Supplementary Material

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Table S1. Brazilian samples mean values for meteorological parameters related to the specific cultivation sites during maturation period (April to June 2021). Maximum temperature (Tmax), minimum temperature (Tmin), mean temperature (Tmean), daylight duration (day_dur), sunshine duration (sun_dur), rainfall (precip), average wind speed (wnd_spd), maximum wind gusts (wnd_gst), shortwave radiation (sw_rad) and evapotranspiration (evap). Data were sourced from Visual Crossing Weather 2020-2021 database (Visual Crossing Corporation).

Sample	Location	Tmax (°C)	Tmin (°C)	Tmean (°C)	day_dur (sec)	sun_dur (sec)	precip (mm)	wnd_spd (km/h)	wnd_gst (km/h)	sw_rad (MJ/m²)	evap (mm)
BRA1	Divisa Nova	24.3	13.2	18.2	40217	35262	0.56	12.8	32.6	16.61	3.2
BRA2	Capelinha	23.9	14.1	18.7	40861	35046	0.36	12.0	29.5	16.43	3.2
BRA3	Patos De Minas	27.1	16.0	21.3	40708	36114	0.41	12.0	28.0	17.42	3.8
BRA4	Araponga	22.0	14.5	17.8	40362	35995	0.93	13.5	34.8	16.18	2.9
BRA5	São Gotardo	24.7	15.0	19.5	40590	36047	0.63	13.0	31.4	17.17	3.6
BRA6	Campestre	22.7	12.5	17.2	40180	35497	0.54	13.7	31.7	16.56	3.2
BRA7	Tapira	24.3	13.9	18.6	40483	36045	0.62	14.2	32.9	17.12	3.5
BRA8	Monte Santo De Minas	25.0	14.6	19.3	40265	35649	0.82	12.7	31.0	16.85	3.5
BRA9	Juruaia	24.2	13.3	18.3	40253	34681	0.75	12.3	30.3	16.37	3.1
BRA10	Cabo Verde	24.3	13.2	18.2	40217	35262	0.56	12.8	32.6	16.61	3.2

Table S2. Brazilian samples mean values for environmental parameters related to the specific cultivation sites during maturation period (April to June 2021). Elevation (elev, above sea level), relative humidity (Rh), cloud cover (Cc), soil temperature at 7, 28, 100, 255 cm depth (sT7, sT28, sT100, sT255), and soil moisture at 7, 28, 100, 255 cm depth (sm7, sm28, sm100, sm255). Data were sourced from Visual Crossing Weather 2020-2021 database (Visual Crossing Corporation).

Sample	Location	elev (m a.s.l.)	Rh (%)	Cc (%)	sT7 (°C)	sT28 (°C)	sT100 (°C)	sT255 (°C)	sm7 (m³/m³)	sm28 (m³/m³)	sm100 (m³/m³)	sm255 (m³/m³)
BRA1	Divisa Nova	894	72.53	25.19	18.4	18.7	19.7	21.1	0.258	0.275	0.312	0.355
BRA2	Capelinha	928	73.86	33.95	19.9	20.2	20.9	21.9	0.312	0.351	0.412	0.332
BRA3	Patos De Minas	841	60.15	24.98	22.9	23.0	23.4	23.8	0.212	0.300	0.355	0.374
BRA4	Araponga	958	77.96	34.49	18.9	19.2	20.0	21.2	0.386	0.379	0.396	0.471
BRA5	São Gotardo	1061	64.02	27.09	20.2	20.4	20.9	21.6	0.195	0.219	0.267	0.373
BRA6	Campestre	1070	70.02	23.13	18.3	18.6	19.5	20.9	0.312	0.359	0.412	0.444
BRA7	Tapira	1088	66.43	24.68	19.5	19.8	20.5	21.5	0.329	0.351	0.390	0.427
BRA8	Monte Santo De Minas	884	64.97	21.53	19.8	20.1	21.0	22.3	0.306	0.333	0.377	0.402
BRA9	Juruaia	874	71.82	26.33	18.8	19.1	20.1	21.6	0.364	0.374	0.411	0.465
BRA10	Cabo Verde	894	72.53	25.19	18.4	18.7	19.7	21.1	0.258	0.275	0.312	0.355

Table S3. Free amino acid content (μg/gFW) in green coffee bean samples from Brazil (BRA1-10), Rwanda (RWA1-4), India (IND1-4), Ethiopia (ETH1-4), Guatemala (GUA1-4), and Honduras (HON1-4). Data are the mean (n = 3) ± SD. Lowercase letters (a, b and c) represent statistically significant differences among samples determined by ANOVA test followed by Tukey post-hoc test ($p < 0.05$) or Kruskal-Wallis test followed by Dunn test ($p < 0.05$).

