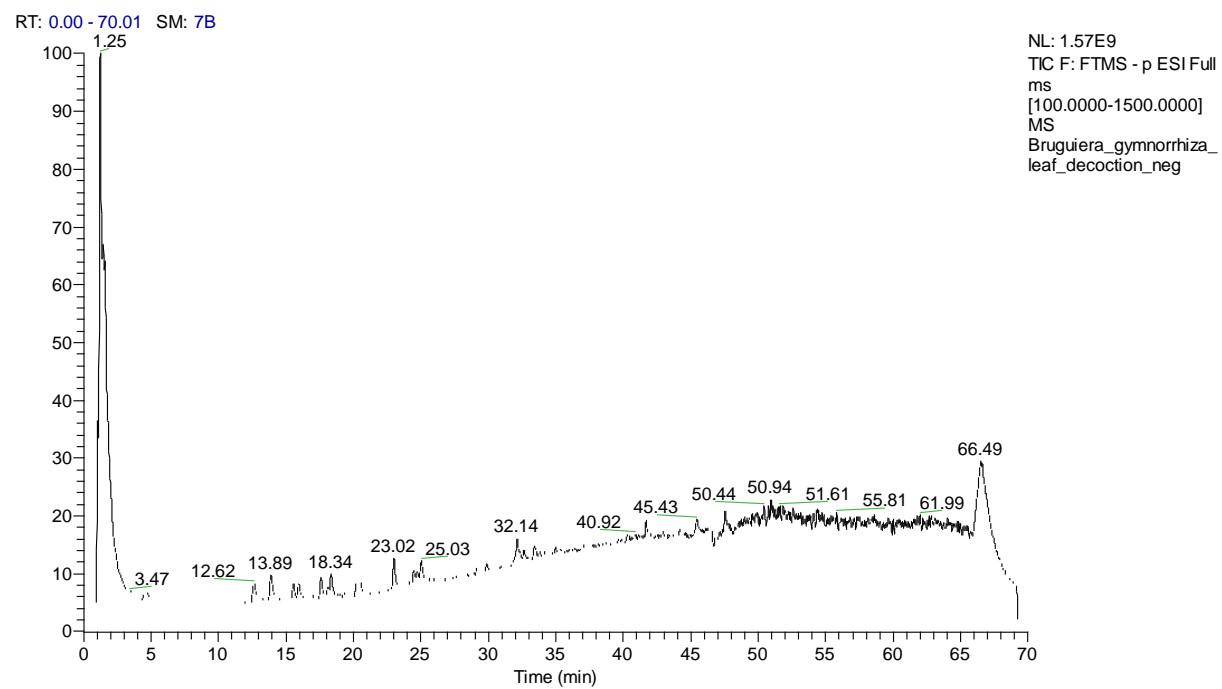


Figure S6. *Bruguiera gymnorrhiza* leaf decoction TIC negative.

