

Supplementary material

Exploration of Rapid Evaporative-Ionization Mass Spectrometry as a Shotgun Approach for the Comprehensive Characterization of *Kigelia Africana* (Lam) Benth. Fruit

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Table S1. S/N comparison of 5 representative ions detected in negative ionization mode between two different power of cutting (DC 10 W and FC 20 W), along with their coefficient of variation (CV%).

m/z	tentative assignment	DC 10 W		FC 20 W	
		S/N	CV%	S/N	CV%
137.0249	4-hydroxybenzoic acid	34.77	10.21	12.72	16.87
281.2486	Octadecenoic acid (C18:1)	160.85	7.88	67.14	4.35
523.147	Verminoside	13.12	21.36	9.96	21.04
671.462	PA (C34:2)	10.18	6.78	-	-
861.5469	PI (C18:2/C18:1)	5.92	14.59	-	-

Table S2. S/N comparison of 7 representative ions detected in positive ionization mode between two different power of cutting (DC 10 W and FC 20 W), along with their coefficient of variation (CV%).

m/z	tentative assignment	DC 10 W		FC 20 W	
		S/N	CV%	S/N	CV%
339.2898	MG (C18:1)	90.15	11.41	25.51	3.81
383.0776	Rosmarinic acid	-	-	10.53	19.87
475.0970	Epigallocatechin-p-coumaroate	-	-	146.49	11.81
549.1154	Piperenol A triacetate	-	-	67.32	2.99
599.5039	DG (C36:4)	43.88	3.70	54.41	16.60
853.7281	TG (52:5)	11.43	4.06	32.86	13.99
877.7289	TG (54:7)	25.21	18.00	86.39	15.16

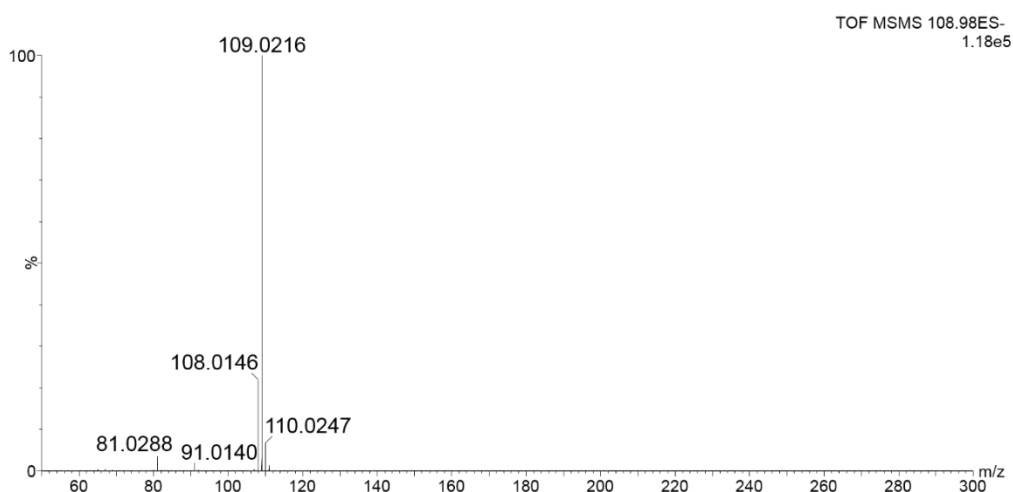


Figure S1. MS/MS spectrum over the range 50-300 of m/z 109.02 (pyrocatechol) obtained in negative ionization mode at a collision energy of 20 eV, by cutting the sample at DC 10 W. The ion at m/z 91.01 corresponds to the loss of water, while the ion at m/z 81.03 corresponds to the loss of ethylene and opening of the aromatic ring.

