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Data Article

Analytical dataset on volatile compounds of cocoa bean shells from different cultivars and geographical origins

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ABSTRACT

This data article describes the analysis of volatile organic compounds (VOCs) in 44 samples of cocoa bean shells (CBS) obtained from cocoa beans of diverse cultivars and collected in different geographical origins. The volatile compounds were extracted by headspace solid-phase microextraction (HS-SPME) method and then analyzed by gas chromatography coupled to a quadrupole mass spectrometry GC-qMS. The retention times, identification and semi-quantification of 101 VOCs are reported. Data collected on the volatile profile of CBS samples using E-nose analysis are also available. Additional data related to physicochemical characteristics and color analysis for CBS samples are reported. Further interpretation and discussion on these datasets can be found in the related article entitled "Assessment of volatile fingerprint by HS-SPME/GC-qMS and E-nose for the classification of cocoa bean shells using chemometrics" (Barbosa-Pereira et al., 2019).

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Abbreviations: CBS, cocoa bean shell; HS-SPME/GC-qMS, headspace solid-phase micro-extraction coupled with gas chromatography-quadrupole mass spectrometry; VOC, volatile organic compound; E-nose, electronic nose; DVB/CAR/PDMS, divinylbenzene/carboxen/ polydimethylsiloxane; ISTD, internal standard.

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Specifications table

Subject area	Chemistry
More specific subject area	Food Chemistry and Technology
Type of data	Table (Microsoft Excel Worksheet)
How data was acquired	HS-SPME/GC-qMS: Autosampler for HS-SPME (SPME COMBI PAL System, CTC Analytics AG, Zwingen, Switzerland) – Gas chromatography (GC-2010, Shimadzu Corporation, Kyoto, Japan) coupled with quadrupole mass spectrometer (QP-2010 Plus, Shimadzu Corporation, Kyoto, Japan) E-nose: Portable electronic nose system PEN3 (Airsense Analytics GmbH., Schwerin, Germany)
Data format	Raw, analyzed and formatted
Experimental factors	Roasting of cocoa beans to obtain the cocoa bean shell (CBS); physical separation of CBSs; grinding of CBSs into a powder with a 250 μm mesh size
Experimental features	Semi-quantification (μg 5-nonanol Eq. kg^{-1} of CBS) of the identified volatile compounds in CBS powders from different geographical origins and cultivars. E-nose sensor responses for CBS powders from different geographical origins and cultivars.
Data source location	GC-qMS and E-nose datasets were obtained at Food Technology Laboratory at the Department of Agriculture, Forestry and Food Sciences (DISAFA), University of Turin, Grugliasco, Italy *Cocoa beans samples from American countries*: Brazil, Colombia, Dominican Republic, Ecuador, Jamaica, Mexico, Peru, Venezuela. *Cocoa beans samples from African countries*: Cameroon, Congo, Ghana, Ivory Coast, Madagascar, São Tomé, Sierra Leone, Tanzania, Togo, Uganda. The cocoa bean samples were kindly supplied by Silvio Bessone S.r.l., ICAM S.p.A., Ferrero International S.A., Guido Gobino S.r.l., Pastiglie Leone S.r.l., and Venchi S.p.A.
Data accessibility	Data are presented in this article and in a Microsoft Excel Worksheet, which is available as supplementary data.
Related research article	Barbosa-Pereira, L., Rojo-Poveda, O., Ferrocino, I., Giordano, M., & Zeppa, G. (2019). Assessment of volatile fingerprint by HS-SPME/GC-qMS and E-nose for the classification of cocoa bean shells using chemometrics. *Food Research International*, 123, 684–696. https://doi.org/10.1016/j.foodres.2019.05.041

Value of the data

- These are the first data on the contents of VOCs in CBSs from different origins and cultivars determined by HS-SPME/GC-qMS
- The dataset allows the selection of CBSs with specific flavor characteristics according to the food application
- The present data contribute to the chemical characterization and add-value of this cocoa by-product as food ingredient
- The data can be used for reference of volatiles quantification and allow other researchers to extend the statistical analysis
- The datasets from both techniques GC-qMS and E-nose may be useful for developing rapid detection methods for CBS origin and cultivar authentication

1. Data

The dataset collected for 44 CBS samples from different cultivars and geographical origins is presented in four segments of data: A) Samples information regarding the cultivar and geographical origin is labeled in Table 1; B) Physicochemical characterization of CBS samples is described in Table 2; C) The experimental retention index, names and contents of the volatile organic compounds (VOCs) identified among the CBSs determined by HS-SPME/GC-qMS are described indetail in Table S1 (Microsoft Excel Worksheet in supplementary material) and the total contents of each categorie of volatile compounds are summarized in Table 3; and D) The dataset obtained from E-nose sensors for CBS samples is described in Table 4.

The data reported in Table 3, Table S1 and Table 4 were used for the assessment of volatile fingerprint and classification of CBSs from different cultivars and geographical origins using chemometrics reported by Barbosa-Pereira et al. (2019) [1].

2. Experimental design, materials and methods

2.1. Samples – CBS

Cocoa beans (n = 44) from different cultivars and countries across the world (Table 1) were purchased from several local chocolate enterprises. Cocoa bean shells were obtained from the cocoa beans after a standardized roasting process according to the procedure described by Barbosa-Pereira et al. (2019) [1] After separation from the respective cocoa beans, the CBS samples were ground into powders with a 250 μm mesh size and stored under a vacuum at −20 °C prior to further analysis. More detailed information related to the origin and description of samples was also reported by Barbosa-Pereira et al. (2019) (see Section 2.2. CBS Samples and Table 1 in Ref. [1]).

