Supplementary Information

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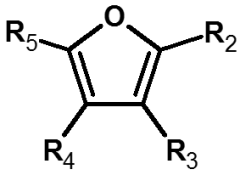
Figure S6: Percent loss of furan (A), 2-methylfuran (B), 3-methylfuran (C) and 2,5-dimethylfuran (D) in coffee brewed from a fully automatic, filter or capsule machine cooled over time in ceramic cups

32 **Table S1:** Structure and boiling points of furan derivatives



Compound	R_2	R_3	R_4	R_5	Bp[1], °C
Furan	H	H	H	H	32
2-methylfuran	CH_3	H	H	H	62
3-methylfuran	H	CH_3	H	H	66
2,5-dimethylfuran	CH_3	H	H	CH_3	94
2,3-dimethylfuran	CH_3	CH_3	H	H	42

[1]Bp = boiling point

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35 **Table S2:** LOD and LOQ for furan for furan, 2-methylfuran, 3-methylfuran and 2,5-dimethylfuran in coffee

36 prepared from a filter, fully automatic or capsule machine

Compound	Concentration in ng/mL					
	Filter		Fully Automatic		Capsule	
	Ceramic	Disposable	Ceramic	Disposable	Ceramic	Disposable
Furan						
LOD	5.77	0.57	7.12	10.88	2.40	3.52
LOQ	17.49	1.72	21.56	32.97	7.28	10.68
2-methylfuran						
LOD	18.99	1.03	16.86	21.24	10.66	6.68
LOQ	57.55	3.13	51.09	64.35	32.30	20.24
3-methylfuran						
LOD	2.55	0.04	0.90	3.70	0.57	0.43
LOQ	7.73	0.13	2.71	11.21	1.73	1.29
2,5-dimethylfuran						
LOD	0.58	0.10	0.48	1.99	0.91	0.30
LOQ	1.75	0.31	1.47	6.02	2.75	0.90

37

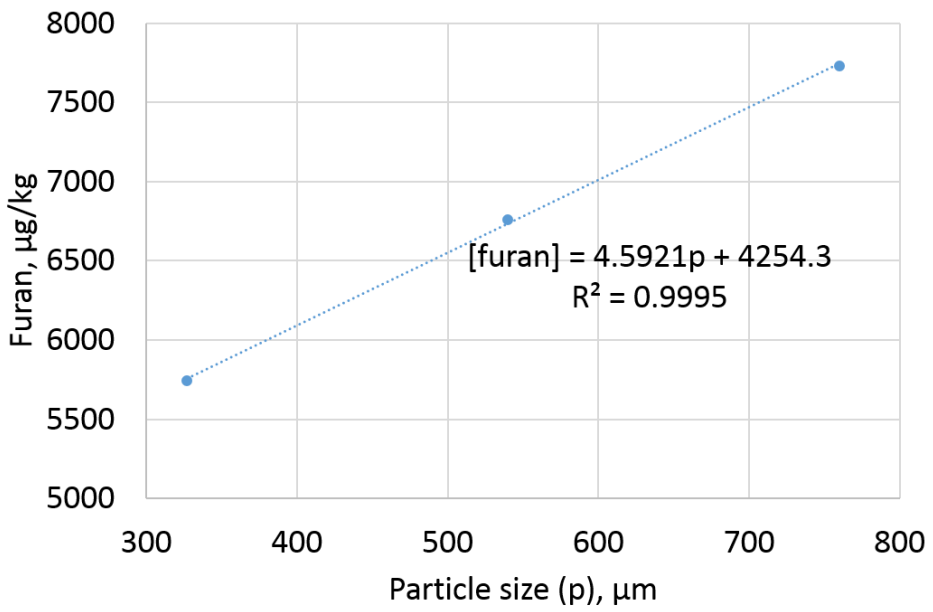


Figure S1: Relationship between mean particle size and furan content found within whole beans

