

Supplementary Table S1. Relative percentage of volatile compounds (%) detected at the beginning and the end of cocoa beans fermentation identified by HS-SPME-GC-MS analysis produced from two different fermentation methods (Box and Heap) under different conditions (inoculated and non-inoculated). Values are expressed as mean \pm SD from triplicate determinations

		BOX									
		At the beginning (%)			At the end (%)						
Group	Compounds	S	ST	C	S	ST	C	S	ST	C	
ESTERS	Ethyl acetate	7.73 \pm 1.37	18.45 \pm 5.58	5.25 \pm 0.45	4.71 \pm 3.37	2.54 \pm 0.65	3.58 \pm 1.13				
	Ethyl octanoate	0.03 \pm 0.00	0.00 \pm 0.00	0.05 \pm 0.01	0.33 \pm 0.06	0.34 \pm 0.06	0.25 \pm 0.07				
	Ethyl caproate	0.21 \pm 0.03	0.18 \pm 0.03	0.11 \pm 0.04	0.45 \pm 0.11	0.43 \pm 0.08	0.29 \pm 0.08				
	Methyl octanoate	0.11 \pm 0.00	0.11 \pm 0.01	0.10 \pm 0.03	0.00 \pm 0.00	0.00 \pm 0.00	0.00 \pm 0.00				
	Ethyl benzoate	0.00 \pm 0.00	0.01 \pm 0.00	0.01 \pm 0.00	0.13 \pm 0.02	0.13 \pm 0.04	0.11 \pm 0.05				
	Ethyl- α -toluate	0.00 \pm 0.00	0.00 \pm 0.00	0.00 \pm 0.00	0.48 \pm 0.07	0.62 \pm 0.19	0.43 \pm 0.10				
	2-Pentanol, acetate	1.42 \pm 0.56	2.55 \pm 0.26	1.75 \pm 0.37	3.93 \pm 0.41	2.45 \pm 0.91	3.85 \pm 0.93				
	Isopentyl alcohol, acetate	1.09 \pm 0.24	0.01 \pm 0.00	1.19 \pm 0.13	4.69 \pm 0.83	3.68 \pm 0.64	6.72 \pm 2.21				
	Hexyl acetate	0.01 \pm 0.01	0.01 \pm 0.00	0.00 \pm 0.00	0.03 \pm 0.01	0.00 \pm 0.00	0.00 \pm 0.00				
	2,3-butanediol diacetate	0.20 \pm 0.10	0.30 \pm 0.08	0.14 \pm 0.03	0.03 \pm 0.01	0.05 \pm 0.01	0.06 \pm 0.02				
	1,2-propanediol, diacetate	6.61 \pm 1.04	8.11 \pm 1.55	4.78 \pm 0.24	1.21 \pm 0.45	2.53 \pm 0.67	1.54 \pm 0.94				
	β -phenylethyl acetate	0.03 \pm 0.01	0.12 \pm 0.04	0.05 \pm 0.01	1.20 \pm 0.20	1.69 \pm 0.57	2.22 \pm 1.60				
	Isoamyl benzoate	0.16 \pm 0.10	0.14 \pm 0.03	0.28 \pm 0.04	0.10 \pm 0.05	0.02 \pm 0.01	0.03 \pm 0.01				
	n-Hexyl butanoate	0.00 \pm 0.00	0.05 \pm 0.02	0.00 \pm 0.00	0.00 \pm 0.00	0.00 \pm 0.00	0.00 \pm 0.00				
		Total ester	17.61 \pm 2.55	30.05 \pm 5.18	13.72 \pm 1.79	17.29 \pm 1.79	14.48 \pm 1.27	19.08 \pm 2.05			
	ALDEHYDES	Hexanal	1.93 \pm 0.02	2.41 \pm 0.12	0.48 \pm 0.03	0.15 \pm 0.04	0.17 \pm 0.04	0.12 \pm 0.03			
		Benzaldehyde	0.41 \pm 0.14	0.55 \pm 0.13	0.17 \pm 0.02	0.63 \pm 0.11	0.73 \pm 0.43	0.78 \pm 0.11			
Benzeneacetaldehyde		5.57 \pm 2.36	6.09 \pm 0.90	2.64 \pm 0.14	3.49 \pm 0.45	5.81 \pm 2.54	4.83 \pm 0.63				
α -ethylidene-benzeneacetaldehyde		0.00 \pm 0.00	0.00 \pm 0.00	0.00 \pm 0.00	0.05 \pm 0.01	0.03 \pm 0.01	0.03 \pm 0.03				
