

Supplementary data

Integrated LC–MS–guided phytochemical profiling, molecular docking, and in vitro validation of *Sauromatum venosum* extracts against colorectal cancer

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Table SI		
Extractive yield of different extracts		
Extract	Solvent	% Yield
Leaf	Hydroalcoholic	13.1
Leaf	Aqueous	9.1
Leaf	Ethyl acetate	7.6
Tuber	Hydroalcoholic	16.4
Tuber	Aqueous	12.3
Tuber	Ethyl acetate	9.3

Table SII		
DPPH radical scavenging activity		
Sample	Concentration (µg/mL)	% Inhibition
Control	-	
Ascorbic acid	200	76.3
	400	77.3
	600	77.6
	800	83.2
	1,000	91.9
Leaf (hydroalcoholic) extract	200	50.3
	400	57.3
	600	61.7
	800	68.1
	1,000	77.8
Leaf (aqueous) extract	200	47.6
	400	50.5
	600	56.9
	800	63.5
	1,000	69.6
Leaf (ethyl acetate) extract	200	34.6
	400	36.7
	600	41.0
	800	47.7
	1,000	61.8
Tuber (hydroalcoholic) extract	200	56.5
	400	62.1
	600	67.5
	800	73.3
	1,000	82.6
Tuber (aqueous) extract	200	51.0
	400	54.3
	600	59.6
	800	63.8
	1,000	78.0
Tuber (ethyl acetate) extract	200	46.4
	400	51.5
	600	56.3
	800	63.6
	1,000	72.3

Table SIII						
Identified bioactive phytoconstituents from hydroalcoholic <i>S. venosum</i> leaf extract						
Peak group	RT range (min)	m/z (observed)	Ion type	Proposed compound	Class	Key fragment/ evidence
1	0.9–1.5	191.0588	[M–H] [–]	Quinic acid	Phenolic acid	Base peak at 191
2	1.2–1.8	353.1015	[M–H] [–]	Chlorogenic acid	Phenolic acid	353 → 191
3	1.3–2.0	169.0152	[M–H] [–]	Gallic acid	Phenolic acid	Typical fragment
4	3.0–3.6	303.0592	[M+H] ⁺	Quercetin	Flavonoid	303 → 179, 151
5	3.6–4.1	287.0645	[M+H] ⁺	Kaempferol	Flavonoid	287 → 153, 165
6	2.4–3.0	315.0836	[M+H] ⁺	Isorhamnetin	Methoxylated flavonoid	+14Da vs quercetin
7	3.5–4.5	449.1263	[M+H] ⁺	Kaempferol glycoside	Flavonoid glycoside	449 → 287
8	3.5–4.5	599.1369	[M–H] [–]	Quercetin glycoside	Flavonoid glycoside	599 → 301
9	3.4–4.0	617.1425	[M+H] ⁺	Quercetin glycoside	Flavonoid glycoside	617 → 303
10	3.5–5.0	757.1162	[M+H] ⁺	Flavonoid diglycoside	Polyphenol	Fragment to 303/287
11	5.0–7.0	801.1239	[M+H] ⁺	Flavonoid conjugate	Polyphenol	Aglycone fragments
12	5.0–8.0	929.1664	[M+H] ⁺	Polyphenolic conjugate	Polyphenol	High MW fragmentation

Table SIV						
Identified bioactive phytoconstituents from hydroalcoholic <i>S. venosum</i> tuber extract						
Peak group	RT range (min)	m/z (observed)	Ion type	Proposed compound	Class	Key fragment ions
1	1.25	191.056	[M–H] [–]	Quinic acid	Phenolic acid	–
2	1.65	353.087	[M–H] [–]	Chlorogenic acid	Phenolic acid	191
3	3.17	303.056	[M+H] ⁺	Quercetin	Flavonoid	179, 151
4	3.63	287.055	[M+H] ⁺	Kaempferol	Flavonoid	153, 165
5	3.83	315.071	[M+H] ⁺	Isorhamnetin	Methoxylated flavonoid	300, 271
6	4.58	433.114	[M+H] ⁺	Quercetin glycoside	Flavonoid glycoside	303
7	5.95	309.101	[M+H] ⁺	Phenolic derivative	Polyphenol	–
8	6.10	287.058	[M+H] ⁺	Kaempferol (repeat)	Flavonoid	–
9	10.80	609.146	[M+H] ⁺	Rutin	Flavonoid glycoside	303
10	11.35	593.151	[M+H] ⁺	Kaempferol glycoside	Flavonoid glycoside	287
11	12.46	637.299	[M+H] ⁺	Diglycoside	Polyphenol	–
12	13.12	621.306	[M+H] ⁺	Diglycoside	Polyphenol	–
13	15.09	563.300	[M+H] ⁺	Polyphenolic conjugate	Polyphenol	–
14	16.15	471.337	[M+H] ⁺	Lipophilic compound	Unknown	–
15	18.27	736.519	[M+H] ⁺	High MW compound	Oligomer/saponin	–

Table SV			
MTT assay			
Sample	Concentration (µg/mL)	% Inhibition	IC ₅₀ (µg/mL)
<i>HT-29 Human Colon Cell line</i>			
Control	-	-	-
5-Fluorouracil	100	17.1	29.9
	50	21.3	
	25	30.7	
	12.5	39.0	
	6.25	46.1	
Leaf (hydroalcoholic) extract	100	35.3	32.0
	50	39.5	
	25	51.9	
	12.5	56.1	
	6.25	58.6	
Leaf (aqueous) extract	100	31.3	20.1
	50	37.0	
	25	52.0	
	12.5	54.9	
	6.25	59.0	
<i>HCT 116 Human Colon Cell line</i>			
Control	-	-	-
5-Fluorouracil	100	22.5	29.9
	50	26.9	
	25	30.7	
	12.5	34.8	
	6.25	53.3	
Tuber (hydroalcoholic) extract	100	35.3	57.0
	50	39.5	
	25	51.9	
	12.5	56.1	
	6.25	58.6	
Tuber (aqueous) extract	100	36.8	36.5
	50	41.2	
	25	52.0	
	12.5	56.2	
	6.25	61.0	