2.2. Physicochemical analysis

2.2.1. Moisture content

The moisture content of the CBS samples was determined by gravimetry, at 110 °C until constant weight, using a Gibertini Eurotherm electronic moisture balance (Gibertini Elettronica, Novate Milanese MI, Italy).

2.2.2. Determination of pH and titratable acidity

Titratable acidity (TA) and pH of the CBS were determined according to AOAC official method described by Nazaruddin, Seng, Hassan, & Said, 2006 [2]. Five grams of CBS powder were homogenised in 100 ml of boiled distilled water by stirring for 30 s and filtered through Whatman no. 4 filter under vacuum. An aliquot (25 mL) was used to measure pH using a pH meter Knick Portamess® 913 (Knick, Berlin, Germany). Then, the same aliquot was titrated with 0.1 mol L^{-1} NaOH standard solution to an endpoint pH of 8.2. All determinations were performed in triplicate. The results of titratable acidity (TA) were expressed as g of acetic acid equivalents/100 g of CBS.

2.2.3. Color analysis – CIELab

The color analysis of CBSs was performed in transmittance mode on a CM-5 spectrophotometer (Konica Minolta, Tokyo, Japan) as reported by Rojo-Poveda et al. (2019) [3]. L^*, a^*, and b^* CIELab parameters were used to measure the color, where L^* is a coefficient of lightness ranging from 0 (black) to 100 (white), a^* indicates the colors red-purple (when positive a^*) and bluish-green (when negative a^*), and b^* denotes the colors yellow (when positive b^*) and blue (negative b^*).

2.3. HS-SPME/GC-qMS analysis

The VOCs from the CBS samples were analysed using a headspace solid phase micro extraction (HS-SPME) coupled with gas chromatography/quadrupole mass spectrometry (GC-qMS) as described by Barbosa-Pereira el al. (2019) [1].

2.3.1. HS-SPME conditions

The extraction of VOCs was performed in a COMBI PAL System Autosampler for SPME (CTC Analytics AG, Zwingen, Switzerland) equipped with an HS-SPME unit. CBS powder (0.1 g) was placed in a 20 mL headspace vial in contact with 2 mL of sodium chloride (40% w/v) and 10 μL of internal standard (IS) 5-nonanol (10 μg mL^{-1}) and equilibrated at 60 °C with stirring at 250 rpm for 10 min. After reach the equilibrium, a SPME fibre coated with divinylbenzene/carboxen/polydimethylsiloxane (DVB/CAR/PDMS) (d_f 50/30 μm, 1 cm) (Supelco, Bellefonte, PA, USA) was exposed to the headspace of the sample for another 30 min with continuous heating and agitation. After extraction, the fibre was desorbed at 260 °C for 2 min in the injection port of the GC system in splitless mode.

2.3.2. GC-qMS instrument and analytical conditions

GC-qMS analyses were performed on a Shimadzu GC-2010 gas chromatograph equipped with a Shimadzu QP-2010 Plus quadrupole mass spectrometer (Shimadzu Corporation, Kyoto, Japan). A

Table 1
Cocoa beans from different cultivars and origin used to obtain the CBSs.

Sample code	Cultivar	Country of origin
BRA	*Trinitario*	Brazil
CAM1	*Forastero*	Cameroon
CAM2	*Trinitario*	Cameroon
COL1	*Forastero*	Colombia
COL2	*Trinitario*	Colombia
CON1	*Forastero*	Congo
CON2	*Forastero*	Congo
DOR1	*Trinitario*	Dominican Republic
DOR2	*Forastero*	Dominican Republic
DOR3	*Trinitario*	Dominican Republic
DOR4	*Trinitario*	Dominican Republic
ECU1	*Forastero*	Ecuador
ECU2	*Trinitario*	Ecuador
ECU3	*Forastero*	Ecuador
ECU4	*Nacional*	Ecuador
ECU5	*Nacional*	Ecuador
ECU6	*Forastero*	Ecuador
ECU7	*Criollo*	Ecuador
GHA	*Forastero*	Ghana
IVC	*Forastero*	Ivory Coast
JAM	*Trinitario*	Jamaica
MAD	*Forastero*	Madagascar
MEX	*Trinitario*	Mexico
PER1	*Forastero*	Peru
PER2	*Trinitario*	Peru
SAT1	*Forastero*	São Tomé
SAT2	*Forastero*	São Tomé
SAT3	*Forastero*	São Tomé
SLE	*Forastero*	Sierra Leone
TAN	*Forastero*	Tanzania
TOG1	*Forastero*	Togo
TOG2	*Forastero*	Togo
UGA1	*Forastero*	Uganda
UGA2	*Forastero*	Uganda
VEN1	*Trinitario*	Venezuela
VEN2	*Trinitario*	Venezuela
VEN3	*Trinitario*	Venezuela
VEN4	*Trinitario*	Venezuela
VEN5	*Criollo*	Venezuela
VEN6	*Trinitario*	Venezuela
VEN7	*Criollo*	Venezuela
VEN8	*Criollo*	Venezuela
VEN9	*Criollo*	Venezuela
VEN10	*Criollo*	Venezuela

30 m × 0.25 mm, 0.25 μm thickness DB-WAXETR capillary column (J&W Scientific Inc., Folsom, CA, USA) was used to separate the VOCs using helium as carrier gas at 1 ml min^{-1}flow rate. The oven time-temperature programme was as follows: initial temperature 40 °C held for 5 min, from 40 °C to 180 °C at the rate of 5 °C min^{-1}, and then to 240 °C at the rate of 10 °C min^{-1}, which was held for 5 min. The MS transfer line was set at 240 °C. The MS fragmentation was performed by electron impact ionization mode (70 eV), and the temperature of the ion source and quadrupole was 240 °C. The data were recorded in full-scan mode in the mass acquisition range of 30–450 *m/z* with 0.30 s scan time. Data were acquired and analysed by using GC-qMS Solution Workstation software (version 4.3) (GC-qMS Solution, Shimadzu Corporation, Kyoto, Japan).