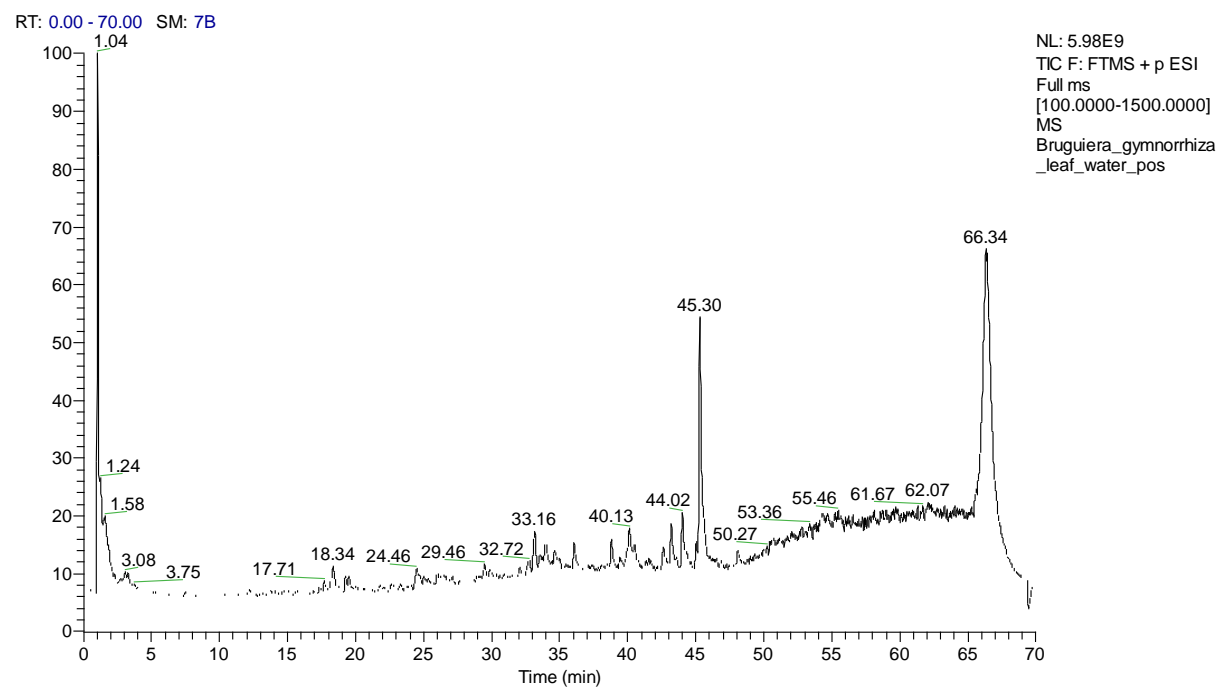


Figure S7. *Bruguiera gymnorhiza* leaf water TIC positive.