<i>trans</i> -2-Undecenal		0.00 \pm 0.00	0.00 \pm 0.00	0.00 \pm 0.00	0.00 \pm 0.00	0.02 \pm 0.01	0.01 \pm 0.00				
Nonanal		0.14 \pm 0.05	0.15 \pm 0.02	0.28 \pm 0.11	0.09 \pm 0.02	0.14 \pm 0.02	0.17 \pm 0.06				
2-methyl-butanal		0.96 \pm 0.09	1.24 \pm 0.15	0.45 \pm 0.01	0.49 \pm 0.15	0.63 \pm 0.35	0.31 \pm 0.11				
		Total aldehyde	9.00 \pm 2.01	10.44 \pm 2.21	4.03 \pm 0.93	4.91 \pm 1.25	7.54 \pm 2.11	6.27 \pm 1.75			
ALCOHOLS	2-Pentanol	47.70 \pm 4.93	25.70 \pm 5.70	52.51 \pm 1.43	3.34 \pm 1.10	2.41 \pm 1.28	4.55 \pm 0.28				
	2-Heptanol	0.39 \pm 0.13	0.54 \pm 0.05	0.34 \pm 0.05	8.97 \pm 3.01	7.77 \pm 1.85	9.10 \pm 2.05				
	(<i>Z</i>)-3-Hexen-1-ol	0.04 \pm 0.01	0.04 \pm 0.01	0.04 \pm 0.01	0.02 \pm 0.00	0.02 \pm 0.00	0.01 \pm 0.01				
	1-Hexanol	0.30 \pm 0.03	0.43 \pm 0.12	0.21 \pm 0.06	0.15 \pm 0.03	0.18 \pm 0.03	0.14 \pm 0.08				
	1-Octen-3-ol	0.04 \pm 0.04	0.05 \pm 0.03	0.00 \pm 0.00	0.00 \pm 0.00	0.00 \pm 0.00	0.19 \pm 0.06				
	1-Heptanol	0.04 \pm 0.01	0.05 \pm 0.01	0.05 \pm 0.01	0.00 \pm 0.00	0.00 \pm 0.00	0.00 \pm 0.00				
	2-ethyl-1-hexanol	0.31 \pm 0.05	0.49 \pm 0.16	0.22 \pm 0.02	0.14 \pm 0.02	0.23 \pm 0.03	0.19 \pm 0.01				
	3-methyl-1-butanol	1.11 \pm 0.05	1.30 \pm 0.08	0.87 \pm 0.21	1.31 \pm 0.57	1.04 \pm 0.29	1.66 \pm 0.35				
		2-Hexanol	0.42 \pm 0.03	0.79 \pm 0.09	0.73 \pm 0.07	0.16 \pm 0.02	0.13 \pm 0.06	0.18 \pm 0.04			

	1-Pentanol	0.43 ± 0.15	0.83 ± 0.08	0.08 ± 0.02	0.10 ± 0.02	0.07 ± 0.03	0.11 ± 0.05
	1-Octanol	0.07 ± 0.01	0.06 ± 0.01	0.10 ± 0.03	0.13 ± 0.05	0.10 ± 0.02	0.11 ± 0.01
	Benzyl alcohol	0.04 ± 0.00	0.05 ± 0.01	0.03 ± 0.01	0.03 ± 0.01	0.06 ± 0.02	0.04 ± 0.00
	Phenylethyl alcohol	0.44 ± 0.05	0.55 ± 0.13	0.25 ± 0.04	3.67 ± 0.47	6.57 ± 2.72	8.42 ± 1.69
	1-Heptadecanol	0.05 ± 0.02	0.03 ± 0.01	0.05 ± 0.02	0.10 ± 0.01	0.11 ± 0.02	0.07 ± 0.02
	Isobutanol	1.54 ± 0.62	0.21 ± 0.07	0.07 ± 0.02	0.07 ± 0.02	0.07 ± 0.02	0.12 ± 0.04
	1-Decanol	0.01 ± 0.00	0.01 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.01 ± 0.00	0.00 ± 0.00
	α -Methylbenzyl alcohol	0.32 ± 0.06	0.29 ± 0.10	0.65 ± 0.05	0.22 ± 0.02	0.33 ± 0.09	0.24 ± 0.05
	1-Dodecanol	0.05 ± 0.02	0.17 ± 0.04	0.23 ± 0.03	0.07 ± 0.02	0.24 ± 0.15	0.07 ± 0.02
	Ethanol	2.17 ± 0.59	3.89 ± 0.58	2.47 ± 0.08	1.59 ± 0.25	1.25 ± 0.29	1.32 ± 0.25
	Decanal	0.03 ± 0.01	0.05 ± 0.01	0.09 ± 0.02	0.02 ± 0.01	0.04 ± 0.02	0.03 ± 0.01
	Total alcohol	55.49 ± 10.59	35.52 ± 5.70	58.99 ± 11.68	20.08 ± 2.17	20.62 ± 2.19	26.57 ± 2.75
	2-Pentanone	2.01 ± 1.08	1.55 ± 0.35	7.49 ± 0.63	1.27 ± 0.43	2.05 ± 0.89	1.74 ± 0.13
