Characterization of volatile compounds in traditional Mexican cocoa-based beverages and their application in flavored milks

Lucía Abadía-García[1], Edgar Ayala-Padilla[1], Pedro A. Vázquez-Landaverde[2], María del Carmen Cortez-Trejo[1], Silvia L. Amaya-Llano[1]*

[1] School of Chemistry, Autonomous University of Querétaro, Santiago de Querétaro 76010, Querétaro, Mexico.

[2] Center for Research in Applied Science and Advanced Technology, National Polytechnic Institute, Querétaro Unit, Santiago de Querétaro, Querétaro 76090, Mexico.

Corresponding author: Silvia L. Amaya Llano. E-mail: samayal@uaq.mx

Supplementary material

Table S1. Flavor proposals for milks. **Table S2**. Descriptors and **Table S3.** phrases to describe traditional Mexican beverages. **Table S4A**. Volatile compound profile of Pozol, **Table S4B** Volatile compound profile of Chilate. **Table S4C.** Volatile compound profile of Cacahuatole.

Table S1. Flavor proposal for milks

FPZ. Flavor proposal for Pozol. **FCH**. Favor proposal for Chilate. **FCA**. Flavor proposal for Cacahuatole.*Code of the flavors provided by the flavor companies.

Beverage	Company	Flavor sample	Components*	Dose/100 mL dairy formula
Pozol	MANE Flavor & Fragrance Manufacturer	FPZ1	E21112234	0.06
	Takasago International Co.	FPZ2	TS-101767	0.1
	DSM Firmenich	FPZ3	0500092285S	0.1
	International Flavors & Fragances Inc.	FPZ4	Chocolate SC1033943	0.1
			Granola SC1033944	0.018
			Canela SC908272	0.018
	International Flavors & Fragances Inc.	FPZ5	Chocolate SC1033943	0.1
			Granola SC1033944	0.018
			Canela SC908272	0.018
			Café SC847452	0.02
	Control	FPZ0	100 mL dairy formula, 33 g Pozol dough and 12 g sugar	-
Chilate	MANE Flavor & Fragrance Manufacturer	FCH1	E21112235	0.06
	Takasago International Co.	FCH2	TS-101768	0.07
	International Flavors & Fragances	FCH3	Tortilla SC1026674	0.03
			Chai SC534636	0.01
			Café SC847452	0.025
	Control	FCH0	100 mL dairy formula, 34 g Chilate dough and 10 g sugar	-
Cacahuatole	MANE Flavor & Fragrance Manufacturer	FCA1	E21154223	0.18
	Takasago International Co.	FCA2	TS-101903	0.06
	International Flavors & Fragances Inc	FCA3	Chocolate SC1033943	0.03
			Cacahuate SC1033946	0.004
	International Flavors & Fragances Inc.	FCA4	Chocolate SC1033943	0.02
			Cacahuate SC1033946	0.005
	Control	FCA0	100 mL dairy formula, 39 g Cacahuatole dough and 14 g sugar	-

Table S2. Descriptors for traditional Mexican beverages

	Pozol	Chilate	Cacahuatole
1	Sweet	Sweet	Sweet
2	Cinnamon	Cinnamon	Cinnamon
3	Soil	Vanilla	Anise
4	Vanilla	Acid	Roasted broad beans
5	Coffee	Bitter	Bitter
6	Piloncillo[a]	Cocoa/Chocolate	Cocoa/Chocolate
7	Roasted cocoa	Rice/Horchata	Corn
8	Cooked Corn	Roasted cocoa	Roasted cocoa
9	Overcooked corn	-	-

[a] Brown sugar.

Table S3. Phrases to describe traditional Mexican beverages.

	Pozol	Chilate	Cacahuatole
1	Not sweet	Not sweet	Not sweet
2	Little sweet taste	Little sweet taste	Little sweet taste
3	Optimal sweet taste	Optimal sweet taste	Optimal sweet taste
4	Excessive sweet taste	Excessive sweet taste	Excessive sweet taste
5	No cinnamon flavor	No cinnamon flavor	No cinnamon flavor
6	Light cinnamon taste	Light cinnamon taste	Light cinnamon taste
7	Optimal cinnamon taste	Optimal cinnamon taste	Optimal cinnamon taste
8	Excessive cinnamon taste	Excessive cinnamon taste	Excessive cinnamon taste
9	No vanilla flavor	No vanilla flavor	No anise flavor
10	Light vanilla taste	Light vanilla taste	Light anise taste
11	Optimal vanilla taste	Optimal vanilla taste	Optimal anise taste
12	Excessive vanilla taste	Excessive vanilla taste	Excessive anise taste
13	No coffee flavor	No acid taste	No toasted broad bean flavor
14	Light coffee taste	Light acid taste	Light toasted broad beantaste
15	Optimal coffe taste	Optimal acid taste	Optimal toasted broad bean taste
16	Excessive coffee taste	Excessive acid taste	Excessive toasted broad bean taste
17	No toasted cocoa flavor	No bitter taste	No bitter taste
18	Light toasted cocoa taste	Light bitter taste	Light bitter taste
19	Optimal toasted cocoa taste	Optimal bitter taste	Optimal bitter taste
20	Excessive toasted cocoa taste	Excessive bitter taste	Excessive bitter taste
21	No cooked corn flavor	No cocoa taste	No cocoa taste
22	Light cooked corn taste	Light cocoa taste	Light cocoa taste
23	Optimal cooked corn taste	Optimal cocoa taste	Optimal cocoa taste
24	Excessive cooked corn taste	Excessive cocoa taste	Excessive cocoa taste
25	No overcooked corn flavor	No rice taste	No corn flavor
26	Light overcooked corn taste	Light rice taste	Light corn taste
27	Optimal overcooked corn taste	Optimal rice taste	Optimal corn taste
28	Excessive overcooked corn taste	Excessive rice taste	Excessive corn taste
29	No earthy taste	No toasted cocoa flavor	No toasted cocoa flavor
30	Light earthy taste	Light toasted cocoa taste	Light toasted cocoa taste
31	Optimal earthy taste	Optimal toasted cocoa taste	Optimal toasted cocoa taste
32	Excessive earthy taste	Excessive toasted cocoa taste	Excessive toasted cocoa taste
33	Less similar to original Pozol flavor	No similar to Chilate	No similar to Cacahuatole
34	Unpleasant to the palate	Slightly similar to Chilate	Slightly similar to Cacahuatole
35	Most similar to original Pozol flavor	Most similar to Chilate	Most similar to Chilate
36	Pleasant to the palate	Unpleasant to the palate	Unpleasant to the palate
37		More or less pleasant to the palate	More or less pleasant to the palate
38		Pleasant to the palate	Pleasant to the palate

Table S4A. Volatile compound profile of Pozol samples.

