Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology. This journal is © The Royal Society of Chemistry 2020

Electronic Supplementary Information

## Mixture effects of drinking water disinfection by-products:

## implications for risk assessment<sup>†</sup>

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Name	Abbreviation	SMILES <sup>a</sup>	CAS# <sup>b</sup>	Purity (%)	Source
halomethanes HMs (+haloe	ethenes)			• • •	
1,1-dichloroethene	1,1-dCE	C=C(CI)CI	75-35-4	99.5	ChemService
dichloromethane	dCM	C(CI)CI	000075-09-2	≥99.8	Sigma-Aldrich
bromochloromethane	BCM	C(Cl)Br	74-97-5	99.5	ChemService
chloroform	tCM	C(CI)(CI)CI	000067-66-3	≥99.0	Sigma-Aldrich
bromodichloromethane	BdCM	C(CI)(CI)Br	000075-27-4	≥99.5	Sigma-Aldrich
bromoform	tBM	C(Br)(Br)Br	000075-25-2	≥99.0	Sigma-Aldrich
dibromochloromethane	dBCM	C(Cl)(Br)Br	000124-48-1	≥99.5	Sigma-Aldrich
dichloroiodomethane	dCIM	C(CI)(CI)I	594-04-7	90-95	CanSyn
bromochloroiodomethane	BCIM	C(Cl)(Br)l	34970-00-8	≥99.5	CanSyn
dibromoiodomethane	dBIM	C(Br)(Br)I	593-94-2	90-95	CanSyn
chlorodiiodomethane	CdIM	C(CI)(I)I	638-73-3	90-95	CanSyn
bromodiiodomethane	BdIM	C(Br)(I)I	557-95-9	90-95	CanSyn
triiodomethane	tIM	C(I)(I)I	75-47-8	≥99.0	Sigma-Aldrich
halonitromethanes HNMs					
trichloronitromethane	tCNM	O=N(=O)C(CI)(CI)CI	76-06-2	≥99.5	Sigma-Aldrich
tribromonitromethane	tBNM	O=N(=O)C(Br)(Br)Br	464-10-8	≥95.0	NovaChem
haloacetonitriles HANs					
dichloroacetonitrile	dCAN	N#CC(CI)CI	003018-12-0	≥99.9	Sigma-Aldrich
trichloroacetonitrile	tCAN	N#CC(CI)(CI)CI	545-06-2	≥99.5	Sigma-Aldrich
bromochloroacetonitrile	BCAN	N#CC(Cl)Br	83463-62-1	≥99.0	NovaChem
dibromoacetonitrile	dBAN	N#CC(Br)Br	3252-43-5	96.3	ChemService
haloketones HKs					
1,1-dichloropropanone	1,1-dCP	O=C(C)C(CI)CI	513-88-2	97.6	ChemService
1,1,1-trichloropropanone	1,1,1-tCP	O=C(C)C(Cl)(Cl)Cl	918-00-3	98.2	ChemService
haloacetic acids HAAs					
chloroacetic acid	CAA	O=C(O)CCI	79-11-8	≥99.0	Sigma-Aldrich
bromoacetic acid	BAA	O=C(O)CBr	000079-08-3	≥99.0	Sigma-Aldrich
iodoacetic acid	IAA	O=C(O)CI	64-69-7	≥99.0	Sigma-Aldrich
dichloroacetic acid	dCAA	O=C(O)C(CI)CI	000079-43-6	≥99.5	Sigma-Aldrich
bromochloroacetic acid	BCAA	O=C(O)C(Cl)Br	5589-96-8	≥98.0	Sigma-Aldrich
dibromoacetic acid	dBAA	O=C(O)C(Br)Br	631-64-1	≥99.5	Sigma-Aldrich
chloroiodoacetic acid	CIAA	O=C(O)C(CI)I	53715-09-6	≥90.0	CanSyn
bromoiodoacetic acid	BIAA	O=C(O)C(Br)I	71815-43-5	≥85.5	CanSyn

# Table S1. DBPs used for this study: abbreviations, SMILES, CAS # (Chemical Abstract Service Number), purity, and source (reprinted from Stalter et al.<sup>1</sup>).

Name	Abbreviation	SMILES <sup>a</sup>	CAS# <sup>b</sup>	Purity (%)	Source
trichloroacetic acid	tCAA	O=C(O)C(CI)(CI)CI	000076-03-9	≥99.0	Sigma-Aldrich
bromodichloroacetic acid	BdCAA	O=C(O)C(Cl)(Cl)Br	71133-14-7	≥99.5	Sigma-Aldrich
dibromochloroacetic acid	dBCAA	O=C(O)C(Cl)(Br)Br	5278-95-5	≥95.0	NovaChem
tribromoacetic acid	tBAA	O=C(O)C(Br)(Br)Br	75-96-7	≥99.5	Sigma-Aldrich
haloacetaldehyde					
chloral hydrate	СН	O=CC(CI)(CI)CI	75-87-6	≥99.5	Sigma-Aldrich
haloacetamides HAcAms					
dichloracetamide	dCAcAm	O=C(N)C(CI)CI	683-72-7	≥99.0	ChemService
bromochloroacetamide	BCAcAm	O=C(N)C(Cl)Br	62872-34-8	≥99.0	CanSyn
dibromoacetamide	dBAcAm	O=C(N)C(Br)Br	598-70-9	≥99.0	CanSyn
chloroiodoacetamide	CIAcAm	O=C(N)C(CI)I	62872–35–9	≥99.0	CanSyn
bromoiodoacetamide	BIAcAm	O=C(N)C(Br)I	62872–36–0	85	CanSyn
diiodoacetamide	dIAcAm	O=C(N)C(I)I	5875-23-0	≥99.0	CanSyn
trichloroacetamide	tCAcAm	O=C(N)C(CI)(CI)CI	594-65-0	99	Sigma-Aldrich
bromodichloroacetamide	BdCAcAm	O=C(N)C(Cl)(Cl)Br	98137-00-9	≥99.0	CanSyn
dibromochloroacetamide	dBCAcAm	O=C(N)C(Cl)(Br)Br	855878-13-6	≥99.0	CanSyn
tribromoacetamide	tBAcAm	O=C(N)C(Br)(Br)Br	594-47-8	≥99.0	CanSyn
nitrosamines					
n-nitrosodimethylamine	NDMA	O=NN(C)C	000062-75-9	≥95.0	NovaChem
n-nitrosodiethylamine	NDEA	O=NN(CC)CC	000055-18-5	≥99.0	Sigma-Aldrich
n-nitrosopiperidine	N-Pip	O=NN1CCCCC1	100-75-4	≥95.0	NovaChem
n-nitrosomorpholine	N-Morph	O=NC1OCCNC1	59-89-2	≥95.0	NovaChem
nitrosodi-n-butylamine	N-But	O=NN(CCCC)CCCC	924-16-3	≥95.0	NovaChem
furanone					
3-chloro-4-(dichloromethyl)-5-					
hydroxy-5H-furan-2-one	MX	O=C1OC(O)C(=C1Cl)C(Cl)Cl	77439-76-0	95	NovaChem

<sup>a</sup> simplified molecular-input line-entry system,

<sup>b</sup> chemical abstracts service number.