	2-Heptanone	0.66 ± 0.05	0.69 ± 0.06	1.28 ± 0.06	1.76 ± 0.42	0.88 ± 1.15	1.57 ± 0.49
	Acetoin	0.39 ± 0.11	0.47 ± 0.02	0.29 ± 0.03	4.42 ± 1.09	5.98 ± 1.39	4.52 ± 0.77
	2-Nonanol	0.05 ± 0.01	0.06 ± 0.01	0.04 ± 0.00	0.78 ± 0.20	0.34 ± 0.07	0.39 ± 0.04
	2-Undecanone	0.04 ± 0.00	0.04 ± 0.01	0.05 ± 0.01	0.02 ± 0.00	0.02 ± 0.00	0.04 ± 0.00
	Acetophenone	1.17 ± 0.32	1.88 ± 0.73	4.94 ± 0.51	0.81 ± 0.18	1.16 ± 0.37	0.84 ± 0.17
	2-Tetradecanone	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
	Dodecanal	0.02 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
KETONE	Total ketone	4.33 ± 0.72	4.68 ± 0.74	14.10 ± 2.86	9.07 ± 1.48	10.44 ± 2.02	9.10 ± 1.53
	β - <i>trans</i> -Ocimene	0.13 ± 0.01	0.34 ± 0.07	0.12 ± 0.02	0.35 ± 0.05	0.06 ± 0.02	0.12 ± 0.06
	Sabinene	0.09 ± 0.01	0.17 ± 0.03	0.05 ± 0.00	0.21 ± 0.04	0.05 ± 0.00	0.08 ± 0.01
	β -Myrcene	2.08 ± 0.30	2.32 ± 0.29	1.99 ± 0.32	1.69 ± 0.11	0.96 ± 0.09	1.22 ± 0.33
	D-Limonene	8.36 ± 1.58	12.37 ± 0.88	5.20 ± 0.49	19.17 ± 3.64	6.43 ± 0.59	12.39 ± 6.26
	<i>cis</i> -furan Linalool oxide	0.10 ± 0.07	0.09 ± 0.01	0.05 ± 0.01	0.09 ± 0.02	0.00 ± 0.00	0.04 ± 0.05
	Limonene epoxide	0.67 ± 0.51	0.90 ± 0.04	0.34 ± 0.01	0.02 ± 0.01	0.00 ± 0.00	0.00 ± 0.00
	α -Citral	0.03 ± 0.02	0.06 ± 0.01	0.01 ± 0.00	0.02 ± 0.00	0.09 ± 0.02	0.10 ± 0.01
	β -Caryophyllene	0.02 ± 0.00	0.02 ± 0.01	0.01 ± 0.00	0.01 ± 0.00	0.02 ± 0.01	0.02 ± 0.01
	α -Caryophyllene	0.08 ± 0.01	0.09 ± 0.02	0.07 ± 0.01	0.07 ± 0.01	0.08 ± 0.03	0.12 ± 0.03
	<i>cis</i> -pyranoid-linalyl oxide	0.11 ± 0.03	0.15 ± 0.04	0.06 ± 0.01	0.06 ± 0.02	0.12 ± 0.03	0.08 ± 0.01
	Carveol	0.04 ± 0.03	0.05 ± 0.00	0.02 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
	<i>cis</i> -Geranylacetone	0.02 ± 0.01	0.04 ± 0.01	0.02 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
	α -Limonene diepoxide	0.01 ± 0.00	0.02 ± 0.01	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
TERPEN	Total terperne	11.74 ± 2.31	16.62 ± 3.39	7.94 ± 1.48	21.69 ± 5.28	7.81 ± 1.77	14.18 ± 3.41
	Acetic acid	0.69 ± 0.32	1.30 ± 0.31	0.72 ± 0.18	22.49 ± 1.74	28.40 ± 8.88	21.09 ± 9.24
	Isobutyric acid	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.09 ± 0.03	0.28 ± 0.02	0.10 ± 0.03
	Isovaleric acid	0.06 ± 0.04	0.10 ± 0.02	0.04 ± 0.01	3.51 ± 0.65	9.20 ± 2.28	2.31 ± 0.42
ACIDS	Hexanoic acid	0.39 ± 0.08	0.23 ± 0.00	0.08 ± 0.01	0.36 ± 0.05	0.46 ± 0.11	0.25 ± 0.02

	Heptanoic acid	0.04 ±	0.01	0.00 ±	0.00	0.02 ±	0.01	0.05 ±	0.01	0.07 ±	0.01	0.04 ±	0.00
	Octanoic Acid	0.04 ±	0.01	0.03 ±	0.00	0.05 ±	0.01	0.15 ±	0.02	0.19 ±	0.05	0.09 ±	0.01
