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DBP Formation from the Chlorination of Organics in Tea and Coffee

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Outline

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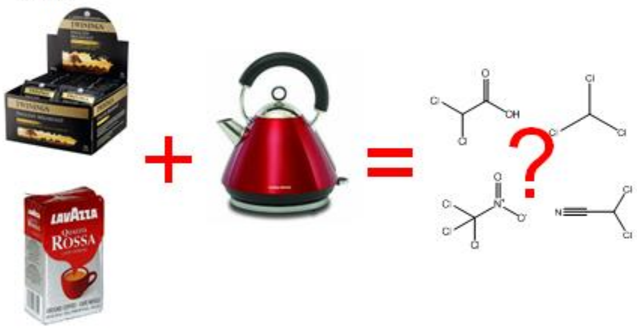
Background

There are multiple papers about the effect of boiling on concentrations of DBPs, but what about DBPs being formed *during* the preparation of tea and coffee?



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Methods

Experiments	Variables	Contact time	Chlorine dose	Method
Chlorine demand	40µM of 9 model compounds	24 h	35 mol/mol	DPD-FAS titration
Chlorine demand	1:100 diluted tea and coffee samples	24 h	200 mg·L^{-1}	
DBPFP	5 µM of 9 model compounds	24 h	35 mol/mol	GC-ECD and modified version of USPEA 551.1
DBPFP	1:100 diluted and cooled tea and coffee	24 h	100 mg·L^{-1}	
Real-life DBP formation	Freshly brewed tea and coffee	5 min	1 and 4 mg·L^{-1}	

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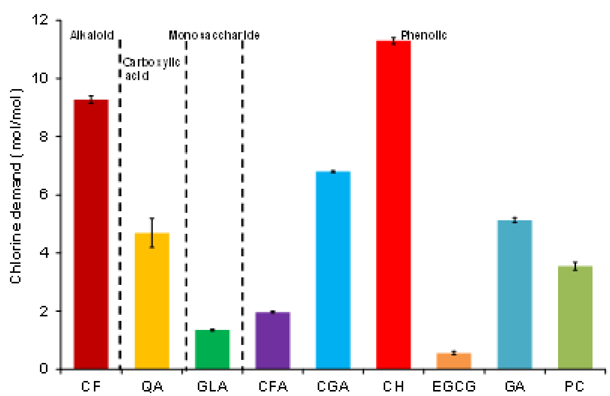
Chlorine demand of model compounds



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Key Findings

- Chlorine at concentrations of 1-10 mg·L^{-1} was reduced by between 5-19% upon boiling, i.e. the majority of aqueous chlorine remained available for reaction.
- DOC concentrations of tea and coffee are at least 100x times more than those typically found in drinking water.
- Chlorine demand and chloroform formation of phenolic surrogates was high and is comparable with reactive DBP precursors found in natural waters.
- DBP formation during preparation of tea and coffee is predicted to be limited by kinetics and chlorine concentrations in tap water. In the UK water companies generally maintain chlorine at <0.5 mg·L^{-1} (DWI, 2010); in the USA up to 4 mg·L^{-1} is permitted (USEPA, 1994).