	POLAR			NON-POLAR								ACIDIC		BASIC			TOTAL
Sample	**ser**	**thr**	**tyr**	**gly**	**ala**	**pro**	**val**	**met**	**ile**	**leu**	**phe**	**asp**	**glu**	**hys**	**arg**	**lys**	
BRA1	113.2^{ab} ± 5.2	8.5^{ab} ±1.8	7.7^{ab} ±0.5	3.6^{abc} ±0.6	32.3^{ab} ±1.7	15.5^{a} ±1.0	13.7^{abc} ±0.5	1.6^{c} ±0.1	8.1^{ab} ±0.4	9.8^{ab} ±0.6	53.0^{ab} ±3.1	92.5^{ab} ±5.5	218.1^{ab} ±12.1	18.3^{ab} ±1.5	26.3^{abc} ±1.6	9.3^{ab} ±0.4	631.5^{abc} ±36.5
BRA2	128.5^{ab} ± 3.2	8.2^{ab} ±0.2	6.8^{a} ±0.3	1.8^{c} ±0.5	32.9^{ab} ±1.7	16.9^{ab} ±1.1	12.8^{abc} ±0.5	1.7^{bc} ±0.1	6.5^{ab} ±1.2	8.2^{ab} ±0.7	47.5^{ab} ±1.4	111.7^{ab} ±2.7	257.7^{ab} ±5.6	14.7^{abc} ±0.9	29.0^{abc} ±2.0	10.0^{ab} ±0.5	695.0^{abc} ±22.5
BRA3	120.8^{ab} ± 10.2	8.6^{ab} ±1.4	6.8^{ab} ±0.9	3.1^{abc} ±1.4	34.7^{ab} ±3.3	17.1^{ab} ±2.4	14.0^{abc} ±1.2	1.9^{abc} ±0.1	8.3^{ab} ±1.0	8.2^{ab} ±0.9	47.2^{ab} ±4.3	113.9^{ab} ±7.1	216.8^{ab} ±13.2	15.6^{abc} ±2.2	28.4^{abc} ±2.4	9.5^{ab} ±0.8	654.8^{abc} ±52.8
BRA4	121.2^{ab} ±10.2	7.1^{ab} ±0.5	7.6^{ab} ±0.2	2.6^{abc} ±0.7	34.6^{ab} ±1.0	16.6^{ab} ±1.4	14.1^{abc} ±0.3	1.9^{abc} ±0.1	7.0^{ab} ±1.1	9.0^{ab} ±0.4	40.1^{ab} ±1.4	108.3^{ab} ±3.8	243.6^{ab} ±6.2	19.0^{abc} ±1.9	31.0^{abc} ±1.1	10.5^{ab} ±0.3	674.4^{abc} ±24.1
BRA5	203.4^{a} ±22.5	9.6^{ab} ±2.0	8.4^{ab} ±1.1	2.8^{abc} ±1.2	50.1^{ab} ±9.3	27.0^{ab} ±1.6	22.4^{ab} ±3.1	1.9^{abc} ±0.2	12.0^{ab} ±2.9	12.3^{ab} ±1.6	60.0^{ab} ±7.4	190.7^{a} ±24.3	314.2^{a} ±43.8	28.1^{a} ±5.3	39.7^{a} ±4.3	14.3^{ab} ±1.6	997.0^{a} ±132.3
BRA6	132.9^{ab} ±3.8	7.1^{ab} ±0.5	7.9^{ab} ±0.3	2.3^{bc} ±0.4	37.6^{ab} ±1.3	16.1^{ab} ±1.8	12.8^{abc} ±0.4	1.5^{c} ±0.1	5.9^{a} ±0.5	8.7^{ab} ±0.3	44.8^{ab} ±1.5	89.6^{ab} ±2.8	280.7^{a} ±8.4	19.5^{abc} ±0.7	29.7^{abc} ±0.7	10.0^{ab} ±0.5	707.1^{abc} ±23.9
BRA7	154.4^{ab} ±12.8	8.8^{ab} ±1.9	8.4^{ab} ±0.8	2.8^{abc} ±1.4	57.7^{ab} ±5.8	16.5^{ab} ±0.8	18.4^{abc} ±1.4	2.2^{abc} ±0.1	11.1^{ab} ±0.8	11.2^{ab} ±0.9	63.3^{a} ±4.9	100.4^{ab} ±6.4	283.1^{a} ±20.8	16.4^{abc} ±5.1	36.2^{ab} ± 4.3	12.6^{ab} ±1.1	803.6^{ab} ±69.2
BRA8	145.4^{ab} ±13.1	8.9^{ab} ±1.6	8.5^{ab} ±0.8	3.8^{abc} ±0.7	56.1^{ab} ±5.5	17.0^{ab} ±2.3	16.8^{abc} ±1.6	2.0^{abc} ±0.2	10.2^{ab} ±1.2	12.8^{ab} ±1.1	52.8^{ab} ±5.8	99.0^{ab} ±7.9	231.3^{ab} ±19.9	14.1^{abc} ±2.3	29.6^{abc} ±4.6	11.8^{ab} ±1.3	720.2^{abc} ±69.9
BRA9	118.4^{ab} ±8.0	6.2^{a} ±1.9	7.3^{ab} ±0.6	3.5^{abc} ±0.4	28.8^{ab} ±1.7	12.8^{a} ±2.1	12.8^{abc} ±0.9	2.0^{abc} ±0.2	7.0^{ab} ±0.8	8.7^{ab} ±0.7	46.8^{ab} ±3.5	100.5^{ab} ±6.7	220.0^{ab} ±15.0	17.2^{abc} ±0.9	24.8^{abc} ±3.9	9.9^{ab} ±0.8	626.6^{abc} ±48.2
BRA10	146.9^{ab} ±5.0	7.4^{ab} ±1.6	7.6^{ab} ±0.4	4.1^{abc} ±0.3	39.1^{ab} ±0.3	13.8^{ab} ±0.8	13.0^{abc} ±0.4	1.6^{c} ±0.1	8.0^{ab} ±0.3	9.2^{ab} ±0.3	55.7^{ab} ±1.7	109.6^{ab} ±3.0	248.2^{ab} ±8.8	22.2^{abc} ±0.4	26.7^{abc} ±2.0	10.2^{ab} ±0.2	723.3^{abc} ±25.6
