

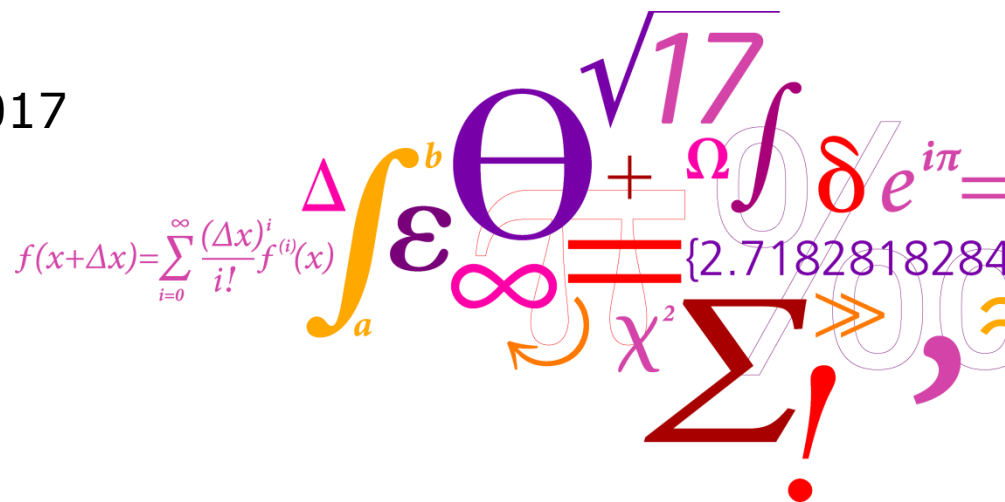
Emerging chemicals in food packaging materials

- toxicological profiling of knowns and unknowns

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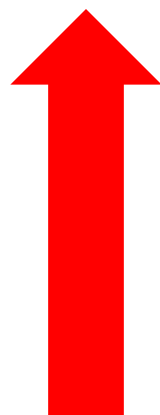
CEHOS Informationsdag, Okt 2017