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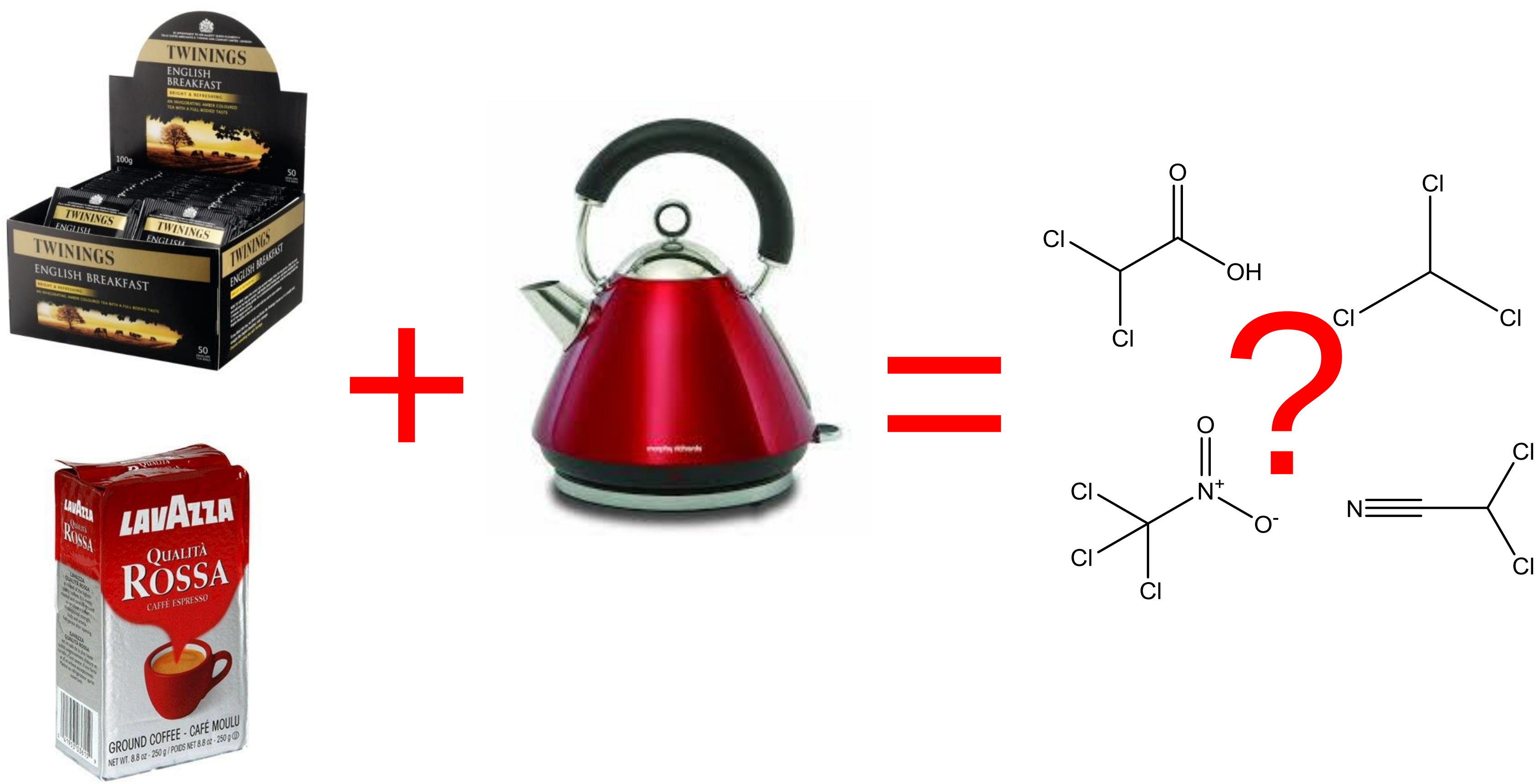

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Objectives

To evaluate the concentrations of DBPs generated from reactions between aqueous chlorine and organics in tea and coffee. More specifically to:

- Summarise the chemical composition of tea and coffee.
- Select model compounds representative of the organics in tea and coffee.
- Evaluate the amount of aqueous chlorine which remains in solution after boiling.
- Measure the chlorine demand of model compounds and authentic tea and coffee samples.
- Measure DBPs generated from model organics and authentic tea and coffee under formation potential conditions.
- Measure DBPs generated from authentic tea and coffee samples under real-life conditions.

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Chemical composition of tea

	Green Tea	Black Tea
Catechins (flavanols)	30-42	3-10
Theaflavin	--	2-6
Simple polyphenols	2	3
Flavonols	2	1
Other polyphenols	6	23
Theanine	3	3
Amino acids	3	3
Sugars	7	7
Caffeine	3-6	3-6

Comparison of green and black tea components in % dry weight (Balentine et al., 1997)

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Chemical composition of coffee

Component	Arabica	Robusta	Constituents
Monosaccharides	0.2-0.5	0.2-0.5	
Oligosaccharides	6-9	3-7	Sucrose (>90%)
Polysaccharides	3-4	3-4	Polymers of galactose (55-65%)
Hemicellulose	5-10	3-4	Polymers of galactose (65-75%)
Cellulose	41-43	32-40	
Non-volatile aliphatic acids	2-2.9	1.3-2.2	Citric acid, malic acid, quinic acid
Chlorogenic acid	6.7-9.2	7.1-12.1	
Lignin	1-3	1-3	
Lipids	15-18	8-12	
Proteins	8.5-12	8.5-12	
Caffeine	0.8-1.4	1.7-4	
Trigonelline	0.6-1.2	0.3-0.9	

Composition of green coffee (weight %), modified from Belitz et al. 2009

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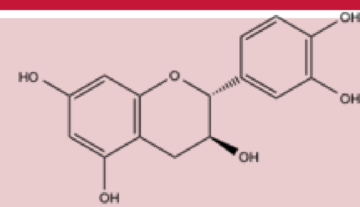
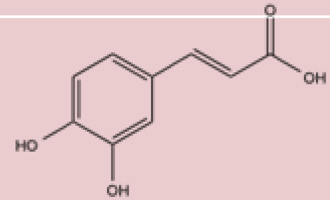
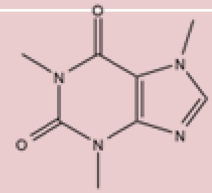
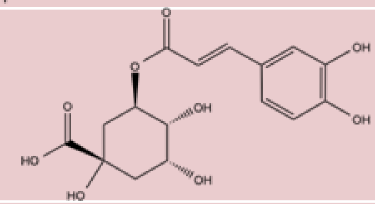
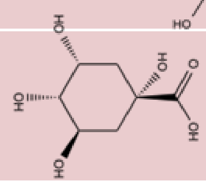
Model Compound Selection