RWA1	75.6^{ab} ±2.0	11.2^{ab} ±0.4	9.1^{ab} ±0.2	5.2^{a} ±0.2	39.7^{ab} ±2.4	26.9^{ab} ±0.5	11.5^{abc} ±0.3	2.8^{ab} ±0.1	7.2^{ab} ±0.1	11.1^{ab} ±0.3	39.1^{ab} ±1.1	35.0^{b} ±1.2	96.5^{b} ±8.1	10.5^{abc} ±0.6	5.8^{c} ±0.3	8.4^{ab} ±0.2	395.7^{c} ±17.9
RWA2	71.9^{ab} ±2.8	11.2^{ab} ±0.5	7.8^{ab} ±0.3	3.0^{abc} ±0.2	25.6^{ab} ±1.7	26.6^{b} ±1.6	10.2^{abc} ±0.5	2.3^{ab} ±0.1	7.5^{ab} ±1.4	8.3^{ab} ±0.8	45.3^{ab} ±2.4	55.9^{ab} ±3.0	172.3^{ab} ±5.4	8.7^{abc} ±0.4	9.1^{abc} ±4.4	7.9^{ab} ±0.6	473.6^{abc} ±26.3
RWA3	75.4^{ab} ±3.0	12.7^{ab} ±0.6	10.3^{ab} ±0.3	3.5^{abc} ±0.3	30.7^{ab} ±1.5	30.6^{b} ±1.4	10.7^{abc} ±0.2	2.7^{ab} ±0.1	8.0^{ab} ±0.3	9.0^{ab} ±0.5	54.0^{ab} ±1.4	67.5^{ab} ±2.7	184.3^{ab} ±7.4	12.4^{abc} ±0.4	11.4^{abc} ±0.4	8.2^{b} ±0.3	531.5^{abc} ±20.8
RWA4	88.6^{ab} ±6.9	12.9^{ab} ±0.2	7.5^{ab} ±0.7	3.2^{abc} ±0.1	29.0^{ab} ±1.3	16.9^{ab} ±1.7	9.5^{c} ±0.4	1.8^{bc} ±0.3	6.9^{ab} ±0.4	7.7^{b} ±0.8	40.5^{ab} ±2.7	54.1^{ab} ±2.1	176.6^{ab} ±7.4	8.7^{abc} ±0.5	10.5^{abc} ±0.9	7.6^{ab} ±0.3	481.8^{bc} ±26.7
IND1	122.1^{b} ±3.4	11.9^{ab} ±0.8	9.3^{ab} ±0.4	4.1^{abc} ±0.8	33.1^{b} ±1.0	30.9^{ab} ±1.7	14.6^{abc} ±0.7	2.7^{abc} ±0.1	9.3^{ab} ±0.4	9.5^{ab}± 0.5	33.8^{ab} ±1.3	96.5^{ab} ±3.4	194.0^{ab} ±7.3	8.2^{abc} ±0.4	13.3^{bc} ±1.4	9.3^{ab} ±0.9	602.7^{bc} ±24.4
IND2	107.4^{ab} ±26.2	10.6^{ab} ±2.6	7.5^{ab} ±1.6	2.9^{abc} ±0.6	26.7^{ab} ±5.0	23.5^{ab} ±6.3	13.1^{bc} ±3.3	2.0^{abc} ±0.5	8.7^{ab} ±1.9	9.5^{ab} ±1.8	32.8^{ab} ±8.3	73.4^{ab} ±15.7	175.2^{ab} ±40.1	7.9^{abc} ±2.3	10.2^{abc} ±3.8	10.0^{ab} ±5.1	521.4^{abc} ±125.3
IND3	116.6^{ab} ±6.2	14.3^{b} ±8.2	9.3^{ab} ±0.2	3.8^{abc} ±0.1	34.3^{ab} ±1.4	19.7^{ab} ±0.6	14.4^{abc} ±0.4	2.4^{abc} ±0.1	10.1^{ab} ±0.5	10.1^{ab} ±0.4	32.0^{ab} ±2.6	95.7^{ab} ±6.2	210.2^{ab} ±13.4	9.3^{abc} ±0.3	13.3^{abc} ±5.6	10.2^{ab} ±0.3	605.5^{abc} ±39.1
IND4	138.8^{ab} ±7.8	8.2^{ab} ±0.3	11.0^{ab} ±0.3	3.9^{abc} ±0.4	42.0^{ab} ±2.3	18.4^{ab} ±01.5	17.2^{abc} ±0.6	2.2^{abc} ±0.2	11.2^{ab} ±0.7	13.2^{ab} ±0.3	32.4^{ab} ±1.4	90.9^{ab} ±4.8	231.0^{ab} ±11.8	8.2^{abc} ±1.4	27.6^{abc} ±1.4	12.3^{ab} ±0.4	668.6^{abc} ±35.5
ETH1	68.4^{b} ±4.3	11.7^{ab} ±1.0	9.7^{ab} ±0.9	4.2^{abc} ±0.9	35.1^{ab} ±0.8	15.8^{ab} ±0.6	11.9± 1.0^{abc}	1.8^{bc} ±0.3	8.6^{ab} ±0.5	10.0^{ab} ±1.3	29.3^{ab} ±2.4	43.2^{b} ±5.0	184.9^{ab} ±18.7	7.6^{abc} ±0.3	14.3^{abc} ±14.3	9.0^{ab} ±0.3	465.7^{bc} ±42.6
ETH2	78.3^{ab} ±5.8	14.6^{b} ±1.3	10.5^{ab} ±1.2	4.1^{abc} ±0.4	43.8^{ab} ±5.6	12.6^{a} ±0.9	12.5± 1.1^{abc}	1.8^{bc} ±0.2	8.5^{ab} ±0.7	11.3^{ab} ±1.0	30.9^{b} ±3.1	53.0^{ab} ±3.4	236.4^{ab} ±10.5	10.8^{abc} ±0.9	23.4^{abc} ±0.9	10.6^{ab} ±0.9	563.3^{abc} ±37.9
ETH3	85.5^{ab} ±6.4	9.2^{ab} ±0.7	11.6^{ab} ±1.1	4.1^{abc} ±0.9	58.2^{ab} ±5.2	15.2^{ab} ±0.5	12.9± 1.1^{abc}	2.0^{abc} ±0.1	8.6^{ab} ±0.6	9.7± 0.9^{ab}	34.3^{ab} ±3.2	65.2^{ab} ±5.5	195.5^{ab} ±14.6	6.4^{c} ±1.1	21.2^{abc} ±1.9	9.8^{ab} ±0.9	549.4^{abc} ±44.6
