

1 *Article*

2 **UPLC-HRMS Polyphenolic Characterization, Contents**
3 **and Antioxidant Activity of *Zingiber officinale* Roscoe**
4 **rhizomes from Costa Rica**

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Table S-1. Profile of the phenolic compounds identified by UPLC-QTOF-ESI MS in *Zingiber officinale* rhizomes from Costa Rica

No.	Rt (min)	Tentative identification	Ion (m/z)	Adduct	Molecular formula	MS2 Fragments	Sample ¹
1	8.20	4-Gingerol	289.1427 249.1501	[M+Na] ⁺ [M+H-H ₂ O] ⁺	C ₁₅ H ₂₂ O ₄ Na C ₁₅ H ₂₁ O ₃	177	NR-1, NR-2, NR-3, NR-4, NR-5, NW-1, NW-2, NW-3, SR-1, WR-2
2	11.71	6-Gingerdiol	319.1875 279.1975 261.1873	[M+Na] ⁺ [M+H-H ₂ O] ⁺ [M+H-2(H ₂ O)] ⁺	C ₁₇ H ₂₈ O ₄ Na C ₁₇ H ₂₇ O ₃ C ₁₇ H ₂₅ O ₂	137	NR-1, NR-2, NR-3, NR-4, NR-5, NW-1, NW-2, NW-3, SR-1, WR-1, WR-2, WR-3
3	12.93	6-Gingerol	317.1722 277.1800	[M+Na] ⁺ [M+H-H ₂ O] ⁺	C ₁₇ H ₂₆ O ₄ Na C ₁₇ H ₂₅ O ₃	179, 177, 145, 137, 117	NR-1, NR-2, NR-3, NR-4, NR-5, NW-1, NW-2, NW-3, SR-1, WR-1, WR-2, WR-3
4	12.98	6-Paradol	279.1949 301.1779	[M+H] ⁺ [M+Na] ⁺	C ₁₇ H ₂₇ O ₃ C ₁₇ H ₂₆ O ₃ Na	137	NR-4, NW-1, NW-2, SR-1, WR-3
5	15.68	3-Acetoxy-6-gingerdiol	339.2177 361.1989 321.2059	[M+H] ⁺ [M+Na] ⁺ [M+H-H ₂ O] ⁺	C ₁₉ H ₃₁ O ₅ C ₁₉ H ₃₀ O ₅ Na C ₁₉ H ₂₉ O ₄	301, 279	NR-1, NR-4, NR-5, NW-1, NW-3, SR-1, WR-1, WR-3
6	15.72	8-Gingerdiol	347.2189 307.2273 289.2173	[M+Na] ⁺ [M+H-H ₂ O] ⁺ [M+H-2(H ₂ O)] ⁺	C ₁₉ H ₃₂ O ₄ Na C ₁₉ H ₃₁ O ₃ C ₁₉ H ₂₉ O ₂	137	NR-1, NW-2, SR-1, WR-2
7	15.82	Methyl-6-Gingerol	331.1897 291.1988	[M+Na] ⁺ [M+H-H ₂ O] ⁺	C ₁₈ H ₂₈ O ₄ Na C ₁₈ H ₂₇ O ₃	191, 177, 151, 145, 137	NR-1, NR-2, NR-3, NR-4, NR-5, NW-1, NW-2, NW-3, SR-1, WR-1, WR-2, WR-3
8	16.74	Diacetoxy-4-gingerdiol	375.1790	[M+Na] ⁺	C ₁₉ H ₂₈ O ₆ Na	293, 233, 177, 163, 137	NR-1, NR-2, NR-3, NR-4, NR-5, NW-1, NW-2, NW-3, SR-1, WR-1, WR-2, WR-3
9	18.19	8-Paradol	307.2272 329.2097	[M+H] ⁺ [M+Na] ⁺	C ₁₉ H ₃₁ O ₃ C ₁₉ H ₃₀ O ₃ Na	137	NR-3, NR-5, SR-1, WR-3