Name	Structure	Significance
(+) catechin hydrate (CH)		Tea
Caffeic acid (CFA)		Coffee
Caffeine (CF)		Tea and coffee
Chlorogenic acid (CGA)		Coffee
D (-) quinic acid (QA)		Coffee

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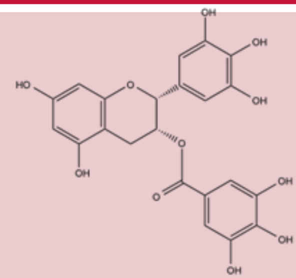
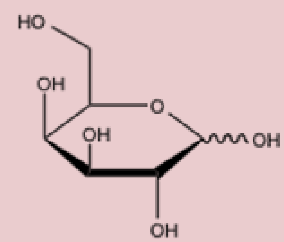
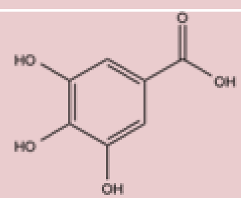
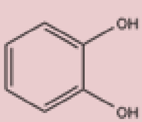
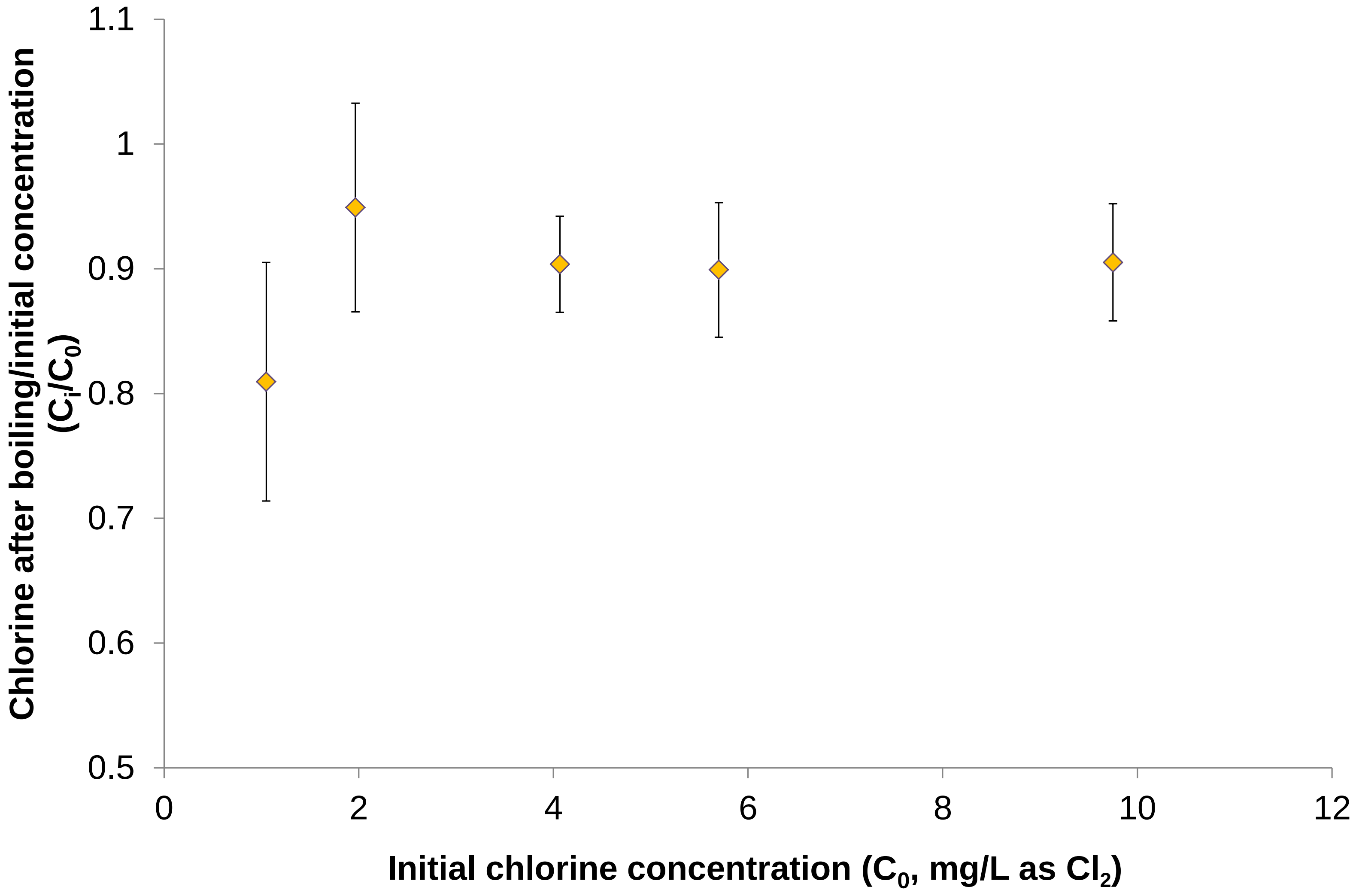
Model Compound Selection

Name	Structure	Significance
Epigallocatechin gallate (EGCG)		More in green tea than black tea
D (+) Galactose (GLA)		Coffee (part of polymers)
Gallic acid (GA)		Tea
Pyrocatechol (PC)		Skeleton present in catechin (tea)

How volatile is aqueous chlorine?