Table S3: Yield of furan derivatives according to brewing method for black coffee prepared in a ceramic cup

Brewing Method	Coffee, g	Brew, mL	Furan			2-methylfuran			3-methylfuran			2,5-dimethyfuran		
			Conc., ng/mL			Conc., ng/mL			Conc.' ng/mL			Conc., ng/mL		
			Theoretical[a]	Actual	Yield, %	Theoretical[a]	Actual	Yield, %	Theoretical[a]	Actual	Yield, %	Theoretical[a]	Actual	Yield, %
Filter	48	804	398.0	47.3	11.9	1029.8	127.8	12.4	49.2	5.8	11.7	63.7	3.9	6.2
Fully Automatic	9	125	480.0	99.0	20.6	1242.0	263.9	21.3	59.4	13.2	22.1	76.8	8.4	11.0
Capsule	6	125	102.8	33.5	32.6	250.8	103.4	41.2	-	4.6	-	23.2	2.6	11.2
Soluble	2	125	11.9	-	0.0	40.0	-	0.0	4.3	-	0.0	3.6	-	0.0

conc. = concentration; [a]-calculated from whole beans

Table S4: Dunn test results demonstrating the significant difference between furan derivative concentrations between brewing methods and vessels

Coffee Preparations	Furan	2-methylfuran	3-methylfuran	2,5-dimethylfuran
Capsule Ceramic	a b	A B	f	F
Capsule Disposable	a	A	f	
Filter Ceramic	C d	B C	g	G
Filter Disposable	b C	B C	g	F G
Fully Automatic Ceramic	e	D	h	H
Fully Automatic Disposable	d e	C D	g h	G

Table S5: Concentration of furan derivatives per cup of freshly brewed coffee

	Concentration of furan derivatives per ceramic cup, µg/125mL (furan ratio[a])		
	Filter [b]	**Fully Automatic** [b]	**Capsule** [c]
furan	5.9	12.4	4.2
2-methylfuran	16.0 (2.70)	33.0 (2.66)	12.9 (3.09)
3-methylfuran	0.7 (0.12)	1.6 (0.13)	0.6 (0.14)
2,5-dimethylfuran	0.5 (0.08)	1.1 (0.09)	0.3 (0.08)
Brew Ratio, g brew/g coffee	16.8	13.9	20.8

[a] furan derivative concentration divided by the concentration of the parent furan; [b]- at 75°C; [c]- at 65°C

