

Supplement

Utilization of Industrial *Rosa damascena* Mill. By-products and Cocoa Pod Husks as Natural Preservatives in Muffins

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Table S1 GC-MS analysis of RDCO2 and CPH extracts: aroma substances

Compound	RI	RDCO2	CPH
		% of TIC	
Hexanal	800	-	9.26 ± 0.21
α -Pinene	940	0.80 ± 0.05 ^a	7.06 ± 0.33 ^b
Benzaldehyde	961	-	1.42 ± 0.08
Sabinene	976	-	7.12 ± 0.12
β -Pinene	980	0.57 ± 0.06 ^a	2.53 ± 0.10 ^b
β -Myrcene	991	0.31 ± 0.10	-
3-Octanol	993	-	0.60 ± 0.06
2-Octanol	998	-	0.34 ± 0.08
α -Phellandrene	1005	-	7.40 ± 0.15
<i>o</i> -Cymene	1022	-	2.85 ± 0.13
Limonene	1029	-	1.50 ± 0.10
β -Phellandrene	1031	-	5.32 ± 0.18
γ -Terpinene	1062	0.83 ± 0.08	-
Terpinolene	1087	0.62 ± 0.11	-
β -Linalool	1097	2.47 ± 0.10 ^a	3.25 ± 0.21 ^b
Phenethyl alcohol	1110	17.22 ± 0.16	-
cis-Rose oxide	1112	0.40 ± 0.07	-
trans-Rose oxide	1127	0.23 ± 0.04	-
Terpin-4-ol	1178	1.24 ± 0.10	-
β -Citronellol	1228	6.45 ± 0.15	-
Nerol	1230	3.47 ± 0.09	-
Geraniol	1255	2.50 ± 0.12	-
Thymol	1289	-	1.62 ± 0.06
Eugenol	1356	0.18 ± 0.04	-
Geranyl acetate	1383	2.60 ± 0.14	-

Compound	RI	RDCO2	CPH	
			% of TIC	
Neryl acetate	1365	1.92 ± 0.18	-	-
Methyl eugenol	1401	0.40 ± 0.04	-	-
β -Bourbonene	1383	2.90 ± 0.09	-	-
β -Cubebene	1389	5.41 ± 0.12	-	-
β -Elemene	1390	0.46 ± 0.06	-	-
β -Caryophyllene	1419	1.45 ± 0.11 ^a	1.25 ± 0.14 ^a	-
α -Humulene (α -Caryophyllene)	1454	0.31 ± 0.07	-	-
Germacrene D	1479	0.36 ± 0.09	-	-
α -Farnesene	1508	0.52 ± 0.10	-	-
β -Bisabolene	1510	0.17 ± 0.02	-	-
trans-Nerolidol	1564	4.39 ± 0.06	-	-
Spathulenol	1575	1.50 ± 0.14	-	-
Caryophyllene oxide	1580	0.30 ± 0.07 ^a	0.15 ± 0.04 ^b	-
γ -Eudesmol	1631	0.27 ± 0.05	-	-
β -Eudesmol	1649	0.23 ± 0.06	-	-
α -Eudesmol	1652	0.81 ± 0.11	-	-
Farnesol	1714	0.31 ± 0.03	-	-
<i>n</i> -Nonadecane	1901	16.69 ± 0.16	-	-
<i>n</i> -Eicosane	2000	0.12 ± 0.04	-	-
10-Heneicosene	2093	3.51 ± 0.08	-	-
<i>n</i> -Heneicosane	2100	5.25 ± 0.15	-	-
<i>n</i> -Docosane	2200	0.68 ± 0.18	-	-
<i>n</i> -Tricosane	2300	4.09 ± 0.21	-	-
<i>n</i> -Tetracosane	2400	1.47 ± 0.14	-	-
<i>n</i> -Pentacosane	2500	1.30 ± 0.10	-	-
<i>n</i> -Hexacosane	2600	1.30 ± 0.09	-	-

RDCO2 - waste from CO₂ extracted *Rosa damascena* Mill.

CPH - Cocoa Pod Husks

RI - Relativ Index (Kovats retention index)

% of TIC - percent of Total Ion Current

The results were expressed as mean ±SD (*n* = 3)

^{a, b} - Values with different letters in superscript (a, b) in a column are statistically significant (ANOVA, Tuckey's post hoc test, *p* < 0.05).