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area					Aroma descriptor[b]
						PZ1	PZ2	PZ3	PZ4	PZ5	
4.447	n-Hexylmethylamine	035161-70-7	-	-	-	2	-	-	-	-	-
4.551	Methanethiol	000074-93-1	-	464	Bonaïti et al. [49]	-	0.61	0.49	-	-	Cabbage, garlic, spicy
4.68-4.70	Ethanol	000064-17-5	-	-	-	1.64	0.88	1.33	8.2	1.79	-
5.03	1,2-Diethoxyethane	000629-14-1	-	-	-	-	-	-	-	0.51	Sweet
5.036	Diethyl ether	000060-29-7	-	-	-	-	-	0.49	-	-	-
6.103	2,3-Butanedione	000431-03-8	-	586	Wu et al. [50]	0.15	-	-	-	-	Butter, pastry, yeast.
6.246-6.278	Hexane	000110-54-3	600.371	601	Insausti et al. [51]	0.61	0.82	1.29	1.89	1.09	-
6.382	2-Methylfuran	000534-22-5	604.393	605	Engel and Ratel [47]	-	0.13	0.41	-	0.19	Spicy, smoky
6.983	Acetic acid	000064-19-7	622.988	625	Avsar et al. [52]	-	-	-	1.45	-	Vinegar
7.74	Butanal, 3-methyl	000590-86-3	645.42	649	Jarunrattanasri et al. [53]	-	0.08	-	-	-	Apples
8.07	Butanal, 2- methyl	000096-17-3	657.905	659	Jarunrattanasri et al. [53]	-	0.1	-	-	-	Unpleasant odor
9.49	3-Methyl-2-butanol	000598-75-4	700.335	692.1	Tret'yakov [54]	-		-	-	0.6	-
9.493	2-Pentanol	006032-29-7	700.75	706	Wu et al. [50]	-	0.24	0.47	-	-	-
9.978	2,5-Dimethylfuran	000625-86-5	708.079	718	Ames et al. [55]	-		0.18	-	-	Spicy,smoky, caustic
10.864	Butanoic acid, methyl ester	000623-42-7	722.225	724	Pino et al. [56]	-	0.14	-	-	-	Apple, ester, sweet
11.55	Oxirane, 2-(1,1-dimethylethyl)-3-ethyl-, cis	036099-44-2	733.178	-	-	-	0.24	-	0.61	-	-
11.556	Oxirane, 2-(1,1-dimethylethyl)-3-methyl	053897-30-6	733.274	-	-	-	-	-	-	0.55	-
11.615	1-Butanol, 3-methyl	000123-51-3	730.819	734	Engel and Ratel [47	0.1	-	-	-	-	Alcohol, Malt
11.777-11.79	1-Butanol, 2-methyl	000137-32-6	736.803	736	Pino et al. [56]	-	0.22	0.61	0.44	0.49	Cooked ,roasted, fruity, alcoholic
12.139	Dimethyl disulfide	000624-92-0	742.583	740	Bonaïti et al. [49]	-	-	0.21	-	0.19	Garlic
15.748	Octane	000111-65-9	799	799	Insausti et al. [51]	-	-	0.14	-	0.14	Gasoline
15.962-15.995	Butanoic acid, ethyl ester	000105-54-4	803.277	802	Pino et al. [56]	-	0.13	0.14	-	0.18	Apple, pineapple

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4A. Volatile compound profile of Pozol samples (Continued).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area					Aroma descriptor[b]
						PZ1	PZ2	PZ3	PZ4	PZ5	
17.327	Pyrazine, methyl	000109-08-0	822.985	826	Nakahara et al. [57]	-	-	0.32	-	-	cocoa, nutty
18.122-18.142	Furfural	000098-01-1	834.652	839	Weissbecker and Holighaus [58]	0.87	0.84	0.76	-	0.9	Almond, baked potatoes, bread, overcooked, spices
19.371	2-Pentanol, acetate	000626-38-0	852.497	843.3	Tret'yakov [54]	-	-	0.33	0.41	0.3	Banana
19.875-19.882	2-Furanmethanol	000098-00-0	859.875	852	Siegmund and Murkovic [59]	-	-	0.33	-	0.31	Overcooked, burnt
20.069	Ethylbenzene	000100-41-4	862.575	857	Kotowska et al. [60]	-	0.12	0.17	-	0.27	Sweet, gasoline
20.619-20.651	Benzene, 1,3-dimethyl	000108-38-3	870.516	868	Isidorov et al. [61]	0.3	0.37	-	-	0.48	Sweet
21.001	2-Hexanal, 2-methyl	028467-88-1	876.032	884	Miyazaki et al. [62]	-	-	0.09	-	-	-
21.201-21.221	1-Butanol, 3-methyl-, acetate	000123-92-2	879.107	876	Pino et al. [56]	0.13	0.49	0.95	0.75	0.73	Apple, banana, Pear
21.369-21.378	1-Butanol, 2-methyl-, acetate	000624-41-9	881.446	880	Pino et al. [56]	-	0.17	-	0.26	0.24	Apple, banana, fruit
22.087-22.1	Styrene	000100-42-5	891.712	890	Pino et al. [56]	0.89	0.56	0.87	1.18	1.73	Sweet and floral
22.741-22.754	2-Heptanol	000543-49-7	901.35	901.4	Tret'yakov [54]	-	0.13	0.35	0.46	0.53	Citrus, herbaceous, lemon, grass
23.459-23.569	Oxime-, methoxy-phenyl	067160-14-9	912.535	-	-	1.68	1.5	-	-	-	-
23.64	Ethylpyrazine	013925-00-3	915.378	915	Siegmund and Murkovic [59]	-	-	0.4	-	0.31	Peanut Butter, nutty
24.513-24.52	Alpha-Thujene	002867-05-2	929.202	826	Benkaci-Ali et al. [63]	0.44	1.58	-	-	1.24	Coriander, citrus
24.946-24.966	1R-Alpha-Pinene	007785-70-8	936.207	935	Zeller & Rychlik [64]	3.63	3.06	-	0.26	3.02	Pine
25.768	Benzene, 2-propenyl	000300-57-2	948.806	947	Rezazadeh et al. [65]	-	-	-	0.63	-	-
25.775	1H-pirrol, 1-butil	000589-33-3	936.916	-	-	-	-	0.3	-	0.37	-
25.768-25.91	Camphene	000079-92-5	951.052	936	Couladis et al. [66]	0.78	1.04	1.17	-	1.02	oil-camphoraceous
26.648-26.654	Benzaldehyde	000100-52-7	962.629	965.6	Zeng et al. [67]	-	0.62	1.09	1.98	-	Sweet, almond

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4A. Volatile compound profile of Pozol samples (Continued).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area					Aroma descriptor[b]
						PZ1	PZ2	PZ3	PZ4	PZ5	
27.262	1-Heptanol	000111-70-6	972.274	972	Rembold et al. [68]	-	-	0.19	-	-	Fatty, aromatic
27.502	Sabinene	003387-41-5	976.138	977	Kundakovic et al. [69]	-	0.44	-	-	0.35	-
27.696-27.709	(-)-Beta-Pinene	000127-91-3	978.982	975	Benkaci-Ali et al. [63]	1.4	0.97	1.05	0.22	0.93	Pine and wood
28.194	Phenol	000108-95-2	986.914	981	Lalel et al. [70]	-	-	0.29	-	-	Sweet
28.569	Beta-Myrcene	000123-35-3	992.805	990	Benkaci-Ali et al. [63]	0.85	1.28	-	-	-	Balsamic, Fruit, Geranium
28.588	Furan, 2-pentyl	003777-69-3	993.103	993	Zeng et al. [67]	-	-	-	1.33	-	Butter, Floral, Fruit, Green Bean
28.802-28.808	2-Furanmethanol, acetate	000623-17-6	996.465	991	Beaulieu and Grim [71]	-	-	1.45	-	0.42	Fruits
29.397-29.423	Alpha-Phellandrene	000099-83-2	1006.936	1001	Benkaci-Ali et al. [63]	2.32	6.34	5.4	-	4.82	Citrus, fresh, mint, pepper, spices and wood
29.476	3-Carene	013466-78-9	1007.864	1010	Kallio et al. [72]	-	0.57	-	-	0.64	Lemon
29.746	Alpha-Terpinene	000099-86-5	1012.594	1015	Benkaci-Ali et al. [63]	0.41	1.49	-	-	-	Lemon
29.85	Benzene, 1,4-dichloro	000106-46-7	1014.415	1014.9	Xu et al. [73]	-	-	-	0.36	-	-
30.141-30.154	2-Carene	000554-61-0	1019.411	-	-	0.42	4.35	0.5	-	2.82	-
30.148	(+) - 4 Carene	029050-33-7	1019.513	1022	Yang et al. [74]	-	-	3.01	-	-	-
30.451	1-etil-3,5-dimetilbenceno	000934-74-7	1024.943	-	-	0.51	0.19	-	-	0.18	-
30.458	Benzene, 4-ethyl-1,2-dimethyl-	000934-80-5	1025.065	-	-	-	-	0.23	-	-	-
30.658	Benzene, 1-methyl-4-(1-methylethyl)	000099-87-6	1024.943	1027	Kallio et al. [72]	9.79	10.23	-	-	-	Fresh, citrus
30.684	Benzene, 1-methyl-3-(1-methylethyl)	000535-77-3	1026.992	1023	Kallio et al. [72]	-	-	12.83	-	-	-
30.71	Benzene, 1-propenyl	000637-50-3	1029.479	-	-	-	-	-	3.93	-	-
30.658	p-Cimene	000099-87-6	1029.024	1027	Kallio et al. [72]	-	-	-	-	10	Fresh, citrus
30.839	D-Limonene	005989-27-5	1031.739	-	-	-	-	-	2.07		Citrus, Mint
30.93-30.949	Beta-Felandrene	000555-10-2	1033.666	1028	Radulović et al. [75]	8.07	17.55	-	-	14.05	-