Toxicological profiling
in silico and in vitro



Known chemicals in food
packaging with **unknown**
effects

- *Bisphenol A analogues*
- *Fluorochemicals*



Unknowns in food packaging



Effect-directed analysis &
analytical chemistry



A

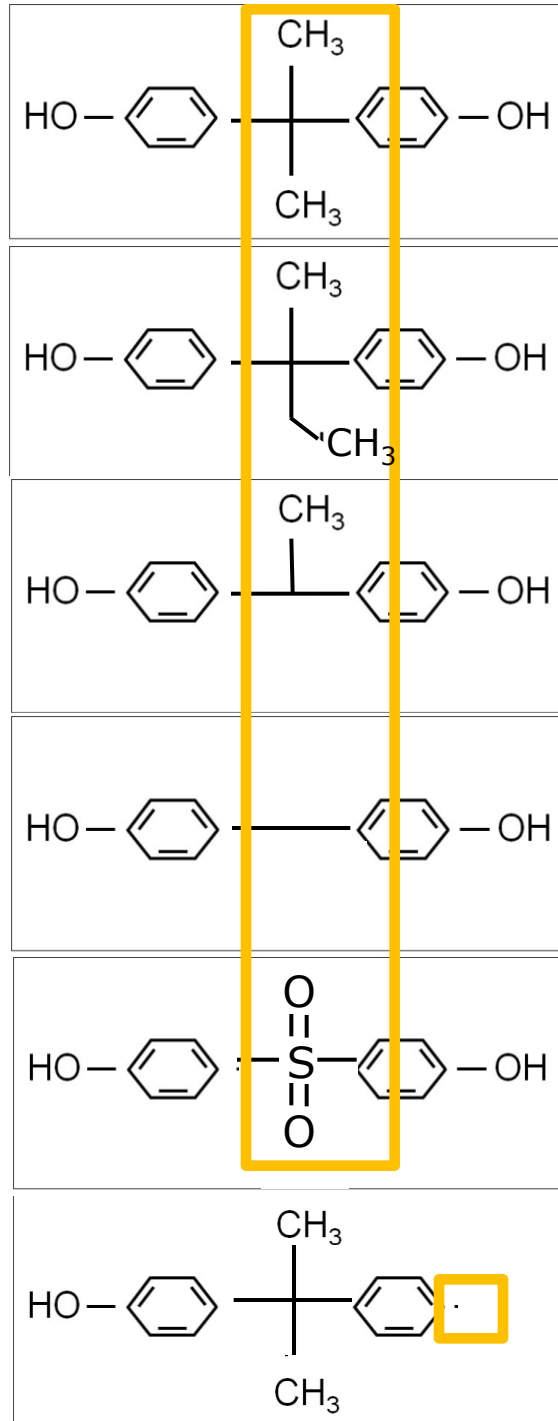
B

E

F

S

CP

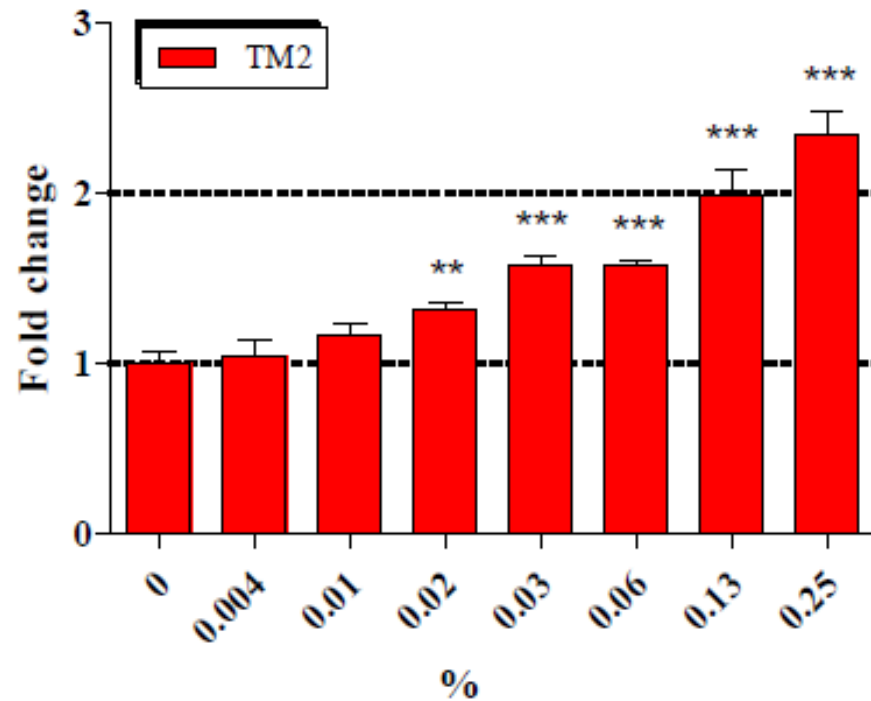


	ER	AR	Steroid hormone synthesis				AhR	PPARα	PPARγ	RAR	Nrf2	p53	Lipid accum
			Prog	Corti coids	Andro -gens	Estro gens							
BPA	↑	↓	↑	↓	↓	↑	↑					↑	↑
BPB	↑	↓	↑	↓	↓	↑	↑					↑	↑
BPE	↑	↓	↑	↑	↓	↑	↑		↑			↑	↑
BPF	↑	↓	↑	↑	↓	↑	↑		↑		↑		↑
BPS	↑	↓	↑	↓	↓				↑				↑
CP	↑	↓	↑	↓	↓	↑							↑

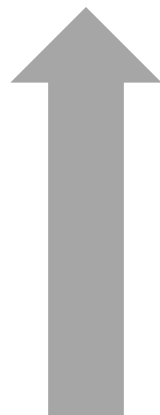


	ER	AR	H295R			AhR	PPARα	PPARγ	RAR	Nrf2	p53
			Prog	Andr	Estr						
8:2 triPAPs			↓	↓	↑	↑					
10:2 diPAPs			↓	↓	↑						
8:2 diPAPs			↓	↓	↑						
8:2monoPAPs	↑		↓	↓	↑	↑					
8:2 FTOH	↑		↓	↓	↑						
6:2 FTOH	↑				↑						
4:2 FTOH	↑										
PFdoDA					↑		↑	↑			
PFunDA					↑		↑	↑			
PFDA					↑		↑	↑			
PFNA					↑		↑	↑			
PFOA					↑		↑	↑			
PFHpA							↑	↑			
PFHxA							↑	↑			
PFPA							↑	↑			
PFBA							↑				

	ER	AR	H295R			AhR	PPAR α	PPAR γ
			Prog	Andr	Estro			
Technical Mixture 1								
Technical Mixture 2	↑				↑			
Technical Mixture 3	↑							



Toxicological profiling
in silico and in vitro



Known chemicals in food
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effects

