Assessment of different isotope dilution strategies and combination with switchable solvent liquid phase microextraction prior to quantification of bisphenol A at trace levels by GC-MS

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Supplementary Material 3

Quadruplicate measurements were carried out by the GC-MS system for all blends. The mean values of the isotope ratios for all blends were utilized in calculating mass fraction of the analyte in the sample. The preparation and combination of the blends are clarified in the relevant tables for the isotope dilution strategies applied in this study.

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Table S1. Notation and description of symbols.

Symbol	Description
A*	Standard of the analyte
A	Sample (containing the analyte)
B	Labelled material of the analyte
$\mathbf{m_x}$	Mass of the standard/sample solution, labelled solution of the analyte or deionized water x: A, A*, B or w
$\mathbf{r_x}$	Ratio of peak areas, x: A*/B or A/B
PA	Peak area of the analyte or its isotope
$\mathbf{w_A}$	Mass fraction of the analyte
E*u*	Mean of experimental mass fraction of the analyte
Et	Theoretical mass fraction of the analyte

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Table S2. Blends preparation for ID^2-GC-MS.

Blends	Code	$m_{A^*, A}$, g	m_B, g	$r_{A^*A/B}$, PA/PA
Calibration Blends	A*B-a	0.604	0.601	2.25
	A*B-b	0.606	0.598	2.42
	A*B-c	0.600	0.598	2.17
Sample Blends	AB-a	0.602	0.596	2.39
	AB-b	0.600	0.598	2.31
	AB-c	0.604	0.600	2.27

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Table S3. Theoretical and experimental concentrations of the analyte, percent recovery results and percent relative standard deviation for ID^2-GC-MS.

Combination, x-y	w_A, µg/g	E*u* (w_A), µg/g	Et (w_A), µg/g	Recovery, %	RSD%
a-a	10.62				
b-a	9.90				
c-a	10.97				
a-b	10.29				
b-b	9.59	10.22	9.99	102.3	5.0
c-b	10.63				
a-c	10.10				
b-c	9.42				
c-c	10.44				

*x-y define the blends, x: a, b or c, y: a, b or c

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Table S4. Blends preparation for ID^3-GC-MS

Blends	Code	$m_{A^*, A}$, g	m_B, g	$r_{A^*A/B}$, PA/PA
Calibration Blends	A*B-1-a	0.801	0.400	3.74
	A*B-1-b	0.804	0.403	3.71
	A*B-1-c	0.801	0.407	3.74
	A*B-2-a	0.603	0.600	2.14
	A*B-2-b	0.601	0.603	2.07
	A*B-2-c	0.603	0.601	2.16
Sample Blends	AB-a	0.601	0.601	2.17
	AB-b	0.601	0.598	2.19
	AB-c	0.603	0.600	2.20

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Table S5. Theoretical and experimental concentrations of the analyte, percent recovery results and percent relative standard deviation for ID^3-GC-MS.

Combination, x-y-z	w_A, µg/g	E*u* (w_A), µg/g	Et (w_A), µg/g	Recovery, %	RSD%
1a-2a-1a	10.23				
1a-2a-1b	10.33				
1a-2a-1c	10.41				
1a-2b-1a	10.56				
1a-2b-1b	10.65				
1a-2b-1c	10.72				
1a-2c-1a	10.29				
1a-2c-1b	10.16				
1a-2c-1c	10.23				
1b-2a-1a	10.24				
1b-2a-1b	10.33				
1b-2a-1c	10.41				
1b-2b-1a	10.56				
1b-2b-1b	10.65	9.99	10.37	103.8	2.1
1b-2b-1c	10.73				
1b-2c-1a	10.06				
1b-2c-1b	10.16				
1b-2c-1c	10.24				
1c-2a-1a	10.23				
1c-2a-1b	10.32				
1c-2a-1c	10.39				
1c-2b-1a	10.54				
1c-2b-1b	10.62				
1c-2b-1c	10.69				
1c-2c-1a	10.06				
1c-2c-1b	10.15				
1c-2c-1c	10.23				

*x-y-z define the blends, x: 1a, 1b or 1c, y: 2a, 2b or 2c, z: 1a, 1b, 1c

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Table S6. Blends preparation for ID^4-GC-MS.