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4A. Volatile compound profile of Pozol samples (Continued).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area					Aroma descriptor[b]
						PZ1	PZ2	PZ3	PZ4	PZ5	
30.956	Beta-Terpinene	000099-84-3	1033.788	1036	Estévez et al. [76]	-	-	12.4	-	-	-
31.189	Benzyl alcohol	000100-51-6	1037.87	1034.4	Zeng et al. [67]	-	-	-	0.31	-	Boiled Cherries, Moss, Toast Bread, Rose
31.318-31.325	(E) -Beta-Ocimene	003779-61-1	1040.129	1046	Belsito et al. [77]	0.13	0.22	-	-	0.26	Floral
31.331	Cyclofencene	000488-97-1	1040.357	1050	Kartal et al. [78]	-	-	0.25	-	-	-
31.538	2-Butyl methylbutanoate	015706-73-7	1043.983	1045	De Pooter et al. [79]	-	0.09	0.11	-	-	-
31.726	Benzeneacetaldehyde	000122-78-1	1047.276	1050	Jarunrattanasri et al. [53]	-	-	0.21	0.62	0.19	-
31.81	1-Propyne, 3-phenyl	010147-11-2	1048.747	-	-	-	-	-	-	-	-
31.926	Beta-Ocimene	013877-91-3	1050.779	1050	Agnihotri et al. [80]	0.09	0.18	-	-	0.13	Floral
31.933	(Z)-Beta-Ocimene	003338-55-4	1050.902	1040	Vagionas et al. [81]	-	-	0.17	-	-	-
32.276	1H-Pyrrole, 1-pentyl	000699-22-9	1056.91	-	-	0.17	0.2	0.33	-	-	-
32.58-32.593	Gamma-Terpinene	000099-85-4	1062.462	1060	Benkaci-Ali et al. [63]	0.48	0.96	0.97	-	-	Bitter and citrus
33.026-33.032	Acetophenone	000098-86-2	1070.275	1069	Kallio et al. [72]	0.15	0.07	0.22	-	0.26	Bitter, wood, almonds, flower, meat and must
33.673	Pyrazine, 3-ethyl-2,5-dimethyl	013360-65-1	1081.526	1078	Cerny and Guntz- Dubini [82]	0.47	0.41	-	0.36	0.86	-
34.087	Pyrazine, tetramethyl	001124-11-4	1088.632	1087.3	-	-	-	-	-	1.31	Cocoa, coffee, mocha, roasted
34.1	Benzene, 1-ethenyl-3-ethyl	007525-62-4	1088.859	-	-	-	-	-	0.31	-	-
34.274	Terpinolene	000586-62-9	1091.907	1089	Benkaci-Ali et al. [63]	-	1.08	-	-	-	Pine
34.31	Phenol, 2-methoxy	000090-05-1	1092.590	1092	Jarunrattanasri et al. [533]	-	-	-	0.49	-	Burnt, phenol, wood
34.313-34.326	Benzene, 1-methyl-4-(1-methylethenyl)	001195-32-0	1092.59	1094.7	Zeng et al. [67]	0.97	-	1.15	-	1.04	Citrus, pine

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4A. Volatile compound profile of Pozol samples (Continued).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area					Aroma descriptor[b]
						PZ1	PZ2	PZ3	PZ4	PZ5	
34.818-34.883	Linalool	000078-70-6	1102.444	1104	Hazzit et al. [83]	2.52	3.6	4.41	0.56	3.26	Coriander,floral, lavender, lemon, rose
35.044	Hexane, 1-(hexyloxy)-3-methyl	074421-18-4	1105.928	-	-	-	-	-	-	0.3	-
35.258	Trans-5-methyl-2-isopropyl-2-hexen-1-al	0035158-25-9	1110.048	-	-	-	-	-	-	0.31	-
35.659-35.672	Phenylethyl alcohol	000060-12-8	1117.767	1118.4	Zeng et al. [67]	0.38	0.29	0.69	0.78	-	Fruit, honey, lilac, rose, wine
36.383	2,4,6-Octatriene, 2,6-dimethyl-, (E, Z)	007216-56-0	1131.703	1131	Andriamahavaro [84]	0.27	-	0.25	-	0.23	-
36.383	Alpha-Pironene	000514-94-3	1131.703	-	-	-	0.19	-	-	-	-
37.069	1,2-Benzenediamine, N,N-dimethyl	002836-03-5	1144.908	1216	-	-	-	-	-	0.19	-
37.418	D-camphor	000464-49-3	1151.626	-	-	-	-	0.32	-	-	-
37.767	Pyrazine, 2,3-diethyl-5-methyl	018138-04-0	1158.344	1158	Steinhaus and Schieberle [85]	-	-	-	-	0.12	Soil, meat, potato, roast
37.916	Pyrazine, 3,5-diethyl-2-methyl	018138-05-1	1161.097	1165	Ames et al. [55]	-	0.09	0.16	-	0.19	Baked, cocoa, roasted, rum
38.046	2,3,5-Trimethyl-6-ethylpyrazine	017398-16-2	1163.715	1169	Ames et al. [55]	-	-	-	-	0.29	-
38.252	3-fenilpropionaldehyde	000104-53-0	1167.68	1162	Buchin et al. [86]	-	-	-	1.25	-	-
38.278	Benzoic acid	000065-85-0	1168.18	1170	Alves et al. [87	-	-	-	-	0.42	Spicy, Sour
38.531	(-)-Borneol	000464-45-9	1173.051	1173	Avsar et al. [52]	0.47	-	-	-	-	Camphor, fragrance, green
38.569	1-Nonanol	000143-08-8	1173.782	1169.2	Zhao et al. [88]	-	-	-	0.69	-	Fat, floral, green, oil
39.081-39.087	Terpinen-4-ol	000562-74-3	1183.753	1175	Skaltsa et al. [89]	0.55	-	0.57	-	-	Soil, must, nutmeg, wood
39.255	1H-Pyrrole, 1-(2-furanylmethyl)	001438-94-4	1186.987	1185	Andriamahavaro [84]	-	-	0.15	-	-	Cocoa, roasted
39.747	3-Cyclohexene-1	000098-55-5	1196.458	1190	Benkaci-Ali et al. [63]	-	-	0.81	-	-	Anise, fresh, mint, oil