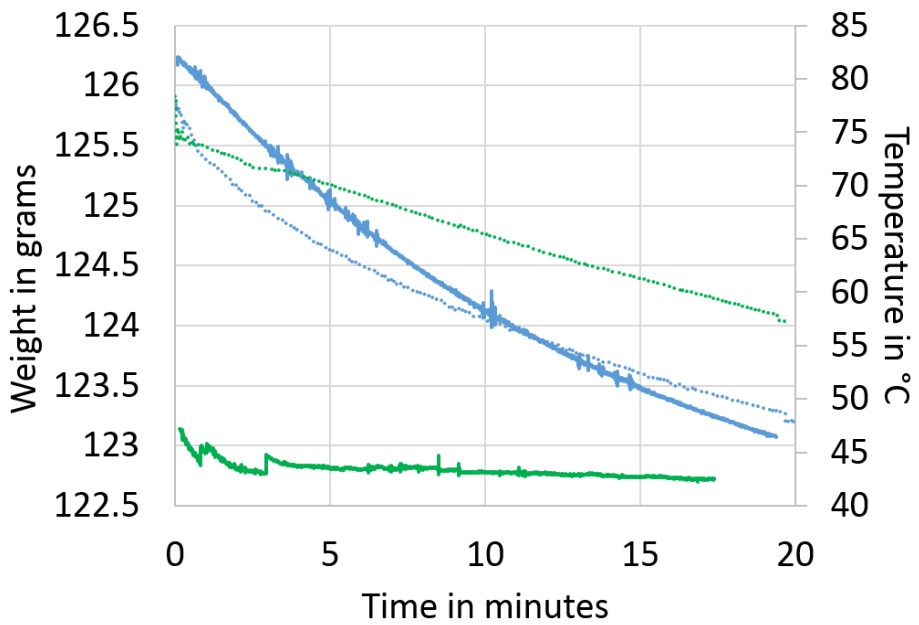
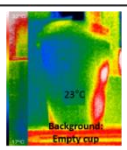
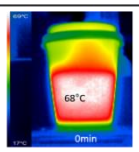
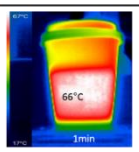
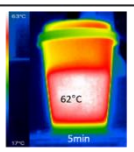
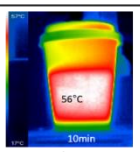
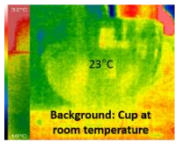
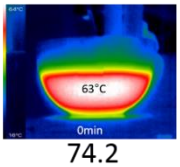
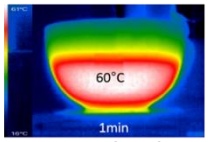
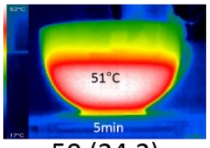
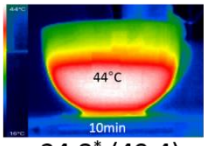
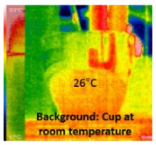
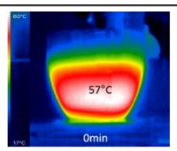
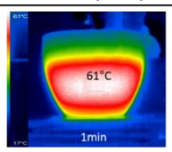
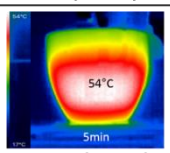
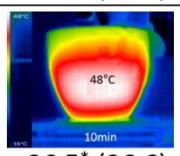
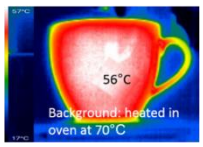
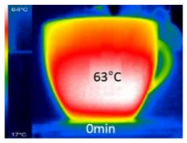
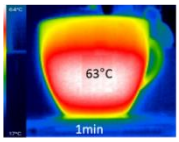
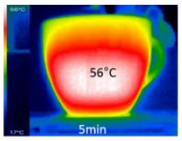
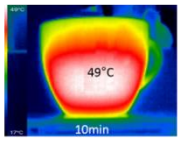


Figure S2: Weight loss (solid line) and temperature (dashed lines) monitored over cooling time of coffee prepared from a fully automatic machine in either a ceramic (blue) or Disposable (green) cup

Table S6: Average concentration of furan derivatives per cup of coffee at 55-60°C

Coffee preparations	Concentration in µg/125 mL				
	furan	**2-methylfuran**	**3-methylfuran**	**2,5-dimethylfuran**	**Total**
Filter Disposable	4.06	9.83	0.54	0.31	14.74
Filter Ceramic	4.78	13.27	0.60	0.41	19.06
Fully Automatic Ceramic	10.52	28.87	1.28	0.98	41.65
Fully Automatic Disposable	6.55	14.83	0.62	0.33	22.33
Capsule Ceramic	4.01	11.67	0.51	0.30	16.49
Capsule Disposable	2.18	5.71	0	0.00	7.89

Table S7: Infrared temperature mapping of external and internal cup temperatures during fully automatic coffee cooling

