SUPPORTING INFORMATION TO:

Development And Pilot Application Of A Wastewater-Based Epidemiology Methodology To Investigate Human Exposure To Bisphenol A, Bisphenol F and Bisphenol S.

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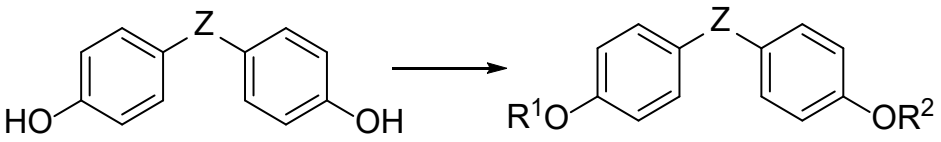
INDEX

	Page
Table S1. Chemical structures of target bisphenols and the corresponding human metabolites considered	3
Table S2. Details on WWTPs sampled. Sampling Mode: time proportional, followed by subsampling interval and volume taken per subsample. Dates presented as DD.MM.YYYY.	4
Table S3. Chromatographic conditions used with the EC 150/2 Nucleodur HILIC and Luna Omega Polar C18 columns	5
Table S4. Chemical formulae, retention time (RT), transitions (Q_n) used for quantification (Q_1) and confirmation (Q_2 and Q_3), ratio between the transitions, optimal collision energy (CE) values and compounds used as internal standards (IS) for bisphenols and their glucuronides.	6
Table S5. Instrumental quantification and detection limits (IQL and IDL) obtained with the EC 150/2 Nucleodur HILIC and the Omega Polar C18 columns.	7
Figure S1. Chromatogram of a 500 $ngmL^{-1}$ standard obtained on the EC 150/2 Nucleodur HILIC column.	8
Figure S2. Chromatograms showing the 3 SRM transitions of a wastewater extract spiked with 500 ng mL^{-1} of BPA-S obtained with the EC 150/2 Nucleodur HILIC column.	9
Figure S3. Absolute recoveries obtained with ultrapure water with the Oasis HLB and Oasis WAX protocols	10
Table S6. Concentration of bisphenols' sulfates in the wastewater samples. BPA-DS was below the MDL in all samples.	11
Table S7. Population normalized daily loads (PNDLs) calculated from the concentrations measured in wastewater (Table S6) after considering WWTP flow data and population served (Table S2).	12
Table S8. Urinary concentration of bisphenol metabolites estimated from PNDLs (Table S7).	13
Table S9. Compilation of literature studies where the excretion factors of sulfate metabolites were investigated.	14
Table S10. Human exposure to bisphenols calculated from the PNDL (Table S7) after considering the correction factor (CF) and human intake for bisphenols calculated from human exposure ,after considering the average European population weight (70.8 kg).	16

Table S1. Chemical structures of target bisphenols and the corresponding human metabolites considered.



Parent compound **Metabolite**

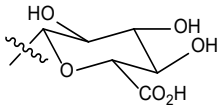
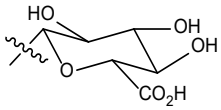
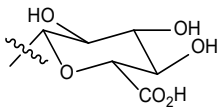
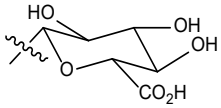
Parent plasticizer	Z	Metabolite	R^1 and R^2
Bisphenol A (BPA)	$-C(CH_3)_2$	**Bisphenol A Monosulfate (BPA-S)**	R^1 -H R^2 -SOH
		Bisphenol A Bissulfate (BPA-DS)	$R^1 = R^2$ $-SO_3H$
		Bisphenol A β-D-Glucuronide (BPA-G)	R^1 -H R^2 
		Bisphenol A Bis-(β-D-Glucuronide) (BPA-G)	$R^1 = R^2$ 
Bisphenol F (BPF)	$-CH_2$	**Bisphenol F Monosulfate (BPF-S)**	R^1 -H R^2 $-SO_3H$
		Bisphenol F β-D-Glucuronide (BPF-G)	R^1 -H R^2 
Bisphenol S (BPS)	$-SO_2$	**Bisphenol S Monosulfate (BPS-S)**	R^1 -H R^2 $-SO_3H$
		Bisphenol S β-D-Glucuronide (BPS-G)	R^1 -H R^2 

Table S2. Details on WWTPs sampled. Sampling Mode: time proportional, followed by subsampling interval and volume taken per subsample. Dates presented as DD.MM.YYYY.