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4A. Volatile compound profile of Pozol samples (Continued).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area					Aroma descriptor[b]
						PZ1	PZ2	PZ3	PZ4	PZ5	
39.74	(-) - Alpha-Terpineol	010482-56-1	1196.323	1187	Skaltsa et al. [89]	-	0.68	-	-	-	Flowers
39.947	Dodecan	000112-40-3	1200.294	-	-	0.08	-	-	0.15	0.14	-
40.167	Pyrazine, 2,5-dimethyl-3- (2-methylpropyl)	032736-94-0	1204.341	1207	Oruna-Concha et al. [90]	-	-	0.14	-	0.15	-
41.06	Benzofuran, 2,3-dihydro	000496-16-2	1220.77	1223	Pino et al. [91]	0.23	-	-	0.19	0.12	-
41.662-41.713	3-Phenyl-1-propanol	000122-97-4	1232.784	1233	Shalit et al. [92]	-	0.14	-	0.6	-	Cinnamon, fruit
42.211	Benzaldehyde, 4-(1-methylethyl)	000122-03-2	1241.946	1246	Lalel et al. [70]	-	-	-	0.33	-	-
42.515	2-isoamyl-6-methylpyrazine	091010-41-2	1247.539	1248	Solina et al. [93]	-	-	-	-	0.33	-
42.884	Acetic acid, 2-phenylethyl ester	000103-45-7	1254.328	1256	Pino et al. [56]	-	-	0.21	-	0.26	Flower, honey, rose
42.891	Butanamide, 2,2,3,3,4,4,4-heptaflu oro-N- (2- phenylethyl)	029723-29-3	1254.456	-	-	-	0.28	-	-	-	-
43.389	Nonanoic acid/ Pelargonic acid	000112-05-0	1263.618	1272.1	Zeng et al. [67]	0.5	0.71	0.46	1.04	0.67	Fat, bitter
43.667	Cinnamaldehyde, (E)	014371-10-9	1268.733	1266	Benkaci-Ali et al. [63]	-	0.11	0.79	-	1.23	Spices
43.693-43.731	2-Propenal, 3-phenyl	000104-55-2	1269.211	1266	Benkaci-Ali et al. [63]	1.99	2.44	-	10.12	-	Spices
44.016	Phenol, 4-ethyl-2-methoxy	002785-89-9	1275.154	1268	Boulanger and Crouzet [94]	0.1	-	0.16	-	-	Clove, Phenol, Spices
44.818	Tridecane	000629-50-5	1289.908	-	-	-	-		-	0.14	-
45.426-45.459	2-Propen-1-ol, 3-phenyl	000104-54-1	1301.223	1309	Mondello et al. [95]	0.57	0.69	0.7	19.73	0.84	-
45.873-45.886	2-Methoxy-4-vinylphenol	007786-61-0	1309.557	1312	Pino et al. [56]	2.07	1.99	0.59	2.45	1.22	Clove, Curry, Spices
47.444	Benzene, 1,3-hexadienyl	041635-77-2	1338.221	-	-	-	-	-	0.46	-	-
48.02	Alpha-Cubebene	017699-14-8	1348.818	1348	Radulović et al. [75]	0.22	-	-	-	0.67	-
48.363-48.376	Eugenol	000097-53-0	1355.257	1362.4	Zhao et al. [88]	0.63	0.71	0.61	0.57	0.93	Burnt, cloves, spices
48.596-48.628	N-decanoic acid	000334-48-5	1360.13	1368.2	Zeng et al. [67]	0.34	0.48	0.28	-	0.3	Dust, Fat, Grass
49.359	(+) - Cyclosativen	022469-52-9	1373.452	1373.6	Zeng et al. [67]	0.31	-	0.24	-	-	-

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4A. Volatile compound profile of Pozol samples (Continued).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area					Aroma descriptor[b]
						PZ1	PZ2	PZ3	PZ4	PZ5	
49.838-49.844	Copaene	003856-25-5	1382.264	1379	Kundakovic et al. [69]	1.54	0.69	1.06	0.94	-	-
51.177	Vanillin	000121-33-5	1403.877	1409	Kundakovic et al. [69]	-	-	-	0.41	-	Vanilla
52.121	Bicyclo[5.2.0]nonane, 2-methylene- 4,8,8-trimethyl- 4-vinyl	242794-76-9	1413.637	-	-	-	-	-	-	0.15	-
52.121-52.128	Isocaryophyllene	000118-65-0	1413.637	-	Benkaci-Ali et al. [63]	-	0.12	0.44	-	-	Fried, Spices, Wood
52.477	Alpha-Bergamotene	017699-05-7	1417.318	1415	Pino et al [96]	0.25	-	-	-	-	-
52.904	Alpha-Santalene	000512-61-8	1421.732	1420	Masoudi et al. [97]	0.24	-	-	-	-	-
53.189-53.202	Caryophyllene	000087-44-5	1424.679	1419	Benkaci-Ali et al. [63]	2.9	3.72	3.03	0.7	4.07	Fried, Spices, Wood
54.741	(+)-Aromadendrene	000489-39-4	1440.725	1440	Saroglou et al. [98]	0.43	-	-	-	-	-
55.213	Phenol, 2-methoxy-4-(1- propenyl)	000097-54-1	1445.605	1448	Paulo et al. [99]	0.15	-	-	-	-	Floral
56.029-56.041	Alpha-Caryophyllene	006753-98-6	1454.042	1455	Benkaci-Ali et al. [63]	0.75	-	0.57	-	0.61	Fried, Spices, Wood
57.044	1-Cycloheptene, 1,4-dimethyl-3-(2-methyl-1-propene-1-yl)-4-vinyl	068480-14-8	1464.536	-	-	-	-	-	1.29	-	-
57.076	Alpha-Gurjunene	000489-40-7	1464.867	1464	Couladis et al. [66]	1.67	-	-	-	-	-
57.995	Gamma-Muurolene	030021-74-0	1474.369	1473	Vagionas et al. [81]	0.21	-	-	-	-	-
61.139	Beta-Bisabolene	00495-61-4	1506.875	1505	Benkaci-Ali et al. [63]	0.22	-	0.23	-	-	-
63.073-63.086	(+) - Delta-Cadinene	000483-76-1	1526.871	1521	Benkaci-Ali et al. [63]	0.57	-	0.28	-	-	-

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4A. Volatile compound profile of Pozol samples (Continued).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area					Aroma descriptor[b]
						PZ1	PZ2	PZ3	PZ4	PZ5	
67.057-67.083	Dodecanoic acid/ Lauric acid	000143-07-7	1568.331	1566.6	Zeng et al. [67]	0.29	0.82	0.39	1.55	1.1	-
68.804-68.817	Spathulenol	006750-60-3	1586.124	1580	Salido et al. [100]	0.59	-	0.25	-	-	-
68.804	Isolongifolene, 9,10-dehydro	067530-11-4	1586.124	-	-	-	-	-	0.31	-	-
71.094	Hexaethylene glycol	002615-15-8	1615.514	-	-	2.48	-	-	-	-	Sweet
89.161	n-Hexadecanoic acid/Palmitic acid	000057-10-3	1966.092	1963	Zeng et al. [67]	0.23	-	-	-	-	-
89.348	Dibutyl phthalate	000084-74-2	1970.663	1968.4	Zhao et al. [88]		-	0.07	-	-	Bitter
96.567	15-Crown-5	033100-27-5	2209.301	-	-	0.7	-	-	-	-	-
96.787	Hexanedioic acid, bis(2-ethylhexyl) ester	000103-23-1	2216.952	-	-	0.55	-	-	-	-	-
96.884	Squalene	007683-64-9	2220.325	-	-	-	0.31	-	-	-	-
100.326	Estigmastan-3,5-diene	1000214-16-4	2340.015	-	-	-	-	0.18	-	-	-
103.579	18-crown-6	017455-13-9	-	-	-	0.29	-	-	-	-	-

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4B. Volatile compounds in Chilate.

