

SUPPORTING INFORMATION

Biomarkers, matrices and analytical methods targeting human exposure to chemicals selected for a European human biomonitoring initiative

Katrin Vorkamp^{a*}, Argelia Castaño^b, Jean-Philippe Antignac^c, Luis D. Boada^d, Enrique Cequier^{e#}, Adrian Covaci^f, Marta Esteban López^b, Line S. Haug^e, Monika Kasper-Sonnenberg^g, Holger M. Koch^g, Octavio Pérez Luzardo^d, Agnese Osīte^h, Loïc Rambaudⁱ, Maria-Teresa Pinorini^{j¤}, Gabriele Sabbioni^{j¤}, Cathrine Thomsen^e

^aAarhus University, Department of Environmental Science, Denmark; ^bInstituto de Salud Carlos III, National Centre for Environmental Health, Spain; ^cOniris, INRAE, LABERCA, Nantes, France; ^dUniversity of Las Palmas de Gran Canaria, Institute for Biomedical and Health Research, Spain; ^eNorwegian Institute of Public Health, Norway; ^fUniversity of Antwerp, Toxicological Centre, Belgium; ^gRuhr University Bochum, Institute for Prevention and Occupational Medicine of the German Social Accident Insurance, Germany; ^hUniversity of Latvia, Department of Analytical Chemistry, Latvia; ⁱSanté Publique France, Department of Environmental Health, France; ^jAlpine Institute of Chemistry and Toxicology, Olivone, Switzerland

* Corresponding author. E-mail: kvo@envs.au.dk. Phone: +45-87158483. Postal address: Aarhus University, Department of Environmental Science, Frederiksborgvej 399, 4000 Roskilde, Denmark

Present address: University of Lleida, Alcalde Rovira Roure 191, 25198 Lleida, Spain

¤ Present address: Università della Svizzera italiana, Research and Transfer Service, 6900 Lugano, Switzerland

Table S1: List of acronyms used in this article

Acronym	Full name
AAS	Atomic absorption spectrometry
ABP	Aminobiphenyl
ADONA	Ammonium 4,8-dioxa-3H-perfluorononanoate
BBOEP	Bis(2-butoxyethyl) phosphate
BzBP	Benzyl butyl phthalate
BCIPHIPP	1-Hydroxy-2-propyl-bis(1-chloro-2-propyl)phosphate
BCIPP	Bis(chloroisopropyl) phosphate; bis(1-chloro-2-propyl) phosphate
BDCIPP	Bis(1,3-dichloroisopropyl) phosphate
BCEP	Bis(2-chloroethyl) phosphate
BDE	Bromodiphenyl ether
BEHP	Bis(2-ethylhexyl) phosphate
BEH-TEBP	Bis(2-ethylhexyl) tetrabromophthalate
BMPP	Biscresyl phosphate (Bis(methylphenyl) phosphate)
BPA	Bisphenol A
BPF	Bisphenol F
BPS	Bisphenol S
BTBPE	1,2-Bis(2,4,6- tribromophenoxy)ethane
CA	Chloroaniline
CAS	Chemical Abstracts Service
5cx-MEPP	Mono-(5-carboxy-2-ethylpentyl) phthalate
cx-MIDP	Carboxy-(mono-isodecyl) phthalate (carboxylated DIDP metabolite)
cx-MINCH	Cyclohexane-1,2-dicarboxylate-mono-carboxyisononyl ester
cx-MINP	Carboxy-(mono-isobutyl) phthalate (carboxylated DINP metabolite)
cx-MPrHpP	Carboxy-(mono-2-propyl-heptyl) phthalate
DBDPE	Decabromodiphenyl ethane
DBE-DBCH	Tetrabromoethylcyclohexane
DBP	Dibutyl phthalate
DCA	Dichloroaniline
DCHP	Dicyclohexyl phthalate
DDC-CO	Dechlorane plus
DEHP	Bis(2-ethylhexyl) phthalate
DEP	Diethyl phthalate / Diethyl phosphate
DIBP	Diisobutyl phthalate
DIDP	Diisodecyl phthalate
DINCH	1,2-cyclohexane dicarboxylic acid diisononyl ester
DINP	Diisononyl phthalate
diPAP	Polyfluoroalkyl phosphoric acid diester
DIPeP	Diisopentyl phthalate
DMA	Dimethylaniline
DMP	Dimethyl phthalate
DNBP	Di-n-butyl phosphate
DNHxP	Di-n-hexyl phthalate
DNOP	Di-n-octyl phthalate
DNPeP	Di-n-pentyl phthalate
DP	Dechlorane plus
DPHP	Diphenyl phosphate
DPrHpP	Di(2-propyl-heptyl) phthalate
DRC	Dynamic reaction cell
EA	Ethylaniline