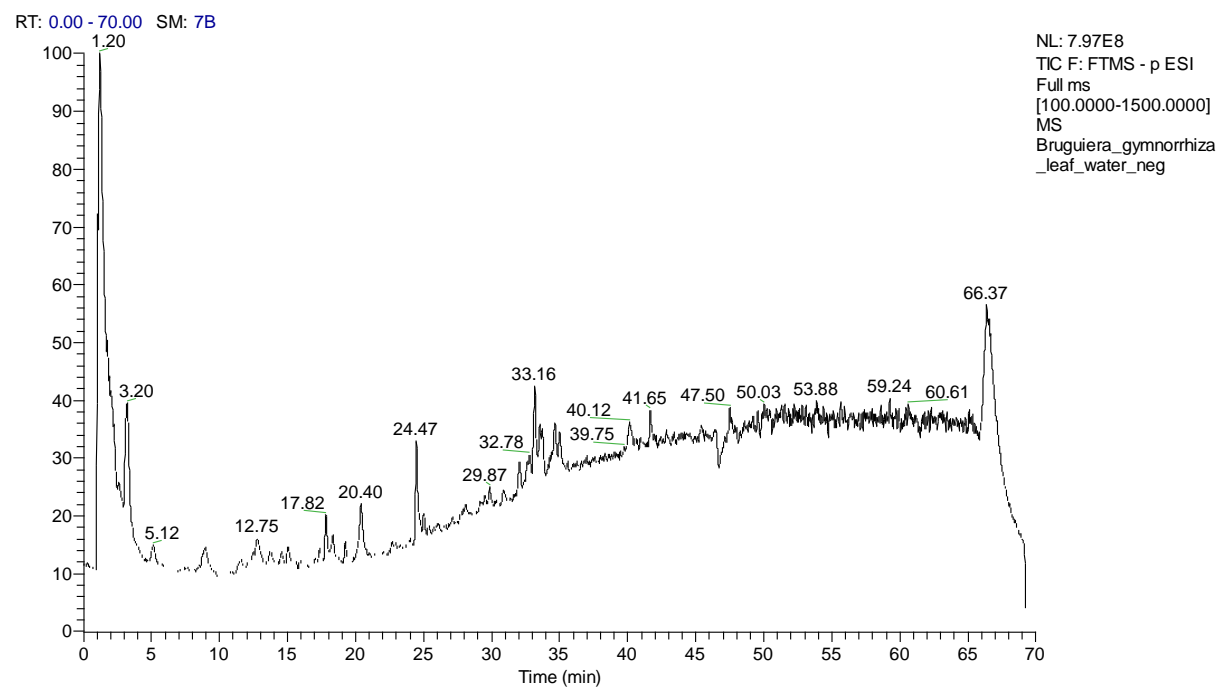


Figure S8. *Bruguiera gymnorhiza* leaf water TIC negative.

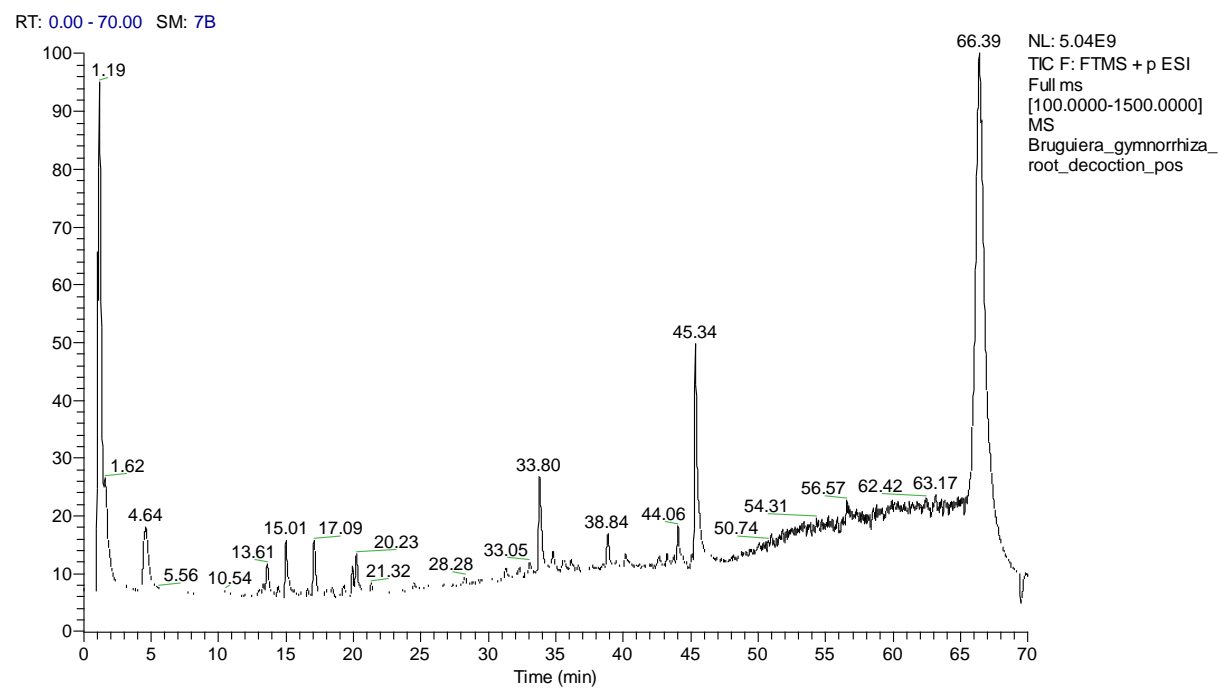


Figure S9. *Bruguiera gymnorhiza* root decoction TIC positive.