Table 2
Moisture, pH, titratable acidity, and CIELab values of the CBSs powders obtained from cocoa beans from different origins and cultivars.

Sample	Moisture[a]	pH	Titratable Acidity[b]	L*	a*	b*
BRA	6.97 ± 0.38	4.06 ± 0.02	0.69 ± 0.00	40.15 ± 1.19	11.46 ± 0.61	22.98 ± 1.98
CAM1	5.46 ± 0.68	5.32 ± 0.01	0.22 ± 0.00	41.63 ± 0.87	11.96 ± 0.13	21.21 ± 0.45
CAM2	9.15 ± 0.27	6.31 ± 0.02	0.11 ± 0.00	36.23 ± 1.36	12.32 ± 0.15	21.01 ± 0.54
COL1	7.48 ± 0.25	4.83 ± 0.44	0.55 ± 0.24	42.88 ± 2.20	12.21 ± 0.34	21.78 ± 1.31
COL2	7.80 ± 0.75	5.42 ± 0.14	0.43 ± 0.05	36.94 ± 0.91	14.92 ± 1.01	26.24 ± 4.93
CON1	7.52 ± 0.30	4.90 ± 0.01	0.38 ± 0.00	43.72 ± 0.94	12.48 ± 0.17	24.58 ± 0.53
CON2	7.25 ± 0.34	5.20 ± 0.07	0.33 ± 0.03	40.22 ± 0.64	12.70 ± 0.23	23.28 ± 1.73
DOR1	6.44 ± 0.12	5.51 ± 0.03	0.47 ± 0.00	40.86 ± 1.42	14.03 ± 0.69	23.47 ± 0.77
DOR2	7.19 ± 0.48	5.58 ± 0.01	0.31 ± 0.05	45.91 ± 0.78	11.63 ± 0.71	22.16 ± 0.98
DOR3	7.85 ± 0.18	4.61 ± 0.01	0.42 ± 0.00	44.84 ± 0.83	12.15 ± 0.17	23.33 ± 0.47
DOR4	7.47 ± 0.27	5.42 ± 0.03	0.37 ± 0.01	32.66 ± 2.37	16.02 ± 1.18	32.20 ± 2.47
ECU1	8.45 ± 0.37	5.05 ± 0.18	0.32 ± 0.02	41.65 ± 1.21	13.61 ± 1.59	23.94 ± 1.30
ECU2	6.89 ± 0.41	4.97 ± 0.04	0.29 ± 0.01	45.81 ± 1.46	10.95 ± 0.77	21.29 ± 1.87
ECU3	6.74 ± 0.96	5.71 ± 0.01	0.34 ± 0.01	42.22 ± 2.01	14.62 ± 0.79	25.29 ± 0.62
ECU4	6.05 ± 0.14	5.71 ± 0.01	0.18 ± 0.00	35.98 ± 5.83	15.13 ± 0.67	30.74 ± 2.83
ECU5	7.12 ± 0.19	5.68 ± 0.01	0.23 ± 0.00	39.48 ± 9.47	14.19 ± 1.60	28.73 ± 4.87
ECU6	8.13 ± 0.38	4.96 ± 0.03	0.38 ± 0.00	47.01 ± 1.62	12.85 ± 0.71	26.22 ± 2.59
ECU7	6.46 ± 0.35	6.34 ± 0.01	0.18 ± 0.00	35.58 ± 0.93	12.89 ± 0.57	18.09 ± 0.89
GHA	9.18 ± 0.33	5.40 ± 0.08	0.18 ± 0.02	40.44 ± 3.39	12.54 ± 1.19	23.63 ± 1.18
IND	7.01 ± 0.18	5.49 ± 0.01	0.20 ± 0.01	42.33 ± 0.22	11.11 ± 0.35	20.72 ± 0.64
IVC	7.39 ± 1.44	5.46 ± 0.11	0.18 ± 0.01	35.45 ± 4.45	11.38 ± 0.29	19.45 ± 2.38
JAM	7.19 ± 0.35	6.32 ± 0.02	0.27 ± 0.00	35.68 ± 0.68	13.05 ± 0.23	21.06 ± 1.65
MAD	6.97 ± 0.36	4.96 ± 0.01	0.53 ± 0.01	43.12 ± 0.78	14.25 ± 0.06	23.92 ± 0.82
MEX	6.02 ± 1.46	5.24 ± 0.09	0.64 ± 0.03	36.34 ± 1.13	15.19 ± 0.55	23.88 ± 2.12
PER1	7.80 ± 1.03	5.57 ± 0.46	0.36 ± 0.23	36.90 ± 5.93	14.41 ± 2.43	24.72 ± 2.78
PER2	6.37 ± 0.67	5.17 ± 0.27	0.64 ± 0.15	39.61 ± 1.88	14.81 ± 0.52	25.29 ± 3.36
SAT1	6.95 ± 0.88	4.97 ± 0.03	0.40 ± 0.01	39.15 ± 1.70	15.92 ± 0.73	28.96 ± 5.04
SAT2	7.99 ± 0.39	5.32 ± 0.03	0.43 ± 0.01	42.36 ± 1.21	13.29 ± 0.41	24.15 ± 0.84
SAT3	6.87 ± 0.40	5.78 ± 0.05	0.35 ± 0.01	38.79 ± 0.92	13.49 ± 0.31	21.76 ± 1.15
SLE	7.12 ± 0.51	4.14 ± 0.02	0.70 ± 0.00	42.30 ± 2.24	11.03 ± 0.26	23.17 ± 0.61
TAN	6.70 ± 0.71	4.68 ± 0.11	0.42 ± 0.01	42.84 ± 0.80	11.93 ± 0.75	23.84 ± 1.61
TOG1	6.67 ± 0.90	4.33 ± 0.05	0.60 ± 0.01	41.48 ± 2.05	12.10 ± 0.76	24.58 ± 0.70
TOG2	7.68 ± 0.24	4.40 ± 0.19	0.28 ± 0.11	41.31 ± 2.21	12.56 ± 0.49	26.00 ± 1.41
UGA1	9.22 ± 0.79	5.19 ± 0.31	0.23 ± 0.09	43.63 ± 1.18	10.89 ± 0.54	22.25 ± 1.10
UGA2	7.92 ± 0.65	5.42 ± 0.04	0.16 ± 0.01	44.47 ± 1.32	11.01 ± 0.64	22.91 ± 1.11
VEN1	6.01 ± 0.81	4.82 ± 0.10	0.32 ± 0.01	46.28 ± 1.73	11.44 ± 0.65	23.08 ± 1.00
VEN2	6.23 ± 1.01	4.58 ± 0.09	0.48 ± 0.01	36.63 ± 0.44	14.34 ± 0.81	30.32 ± 1.63
VEN3	7.43 ± 0.88	6.02 ± 0.14	0.21 ± 0.02	37.89 ± 0.40	14.71 ± 0.21	26.46 ± 0.77
VEN4	6.30 ± 1.44	5.01 ± 0.31	0.36 ± 0.02	37.81 ± 1.22	13.85 ± 0.39	28.72 ± 1.56
VEN5	7.34 ± 0.80	5.94 ± 0.04	0.22 ± 0.03	35.36 ± 1.06	12.26 ± 0.36	20.83 ± 2.23
VEN6	7.44 ± 1.27	5.26 ± 0.02	0.39 ± 0.02	39.29 ± 2.82	14.29 ± 0.98	26.71 ± 4.44
VEN7	5.46 ± 0.45	5.95 ± 0.01	0.25 ± 0.00	37.97 ± 0.50	13.64 ± 0.28	19.86 ± 0.41
VEN8	5.63 ± 0.11	6.02 ± 0.01	0.27 ± 0.00	36.63 ± 1.02	13.56 ± 0.22	18.48 ± 0.54
VEN9	5.68 ± 0.11	5.49 ± 0.01	0.32 ± 0.00	40.78 ± 0.91	12.95 ± 0.13	21.35 ± 0.26
VEN10	5.74 ± 0.12	4.65 ± 0.02	0.55 ± 0.00	40.83 ± 0.87	12.37 ± 0.22	20.69 ± 0.41