ETH4	98.3^{ab} ±13.7	8.6^{ab} ±0.8	13.8^{ab} ±2.4	4.9^{ab} ±2.8	50.8^{ab} ±6.4	16.1^{ab} ±2.9	15.8± 1.8^{abc}	2.2^{abc} ±0.2	10.0^{ab} ±2.1	13.2$_{ab}$ ±2.9	37.6^{ab} ±3.2	70.5^{ab} ±7.3	235.4^{ab} ±15.4	10.6^{abc} ±0.9	30.1^{abc} ±1.8	13.5^{ab} ±1.8	631.3^{abc} ±66.3
GUA1	145.7^{ab} ±4.7	7.5^{ab} ±1.1	11.9^{ab} ±0.4	3.4^{abc} ±0.4	44.8^{ab} ±1.4	22.6^{ab} ±0.7	17.6± 3.8^{abc}	2.5^{ab} ±0.1	12.2^{ab} ±0.3	15.0^{ab} ±0.4	42.6^{ab} ±2.0	99.5^{ab} ±3.6	231.5^{ab} ±8.7	14.8^{abc} ±0.7	24.7^{abc} ±0.9	13.9^{ab} ±0.3	710.0^{abc} ±29.4
GUA2	140.2^{ab} ±13.8	7.5^{ab} ±0.6	10.9^{ab} ±0.8	3.4^{abc} ±0.3	47.4^{ab} ±3.9	15.6^{ab} ±1.6	19.0± 1.5^{abc}	2.1^{abc} ±0.2	12.1^{ab} ±0.9	15.0^{ab} ±1.2	40.9^{ab} ±3.3	102.8^{ab} ±9.1	225.4^{ab} ±16.8	14.8^{abc} ±1.4	29.3^{abc} ±2.4	15.3^{ab} ±1.2	701.6^{abc} ±59.1
GUA3	179.6^{a} ±11.8	7.7^{ab} ±1.1	14.3^{b} ±0.9	5.0^{ab} ±1.6	57.0^{ab} ±4.8	21.8^{ab} ±2.7	25.2± 1.9^{a}	3.0^{a} ±0.2	16.7^{b} ±1.7	19.2^{ab} ±1.5	42.7^{ab} ±3.1	117.4^{ab} ±7.5	211.9^{ab} ±13.8	14.6^{abc} ±2.3	28.6^{abc} ±1.9	16.6^{a} ±1.2	781.2^{abc} ±58.3
GUA4	148.3^{ab} ±18.3	8.1^{ab} ±1.2	9.9^{ab} ±0.9	4.2^{abc} ±0.6	39.3^{ab} ±4.7	19.9^{ab} ±1.6	17.3± 2.0^{abc}	2.1^{abc} ±0.3	10.8^{ab} ±1.3	11.9^{a} ±1.5	35.6^{ab} ±4.5	109.1^{ab} ±13.1	193.7^{ab} ±22.0	12.0^{abc} ±1.7	28^{abc} ± 5.1	12.3^{ab} ±1.5	662.4^{abc} ±80.4
HON1	144.1^{ab} ±3.4	10.4^{ab} ±0.4	10.9^{ab} ±0.3	4.5^{abc} ±0.2	45.5^{ab} ±4.8	17.9^{ab} ±0.5	18.0± 0.6^{abc}	2.2^{abc} ±0.1	11.8^{ab} ±0.4	14.6^{ab} ±0.5	37.9^{ab} ±1.0	91.5^{ab} ±9.3	185.0^{ab} ±21.0	11.7^{abc} ±0.7	26.5^{abc} ±0.7	12.6^{ab} ±0.8	645.3^{abc} ±44.8
HON2	143.5^{ab} ±8.0	8.7^{ab} ±0.9	13.0^{ab} ±0.6	5.2^{ab} ±0.5	61.2^{a} ±3.5	20.6^{ab} ±0.8	22.2± 1.0^{ab}	3.0^{a} ±0.1	15.1^{b} ±0.7	17.9^{ab} ±0.7	41.2^{ab} ± 1.8	102.5^{ab} ±3.8	202.1^{ab} ±11.0	12.9^{abc} ±1.3	27.3^{abc} ±1.2	16.0^{a} ±0.6	712.4^{abc} ±36.7
HON3	147.2^{ab} ±12.7	7.6^{ab} ±1.0	11.4^{ab} ±1.0	5.7^{a} ±0.4	51.3^{ab} ±9.6	21.6^{ab} ±2.7	18.7± 1.8^{abc}	2.2^{abc} ±0.2	12.4^{ab} ±0.8	14.7^{ab} ±1.3	35.9^{ab} ± 3.5	99.8^{ab} ±10.4	193.4^{ab} ±21.8	8.0^{abc} ±0.4	25.3^{abc} ±1.3	13.7^{ab} ±1.3	668.8^{abc} ±70.3
HON4	125.3^{ab} ±23.7	6.3^{a} ±1.1	11.8^{ab} ±2.7	5.2^{ab} ±1.3	56.5^{ab} ±4.8	21.3^{ab} ±4.5	18.6± 3.7^{abc}	2.3^{abc} ±0.4	12.4^{ab} ±2.6	14.6^{ab} ±2.8	35.0^{ab} ±6.7	91.7^{ab} ±17.5	196.2^{ab} ±37.9	9.1^{abc} ±1.8	24.0^{abc} ±3.6	12.8^{ab} ±2.2	643.1^{abc} ±117.1

Figure S1. Principal Component Analysis (PCA) score plots for specific compound subsets: (**a**), 3-, 5-, 4-caffeoylquinic acids; (**b**) caffeine and trigonelline; (**c**) free amino acids (ser, thr, tyr, gly, ala, pro, val, met, ile, leu, phe, asp, glu, hys, arg, lys). Each point represents sample replicates and the ellipses indicate 95% confidence intervals around the mean data of each country. The analyses were conducted using R program (R Core Team version 4.1.2, 2022). The *prcomp()* function was used for principal component computation. The *factoextra* package was employed for plot visualization.