EB	Exposure biomarker
ECNI	Electron capture negative ionization
EHDHPHP	2-Ethylhexyl diphenyl phosphate
EH-TBB	2-Ethylhexyl-2,3,4,5-tetrabromobenzoate
EI	Electron ionization
EtFOSAA	N-ethyl-perfluorooctane sulfonamidoacetate
EtFOSE	N-ethyl-perfluorooctane sulfonamidoethanol
FOSA	Perfluoroalkyl sulfonamide
FOSE	Perfluoroalkyl sulfonamidoethanol
FR	Flame retardant
FTCA	Fluorotelomer carboxylic acid
FTOH	Fluorotelomer alcohol
FTSA	Fluorotelomer sulfonic acid
FTUCA	Fluorotelomer unsaturated carboxylic acid
GC	Gas chromatography
GC-MS	Gas chromatography-mass spectrometry
GC-MS/MS	Gas chromatography-tandem mass spectrometry
GPC	Gel permeation chromatography
Hb	Haemoglobin
HBB	Hexabromobenzene
HBCDD	Hexabromocyclododecane
HBM4EU	Human Biomonitoring for Europe
HFR	Halogenated flame retardant
HPLC	High performance liquid chromatography
HRMS	High resolution mass spectrometry
ICP-MS	Inductively coupled plasma-mass spectrometry
i,p-PHPHP	Isopropylphenyl phenyl phosphate
i,p-TPHP	Isopropyl triphenyl phosphate
LC	Liquid chromatography
LC-MS/MS	High performance liquid chromatography-tandem mass spectrometry
LLE	Liquid-liquid extraction
LOD	Limit of detection
LRMS	Low resolution mass spectrometry
M	Matrix
MA	Methylaniline
MBzP	Monobenzyl phthalate
MCHP	Monocyclohexyl phthalate
MDA	4,4-Methylenedianiline
MDL	Method detection limit
MECPP	Mono(2-ethyl-5-carboxypentyl) phthalate
MeFOSAA	N-methyl-perfluorooctane sulfonamidoacetate
MeFOSE	N-methyl-perfluorooctane sulfonamidoethanol
MEHHP	Mono(2-ethyl-5-hydroxyhexyl) phthalate
MEP	Monoethyl phthalate
MeOA	Methoxyaniline
MEOHP	Mono(2-ethyl-5-oxo-hexyl) phthalate
MIBP	Monoisobutyl phthalate
MIPeP	Monoisopentyl phthalate
MMP	Monomethyl phthalate
MNBP	Mono-n-butyl phthalate
MNHxP	Mono-n-hexyl phthalate

MNOP	Mono-n-octyl phthalate
MNPeP	Mono-n-pentyl phthalate
MOCA	4,4-Methylenebis(2-chloroaniline)
monoPAP	Polyfluoroalkyl phosphoric acid monoester
NA	Naphthylamine
N-EtFOSA	N-ethyl-perfluoro-1-octanesulfonamide
NHANES	National Health and Nutrition Examination Survey
N-MeFOSA	N-methyl-perfluoro-1-octane sulfonamide
5OH-MEHP	Mono(2-ethyl-5-hydroxyhexyl) phthalate
OH-MIDP	OH-mono-isodecyl phthalate
OH-MINCH	Cyclohexane-1,2-dicarboxylate-mono-hydroxyisonyl ester
OH-MINP	OH-mono-isonyl phthalate
OH-MPrHpP	OH-mono-2-propyl-heptyl phthalate
OPFR	Organophosphorous flame retardant
5oxo-MEHP	Mono(2-ethyl-5-oxo-hexyl) phthalate
Oxo-MIDP	Oxo-mono-isodecyl phthalate
Oxo-MINCH	Cyclohexane-1,2-dicarboxylate-mono-oxoisonyl ester
Oxo-MINP	Oxo-mono-isonyl phthalate
Oxo-MPrHpP	Oxo-mono-2-propyl-heptyl phthalate
PAH	Polycyclic aromatic hydrocarbon
PBDE	Polybrominated diphenyl ether
PBEB	Pentabromoethylbenzene
PBT	Pentabromotoluene
PDA	Phenylenediamine
PFAS	Per- and polyfluoroalkyl substance
PFBA	Perfluorobutanoic acid
PFBS	Perfluorobutane sulfonate
PFCA	Perfluoralkyl carboxylic acids
PFDA	Perfluorodecanoic acid
PFDoDA	Perfluorododecanoic acid
PFDPa	Perfluorodecyl phosphonic acid
PFDS	Perfluorodecane sulfonate
PFHpA	Perfluoroheptanoic acid
PFHpS	Perfluoroheptane sulfonate
PFHxA	Perfluorohexanoic acid
PFHxDA	Perfluorohexadecanoic acid
PFHxPA	Perfluorohexyl phosphonic acid
PFHxS	Perfluorohexane sulfonate
PFNA	Perfluorononanoic acid
PFOA	Perfluorooctanoic acid
PFODA	Perfluorooctadecanoic acid
PFOPA	Perfluorooctyl phosphonic acid
PFOS	Perfluorooctane sulfonate
PFPeA	Perfluoropentanoic acid
PPPiA	Perfluorophosphinic acid
PFSA	Perfluoroalkane sulfonic acid
PFTeDA	Perfluorotetradecanoic acid
PFTrDA	Perfluorotridecanoic acid
PFUnDA	Perfluoroundecanoic acid
POP	Persistent organic pollutant
PTFE	Polytetrafluoroethylene