Code	Location 1	Location 2	Location 3	Location 4
Country	Spain	Spain	Spain	Portugal
Population served	860,237	136,500	255,052	150,000
Sampling date 1	20.10.2021	19.10.2021	19.10.2021	21.04.2021
Sampling date 2	21.10.2021	20.10.2021	20.10.2021	22.04.2021
Sampling date 3	22.10.2021	21.10.2021	21.10.2021	23.04.2021
Sampling date 4	23.10.2021	22.10.2021	22.10.2021	24.04.2021
Sampling date 5	24.10.2021	23.10.2021	23.10.2021	25.04.2021
Sampling date 6	25.10.2021	24.10.2021	24.10.2021	26.04.2021
Sampling date 7	26.10.2021	25.10.2021	25.10.2021	27.04.2021
Flow (m^3day^{-1}) day 1	205916	39866	70100	31670
Flow (m^3day^{-1}) day 2	203351	42948	70400	36500
Flow (m^3day^{-1}) day 3	231651	39397	67300	36170
Flow (m^3day^{-1}) day 4	191835	36981	68000	35110
Flow (m^3day^{-1}) day 5	191507	40300	66000	37780
Flow (m^3day^{-1}) day 6	194848	41486	61200	35370
Flow (m^3day^{-1}) day 7	200330	42081	66200	35460
Sampling mode	60 min, 100 mL	10 min, 150 mL	10 min, 150 mL	15 min, 125 mL

Table S3. Chromatographic conditions used with the EC 150/2 Nucleodur HILIC and Luna Omega Polar C18 columns.

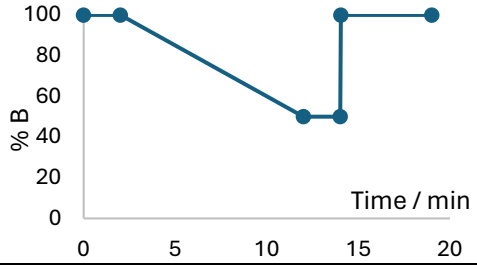
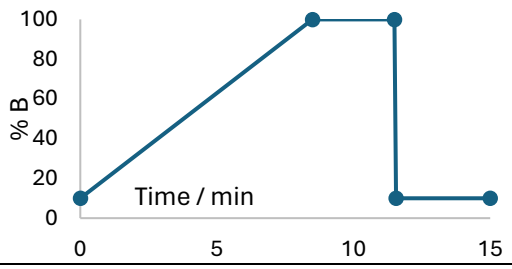
Mobile Phase A	5 mM of ammonium formiate in ultrapure water: acetonitrile 95: 5 at pH 4	5 mM of ammonium acetate in ultrapure water
Mobile Phase B	5 mM of ammonium formiate in ultrapure water: acetonitrile 5: 95 at pH 4	5 mM of ammonium acetate in MeOH
Injection Volume	2 µL	2 µL
Flow rate	0.3 mL min^{-1}	0.4 mL min^{-1}
Chromatographic gradient		
Target analytes	BPA-S, BPA-DS, BPA-G, BPA-DG BPS-S, BPS-G BPF-S, BPF-G	BPA, BPS and BPF

Table S4. Chemical formulae, retention time (RT), transitions (Q_n) used for quantification (Q_1) and confirmation (Q_2 and Q_3), ratio between the transitions, optimal collision energy (CE) values and compounds used as internal standards (IS) for bisphenols and their glucuronides.