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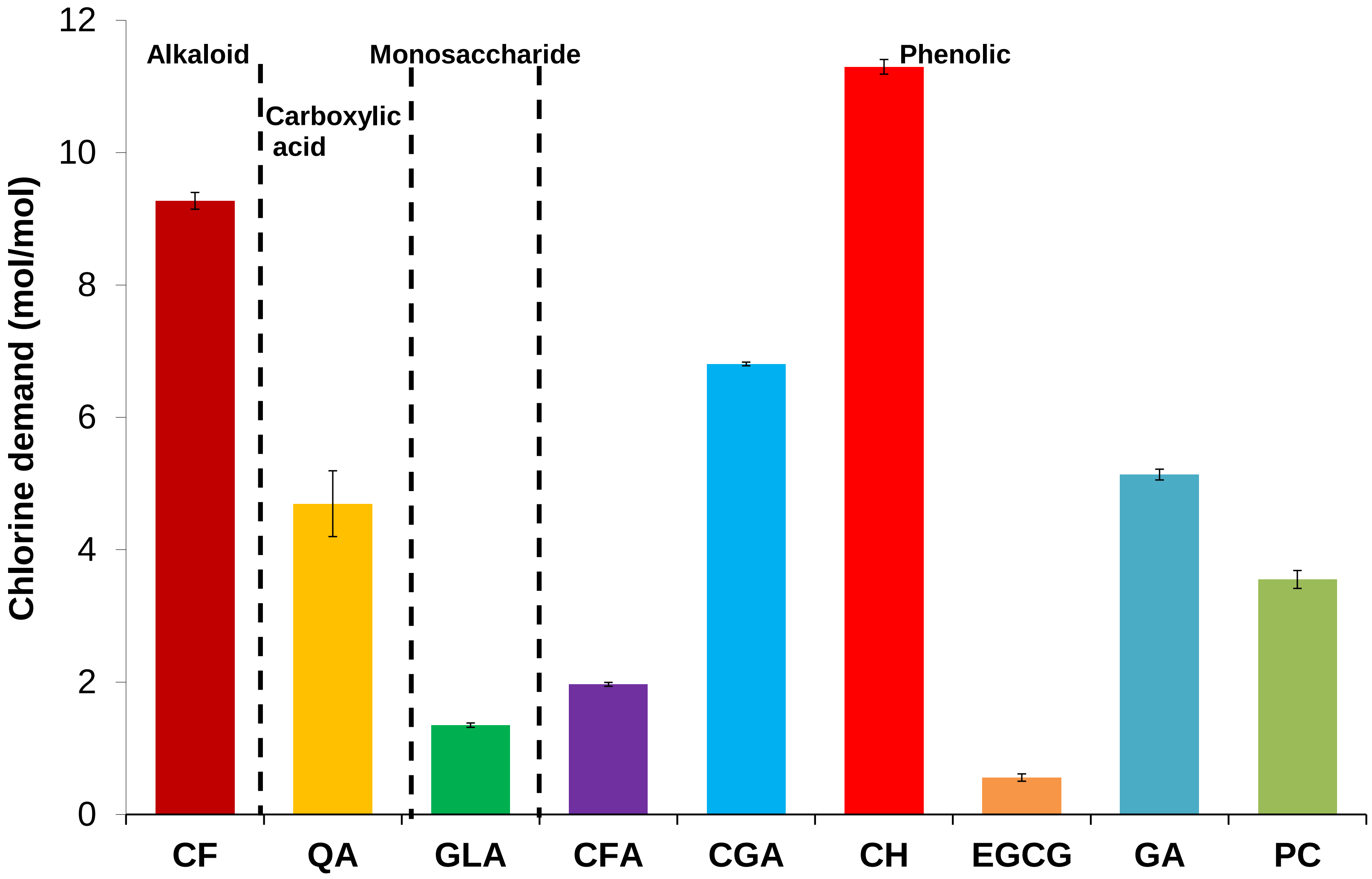
Chlorine demand of model compounds



