

Table S1. LC-ESI-UHR-QqTOF-MS data of organic acids and phenolic compounds identified in ethanolic extracts obtained from sugarcane straw.

Name	Formula- H	m/z Measured [M-H]-	MS/MS fragments (m/z)
Organic acids			
Quinic acid	C ₇ H ₁₁ O ₆	191.0	85, 75, 59
Malic acid	C ₄ H ₆ O ₅	133.0	71, 115, 59
Citric acid	C ₆ H ₇ O ₇	191.1	111, 87, 57, 67
Sebacic acid	C ₁₀ H ₁₇ O ₄	201.1	139, 183, 201
Azelaic acid	C ₉ H ₁₆ O ₄	187.1	125, 169, 187
Aconitic acid	C ₆ H ₆ O ₆	173.0	
Hydroxybenzoic acids			
1-O-Vanilloyl-β-D-glucose	C ₁₄ H ₁₇ O ₉	329.0	167
Vanillic acid	C ₈ H ₇ O ₄	167.0	108, 119, 152
Protocatechuic acid	C ₇ H ₅ O ₄	153.0	109, 153
2,5-Dihydrobenzoic acid	C ₇ H ₅ O ₄	153.0	109, 153
2,4 Dihydrobenzoic acid	C ₇ H ₅ O ₄	153.0	109, 153
Gentisic acid 2-O-β-glucoside	C ₁₃ H ₁₅ O ₉	315.1	108, 152
Gentisic acid 5-O-β-glucoside	C ₁₃ H ₁₅ O ₉	315.1	109, 153
Protocatechuic acid 4-β-glucoside	C ₁₃ H ₁₅ O ₉	315.1	109, 153
4-Hydroxybenzoic acid	C ₇ H ₅ O ₃	137.0	137
3,4-Dihydroxybenzaldehyde	C ₇ H ₅ O ₃	137.0	93, 137
4-Hydroxybenzaldehyde	C ₇ H ₅ O ₂	121.0	121
Hydroxybenzoic-4- β-glucoside	C ₁₃ H ₁₅ O ₈	299.1	108, 152
Hydroxycinnamic acids			
Neochlorogenic acid	C ₁₆ H ₁₇ O ₉	353.1	135, 179, 191
Chlorogenic acid	C ₁₆ H ₁₇ O ₉	353.1	191
4-Caffeoylquinic acid isomer 1	C ₁₆ H ₁₇ O ₉	353.1	135, 173, 179, 191
4-Caffeoylquinic acid isomer 2	C ₁₆ H ₁₇ O ₉	353.1	191
cis-5-O-p-Coumaroylquinic acid isomer 1	C ₁₆ H ₁₇ O ₈	337.1	119, 163
cis-5-O-p-Coumaroylquinic acid isomer 2	C ₁₆ H ₁₇ O ₈	337.1	93, 163, 173, 191
cis-5-O-p-Coumaroylquinic acid isomer 3	C ₁₆ H ₁₇ O ₈	337.1	191
3-O-Feruloylquinic acid	C ₁₇ H ₁₉ O ₉	367.1	134, 193
trans-3-Feruloylquinic acid	C ₁₇ H ₁₉ O ₉	367.1	173
Caffeic acid	C ₉ H ₈ O ₄	179.0	135, 179
Ferulic acid	C ₁₀ H ₉ O ₄	193.1	134
Isoferulic acid	C ₁₀ H ₉ O ₄	193.0	134, 161, 193
p-Coumaric acid	C ₉ H ₇ O ₃	163.0	119
p-Coumaric acid isomer	C ₉ H ₇ O ₃	163.0	119
Caffeoylquinic acid	C ₁₆ H ₁₈ O ₉	515.1	515
1,3-Dicaffeoylquinic acid	C ₂₅ H ₂₃ O ₁₂	515.1	173, 179, 191, 335, 353
Caffeoylshikimic acid	C ₂₅ H ₂₃ O ₁₄	335.1	135, 161, 179
1,3-Dicaffeoylquinic acid	C ₂₅ H ₂₄ O ₁₂	335.1	135, 161, 179
Flavones			
Apigenin-8-C-glucoside isomer 1	C ₂₁ H ₁₉ O ₁₀	431.1	89, 179

Apigenin-8-C-glucoside isomer 2	C ₂₁ H ₁₉ O ₁₀	431.1	311, 341, 431
Apigenin-6-C-glucoside	C ₂₁ H ₁₉ O ₁₀	431.1	311, 341
Isoschaftoside	C ₂₆ H ₂₇ O ₁₄	563.1	353, 473
Neoschaftoside	C ₂₆ H ₂₇ O ₁₄	563.1	399, 473
Apigenin-6-C-arabinoside-8-C-glucoside	C ₂₆ H ₂₇ O ₁₄	563.1	293, 413
Luteolin-8-C-glucoside	C ₂₁ H ₁₉ O ₁₁	447.1	327, 357
Vitexin 2''-O-beta-L-rhamnoside	C ₂₇ H ₂₉ O ₁₄	577.2	293, 413
Apigenin 7-O-neohesperidoside isomer 1	C ₂₇ H ₂₉ O ₁₄	577.2	293, 413, 473
Apigenin 7-O-neohesperidoside isomer 2	C ₂₇ H ₂₉ O ₁₄	577.2	293, 413, 474
6-Methoxyluteolin 7-rhamnoside	C ₂₂ H ₂₁ O ₁₁	461.1	461
Tricin-O-neohesperoside isomer 1	C ₂₉ H ₃₃ O ₁₆	637.2	329
Tricin-O-neohesperoside isomer 2	C ₂₉ H ₃₃ O ₁₆	637.2	329
Tricin-7-O-glucoside	C ₂₅ H ₃₁ O ₁₀	491.2	329
Tricin-7-O-rhamnosyl-glucuronide	C ₂₉ H ₃₁ O ₁₇	651.2	329
Tricin-4-(O-erythro) ether glucoside isomer 1	C ₃₃ H ₃₅ O ₁₆	687.2	165, 195, 329, 491, 525
Tricin-4-(O-erythro) ether glucoside isomer 2	C ₃₃ H ₃₅ O ₁₆	687.2	165, 195, 329, 491, 526
Tricin	C ₁₇ H ₁₃ O ₇	329.1	299

Figure S1. LC-ESI-UHR-QqTOF-MS chromatogram of organic acids and phenolic compounds identified in the sugarcane straw extract-based ingredient.