Compound	Chemical formulae	RT (min)	Q_1 (*m/z*)	CE (eV)	Q_2 (*m/z*)	CE (eV)	Q_3 (*m/z*)	CE (eV)	IS
BPA	$C_{15}H_{16}O_2$	5.05 [a]	227 > 211	37	227 > 133	25	227 > 93	57	BPA-d6
BPF	$C_{13}H_{12}O_2$	4.27 [a]	199 > 93	21	199 > 105	21	199 > 77	29	BPF-d10
BPS	$C_{12}H_{10}O_4S$	3.13 [a]	249 > 108	29	249 > 156	21	249 > 92	37	BPS-d8
BPA-d6	$C_{15}H_{10}{}^2H_6O_2$	5.05 [a]	233 > 138	25	-	-	-	-	-
BPS-d8	$C_{12}H_2{}^2H_8O_4S$	3.13 [a]	257 > 112	29	-	-	-	-	-
BPF-d10	$C_{13}H_2{}^2H_{10}O_2$	4.27 [a]	209 > 97	21	-	-	-	-	-
BPA-G	$C_{21}H_{24}O_8$	7.35 [b]	403 > 227	29	403 > 175	13	403 > 113	17	$^{13}C_{12}$BPA-G
BPA-DG	$C_{27}H_{32}O_{14}$	10.1 [b]	579 > 403	21	579 > 113	33	579 > 227	49	$^{13}C_{12}$BPA-G
BPS-G	$C_{18}H_{18}O_{10}S$	7.90 [b]	425 > 249	25	425 > 156	49	425 > 113	17	$^{13}C_{12}$BPA-G
BPF-G	$C_{19}H_{20}O_8$	7.65 [b]	375 > 199	33	375 > 175	9	375 > 113	13	$^{13}C_{12}$BPA-G
$^{13}C_{12}$BPA-G	$C_9{}^{13}C_{12}H_{24}O_8$	7.35 [b]	415 > 113	17	-	-	-	-	-

[a]: referred to Omega Polar C18 column.

[b]: referred to EC 150/2 Nucleodur HILIC column .

Table S5. Instrumental quantification and detection limits (IQL and IDL) obtained with the EC 150/2 Nucleodur HILIC and the Omega Polar C18 columns.

	Compounds	IDL (ng mL^{-1})	IQL (ng mL^{-1})
EC 150/2 Nucleodur HILIC	**BPA-S**	0.41	1.39
	BPA-DS	0.53	1.77
	BPA-G	0.32	1.08
	BPA-DG	0.69	2.31
	BPS-S	0.06	0.20
	BPS-G	0.18	0.61
	BPF-S	0.05	0.17
	BPF-G	0.23	0.76
Omega Polar C18	**BPA**	12	40
	BPS	0.13	0.43
	BPF	7.4	24.8

