

Supplementary Information

Ion mobility-high resolution mass spectrometry (IM-HRMS) for the analysis of Contaminants of Emerging Concern (CECs): Database compilation and application to urine samples

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Table S6: $^{DT}CCS_{N2}$ database compiled within this study. The compound name, abbreviation, SMILES, molecular formula, mass-to-charge ratio (m/z), adduct species, average observed $^{DT}CCS_{N2}$ values, standard deviation (SD), relative standard deviation (RSD), InChI, InChI Key and compound class are reported.

(available as separate CSV and XLSX files)

Table S2: Comparison of experimentally determined $^{DT}CCS_{N2}$ values ($^{DT}CCS_{N2exp.}$) and data available from literature ($CCS_{N2lit.}$). For each compound, the absolute percentage of error was calculated. $^{DT}CCS_{N2}$ derived from reference [35] for PFAS and reference [42] for di(2-ethylhexyl) phthalate. $^{TW}CCS_{N2}$ for OPs derived from reference [38].

Table S3: $^{DT}CCS_{N2}$ values of 15 organophosphate metabolites acquired in spiked human urine. Pooled urine spiked at two concentration levels (20 ng/mL and 50 ng/mL) was analyzed in triplicate. Average measured m/z ratios and $^{DT}CCS_{N2}$ values are reported. Also, the calculated mass error and absolute percent error of the experimental $^{DT}CCS_{N2}$ values in comparison with database values are given. Bis(2-chloropropyl) hydrogen phosphate and bis(2-chloroethyl) phosphate were spiked in urine but not detected after sample preparation. Therefore, no data is reported for these compounds. n.d. = not detected

Table S9: $^{DT}CCS_{N2}$ values of 15 alternative plasticizers metabolites acquired in spiked human urine. Pooled urine spiked at two concentration levels (20 ng/mL and 50 ng/mL) were analyzed in triplicate. Average measured m/z ratios and $^{DT}CCS_{N2}$ values are reported. Also, the calculated mass error and absolute percent error of the experimental $^{DT}CCS_{N2}$ values in comparison with database values are given. Mono-hydroxy-isononyl phthalate, mono-carboxy-isononyl phthalate and mono(2-ethyl-5-carboxypentyl) adipate were spiked in urine but not detected after sample preparation. Therefore, no data is reported for these compounds. n.d. = not detected

Figure S1: Number of observed ions for the studied compounds.

Figure S2: Depiction of $^{DT}CCS_{N2}$ vs. m/z for organophosphates (OPs) and metabolites. The trendline calculated for all OPs and their metabolites ($n = 37$) is indicated. The subclass of alkyl OPs is marked separately with the corresponding trendline indicated in grey. For comparison, all acquired $^{DT}CCS_{N2}$ values are also displayed in grey.

Table S4: Compound classes included in the ^{DT}CCSN₂ database.

Compound or compound class investigated in this study	Company
Bisphenols (except for bisphenol B)	Sigma Aldrich Chemie GmbH (Steinheim, Germany)
Bisphenol B (BPB)	Tokyo Chemical Industry Co., LTD (Tokyo, Japan)
Benzotriazoles	Sigma Aldrich Chemie GmbH (Steinheim, Germany) Alfa Aesar (Kandel, Germany)
Benzothiazoles	Sigma Aldrich Chemie GmbH (Steinheim, Germany)
Organophosphates	Chiron AS (Trondheim, Norway) AccuStandard (New Heaven, CT, USA) TCI Europe (Zwijndrecht, Belgium)
Organophosphates' metabolites	Sigma Aldrich Chemie GmbH (Steinheim, Germany) Provided by Dr. V. N. Belov (Max Planck Institute, Göttingen, Germany)
Plasticizers	AccuStandard (New Heaven, CT, USA)
Plasticizers' metabolites	SynChem Inc. (Elk Grove Village, IL, USA) BASF (Ludwigshafen, Germany) Cambridge Isotope Laboratories (Tewksbury, MA, USA) Provided by Dr. V. N. Belov (Max Planck Institute, Göttingen, Germany)
Per- and polyfluoroalkyl substances	Wellington Laboratories (Guelph, Canada)
Other chemicals	Sigma Aldrich Chemie GmbH (Steinheim, Germany) Wellington Laboratories (Guelph, Canada)

Table S5: Drift Tube settings applied for all IM-MS measurements in positive (ESI+) and negative (ESI-) ionization modes.

	ESI+	ESI-
Drift Tube Entrance [V]	1574	-1574
Drift Tube Exit [V]	224	-224
Rear Funnel Entrance [V]	217.5	-217.5
Rear Funnel Exit [V]	45	-45
Trap Funnel RF [V]	120	120
Acquisition mode	4-bit multiplexing	4-bit multiplexing
Trap Fill Time [μ s]	3000	3000
Trap Release Time [μ s]	250	250
Max. Drift Time [ms]	60	60
IM Transient Rate [transients/frame]	16	16
Frame Rate [frame/sec]	1	1

Table S6: Chromatographic method used for the acquisition of PFAS data. Settings for the Agilent Jet Stream ESI source, as well as the applied DTIMS conditions, were identical to the parameters used for the other compound classes.