[a] Moisture expressed as % wt/wt.

[b] Titratable acidity (% acetic acid wt/wt) =((N*V*Eqwt)/(wt*1000)) *100.

2.3.3. *Qualitative and quantitative analysis*

The identification of the volatile organic compounds, focused on 101 molecules, was performed by comparing the EI-MS fragmentation pattern of each compound with those available on the National Institute of Standards and Technology (NIST05) mass-spectral library and on our home-based library as reported by Barbosa-Pereira et al. (2019) (see section 2.3.2 and Table 2 in Ref [1]). The semi-quantitative concentrations of the VOCs identified were calculated as the area of the volatile marker component divided by the response factor of the ISTD 5-nonanol and expressed as micrograms of 5-nonanol equivalents per kg of sample (μg 5-nonanol Eq. kg^{-1} of CBS). CBS sample were analysed in triplicate

Table 3

Total contents of the different categories of volatile compounds determined in CBS powders from different geographical origins and cultivars.

Sample	Concentration[a] (μg kg^{-1} of CBS)													
	∑ Aldehydes	∑ Ketones	∑ Sulfur compounds	∑ Esters	∑ Hydrocarbons	∑ Furan derivates	∑ Pyrazines	∑ Alcohols	∑ Pyrroles	∑ Terpenes/ Isoprenoids	∑ Acids	∑ Lactones	∑ Others	∑ Total
BRA	2621.6	411.0	18.6	106.1	324.0	2225.5	405.4	348.5	467.5	349.3	462.9	99.2	25.8	7865.3
CAM1	2151.5	574.5	39.6	83.5	268.3	299.0	746.1	383.6	112.8	77.9	210.5	58.9	20.5	5026.7
CAM2	2353.0	995.8	23.1	90.9	569.1	279.6	499.0	696.8	143.6	68.5	100.4	133.5	60.2	6013.3
COL1	3088.4	638.0	68.3	282.6	119.0	418.5	865.1	682.2	167.3	126.2	1351.6	79.2	52.0	7604.7
COL2	4164.0	705.4	227.7	207.7	348.4	162.1	2240.4	619.5	112.6	111.9	490.5	32.9	116.4	9268.4
CON1	2948.6	763.4	82.4	297.8	205.8	436.2	1140.8	903.4	185.1	136.7	1189.4	87.2	27.8	7849.5
CON2	3773.8	665.6	76.5	199.4	290.5	534.8	1125.7	428.5	157.6	109.6	526.8	68.2	30.7	7907.8
DOR1	5123.9	546.1	577.4	158.1	242.5	193.9	2671.0	477.5	133.7	139.7	818.2	12.6	47.9	11013.4
DOR2	3820.2	605.5	181.4	178.3	244.0	304.0	1902.3	424.9	114.4	166.5	543.3	33.8	36.0	8478.2
DOR3	1894.5	597.4	11.9	359.7	298.2	677.7	505.5	759.2	111.5	270.2	795.3	49.5	18.2	5938.1
DOR4	4544.6	695.8	365.1	188.3	309.8	137.6	3272.7	824.6	214.3	120.6	1807.6	227.3	47.1	12279.3
ECU1	2244.0	564.8	37.6	199.1	261.3	345.0	689.3	514.1	142.5	93.4	871.6	33.3	20.6	5851.0
ECU2	2520.8	624.0	21.0	167.0	376.5	474.5	685.4	869.6	165.1	103.8	442.0	65.5	29.4	6023.6
ECU3	2871.3	431.1	184.3	176.2	137.7	196.6	1070.3	329.9	70.5	87.3	359.1	5.4	21.5	5959.7
ECU4	3883.3	990.1	113.4	312.5	251.7	164.4	1377.1	1908.8	200.6	107.3	1692.7	201.7	32.5	9675.7