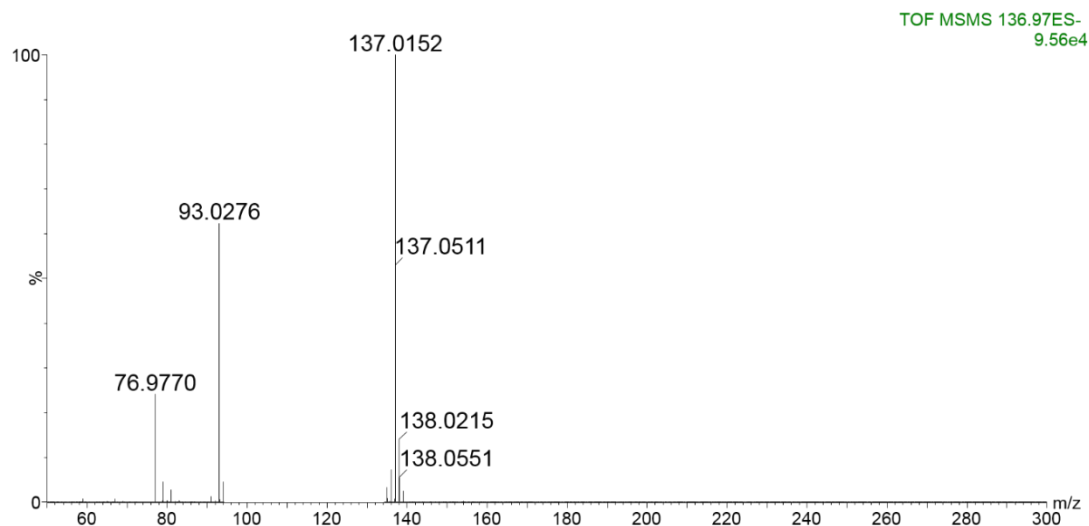


Figure S2. MS/MS spectrum over the range 50-300 of m/z 137.01 (4-hydroxybenzoic acid) obtained in negative ionization mode at a collision energy of 20 eV, by cutting the sample at DC 10 W. The ion at m/z 93.03 corresponds to the loss of the carboxyl group, while the ion at m/z 76.98 corresponds to the further removal of the hydroxyl group.

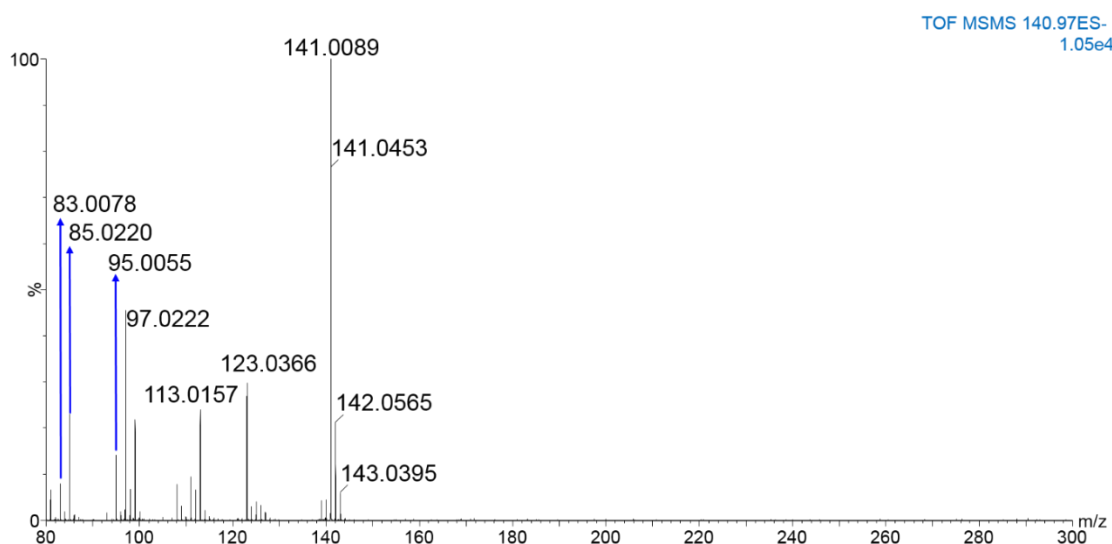


Figure S3. MS/MS spectrum over the range 80-300 of m/z 141.01 (kojic acid) obtained in negative ionization mode at a collision energy of 20 eV, by cutting the sample at DC 10 W. The ion at m/z 123.04 corresponds to the loss of water, while the ion at m/z 113.02 corresponds to the loss of a carbonyl group after the opening of the pyranone ring and m/z 95.01 corresponds to the loss of the $-\text{CH}_2\text{OH}$ chain followed by the opening of the ring and the loss of an additional alkyl group.