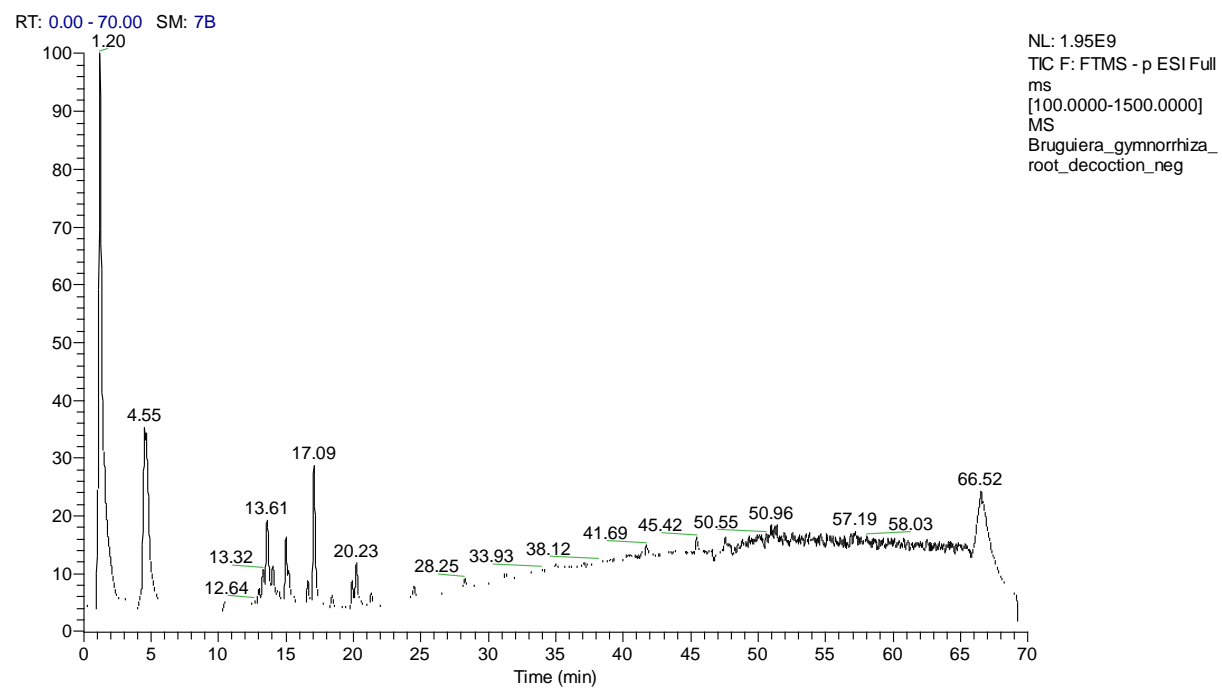


Figure S10. *Bruguiera gymnorrhiza* root decoction TIC negative.