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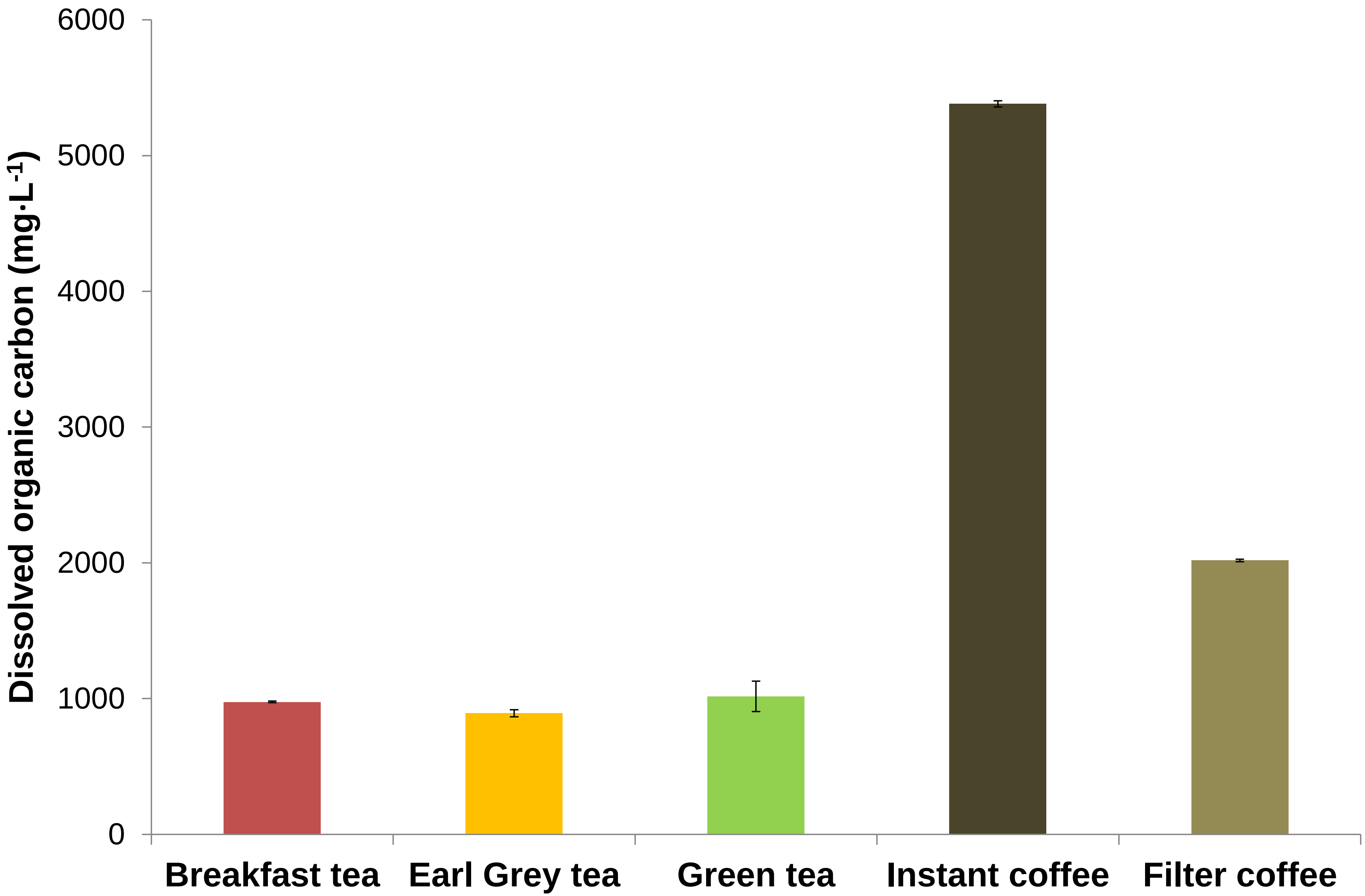
DOC concentration of tea and coffee