With the letter a are denoted the highest determined value, and with the letter b – the lowest value. The values denoted with different letters (a, b) are different with level of significance *p* < 0.05, meaning that 95 % of the determined results differ.

Table S2 GC-MS analysis of RDCO2 and CPH extracts: non-volatile substances

Compound	RI	RDCO2	CPH	
			% of TIC	
<i>L</i> -Valine	1228	0.67 ± 0.12 ^a	1.83 ± 0.14 ^b	-
Glycerol	1266	0.80 ± 0.14 ^a	2.91 ± 0.09 ^b	-
<i>L</i> -Leucine	1272	0.44 ± 0.08 ^a	2.00 ± 0.10 ^b	-
Phosphoric acid	1278	7.56 ± 0.32	-	-
<i>L</i> -Isoleucine	1299	0.31 ± 0.04 ^a	1.55 ± 0.08 ^b	-
<i>L</i> -Proline	1307	1.74 ± 0.09 ^a	2.88 ± 0.15 ^b	-
Succinic acid	1310	5.02 ± 0.11 ^a	9.94 ± 0.19 ^b	-
<i>o</i> -Hydroxybenzoic acid	1326	-	7.76 ± 0.12	-
Fumaric acid	1355	1.11 ± 0.06 ^a	5.10 ± 0.10 ^b	-
Serine	1362	0.81 ± 0.10 ^a	1.53 ± 0.11 ^b	-
<i>L</i> -Threonine	1390	0.37 ± 0.07 ^a	1.19 ± 0.09 ^b	-
<i>L</i> -Homoserine	1446	0.19 ± 0.03	-	-
Malic acid	1488	8.38 ± 0.15 ^a	6.68 ± 0.19 ^b	-
Salicylic acid	1516	0.51 ± 0.10	-	-

Compound	RI	RDCO2	CPH
			% of TIC
Pyroglutamic acid	1512	0.63 ± 0.06 ^a	8.49 ± 0.08 ^b
<i>L</i> -Aspartic acid	1531	0.69 ± 0.09 ^a	7.84 ± 0.12 ^b
<i>L</i> -Threonic acid	1528	0.33 ± 0.04	-
4-Aminobutyric acid	1542	-	15.43 ± 0.18
<i>p</i> -Hydroxybenzoic acid	1621	-	7.66 ± 0.21
<i>L</i> -Glutamic acid	1629	-	10.41 ± 0.16
<i>L</i> -Phenylalanine	1646	1.17 ± 0.11 ^a	6.18 ± 0.19 ^b
<i>L</i> -Asparagine	1682	0.11 ± 0.02	-
<i>L</i> -Lysine	1737	0.17 ± 0.05	-
Ribonic acid	1756	0.71 ± 0.09	-
Vanillic acid	1758	0.53 ± 0.10 ^a	16.11 ± 0.17 ^b
Protocatechuic acid	1813	0.65 ± 0.08 ^a	32.51 ± 0.28 ^b
Isocitric acid	1839	-	7.22 ± 0.17
Quinic acid	1843	0.34 ± 0.07	-
Fructose isomer	1862	25.06 ± 0.23 ^a	7.78 ± 0.34 ^b
Fructose isomer	1868	38.55 ± 0.41 ^a	4.49 ± 0.47 ^b
Fructose isomer	1875	13.04 ± 0.20	-
Galactose isomer	1884	26.37 ± 0.19 ^a	6.55 ± 0.29 ^b
Syringic acid	1888	8.65 ± 0.11	-
Glucose isomer	1896	90.09 ± 0.28 ^a	17.77 ± 0.34 ^b
Galactose isomer	1907	14.42 ± 0.21 ^a	3.67 ± 0.35 ^b
Glucose isomer	1916	12.63 ± 0.19 ^a	13.40 ± 0.30 ^a
<i>p</i> -Coumaric acid	1920	-	15.91 ± 0.18
Glucitol	1930	64.65 ± 0.24 ^a	9.72 ± 0.29 ^b
Gallic acid	1968	35.96 ± 0.18	-
Gluconic acid	1991	26.57 ± 0.26	-
Palmitic acid	2039	5.61 ± 0.17 ^a	8.46 ± 0.26 ^b
Glucaric acid	2013	10.58 ± 0.15 ^a	8.75 ± 0.24 ^b
Ferulic acid	2069	-	23.16 ± 0.31
Myo-Inositol	2090	19.42 ± 0.20	-
Stearic acid	2132	0.99 ± 0.14 ^a	7.43 ± 0.19 ^b
Caffeic acid	2140	4.61 ± 0.16 ^a	16.32 ± 0.24 ^b
Linoleic acid	2209	8.41 ± 0.26	-
Linolenic acid	2217	6.73 ± 0.12	-
Sucrose isomer; α -D-Glc-(1,2)- β -D-Fru	2649	2.17 ± 0.14 ^a	39.01 ± 0.31 ^b
Sucrose isomer; α -D-Glc-(1,2)- β -D-Fru	2660	4.24 ± 0.10 ^a	15.76 ± 0.29 ^b
Sucrose isomer; α -D-Glc-(1,2)- β -D-Fru	2674	1.31 ± 0.11	-
Catechin	3222	3.64 ± 0.14 ^a	55.38 ± 0.41 ^b
Epicatechin	3228	-	45.71 ± 0.21
Stigmasterol	3315	1.91 ± 0.12	-
β -Sitosterol	3355	2.05 ± 0.13	-