ECU5	2772.7	1181.0	50.3	288.7	191.9	129.9	2784.3	1068.1	86.6	134.2	1255.1	30.8	33.8	9287.9
ECU6	2596.9	746.0	44.0	582.2	248.7	117.6	2112.0	779.9	92.1	52.1	1012.7	49.6	16.2	8018.6
ECU7	4405.9	1362.2	103.4	524.9	10.9	116.2	1916.0	2310.2	62.5	228.0	2124.0	4.4	37.6	11244.4
GHA	2020.7	832.8	29.3	112.2	413.7	233.7	940.0	667.3	116.2	221.8	1159.9	452.8	28.4	6909.8
IVC	2542.1	1076.1	31.3	73.4	1108.5	404.1	1263.5	876.3	235.3	124.1	1154.3	565.7	29.5	8956.4
JAM	4244.8	818.7	159.1	148.1	176.4	135.8	1697.8	1000.3	91.1	186.0	327.2	18.4	151.1	8503.0
MAD	4398.3	628.4	371.2	478.6	292.4	166.0	5140.7	277.1	198.8	66.5	1895.2	20.3	82.8	14087.7
MEX	4425.8	797.5	280.1	586.7	584.1	157.8	4353.5	319.2	79.3	48.8	1299.0	14.2	88.8	13034.6
PER1	4112.6	1044.0	197.8	1036.6	128.7	193.4	3031.1	1309.3	180.8	87.8	2155.1	214.8	34.1	13726.0
PER2	4951.5	979.8	281.1	830.8	319.8	227.0	4515.2	1084.9	183.6	74.4	1257.7	241.2	41.4	14988.4
SAT1	3163.1	343.8	150.7	127.9	200.2	213.0	1009.9	135.8	175.5	76.1	508.2	6.4	77.5	6188.1
SAT2	3669.2	514.0	158.6	312.9	145.7	153.7	1851.9	384.0	61.1	70.6	747.8	12.7	87.9	8170.2
SAT3	5122.6	846.7	284.3	195.8	370.9	174.3	2801.4	364.2	71.0	65.6	436.0	14.1	116.1	10863.0

SLE	1698.4	461.5	26.3	236.9	349.1	2004.0	198.3	474.0	157.0	133.7	1148.1	74.2	14.9	6976.5
TAN	3335.2	642.2	97.4	868.4	391.6	920.7	1131.5	934.5	277.2	154.8	1494.7	100.1	32.5	10380.7
TOG1	1712.2	291.7	29.3	316.6	318.2	2081.0	309.4	428.6	203.9	222.4	1404.0	367.8	16.9	7701.9
TOG2	1444.8	375.3	24.7	434.8	218.8	1918.9	272.5	439.5	182.0	183.7	1121.5	572.7	20.8	7210.2
UGA1	2666.4	747.9	33.6	385.6	635.9	399.8	1359.1	1032.2	161.7	119.4	1404.7	32.7	27.9	9007.0
UGA2	2849.8	826.1	28.5	201.8	227.7	354.2	792.6	880.5	142.4	114.8	421.1	13.5	26.5	6879.5
VEN1	1731.1	373.8	40.0	255.6	162.9	486.3	1176.0	266.6	112.0	65.7	832.5	25.4	20.8	5548.7
VEN2	2657.9	275.9	166.9	259.4	282.6	449.3	838.7	296.3	267.9	92.7	826.6	46.8	18.1	6479.0
VEN3	2621.5	421.0	43.3	146.1	142.8	101.1	665.2	302.6	48.7	43.4	338.6	6.7	29.6	4910.2
VEN4	1690.7	419.0	58.9	205.9	161.5	330.0	1138.0	514.6	118.4	124.0	503.6	11.8	16.5	5292.9
VEN5	4536.5	1115.8	115.4	308.1	536.7	294.3	3167.8	1046.2	114.0	174.5	329.7	49.9	55.3	11844.2
VEN6	2309.5	467.9	87.2	230.6	89.4	98.8	1702.0	492.5	67.3	102.3	484.1	11.2	20.5	6163.3
VEN7	4260.7	726.7	186.3	356.7	20.3	153.2	3918.3	1355.8	119.0	91.8	1654.9	10.3	40.6	12894.7
VEN8	4843.8	715.6	146.2	604.7	16.7	112.1	3731.4	891.2	84.6	47.0	1354.1	3.3	52.6	12603.4
VEN9	2977.5	593.9	132.5	760.0	21.0	487.9	5285.7	895.2	101.9	66.7	2100.8	29.2	26.8	13479.0