QA/QC	Quality assurance/quality control
REACH	European Regulation on Registration, Evaluation, Authorisation and Restriction of Chemicals
RoHS	Restriction of Hazardous Substances Directive
SPE	Solid phase extraction
SVHC	Substances of Very High Concern
TBBPA	Tetrabromobisphenol A
TBOEP	Tris(2-butoxyethyl) phosphate
TBX	2,3,5,6-Tetrabromoxylene
TCEP	Tri(2-chloroethyl) phosphate
TCIPP	Tri(chloroisopropyl) phosphate
TDA	Toluenediamine
TDCIPP	Tri(1,3-dichloroisopropyl) phosphate
TEP	Triethyl phosphate
TEHP	Tris(2-ethylhexyl) phosphate
TMPP	Tricresyl phosphate (Tris(methylphenyl) phosphate)
TNBP	Tri-n-butyl phosphate
TOPA	Total oxidizable precursor analysis
TPHP	Triphenyl phosphate

Table S2: Chemical structures of some phthalates and DINCH

Compound name	Acronym	CAS no.	Structure
Dibutyl phthalate	DBP	84-74-2	
Diisobutyl phthalate	DIBP	84-69-5	
Benzyl butyl phthalate	BzBP	85-68-7	
Bis(2-ethylhexyl)phthalate	DEHP	117-81-7	
Di-n-octyl phthalate	DNOP	117-84-0	
Diisononyl phthalate	DINP*	28553-12-0 and 68515-48-0	
1,2-cyclohexane dicarboxylic acid diisononyl ester	DINCH*	166412-78-8	

* One of many alkyl chain isomers shown.

Table S3: Chemical structures of bisphenols A, S and F

Compound name	Acronym	CAS no.	Structure
Bisphenol A	BPA	80-05-7	
Bisphenol S	BPS	80-09-1	
Bisphenol F (4,4-Bisphenol F)	BPF	620-92-8	

Table S4: Chemical structures of some per- and polyfluoroalkyl substances (PFASs) mentioned in the article

Compound name	Acronym	CAS no.	Structure
Perfluorohexane sulfonate	PFHxS	355-46-4	
Perfluorooctane sulfonate	PFOS	1763-23-1	
Perfluorooctanoic acid	PFOA	335-67-1	
Perfluorononanoic acid	PFNA	375-95-1	
Perfluoro-1-octapefluoro-1-octane sulfonamide	FOSA	754-91-6	
N-ethylperfluoro-1-octane sulfonamide	N-EtFOSA	4151-50-2	

Table S5: Chemical structures of some halogenated flame retardants (HFRs) mentioned in the article

Compound name	Acronym	CAS no.	Structure
2,2',4,4'-Tetrabromodiphenyl ether	BDE-47	5436-43-1	
2,2',4,4',5,5'-Hexabromodiphenyl ether	BDE-153	68631-49-2	
Decabromodiphenyl ether	BDE-209	1163-19-5	
Hexabromocyclododecane	HBCDD	α -HBCDD: 134237-50-6; γ -HBCDD: 134-237-52-8	
Tetrabromobisphenol A	TBBPA	79-94-7	
Bis(2-ethylhexyl)tetra(bromophthalate)	BEH-TEBP	26040-51-7	
2-Ethylhexyl-2,3,4,5-tetrabromobenzoate	EH-TBB	183658-27-7	
Decabromodiphenyl ethane	DBDPE	84852-53-9	
Dechlorane plus	DP; DDC-CO	13560-89-9	

Table S6: Chemical structures of some organophosphorous flame retardants (OPFRs) mentioned in the article. The side chains R can differ (R1-R3) for other compounds.