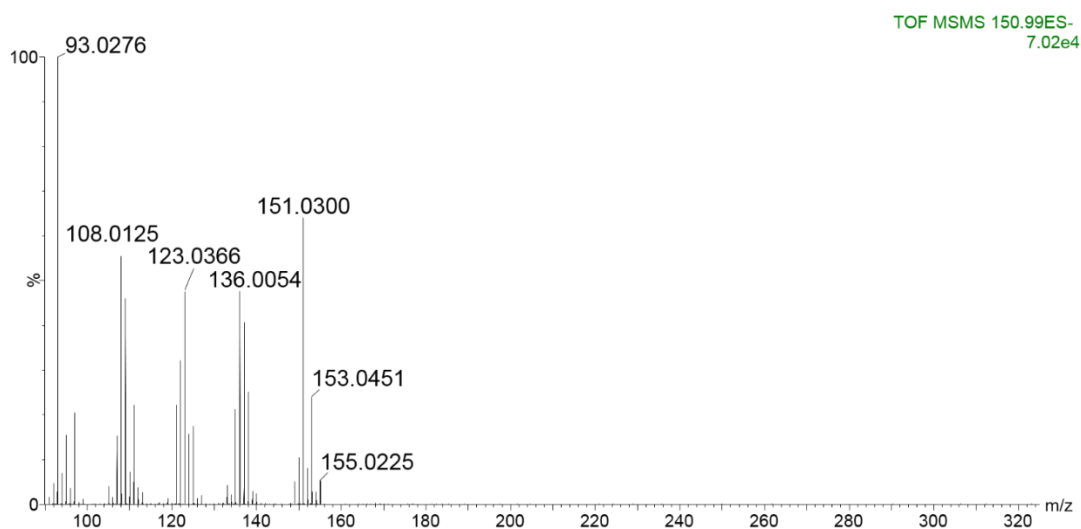


Figure S4. MS/MS spectrum over the range 90-325 of m/z 151.03 (vanillin) obtained in negative ionization mode at a collision energy of 30 eV, by cutting the sample at DC 10 W. The ion at m/z 136.00 corresponds to the loss of the methyl group, the ion at m/z 123.04 corresponds to the loss of the carbonyl group, the ion at m/z 108.01 corresponds to the loss of both the methyl and the carbonyl group and the ion at m/z 93.03 corresponds to the deprotonated phenol.

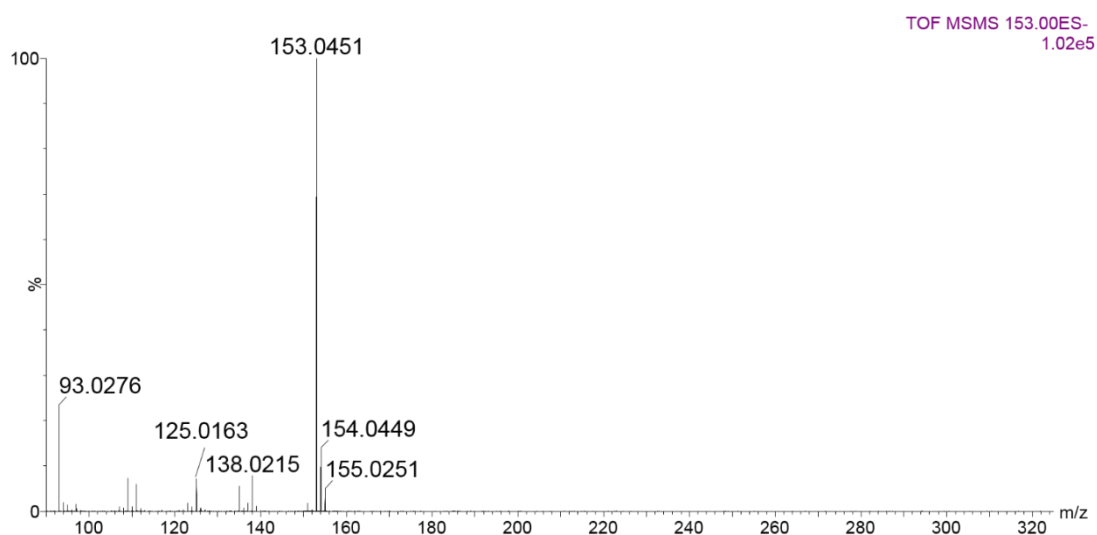


Figure S5. MS/MS spectrum over the range 90-325 of m/z 153.04 (vanillin alcohol) obtained in negative ionization mode at a collision energy of 20 eV, by cutting the sample at DC 10 W. The ion at m/z 138.00 corresponds to the loss of the methyl group, the ion at m/z 135.04 is the loss of water, the ion at m/z 125.04 corresponds to the loss of a carbonyl group (followed by rearrangement) and the ion at m/z 93.03 corresponds to the deprotonated phenol.