- *Bisphenol analogues*
- *Fluorochemicals*

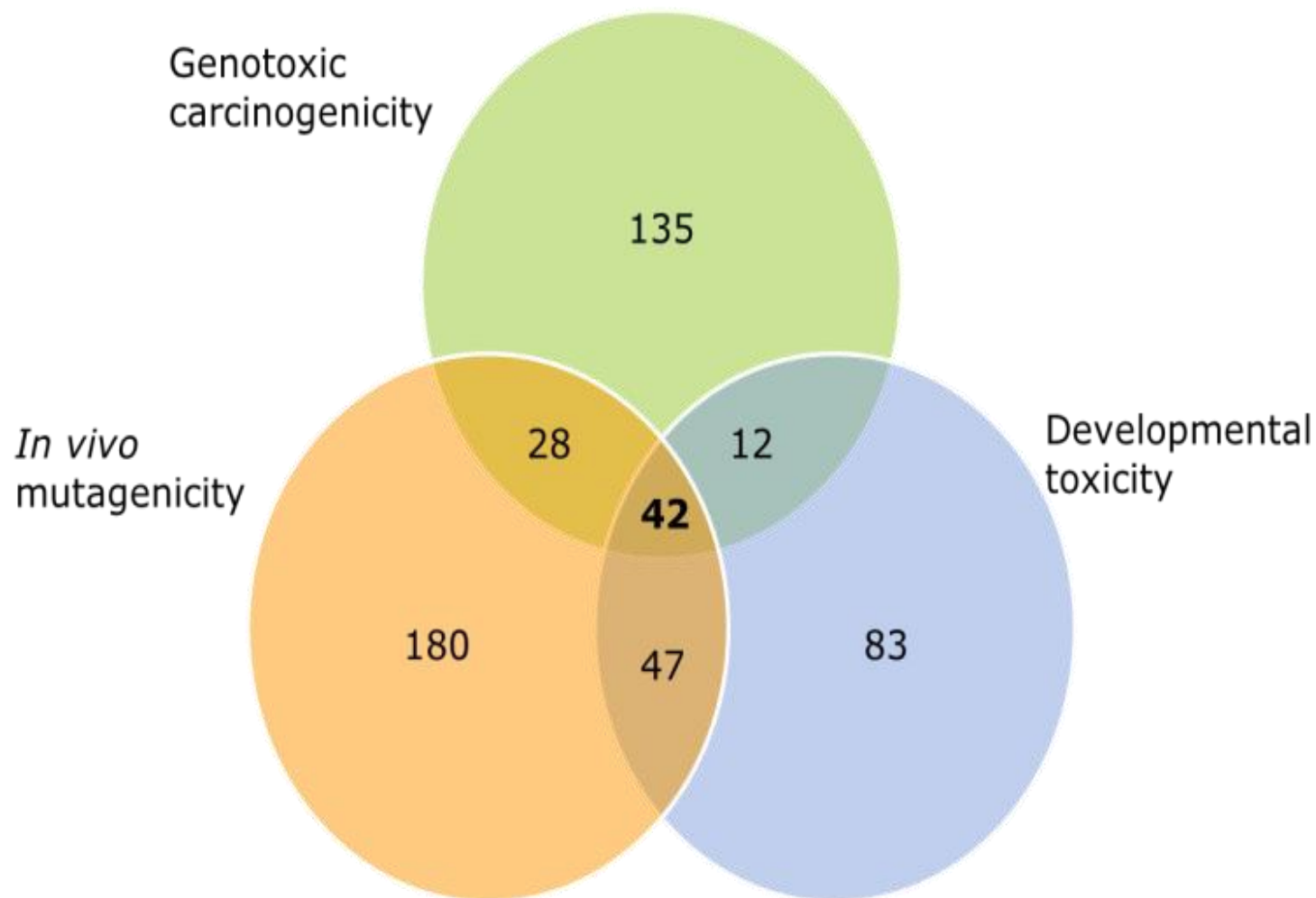


Unknowns in food packaging

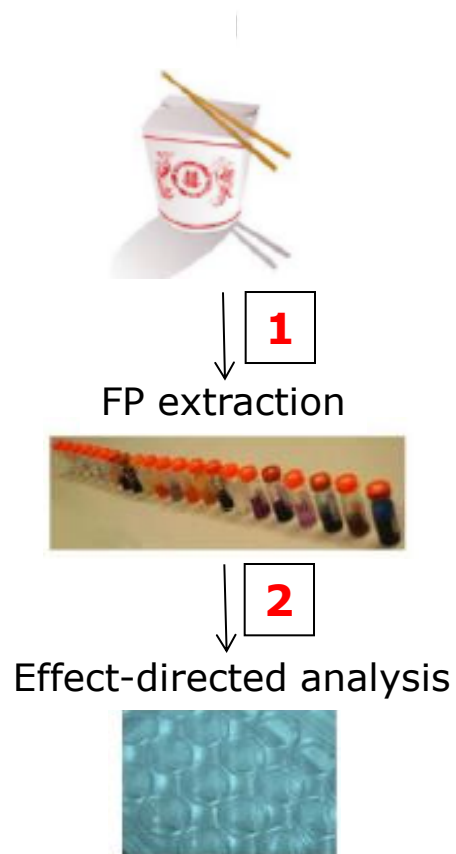