	Total acids	1.23 ±	0.28	1.67 ±	0.51	0.91 ±	0.28	26.66 ±	8.94	38.58 ±	11.34	23.88 ±	8.43
	Phenol	0.02 ±	0.00	0.03 ±	0.00	0.02 ±	0.00	0.02 ±	0.00	0.06 ±	0.02	0.03 ±	0.00
	o-Guaiacol	0.00 ±	0.00	0.00 ±	0.00	0.00 ±	0.00	0.02 ±	0.00	0.04 ±	0.01	0.02 ±	0.01
PHENOLS	Total phenols	0.02 ±	0.01	0.03 ±	0.02	0.02 ±	0.01	0.04 ±	0.01	0.10 ±	0.01	0.05 ±	0.01
	2-butoxy-ethanol	0.57 ±	0.22	0.97 ±	0.14	0.30 ±	0.02	0.24 ±	0.04	0.40 ±	0.09	0.85 ±	0.29
	trans-methyl dihydro jasmonate	0.03 ±	0.02	0.04 ±	0.00	0.02 ±	0.15	0.02 ±	0.00	0.02 ±	0.01	0.01 ±	0.00
OTHERS	Total others	0.60 ±	0.38	1.01 ±	0.66	0.32 ±	0.20	0.25 ±	0.15	0.42 ±	0.27	0.86 ±	0.59

		HEAP											
		At the beginning (%)						At the end (%)					
Groups	Compounds	S		ST		C		S		ST		C	
	Ethyl acetate	11.92 ±	0.66	5.92 ±	0.63	5.52 ±	0.74	4.67 ±	1.24	4.88 ±	1.22	0.96 ±	0.43
	Ethyl octanoate	0.06 ±	0.00	0.03 ±	0.01	0.36 ±	0.04	0.33 ±	0.09	0.85 ±	0.26	0.34 ±	0.15
	Ethyl caproate	0.30 ±	0.00	0.22 ±	0.01	1.17 ±	0.05	0.53 ±	0.13	0.94 ±	0.16	0.09 ±	0.02
	Methyl octanoate	0.17 ±	0.01	0.15 ±	0.01	0.00 ±	0.00	0.00 ±	0.00	0.00 ±	0.00	0.00 ±	0.00
	Ethyl benzoate	0.04 ±	0.02	0.02 ±	0.01	1.38 ±	0.18	0.21 ±	0.06	0.24 ±	0.04	0.14 ±	0.01
	Ethyl- <i>α</i> -toluate	0.03 ±	0.06	0.00 ±	0.00	0.00 ±	0.00	0.33 ±	0.10	0.50 ±	0.08	1.02 ±	0.19
	2-Pentanol, acetate	0.97 ±	0.03	1.52 ±	0.49	1.42 ±	0.65	1.78 ±	0.42	2.80 ±	0.13	0.37 ±	0.18
	Isopentyl alcohol, acetate	1.11 ±	0.06	0.94 ±	0.22	0.23 ±	0.02	2.53 ±	0.46	4.35 ±	0.04	0.05 ±	0.02
	Hexyl acetate	0.02 ±	0.00	0.00 ±	0.00	0.04 ±	0.00	0.04 ±	0.01	0.00 ±	0.00	0.00 ±	0.00
	2,3-butanediol diacetate	0.20 ±	0.02	0.15 ±	0.04	3.26 ±	0.43	1.20 ±	0.32	0.03 ±	0.01	1.90 ±	0.24
	1,2-propanediol, diacetate	10.49 ±	0.78	7.78 ±	2.22	2.27 ±	0.09	2.22 ±	0.56	1.88 ±	0.13	3.65 ±	0.44
	β -phenylethyl acetate	0.33 ±	0.08	0.05 ±	0.00	0.12 ±	0.02	0.85 ±	0.24	0.73 ±	0.07	1.19 ±	0.14
	Isoamyl benzoate	0.06 ±	0.00	0.10 ±	0.02	0.06 ±	0.00	0.56 ±	0.15	0.09 ±	0.02	0.13 ±	0.03
	n-Hexyl butanoate	0.11 ±	0.05	0.02 ±	0.01	0.00 ±	0.00	0.00 ±	0.00	0.00 ±	0.00	0.00 ±	0.00
ESTERS	Total ester	25.82 ±	3.99	16.89 ±	2.46	15.82 ±	1.61	15.26 ±	1.32	17.29 ±	1.65	9.84 ±	1.03
	Hexanal	0.39 ±	0.01	0.40 ±	0.11	2.77 ±	0.13	0.21 ±	0.03	0.24 ±	0.02	0.30 ±	0.04
	Benzaldehyde	0.68 ±	0.11	0.21 ±	0.04	0.76 ±	0.05	0.75 ±	0.24	0.59 ±	0.09	1.20 ±	0.26
	Benzeneacetaldehyde	7.25 ±	0.30	4.06 ±	0.59	5.24 ±	0.15	12.37 ±	3.88	5.71 ±	0.83	11.95 ±	1.43
	α -ethylidene-benzeneacetaldehyde	0.00 ±	0.00	0.00 ±	0.00	0.00 ±	0.00	0.00 ±	0.00	0.03 ±	0.00	0.01 ±	0.01
	<i>trans</i> -2-Undecenal	0.00 ±	0.00	0.01 ±	0.01	0.00 ±	0.00	0.03 ±	0.01	0.05 ±	0.01	0.05 ±	0.01