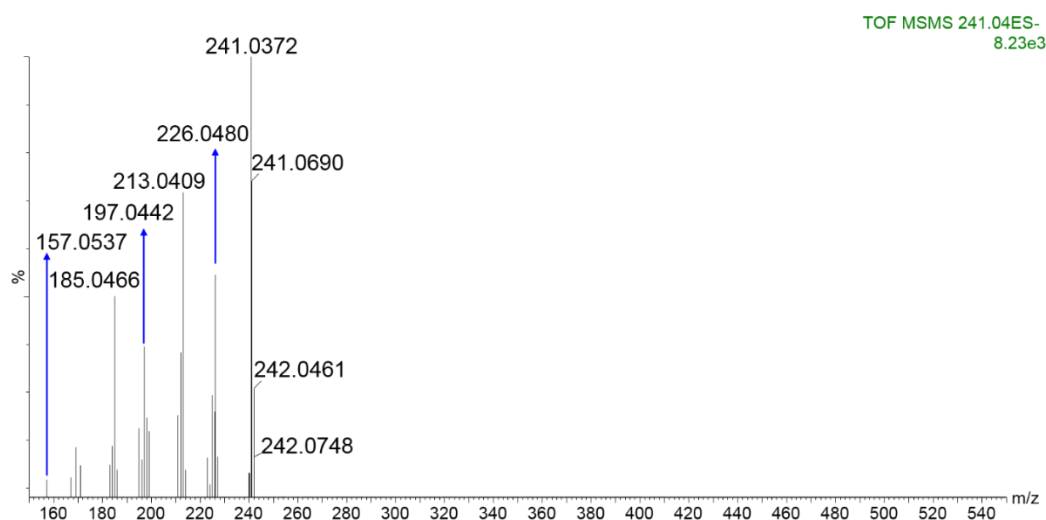


Figure S6. MS/MS spectrum over the range 150-550 of m/z 241.03 (lapachol) obtained in negative ionization mode at a collision energy of 20 eV, by cutting the sample at DC 10 W. The ion at m/z 226.05 corresponds to the loss of the methyl group, the ion at m/z 213.04 corresponds to the loss of ethylene from the side chain, the ion at m/z 197.04 could be generated by the simultaneous loss of ethylene and a hydroxyl group, the ion at m/z 185.05 is probably related to the cleavage of the side chain and the ion at m/z 157.05 corresponds to the deprotonated naphtoquinone.

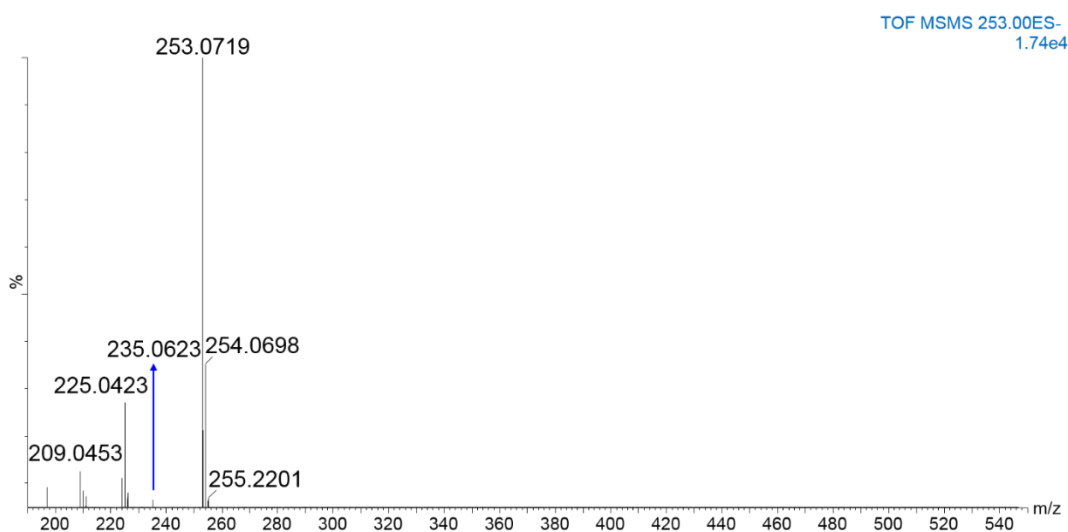


Figure S7. MS/MS spectrum over the range 190-550 of m/z 253.07 (daidzein) obtained in negative ionization mode at a collision energy of 20 eV, by cutting the sample at DC 10 W. The ion at m/z 235.06 corresponds to the loss of water, while the ion at m/z 225.04 is the loss of the carbonyl group after the opening of the pyranone ring.