[a] The total amounts of each category of volatile compounds semi-quantified as 5-nonanol equivalents (μg $kg^{-1}$of CBS). Data are presented as the sum ($\sum$) of the means of the different molecules ($n = 6$) for each category.

Table 4
Average of E-nose sensor responses G/G0 (area under the curve; G and G0 stand for the conductance of the MOS connected with the sample and clean gas, respectively), expressed as resistivity (Ohm), for CBS powders from different geographical origins and cultivars.

Sample	E-nose Sensors									
	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
BRA	21.67 ± 2.71	7066.91 ± 1413.30	25.19 ± 3.39	92.05 ± 1.00	28.58 ± 4.00	1640.40 ± 280.07	2553.81 ± 476.52	662.21 ± 154.87	1335.16 ± 217.20	101.07 ± 2.77
CAM1	24.32 ± 0.54	6471.08 ± 88.20	28.25 ± 0.42	89.67 ± 0.46	31.76 ± 0.37	1319.07 ± 16.36	1820.72 ± 68.53	481.43 ± 3.10	968.75 ± 47.29	98.44 ± 0.79
CAM2	19.44 ± 0.95	7476.53 ± 298.55	22.38 ± 0.72	93.80 ± 0.77	25.06 ± 0.59	1845.28 ± 72.22	2545.55 ± 249.02	764.69 ± 127.89	1291.37 ± 135.09	104.36 ± 0.74
COL1	21.82 ± 3.63	7363.27 ± 2195.01	25.39 ± 4.30	89.32 ± 0.98	28.52 ± 5.11	1586.49 ± 310.26	2746.75 ± 698.52	642.11 ± 166.67	1446.12 ± 309.88	97.98 ± 1.68
COL2	21.56 ± 2.58	7984.51 ± 1821.07	25.27 ± 3.04	90.98 ± 0.76	28.77 ± 3.38	1671.50 ± 269.72	2684.13 ± 479.19	634.39 ± 98.26	1423.07 ± 177.29	105.14 ± 3.46
CON1	19.13 ± 0.19	9443.36 ± 142.67	21.85 ± 0.17	89.55 ± 0.15	24.02 ± 0.12	1783.55 ± 5.68	3202.33 ± 74.91	698.94 ± 4.27	1655.81 ± 39.61	95.44 ± 0.29
CON2	18.68 ± 0.32	7708.13 ± 391.41	22.23 ± 0.74	92.90 ± 3.38	24.37 ± 0.96	2028.79 ± 338.99	2747.88 ± 198.67	788.78 ± 110.15	1375.48 ± 99.26	102.99 ± 8.56
DOR1	16.56 ± 2.26	11829.35 ± 2456.92	19.06 ± 2.66	92.44 ± 1.10	20.69 ± 3.62	2214.38 ± 211.63	3502.73 ± 442.91	924.91 ± 174.36	1687.11 ± 144.54	104.98 ± 2.07
DOR2	17.31 ± 2.33	10941.95 ± 2082.60	19.88 ± 2.78	93.02 ± 1.15	21.94 ± 3.82	2103.86 ± 257.59	3287.51 ± 478.67	892.91 ± 218.62	1601.99 ± 193.46	107.83 ± 1.92
DOR3	18.92 ± 0.09	8003.06 ± 28.39	21.80 ± 0.10	89.65 ± 0.19	23.68 ± 0.12	1790.95 ± 7.24	2610.91 ± 9.35	689.22 ± 4.38	1352.05 ± 12.65	93.67 ± 0.46
DOR4	18.70 ± 0.30	9687.95 ± 151.09	21.39 ± 0.28	89.04 ± 0.17	22.98 ± 0.32	1688.86 ± 15.24	2735.65 ± 138.98	723.46 ± 39.29	1474.48 ± 93.49	94.81 ± 0.42
ECU1	19.25 ± 0.66	8914.25 ± 235.90	22.29 ± 0.66	92.37 ± 0.95	25.19 ± 1.02	1896.56 ± 51.70	2971.79 ± 263.95	770.30 ± 119.21	1484.32 ± 125.55	108.43 ± 4.02
ECU2	21.48 ± 2.38	7361.28 ± 1716.64	25.02 ± 2.93	92.16 ± 1.60	28.38 ± 3.22	1627.18 ± 224.41	2601.30 ± 687.30	674.54 ± 171.02	1328.67 ± 327.70	104.41 ± 5.57