	ARE	c32	ARE	-bla	p53-	bla	Mic	rotox	ur	muC
THMs	EC <sub>IR1.5</sub> (M)	<b>REP<sub>dBAN</sub></b>	EC <sub>IR1.5</sub> (M)	<b>REP<sub>dBAN</sub></b>	EC <sub>IR1.5</sub> (M)	<b>REP<sub>dBAN</sub></b>	EC <sub>50</sub> (M)	<b>REP<sub>dBAN</sub></b>	EC <sub>IR1.5</sub> (M)	<b>REP<sub>dBAN</sub></b>
tCM	1.4E-02	1.1E-05	n.eª.≤4E-2		n.e.≤3E-2		6.8E-03	1.3E-03	1.3E-02	3.2E-03
BdCM	6.1E-03	2.5E-05	n.e.≤4E-2		n.e.≤1E-2		1.8E-03	4.7E-03	1.4E-03	2.9E-02
tBM	1.4E-03	1.1E-04	n.e.≤4E-2		n.e.≤6E-3		2.3E-04	3.7E-02	5.2E-04	8.0E-02
dBCM	1.9E-03	7.9E-05	1.6E-02	4.4E-04	n.e.≤1E-2		1.0E-03	8.5E-03	5.5E-04	7.5E-02
dCIM	1.6E-04	9.4E-04	2.7E-03	2.6E-03	2.3E-03	5.7E-03	3.2E-04	2.7E-02	2.1E-04	2.0E-01
BCIM	1.2E-04	1.3E-03	2.8E-03	2.5E-03	2.9E-03	4.5E-03	9.7E-05	8.8E-02	1.8E-04	2.3E-01
dBIM	9.2E-05	1.6E-03	1.8E-03	3.9E-03	1.8E-03	7.2E-03	8.9E-05	9.6E-02	5.4E-05	7.7E-01
CdIM	2.7E-05	5.6E-03	2.8E-04	2.5E-02	2.6E-04	5.0E-02	7.1E-05	1.2E-01	5.6E-05	7.4E-01
BdIM	5.5E-05	2.7E-03	5.2E-04	1.3E-02	6.5E-05	2.0E-01	2.2E-05	3.9E-01	2.6E-05	1.6E+00
tIM	2.6E-05	5.8E-03	2.3E-04	3.0E-02	1.7E-05	7.6E-01	9.4E-06	9.0E-01	1.9E-05	2.2E+00
HNMs										
tCNM	8.1E-06	1.9E-02	n.e.≤4E-4		6.9E-05	1.9E-01	3.8E-08	2.2E+02	1.3E-05	3.3E+00
tBNM	4.9E-06	3.1E-02	n.e.≤4E-4		6.2E-05	2.1E-01	3.0E-07	2.8E+01	1.2E-06	3.4E+01
HANs										
dCAN	7.7E-06	1.9E-02	4.8E-05	1.5E-01	2.7E-05	4.8E-01	4.9E-05	1.7E-01	6.0E-05	6.9E-01
tCAN	1.4E-05	1.1E-02	1.5E-04	4.7E-02	1.4E-05	9.3E-01	2.5E-06	3.4E+00	1.7E-05	2.4E+00
BCAN	2.2E-06	6.8E-02	1.1E-05	6.4E-01	1.3E-05	1.0E+00	1.3E-05	6.5E-01	3.7E-05	1.1E+00
dBAN	1.5E-07	1.0E+00	7.0E-06	1.0E+00	1.3E-05	1.0E+00	8.5E-06	1.0E+00	4.1E-05	1.0E+00
HKs										
1,1-dCP	6.8E-07	2.2E-01	n.e.<4E-3		3.4E-05	3.8E-01	3.0E-04	2.8E-02	1.1E-04	3.9E-01
1,1,1-tCP	1.5E-05	1.0E-02	n.e.<4E-3		7.3E-05	1.8E-01	2.2E-04	3.9E-02	1.7E-04	2.5E-01
HAAs										
CAA	2.7E-04	5.6E-04	2.5E-04	2.8E-02	1.7E-04	7.6E-02	3.8E-03	2.2E-03	n.e.≤8E-3	
BAA	5.2E-06	2.9E-02	1.1E-05	6.4E-01	9.5E-06	1.4E+00	3.8E-05	2.2E-01	n.e.≤2E-4	
IAA	3.6E-06	4.2E-02	5.1E-06	1.4E+00	4.7E-06	2.8E+00	1.7E-05	5.0E-01	n.e.≤2E-4	
dCAA	6.0E-03	2.5E-05	1.6E-02	4.4E-04	n.e.≤3E-2		3.7E-03	2.3E-03	n.e.≤2E-2	
BCAA	1.4E-04	1.1E-03	4.6E-04	1.5E-02	2.3E-04	5.7E-02	1.2E-03	7.1E-03	3.4E-04	1.2E-01
dBAA	1.2E-04	1.3E-03	2.5E-04	2.8E-02	2.6E-04	5.0E-02	8.5E-04	1.0E-02	3.9E-04	1.1E-01
CIAA	2.2E-05	6.8E-03	1.0E-04	7.0E-02	1.1E-04	1.2E-01	3.1E-05	2.7E-01	1.9E-04	2.1E-01
BIAA	2.6E-05	5.8E-03	5.3E-05	1.3E-01	1.1E-04	1.2E-01	1.6E-04	5.3E-02	1.1E-04	3.7E-01
tCAA							1.3E-02			
BdCAA	2.0E-03	7.5E-05	4.0E-03	1.8E-03	n.e.≤3E-3		6.1E-04	1.4E-02	1.1E-04	3.7E-01

Table S2. Effect concentrations (EC) and relative effect potencies (REP, relative to dibromoacetonitrile (dBAN)) of DBPs used for this study (reprinted from Stalter et al.<sup>1</sup>).