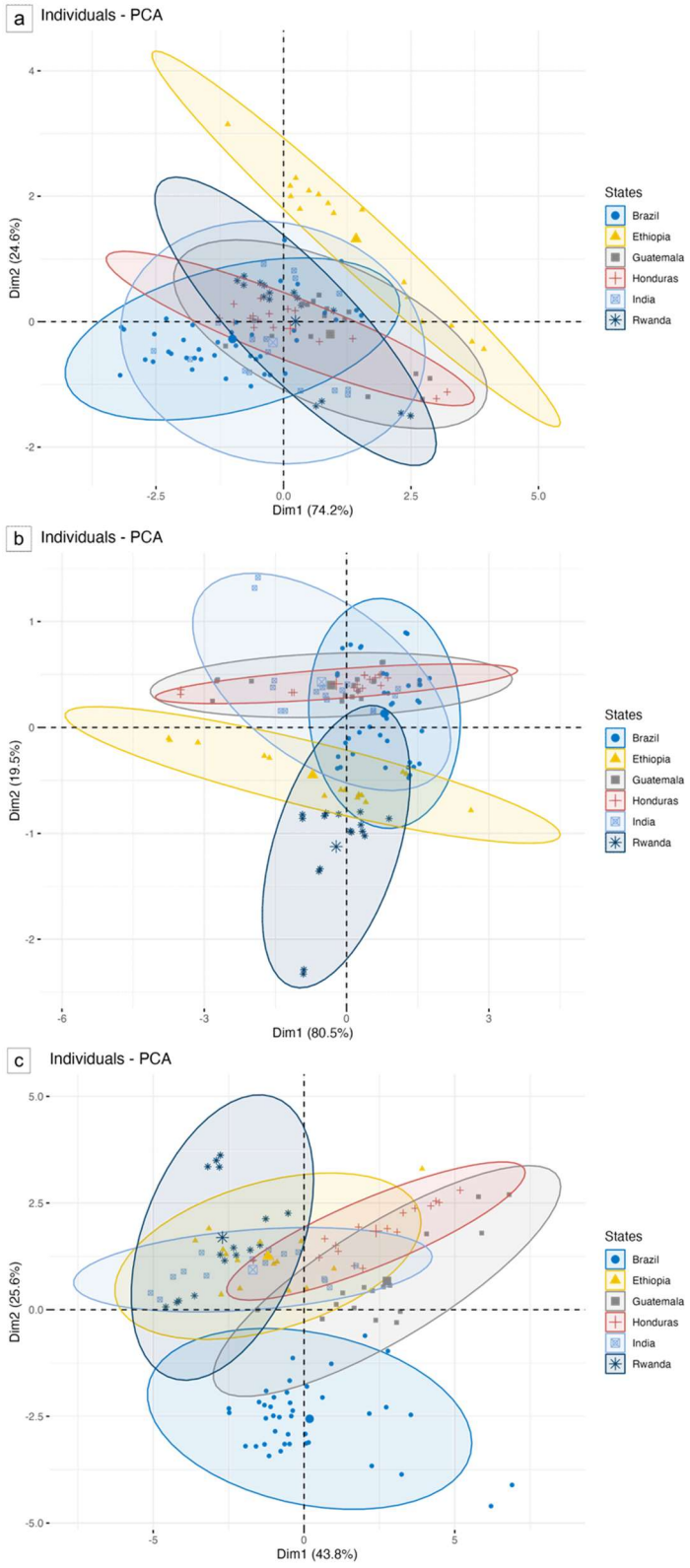

Table S4. Matrix including Pearson correlation coefficients between phytochemical data of green coffee beans from Brazil (BRA1-10) and meteorological parameters of cultivation sites (Table S1). TOTP, total polyphenols; 3-CQA, 5-CQA, 4-CQA: 3-, 5-, 4-caffeoylquinic acids; CAF, caffeine; TRI, trigonelline; SUC, sucrose; POLAR, NON-POLAR, ACIDIC, BASIC: free polar, non-polar, acidic and basic amino acids; PUT, putrescine; SPD, spermidine; SPM, spermine; TRP, tryptamine; Tmax, Tmin, Tmean: maximum, minimum and mean temperatures; day_dur, daylight duration; sun_dur, sunshine duration; precip, rainfall; wnd_spd, average wind speed; wnd_gst, maximum wind gusts; sw_rad, shortwave radiation; evap, evapotranspiration. To indicate the significance of correlations, asterisks were assigned: $p < 0.001$ (highly significant, ***), $p < 0.01$ (**), $p < 0.05$ (*), $p \geq 0.05$ (not significant, no asterisk).