ECU3	19.20 ± 0.17	9074.20 ± 990.59	21.98 ± 0.27	92.43 ± 0.32	24.84 ± 0.49	1861.96 ± 33.03	3179.05 ± 173.82	745.17 ± 86.90	1625.42 ± 92.66	102.99 ± 0.65
ECU4	19.31 ± 0.35	9609.19 ± 149.24	21.66 ± 0.36	90.40 ± 0.06	22.98 ± 0.35	1601.76 ± 9.61	2313.98 ± 33.13	682.87 ± 3.95	1278.82 ± 26.81	93.15 ± 0.33
ECU5	19.67 ± 0.24	9341.42 ± 548.90	22.11 ± 0.22	89.85 ± 0.48	23.72 ± 0.18	1560.93 ± 21.72	2513.20 ± 60.96	699.18 ± 40.12	1434.21 ± 79.14	93.54 ± 0.42
ECU6	21.94 ± 5.00	8693.98 ± 1899.47	25.73 ± 5.29	90.12 ± 1.78	29.65 ± 6.17	1681.91 ± 457.92	3156.50 ± 804.72	673.04 ± 249.26	1631.93 ± 327.72	105.49 ± 4.77
ECU7	55.71 ± 3.48	1514.15 ± 270.69	57.24 ± 2.92	89.38 ± 0.15	55.23 ± 2.88	574.67 ± 47.85	1646.82 ± 105.21	242.67 ± 12.20	620.72 ± 11.39	90.93 ± 0.14
GHA	18.93 ± 0.36	8274.79 ± 644.82	21.89 ± 0.35	91.25 ± 0.60	24.46 ± 0.64	1890.14 ± 35.03	2797.61 ± 134.52	750.80 ± 85.80	1437.51 ± 99.64	102.10 ± 1.30
IND	25.30 ± 0.38	4874.39 ± 190.58	29.38 ± 0.17	89.00 ± 0.18	33.11 ± 0.16	1267.68 ± 21.82	1860.06 ± 176.65	490.07 ± 58.38	1011.30 ± 94.65	95.67 ± 1.32
IVC	17.69 ± 1.56	10417.91 ± 1928.62	20.13 ± 2.10	92.39 ± 1.03	21.78 ± 3.07	1984.29 ± 149.63	3021.47 ± 257.57	806.68 ± 112.71	1463.84 ± 52.88	103.01 ± 1.00
JAM	21.28 ± 2.66	8305.77 ± 890.69	24.61 ± 3.32	90.71 ± 1.13	27.63 ± 3.90	1657.18 ± 277.15	2551.96 ± 390.84	625.90 ± 106.84	1318.46 ± 165.16	101.70 ± 1.82
MAD	13.60 ± 0.84	14944.91 ± 211.24	15.86 ± 0.72	96.09 ± 2.33	16.73 ± 0.61	2685.12 ± 243.43	4464.91 ± 292.33	1188.71 ± 126.59	2072.15 ± 209.74	110.69 ± 2.45
MEX	21.34 ± 2.60	8754.26 ± 1136.11	25.38 ± 2.72	88.62 ± 1.49	29.06 ± 2.95	1768.73 ± 244.89	3489.61 ± 318.57	711.20 ± 127.84	1833.66 ± 136.42	103.28 ± 4.36
PER1	18.77 ± 0.74	9253.63 ± 1623.86	21.81 ± 0.70	90.92 ± 1.92	24.29 ± 0.89	1880.98 ± 57.96	3181.73 ± 472.45	747.68 ± 78.93	1615.90 ± 224.08	99.39 ± 1.56
PER1	20.64 ± 1.96	7902.55 ± 518.35	24.35 ± 2.86	89.04 ± 1.60	27.48 ± 4.08	1660.89 ± 130.46	3012.20 ± 370.89	648.06 ± 62.76	1603.76 ± 215.80	97.88 ± 2.80
SAT1	19.27 ± 0.64	10015.39 ± 226.20	22.80 ± 0.67	92.18 ± 0.53	25.83 ± 0.67	1935.85 ± 74.23	3239.05 ± 294.67	739.29 ± 96.39	1618.85 ± 135.67	107.17 ± 4.15
SAT2	17.86 ± 0.31	8806.54 ± 316.45	21.02 ± 0.21	89.04 ± 0.21	23.17 ± 0.18	1891.34 ± 58.48	3252.55 ± 346.96	756.60 ± 81.73	1685.34 ± 174.02	95.69 ± 0.61
SAT3	21.71 ± 3.10	7747.48 ± 2194.60	25.27 ± 3.67	90.38 ± 2.17	28.59 ± 3.98	1629.68 ± 315.13	2614.14 ± 612.93	616.95 ± 146.59	1367.30 ± 262.75	104.55 ± 7.31