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	ARE	c32	ARE-bla		p53	-bla	Mic	rotox	um	uC
THMs	EC <sub>IR1.5</sub> (M)	<b>REP<sub>dBAN</sub></b>	EC <sub>IR1.5</sub> (M)	<b>REP<sub>dBAN</sub></b>	EC <sub>IR1.5</sub> (M)	<b>REP<sub>dBAN</sub></b>	EC <sub>50</sub> (M)	<b>REP<sub>dBAN</sub></b>	EC <sub>IR1.5</sub> (M)	<b>REP<sub>dBAN</sub></b>
dBCAA	4.9E-03	3.1E-05	2.2E-03	3.2E-03	n.e.≤2E-3		4.2E-04	2.0E-02	1.1E-04	3.8E-01
tBAA	4.4E-04	3.4E-04	6.7E-04	1.0E-02	n.e.≤5E-4		1.3E-04	6.5E-02	7.0E-06	5.9E+00
Chloralhydrate										
СН	1.7E-04	8.8E-04	6.1E-04	1.1E-02	9.8E-03	1.3E-03	1.5E-02	5.7E-04		
HAcAms										
dCAcAm	1.2E-03	1.3E-04	1.8E-03	3.9E-03	n.e.≤3E-2		3.7E-02	2.3E-04		
BCAcAm	1.4E-05	1.1E-02	3.7E-05	1.9E-01	3.1E-04	4.2E-02	2.7E-03	3.1E-03	2.7E-03	1.5E-02
dBAcAm	4.7E-06	3.2E-02	2.1E-05	3.3E-01	2.4E-05	5.4E-01	1.8E-05	4.7E-01	1.7E-05	2.5E+00
CIAcAm	5.1E-06	2.9E-02	6.4E-05	1.1E-01	6.0E-05	2.2E-01	5.1E-04	1.7E-02	3.4E-04	1.2E-01
BIAcAm	3.3E-06	4.5E-02	1.6E-05	4.4E-01	4.4E-05	3.0E-01	2.1E-03	4.0E-03	4.4E-04	9.4E-02
dIAcAm	5.4E-07	2.8E-01	2.7E-06	2.6E+00	4.9E-05	2.7E-01	1.9E-03	4.5E-03	1.5E-04	2.8E-01
tCAcAm	1.2E-03	1.3E-04	4.7E-03	1.5E-03	n.e.≤6E-3		1.4E-04	6.1E-02	3.2E-03	1.3E-02
BdCAcAm	3.2E-06	4.7E-02	2.0E-05	3.5E-01	2.4E-05	5.4E-01	4.9E-05	1.7E-01	2.2E-05	1.9E+00
dBCAcAm	1.2E-06	1.3E-01	1.3E-05	5.4E-01	3.5E-03	3.7E-03	4.2E-05	2.0E-01	1.3E-05	3.2E+00
tBAcAm	6.6E-06	2.3E-02	8.8E-06	8.0E-01	2.2E-05	5.9E-01	6.9E-06	1.2E+00	1.0E-05	4.1E+00
Halofuranones										
MX	6.5E-06	2.3E-02	4.7E-05	1.5E-01	5.3E-06	2.5E+00	9.8E-07	8.7E+00	1.3E-08	3.1E+03

<sup>a</sup>n.e. = no effect.

		mix1 <sub>AREc32</sub>	mix2 <sub>AREc32</sub>	<b>mix3<sub>AREc32</sub></b>	<b>mix4</b> <sub>AREc32</sub>	mix5 <sub>AREc32</sub>	mix6 <sub>AREc32</sub>	
		except non- ITHMs	WTP1-3 + monoHAAs	monoHAAs + HacAm	monoHAAs + HacAm + MX	mono HAAs	HAcAms	
DBPs in mixture	#of DBPs in mixtures:	14	17	23	24	3	8	EC <sub>IR1.5</sub> (M) <sup>1</sup>
dBIM		1.393%	1.338%	0.994%	0.993%			9.2E-05
CdIM		0.412%	0.395%	0.294%	0.294%			2.7E-05
tCNM		0.123%	0.118%	0.087%	0.087%			8.1E-06
tBNM		0.073%	0.070%	0.052%	0.052%			4.9E-06
dCAN		0.117%	0.112%	0.083%	0.083%			7.7E-06
tCAN		0.219%	0.210%	0.156%	0.156%			1.5E-05
BCAN		0.034%	0.032%	0.024%	0.024%			2.2E-06
dBAN		0.002%	0.002%	0.002%	0.002%			1.5E-07
1,1-dCP	a	0.010%	0.010%	0.007%	0.007%			6.8E-07
1,1,1-tCP	L N	0.231%	0.222%	0.165%	0.165%			1.5E-05
BAA	ixt		0.075%	0.056%	0.056%	1.896%		5.2E-06
BCAA	E	2.126%	2.041%	1.517%	1.516%			1.4E-04
CAA	2.		3.839%	2.853%	2.851%	96.800%		2.7E-04
dBAA	Ps	1.741%	1.672%	1.242%	1.241%			1.2E-04
dCAA	B	90.917%	87.311%	64.876%	64.831%			6.0E-03
ΙΑΑ	of		0.052%	0.038%	0.038%	1.304%		3.6E-06
СН	5	2.604%	2.500%	1.858%	1.857%			1.7E-04
BCAcAm	tio			0.147%	0.147%		35.678%	1.4E-05
dBAcAm	ac			0.051%	0.051%		12.322%	4.7E-06
CIAcAm	fr						13.357%	5.1E-06
BdCAcAm				0.034%	0.034%		8.225%	3.2E-06
BIAcAm							8.731%	3.4E-06
dBCAcAm							3.070%	1.2E-06
tBAcAm				0.071%	0.071%		17.214%	6.6E-06
dIAcAm							1.404%	5.4E-07
tCAcAm				12.863%	12.854%			1.2E-03
dCAcAm				12.530%	12.521%			1.2E-03
MX					0.070%			6.5E-06
EC <sub>IR1.5</sub> (M) in sum of molar		6 63E-03	6 90F-03	9 29F-03	9 30F-03	2 70F-04	3 80F-05	
concentrations for each mixture		0.032 03	0.002 00	5.252 05	5.502 05	2.702 04	3.002 05	

Table S3: Molar fractions of DBPs in equipotent mixtures based on AREc32 effect concentrations (EC<sub>IR1.5</sub> from Stalter et al.<sup>1</sup>).

		mix1 <sub>p53-bla</sub>	mix2 <sub>p53-bla</sub>	mix3 <sub>p53-bla</sub>	mix4 <sub>p53-bla</sub>	mix5 <sub>p53-bla</sub>	mix6 <sub>p53-bla</sub>	
		found at WTP1-3 except non- ITHMs	WTP1-3 + monoHAAs	WTP1-3 + monoHAAs + HacAm	WTP1-3 + monoHAAs + HacAm + MX	mono HAAs	HAcAms	
DBPs in mixture	#of DBPs in mixtures:	13	16	20	21	3	8	EC <sub>IR1.5</sub> (M) <sup>b</sup>
dBIM		13.914%	13.717%	13.321%	13.316%			1.8E-03
CdIM		2.064%	2.035%	1.977%	1.976%			2.6E-04
tCNM		0.545%	0.537%	0.521%	0.521%			6.9E-05
tBNM		0.491%	0.484%	0.470%	0.470%			6.2E-05
dCAN		0.216%	0.213%	0.207%	0.207%			2.7E-05
tCAN		0.110%	0.109%	0.106%	0.106%			1.4E-05
BCAN		0.103%	0.102%	0.099%	0.099%			1.3E-05
dBAN		0.102%	0.100%	0.097%	0.097%			1.3E-05
1,1-dCP	۵	0.269%	0.265%	0.257%	0.257%			3.4E-05
1,1,1-tCP		0.574%	0.566%	0.549%	0.549%			7.3E-05
BAA	ixt		0.074%	0.072%	0.072%	5.249%		9.5E-06
BCAA	Ē	1.800%	1.775%	1.724%	1.723%			2.3E-04
CAA	Ľ.		1.301%	1.263%	1.263%	92.152%		1.7E-04
dBAA	Ps	2.091%	2.061%	2.002%	2.001%			2.6E-04
dCAA	DB	no effect	no effect	no effect	no effect			no effect
ΙΑΑ	of		0.037%	0.036%	0.036%	2.599%		4.7E-06
СН	Ē	77.721%	76.624%	74.409%	74.380%			9.8E-03
BCAcAm	tio			2.364%	2.363%		7.707%	3.1E-04
dBAcAm	ä			0.181%	0.181%		0.590%	2.4E-05
CIAcAm	fr						1.478%	6.0E-05
BdCAcAm				0.179%	0.179%		0.584%	2.4E-05
BIAcAm							1.087%	4.4E-05
dBCAcAm							86.812%	3.5E-03
tBAcAm				0.166%	0.166%		0.540%	2.2E-05
dIAcAm							1.202%	4.9F-05
tCAcAm				no effect	no effect		,	no effect
dCAcAm				no effect	no effect			no effect
MX					0.040%			5.3F-06
EC <sub>IR1.5</sub> (M) in sum of molar		1.27E-02	1.28E-02	1.32E-02	1.30E-02	1.80E-04	4.10E-03	5.52 00
concentrations for each mixture								