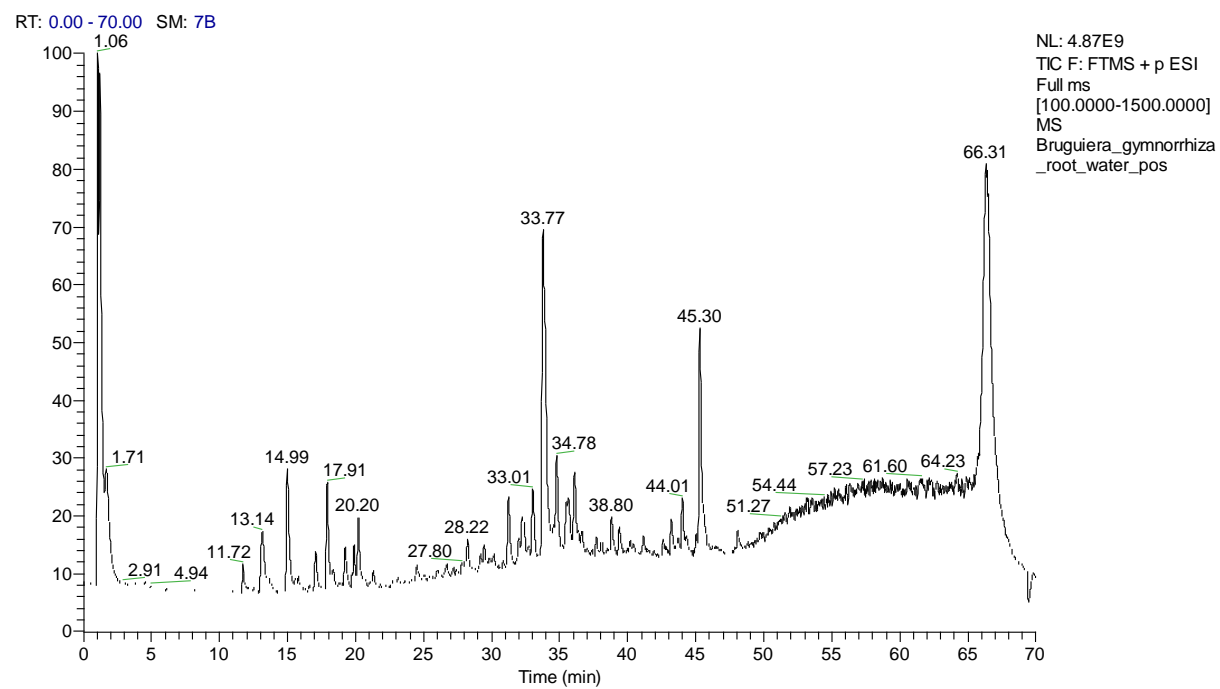


Figure S11. *Bruguiera gymnorhiza* root water TIC positive.

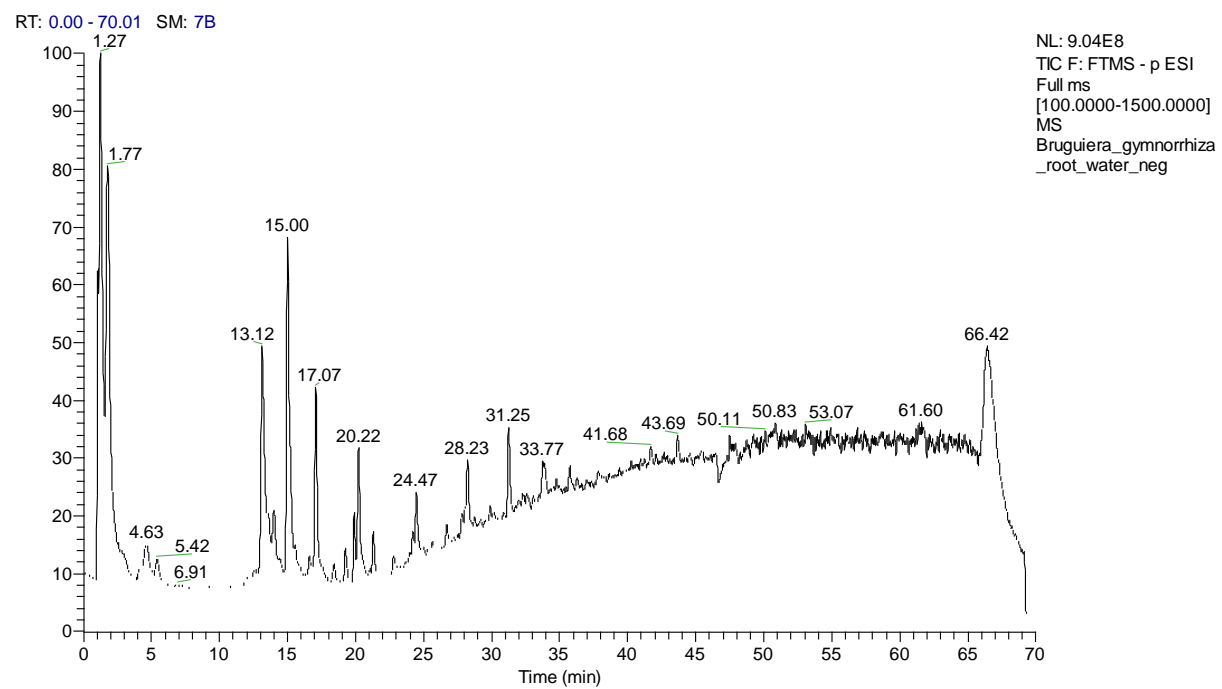


Figure S12. *Bruguiera gymnorhiza* root water TIC negative.