No.	Rt (min)	Tentative identification	Ion (m/z)	Adduct	Molecular formula	MS2 Fragments	Sample ¹
10	18.23	8-Gingerol	345.2051 305.2136	[M+Na] ⁺ [M+H-H ₂ O] ⁺	C ₁₉ H ₃₀ O ₄ Na C ₁₉ H ₂₉ O ₃	179, 177, 145, 137, 117	NR-1, NR-2, NR-3, NR-4, NR-5, NW-1, NW-2, NW-3, SR-1, WR-1, WR-2, WR-3
11	18.27	6-Shogaol	277.1795	[M+H] ⁺	C ₁₇ H ₂₅ O ₃	137	NR-1, NR-2, NR-3, NR-4, NR-5, NW-1, NW-2, NW-3, SR-1, WR-1, WR-2, WR-3
12	18.42	Acetoxy-6-gingerol	359.1815	[M+Na] ⁺	C ₁₉ H ₂₈ O ₅ Na	299	NR-1, NR-3, NR-4, NR-5, NW-1, NW-2, SR-1, WR-1, WR-2, WR-3
13	18.77	7-Paradol	293.2095 315.1941	[M+H] ⁺ [M+Na] ⁺	C ₁₈ H ₂₉ O ₃ C ₁₈ H ₂₈ O ₃ Na	137	NR-3, NR-4, NR-5, NW-1, NW-2, NW-3, SR-1, WR-1, WR-2, WR-3
14	18.82	Methyl-5-acetoxy-6-gingerdiol	353.2322 375.2150 335.2222	[M+H] ⁺ [M+Na] ⁺ [M+H-H ₂ O] ⁺	C ₂₀ H ₃₃ O ₅ C ₂₀ H ₃₂ O ₅ Na C ₂₀ H ₃₁ O ₄	293, 151	NR-3, NR-4, SR-1
15	19.79	Methyl-diacetoxy-4-gingerdiol	389.1938	[M+Na] ⁺	C ₂₀ H ₃₀ O ₆ Na	307, 247, 191, 151	NR-2, NR-4, NR-5, NW-1, SR-1, WR-1, WR-3
16	21.18	Methyl acetoxy-6-gingerol	351.2173 373.2003	[M+H] ⁺ [M+Na] ⁺	C ₂₀ H ₃₁ O ₅ C ₂₀ H ₃₀ O ₅ Na	151	NR-1, NR-2, NR-4, NR-5, NW-1, NW-2, NW-3, SR-1, WR-1, WR-3
17	21.23	10-Gingerdiol	375.2521 335.2585 317.2487	[M+Na] ⁺ [M+H-H ₂ O] ⁺ [M+H-2(H ₂ O)] ⁺	C ₂₁ H ₃₆ O ₄ Na C ₂₁ H ₃₅ O ₃ C ₂₁ H ₃₃ O ₂	137	NR-3, NR-4, NR-5, NW-1, NW-2, NW-3, SR-1, WR-1, WR-2, WR-3
18	21.57	Diacetoxy-6-gingerdiol	403.2099	[M+Na] ⁺	C ₂₁ H ₃₂ O ₆ Na	321, 261, 177, 163, 137	NR-1, NR-2, NR-3, NR-4, NR-5, NW-1, NW-2, NW-3, SR-1, WR-1, WR-2, WR-3
19	22.53	1-Dehydro-6-gingerdione	291.1596	[M+H] ⁺	C ₁₇ H ₂₃ O ₄	177	NR-1, NR-2, NR-3, NR-4, NR-5, NW-1, NW-2, NW-3, SR-1, WR-1, WR-2, WR-3

