

An integrated human health risk assessment framework for alkylphenols due to drinking water and crops' food consumption

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Supplementary Materials

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Section S1: Stochastic simulations

In this section the methodologies adopted for the fitting statistical distributions of NP and BPA data and the application of uncertainty analysis are explained. These methodologies were applied throughout the different steps of the developed probabilistic QCRA procedure.

Section S1.1: Definition of input and output distributions

For each collected input and estimated output, the dataset available was used to fit their statistical distributions. Fits to different statistical distributions were tested, in particular lognormal, normal, logistic, Weibull, gamma, beta, Rayleigh, uniform and triangular were the chosen distributions. The fit function in the R *fitdistrplus* package, which applies a Maximum Likelihood Estimation (MLE) method, was selected to fit data to specific distributions. Then, the statistical distribution having the minimum Akaike Information Criterion (AIC) was selected. Since, for C_{EXP} data, a high percentage of censored data were present, the method explained in [1] was used for the inclusion of left-censored in the fitted statistical distributions, namely the Maximum Likelihood Estimation method for left-censored data (MLE_{LC}).

Section S1.2: Uncertainty analysis

Uncertainty analyses were performed in different steps of the developed QCRA procedure, for the estimation of Dose_{EXP} values first, and of BQ, then. A Monte Carlo simulation method was applied, which allowed for the simultaneous forward propagation of all the inputs uncertainties into the output distribution [2]. For the Dose_{EXP,i,j} estimation (i referred to the contaminant, j to the exposure source), all the obtained $C_{EXP,i,j}$ and IR_j were simultaneously sampled from their estimated statistical distributions and randomly combined together, resulting in 1,000 values of Dose_{EXP,i,j}. Then the same procedure was applied to obtain 1,000 values of BQ, starting from Dose_{EXP,i,j} and HBGV_i estimated statistical distributions. As confirmed by the two previous work [2, 3], 1,000 simulations were enough to get stable outputs.

Section S2: Exposure assessment

Table S1: Summary of the C_{EXP} collected from literature for BPA and NP for each compartment, reporting: number of available data and studies, concentration data range and study's reference.

Compartment	Contaminant	# available data	# available studies	Range	Unit	Reference
Groundwater	BPA	10	9	0.01 – 2.30	µg L ⁻¹	[4]–[12]
	NP	8	8	0.02 – 3.85	µg L ⁻¹	[4]–[11]
Surface water	BPA	95	55	0.0055 – 46.70	µg L ⁻¹	[4], [5], [7]–[60]
	NP	37	13	0.0012 – 2.55	µg L ⁻¹	[4], [5], [7], [16], [21], [22], [26], [27], [39], [41], [46], [59], [61]
Treated drinking water	BPA	37	12	0.0005 – 3.57	µg L ⁻¹	[38], [62]–[74]
	NP	34	11	<0.0001 – 1.10	µg L ⁻¹	[62], [65]–[69], [71], [73]–[76]
Consumed tap water	BPA	88	27	<0.0001 – 3.61	µg L ⁻¹	[8], [11], [16], [23], [26], [29], [39], [62], [71], [72], [77]–[93]
	NP	95	17	<0.0001 – 6.19	µg L ⁻¹	[16], [23], [26], [39], [62], [71], [75], [77], [79], [80], [82]–[85], [90], [92], [94]
Consumed bottled water	BPA	54	13	<0.00001 – 1.18	µg L ⁻¹	[77], [83], [84], [88], [95]–[103]
	NP	42	11	<0.006 – 0.54	µg L ⁻¹	[77], [83], [84], [96], [99]–[101], [103]–[106]
Untreated wastewater	BPA	32	14	<0.005 – 29.74	µg L ⁻¹	[7], [11], [15], [21], [39], [57], [73], [107]–[113]
	NP	7	5	0.0176 – 14.18	µg L ⁻¹	[7], [21], [39], [73], [112]
Treated wastewater	BPA	31	14	0.0104 – 9.40	µg L ⁻¹	[5]–[7], [11], [15], [21], [57], [73], [107], [109], [110], [112], [114], [115]
	NP	10	7	0.0006 – 4.20	µg L ⁻¹	[4], [5], [7], [21], [73], [112], [116]
Biosolids	BPA	21	7	63.60 – 236,000	µg kg ⁻¹	[15], [107], [110], [117]–[120]
	NP	6	3	2,000 – 1,359,000	µg kg ⁻¹	[121]–[123]
Agricultural soil	BPA	55	16	<0.0042 – 167.90	µg kg ⁻¹	[4], [5], [20], [35], [81], [119], [120], [124]–[133]
	NP	8	5	4.43 – 542.00	µg kg ⁻¹	[4]–[6], [134], [135]
Food – Cereals	BPA	22	5	1.60 – 1,740	µg kg ⁻¹	[4], [78], [81], [136], [137]
	NP	18	2	<0.06 – 440	µg kg ⁻¹	[4], [136]
Food – Fruits and vegetables	BPA	62	11	<0.0009 – 1,188	µg kg ⁻¹	[4], [35], [36], [81], [131], [137]–[142]
	NP	42	5	<0.0007 – 700.00	µg kg ⁻¹	[4], [134], [140], [141], [143]

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