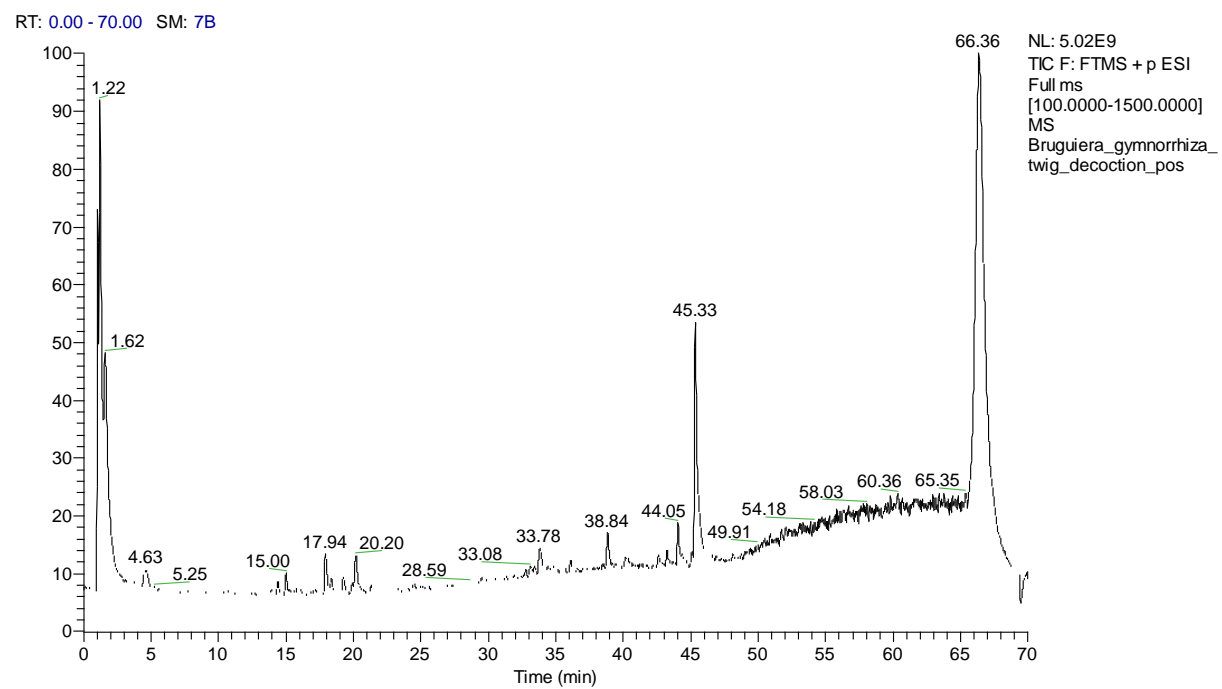


Figure S13. *Bruguiera gymnorrhiza* twig decoction TIC positive.