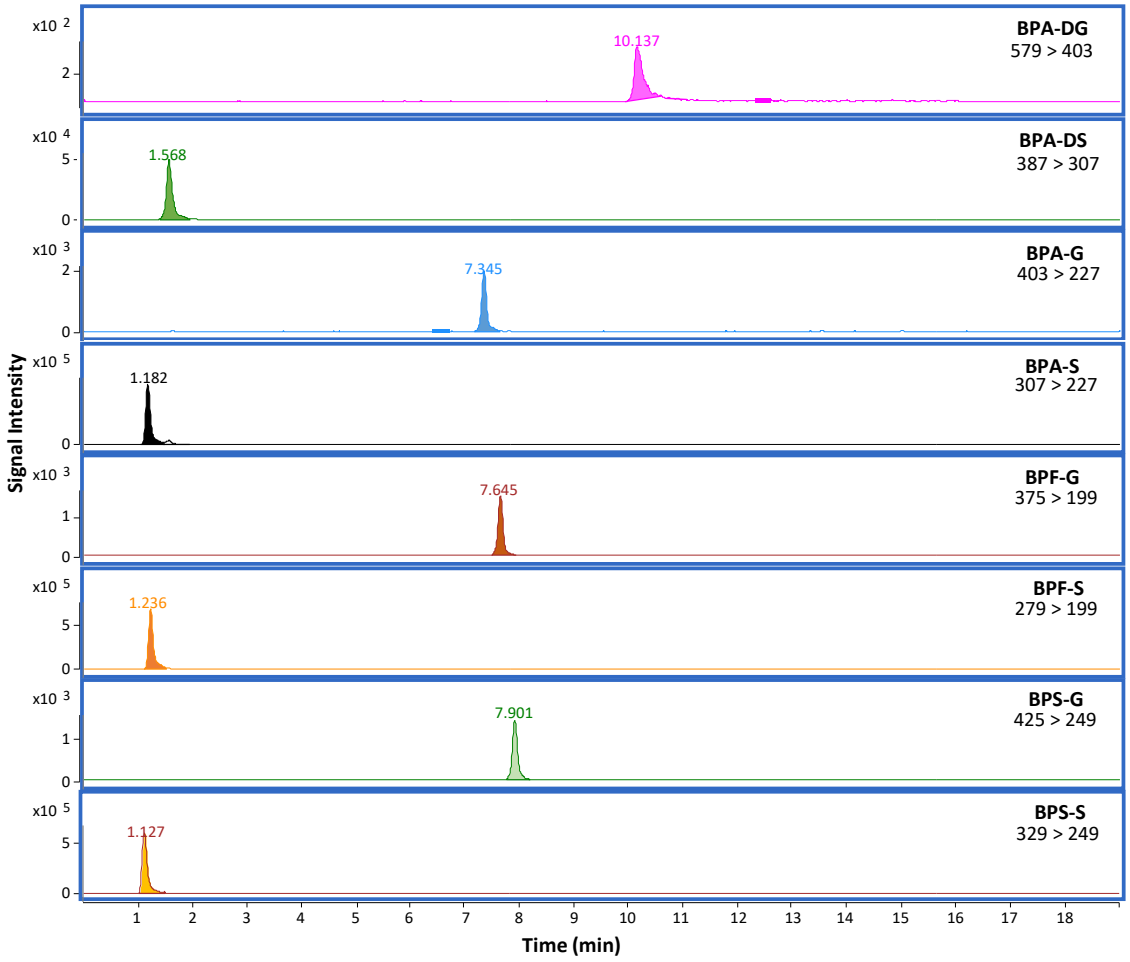


Figure S1. Chromatogram of a 500 ng mL^{-1} standard obtained on the EC 150/2 Nucleodur HILIC column.