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area					Aroma descriptor[b]
						CH1	CH2	CH3	CH4	CH5	
4.68	Ethanol	000064-17-5	-	-	-	3.27	0.53	2.72	9.04	7.71	-
5.023	Ethyl ether	000060-29-7	-	-	-	0.42	0.18	-	-	-	-
6.077	2,3-Butanedione	000431-03-8	-	586	Wu et al. [50]	-	0.22	-	0.88	0.59	Butter, pastry, yeast
6.239-6.252	Hexane	000110-54-3	600.185	-	-	0.64	0.39	0.19	0.56	1.32	-
6.724	Acetic acid	000064-19-7	628.186	625	Isidorov et al. [61]; Avsar et al. [52]	-	0.47	1.21	1.24	2.88	Acid, fruit, spicy, sour, vinegar
6.951	Butanoic acid, 3-hydroxy	000300-85-6	629.998	-	-	0.81	-	-	-	-	-
8.051-8.076	Butanal, 2-methyl	000096-17-3	656.033	659	Jarunrattanasri et al. [53]	0.2	0.19	-	-	-	Herbaceous, fruit and nut
9.519	2-Pentanol	006032-29-7	700.75	706	Wu et al. [50]	-	-	0.51	-	-	-
10.224	2-Butanone, 3-hydroxy	000513-86-0	712.007	715	-	-	-	-	-	1.68	Butter, creamy, green pepper
11.544	2-Pentene	000109-68-2	733.083	-	-	0.27	-	-	-	-	-
11.589	1-Butanol, 3-methyl	000123-51-3	730.819	734	Engel and Ratel [47]	-	-	-	0.13	-	Alcohol, malt
11.595	Oxirane, 2-(1,1-dimethylethyl)-3-ethyl-	036099-44-2	733.897	-	-	-	-	0.18	-	0.27	-
15.729	Octane	000111-65-9	799.904	-	-	-	-	-	-	0.49	Gasoline
18.129	Furfural	000098-01-1	834.565	839	Weissbecker and Holighaus [58]	-	0.21	-	-	-	almond, baked potatoes, bread, burnt, spices
20.625	Benzene, 1,3-dimethyl-	000108-38-3	870.242	868	Isidorov et al. [101]	-	-	0.32	-	2.12	-
20.671-20.71	1-Hexanol	000111-27-3	871.83	874	Weissbecker and Holighaus [58]	1.17	-	-	0.47	-	Banana, flower, herb, grass
21.202	1-Butanol, 3-methyl-, acetate	000123-92-2	878.934	876	Pino et al. [56]	-	-	-	-	1.85	Apple, banana, pear
22.068-22.094	Styrene	000100-42-5	891.726	890	Pino et al. [56] Isidorov et al. [101]	0.5	0.26	0.45	0.38	1.11	Sweet and floral

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4B. Volatile compounds in Chilate (Continued).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area					Aroma descriptor[b]
						CH1	CH2	CH3	CH4	CH5	
22.76-22.858	2-Heptanol	000543-49-7	901.759	901.4	Tret'yakov [54]	0.25	-	0.22	-	1.01	Citrus, herbaceous, lemon, grass
23.433	Pyrazine, 2,5-dimethyl	000123-32-0	912.126	911	Pino et al. [56]	-	-	-	-	0.86	Cocoa, roast beef, toasted walnut
23.938	Pyrazine, 2,3-dimethyl	005910-89-4	920.059	918	Boulanger and Crouzet [94]	-	-	-	-	0.21	Caramel, cocoa, hazelnut, peanut butter, roasted
24.501-24.526	Alpha-Thujene	002867-05-2	929.202	926	Benkaci-Ali et al. [63]	0.95	0.72	1.75	1.03	0.71	Coriander, citrus
25.959-25.917	Camphene	000079-92-5	950.942	936	Couladis et al. [66]	0.92	1.67	1.12	0.63	0.56	oil-camphoraceous
26.635-26.654	Benzaldehyde	000100-52-7	962.723	965.6	Zeng et al. [67]	1.14	0.71	0.69	0.77	0.26	Sweet, almond
27.495-27.502	Sabinene	003387-41-5	975.934	977	Kundakovic et al. [69]	0.27	3.43	-	0.32	-	-
27.508	Beta-Thujene	028634-89-1	975.84	968	Radulović et al. [75]	-	-	-	0.47	0.29	-
27.508-27.689	Beta-Pinene	000127-91-3	978.887	975	Benkaci-Ali et al. [63]	0.68	0.17	0.87	0.97	0.44	Pine and wood
27.709-28.575	Beta-Myrcene	000123-35-3	992.899	990	-	1.33	0.59	1.21	0.54	-	Balsamic, fruit, geranium, herb
28.575-29.384	Alpha-Phellandrene	000099-83-2	1006.708	1001	Benkaci-Ali et al. [63]	6.31	0.99	6.44	5.59	3.43	Citrus, fresh, mint, pepper, spices and wood
29.74	(+)-3-Carene	000498-15-7	1012.489	-	Benkaci-Ali et al. [63]	0.52	4.54	0.46	-	-	Lemon
29.753	Delta-3-carene	013466-78-9	1012.821	1013	Kallio et al. [72]	-	0.32	-	-	-	Lemon
29.87	Hexyl acetate	000142-92-7	1014.766	1013	Shalit et al. [92]	-	-	-	-	0.27	Apple, banana, grass, herb, pear
30.122-30.141	(+) - 4-Carene	029050-33-7	1019.18	1022	Yang et al. [74]	4.25	-	-	-	2.31	-
30.154	2-Carene	000554-61-0	1019.74	-	-	-	-	-	4.95	-	-

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4B. Volatile compounds in Chilate (Continued).

Rt	Compound	CAS	Calculated IR	Reported IR	References[a]	% Area					Aroma descriptor[b]
						CH1	CH2	CH3	CH4	CH5	
30.173	Alpha-Terpinene	000099-86-5	1020.073	1015	Benkaci-Ali et al. [63]	-	-	5.4	-	-	Lemon
30.458	Benzene, 1-methyl-3-(1-methylethyl)	000535-77-3	1025.065	1023	Kallio et al. [72]	-	-	-	0.18	-	-
30.607-30.742	Benzene, 1-methyl-4-(1-methylethyl)	000099-87-6	1028.568	1027	Kallio et al. [72]	12.27	2.17	14.41	11.09	4.44	Fresh, citrusy
30.905-30.949	Beta.-Phellandrene	000555-10-2	1033.666	1028	Radulović et al. [75]	14.56	-	-	18.78	8.66	-
30.969-31.033	Beta-Terpinene	000099-84-3	1035.137	1036	Estévez et al. [76]	-	9.14	21.75	-	-	-
31.312-31.344	1(E) -Beta-Ocimene	003779-61-1	1040.357	1046	Belsito et al. [77]	0.29	0.28	0.3	0.29	0.22	Floral
31.707-31.732	Benzene Acetaldehyde	000122-78-1	1047.153	1050	Jarunrattanasri et al. [53]	0.43	-	0.23	0.24	0.27	-
31.745	(Z)-Beta-Ocimene	003338-55-4	1047.609	1050	Jarunrattanasri et al. [53]	-	0.99	-	-	-	-
31.92	Alpha-Ocimene	000502-99-8	1050.674	1052	Liu et al. [102]	-	-	-	-	0.17	-
31.931-31.933	Beta-Ocimene	013877-91-3	1050.902	1050	Agnihotri et al. [80]	0.31	-	0.31	0.28	-	Floral
31.925-31.931	Octane, 2,6-dimethyl	003338-55-4	1051.007	1040	Vagionas et al. [81]	-	0.36	0.25	-	-	-
32.275-32.605	Gamma-Terpinene	000099-85-4	1062.445	1060	Benkaci-Ali et al. [63]	0.64	0.3	0.83	0.75	0.63	Bitter and citrusy
32.774-32.786	Undecane, 2,9-dimethyl	017301-26-7	1065.843	-	-	-	-	0.24	0.21	-	-
33.007-33.019	Acetophenone	000098-86-2	1069.714	1069	Kallio et al. [72]	0.34	0.28	-	-	0.27	Bitter, wood, almonds, flower, meat, must
33.479	Sulfurous acid, 2-propyl tetradecyl ester	1000309-15-6	1077.982	-	-	-	-	0.4	-	-	-
33.68	Pyrazine, 2-ethyl-3,5-dimethyl	013925-07-0	1081.502	1081	Majcher and Jeleń [103]	-	-	-	-	0.54	Soil, Must, Walnut, Potato, Roast
34.119-34.125	Pyrazine, tetramethyl	001124-11-4	1088.859	1087.3	Andriamahavaro [84]	0.73	0.67	0.61	0.48	1.2	Cocoa, Coffee, Green, Moca, Roasted