Table S4: Molar fractions of equipotent mixtures based on p53-bla effect concentrations (EC<sub>IR1.5</sub> from Stalter et al.<sup>1</sup>).



**Figure S1. Mixture effects of DBPs in the Microtox assay on cytotoxicity**: Experimental effects (Exp, symbols and green lines) versus effects predicted with the model for concentration addition (CA, blue lines). Mixtures A – F: concentration ratios equipotent to effect concentrations in the AREc32 assay (Table S1); Mixtures G – L: concentration ratios equipotent to effect concentrations in the p53-bla assay (Table S2). Standard deviation of each experimental data point is displayed as vertical error bar and the 95% confidence intervals of the modeled and experimental dose-response curves are displayed as dotted black lines.



**Figure S2. Mixture effects of DBPs in the AREc32 assay on oxidative stress**: Experimental effects (Exp, symbols and green lines) versus effects predicted with the model for concentration addition (CA, blue lines). Mixtures A – F: concentration ratios equipotent to effect concentrations in the AREc32 assay (Table S1); Mixtures G – L: concentration ratios equipotent to effect concentrations in the p53-bla assay (Table S2). Standard deviation of each experimental data point is displayed as vertical error bar, for the modeled effects as transparent blue band and the 95% confidence interval for the linear regression of the experimental data is displayed in light green.







**Figure S4. Mixture effects of DBPs in the p53-bla assay on genotoxicity**: Experimental effects (Exp, symbols and green lines) versus effects predicted with the model for concentration addition (CA, blue lines). Mixtures A – F: concentration ratios equipotent to effect concentrations in the AREc32 assay (Table S1); Mixtures G – L: concentration ratios equipotent to effect concentrations in the p53-bla assay (Table S2). Standard deviation of each experimental data point is displayed as vertical error bar, for the modeled effects as transparent blue band and the 95% confidence interval for the linear regression of the experimental data is displayed in light green.

Table S5: Relative effect potencies (REP, equation 5, molar ratios) of DBPs and DBP concentrations in 16 different samples based on literature data (see references in the table legend below) plus four hypothetical mixtures (abbreviations of chemical names according to Table S1 and Figure 3; n.a., not analyzed; n.i., not included). Samples: 1 (Neale et al.<sup>2</sup>); 2 – 7 (Farré et al.<sup>3</sup>); 8 – 10 (Stalter et al.<sup>4</sup>); 11 – 12 (Miltner et al. <sup>5</sup>(; 13 (Wei et al.<sup>6</sup>); 14 – 16 (Weinberg et al.<sup>7</sup>); 17, hypothetical mixture 1 (no MX, no mono-HAAs, no HAcAms); 18, hypothetical mixture 2 (+ MX, no mono-HAAs, no HAcAms); 19, hypothetical mixture 3 (+ MX, + mono-HAAs, no HAcAms); 20, hypothetical mixture 4 (+ MX, + mono-HAAs, + HAcAms).

	Concentrations (µg/L) in samples																								
	REP <sub>AREc32</sub>	<b>REP</b> ARE-bla	REP <sub>AREc32</sub>	REPumUC	REP <sub>Microtox</sub>	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
THMs																									
tCM	1.07E-05			3.16E-03	1.25E-03	25	270	15	57	6	50	6.3	22	18	23	60	30	6.5	7	14	27	100	100	100	100
BdCM	2.46E-05			2.91E-02	4.72E-03	46	48	7.5	18	1.7	42	6	15	16	18	40	30	3.7	13	8	9	50	50	50	50
tBM	1.07E-04			7.99E-02	3.70E-02	17	<0.1	<0.1	<0.1	<0.1	1.8	0.5	1.1	3.9	1.9	3	4	1.9	2	0.1	<0.1	20	20	20	20
dBCM	7.89E-05	4.38E-04		7.54E-02	8.50E-03	57	4.3	0.8	3.3	0.2	16	2.3	7.7	16	16	20	20	2.4	10	2	1	50	50	50	50
dCIM	9.38E-04	2.59E-03	5.65E-03	1.97E-01	2.66E-02	1.2	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	0.1	0.9	0.2	0.6	0.3	n.a.	4	0.5	<0.1	10	10	10	10
BCIM	1.25E-03	2.50E-03	4.48E-03	2.32E-01	8.76E-02	n.a.	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	0.2	<0.1	n.a.	1	<0.1	<0.1	10	10	10	10
dBIM	1.63E-03	3.89E-03	7.22E-03	7.72E-01	9.55E-02	n.a.	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	n.a.	0.5	<0.53	<0.53	10	10	10	10
CdIM	5.56E-03	2.50E-02	5.00E-02	7.36E-01	1.20E-01	n.a.	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	n.a.	0.5	<0.1	<0.1	10	10	10	10
BdIM	2.73E-03	1.35E-02	2.00E-01	1.60E+00	3.86E-01	n.a.	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	n.a.	n.a.	<0.1	<0.1	1	1	1	1
tIM	5.77E-03	3.04E-02	7.65E-01	2.21E+00	9.04E-01	n.a.	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	n.a.	n.a.	<0.1	<0.1	1	1	1	1
												Со	ncer	ntrat	ions	(µg	/L) i	n sar	nple	S					
	REP <sub>AREc32</sub>	<b>REP</b> ARE-bla	REP <sub>AREc32</sub>	REPumUC	REPMicrotox	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
HNMs																									
tCNM	1.85E-02		1.88E-01	3.25E+00	2.24E+02	0.2	1.3	1.5	0.2	0.3	0.1	0.3	<0.1	0.2	0.2	0.8	3	n.a.	0.2	0.3	<0.1	2	2	2	2
tBNM	3.06E-02		2.10E-01	3.41E+01	2.83E+01	n.a.	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	0.8	1.8	<0.1	<0.1	n.a.	<0.5	<0.5	<0.5	2	2	2	2
HANs																									
dCAN	1.95E-02	1.46E-01	4.81E-01	6.94E-01	1.73E-01	2.1	13	4.8	2.8	1	3.3	1.2	<0.1	2	1.5	5	3	0.6	2	2	8	2	2	2	2
tCAN	1.07E-02	4.67E-02	9.29E-01	2.42E+00	3.40E+00	0.2	5.6	0.7	1.6	0.4	2.2	<0.1	<0.1	<0.1	<0.1	0.2	0.1	0.1	<0.1	<0.1	<0.1	2	2	2	2
BCAN	6.82E-02	6.36E-01	1.00E+00	1.11E+00	6.54E-01	4.8	2.2	0.6	1	0.2	3.7	0.8	<0.1	2.3	1.8	4	3	0.9	2	0.6	1	2	2	2	2
dBAN	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	3.1	0.2	0.2	0.3	0.2	1.2	0.3	<0.1	2.5	2.3	2	2	0.9	2	0.2	0.4	2	2	2	2
HKs																									
1,1-dCP	2.21E-01		3.82E-01	3.86E-01	2.83E-02	0.4	1.2	4.7	0.3	1	0.5	0.7	<0.1	0.5	1.6	<0.1	<0.1	0.7	0.7	2	1	5	5	5	5
1,1,1-tCP	1.00E-02		1.78E-01	2.46E-01	3.86E-02	1.9	13	0.7	2.7	0.2	11	0.2	<0.1	<0.1	0.5	4	8	0.5	1	1	6	5	5	5	5
HAAs																									
CAA	5.56E-04	2.80E-02	7.65E-02		2.24E-03	n.a.	<5	<5	<5	5	7	n.a.	<2	5.3	7.8	n.i.	n.i.	10	10						
BAA	2.88E-02	6.36E-01	1.37E+00		2.24E-01	n.a.	<5	<5	<5	6.4	4.5	n.a.	<1	3.5	<1	n.i.	n.i.	10	10						
IAA	4.17E-02	1.37E+00	2.77E+00		5.00E-01	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.i.	n.i.	3	3								