Blends	Code	$m_{A^*, A}$, g	m_B, g	$r_{A^*A/B}$, PA/PA
Calibration Blends	A*B-1-a	0.801	0.398	2.99
	A*B-1-b	0.806	0.400	3.05
	A*B-1-c	0.809	0.398	3.08
	A*B-2-a	0.600	0.599	1.86
	A*B-2-b	0.603	0.599	1.86
	A*B-2-c	0.600	0.602	1.85
	A*B-3-a	0.400	0.795	0.87
	A*B-3-b	0.399	0.799	0.91
	A*B-3-c	0.404	0.807	0.92
Sample Blends	AB-a	0.607	0.602	1.86
	AB-b	0.606	0.599	1.83
	AB-c	0.602	0.600	1.82

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Table S7. Theoretical and experimental concentrations of the analyte, percent recovery results and percent relative standard deviation for ID^4-GC-MS.

Combination, x-y-z-t	w_A, µg/g	E*u* (w_A), µg/g	Et (w_A), µg/g	Recovery, %	RSD%
1a-2a-3a-1a	10.15				
1a-2a-3a-1b	9.85				
1a-2a-3a-1c	9.95				
1a-2a-3b-1a	10.15				
1a-2a-3b-1b	9.96				
1a-2a-3b-1c	9.98				
1a-2a-3c-1a	10.15				
1a-2a-3c-1b	9.96				
1a-2a-3c-1c	9.98				
1a-2b-3a-1a	10.21				
1a-2b-3a-1b	9.97				
1a-2b-3a-1c	9.99				
1a-2b-3b-1a	10.21				
1a-2b-3b-1b	10.02	10.06	10.02	100.4	1.0
1a-2b-3b-1c	10.04				
1a-2b-3c-1a	10.21				
1a-2b-3c-1b	10.02				
1a-2b-3c-1c	10.04				
1a-2c-3a-1a	10.20				
1a-2c-3a-1b	10.01				
1a-2c-3a-1c	10.03				
1a-2c-3b-1a	10.20				
1a-2c-3b-1b	10.01				
1a-2c-3b-1c	10.03				
1a-2c-3c-1a	10.20				
1a-2c-3c-1b	10.01				
1a-2c-3c-1c	10.03				

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1b-2a-3a-1a	10.15
1b-2a-3a-1b	9.86
1b-2a-3a-1c	9.96
1b-2a-3b-1a	10.15
1b-2a-3b-1b	9.97
1b-2a-3b-1c	9.99
1b-2a-3c-1a	10.15
1b-2a-3c-1b	9.96
1b-2a-3c-1c	9.98
1b-2b-3a-1a	10.21
1b-2b-3a-1b	9.97
1b-2b-3a-1c	9.99
1b-2b-3b-1a	10.21
1b-2b-3b-1b	10.02
1b-2b-3b-1c	10.04
1b-2b-3c-1a	10.21
1b-2b-3c-1b	10.02
1b-2b-3c-1c	10.04
1b-2c-3a-1a	10.20
1b-2c-3a-1b	10.02
1b-2c-3a-1c	10.04
1b-2c-3b-1a	10.20
1b-2c-3b-1b	10.01
1b-2c-3b-1c	10.03
1b-2c-3c-1a	10.20
1b-2c-3c-1b	10.01
1b-2c-3c-1c	10.03
1c-2a-3a-1a	10.15
1c-2a-3a-1b	9.86
1c-2a-3a-1c	9.96
1c-2a-3b-1a	10.15
1c-2a-3b-1b	9.97

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1c-2a-3b-1c	9.99
1c-2a-3c-1a	10.15
1c-2a-3c-1b	9.97
1c-2a-3c-1c	9.99
1c-2b-3a-1a	10.21
1c-2b-3a-1b	9.97
1c-2b-3a-1c	9.99
1c-2b-3b-1a	10.21
1c-2b-3b-1b	10.02
1c-2b-3b-1c	10.04
1c-2b-3c-1a	10.21
1c-2b-3c-1b	10.02
1c-2b-3c-1c	10.04
1c-2c-3a-1a	10.20
1c-2c-3a-1b	10.02
1c-2c-3a-1c	10.04
1c-2c-3b-1a	10.20
1c-2c-3b-1b	10.01
1c-2c-3b-1c	10.03
1c-2c-3c-1a	10.20
1c-2c-3c-1b	10.01
1c-2c-3c-1c	10.03

*x-y-z-t define the blends, x: 1a, 1b or 1c, y: 2a, 2b or 2c, z: 3a, 3b, 3c, t: 1a, 1b, 1c

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Table S8. Blends preparation for SA-ID^2-GC-MS.