Effect-directed analysis &
analytical chemistry

QSAR predictions for 2,076 substances used in food packaging



Food packaging test strategy



ASSAYS

ER

AR

AhR

GR

RAR

PPAR γ

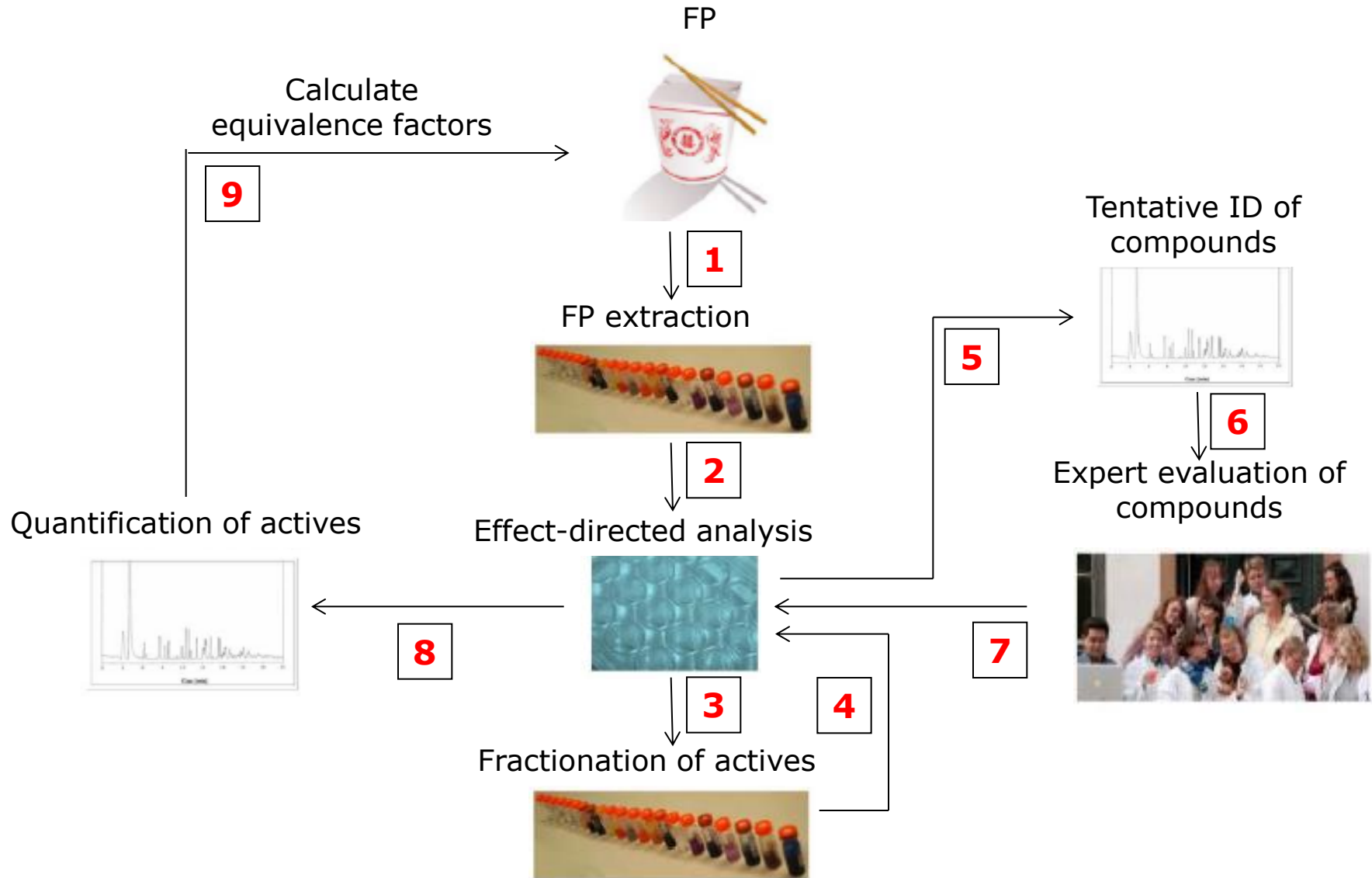
Nrf2

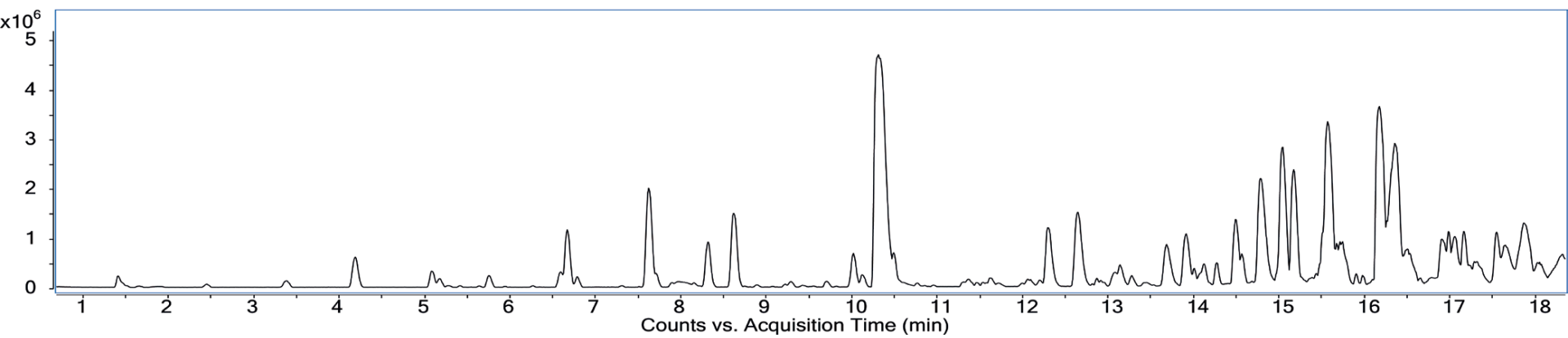
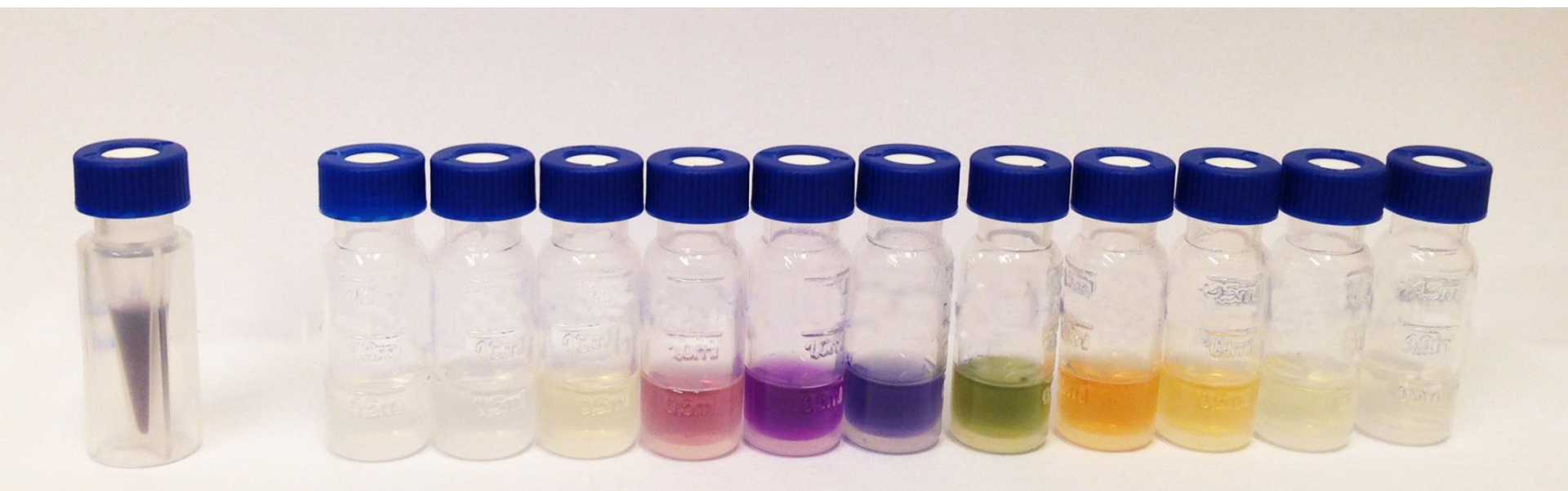
p53