Column:	InfinityLab Poroshell 120 EC-C18; 2.1x50 mm, 1.8 µm particle size		
Temperature:	40 °C		
Injection volume:	2 µL		
Flow rate:	0.25 mL/min		
Mobile phases:	(A) H ₂ O + 2 mM ammonium acetate (B) MeOH		
Gradient	Time [min]	(A) [%]	(B) [%]
	0	70	30
	1.5	70	30
	6	30	70
	8	15	85
	10	5	95
	12	1	99
	13	1	99
	14	70	30
	20	70	30

Table S7: Detailed report of the comparison between experimental ^{DT}CCS_{N2} values (CCS_{exp.}) and literature CCS values (CCS_{lit.}) acquired by Stow et al. for QA compounds. For each of the sample batches acquired data is reported separately.

QA compound	Molecular formula	Batch nr.	Adduct	Exact m/z values	CCS _{exp.} (SD) [Å ²]	%RSD	CCS _{lit.} [Å ²]	%Error
Creatinine	C ₄ H ₇ N ₃ O	1.	[M+H] ⁺	114.0662	122.99 (0.06)	0.05	122.98	0.01
		2.	[M+H] ⁺		123.49 (0.07)	0.06		0.41
		3.	[M+H] ⁺		122.81 (0.02)	0.02		0.14
		4.	[M+H] ⁺		123.05 (0.02)	0.01		0.06
Glucose	C ₆ H ₁₂ O ₆	1.	[M+Na] ⁺	203.0526	147.17 (0.04)	0.03	146.94	0.15
		2.	[M+Na] ⁺		147.23 (0.10)	0.07		0.20
		3.	[M+Na] ⁺		146.95 (0.15)	0.10		0.01
		4.	[M+Na] ⁺		146.75 (0.07)	0.05		0.13
Cortisol	C ₂₁ H ₃₀ O ₅	1.	[M+H] ⁺	363.2166	188.49 (0.05)	0.03	188.34	0.08
			[M+Na] ⁺		212.16 (0.14)	0.07		0.30
		2.	[M+H] ⁺	385.1985	189.88 (0.07)	0.04		0.82
			[M+Na] ⁺		212.56 (0.11)	0.05		0.11
		3.	[M+H] ⁺		188.57 (0.02)	0.01		0.12
			[M+Na] ⁺		212.55 (0.16)	0.08		0.11
		4.	[M+H] ⁺		188.71 (0.02)	0.01		0.20
			[M+Na] ⁺		212.43 (0.12)	0.06		0.17
L-Phenylalanine	C ₉ H ₁₁ NO ₂	1.	[M+H] ⁺	166.0863	144.44 (0.03)	0.02	140.3	0.10
		2.	[M+H] ⁺		140.85 (0.09)	0.07		0.39
		3.	[M+H] ⁺		140.33 (0.03)	0.02		0.02
		4.	[M+H] ⁺		140.23 (0.05)	0.03		0.05
		1.	[M-H] ⁻	164.0717	140.63 (0.03)	0.02	139.94	0.49
		2.	[M-H] ⁻		139.81 (0.04)	0.03		0.09
		3.	[M-H] ⁻		139.70 (0.11)	0.08		0.17
		4.	[M-H] ⁻		139.82 (0.02)	0.01		0.09
		5.	[M-H] ⁻		139.71 (0.10)	0.07		0.17
L-Cystine	C ₆ H ₁₂ N ₂ O ₄ S ₂	1.	[M+H] ⁺	241.0311	149.50 (0.02)	0.01	149.48	0.01
			[M+Na] ⁺		263.0131	0.07		0.07
		2.	[M+H] ⁺		149.26 (0.03)	0.02		0.15
			[M+Na] ⁺		151.60 (0.03)	0.02		0.22
		3.	[M+H] ⁺		149.45 (0.05)	0.04		0.02
			[M+Na] ⁺		151.32 (0.13)	0.08		0.04
		4.	[M+H] ⁺		149.36 (0.05)	0.03		0.08
			[M+Na] ⁺		151.12 (0.06)	0.03		0.09
L-Tyrosine	C ₉ H ₁₁ NO ₃	1.	[M+H] ⁺	182.0812	145.68 (0.04)	0.03	145.58	0.07
		2.	[M+H] ⁺		146.03 (0.08)	0.05		0.31
		3.	[M+H] ⁺		145.50 (0.02)	0.01		0.05
		4.	[M+H] ⁺		145.53 (0.02)	0.01		0.04
		1.	[M-H] ⁻	180.0666	145.16 (0.03)	0.02	144.42	0.51
		2.	[M-H] ⁻		144.31 (0.07)	0.05		0.08
		3.	[M-H] ⁻		144.20 (0.09)	0.06		0.16
		4.	[M-H] ⁻		144.29 (0.04)	0.02		0.09
		5.	[M-H] ⁻		144.20 (0.02)	0.01		0.15
Pyridoxalphosphate	C ₈ H ₁₀ NO ₆ P	1.	[M-H] ⁻	246.0173	149.37 (0.04)	0.03	149.35	0.02
		2.	[M-H] ⁻		149.42 (0.05)	0.03		0.05
		3.	[M-H] ⁻		149.36 (0.04)	0.02		0.01
		4.	[M-H] ⁻		149.50 (0.05)	0.03		0.10
		5.	[M-H] ⁻		149.43 (0.04)	0.03		0.05
L-Histidine	C ₆ H ₉ N ₃ O ₂	1.	[M-H] ⁻	154.0622	128.60 (0.04)	0.03	128.83	0.18
		2.	[M-H] ⁻		128.53 (0.03)	0.03		0.23
		3.	[M-H] ⁻		128.50 (0.10)	0.08		0.26
		4.	[M-H] ⁻		128.58 (0.03)	0.02		0.19
		5.	[M-H] ⁻		128.56 (0.08)	0.06		0.21
Uric acid	C ₅ H ₄ N ₄ O ₃	1.	[M-H] ⁻	167.0211	125.82 (0.27)	0.21	125.55	0.21
		2.	[M-H] ⁻		125.61 (0.07)	0.05		0.05
		3.	[M-H] ⁻		125.66 (0.05)	0.04		0.09
		4.	[M-H] ⁻		125.63 (0.04)	0.03		0.06
		5.	[M-H] ⁻		125.72 (0.09)	0.07		0.13