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4B. Volatile compounds in Chilate (Continued).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area					Aroma descriptor[b]
						CH1	CH2	CH3	CH4	CH5	
34.261-34.274	Terpinolene	000586-62-9	1091.907	1089	Benkaci-Ali et al. [63]	1.06	-	1.05	1.04	-	Pine
34.326	Guaiacol	000090-05-1	1092.59	1092	Jarunrattanasri et al. [53]	-	1.15	-	-	-	Burnt, phenol, wood
34.346	2-Nonanone	000821-55-6	1093.168	1091	Skaltsa et al. [89]	-	-	-	-	1.11	Fruit
34.837-34.987	Linalool	000078-70-6	1102.329	1104	Hazzit et al. [83]	3.53	10.39	5.77	4.41	3.7	Coriander, Floral, Lavender, Lemon, Rose
35.031	n-Amyl isovalerate	025415-62-7	1105.678	1107	Tuberoso et al. [104]	0.22	-	-	-	-	Fruits
35.038	Butanoic acid, 2-methyl-, 2-methylbutyl ester	002445-78-5	1105.813	1106.1	Andriamahavaro [84]	-	-	-	0.12	-	Apple, berry, rum
35.678-35.821	Phenylethyl alcohol	000060-12-8	1118.498	1118.4	Zeng et al. [67]	1.08	0.83	0.71	0.66	0.84	Fruit, Honey, Lilac, Rose, Wine
36.396-37.056	2,4,6-Octatriene, 2,6-dimethyl-	007216-56-0	1131.703	1131	Andriamahavaro [84]	0.28	0.19	0.26	0.21	-	-
37.069	Allocimene	000673-84-7	1144.658	1142	Saroglou et al. [105]	-	0.07	-	-	-	-
38.052	2,3,5-Trimetil-6-etilpyrazine	017398-16-2	1163.83	1169	Ames et al. [55]	-	-	-	-	0.19	-
38.246-38.259	Benzenepropanal	000104-53-0	1167.68	1162	Buchin et al. [86]	0.76	-	0.3	0.27	-	-
39.074-39.08	Terpinen-4-ol	000562-74-3	1183.618	1175	Skaltsa et al. [89]	0.47	0.36	0.52	0.56	-	Soil, must, nutmeg, wood
39.553	2-Cyclohexen-1-one, 4-(1-methylethyl)	000500-02-7	1192.723	1186	Tsiri et al. [106]	-	-	0.14	-	-	Spices
39.734-39.74	Alpha-Terpineol	000098-55-5	1196.323	1190	Benkaci-Ali et al. [63]	0.45	0.68	0.51	0.47	-	Anise, fresh, mint, oil
39.941-39.947	Dodecan	000112-40-3	1200.294	-	-	-	0.07	0.1	0.08	0.61	-
41.771-41.797	3-Phenyl-1-propanol	000122-97-4	1234.329	1233	Shalit et al. [92]	-	0.22	0.26	0.21	-	Cinnamon, fruit
42.276	Phenyl ethyl acetate	000101-97-3	1243.142	1244	Pino et al. [56]	-	-	-	-	0.16	Floral, fruit, honey, roses

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4B. Volatile compounds in Chilate (Continued).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area					Aroma descriptor[b]
						CH1	CH2	CH3	CH4	CH5	
42.373	D-Carvone	002244-16-8	1244.926	1242	-	0.07	-	-	-	-	Basil, bitter, caraway, fennel, mint
42.878	2-Phenylethyl Acetate	000103-45-7	1254.217	1256	Pino et al. [56]	-	-	-	-	1.65	Flower, honey, rose
43.234-43.466	Nonanoic Acid	000112-05-0	1260.767	1272.1	Zeng et al. [67]	-	0.23	-	1.06	0.53	Fat and bitter
43.648-43.706	2-Propenal, 3-phenyl	000104-55-2	1268.383	1266	Benkaci-Ali et al. [63]	-	25.13	-	3.64	1.31	Spices
43.731-43.732	Cinamaldehyde, (E)	014371-10-9	1269.929	1266	Benkaci-Ali et al. [63]	6.15	-	3.86	-	-	Spices
44.547	2-Undecanone	000112-12-9	1284.923	1288	Shang et al. [107]	-	-	-	-	0.3	Fresh, green, orange
44.579	Safrole	000094-59-7	1285.511	1291.4	Zhao et al. [88]	0.11	-	-	-	-	Sweet
45.459-45.491	2-Propen-1-ol, 3-phenyl	000104-54-1	1301.701	1309	Mondello et al. [95]	-	1.16	1.48	4.04	-	-
45.776	Pyrazine, 2,5-dimethyl-3-propyl	018433-97-1	1307.533	-	-	-	-		-	0.3	-
48.337-48.421	Eugenol	000097-53-0	1354.65	1362.4	Zhao et al. [108]	0.82	1.81	-	-	0.44	Burnt, cloves, spices
48.369	Phenol, 2-methoxy-3-(2-propenyl)	001941-12-4	1355.238	1362	Mevy et al. [109]	-	-	0.69	0.69	-	-
48.642-48.735	N-decanoic acid	000334-48-5	1360.261	1368.2	Zeng et al. [67]	0.45	-	-	0.94	1.19	Dust, Fat, Grass
49.081	3-Phenyl-1-propanol, acetate	000122-72-5	1368.337	1373	Beaulieu and Grim [71]	-	-	-	-	0.25	Flowers
49.806-49.838	Alpha-Copaene	003856-25-5	1382.264	1379	Kundakovic et al. [68]	-	0.31	-	-	-	-
49.831	Alpha -Cubebene	017699-14-8	1382.136	1348	Radulović et al. [75]	1.17	-	-	0.63	0.36	-
50.84	Tetradecane	000629-59-4	1400.392	-	-	-	0.09	0.13	-	-	-
52.121-52.134	Isocaryophyllene	000118-65-0	1400.465	-	Benkaci-Ali et al. [63]	0.29	0.12	0.18	-	-	Fried, Spices
53.137	Caryophyllene	000087-44-5	1424.741	1419	Benkaci-Ali et al. [63]	4.9	7.03	5.54	-	1.61	Fried, Spices, Wood
55.194	Humulen-(v1)	005912-86-7	1445.409	1447	-	-	0.18	-	-	-	-

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4B. Volatile compounds in Chilate (Continued).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area					Aroma descriptor[b]
						CH1	CH2	CH3	CH4	CH5	
55.588-56.797	Alpha-Caryophyllene	006753-98-6	1461.983	1455	Benkaci-Ali et al. [63]	0.17	0.12	0.82	0.67	0.27	Fried, Spices, Wood
56.048	2-Propenal, 3-(2-methoxyphenyl)	001504-74-1	1454.239	1455	Benkaci-Ali et al. [63]	-	0.93	-	-	-	Fried, Spices, Wood
66.986-67.122	Dodecanoic acid/ Lauric acid	000143-07-7	1568.734	1566.6	Zeng et al. [67]	0.42	0.33	-	1.01	0.85	Spices

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4C. Volatile compounds in Cacahuatole.