Cup Type	Background	Temperature of coffee (below IR picture) versus cup temperature (on IR picture) in °C ($\Delta T = T_{t=0}-T_t$)			
Disposable cup with lid		 78.3	 75.1 (3.2)	 65.0 (13.3)	 54.8* (23.5)
Café au lait		 74.2	 66.4 (7.8)	 50 (24.2)	 24.8* (49.4)
Experiment Cups: 26°C cup		 73.1	 68.5 (4.6)	 55.4 (17.7)	 36.5* (36.6)
Experiment Cups: Cup heated at 70°C cup		 77.7	 72.2 (5.5)	 57.2 (20.5)	 36.5* (41.2)

*** calculated from trendlines fitted to cooling curves obtained from thermocouple monitoring**

Table S8: Dunn test results demonstrating the significant difference between percent loss of furan derivative between brewing methods and vessels

Coffee Preparations	Furan				2-methylfuran				3-methylfuran		2,5-dimethylfuran	
Capsule Ceramic	a		A						c		F	
Capsule Disposable	a	b	A	B					c	d		
Filter Ceramic		b		B	C	D			c	d	F	G
Filter Disposable		b			C	D				d	F	G
Fully Automatic Ceramic		b				D	E		c	d	F	G
Fully Automatic Disposable		b					E			d		G

Table S9: Dunn test results demonstrating the significant difference between furan derivative loss upon cooling

Temperature, °C	Furan				2-methylfuran				3-methylfuran				2,5-dimethylfuran			
75	a				A				e				F			
70	a	b			A	B			e	f			F	G		
65	a	b				B	C			f	g		F	G	H	
60		b	c			B	C	D			g	h		G	H	I
55			c	d			C	D	E		g	h			H	I
50			c	d				D	E			h			H	I
35				d					E			h				I

Table S10: Dunn test results demonstrating the significant difference between furan derivative concentrations upon cooling

Temperature, °C	Furan				2-methylfuran				3-methylfuran				2,5-dimethylfuran			
75	a				A				e				F			
70	a	b			A	B			e	f			F	G		
65	a	b				B	C			f	g		F	G	H	
60		b	c			B	C	D			g	h		G	H	I
55			c	d			C	D	E		g	h			H	I
50			c	d				D	E			h			H	I
35				d					E			h				I