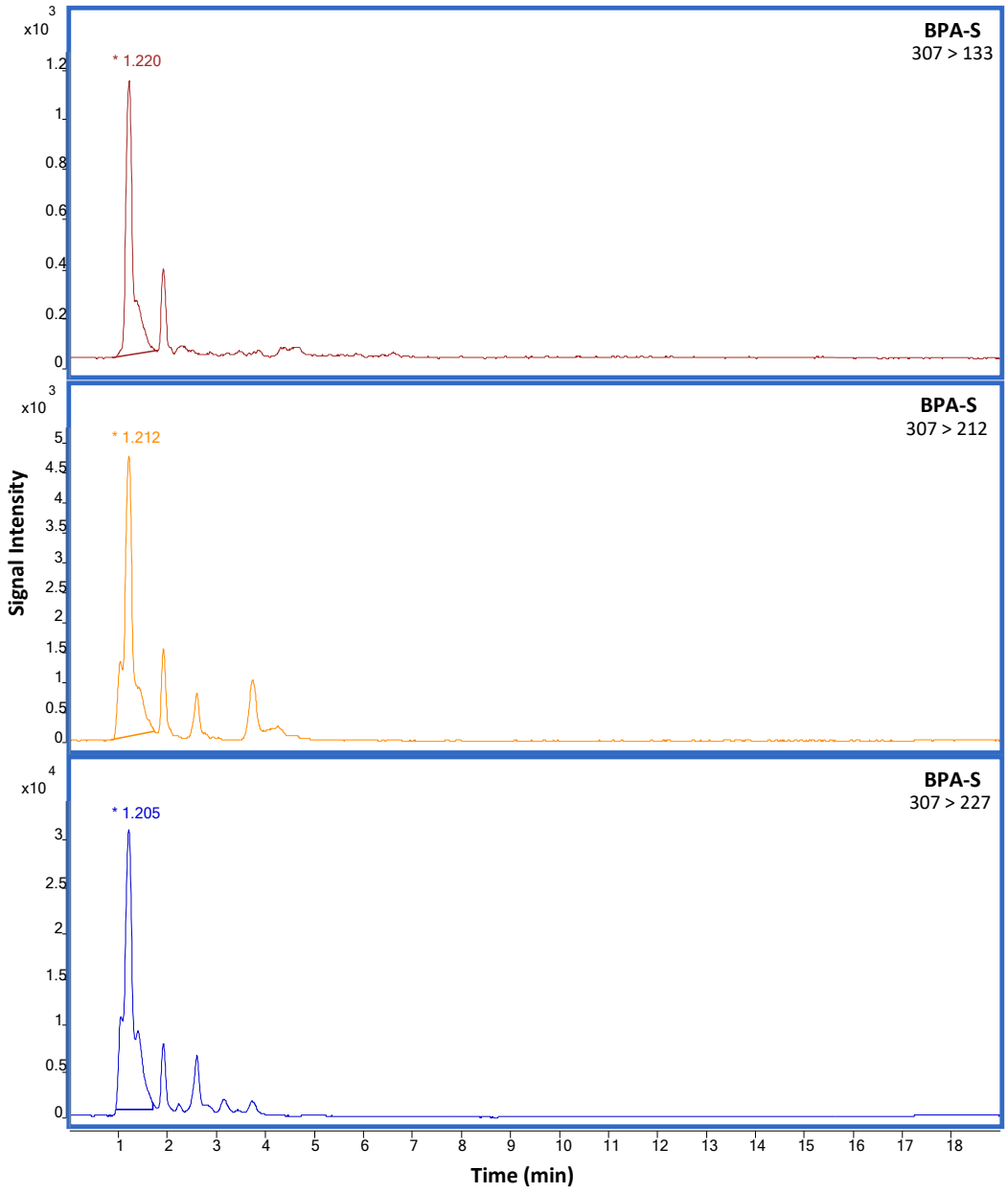


Figure S2. Chromatograms showing the 3 SRM transitions of a wastewater extract spiked with 500 ng mL^{-1} of BPA-S obtained with the EC 150/2 Nucleodur HILIC column.

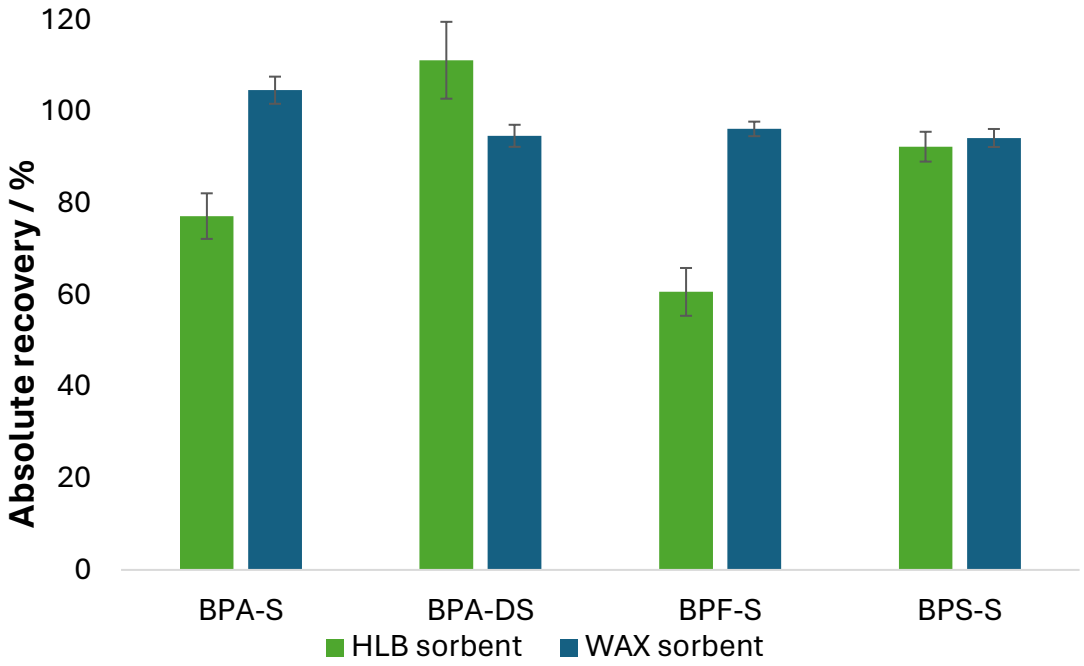


Figure S3. Absolute recoveries obtained with ultrapure water with the Oasis HLB and Oasis WAX protocols.

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Table S6. Concentration of bisphenols' sulfates in the wastewater samples. BPA-DS was below the MDL in all samples.