No.	Rt (min)	Tentative identification	Ion (m/z)	Adduct	Molecular formula	MS2 Fragments	Sample ¹
20	23.34	8-Shogaol	305.2117	[M+H] ⁺	C ₁₉ H ₂₉ O ₃	137	NR-1, NR-2, NW-1, NW-2, SR-1, WR-1, WR-2, WR-3
21	23.40	Acetoxy-8-gingerol	387.2158	[M+Na] ⁺	C ₂₁ H ₃₂ O ₅ Na	327	NR-1, NR-2, NW-3, SR-1, WR-3
22	23.48	10-Paradol	335.2590 357.2416	[M+H] ⁺ [M+Na] ⁺	C ₂₁ H ₃₅ O ₃ C ₂₁ H ₃₄ O ₃ Na	137	NR-2, NR-3, NR-4, SR-1, WR-3
23	23.52	10-Gingerol	373.2359 333.2457	[M+Na] ⁺ [M+H-H ₂ O] ⁺	C ₂₁ H ₃₄ O ₄ Na C ₂₁ H ₃₃ O ₃	179, 177, 145, 137, 117	NR-1, NR-2, NR-3, NR-4, NR-5, NW-1, NW-2, NW-3, SR-1, WR-1, WR-2, WR-3
24	24.51	Methyl diacetoxy-6-gingerdiol	417.2252	[M+Na] ⁺	C ₂₂ H ₃₄ O ₆ Na	357, 335, 297, 275, 191, 177, 151	NR-1, NR-2, NR-3, NR-4, NR-5, NW-1, NW-2, NW-3, SR-1, WR-1, WR-2, WR-3
25	24.76	Methyl-8-Gingerol	359.2199 319.2277	[M+Na] ⁺ [M+H-H ₂ O] ⁺	C ₂₀ H ₃₂ O ₄ Na C ₂₀ H ₃₁ O ₃	191, 177, 151	NR-1, NR-2, NR-3, NR-4, NR-5, NW-3, SR-1, WR-1, WR-2, WR-3
26	26.34	Diacetoxy-8-gingerdiol	431.2443	[M+Na] ⁺	C ₂₃ H ₃₆ O ₆ Na	349, 289, 177, 163, 137	NR-1, NR-2, NR-3, NR-4, NR-5, NW-1, NW-2, NW-3, SR-1, WR-1, WR-2, WR-3
27	27.37	1-Dehydro-8-gingerdiona	319.1909	[M+H] ⁺	C ₁₉ H ₂₇ O ₄	177	NR-1, NR-2, NR-3, NR-4, NW-2, NW-3, SR-1
28	27.94	10-Shogaol	333.2430	[M+H] ⁺	C ₂₁ H ₃₃ O ₃	137	NR-1, NR-2, NR-3, NW-1, NW-2, NW-3, SR-1, WR-1, WR-2, WR-3
29	27.99	Acetoxy-10-gingerol	415.2458	[M+Na] ⁺	C ₂₃ H ₃₆ O ₅ Na	355	NR-4, NW-1, NW-2, NW-3, SR-1, WR-3
30	28.43	12-Gingerol	401.2653 361.2740	[M+Na] ⁺ [M+H-H ₂ O] ⁺	C ₂₃ H ₃₈ O ₄ Na C ₂₃ H ₃₇ O ₃	179, 177, 145, 137	NR-2, NR-3, NW-2, NW-3, SR-1, WR-2
31	28.96	Methyl diacetoxy-8-gingerdiol	445.2567	[M+Na] ⁺	C ₂₄ H ₃₈ O ₆ Na	363, 325, 303, 191, 151	NR-1, NR-2, NR-3, NR-4, NW-1, NW-2, NW-3, SR-1, WR-3

No.	Rt (min)	Tentative identification	Ion (m/z)	Adduct	Molecular formula	MS2 Fragments	Sample ¹
32	30.49	Diacetoxy-10-gingerdiol	459.2726	[M+Na] ⁺	C ₂₅ H ₄₀ O ₆ Na	377, 317, 177, 163, 137	NR-1, NR-4, NW-1, NW-2, NW-3, SR-1
33	30.87	Methyl diacetoxy-10-gingerdiol	473.2862	[M+Na] ⁺	C ₂₆ H ₄₂ O ₆ Na	391, 331, 353, 191, 151	NR-2, NR-3, NW-3, SR-1
34	31.37	1-Dehydro-10-gingerdiona	347.2220	[M+H] ⁺	C ₂₁ H ₃₁ O ₄	177	NR-3, NR-4, SR-1

¹ Regions: Northern (NR), Northwestern (NW), Western (WR), Southern (SR).