RDCO2 - waste from CO₂ extracted *Rosa damascena* Mill.

CPH - Cocoa Pod Husks

RI - Relativ Index (Kovats retention index)

% of TIC- percent of Total Ion Current

The results were expressed as mean ±SD ($n = 3$)

^{a, b} - Values with different letters in superscript (a, b) in a column are statistically significant (ANOVA, Tuckey's post hoc test, $p < 0.05$). With the letter a are denoted the highest determined value, and with the letter b – the lowest value. The values denoted with different letters (a, b) are different with level of significance $p < 0.05$, meaning that 95 % of the determined results differ.

Table S3 Inhibition of microorganisms' development in presence of extracts of RDCO2 and CPH waste

Microorganism		Control	RDCO2	CPH
<i>Escherichia coli</i> ATCC 25922, 1.0×10^{12} cfu/cm ³	IZ, mm	-	10.0 ± 0.3 ^a	9.0 ± 0.5 ^a
	MIC, µg/ml	-	60	600
<i>Proteus vulgaris</i> ATCC 6380, 5.0×10^{11} cfu/cm ³	IZ, mm	-	10.0 ± 0.3 ^a	9.0 ± 0.0 ^b
	MIC, µg/ml	-	> 60	600
<i>Pseudomonas aeruginosa</i> NBIMCC 1370, 7.5×10^{11} cfu/cm ³	IZ, mm	-	9.0 ± 0.0 ^a	10.0 ± 0.2 ^b
	MIC, µg/ml	-	600	600
<i>Staphylococcus aureus</i> ATCC 25923, 4.0×10^8 cfu/cm ³	IZ, mm	-	11.0 ± 1.0 ^a	9.0 ± 0.5 ^b
	MIC, µg/ml	-	< 600	600
<i>Enterococcus faecalis</i> ATCC 19433, 8.0×10^{11} cfu/cm ³	IZ, mm	-	10.5 ± 0.5 ^a	10.0 ± 0.7 ^a
	MIC, µg/ml	-	60	600
<i>Listeria monocytogenes</i> ATCC 19111, 4.9×10^9 cfu/cm ³	IZ, mm	-	17.0 ± 1.0 ^a	10.0 ± 0.2 ^b
	MIC, µg/ml	-	60	600
<i>Salmonella abony</i> NTCC 6017, 2.0×10^8 cfu/cm ³	IZ, mm	-	10.0 ± 0.2 ^a	9.0 ± 0.5 ^a
	MIC, µg/ml	-	600	600
<i>Candida albicans</i> NBIMCC 74, 2.0×10^{10} cfu/cm ³	IZ, mm	-	9.5 ± 0.5 ^a	9.0 ± 0.0 ^a
	MIC, µg/ml	-	600	600
<i>Candida utilis</i> ATCC 42402, 4.6×10^8 cfu/cm ³	IZ, mm	-	13.5 ± 0.2 ^a	10.0 ± 0.2 ^b
	MIC, µg/ml	-	< 600	600
<i>Aspergillus niger</i> ATCC 1015, 1.4×10^7 cfu/cm ³	IZ, mm	-	10.0 ± 0.0 ^a	9.5 ± 0.5 ^a
	MIC, µg/ml	-	600	600
<i>Penicillium chrysogenum</i> ATCC 28089, 1.5×10^7 cfu/cm ³	IZ, mm	-	9.5 ± 0.5 ^a	9.5 ± 0.5 ^a
	MIC, µg/ml	-	600	600
<i>Bacillus subtilis</i> ATCC 19659, 1.0×10^9 cfu/cm ³	IZ, mm	-	10.5 ± 0.5 ^a	11.0 ± 0.0 ^a
	MIC, µg/ml	-	60	60
<i>Fusarium moniliforme</i> ATCC 38932, 1.0×10^7 cfu/cm ³	IZ, mm	-	10.0 ± 0.0 ^a	11.0 ± 0.2 ^b
	MIC, µg/ml	-	600	< 600
<i>Rhizopus arrhizus</i> ATCC 11145, 4.0×10^6 cfu/cm ³	IZ, mm	-	9.5 ± 0.5 ^a	9.5 ± 0.5 ^a
	MIC, µg/ml	-	600	600