	Nonanal	0.16 ±	0.01	0.16 ±	0.07	0.52 ±	0.22	0.12 ±	0.02	0.13 ±	0.05	0.26 ±	0.07
	2-methyl-butanal	1.16 ±	0.08	0.70 ±	0.05	1.02 ±	0.14	1.46 ±	0.34	0.73 ±	0.01	1.34 ±	0.06
ALDEHYDES	Total aldehyde	9.65 ±	2.62	5.53 ±	1.46	10.30 ±	1.91	14.94 ±	4.54	7.49 ±	2.07	15.11 ±	4.35
	2-Pentanol	20.89 ±	0.67	44.15 ±	2.25	0.72 ±	0.14	1.52 ±	0.31	4.32 ±	0.12	0.13 ±	0.01
	2-Heptanol	0.47 ±	0.02	0.35 ±	0.06	1.94 ±	0.10	2.48 ±	0.58	7.99 ±	0.43	0.07 ±	0.03
	(<i>Z</i>)-3-Hexen-1-ol	0.05 ±	0.00	0.04 ±	0.00	0.12 ±	0.00	0.02 ±	0.01	0.01 ±	0.00	0.01 ±	0.00
	1-Hexanol	0.32 ±	0.02	0.21 ±	0.00	1.32 ±	0.04	0.18 ±	0.04	0.22 ±	0.01	0.20 ±	0.01
	1-Octen-3-ol	0.05 ±	0.00	0.03 ±	0.00	0.00 ±	0.00	0.18 ±	0.05	0.00 ±	0.00	0.00 ±	0.00
	1-Heptanol	0.04 ±	0.01	0.05 ±	0.02	0.16 ±	0.01	0.00 ±	0.00	0.00 ±	0.00	0.00 ±	0.00
	2-ethyl-1-hexanol	0.50 ±	0.01	0.38 ±	0.05	1.00 ±	0.02	0.28 ±	0.07	0.34 ±	0.01	0.65 ±	0.04
	3-methyl-1-butanol	1.42 ±	0.06	1.11 ±	0.03	1.23 ±	0.15	0.88 ±	0.17	1.86 ±	0.05	0.19 ±	0.05
	2-Hexanol	0.74 ±	0.02	1.13 ±	0.05	0.00 ±	0.00	0.07 ±	0.01	0.18 ±	0.01	0.02 ±	0.00
	1-Pentanol	0.29 ±	0.07	0.13 ±	0.04	0.78 ±	0.21	0.14 ±	0.03	0.14 ±	0.07	0.28 ±	0.13
	1-Octanol	0.07 ±	0.00	0.09 ±	0.01	0.49 ±	0.01	0.09 ±	0.02	0.17 ±	0.02	0.23 ±	0.01
	Benzyl alcohol	0.06 ±	0.00	0.04 ±	0.01	0.08 ±	0.00	0.06 ±	0.02	0.07 ±	0.01	0.11 ±	0.02
ALCOHOLS	Phenylethyl alcohol	1.26 ±	0.12	0.31 ±	0.04	0.74 ±	0.04	4.52 ±	1.26	5.61 ±	0.89	8.29 ±	1.39

	1-Heptadecanol	0.10 ± 0.06	0.10 ± 0.08	0.12 ± 0.03	0.06 ± 0.02	0.21 ± 0.02	0.21 ± 0.07
	Isobutanol	0.14 ± 0.03	0.10 ± 0.05	2.23 ± 0.20	0.06 ± 0.02	0.14 ± 0.07	0.03 ± 0.02
	1-Decanol	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.00
	<i>α</i>-Methylbenzyl alcohol	0.57 ± 0.02	0.55 ± 0.07	0.53 ± 0.01	0.30 ± 0.08	0.34 ± 0.05	0.52 ± 0.08
	1-Dodecanol	0.06 ± 0.02	0.02 ± 0.01	0.54 ± 0.15	0.05 ± 0.01	0.38 ± 0.17	0.49 ± 0.23
	Ethanol	3.72 ± 0.09	3.08 ± 0.32	2.52 ± 0.32	2.78 ± 0.52	3.81 ± 0.19	0.45 ± 0.07
	Decanal	0.08 ± 0.01	0.06 ± 0.02	0.09 ± 0.04	0.02 ± 0.00	0.03 ± 0.00	0.05 ± 0.02
	Total alcohol	30.85 ± 4.63	51.93 ± 9.81	14.61 ± 0.77	13.70 ± 1.22	25.83 ± 2.28	11.93 ± 1.82
	2-Pentanone	1.75 ± 0.15	9.73 ± 1.21	0.96 ± 0.06	1.01 ± 0.23	2.23 ± 0.07	3.52 ± 0.24
	2-Heptanone	0.93 ± 0.04	1.28 ± 0.05	1.07 ± 0.17	1.97 ± 0.41	3.61 ± 0.32	0.13 ± 0.03
	Acetoin	0.48 ± 0.05	0.38 ± 0.01	1.88 ± 0.09	1.23 ± 0.24	2.65 ± 0.02	4.09 ± 0.24
	2-Nonanol	0.07 ± 0.00	0.04 ± 0.00	0.08 ± 0.01	0.16 ± 0.04	0.46 ± 0.05	1.21 ± 0.16
	2-Undecanone	0.08 ± 0.00	0.05 ± 0.01	0.14 ± 0.01	0.03 ± 0.01	0.00 ± 0.00	0.14 ± 0.02