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area			Aroma descriptor[b]
						CA1	CA2	CA3	
4.667-4.668	Ethanol	000064-17-5	-	-	-	1.28	2.75	1.29	-
6.207-6.22	Hexane	000110-54-3	599.381	-	-	0.08	0.26	-	-
7.708	Butanal, 3-methyl	000590-86-3	645.42	649	Jarunrattanasri et al. [53]	-	0.05	-	Apples
8.051	Butanal, 2-methyl	000096-17-3	656.033	659	Jarunrattanasri et al. [53]	0.08	-	-	-
9.454	2-Pentanol	006032-29-7	699.443	706	Wu et al. [50]	-	0.26	-	-
11.492	2-Pentene, (E)	000646-04-8	732.252	-	-	-	-	0.06	
11.511	Oxirane, 2-(1,1dimethylethyl)-3-methyl	053897-30-6	732.556	-	-	-	0.08	-	-
15.677-15.696	Octane	000111-65-9	799.377	-	-	-	0.2	0.21	Gasoline
15.761	Hexanal	000066-25-1	800.375	799	Jarunrattanasri et al. [53]	0.15	-	-	Apple, fat, oil
17.249-17.288	Pyrazine, methyl	000109-08-0	822.422	826	Cerny and Guntz- Dubini [82]	0.32	0.31	0.38	Cocoa, nutty
18.077-18.083	Furfural	000098-01-1	833.901	839	Weissbecker and Holighaus [58]	0.81	0.4	-	Almond, baked potatoes, bread, burnt, spices
19.824-19.882	2-Furanmethanol	000098-00-0	859.875	852	Siegmund and Murkovic [57]	0.22	0.46	0.3	Overcooked, burnt
19.992-20.024	Ethylbenzene	000100-41-4	861.464	857	Kotowska et al. [60]	0.05	-	0.06	Sweet, gasoline
20.542	Benzene, 1,3-dimethyl	000108-38-3	869.867	868	Isidorov et al. [101]	0.24	-	0.33	Sweet
21.169	1-Butanol, 3-methyl-, acetate	000123-92-2	878.457	876	Pino et al. [56]	-	0.12	-	Apple, banana, pear
22.029-22.042	Styrene	000100-42-5	891.062	890	Pino et al. [56]	0.29	0.62	0.23	Sweet and floral
22.146-22.178	o-Xylene	000095-47-6	892.564	894	Pino et al. [56]	0.09	-	0.1	Sweet
22.709	2-Heptanol	000543-49-7	900.754	901.4	Tret'yakov [54]	-	0.51	0.09	Citrus, herbaceous, lemon, grass
23.278-23.304	Pyrazine, 2,5-dimethyl	000123-32-0	909.692	911	Pino et al. [56]	1.29	1.38	0.92	Cocoa, roast beef, toasted Walnut
23.595-23.624	Pyrazine, ethyl	013925-00-3	914.671	915	Siegmund and Murkovic [59]	0.45	0.44	0.38	Peanut butter, nutty
23.834-23.86	Pyrazine, 2,3-dimethyl	005910-89-4	918.426	918	Boulanger and Crouzet [94]	0.15	0.16	0.14	Caramel, cocoa, hazelnut, peanut butter, toasted

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4C. Volatile compounds in Cacahuatole (Continue).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area			Aroma descriptor[b]
						CA1	CA2	CA3	
24.449-24.474	Alpha-Thujene	002867-05-2	928.086	926	Benkaci-Ali et al. [63]	0.33	1.25	0.33	Coriander, citrus
24.882	Alpha-Pinene	000080-56-8	934.888	934	Benkaci-Ali et al. [63]	-	-	0.56	Pine
24.908	1R-Alpha-Pinene	007785-70-8	935.296	935	Zeller & Rychlik [64]	0.54	2.77	-	Pine
25.846-25.859	Camphene	000079-92-5	950.235	936	Couladis et al. [66]	0.19	0.8	0.22	oil-camphoraceous
26.35	Cyclobut-1-enylmethanol	089182-08-1	957.948	-	-	0.08	-	-	-
26.577-26.603	Benzaldehyde	000100-52-7	961.922	965.6	Zeng et al. [67]	0.41	0.5	0.47	Sweet, almond
26.803	2-Furancarboxaldehyde, 5-methyl	000620-02-0	965.064	964	Pino et al. [56]	0.29	-	-	Caramel
27.437-27.456	Sabinene	003387-41-5	975.322	977	Kundakovic et al. [69]	0.09	0.2	0.11	-
27.638	(-)-Beta-Pinene	018172-67-3	978.023	979	-	-	-	0.21	-
27.651-27.657	Beta-Pinene	000127-91-3	978.479	975	Benkaci-Ali et al. [63]	0.19	0.8	-	Pine, wood
27.812-27.799	1-Octene-3-ol	003391-86-4	980.71	986	Hazzit et al. [83]	-	0.31	0.37	Cucumber, earth, fat, floral, mushroom
28.09	2,3-Octanedione	000585-25-1	985.281	980	Engel and Ratel [47]	0.13	-	-	Green
28.517	Beta-Terpinene	000099-84-3	991.988	1036	Estévez et al. [76]	-	0.86	-	-
28.66-28.685	Benzene, 1,2,4-trimethyl	000095-63-6	994.627	991	-	0.14	-	0.26	-
28.673	Benzene, 1,2,3-trimethyl	000526-73-8	994.439	994	Molo et al. [110]	-	0.26	-	-
29.339-29.378	Alpha-Phellandrene	000099-83-2	1005.692	1001	Benkaci-Ali et al. [63]	1.42	6.2	1.34	Citrus, fresh, mint, pepper, spices and wood
29.695	3-Carene	013466-78-9	1011.7	1010	Kallio et al. [72]	-	0.61	-	Lemon
29.792	Benzene, 1,3-dichloro	000541-73-1	1013.399	1014.97	Harangi [111]	-	-	0.16	-
30.07-30.08	Alpha-Terpinene	000099-86-5	1018.602	1015	Benkaci-Ali et al. [63]	0.89	-	0.85	Lemon
30.089	Beta-Terpinene	000099-86-5	1018.602	1015	Benkaci-Ali et al. [63]	-	1.81	-	Lemon

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4C. Volatile compounds in Cacahuatole (Continue).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area			Aroma descriptor[b]
						CA1	CA2	CA3	
30.555	Benzene, 1-methyl-2-(1-methylethyl)	000527-84-4	1026.764	1026	Vagionas et al. [81]	-	-	1.53	-
30.568	Benzene, 1-methyl-3-(1-methylethyl)	000535-77-3	1026.992	1023	Kallio et al. [72]	1.15	-	-	-
30.594	Benzene, 1-methyl-4-(methylethyl)	000099-87-6	1027.447	1027	Kallio et al. [72]	-	6.73	-	Fresh, citrus
30.846-30.885	Beta-Phellandrene	000555-10-2	1032.194	1028	Radulović et al. [75]	3.52	7.96	3.44	-
31.092	Decane, 3,7-dimethyl	017312-54-8	1036.171	-	-	0.31	-	-	-
31.098	Heptadecane, 2,6,10,15-tetramethyl	054833-48-6	1036.276	-	-	-	0.64	-	-
31.292	(E) -Beta-Ocimene	003779-61-1	1039.674	1046		-	0.31	-	Floral
31.668-31.674	Benzene Acetaldehyde	000122-78-1	1046.365	1050	Jarunrattanasri et al. [53]	0.23	0.31	0.21	-
31.881-31.887	Beta-Ocimene	013877-91-3	1049.991	1050	Agnihotri et al. [81]	0.07	-	0.12	Floral
31.887	Alpha-Ocimene	000502-99-8	1050.096	1052	Liu et al. [102)	-	0.2	-	-
32.217	Octane, 2,6-dimethyl	002051-30-1	1055.876	-	-	-	0.64	0.82	-
32.528-32.541	Gamma-Terpinene	000099-85-4	1061.551	1060	Benkaci-Ali et al. [63]	0.22	0.58	0.59	Bitter and citrusy
32.735	2,2,7,7-Tetramethyloctane	001071-31-4	1064.95	-	-	-	0.61	-	-
32.968-32.981	Acetophenone	000098-86-2	1069.031	1069	Kallio et al. [72]	0.26	0.37	-	Bitter, wood, almonds, flower, meat and must
33.427-33.433	Undecane, 2,8-dimethyl	017301-25-6	1077.071	-	-	0.29	0.62	-	-
33.628-33.634	Pyrazine, 3-ethyl-2,5-dimethyl	013360-65-1	1080.592	1078	Cerny and Guntz- Dubini [82]	0.92	0.9	-	-
33.621-34.061	Pyrazine, 2-ethyl-3,5-dimethyl	013925-07-0	1088.176	1088	Ames et al. [55]	0.33	-	1.15	Earth, nut, potato, roasted
33.932	Pyrazine, 2,6-diethyl	013067-27-1	1085.917	1089	Ames et al. [55]	0.19	-	-	-
34.048	Pyrazine, 3-ethyl-3,5-dimethyl	013925-07-0	1087.948	1081	Majcher and Jeleń [103]	-	-	0.73	Earth, must, walnut, potato, roast
34.21	2-Carene	000554-61-0	1090.786	-	-	-	0.28	0.41	-
34.223	Terpinolene	000586-62-9	1091.014	1089	Benkaci-Ali et al. [63]	0.38	0.96	-	Pine