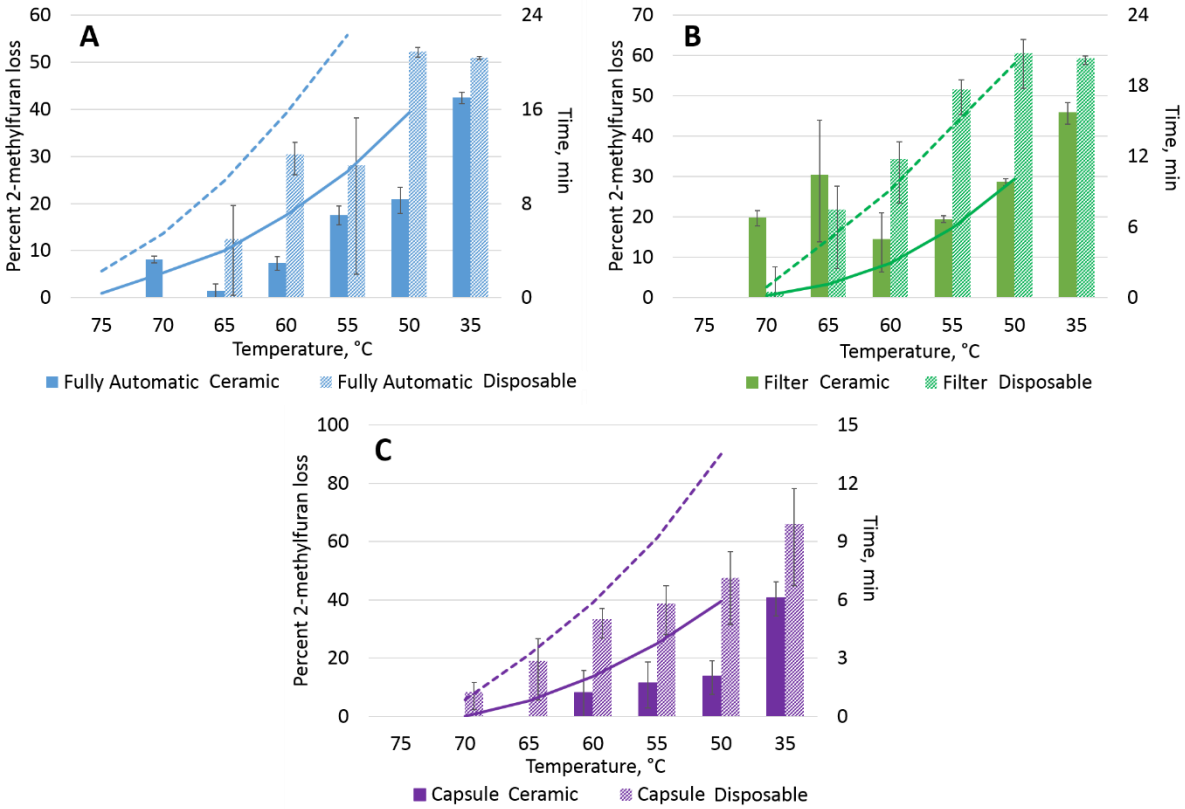


Figure S3: 2-methylfuran loss in coffee upon cooling comparison between ceramic and disposable cups prepared from either a fully automatic (A), filter (B) or capsule (C) machine