RDCO2 - waste from CO₂ extracted *Rosa damascena* Mill.

CPH - Cocoa Pod Husks

IZ - Inhibition Zone

MIC - Minimal Inhibition Concentration

cfu - colony forming units

The results were averaged of 4 repetitions ±SD

^{a,b} - Values with different letters in superscript (a, b) in a column are statistically significant (ANOVA, Tuckey's post hoc test, $p < 0.05$).

With the letter a are denoted the highest determined value, and with the letter b – the lowest value. The values denoted with different letters (a, b) are different with level of significance $p < 0.05$, meaning that 95 % of the determined results differ.

Table S4 Shear stress range (D); yield stress (τ_0), consistency index (k), flow index (n) and coefficient of determination (R^2) of muffin batters

Sample	D , s ⁻¹	τ_0 , Pa	k , Pa · s ⁿ	n	R^2 , %
C1	0.17 ÷ 3.4	5.45 ± 0.11 ^a	68.53 ± 0.26 ^a	0.49 ± 0.08	99.8
C2	0.17 ÷ 3.4	3.26 ± 0.08 ^b	46.21 ± 0.33 ^b	0.43 ± 0.07	99.9
V1	0.17 ÷ 3.4	3.23 ± 0.10 ^b	44.31 ± 0.35 ^b	0.44 ± 0.06	99.9
V2	0.17 ÷ 3.4	6.39 ± 0.11 ^c	51.43 ± 0.29 ^c	0.45 ± 0.09	99.9
V3	0.17 ÷ 3.4	7.18 ± 0.12 ^d	50.75 ± 0.28 ^c	0.51 ± 0.08	99.8

The results were expressed as mean ±SD ($n = 3$)

^{a,b,c,d} - Values with different letters in superscript (a, b, c, d) in a column are statistically significant (ANOVA, Tuckey's post hoc test, $p < 0.05$). With the letter a are denoted the highest determined value, and with the letter d – the lowest value; the others denotes values in between a and d. The values denoted with different letters (a, b, c, d) are different with level of significance $p < 0.05$, meaning that 95 % of the determined results differ.

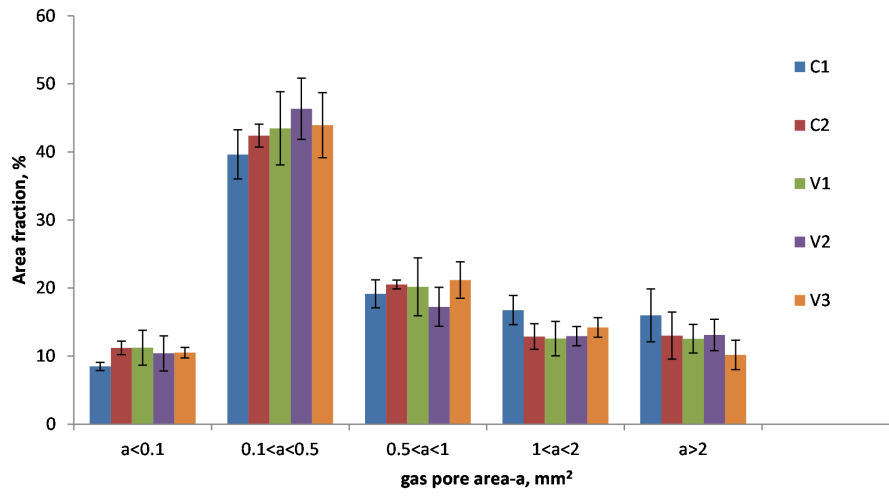


Fig. S1 Image analysis of muffins: gas pore area distribution pattern