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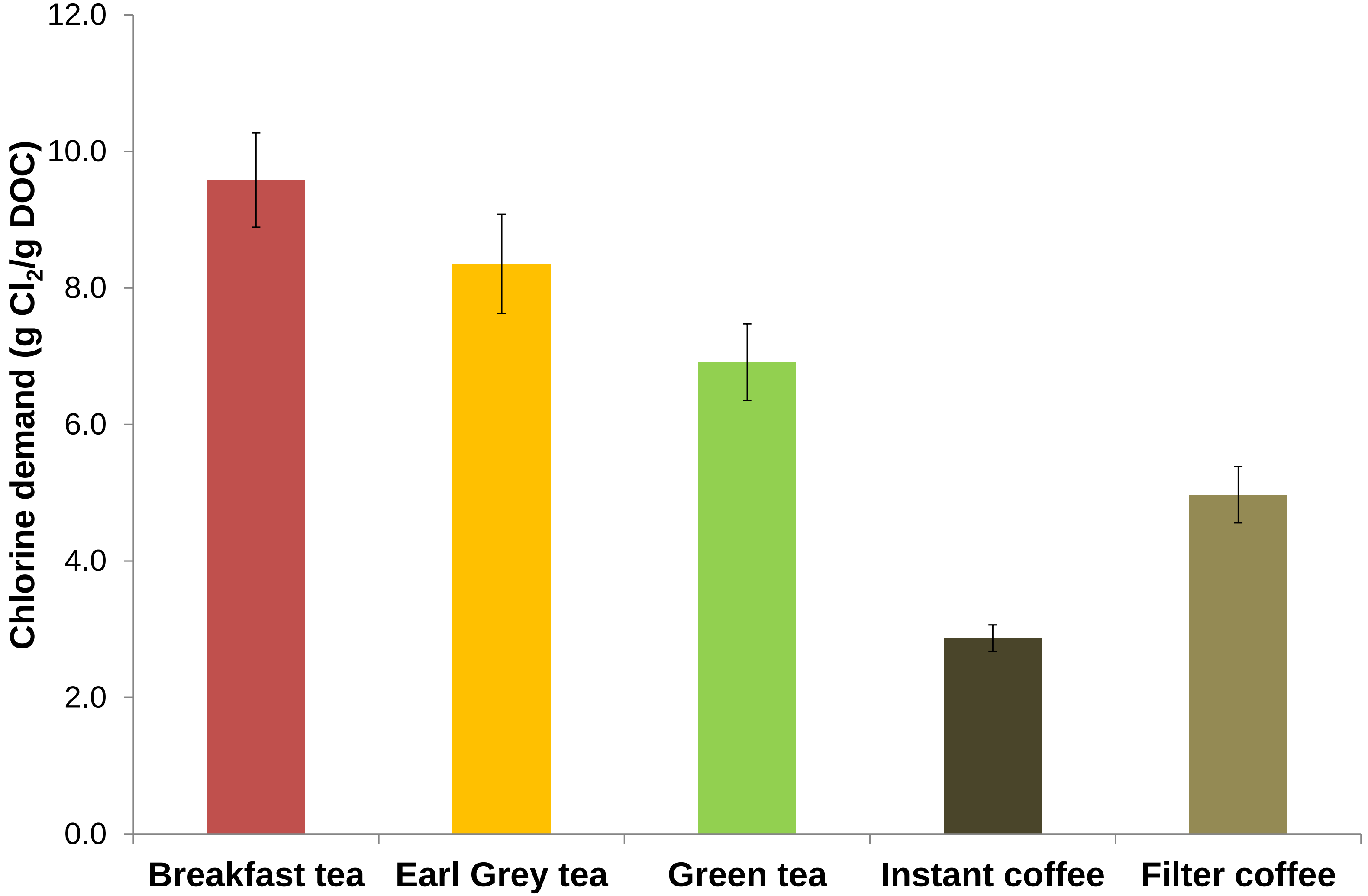
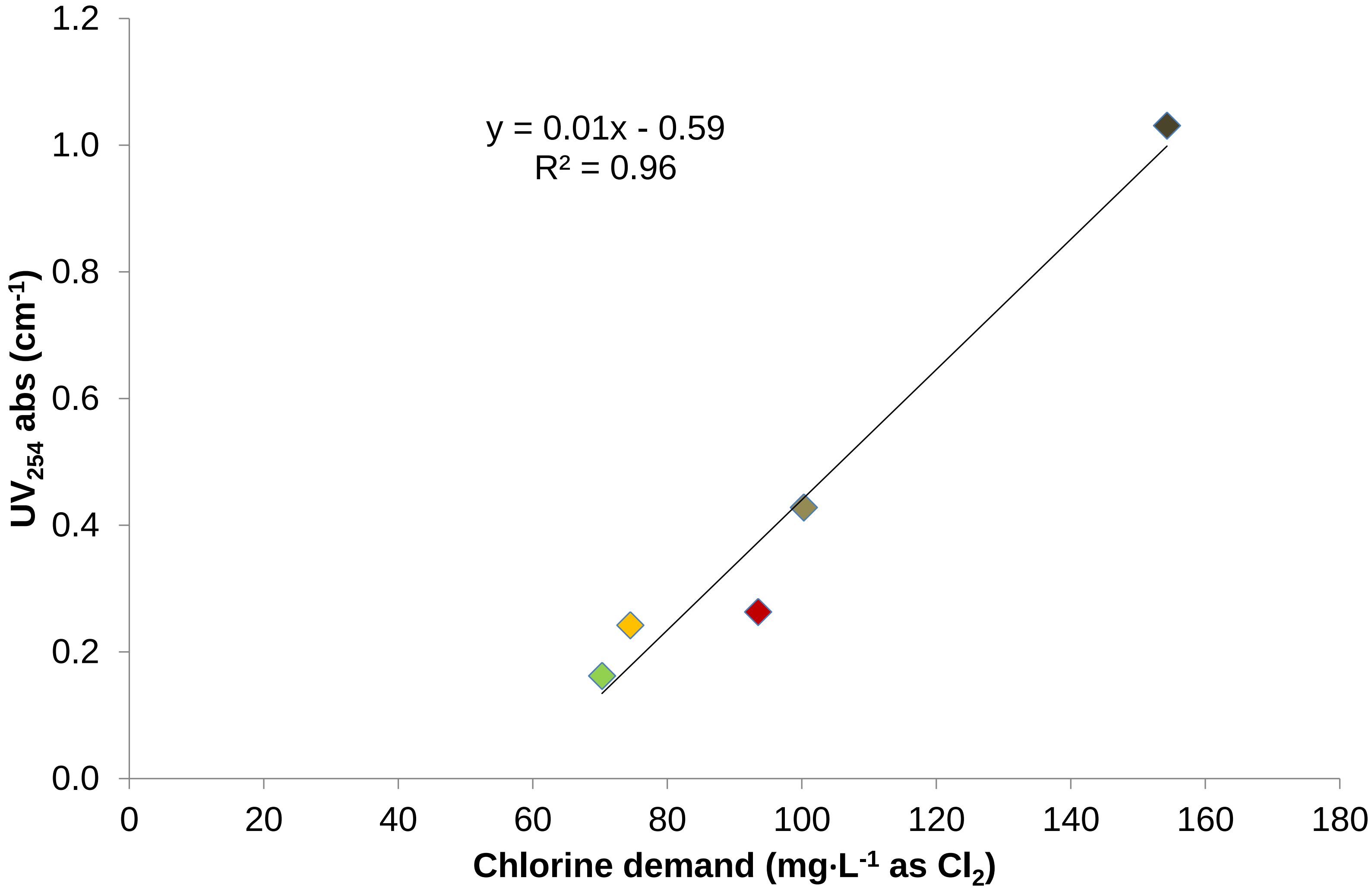