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4C. Volatile compounds in Cacahuatole (Continue).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area			Aroma descriptor[b]
						CA1	CA2	CA3	
34.798-34.818	Linalool	000078-70-6	1101.193	1104	Hazzit et al. [83]	1.77	1.98	2.01	Coriander, floral, lavender, lemon, rose
35.018	Nonanal	000124-19-6	1105.428	1102	Saroglou et al. [98]	1.09	-	-	Fat, floral, green, lemon
35.607	Phenylethyl alcohol	000060-12-8	1116.766	1118.4	Zeng et al. [67]	-	0.47	-	Fruit, honey, lilac, rose, wine
36.04	Octanoic acid, methyl ester	000111-11-5	1125.101	1126	Pino et al. [56]	-	0.23	-	Fruit, orange, wax, wine
36.331	2,4,6-Octatriene, 2,6-dimethyl-, (E, Z)	007216-56-0	1130.702	1131	Andriamahavaro [84]	-	0.15	-	-
36.648	Pyrazine, 2-methyl-5-propyl	029461-03-8	1136.804	-	-	-	-	0.06	-
37.729-37.742	Pyrazine, 2,3-diethyl-5-methyl	018138-04-0	1157.728	1158	Steinhaus and Schieberle [85]	0.12	0.09	0.14	Earth, meat, potato,toasted
37.871-37.884	Pyrazine, 3,5-diethyl-2-methyl	018138-05-1	1160.346	1165	Ames et al. [55]	0.41	0.18	0.22	Baked, cocoa, toasted, rum
38.499	1-Decanol	000112-30-1	1172.435	-	-	-	-	0.62	Fat, oil
39.204-39.21	1H-Pyrrole, 1-(2-furanylmethyl)	001438-94-4	1186.121	1185	Andriamahavaro [84]	0.15	-	0.14	Cocoa, toasted
39.404-39.411	Naphthalene	000091-20-3	1189.855	1190.9	Zeng et al. [67]	-	0.1	0.19	-
39.682	Alpha-Terpineol	000098-55-5	1195.206	1190	Benkaci-Ali et al. [63]	-	-	0.12	Anise, fresh, mint, oil
40.038-40.064	Estragole	000140-67-0	1201.968	1198	Bruni et al. [112]	1.61	4.74	1.56	Anise, licorice
40.251	Decanal	000112-31-2	1205.887	1203	Saroglou et al. [98]	0.11	-	-	Floral, fried, orange peel
42.839-48.878	Benzaldehyde, 4-methoxy	000123-11-5	1254.217	1251	Pino et al. [56] Zeng et al. [67]	0.24	-	0.1	Almond, anise, mint
42.839-43.311	Nonanoic acid/ Pelargonic acid	000112-05-0	1262.183	1272.1	Zeng et al. [67]	0.22	0.11	-	Fat and bitter
43.66	Cinnamaldehyde, (E)	014371-10-9	1271.235	1266	Benkaci-Ali et al. [63]	2.06	0.98	0.26	Spices
44.495-44.637	Benzene, 1-methoxy-4-(1-propenyl)	000104-46-1	1287.406	1289.3	Zeng et al. [67]	58.24	24.19	56.18	Almond, anise, mint
45.362-45.407	2-Propen-1-ol, 3-phenyl	000104-54-1	1299.917	1309	Mondello et al. [95]	0.32	0.51	0.27	-
45.776-45.801	2-Methoxy-4-vinylphenol	007786-61-0	1307.993	1312	Pino et al. [56]	0.32	0.31	0.27	Clove, curry, spices

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4C. Volatile compounds in Cacahuatole (Continue).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area			Aroma descriptor[b]
						CA1	CA2	CA3	
47.238-47.244	Delta-Elemene	020307-84-0	1334.541	1339	Radulović et al. [75]	0.14	-	0.08	-
48.298-48.311	Eugenol	000097-53-0	1354.171	1362.4	Zhao et al. [108]	0.55	0.95	0.5	Burnt, cloves, spices
49.366-49.405	Propanoic acid, 2-methyl-, 2-ethyl-3-hydroxyhexyl ester	074367-31-0	1375.581	1373	Gómez et al.[113]	-	0.2	0.24	-
49.773	Alpha.-Cubebene	017699-14-8	1381.179	1348	Radulović et al. [75]	0.12	-	-	-
49.76-49.767	Copaene	003856-25-5	1380.829	1379	Kundakovic et al. [69]	-	0.57	0.13	-
50.032-50.038	2-Propanone, 1- (4-methoxyphenyl)	000122-84-9	1385.833	1384	Zeller & Rychlik [64]	0.07	-	0.06	-
52.089	2,4,7,9-Tetramethyl-5-decyn-4,7-diol	000126-86-3	1413.306	1407.3	-	0.13	-	-	-
53.072-53.105	Caryophyllene	000087-44-5	1423.542	1419	Benkaci-Ali et al. [63]	0.53	2.82	0.54	Fried, spices, wood
54.534-54.554	2-Propen-1-ol, 3-phenyl-, acetate	000103-54-8	1438.792	1440	Vahirua-Lechat et al. [114]	0.37	0.12	0.22	Floral, fruit, honey
55.595	1H-Benzocycloheptene, 2,4a, 5,6,7,8, 9,9a-octahydro-3,5,5-trimethyl-9-methylene	080923-88-2	1449.555	-	-	-	-	0.15	-
55.601	(-) - Alpha-Himachalen	003853-83-6	1449.617	1450	Benkaci-Ali et al. [63]	0.17	-	-	-
55.925-55.931	Alpha-Caryophyllene	006753-98-6	1453.029	1455	Benkaci-Ali et al. [63]	0.08	0.37	-	Fried, spices, wood
58.26	Dodecanoic acid/ Lauric acid	000143-07-7	1477.109	1477	-	-	0.56	-	-
58.286	(-) - Alloaromadendrene	025246-27-9	1477.378	1477	-	1.13	-	-	-
59.547	(-) - Zingiberene	000495-60-3	1490.415	1493	-	0.16	-	-	-
66.708	Hexadecanoic acid, methyl ester	000143-07-7	1564.454	1566.6	-	-	0.13	-	-
87.757	1,2-Benzenedicarboxylic acid, butyl	000112-39-0	1931.768	1928.1	-	-	0.06	-	Oil

[a] References for reported RI. [b] Most frequently associated odors [37].

Table S4C. Volatile compounds in Cacahuatole (Continue).

Rt	Compound	CAS	Calculated RI	Reported RI	References[a]	% Area			Aroma descriptor[b]
						CA1	CA2	CA3	
89.057	Ácido n-hexadecanoico/Palmitico	000057-10-3	1963.549	1963	-	0.06	-	-	-
89.303	11-octadecenoic acid, methyl ester	017851-53-5	1969.563	-	-	-	0.06	-	-
94.426	9,12-Octadecadienoic acid, methyl ester, (E, E)	002566-97-4	-	-	-	-	-	0.23	-
94.679	9-Octadecenoic acid (Z)-, methyl ester	000112-62-9	-	-	-	-	-	0.31	-
94.679	9-Octadecenoic acid, methyl ester, (E)	001937-62-8	2143.649	2110.9	Tret'yakov [54]	0.07	-	-	-
94.685	Methyl 11-octadecenoate	001937-63-9	-	-	Tret'yakov [54]	-	0.49	-	-

[a] References for reported RI. [b] Most frequently associated odors [37].