Pearson Correlation Matrix

	TOTP	3-CQA	5-CQA	4-CQA	CAF	TRI	SUC	POLAR	NON-POLAR	ACIDIC	BASIC	PUT	SPD	SPM	TRP	Tmax	Tmin	Tmean	day_dur	sun_dur	precip	wnd_spd	wnd_gst	sw_rad	evap
TOTP	1NA	-0.102	0.006	-0.028	-0.128	-0.076	0.176	0.06	-0.056	0.113	0	0.049	0.117	0.105	-0.068	0.052	-0.08	0.013	-0.166	-0.002	-0.111	-0.018	-0.227	0.089	0.112
3-CQA	-0.102	1NA	0.494**	0.953***	0.321*	0.536***	0.212	0.373*	0.48**	0.144	0.146	0.333*	0.272	0.288	0.47**	0.611***	0.266	0.481**	0.148	-0.079	-0.002	-0.301	-0.388*	0.48**	0.545***
5-CQA	0.006	0.494**	1NA	0.604***	0.835***	0.371*	-0.03	0.439**	0.436**	0.362*	0.374*	-0.208	-0.333*	-0.294	0.286	-0.085	-0.234	-0.161	-0.128	0.014	0.097	0.379*	0.048	0.203	0.174
4-CQA	-0.028	0.953***	0.604***	1NA	0.427**	0.559***	0.211	0.386*	0.495**	0.16	0.147	0.277	0.205	0.209	0.43**	0.473**	0.136	0.336*	0.103	-0.112	0.029	-0.157	-0.329*	0.409**	0.462**
CAF	-0.128	0.321*	0.835***	0.427**	1NA	0.37*	-0.101	0.379*	0.422**	0.34*	0.4*	-0.225	-0.363*	-0.298	0.072	-0.258	-0.318*	-0.318*	-0.191	-0.025	0.246	0.487**	0.263	0.026	-0.03
TRI	-0.076	0.536***	0.371*	0.559***	0.37*	1NA	0.201	-0.074	0.201	-0.34*	-0.266	-0.183	-0.071	-0.072	0.058	0.285	-0.343*	-0.032	-0.325*	-0.404**	-0.073	-0.115	-0.143	0.088	0.14
SUC	0.176	0.212	-0.03	0.211	-0.101	0.201	1NA	-0.07	-0.073	-0.059	-0.152	0.641***	0.672***	0.623***	-0.192	0.491**	-0.124	0.24	0.224	-0.209	-0.743***	-0.221	-0.464**	0.374*	0.375*
POLAR	0.06	0.373*	0.439**	0.386*	0.379*	-0.074	-0.07	1NA	0.874***	0.918***	0.908***	0.258	-0.01	0.047	0.572***	0.112	0.218	0.189	0.175	0.413**	0.035	0.283	0.087	0.462**	0.413**
NON-POLAR	-0.056	0.48**	0.436**	0.495**	0.422**	0.201	-0.073	0.874***	1NA	0.682***	0.76***	0.176	-0.071	-0.083	0.445**	0.249	0.245	0.272	0.094	0.492**	0.117	0.373*	0.125	0.585***	0.526***
ACIDIC	0.113	0.144	0.362*	0.16	0.34*	-0.34*	-0.059	0.918***	0.682***	1NA	0.925***	0.252	-0.034	0.049	0.409**	-0.055	0.205	0.095	0.322*	0.386*	-0.069	0.268	0.083	0.318*	0.26
BASIC	0	0.146	0.374*	0.147	0.4*	-0.266	-0.152	0.908***	0.76***	0.925***	1NA	0.22	-0.062	-0.006	0.381*	-0.077	0.181	0.06	0.138	0.476**	0.107	0.404**	0.258	0.326*	0.242
PUT	0.049	0.333*	-0.208	0.277	-0.225	-0.183	0.641***	0.258	0.176	0.252	0.22	1NA	0.91***	0.88***	0.097	0.567***	0.433**	0.564***	0.456**	0.207	-0.373*	-0.254	-0.366*	0.509***	0.502***
SPD	0.117	0.272	-0.333*	0.205	-0.363*	-0.071	0.672***	-0.01	-0.071	-0.034	-0.062	0.91***	1NA	0.941***	-0.02	0.569***	0.328*	0.506***	0.301	0.028	-0.354*	-0.384*	-0.426**	0.369*	0.393*
SPM	0.105	0.288	-0.294	0.209	-0.298	-0.072	0.623***	0.047	-0.083	0.049	-0.006	0.88***	0.941***	1NA	0.054	0.502***	0.292	0.448**	0.317*	-0.047	-0.352*	-0.427**	-0.417**	0.291	0.324*
TRP	-0.068	0.47**	0.286	0.43**	0.072	0.058	-0.192	0.572***	0.445**	0.409**	0.381*	0.097	-0.02	0.054	1NA	0.187	0.21	0.213	-0.038	0.195	0.171	-0.025	0.024	0.282	0.298
Tmax	0.052	0.611***	-0.085	0.473**	-0.258	0.285	0.491**	0.112	0.249	-0.055	-0.077	0.567***	0.569***	0.502***	0.187	1NA	0.594***	0.903***	0.389*	0.183	-0.446**	-0.552***	-0.743***	0.795***	0.872***
Tmin	-0.08	0.266	-0.234	0.136	-0.318*	-0.343*	-0.124	0.218	0.245	0.205	0.181	0.433**	0.328*	0.292	0.21	0.594***	1NA	0.878***	0.672***	0.634***	-0.026	-0.337*	-0.419**	0.594***	0.632***
Tmean	0.013	0.481**	-0.161	0.336*	-0.318*	-0.032	0.24	0.189	0.272	0.095	0.06	0.564***	0.506***	0.448**	0.213	0.903***	0.878***	1NA	0.604***	0.456**	-0.312*	-0.496**	-0.682***	0.8***	0.864***
day_dur	-0.166	0.148	-0.128	0.103	-0.191	-0.325*	0.224	0.175	0.094	0.322*	0.138	0.456**	0.301	0.317*	-0.038	0.389*	0.672***	0.604***	1NA	0.276	-0.532***	-0.372*	-0.542***	0.391*	0.427**
