

Supplementary Table 1. Volatile compounds of cocoa beans after treatment with papain (concentration 3.3 U/mL for 10 hours incubation) compared with that of unfermented and fermented cocoa.

Compounds	KI ^{exp}	KI ^{lit}	Concentration (ng/g)			*Odor description
			Unfermented	Fermented	Papain treatment	
Pyrazine						
2,5-dimethyl- Pyrazine	1,320	1,323	0.16 ± 0.00^a	0.30 ± 0.05^c	0.22 ± 0.00^b	Chocolate, nutty
2,6-dimethyl-Pyrazine	1,325	1,328	0.02 ± 0.00 ^a	0.13 ± 0.15 ^b	0.03 ± 0.00 ^a	Nutty, coffee
ethyl-Pyrazine	1,330	-	0.01 ± 0.00^a	0.11 ± 0.09^c	0.04 ± 0.01^b	Peanut-butter, nutty
2,3-dimethyl- Pyrazine	1,339	1,315-1,345	0.04 ± 0.00^a	0.31 ± 0.33^c	0.14 ± 0.01^b	Cocoa, caramel
2-ethyl-5-methyl-Pyrazine	1,372	1,386	0.01 ± 0.00^a	0.12 ± 0.01^c	0.03 ± 0.00^b	Nutty, raw potato
trimethyl-Pyrazine	1,390	1,395-1,403	0.02 ± 0.00^a	1.67 ± 0.17^c	0.08 ± 0.00^b	Cocoa, roasted nuts, peanut
3-ethyl-2,5-dimethyl-Pyrazine	1,444	-	0.03 ± 0.00^a	0.39 ± 0.26^c	0.07 ± 0.00^b	cocoa roasted, nutty
tetramethyl-Pyrazine	1,460	1,438-1,465	0.05 ± 0.01^a	7.08 ± 0.40^c	0.17 ± 0.00^b	chocolate, cocoa, roasted
Total			0.34	10.66	0.78	
Aldehyd						
3-methylbutanal*	916	912-937	-	4.05 ± 0.087^a	1.6 ± 0.10^b	Cocoa, chocolate
Benzaldehyde	1,498	1,495-1,499	0.06 ± 0.04^a	3.73 ± 0.61^c	0.69 ± 0.01^b	Sweet, almond, cherry, bitter
Benzeneacetaldehyde	1,621	1,609-1,671	0.12 ± 0.03^a	1.64 ± 0.67^c	0.68 ± 0.12^b	Almond, fruity, nutty
2-Phenyl-2-butenal	1,925	1,896-1,972	-	0.70 ± 0.22^a	0.05 ± 0.01^b	Sweet chocolate
Total			0.18	11.89	3.02	
Ester						
Isobutyl acetate	1,011	1,008	0.02 ± 0.01 ^a	0.07 ± 0.01 ^b	0.03 ± 0.00 ^a	Fruity

2-pentyl acetate	1,071	1,073-1,080	0.02 ± 0.06^b	0.67 ± 0.62^a	0.18 ± 0.01^a	Fruity, orange, tropical
Isoamyl acetate	1,122	1,118-1,137	-	2.74 ± 0.45^a	0.89 ± 0.07^b	Banana, fruity
Total			0.04	5.19	1.1	
Alcohol						
2-Ethyl-1-pentanol	1,297	-	0.04 ± 0.01 ^a	0.08 ± 0.02 ^b	0.04 ± 0.01 ^a	-
2-Heptanol	1,322	1,315-1,326	0.02 ± 0.01 ^a	0.54 ± 0.34 ^b	0.03 ± 0.00 ^a	Citrus, fruity, lemon grass
2-Nonanol	1,509	-	-	0.82 ± 0.44^b	0.03 ± 0.00^a	Citrus, orange, waxy
2-Hexanol	1,528	-	-	0.23 ± 0.09^b	0.03 ± 0.01^a	Fruity, green, herbal
Benzyl alcohol	1,869	1,840-1,864	0.04 ± 0.01 ^a	0.23 ± 0.16 ^b	0.04 ± 0.01 ^a	Sweet, flowery
Phenylethyl alcohol	1,907	-	0.18 ± 0.08^a	3.39 ± 0.59^c	1.48 ± 0.33^b	Floral, sweet, and bready
Isoamyl alcohol	1,211	-	0.04 ± 0.08^a	0.24 ± 0.28^b	0.55 ± 0.15^c	Banana, fruity, fermented
2,3 butanediol	1,575	1,516-1,582	0.03 ± 0.04^a	0.77 ± 0.27^c	0.05 ± 0.02^b	fruity, sweet, butter
Total			0.35	6.3	2.25	
ketones						
2-Heptanone	1,183	1,145-1,216	0.08 ± 0.01 ^a	0.31 ± 0.23 ^c	0.11 ± 0.02 ^b	Fruity, coconut, floral, cheesy
Acetoin	1,284	1,250-1,255	0.03 ± 0.00^a	0.56 ± 0.25^c	0.09 ± 0.02^b	Buttery and creamy
2-Nonanone	1,376	1,347-1,420	0.01 ± 0.02 ^a	1.2 ± 0.45 ^c	0.04 ± 0.01 ^b	Fruity, fresh, sweet
Acetophenone	1,631	1,600-1,655	0.30 ± 0.02^a	1.03 ± 0.20^c	0.73 ± 0.03^b	Floral, flowery, sweet
Total			0.42	3.1	0.97	
Acids						
Acetic acid	1,430	1,430-1,452	0.13 ± 0.04^a	3.50 ± 0.77^c	1.80 ± 0.59^b	Sour, astringent, vinegar

Propanoic acid	1,521	1,514-1,523	-	0.12 ± 0.07^a	0.04 ± 0.00^b	Pungent and rancid
Isovaleric acid	1,660	-	0.12 ± 0.06^a	3.06 ± 0.65^c	0.26 ± 0.04^b	Sweat, acid and rancid
3-methylpentanoic acid	1,845	-	-	0.39 ± 0.18^a	0.09 ± 0.01^b	-
Total			0.25	7.07	2.19	
Other						
2-Acetylpyrrole	1,964	1,930-2,020	0.06 ± 0.03	0.55 ± 0.29	0.08 ± 0.02	cocoa, chocolate, hazelnut, roasted
Furaneol	2,343	-	0.03 ± 0.01	0.13 ± 0.01	0.06 ± 0.02	caramel-like, sweet
Total			0.25	7.07	2.19	

Significance: Value with different letters represent significant differences ($\alpha = 0.05$) in between samples; $KI^{(exp)}$: Kovat retention Index on the DB-WAX column; $KI^{(lit)}$: Kovat retention Index literature sourced from <http://www.pherobase.com> accessed on March 2023 (Hinne et al., 2018; Tuenter et al., 2020); *odor description from Afoakwa et al. (2008), Aprotosoai et al. (2016), Rottiers et al. (2019), and <http://www.thegoodscentscompany.com> accessed on March 2023