dCAA	2.50E-05	4.38E-04			2.30E-03	n.a.	5	18	38	29	20	2.7	12	40	25	50	50	50	50						
BCAA	1.07E-03	1.52E-02	5.65E-02	1.20E-01	7.08E-03	n.a.	<5	12	23	14	12	n.a.	11	12	4.9	20	20	20	20						
dBAA	1.25E-03	2.80E-02	5.00E-02	1.07E-01	1.00E-02	n.a.	<5	<5	<5	3.1	3.8	0.6	6.2	1.7	<1	10	10	10	10						
CIAA	6.82E-03	7.00E-02	1.18E-01	2.14E-01	2.74E-01	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	3	3	3	3							
BIAA	5.77E-03	1.32E-01	1.18E-01	3.72E-01	5.31E-02	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	3	3	3	3							
BdCAA	7.50E-05	1.75E-03		3.72E-01	1.39E-02	n.a.	<5	16	15	12	7.3	n.a.	7.8	8.1	7.3	20	20	20	20						
dBCAA	3.06E-05	3.18E-03		3.75E-01	2.02E-02	n.a.	<5	<5	<5	3.4	3.4	n.a.	3.6	1.3	1.2	20	20	20	20						
tBAA	3.41E-04	1.04E-02		5.91E+00	6.54E-02	n.a.	n.a.	n.a.	4	4	n.a.	<2	<2	<2	10	10	10	10							
Chloralhydrate																									
СН	8.82E-04	1.15E-02	1.33E-03		5.67E-04	3.2	0.2	0.2	0.3	0.2	1.2	0.3	1.5	3.5	6	20	25	0.5	2	4	4	10	10	10	10
HAcAms																									
dCAcAm	1.25E-04	3.89E-03			2.30E-04	n.a.	< 0.1	<0.1	<0.1	n.a.	n.a.	n.a.	3.9	4.1	<0.1	n.i.	n.i.	n.i.	5						
BCAcAm	1.07E-02	1.89E-01	4.19E-02	1.52E-02	3.15E-03	n.a.	<0.1	<0.1	<0.1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.i.	n.i.	n.i.	5						
dBAcAm	3.19E-02	3.33E-01	5.42E-01	2.49E+00	4.72E-01	n.a.	<0.1	<0.1	<0.1	n.a.	n.a.	n.a.	0.8	0.2	<0.1	n.i.	n.i.	n.i.	5						
CIAcAm	2.94E-02	1.09E-01	2.17E-01	1.23E-01	1.67E-02	n.a.	<0.1	<0.1	<0.1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.i.	n.i.	n.i.	5						
BIAcAm	4.55E-02	4.38E-01	2.95E-01	9.39E-02	4.05E-03	n.a.	<0.1	<0.1	<0.1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.i.	n.i.	n.i.	5						
dIAcAm	2.78E-01	2.59E+00	2.65E-01	2.83E-01	4.47E-03	n.a.	< 0.1	<0.1	<0.1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.i.	n.i.	n.i.	5						
tCAcAm	1.25E-04	1.49E-03		1.31E-02	6.07E-02	n.a.	<0.1	<0.1	<0.1	n.a.	n.a.	n.a.	0.3	1.1	<0.1	n.i.	n.i.	n.i.	5						
BdCAcAm	4.69E-02	3.50E-01	5.42E-01	1.91E+00	1.73E-01	n.a.	<0.1	<0.1	<0.1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.i.	n.i.	n.i.	5						
dBCAcAm	1.25E-01	5.38E-01	3.71E-03	3.20E+00	2.02E-01	n.a.	<0.1	<0.1	<0.1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.i.	n.i.	n.i.	5						
tBAcAm	2.27E-02	7.95E-01	5.91E-01	4.14E+00	1.23E+00	n.a.	<0.1	<0.1	<0.1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.i.	n.i.	n.i.	5						
Halofuranones																									
MX	2.31E-02	1.49E-01	2.45E+00	3.11E+03	8.67E+00	n.a.	n.a.	n.a.	<0.02	<0.02	n.a.	0.1	0.3	<0.02		0.3	0.3	0.3							

#### Electronic Supplementary Information

Table S6: DBP concentrations ( $\mu$ g/L) in the sample extracts used to calculate the effect of known DBPs (BEQ<sub>chem</sub>) versus the effect of the sample extract (BEQ<sub>bio</sub>). TW1 – 3<sub>SPE</sub>: three tap waters (TW) from three different taps in the Brisbane area were sampled at two different time points (e.g., TW1-1 and TW1-2: sampled from the same tap at two different time points) and extracted with solid phase extraction (SPE); TW1-1<sub>P&T</sub>, TW2-1<sub>P&T</sub>, and TW3-1<sub>P&T</sub>: same samples as TW1-1<sub>SPE</sub>, etc., extracted with a purge and trap method (P&T) before SPE to capture the volatile DBP fraction (Stalter et al.<sup>4</sup>); WTP1 – 3: final drinking water collected directly from three different drinking water treatment plants from the greater Brisbane area (Queensland, Australia); n.a.: not analyzed; <LOD: below limit of detection; for DBP abbreviations see Table S1. DBP concentrations were from a previous study (Stalter et al.<sup>4</sup>).