Correlation between chlorine demand and UV_{254} abs.



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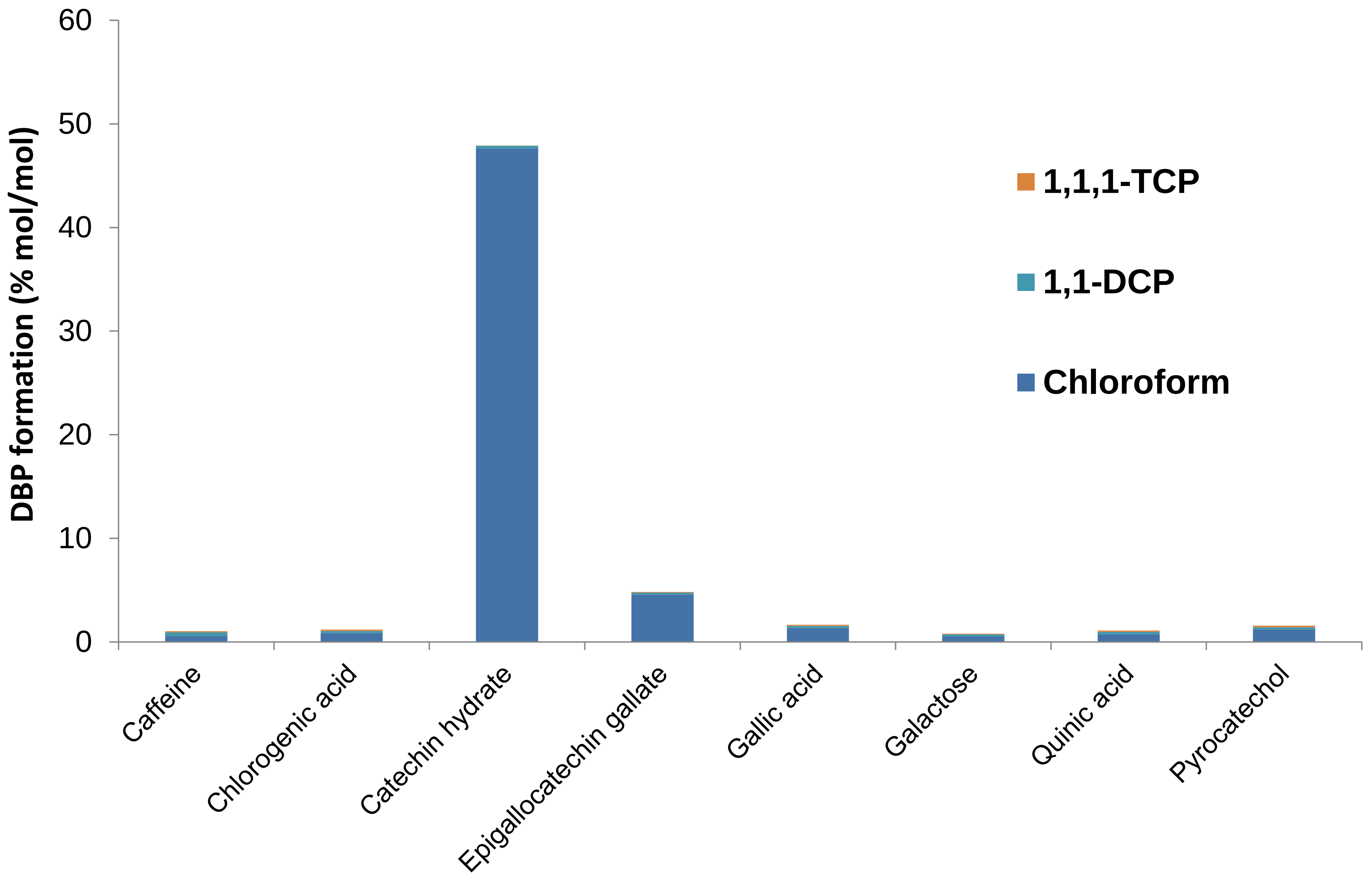
DBP formation potential tests from model compounds