	Acetophenone	2.29 ± 0.04	3.06 ± 0.59	1.46 ± 0.04	1.79 ± 0.55	2.31 ± 0.43	1.23 ± 0.25
	2-Tetradecanone	0.01 ± 0.00	0.00 ± 0.00	0.01 ± 0.01	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
	Dodecanal	0.04 ± 0.00	0.00 ± 0.00	0.03 ± 0.01	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00
KETONE	Total ketone	5.65 ± 0.88	14.54 ± 3.37	5.63 ± 0.74	6.20 ± 0.83	11.28 ± 1.45	10.32 ± 1.64
	<i>β</i>-trans-Ocimene	0.32 ± 0.01	0.08 ± 0.01	0.28 ± 0.02	0.51 ± 0.12	0.37 ± 0.04	0.04 ± 0.01
	Sabinene	0.21 ± 0.01	0.05 ± 0.00	0.25 ± 0.05	0.30 ± 0.06	0.17 ± 0.02	0.02 ± 0.01
	<i>β</i>-Myrcene	4.50 ± 0.13	1.98 ± 0.16	3.51 ± 0.21	3.14 ± 0.63	2.31 ± 0.43	3.26 ± 0.27
	D-Limonene	18.46 ± 0.81	6.65 ± 0.63	38.55 ± 1.85	30.60 ± 6.00	17.38 ± 2.88	4.56 ± 0.62
	<i>cis</i>-furan Linalool oxide	0.04 ± 0.00	0.03 ± 0.01	0.18 ± 0.00	0.10 ± 0.02	0.10 ± 0.04	0.10 ± 0.02
	Limonene epoxide	0.62 ± 0.06	0.29 ± 0.10	5.04 ± 0.22	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
	<i>α</i>-Citral	0.07 ± 0.00	0.10 ± 0.02	0.07 ± 0.03	0.08 ± 0.02	0.15 ± 0.02	0.19 ± 0.02
	<i>β</i>-Caryophyllene	0.03 ± 0.00	0.02 ± 0.01	0.10 ± 0.00	0.02 ± 0.00	0.03 ± 0.02	0.12 ± 0.01
	<i>α</i>-Caryophyllene	0.15 ± 0.00	0.09 ± 0.05	0.41 ± 0.01	0.12 ± 0.03	0.18 ± 0.02	0.86 ± 0.09
	<i>cis</i>- pyranoid-linalylol oxide	0.14 ± 0.01	0.10 ± 0.03	0.18 ± 0.01	0.13 ± 0.03	0.17 ± 0.02	0.24 ± 0.04
	Carveol	0.03 ± 0.00	0.01 ± 0.00	0.54 ± 0.04	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
	<i>cis</i>-Geranylacetone	0.00 ± 0.00	0.02 ± 0.01	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
	<i>α</i>-Limonene diepoxide	0.04 ± 0.01	0.00 ± 0.00	0.05 ± 0.01	0.01 ± 0.00	0.02 ± 0.00	0.00 ± 0.00
TERPEN	Total terperne	24.62 ± 5.12	9.42 ± 1.86	49.17 ± 10.56	35.00 ± 8.43	20.86 ± 4.78	9.40 ± 1.46
	Acetic acid	1.00 ± 0.16	0.68 ± 0.27	1.06 ± 0.39	4.33 ± 1.25	6.35 ± 0.74	17.88 ± 3.14
	Isobutyric acid	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.46 ± 0.11	0.46 ± 0.07	0.48 ± 0.21
	Isovaleric acid	0.09 ± 0.02	0.05 ± 0.01	0.19 ± 0.04	8.07 ± 2.00	8.09 ± 0.33	22.33 ± 3.88
	Hexanoic acid	0.96 ± 0.19	0.20 ± 0.08	0.62 ± 0.31	0.43 ± 0.09	0.38 ± 0.08	0.83 ± 0.23
	Heptanoic acid	0.13 ± 0.03	0.00 ± 0.00	0.07 ± 0.04	0.08 ± 0.03	0.09 ± 0.02	0.14 ± 0.05
	Octanoic Acid	0.07 ± 0.04	0.06 ± 0.02	0.11 ± 0.07	0.11 ± 0.07	0.27 ± 0.06	0.34 ± 0.11
ACIDS	Total acids	2.26 ± 0.47	0.99 ± 0.26	2.06 ± 0.42	13.49 ± 3.29	15.64 ± 3.62	41.99 ± 10.25
PHENOLS	Phenol	0.04 ± 0.00	0.03 ± 0.01	0.03 ± 0.00	0.35 ± 0.09	0.37 ± 0.05	0.27 ± 0.04