	TW1-1 <sub>SPE</sub>	TW2-1 <sub>SPE</sub>	TW3-1 <sub>SPE</sub>	TW1-1 <sub>P&amp;T</sub>	TW2-1 <sub>P&amp;T</sub>	TW3-1 <sub>P&amp;T</sub>	TW1-2 <sub>SPE</sub>	TW2-2 <sub>SPE</sub>	TW3-2 <sub>SPE</sub>	WTP1 <sub>SPE</sub>	WTP2 <sub>SPE</sub>	WTP3 <sub>SPE</sub>
THMs												
tCM	<lod< td=""><td><lod< td=""><td><lod< td=""><td>12.4</td><td>10.08</td><td>11.09</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.15</td><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td>12.4</td><td>10.08</td><td>11.09</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.15</td><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td>12.4</td><td>10.08</td><td>11.09</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.15</td><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	12.4	10.08	11.09	<lod< td=""><td><lod< td=""><td><lod< td=""><td>0.15</td><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td>0.15</td><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td>0.15</td><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<>	0.15	<lod< td=""><td><lod< td=""></lod<></td></lod<>	<lod< td=""></lod<>
BdCM	<lod< td=""><td>0.08</td><td>0.01</td><td>7.07</td><td>8.00</td><td>7.82</td><td>0.23</td><td>0.06</td><td>0.09</td><td>0.15</td><td>0.22</td><td>0.03</td></lod<>	0.08	0.01	7.07	8.00	7.82	0.23	0.06	0.09	0.15	0.22	0.03
tBM	<lod< td=""><td><lod< td=""><td>0.04</td><td>0.32</td><td>1.63</td><td>1.48</td><td>0.05</td><td>0.41</td><td>0.04</td><td><lod< td=""><td>0.042</td><td></td></lod<></td></lod<></td></lod<>	<lod< td=""><td>0.04</td><td>0.32</td><td>1.63</td><td>1.48</td><td>0.05</td><td>0.41</td><td>0.04</td><td><lod< td=""><td>0.042</td><td></td></lod<></td></lod<>	0.04	0.32	1.63	1.48	0.05	0.41	0.04	<lod< td=""><td>0.042</td><td></td></lod<>	0.042	
dBCM	0.03	0.1	0.04	4.42	10.35	9.48	0.27	0.23	0.16	0.05	0.15	0.04
dCIM	<lod< td=""><td><lod< td=""><td><lod< td=""><td>0.06</td><td>0.39</td><td>0.33</td><td><lod< td=""><td>0.03</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td>0.06</td><td>0.39</td><td>0.33</td><td><lod< td=""><td>0.03</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td>0.06</td><td>0.39</td><td>0.33</td><td><lod< td=""><td>0.03</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	0.06	0.39	0.33	<lod< td=""><td>0.03</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	0.03	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<>	<lod< td=""></lod<>
BCIM	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.31</td><td>0.18</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td>0.31</td><td>0.18</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td>0.31</td><td>0.18</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td>0.31</td><td>0.18</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	0.31	0.18	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<>	<lod< td=""></lod<>
dBIM	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.03</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.04</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td>0.03</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.04</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td>0.03</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.04</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td>0.03</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.04</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	0.03	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.04</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.04</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td>0.04</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td>0.04</td><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td>0.04</td><td><lod< td=""></lod<></td></lod<>	0.04	<lod< td=""></lod<>
CdIM	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<>	<lod< td=""></lod<>
BdIM	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<>	<lod< td=""></lod<>
tIM	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<>	<lod< td=""></lod<>
HNMs												
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HANs												
dCAN	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.63</td><td>0.46</td><td>0.06</td><td>0.09</td><td>0.05</td><td>0.06</td><td>0.08</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td>0.63</td><td>0.46</td><td>0.06</td><td>0.09</td><td>0.05</td><td>0.06</td><td>0.08</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td>0.63</td><td>0.46</td><td>0.06</td><td>0.09</td><td>0.05</td><td>0.06</td><td>0.08</td><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td>0.63</td><td>0.46</td><td>0.06</td><td>0.09</td><td>0.05</td><td>0.06</td><td>0.08</td><td><lod< td=""></lod<></td></lod<>	0.63	0.46	0.06	0.09	0.05	0.06	0.08	<lod< td=""></lod<>
tCAN	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<>	<lod< td=""></lod<>
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dBAN	<lod< td=""><td>0.15</td><td>0.16</td><td><lod< td=""><td>0.15</td><td>0.29</td><td>0.13</td><td><lod< td=""><td>0.42</td><td><lod< td=""><td>0.08</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	0.15	0.16	<lod< td=""><td>0.15</td><td>0.29</td><td>0.13</td><td><lod< td=""><td>0.42</td><td><lod< td=""><td>0.08</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	0.15	0.29	0.13	<lod< td=""><td>0.42</td><td><lod< td=""><td>0.08</td><td><lod< td=""></lod<></td></lod<></td></lod<>	0.42	<lod< td=""><td>0.08</td><td><lod< td=""></lod<></td></lod<>	0.08	<lod< td=""></lod<>
HKs												
1,1-dCP	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.11</td><td><lod< td=""><td>0.05</td><td>0.03</td><td><lod< td=""><td>0.09</td><td>0.09</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td>0.11</td><td><lod< td=""><td>0.05</td><td>0.03</td><td><lod< td=""><td>0.09</td><td>0.09</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td>0.11</td><td><lod< td=""><td>0.05</td><td>0.03</td><td><lod< td=""><td>0.09</td><td>0.09</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td>0.11</td><td><lod< td=""><td>0.05</td><td>0.03</td><td><lod< td=""><td>0.09</td><td>0.09</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	0.11	<lod< td=""><td>0.05</td><td>0.03</td><td><lod< td=""><td>0.09</td><td>0.09</td><td><lod< td=""></lod<></td></lod<></td></lod<>	0.05	0.03	<lod< td=""><td>0.09</td><td>0.09</td><td><lod< td=""></lod<></td></lod<>	0.09	0.09	<lod< td=""></lod<>
1,1,1-tCP	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.04</td><td>0.13</td><td>0.03</td><td><lod< td=""><td>0.12</td><td>0.15</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.04</td><td>0.13</td><td>0.03</td><td><lod< td=""><td>0.12</td><td>0.15</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td>0.04</td><td>0.13</td><td>0.03</td><td><lod< td=""><td>0.12</td><td>0.15</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td>0.04</td><td>0.13</td><td>0.03</td><td><lod< td=""><td>0.12</td><td>0.15</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td>0.04</td><td>0.13</td><td>0.03</td><td><lod< td=""><td>0.12</td><td>0.15</td><td><lod< td=""></lod<></td></lod<></td></lod<>	0.04	0.13	0.03	<lod< td=""><td>0.12</td><td>0.15</td><td><lod< td=""></lod<></td></lod<>	0.12	0.15	<lod< td=""></lod<>
HAAs												
CAA	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<>	<lod< td=""></lod<>
BAA	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<>	<lod< td=""></lod<>
IAA	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
dCAA	1.5	6.13	5	<lod< td=""><td><lod< td=""><td><lod< td=""><td>7.13</td><td>1.38</td><td>3.25</td><td>42</td><td>21</td><td>6</td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td>7.13</td><td>1.38</td><td>3.25</td><td>42</td><td>21</td><td>6</td></lod<></td></lod<>	<lod< td=""><td>7.13</td><td>1.38</td><td>3.25</td><td>42</td><td>21</td><td>6</td></lod<>	7.13	1.38	3.25	42	21	6
BCAA		8.13	5	<lod< td=""><td><lod< td=""><td><lod< td=""><td>13.25</td><td>1.88</td><td>6.75</td><td>14</td><td>17</td><td>7</td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td>13.25</td><td>1.88</td><td>6.75</td><td>14</td><td>17</td><td>7</td></lod<></td></lod<>	<lod< td=""><td>13.25</td><td>1.88</td><td>6.75</td><td>14</td><td>17</td><td>7</td></lod<>	13.25	1.88	6.75	14	17	7