Ames

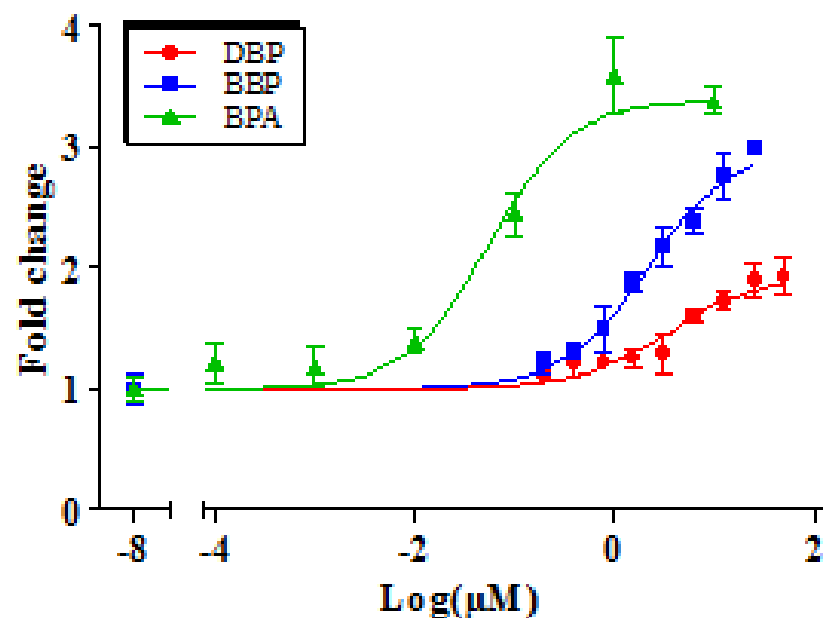
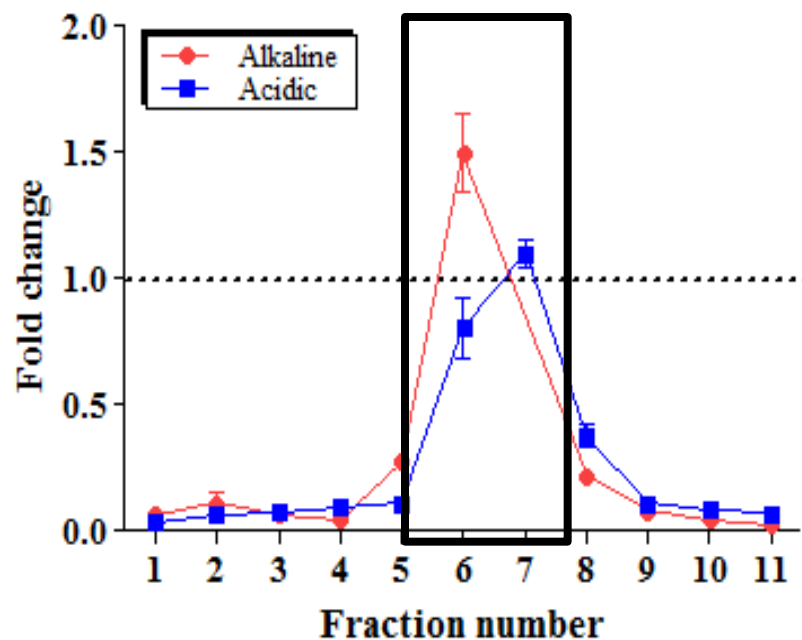
[illegible]