SLE	19.64 ± 0.41	8540.30 ± 429.64	22.36 ± 0.36	89.93 ± 0.12	24.78 ± 0.41	1710.06 ± 9.25	3138.62 ± 263.82	725.62 ± 94.95	1671.07 ± 158.77	93.93 ± 0.38
TAN	21.13 ± 3.55	7226.23 ± 1776.82	24.68 ± 4.17	89.28 ± 0.24	27.58 ± 5.02	1579.49 ± 237.78	2577.40 ± 619.43	631.37 ± 130.42	1381.09 ± 342.89	96.31 ± 0.57
TOG1	18.42 ± 0.25	9096.71 ± 226.91	21.47 ± 0.19	90.55 ± 0.32	23.92 ± 0.24	1949.76 ± 22.78	3190.16 ± 163.26	759.22 ± 68.24	1616.83 ± 85.04	100.49 ± 0.46
TOG2	18.04 ± 0.38	9144.50 ± 648.34	21.21 ± 0.40	90.01 ± 0.38	23.57 ± 0.57	1913.86 ± 42.76	3269.53 ± 256.43	754.92 ± 72.44	1690.98 ± 143.82	96.44 ± 0.62
UGA1	18.67 ± 0.59	8883.83 ± 605.31	21.60 ± 0.53	90.86 ± 0.23	23.98 ± 0.65	1910.96 ± 51.92	2972.22 ± 200.97	750.44 ± 74.80	1489.62 ± 96.00	100.91 ± 0.10
UGA2	18.81 ± 0.40	7748.48 ± 512.48	21.64 ± 0.39	91.36 ± 0.84	23.57 ± 0.61	1741.24 ± 33.06	2514.97 ± 110.86	696.66 ± 56.16	1331.73 ± 92.41	94.93 ± 0.70
VEN1	18.49 ± 0.29	9322.05 ± 407.03	21.54 ± 0.40	92.34 ± 0.21	24.50 ± 0.71	2058.22 ± 45.29	3233.22 ± 257.10	808.82 ± 99.68	1629.05 ± 148.69	105.62 ± 0.72
VEN2	18.76 ± 1.04	12279.52 ± 340.46	22.22 ± 0.95	91.30 ± 0.68	25.54 ± 1.24	1943.82 ± 153.76	3815.66 ± 368.50	758.72 ± 112.61	1886.10 ± 163.19	107.07 ± 0.89
VEN3	19.30 ± 0.45	8369.49 ± 276.09	22.62 ± 0.37	91.98 ± 0.41	25.87 ± 0.43	1915.56 ± 59.49	2746.92 ± 218.96	754.34 ± 106.30	1400.97 ± 108.24	108.49 ± 0.97
VEN4	18.93 ± 0.36	9151.03 ± 178.30	22.15 ± 0.43	92.52 ± 0.27	25.34 ± 0.62	1964.55 ± 25.49	3058.53 ± 264.09	782.13 ± 116.28	1526.11 ± 132.82	109.71 ± 0.38
VEN5	21.03 ± 2.71	7408.06 ± 1578.26	24.48 ± 3.39	90.95 ± 1.43	27.63 ± 3.90	1710.84 ± 300.91	2658.24 ± 496.27	689.56 ± 168.85	1381.97 ± 217.53	101.56 ± 2.34
VEN6	23.26 ± 4.43	8058.15 ± 1845.73	26.77 ± 4.80	91.10 ± 1.07	30.30 ± 5.32	1561.91 ± 395.52	2547.69 ± 615.04	610.96 ± 145.44	1340.39 ± 228.82	105.14 ± 5.51
VEN7	57.71 ± 1.33	4055.88 ± 116.29	58.42 ± 1.25	88.99 ± 0.31	55.57 ± 1.39	582.72 ± 25.23	1746.05 ± 47.27	216.82 ± 7.81	727.72 ± 21.74	90.95 ± 0.04
VEN8	56.64 ± 2.34	2684.49 ± 119.20	57.39 ± 2.30	88.57 ± 0.06	54.95 ± 2.17	583.64 ± 40.85	1657.69 ± 78.70	226.60 ± 10.67	654.89 ± 19.80	91.00 ± 0.24
VEN9	55.58 ± 1.67	4277.87 ± 253.80	57.58 ± 1.79	88.54 ± 0.33	56.97 ± 4.62	577.43 ± 77.01	1997.31 ± 324.73	227.75 ± 14.88	756.53 ± 205.78	91.00 ± 0.09
VEN10	57.01 ± 0.86	3909.49 ± 255.19	57.15 ± 0.80	89.07 ± 0.17	54.64 ± 0.84	608.08 ± 16.61	1938.36 ± 36.70	226.49 ± 3.61	798.33 ± 19.07	91.35 ± 0.16

Data are presented as the mean (n = 6) ± standard deviation.

and the data of the sum of each class of compound are shown in Table 3, while the data for a single molecule are detailed in Table S1 (Microsoft Excel Worksheet in supplementary material).

2.4. E-nose analysis

E-nose data were recorded using a portable electronic nose system PEN3 (Airsense Analytics GmbH., Germany). The system consists of a sampling unit and the gas detection system composed of 10 Metal Oxide Semiconductor (MOS) sensors, which are differentially sensitive to each characteristic volatile compound or group of compounds [4]. The analyses were performed as described by Barbosa-Pereira et al. (2019) [1]. Briefly, CBS powders (2 g) were placed in a 20-mL glass vial and incubated at 30 °C for 30 min to reach the headspace equilibrium. After, the gas headspace was injected into the E-nose for 90 s at a constant flow rate of 400 mL min^{-1}. The sensor signals were recorded at each second by the pattern recognition software (WinMuster, v.1.6, Airsense Analytics GmbH., Germany). Each CBS sample was independently analysed in triplicates and the average of sensor responses (area under the curve) is shown in Table 4.

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Authors contributions

Conceptualization, L.B.P, G.Z; Validation, M.G, G.Z; Investigation, O.R.P, L.B.P, I.F; Writing-original Draft Preparation, L.B.P; Review and Editing, O.R.P, I.F, M.G, G.Z; Supervision, L.B.P., M.G, G.Z; Project Administration, L.B.P, G.Z.

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Conflict of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2019.104268.

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