dBAA	<lod< th=""><th><lod< th=""><th><lod< th=""><th><lod< th=""><th><lod< th=""><th><lod< th=""><th>8</th><th>1.75</th><th>5.75</th><th><lod< th=""><th>6</th><th>8</th></lod<></th></lod<></th></lod<></th></lod<></th></lod<></th></lod<></th></lod<>	<lod< th=""><th><lod< th=""><th><lod< th=""><th><lod< th=""><th><lod< th=""><th>8</th><th>1.75</th><th>5.75</th><th><lod< th=""><th>6</th><th>8</th></lod<></th></lod<></th></lod<></th></lod<></th></lod<></th></lod<>	<lod< th=""><th><lod< th=""><th><lod< th=""><th><lod< th=""><th>8</th><th>1.75</th><th>5.75</th><th><lod< th=""><th>6</th><th>8</th></lod<></th></lod<></th></lod<></th></lod<></th></lod<>	<lod< th=""><th><lod< th=""><th><lod< th=""><th>8</th><th>1.75</th><th>5.75</th><th><lod< th=""><th>6</th><th>8</th></lod<></th></lod<></th></lod<></th></lod<>	<lod< th=""><th><lod< th=""><th>8</th><th>1.75</th><th>5.75</th><th><lod< th=""><th>6</th><th>8</th></lod<></th></lod<></th></lod<>	<lod< th=""><th>8</th><th>1.75</th><th>5.75</th><th><lod< th=""><th>6</th><th>8</th></lod<></th></lod<>	8	1.75	5.75	<lod< th=""><th>6</th><th>8</th></lod<>	6	8
	TW1-1 <sub>SPE</sub>	TW2-1 <sub>SPE</sub>	TW3-1 <sub>SPE</sub>	TW1-1 <sub>P&amp;T</sub>	TW2-1 <sub>P&amp;T</sub>	TW3-1 <sub>P&amp;T</sub>	TW1-2 <sub>SPE</sub>	TW2-2 <sub>SPE</sub>	TW3-2 <sub>SPE</sub>	WTP1 <sub>SPE</sub>	WTP2 <sub>SPE</sub>	WTP3 <sub>SPE</sub>
CIAA	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
BIAA	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
tCAA	0.63	6.5	3.75	<lod< td=""><td><lod< td=""><td><lod< td=""><td>6.5</td><td>1.88</td><td>3.13</td><td>58</td><td>19</td><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td>6.5</td><td>1.88</td><td>3.13</td><td>58</td><td>19</td><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td>6.5</td><td>1.88</td><td>3.13</td><td>58</td><td>19</td><td><lod< td=""></lod<></td></lod<>	6.5	1.88	3.13	58	19	<lod< td=""></lod<>
BdCAA	1	7.25	2.88	<lod< td=""><td><lod< td=""><td><lod< td=""><td>10.88</td><td>3</td><td>6.75</td><td>18</td><td>14</td><td>7</td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td>10.88</td><td>3</td><td>6.75</td><td>18</td><td>14</td><td>7</td></lod<></td></lod<>	<lod< td=""><td>10.88</td><td>3</td><td>6.75</td><td>18</td><td>14</td><td>7</td></lod<>	10.88	3	6.75	18	14	7
dBCAA	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>4.63</td><td>1.63</td><td>4</td><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>4.63</td><td>1.63</td><td>4</td><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>4.63</td><td>1.63</td><td>4</td><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td>4.63</td><td>1.63</td><td>4</td><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td>4.63</td><td>1.63</td><td>4</td><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td>4.63</td><td>1.63</td><td>4</td><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	4.63	1.63	4	<lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<>	<lod< td=""></lod<>
tBAA	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<>	<lod< td=""></lod<>
Chloralhydrate	e											
СН	<lod< td=""><td>0.22</td><td>0.77</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td>0.7</td><td>0.1</td><td>0.81</td><td>2.04</td><td>0.74</td><td>0.21</td></lod<></td></lod<></td></lod<></td></lod<>	0.22	0.77	<lod< td=""><td><lod< td=""><td><lod< td=""><td>0.7</td><td>0.1</td><td>0.81</td><td>2.04</td><td>0.74</td><td>0.21</td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td>0.7</td><td>0.1</td><td>0.81</td><td>2.04</td><td>0.74</td><td>0.21</td></lod<></td></lod<>	<lod< td=""><td>0.7</td><td>0.1</td><td>0.81</td><td>2.04</td><td>0.74</td><td>0.21</td></lod<>	0.7	0.1	0.81	2.04	0.74	0.21
HAcAms												
dCAcAm	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<>	<lod< td=""></lod<>
BCAcAm	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<>	<lod< td=""></lod<>
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BIAcAm	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
dIAcAm	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
tCAcAm	<lod< td=""><td>0.5</td><td>1.44</td><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	0.5	1.44	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""><td><lod< td=""></lod<></td></lod<></td></lod<>	<lod< td=""><td><lod< td=""></lod<></td></lod<>	<lod< td=""></lod<>
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AREc32 assay												
BEQ <sub>chem</sub> <sup>a</sup>	6.63E-13	8.23E-10	8.52E-10	4.25E-12	1.26E-09	1.81E-09	9.57E-10	1.96E-10	2.27E-09	2.88E-10	7.35E-10	9.41E-11
EC <sub>sample</sub> <sup>b</sup>	2.1	1.5	2.2	94.3	10.1	24.4	6.3	18.2	3.5	4.6	5.1	11.5
BEQ <sub>bio</sub> <sup>c</sup>	7.14E-08	1E-07	6.82E-08	1.59E-09	1.49E-08	6.15E-09	2.38E-08	8.24E-09	4.29E-08	3.27E-08	2.95E-08	1.3E-08
explained <sup>d</sup>	0.001%	0.82%	1.25%	0.27%	8.47%	29.44%	4.02%	2.38%	5.29%	0.88%	2.49%	0.72%
P53-bla assay												
BEQ <sub>chem</sub> <sup>a</sup>	0	3.6E-09	2.57E-09	1.61E-12	6.59E-09	7.27E-09	8.19E-09	2.96E-09	6.77E-09	5.25E-09	8.11E-09	4.12E-09
EC <sub>sample</sub> <sup>b</sup>	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	44.95	57.93	108.6
BEQ <sub>bio</sub> <sup>c</sup>	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	2.89E-07	2.24E-07	1.2E-07
explained <sup>d</sup>	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	1.81%	3.62%	3.44%
umuC assav												
BEQ <sub>chem</sub> <sup>a</sup>	1.8E-09	1.97E-08	9.72E-09	3.34E-09	1.7E-08	1.65E-08	4.88E-08	2.27E-08	2.91E-08	4.28E-08	4.12E-08	2.13E-08
EC <sub>sample</sub> <sup>b</sup>	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	27.09	38.18	65.85
BEQ <sub>bio</sub> <sup>c</sup>	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	1.52E-06	1.08E-06	6.27E-07