sun_dur	-0.002	-0.079	0.014	-0.112	-0.025	-0.404**	-0.209	0.413**	0.492**	0.386*	0.476**	0.207	0.028	-0.047	0.195	0.183	0.634***	0.456**	0.276	1NA	0.121	0.464**	0.177	0.629***	0.525***
precip	-0.111	-0.002	0.097	0.029	0.246	-0.073	-0.743***	0.035	0.117	-0.069	0.107	-0.373*	-0.354*	-0.352*	0.171	-0.446**	-0.026	-0.312*	-0.532***	0.121	1NA	0.363*	0.615***	-0.371*	-0.401*
wnd_spd	-0.018	-0.301	0.379*	-0.157	0.487**	-0.115	-0.221	0.283	0.373*	0.268	0.404**	-0.254	-0.384*	-0.427**	-0.025	-0.552***	-0.337*	-0.496**	-0.372*	0.464**	0.363*	1NA	0.758***	-0.002	-0.171
wnd_gst	-0.227	-0.388*	0.048	-0.329*	0.263	-0.143	-0.464**	0.087	0.125	0.083	0.258	-0.366*	-0.426**	-0.417**	0.024	-0.743***	-0.419**	-0.682***	-0.542***	0.177	0.615***	0.758***	1NA	-0.452**	-0.594***
sw_rad	0.089	0.48**	0.203	0.409**	0.026	0.088	0.374*	0.462**	0.585***	0.318*	0.326*	0.509***	0.369*	0.291	0.282	0.795***	0.594***	0.8***	0.391*	0.629***	-0.371*	-0.002	-0.452**	1NA	0.982***
evap	0.112	0.545***	0.174	0.462**	-0.03	0.14	0.375*	0.413**	0.526***	0.26	0.242	0.502***	0.393*	0.324*	0.298	0.872***	0.632***	0.864***	0.427**	0.525***	-0.401*	-0.171	-0.594***	0.982***	1NA

Table S5. Matrix including Pearson correlation coefficients between phytochemical data of green coffee beans from Brazil (BRA1-10) and environmental parameters of cultivation sites (Table S2). TOTP, total polyphenols; 3-CQA, 5-CQA, 4-CQA: 3-, 5-, 4-caffeoylquinic acids; CAF, caffeine; TRI, trigonelline; SUC, sucrose; POLAR, NON-POLAR, ACIDIC, BASIC: free polar, non-polar, acidic and basic amino acids; PUT, putrescine; SPD, spermidine; SPM, spermine; TRP, tryptamine; elev, altitude above sea level; Rh, relative humidity; Cc, cloud cover; sT7, sT28, sT100, sT255: soil temperature at 7, 28, 100, 255 cm depth; sm7, sm28, sm100, sm255: soil moisture at 7, 28, 100, 255 cm depth. To indicate the significance of correlations, asterisks were assigned: $p < 0.001$ (highly significant, ***), $p < 0.01$ (**), $p < 0.05$ (*), $p \geq 0.05$ (not significant, no asterisk).

Pearson Correlation Matrix

	TOTP	3-CQA	5-CQA	4-CQA	CAF	TRI	SUC	POLAR	NON-POLAR	ACIDIC	BASIC	PUT	SPD	SPM	TRP	elev	Rh	Cc	sT7	sT28	sT100	sT255	sm7	sm28	sm100	sm255
TOTP	1NA	-0.102	0.006	-0.028	-0.128	-0.076	0.176	0.06	-0.056	0.113	0	0.049	0.117	0.105	-0.068	0.029	-0.207	-0.303	0.073	0.073	0.085	0.098	-0.083	0.073	0.133	0.181
X3.CQA	-0.102	1NA	0.494**	0.953***	0.321*	0.536***	0.212	0.373*	0.48**	0.144	0.146	0.333*	0.272	0.288	0.47**	-0.162	-0.539***	-0.383*	0.295	0.29	0.293	0.335*	-0.328*	-0.368*	-0.325*	-0.24
X5.CQA	0.006	0.494**	1NA	0.604***	0.835***	0.371*	-0.03	0.439**	0.436**	0.362*	0.374*	-0.208	-0.333*	-0.294	0.286	0.583***	-0.269	-0.364*	-0.191	-0.202	-0.229	-0.276	-0.004	-0.064	-0.023	0.199
X4.CQA	-0.028	0.953***	0.604***	1NA	0.427**	0.559***	0.211	0.386*	0.495**	0.16	0.147	0.277	0.205	0.209	0.43**	-0.018	-0.483**	-0.398*	0.189	0.185	0.188	0.23	-0.159	-0.188	-0.139	-0.11
CAF	-0.128	0.321*	0.835***	0.427**	1NA	0.37*	-0.101	0.379*	0.422**	0.34*	0.4*	-0.225	-0.363*	-0.298	0.072	0.6***	-0.046	-0.197	-0.344*	-0.354*	-0.382*	-0.431**	0.199	0.06	0.042	0.33*
TRI	-0.076	0.536***	0.371*	0.559***	0.37*	1NA	0.201	-0.074	0.201	-0.34*	-0.266	-0.183	-0.071	-0.072	0.058	-0.246	-0.159	-0.584***	-0.198	-0.194	-0.158	-0.007	-0.025	-0.04	-0.004	-0.236
SUC	0.176	0.212	-0.03	0.211	-0.101	0.201	1NA	-0.07	-0.073	-0.059	-0.152	0.641***	0.672***	0.623***	-0.192	-0.094	-0.28	-0.252	0.225	0.217	0.215	0.228	-0.378*	-0.207	-0.101	-0.389*