FP test strategy





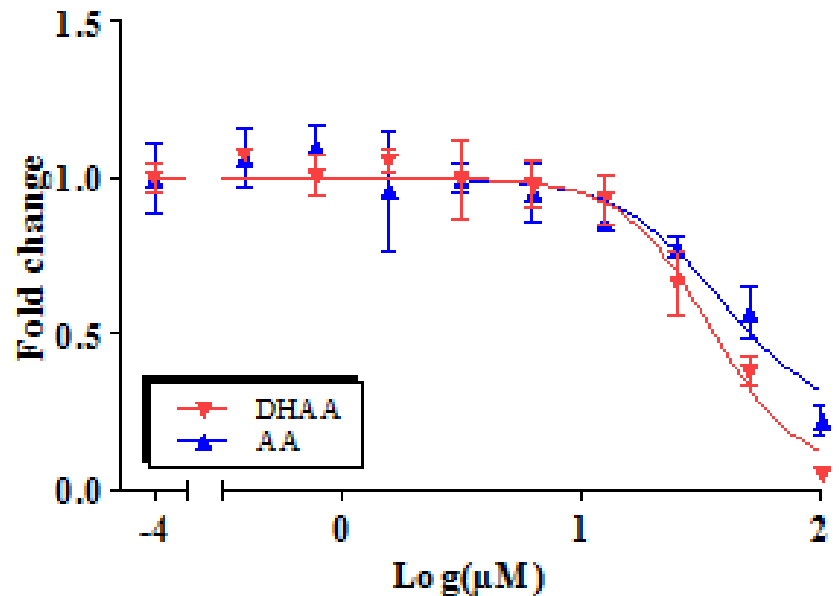
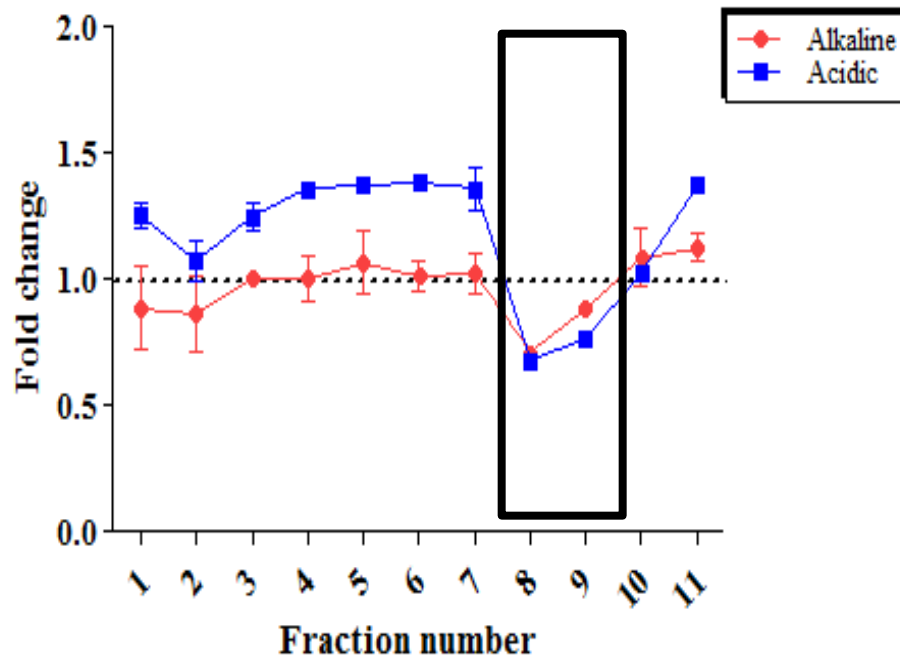
Estrogenic activity in pizza box



BPA, DBP & BBP responsible for estrogenic activity

BPA			DBP			BBP			EEQ	
Ex-tract μM	EC ₅₀ μM	EEQ	Extract μM	EC ₅₀	EEQ	Extract μM	EC ₅₀	EEQ	Predic- ted	Obser- ved
0.08	0.1	1x10 ⁻⁵	0.19	3.6	2x10 ⁻⁷	0.07	2.1	2x10 ⁻⁷	14x10 ⁻⁶	2x10 ⁻⁶