explained <sup>d</sup>	n.d.	2.81%	3.81%	3.40%								
Microtox assay	y											
BEQ <sub>chem</sub> <sup>a</sup>	9.50E-11	2.00E-09	1.92E-09	5.68E-10	1.68E-07	1.42E-07	9.17E-09	1.02E-08	4.17E-09	2.69E-09	2.87E-09	1.23E-09
EC <sub>sample</sub> <sup>b</sup>	17.4	13.9	26.0	200.5	1.8	55.2	9.7	17.9	21.9	42.5	25.6	97.7
BEQ <sub>bio</sub> <sup>c</sup>	4.89E-07	6.12E-07	3.27E-07	4.24E-08	4.72E-06	1.54E-07	8.76E-07	4.75E-07	3.88E-07	2.00E-07	3.32E-07	8.70E-08
explained <sup>d</sup>	0.0194%	0.3275%	0.5888%	1.34%	3.56%	92.02%	1.05%	2.15%	1.08%	1.34%	0.86%	1.41%

a: Bioanalytical equivalent concentrations calculated based on DBPs detected in the respective sample with dBAN as reference compound ( $\rightarrow$  dBAN-EQ<sub>chem</sub>, equation 6 (main manuscript)).

b: Effect concentration of the water extracts determined with the respective bioassay, i.e., sample enrichment factor causing 50% cytotoxicity EC<sub>50</sub> (Microtox) or activating IR 1.5, EC<sub>IR1.5</sub> (AREc32, p53-bla, umuC).

c: Bioanalytical equivalent concentrations calculated based on the bioassay results (b) with dBAN as reference compound ( $\rightarrow$  dBAN-EQ<sub>bio</sub>) according to equation 7 (main manuscript).

d: Percent BEQ in the sample that can be explained by the detected DBPs (% BEQ explained = (BEQ<sub>chem</sub> / BEQ<sub>bio</sub>) x 100).



**Figure S5. Distribution of index on prediction quality IPQ** for the 12 mixtures given in Table S5.

**Table S7: Index on prediction quality (IPQ)** as a measure of the deviation between the observed and predicted effect concentration ( $EC_{50}$  or  $EC_{IR1.5}$ ) calculated according to equations 3 and 4 in the main manuscript. The IPQ is zero if there is perfect agreement and is positive if the prediction for concentration addition (CA) resulted in a higher effect concentration than the experimental data (Exp) and negative if it is the other way around.

	Microtox			AREc32			ARE-bla			p53-bla			
mixtures	EC <sub>50</sub> CA	EC <sub>50</sub> Exp	IPQ	ECIR1.5 CA	EC <sub>IR1.5</sub> Exp	IPQ	ECIR1.5 CA	EC <sub>IR1.5</sub> Exp	IPQ	ECIR1.5 CA	EC <sub>IR1.5</sub> Exp	IPQ	
mix1 <sub>AREc32</sub>	2.7E-05	5.9E-05	-1.16	4.7E-04	5.0E-04	-0.05	3.2E-03	3.1E-03	0.05	2.1E-03	1.3E-03	0.59	
mix2 <sub>AREc32</sub>	2.9E-05	4.2E-05	-0.46	4.1E-04	2.4E-04	0.72	1.6E-03	1.4E-03	0.17	1.1E-03	1.0E-03	0.13	
mix3 <sub>AREc32</sub>	3.7E-05	7.6E-05	-1.06	4.0E-04	3.0E-04	0.36	1.6E-03	1.4E-03	0.17	1.4E-03	1.0E-03	0.34	
mix4 <sub>AREc32</sub>	3.6E-05	5.4E-05	-0.50	3.9E-04	2.8E-04	0.36	1.4E-03	1.7E-03	-0.22	1.2E-03	9.0E-04	0.30	
mix5 <sub>AREc32</sub>	6.6E-04	4.5E-04	0.46	9.1E-05	5.3E-05	0.72	1.2E-04	1.3E-04	-0.10	9.5E-05	7.5E-05	0.26	
mix6 <sub>AREc32</sub>	2.8E-05	4.9E-05	-0.72	4.8E-06	5.5E-06	-0.13	1.8E-05	1.5E-05	0.21	4.5E-05	3.9E-05	0.17	
mix1 <sub>p53-bla</sub>	6.1E-06	6.8E-06	-0.11	4.8E-05	4.6E-05	0.04	5.4E-04	2.7E-04	1.03	9.7E-04	6.3E-04	0.56	
mix2 <sub>p53-bla</sub>	6.2E-06	5.2E-06	0.19	4.8E-05	4.0E-05	0.18	5.0E-04	4.0E-04	0.26	8.0E-04	6.5E-04	0.23	
mix3 <sub>p53-bla</sub>	6.4E-06	5.9E-06	0.08	4.3E-05	4.2E-05	0.02	3.4E-04	2.4E-04	0.40	6.6E-04	5.1E-04	0.30	
mix4 <sub>p53-bla</sub>	6.4E-06	1.0E-05	-0.63	4.3E-05	5.1E-05	-0.18	3.4E-04	2.4E-04	0.42	6.3E-04	4.1E-04	0.54	
mix5 <sub>p53-bla</sub>	3.2E-04	1.5E-04	1.15	4.8E-05	2.6E-05	0.84	7.4E-05	1.2E-04	-0.59	6.0E-05	4.0E-05	0.35	
mix6 <sub>p53-bla</sub>	4.5E-05	3.4E-05	0.32	1.3E-06	1.7E-06	-0.34	1.3E-05	2.4E-05	-0.83	5.1E-04	4.2E-04	0.21	
mean			-0.20			0.21			0.08			0.33	
95% CI		-0.	63 to 0.23		-0.	03 to 0.45		-0.22 to 0.39			-0.3 to 0.23		

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