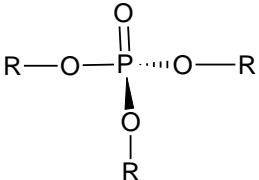
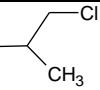
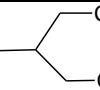
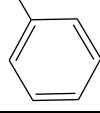
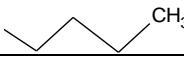
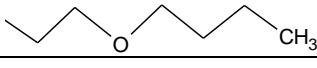
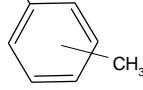
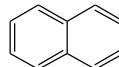
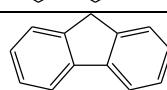
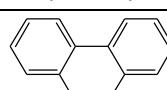
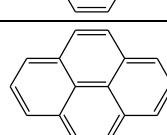
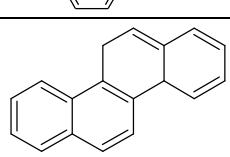
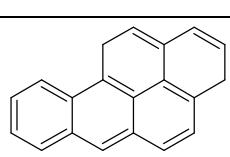
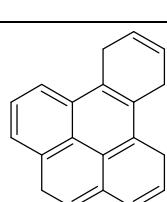
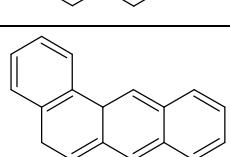
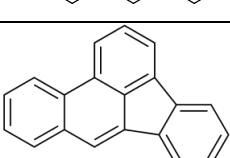
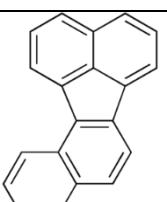
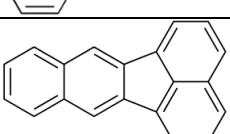
General structure			
Compound name	Acronym	CAS no.	R
Tri(2-chloroethyl) phosphate	TCEP	115-96-8	
Tri(1-chloroisopropyl) phosphate	TCIPP	13674-84-5	
Tri(1,3-dichloro-isopropyl) phosphate	TDCIPP	13674-87-8	
Triphenyl phosphate	TPHP	115-86-6	
Tris-n-butyl phosphate	TNBP	126-73-8	
Tris(2-butoxyethyl) phosphate	TBOEP	78-51-3	
Tris Cresylphosphate	TMPP	1330-78-5	

Table S7: Chemical structures of some polycyclic aromatic hydrocarbons (PAHs) mentioned in the article

Compound name	CAS no.	Structure
Naphthalene	91-20-3	
Fluorene	86-73-7	
Phenanthrene	85-01-8	
Pyrene	129-00-0	
Chrysene	218-01-9	
Benzo[a]pyrene	50-32-8	
Benzo[e]pyrene	192-97-2	
Benz[a]anthracene	56-55-3	
Benzo[b]fluoranthene	205-99-2	
Benzo[j]fluoranthene	205-82-3	
Benzo[k]fluoranthene	207-08-9	

Dibenzo[a,h]anthracene

53-70-3

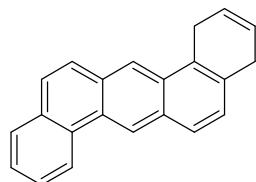


Table S8: Chemical structures of some arylamines mentioned in the article

Compound name	Acronym	CAS no.	Structure
4,4-Methylenedianiline	MDA	101-77-9	
4,4-Methylenebis(2-chloroaniline)	MOCA	101-14-4	
2,4-Toluenediamine	2,4-TDA	95-80-7	
2,6-Toluenediamine	2,6-TDA	823-40-5	
2,5-Toluenediamine	2,5-TDA	95-70-5	
1,4-Phenylenediamine	1,4-PDA	106-50-3	
Aniline	-	62-53-3	
2-Methylaniline	2-MA	95-53-4	
4-Methylaniline	4-MA	106-49-0	
2-Methoxyaniline	2-MeOA	90-04-0	
4-Chloroaniline	4-CA	106-47-8	
3,4-Dichloroaniline	3,4-DCA	95-76-1	