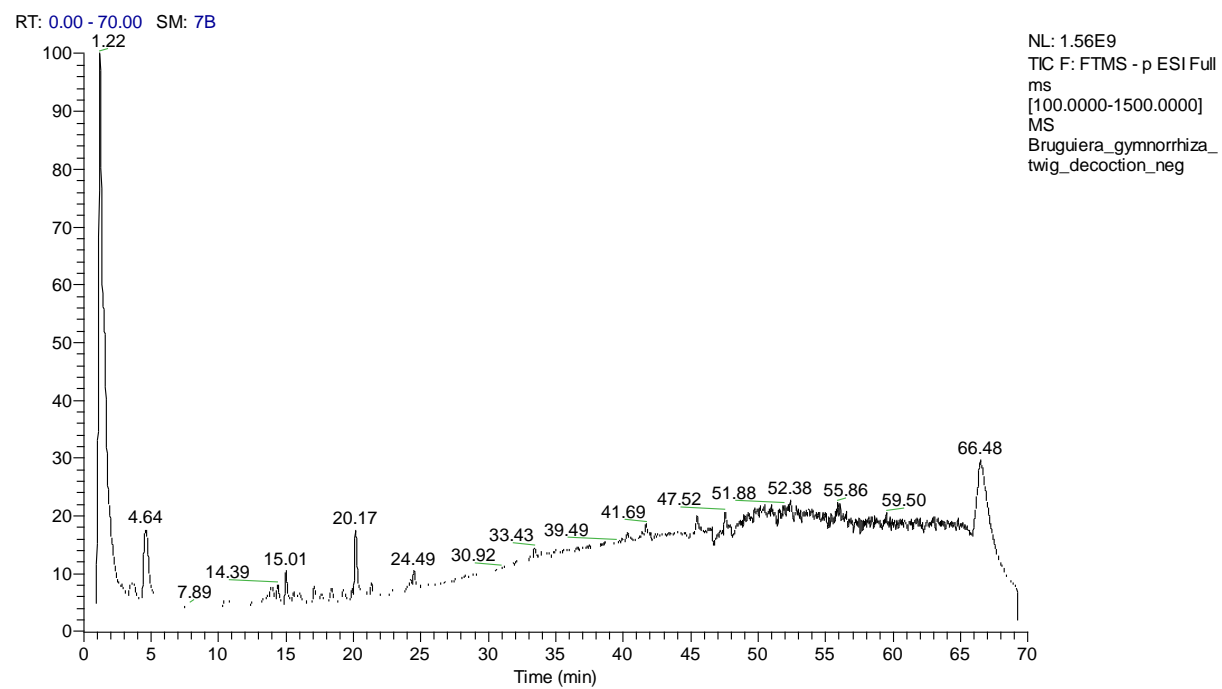


Figure S14. *Bruguiera gymnorrhiza* twig decoction TIC negative.