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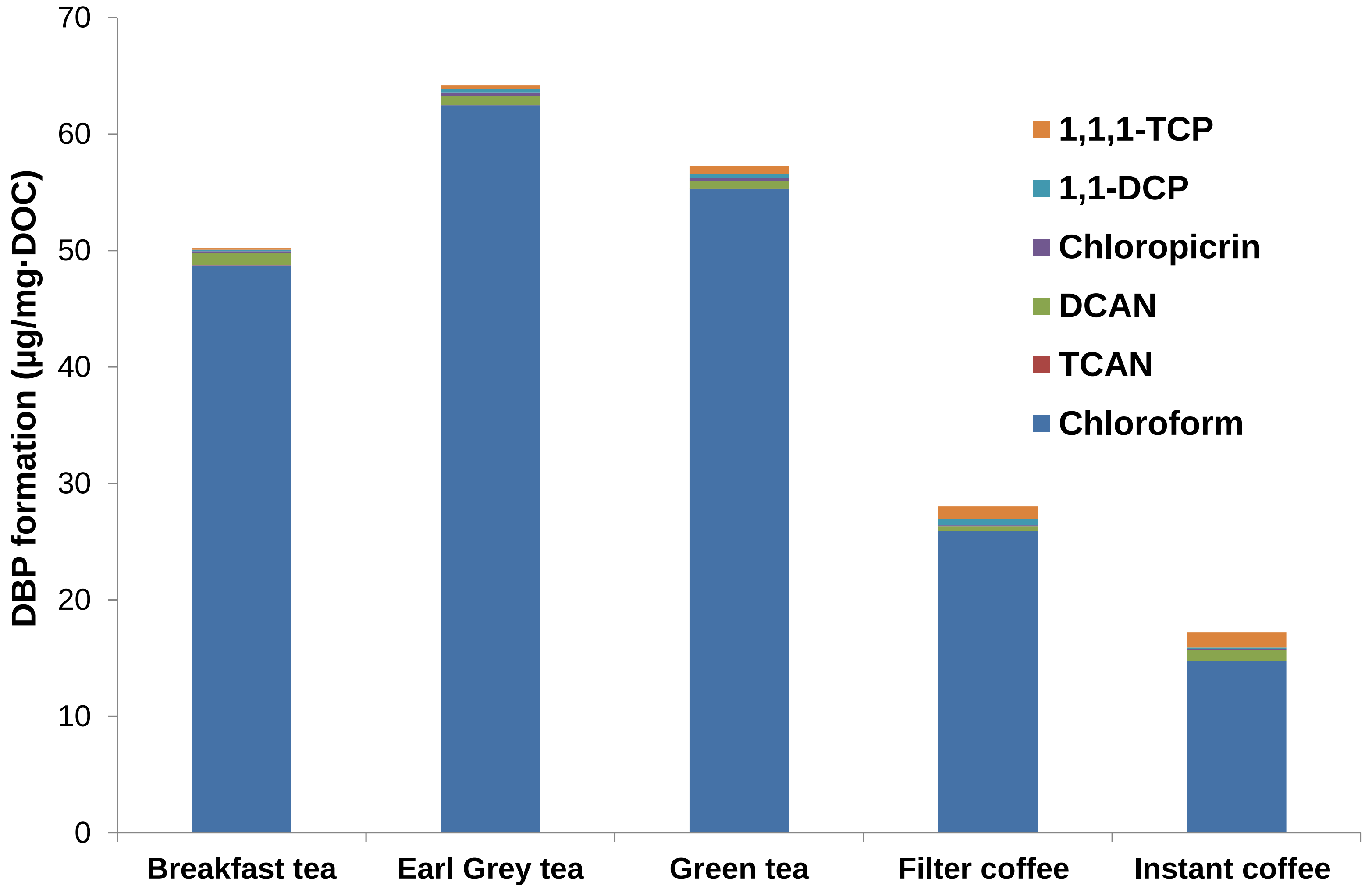

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References

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- UK Drinking Water Inspectorate, 2010. Chlorine. [online] Available from: http://dwi.defra.gov.uk/consumers/advice-leaflets/chlorine.pdf [accessed 12th January 2014].
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- USEPA. Disinfectants/Disinfection Byproduct Rule. Fed. Reg. 1994, 59, 145, 38668-38829.

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Any Questions?

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