POLAR	0.06	0.373*	0.439**	0.386*	0.379*	-0.074	-0.07	1NA	0.874***	0.918***	0.908***	0.258	-0.01	0.047	0.572***	0.543***	-0.415**	-0.161	0.113	0.096	0.041	-0.086	-0.445**	-0.56***	-0.534***	-0.179
NON.POLAR	-0.056	0.48**	0.436**	0.495**	0.422**	0.201	-0.073	0.874***	1NA	0.682***	0.76***	0.176	-0.071	-0.083	0.445**	0.45**	-0.523***	-0.356*	0.16	0.147	0.105	0.031	-0.355*	-0.451**	-0.446**	-0.149
ACIDIC	0.113	0.144	0.362*	0.16	0.34*	-0.34*	-0.059	0.918***	0.682***	1NA	0.925***	0.252	-0.034	0.049	0.409**	0.63***	-0.246	0.118	0.105	0.087	0.021	-0.153	-0.376*	-0.466**	-0.431**	-0.132
BASIC	0	0.146	0.374*	0.147	0.4*	-0.266	-0.152	0.908***	0.76***	0.925***	1NA	0.22	-0.062	-0.006	0.381*	0.614***	-0.236	0.019	0.034	0.017	-0.046	-0.205	-0.332*	-0.471**	-0.488**	-0.018
PUT	0.049	0.333*	-0.208	0.277	-0.225	-0.183	0.641***	0.258	0.176	0.252	0.22	1NA	0.91***	0.88***	0.097	-0.136	-0.391*	0.029	0.535***	0.526***	0.508***	0.456**	-0.428**	-0.338*	-0.305	-0.274
SPD	0.117	0.272	-0.333*	0.205	-0.363*	-0.071	0.672***	-0.01	-0.071	-0.034	-0.062	0.91***	1NA	0.941***	-0.02	-0.364*	-0.304	-0.04	0.474**	0.471**	0.477**	0.489**	-0.326*	-0.2	-0.17	-0.224
SPM	0.105	0.288	-0.294	0.209	-0.298	-0.072	0.623***	0.047	-0.083	0.049	-0.006	0.88***	0.941***	1NA	0.054	-0.338*	-0.235	0.036	0.411**	0.407**	0.409**	0.409**	-0.338*	-0.247	-0.212	-0.262
TRP	-0.068	0.47**	0.286	0.43**	0.072	0.058	-0.192	0.572***	0.445**	0.409**	0.381*	0.097	-0.02	0.054	1NA	0.096	-0.317*	-0.233	0.065	0.057	0.035	0.003	-0.433**	-0.567***	-0.565***	-0.248
elev	0.029	-0.162	0.583***	-0.018	0.6***	-0.246	-0.094	0.543***	0.45**	0.63***	0.614***	-0.136	-0.364*	-0.338*	0.096	1NA	-0.044	-0.01	-0.257	-0.272	-0.337*	-0.503***	0.063	-0.004	0.004	0.268
Rh	-0.207	-0.539***	-0.269	-0.483**	-0.046	-0.159	-0.28	-0.415**	-0.523***	-0.246	-0.236	-0.391*	-0.304	-0.235	-0.317*	-0.044	1NA	0.622***	-0.745***	-0.737***	-0.725***	-0.696***	0.651***	0.431**	0.312*	0.21
Cc	-0.303	-0.383*	-0.364*	-0.398*	-0.197	-0.584***	-0.252	-0.161	-0.356*	0.118	0.019	0.029	-0.04	0.036	-0.233	-0.01	0.622***	1NA	-0.027	-0.023	-0.041	-0.131	0.35*	0.262	0.215	-0.008
sT7	0.073	0.295	-0.191	0.189	-0.344*	-0.198	0.225	0.113	0.16	0.105	0.034	0.535***	0.474**	0.411**	0.065	-0.257	-0.745***	-0.027	1NA	1***	0.995***	0.946***	-0.511***	-0.234	-0.122	-0.298
sT28	0.073	0.29	-0.202	0.185	-0.354*	-0.194	0.217	0.096	0.147	0.087	0.017	0.526***	0.471**	0.407**	0.057	-0.272	-0.737***	-0.023	1***	1NA	0.997***	0.953***	-0.496**	-0.216	-0.105	-0.292
sT100	0.085	0.293	-0.229	0.188	-0.382*	-0.158	0.215	0.041	0.105	0.021	-0.046	0.508***	0.477**	0.409**	0.035	-0.337*	-0.725***	-0.041	0.995***	0.997***	1NA	0.974***	-0.465**	-0.177	-0.067	-0.279
sT255	0.098	0.335*	-0.276	0.23	-0.431**	-0.007	0.228	-0.086	0.031	-0.153	-0.205	0.456**	0.489**	0.409**	0.003	-0.503***	-0.696***	-0.131	0.946***	0.953***	0.974***	1NA	-0.402*	-0.109	-0.002	-0.274
sm7	-0.083	-0.328*	-0.004	-0.159	0.199	-0.025	-0.378*	-0.445**	-0.355*	-0.376*	-0.332*	-0.428**	-0.326*	-0.338*	-0.433**	0.063	0.651***	0.35*	-0.511***	-0.496**	-0.465**	-0.402*	1NA	0.913***	0.811***	0.714***
sm28	0.073	-0.368*	-0.064	-0.188	0.06	-0.04	-0.207	-0.56***	-0.451**	-0.466**	-0.471**	-0.338*	-0.2	-0.247	-0.567***	-0.004	0.431**	0.262	-0.234	-0.216	-0.177	-0.109	0.913***	1NA	0.971***	0.664***
sm100	0.133	-0.325*	-0.023	-0.139	0.042	-0.004	-0.101	-0.534***	-0.446**	-0.431**	-0.488**	-0.305	-0.17	-0.212	-0.565***	0.004	0.312*	0.215	-0.122	-0.105	-0.067	-0.002	0.811***	0.971***	1NA	0.546***
sm255	0.181	-0.24	0.199	-0.11	0.33*	-0.236	-0.389*	-0.179	-0.149	-0.132	-0.018	-0.274	-0.224	-0.262	-0.248	0.268	0.21	-0.008	-0.298	-0.292	-0.279	-0.274	0.714***	0.664***	0.546***	1NA