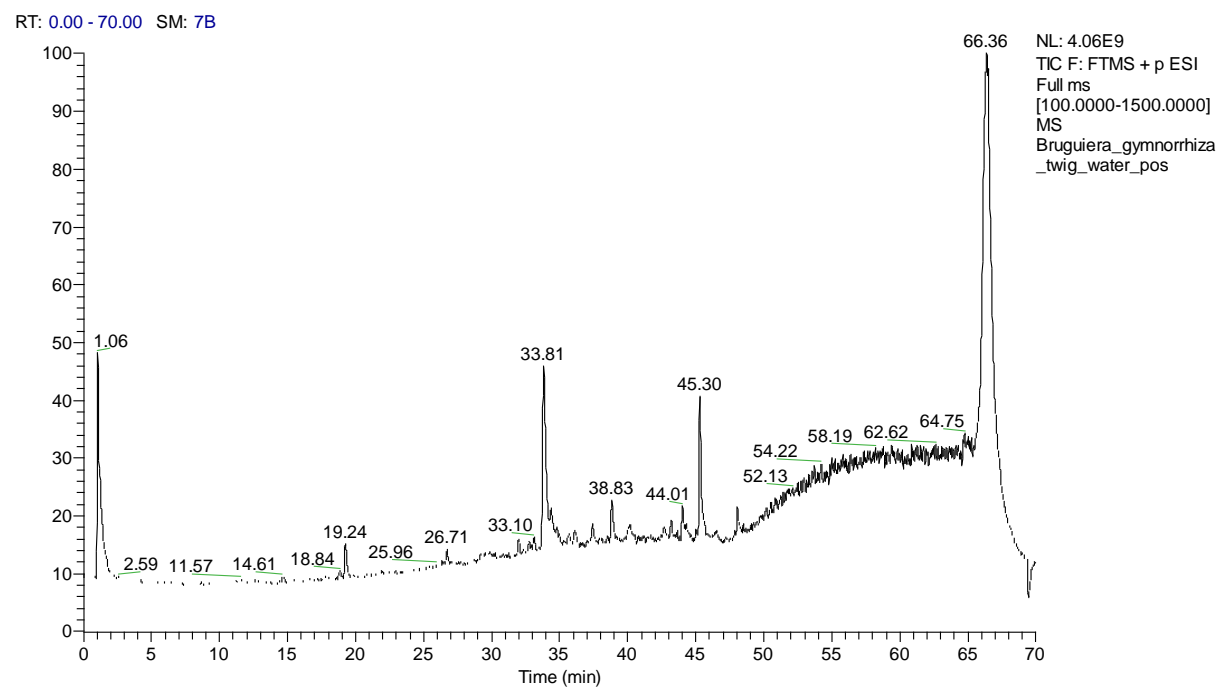


Figure S15. *Bruguiera gymnorrhiza* twig water TIC positive.

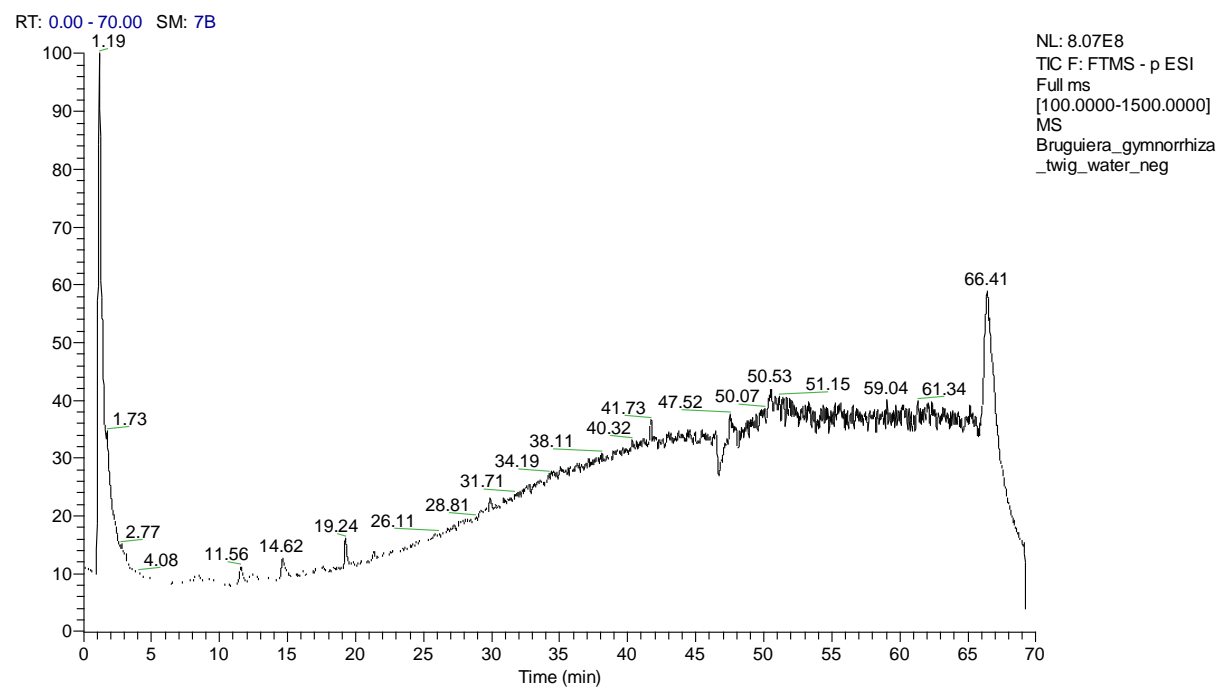


Figure S16. *Bruguiera gymnorhiza* twig water TIC negative.