Location	Date (DD.MM.YYYY)	Concentration (ng L^{-1})			
		BPA-S	**BPA-DS**	**BPS-S**	**BPF-S**
Location 1	20.10.2021	44.0	<MDL	35.1	56.7
	21.10.2021	63.1	<MDL	38.6	57.5
	22.10.2021	196	<MDL	14.8	139
	23.10.2021	121	<MDL	17.0	102
	24.10.2021	36.2	<MDL	17.3	24.3
	25.10.2021	500	<MDL	17.2	142
	26.10.2021	172	<MDL	17.7	63.7
	Average ± SD	**162 ± 162**	**<MDL**	**22.5 ± 9.9**	**83.7 ± 45.1**
Location 2	19.10.2021	1.53	<MDL	3.58	<MDL
	20.10.2021	3.74	<MDL	2.37	<MDL
	21.10.2021	6.14	<MDL	<MDL	<MDL
	22.10.2021	5.59	<MDL	<MDL	<MDL
	23.10.2021	4.00	<MDL	2.04	<MDL
	24.10.2021	<MQL	<MDL	<MDL	<MDL
	25.10.2021	5.60	<MDL	6.78	<MDL
	Average ± SD	**3.91 ± 2.09** [a]	**<MDL**	**2.19 ± 2.42** [a]	**<MDL**
Location 3	19.10.2021	151	<MDL	<MDL	12.9
	20.10.2021	95.8	<MDL	<MDL	7.56
	21.10.2021	109	<MDL	<MDL	5.32
	22.10.2021	170	<MDL	<MDL	19.4
	23.10.2021	264	<MDL	<MDL	20.2
	24.10.2021	57.3	<MDL	<MDL	18.2
	25.10.2021	120	<MDL	<MDL	8.34
	Average ± SD	**138 ± 66**	**<MDL**	**<MDL**	**13.4 ± 6.2**
Location 4	21.04.2021	16.2	<MDL	5.10	<MDL
	22.04.2021	8.48	<MDL	3.28	<MDL
	23.04.2021	29.0	<MDL	<MDL	<MDL
	24.04.2021	6.78	<MDL	4.76	<MDL
	25.04.2021	8.96	<MDL	<MDL	<MDL
	26.04.2021	11.3	<MDL	2.88	<MDL
	27.04.2021	9.60	<MDL	5.10	<MDL
	Average ± SD	**12.9 ± 7.7**	**<MDL**	**2.37 ± 2.18** [a]	**<MDL**

[a] Average and standard deviation calculated by substituting the values <MQL and <MDL by MQL/2 and MDL/2, respectively. MDL/MQL: method detection/quantification limit.

Table S7. Population normalized daily loads (PNDLs) calculated from the concentrations measured in wastewater (Table S6) after considering WWTP flow data and population served (Table S2).

Location	Date (DD.MM.YYYY)	PNDL (µg day^{-1} inhabitant^{-1})			
		BPA-S	BPA-DS	BPS-S	BPF-S
Location 1	20.10.2021	11	<MDL	8.4	14
	21.10.2021	15	<MDL	9.1	14
	22.10.2021	53	<MDL	4.0	37
	23.10.2021	27	<MDL	3.8	23
	24.10.2021	8.1	<MDL	3.9	5.4
	25.10.2021	113	<MDL	3.9	32
	26.10.2021	40	<MDL	4.1	15
	Average ± SD	**38 ± 37**	**<MDL**	**5.3 ± 2.4**	**20 ± 11**
Location 2	19.10.2021	0.45	<MDL	1.0	<MDL
	20.10.2021	1.2	<MDL	0.74	<MDL
	21.10.2021	1.8	<MDL	<MDL	<MDL
	22.10.2021	1.5	<MDL	<MDL	<MDL
	23.10.2021	1.2	<MDL	0.60	<MDL
	24.10.2021	<MQL	<MDL	<MDL	<MDL
	25.10.2021	1.7	<MDL	2.1	<MDL
	Average ± SD	**1.1 ± 0.6** [a]	**<MDL**	**0.66 ± 0.74** [a]	**<MDL**
Location 3	19.10.2021	42	<MDL	<MDL	3.5
	20.10.2021	26	<MDL	<MDL	2.1
	21.10.2021	29	<MDL	<MDL	1.4
	22.10.2021	45	<MDL	<MDL	5.2
	23.10.2021	68	<MDL	<MDL	5.2
	24.10.2021	14	<MDL	<MDL	4.4
	25.10.2021	31	<MDL	<MDL	2.2
	Average ± SD	**37 ± 18**	**<MDL**	**<MDL**	**3.4 ± 1.6**
Location 4	21.04.2021	3.4	<MDL	1.1	<MDL
	22.04.2021	2.1	<MDL	0.80	<MDL
	23.04.2021	7.0	<MDL	<MDL	<MDL
	24.04.2021	1.6	<MDL	1.1	<MDL
	25.04.2021	2.3	<MDL	<MDL	<MDL
	26.04.2021	2.7	<MDL	0.68	<MDL
	27.04.2021	2.3	<MDL	<MDL	<MDL
	Average ± SD	**3.0 ± 1.8**	**<MDL**	**0.54 ± 0.49** [a]	**<MDL**