	o-Guaiacol	0.00 ±	0.00	0.01 ±	0.00	0.00 ±	0.00	0.58 ±	0.17	0.62 ±	0.09	0.23 ±	0.04
	Total phenols	0.04 ±	0.02	0.04 ±	0.02	0.03 ±	0.02	0.93 ±	0.16	0.99 ±	0.18	0.50 ±	0.03
	2-butoxy-ethanol	1.10 ±	0.12	0.67 ±	0.08	2.36 ±	0.65	0.45 ±	0.11	0.58 ±	0.05	0.86 ±	0.04
	trans-methyl dihydro jasmonate	0.05 ±	0.03	0.02 ±	0.01	0.05 ±	0.01	0.02 ±	0.01	0.04 ±	0.00	0.04 ±	0.01
OTHERS	Total others	1.15 ±	0.74	0.69 ±	0.46	2.40 ±	1.63	0.47 ±	0.30	0.62 ±	0.39	0.90 ±	0.58

S2. Yeast community of fermented cocoa beans

Samples	Type	Time	Condition	Chao1	Shannon index (H')	Observed species	ESC (%)
A1T2	Box	T48	<i>S. cerevisiae</i>	736.42	3.32	310	97.17
A1T4	Box	T96	<i>S. cerevisiae</i>	665.32	3.29	255	97.64
A1T5	Box	T120	<i>S. cerevisiae</i>	667	3.56	243	97.64
A3T0	Heap	T0	<i>S. cerevisiae</i>	813.47	3.19	270	97.24
A3T2	Heap	T48	<i>S. cerevisiae</i>	1135.47	3.01	259	97.3
A3T4	Heap	T96	<i>S. cerevisiae</i>	720.06	2.48	188	98.01
A3T5	Heap	T120	<i>S. cerevisiae</i>	530.5	2.45	203	98.07
B1T2	Box	T48	<i>S. cerevisiae_T.delbrueckii</i>	614	3.53	276	97.51
B1T4	Box	T96	<i>S. cerevisiae_T.delbrueckii</i>	771.61	3.73	315	97.14
B1T5	Box	T120	<i>S. cerevisiae_T.delbrueckii</i>	705.92	4.62	302	97.37
B3T0	Heap	T0	<i>S. cerevisiae_T.delbrueckii</i>	828.09	3.55	284	97.2
B3T2	Heap	T48	<i>S. cerevisiae_T.delbrueckii</i>	851.24	3.71	277	97.3
B3T5	Heap	T120	<i>S. cerevisiae_T.delbrueckii</i>	1418.25	4.16	402	96
C1T0	Box	T0	<i>Non_inoculated</i>	451.81	2.94	230	97.98
C1T2	Box	T48	<i>Non_inoculated</i>	718.9	3.36	298	97.29
C1T4	Box	T96	<i>Non_inoculated</i>	744.06	4.12	342	97.06
C1T5	Box	T120	<i>Non_inoculated</i>	672.6	3.21	267	97.51
C3T0	Heap	T0	<i>Non_inoculated</i>	565.33	2.94	264	97.54
C3T2	Heap	T48	<i>Non_inoculated</i>	455.89	2.15	187	98.21
C3T4	Heap	T96	<i>Non_inoculated</i>	1541	4.51	471	95.26
C3T5	Heap	T120	<i>Non_inoculated</i>	1279.44	3.77	353	96.4
A2T0	Box	T0	<i>S. cerevisiae</i>	900.88	4.41	347	96.89
A2T2	Box	T48	<i>S. cerevisiae</i>	876.75	3.69	282	97.3
A2T4	Box	T96	<i>S. cerevisiae</i>	606.72	3.57	264	97.58
A2T5	Box	T120	<i>S. cerevisiae</i>	916.47	3.85	307	97.08
B2T0	Box	T0	<i>S. cerevisiae_T.delbrueckii</i>	796.18	3.83	286	97.29
B2T2	Box	T48	<i>S. cerevisiae_T.delbrueckii</i>	737.38	3.38	242	97.62
B2T4	Box	T96	<i>S. cerevisiae_T.delbrueckii</i>	736.75	3.15	233	97.7
B2T5	Box	T120	<i>S. cerevisiae_T.delbrueckii</i>	819.03	3.65	288	97.4
C2T0	Box	T0	<i>Non_inoculated</i>	982.6	4.5	403	96.27
C2T2	Box	T48	<i>Non_inoculated</i>	785.65	3.35	303	97.09
C2T4	Box	T96	<i>Non_inoculated</i>	1098.38	4.18	393	96.19