AR antagonistic activity in sandwich wrapper

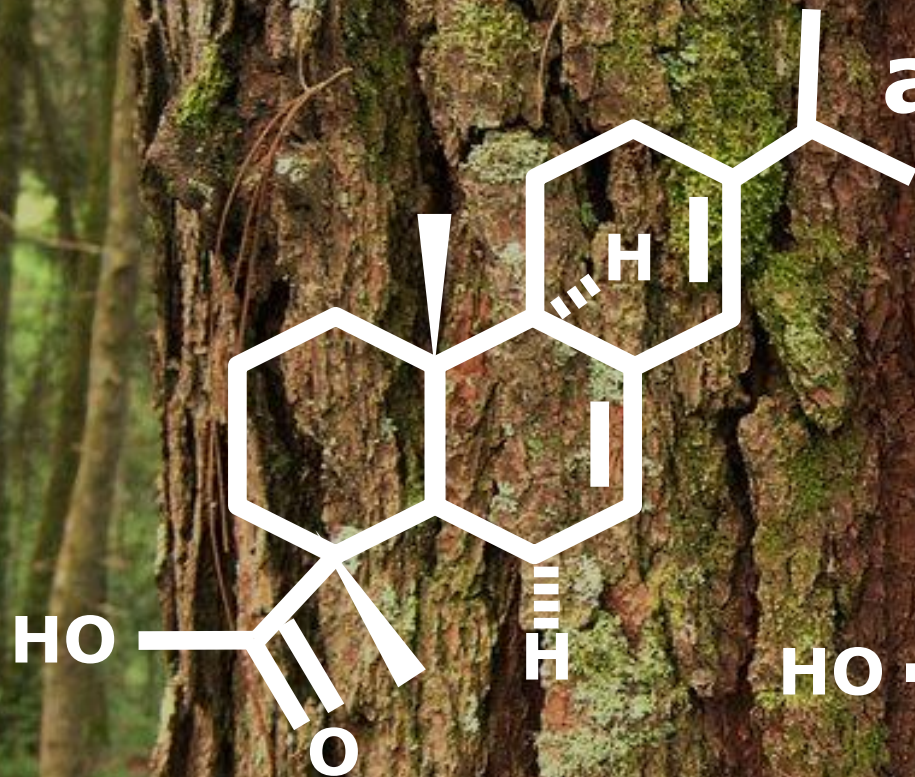


Abietic acid & dehydroabietic acid responsible for activity

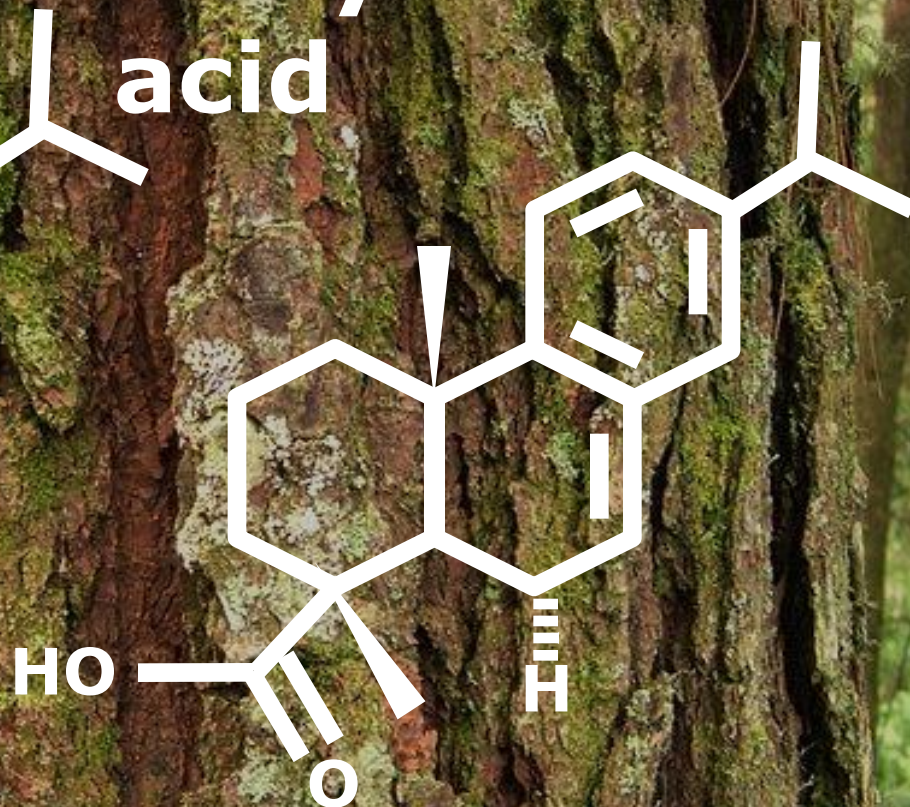
Abietic acid			Dehydroabietic acid			AAEQ	
Extract, μM	EC_{50} μM	AAEQ	Extract, μM	EC_{50}	AAEQ	Predicted	Observed
485	38	1×10^{-1}	3.9	34	2×10^{-4}	15×10^{-2}	9×10^{-2}

Rosenmai et al. Food Chemistry and Toxicology, in press

Abietic acid



Dehydroabietic acid



Take home messages

- More focus on FP is needed as it is a significant source of human exposure to EDCs
- Our method for identifying emerging chemicals in FP is effect-based and quantitative and proved to be valuable
- AA and DHAA identified as AR antagonists in sandwich wrapper; The estrogenic BPA and phthalates were found in a recycled pizza box
- Alternative bisphenols have similar toxicity profile as BPA. Substitution of BPA with BP analogues does not seem appropriate

Thanks!

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