[a] Average and standard deviation calculated by substituting the values <MQL and <MDL by MQL/2 and MDL/2, respectively. MDL/MQL: method detection/quantification limit.

Table S8. Urinary concentration of bisphenol metabolites estimated from PNDLs (Table S7).

Location	Date (DD.MM.YYYY)	Urinary concentration (µg L^{-1})		
		BPA-S	**BPS-S**	**BPF-S**
Location 1	20.10.2021	6.7	5.4	8.6
	21.10.2021	9.5	5.8	8.7
	22.10.2021	34	2.5	24
	23.10.2021	17	2.4	14.5
	24.10.2021	5.1	2.5	3.4
	25.10.2021	72	2.5	21
	26.10.2021	26	2.6	9.5
	Average ± SD	**24.3 ± 25.3**	**3.4 ± 1.5**	**12.7 ± 7.3**
Location 2	19.10.2021	0.28	0.67	<MDL
	20.10.2021	0.75	0.47	<MDL
	21.10.2021	1.1	<MDL	<MDL
	22.10.2021	0.96	<MDL	<MDL
	23.10.2021	0.75	0.38	<MDL
	24.10.2021	0.15	<MDL	<MDL
	25.10.2021	1.1	1.3	<MDL
	Average ± SD	**0.73 ± 0.39** [a]	**0.59 ± 0.34** [a]	**<MDL**
Location 3	19.10.2021	26	<MDL	2.3
	20.10.2021	17	<MDL	1.3
	21.10.2021	18	<MDL	0.89
	22.10.2021	29	<MDL	3.3
	23.10.2021	44	<MDL	3.3
	24.10.2021	8.8	<MDL	2.8
	25.10.2021	20	<MDL	1.4
	Average ± SD	**23.2 ± 11.1**	**<MDL**	**2.2 ± 1.0**
Location 4	21.04.2021	2.2	0.69	<MDL
	22.04.2021	1.3	0.51	<MDL
	23.04.2021	4.5	<MDL	<MDL
	24.04.2021	1.0	0.71	<MDL
	25.04.2021	1.4	<MDL	<MDL
	26.04.2021	1.7	0.43	<MDL
	27.04.2021	1.4	<MDL	<MDL
	Average ± SD	**1.9 ± 1.2**	**0.55 ± 0.10** [a]	**<MDL**

[a] Average and standard deviation calculated by substituting the values <MQL and <MDL by MQL/2 and MDL/2, respectively. MDL/MQL: method detection/quantification limit.

Table S9. Compilation of literature studies where the excretion factors of sulfate metabolites were investigated.

Bisphenol	Metabolite(s)	Number of individuals	Study model	Molar excretion percentage (in 24 hours)	Reference *
BPA	**BPA-S**	5	Rats	3	Pottenger, 2000
BPA	**BPA-S**	-	*In-vitro* (Human hepatocytes)	7.5	Pritchett, 2002
BPA	**BPA-S + BPA-DS**	4	Monkeys	15	Doerge, 2010
BPA	**BPA-S**	-	*In-vitro* (Human hepatocytes)	9	Kurebayashi, 2010
		-	*In-vitro* (Monkeys hepatocytes)	20	
		-	*In-vitro* (Rats hepatocytes)	18	
BPA	**BPA-S + BPA-DS**	30	Humans	21	Ye, 2005
BPA	**BPA-S + BPA-DS**	140	Humans	6.25	Ho, 2017
BPA	**BPA-S**	14	Humans	3	Thayer, 2015
BPA	**BPA-S**	10	Humans	12	Teeguarden, 2015
BPS	**BPS-S**	-	*In-vitro* (Human hepatocytes)	10.5	Le Fol, 2015
BPS	**BPS-S**	24	Mice	7.9-20.7	Song, 2017
BPS	**BPS-S**	9	Rats	18-21	Waidyanatha, 2018
BPS	**BPS-S**	9	Mice	4	Waidyanatha, 2018
BPS	**BPS-S**	9	Rats	4	Sonker, 2021
BPS	**BPS-S**	30	Rats	16	Mao, 2022
BPF	**BPF-S**	18	Rats	> 50	Cabaton, 2006
BPF	**BPF-S**	-	*In-vitro* (Human hepatocytes)	54.1	Dumont, 2011