Blends	Code	m_A, g	m_{A^*}, g	m_B, g	m_w, g	$r_{A^*A/B}$, PA/PA
Calibration/Sample Blends	AA*B-1-a	0.400	-	0.397	0.401	2.50
	AA*B-1-b	0.398	-	0.397	0.401	2.50
	AA*B-1-c	0.400	-	0.401	0.402	2.50
	AA*B-2-a	0.400	0.400	0.399	-	5.14
	AA*B-2-b	0.401	0.401	0.401	-	4.86
	AA*B-2-c	0.404	0.402	0.394	-	4.94

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Table S9. Theoretical and experimental concentrations of the analyte, percent recovery results and percent relative standard deviation for SA-ID^2-GC-MS

Combination, x-y	w_A, µg/g	E*u* (w_A), µg/g	Et (w_A), µg/g	Recovery, %	RSD%
1a-2a	9.30				
1a-2b	10.33				
1a-2c	10.49				
1b-2a	9.41				
1b-2b	10.46	10.16	9.99	101.7	5.7
1b-2c	10.62				
1c-2a	9.50				
1c-2b	10.56				
1c-2c	10.73				

*x-y-z define the blends, x: 1a, 1b or 1c, y: 2a, 2b or 2c

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Table S10. Blends preparation for SA-ID^3-GC-MS.

Blends	Code	m_A, g	m_{A^*}, g	m_B, g	m_w, g	$r_{A^*A/B}$, PA/PA
Calibration/Sample Blends	AA*B-1-a	0.402	-	0.396	0.404	1.99
	AA*B-1-b	0.399	-	0.399	0.399	1.98
	AA*B-1-c	0.403	-	0.408	0.401	1.93
	AA*B-2-a	0.402	0.398	0.393	-	4.56
	AA*B-2-b	0.401	0.401	0.399	-	4.53
	AA*B-2-c	0.401	0.403	0.406	-	4.65
	AA*B-3-a	0.402	0.202	0.598	-	2.00
	AA*B-3-b	0.402	0.201	0.603	-	1.98
	AA*B-3-c	0.403	0.200	0.592	-	2.00

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Table S11. Theoretical and experimental concentrations of the analyte, percent recovery results and percent relative standard deviation for SA-ID^3-GC-MS.

Combination, x-y-z	w_A, µg/g	E*u* (w_A), µg/g	Et (w_A), µg/g	Recovery, %	RSD%
1a-2a-3a	9.96				
1a-2a-3b	9.90				
1a-2a-3c	10.26				
1a-2b-3a	9.96				
1a-2b-3b	9.90				
1a-2b-3c	10.26				
1a-2c-3a	9.96				
1a-2c-3b	9.89				
1a-2c-3c	10.26				
1b-2a-3a	10.23				
1b-2a-3b	10.16				
1b-2a-3c	10.55				
1b-2b-3a	10.23				
1b-2b-3b	10.16	10.16	10.02	101.4	2.1
1b-2b-3c	10.55				
1b-2c-3a	10.25				
1b-2c-3b	10.17				
1b-2c-3c	10.57				
1c-2a-3a	10.00				
1c-2a-3b	9.93				
1c-2a-3c	10.33				
1c-2b-3a	10.01				
1c-2b-3b	9.94				
1c-2b-3c	10.34				
1c-2c-3a	10.08				
1c-2c-3b	9.99				
1c-2c-3c	10.41				

*x-y-z define the blends, x: 1a, 1b or 1c, y: 2a, 2b or 2c, z: 3a, 3b, 3c

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