C2T5	Box	T120	<i>Non_inoculated</i>	826.95	3.21	298	97.03
			Average	817.28 ± 246.85	3.53 ± 0.59	292.18 ± 62.52	97.22 ± 0.62

S3. Bacterial community of fermented cocoa beans

Samples	Type	Time	Condition	Chao1	Shannon index (H')	Observed species	ESC (%)
A1T0	Box	T0	<i>S. cerevisiae</i>	636.25	4.13	184	87.06
A1T2	Box	T48	<i>S. cerevisiae</i>	534.11	4.18	128	91.75
A1T4	Box	T96	<i>S. cerevisiae</i>	282.14	3.73	124	92.14
A1T5	Box	T120	<i>S. cerevisiae</i>	274	2.48	91	94.15
C1T0	Box	T0	<i>Non_inoculated</i>	502.8	3.16	120	91.56
C1T2	Box	T48	<i>Non_inoculated</i>	473.11	4.6	122	92.33
C1T4	Box	T96	<i>Non_inoculated</i>	453.93	3.71	135	90.89
C1T5	Box	T120	<i>Non_inoculated</i>	308.57	2.35	105	92.71
A3T0	Heap	T0	<i>S. cerevisiae</i>	296	2.65	111	92.81
A3T2	Heap	T48	<i>S. cerevisiae</i>	626.2	4.72	166	88.69
A3T4	Heap	T96	<i>S. cerevisiae</i>	809.5	4	154	88.97
A3T5	Heap	T120	<i>S. cerevisiae</i>	670.23	4.17	166	88.97
B1T0	Box	T0	<i>S. cerevisiae_T.delbrueckii</i>	315.89	3.04	128	91.85
B1T2	Box	T48	<i>S. cerevisiae_T.delbrueckii</i>	332	4.16	146	91.08
B1T4	Box	T96	<i>S. cerevisiae_T.delbrueckii</i>	433.18	3.71	142	90.41
B1T5	Box	T120	<i>S. cerevisiae_T.delbrueckii</i>	529.46	3.4	141	90.32
B3T0	Heap	T0	<i>S. cerevisiae_T.delbrueckii</i>	354.35	2.72	124	91.47
B3T2	Heap	T48	<i>S. cerevisiae_T.delbrueckii</i>	501.2	4.36	151	90.12
B3T4	Heap	T96	<i>S. cerevisiae_T.delbrueckii</i>	372	3.57	123	91.95
B3T5	Heap	T120	<i>S. cerevisiae_T.delbrueckii</i>	475.79	4.75	166	89.55
B3T6	Heap	T144	<i>S. cerevisiae_T.delbrueckii</i>	657.05	5.47	202	86.39
C3T0	Heap	T0	<i>Non_inoculated</i>	247	2.91	103	93.86
C3T2	Heap	T48	<i>Non_inoculated</i>	347.13	3.66	124	91.85
C3T4	Heap	T96	<i>Non_inoculated</i>	396	3.69	129	91.37
C3T5	Heap	T120	<i>Non_inoculated</i>	771.91	4.19	155	88.78
A2T0	Box	T0	<i>S. cerevisiae</i>	587	3.51	137	90.41
A2T2	Box	T48	<i>S. cerevisiae</i>	394	4.27	124	92.23
A2T4	Box	T96	<i>S. cerevisiae</i>	275.67	3.42	110	93.19
A2T5	Box	T120	<i>S. cerevisiae</i>	500.13	3.97	115	92.43
B2T0	Box	T0	<i>S. cerevisiae_T.delbrueckii</i>	1003.43	3.55	147	89.45
B2T2	Box	T48	<i>S. cerevisiae_T.delbrueckii</i>	284.08	4.31	114	93.58
B2T4	Box	T96	<i>S. cerevisiae_T.delbrueckii</i>	370.8	3.02	108	93
B2T5	Box	T120	<i>S. cerevisiae_T.delbrueckii</i>	300.56	3.99	125	92.33
C2T0	Box	T0	<i>Non_inoculated</i>	400.09	3.27	120	92.43
C2T2	Box	T48	<i>Non_inoculated</i>	635.91	4.28	149	90.03
C2T4	Box	T96	<i>Non_inoculated</i>	448.1	3.9	116	92.14
C2T5	Box	T120	<i>Non_inoculated</i>	346.91	3.21	108	93
Average				463.42 ± 172.66	3.73 ± 0.68	132.78 ± 23.78	91.22 ± 1.83