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Table S10. Human exposure to bisphenols calculated from the PNDL (Table S7) after considering the correction factor (CF) and human intake for bisphenols calculated from human exposure ,after considering the average European population weight (70.8 kg).

Location	Date (DD.MM.YYYY)	Human exposure (µg day^{-1} inhabitant^{-1})			Human intake (µg kg^{-1} day^{-1})		
		BPA from BPA-S	BPS from BPS-S	BPF from BPF-S	BPA from BPA-S	BPS from BPS-S	BPF from BPF-S
Location 1	20.10.2021	113	92	140	1.6	2.0	1.3
	21.10.2021	160	100	140	2.3	2.0	1.4
	22.10.2021	565	44	387	8.0	5.5	0.62
	23.10.2021	288	41	235	4.1	3.3	0.59
	24.10.2021	86	42	56	1.2	0.79	0.60
	25.10.2021	1213	43	333	17	4.7	0.60
	26.10.2021	430	45	153	6.1	2.2	0.64
	Average ± SD	**408 ± 396**	**58 ± 26**	**206 ± 118**	**5.8 ± 5.6**	**2.9 ± 1.7**	**0.82 ± 0.37**
Location 2	19.10.2021	4.8	11	<MDL	0.068	0.16	<MDL
	20.10.2021	13	8.2	<MDL	0.18	0.12	<MDL
	21.10.2021	19	<MDL	<MDL	0.27	<MDL	<MDL
	22.10.2021	16	<MDL	<MDL	0.23	<MDL	<MDL
	23.10.2021	13	6.6	<MDL	0.18	0.093	<MDL
	24.10.2021	<MQL	<MDL	<MDL	<MQL	<MDL	<MDL
	25.10.2021	18	23	<MDL	0.26	0.32	<MDL
	Average ± SD	**12 ± 6** [a]	**7.3 ± 8.1** [a]	**<MDL**	**0.17 ± 0.09** [a]	**0.10 ± 0.11** [a]	**<MDL**
Location 3	19.10.2021	455	<MDL	37	6.3	<MDL	0.52
	20.10.2021	283	<MDL	22	4.0	<MDL	0.30
	21.10.2021	307	<MDL	14	4.3	<MDL	0.20
	22.10.2021	486	<MDL	53	6.9	<MDL	0.76
	23.10.2021	733	<MDL	54	10	<MDL	0.76
	24.10.2021	147	<MDL	45	2.1	<MDL	0.64
	25.10.2021	334	<MDL	22	4.7	<MDL	0.32
	Average ± SD	**391± 187**	**<MDL**	**35 ± 16**	**5.5 ± 2.6**	**<MDL**	**0.50 ± 0.23**
Location 4	21.04.2021	37	12	<MDL	0.52	0.17	<MDL
	22.04.2021	22	8.5	<MDL	0.31	0.12	<MDL
	23.04.2021	75	<MDL	<MDL	1.1	<MDL	<MDL
	24.04.2021	17	12	<MDL	0.24	0.17	<MDL
	25.04.2021	24	<MDL	<MDL	0.34	<MDL	<MDL
	26.04.2021	29	7.3	<MDL	0.40	0.11	<MDL
	27.04.2021	24	<MDL	<MDL	0.34	<MDL	<MDL
	Average ± SD	**33 ± 20**	**6.0 ± 5.4** [a]	**<MDL**	**0.46 ± 0.28**	**0.084 ± 0.076** [a]	**<MDL**

[a] Average and standard deviation calculated by substituting the values <MQL and <MDL by MQL/2 and MDL/2, respectively. MDL/MQL: method detection/quantification limit.