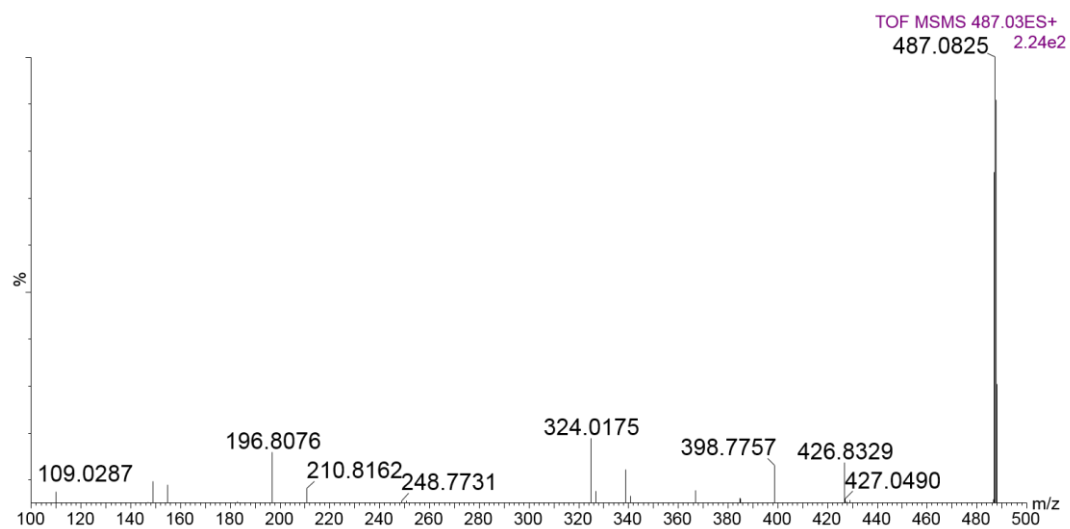


Figure S8. MS/MS spectrum over the range 100-500 of m/z 487.08 obtained in positive ionization mode at a collision energy of 30 eV, by cutting the sample at FC 20 W.

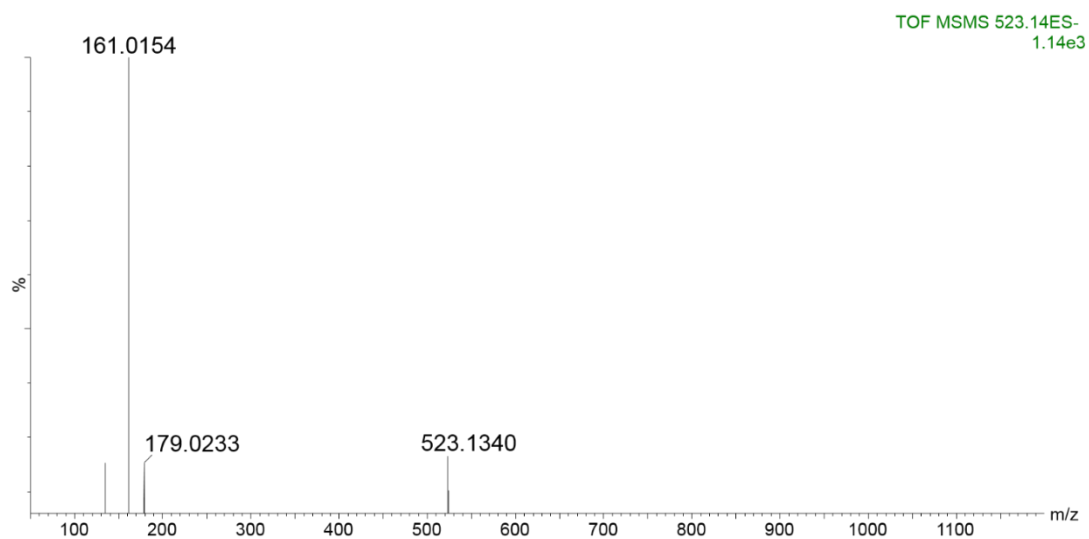


Figure S9. MS/MS spectrum over the range 50-1200 of m/z 523.14 obtained in negative ionization mode at a collision energy of 30 eV, by cutting the sample at DC 10 W.