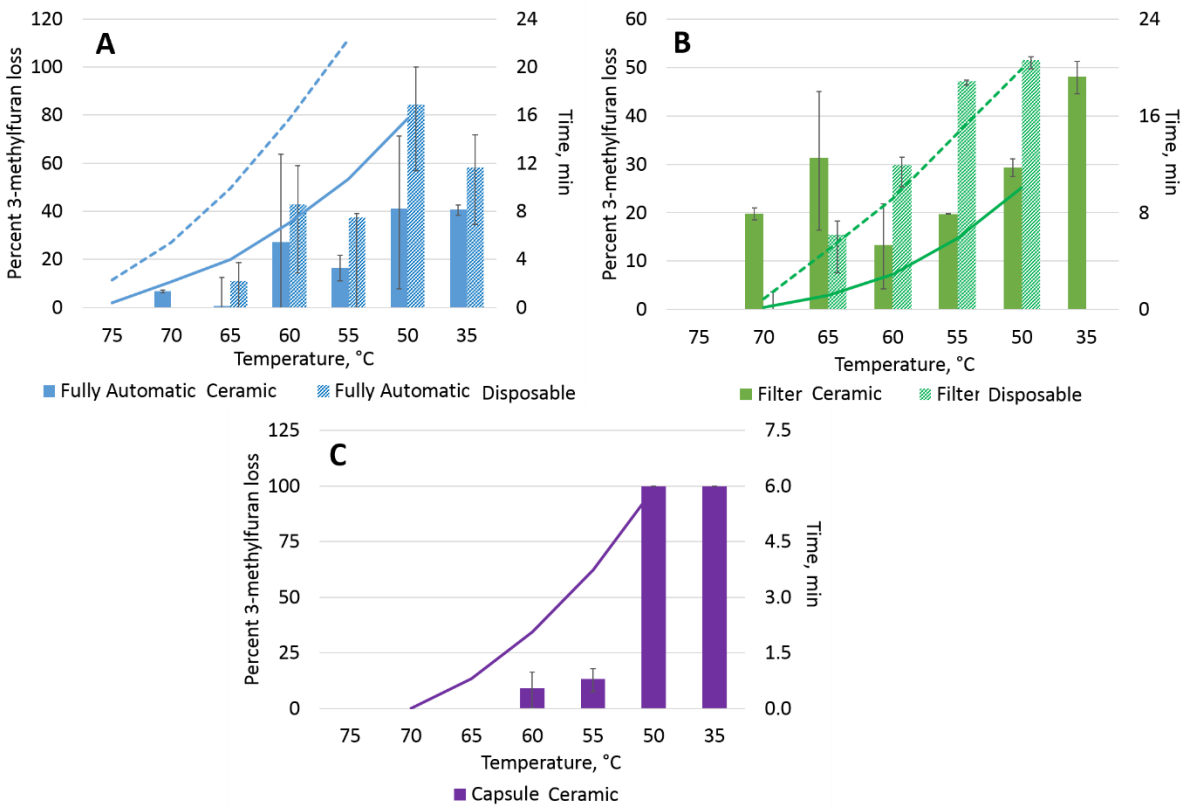


Figure S4: 3-methylfuran loss in coffee upon cooling comparison between ceramic and disposable cups prepared from either a fully automatic (A), filter (B) or capsule (C) machine

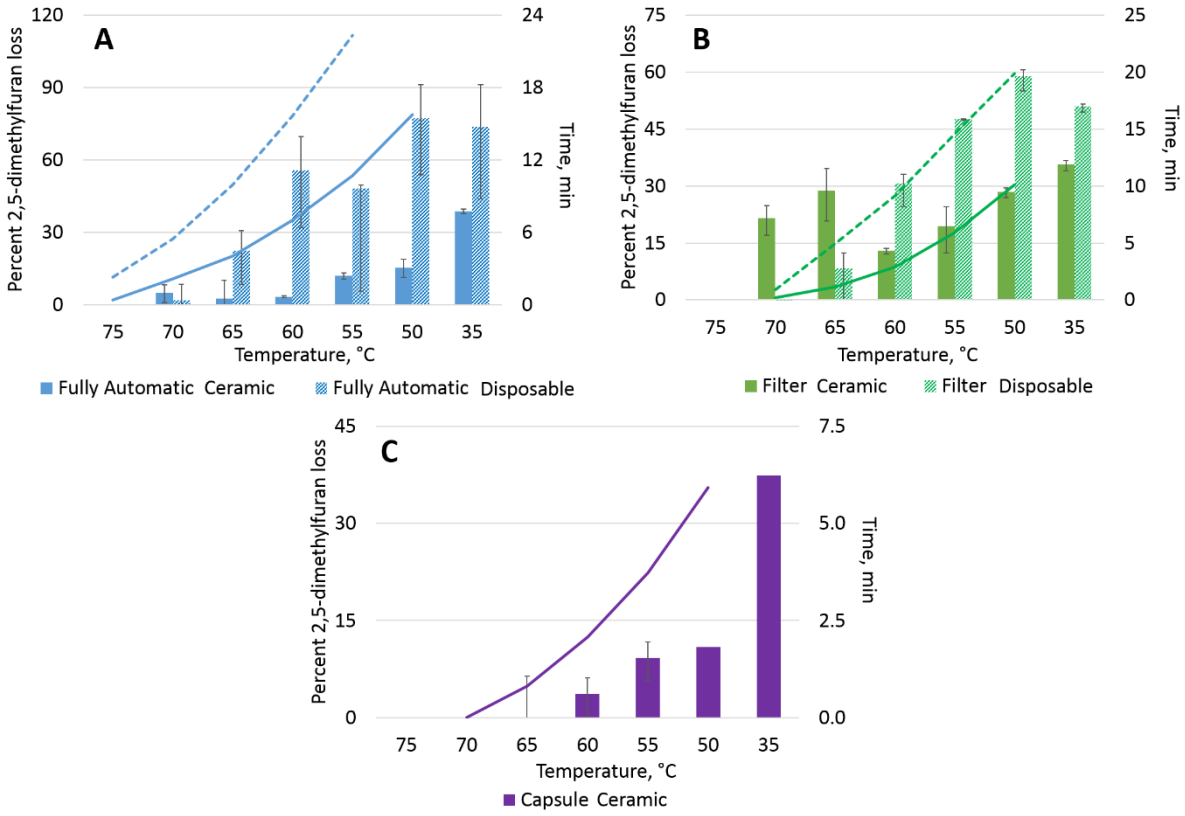


Figure S5: 2,5-dimethylfuran loss in coffee upon cooling comparison between ceramic and disposable cups prepared from either a fully automatic (A), filter (B) or capsule (C) machine

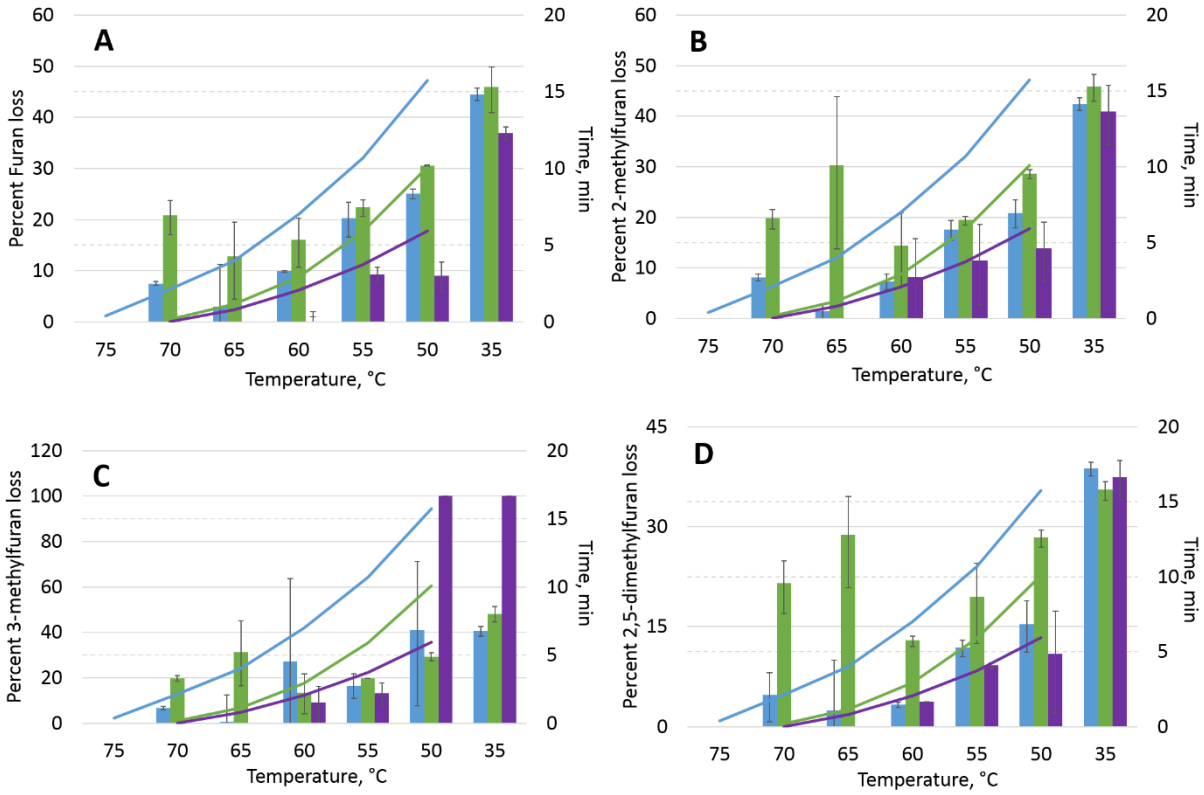


Figure S6: Percent loss of furan (A), 2-methylfuran (B), 3-methylfuran (C) and 2,5-dimethylfuran (D) in coffee brewed from a fully automatic (■), filter (■) or capsule (■) machine cooled over time (▬) in ceramic cups