Table S8: Summary of the ^{DT}CCSN₂ database compiled within this study. The compound name, abbreviation, molecular formula, mass-to-charge ratio (*m/z*), adduct species, average observed ^{DT}CCSN₂ values, standard deviation (SD), relative standard deviation (RSD) and average observed mass error are reported. *Compounds whose ^{DT}CCSN₂ values are reported for the first time. #Ions for which ^{DT}CCSN₂ values are reported for the first time. For these compounds ^{DT}CCSN₂ values for additional ions were reported here.

Compound name	Abbreviation	Molecular formula	<i>m/z</i>	Ion	^{DT} CCSN ₂ (±SD) [Å ²]	RSD [%]	Aver. mass error [ppm]
Bisphenol A	BPA	C ₁₅ H ₁₆ O ₂	227.1078	[M-H] ⁻ #	163.50 (0.01)	0.01	2.53
Bisphenol AF*	BPAF	C ₁₅ H ₁₀ F ₆ O ₂	335.0512 671.1097	[M-H] ⁻ [2M-H] ⁻	166.06 (0.03) 230.13 (0.09)	0.02 0.04	3.47 0.17
Bisphenol AP*	BPAP	C ₂₀ H ₁₈ O ₂	289.1234	[M-H] ⁻	179.95 (0.04)	0.02	1.99
Bisphenol B*	BPB	C ₁₆ H ₁₈ O ₂	241.1234	[M-H] ⁻	167.17 (0.05)	0.03	0.56
Bisphenol C*	BPC	C ₁₄ H ₁₀ Cl ₂ O ₂	278.9985	[M-H] ⁻	165.30 (0.04)	0.02	2.06
Bisphenol P*	BPP	C ₂₄ H ₂₆ O ₂	345.1860	[M-H] ⁻	180.64 (0.03)	0.01	1.26
Bisphenol Z*	BPZ	C ₁₈ H ₂₀ O ₂	267.1390	[M-H] ⁻	174.21 (0.03)	0.02	0.65
Bisphenol F*	BPF	C ₁₃ H ₁₂ O ₂	199.0764	[M-H] ⁻	155.05 (0.05)	0.03	0.28
Bisphenol S*	BPS	C ₁₂ H ₁₀ O ₄ S	249.0227 499.0527	[M-H] ⁻ [2M-H] ⁻	155.49 (0.03) 202.35 (0.05)	0.02 0.03	1.38 1.33
Benzotriazole*	BTR	C ₆ H ₅ N ₃	120.0556 ¹ 118.0411	[M+H] ⁺ [M-H] ⁻	122.42 (0.03) 118.30 (0.02)	0.03 0.02	8.14 1.60
4-Methylbenzotriazole*	4-Me-BTR	C ₇ H ₇ N ₃	134.0713 ¹ 132.0567	[M+H] ⁺ [M-H] ⁻	126.79 (0.04) 123.70 (0.07)	0.03 0.05	5.79 3.12
5-methyl-1 <i>H</i> -benzotriazole*	5-Me-BTR	C ₇ H ₇ N ₃	132.0567	[M-H] ⁻	124.64 (0.02)	0.01	1.18
5,6-Dimethylbenzotriazole*	5,6-diMe-BTR	C ₈ H ₉ N ₃	148.0869 146.0724	[M+H] ⁺ [M-H] ⁻	131.25 (0.02) 130.84 (0.11)	0.01 0.08	0.52 2.04
5-Chlorobenzotriazole*	5Cl-BTR	C ₆ H ₄ ClN ₃	154.0167 152.0021	[M+H] ⁺ [M-H] ⁻	131.88 (0.03) 122.49 (0.04)	0.03 0.03	1.63 1.45
Benzo[thiazole]*	BTH	C ₇ H ₅ NS	158.0035	[M+Na] ⁺	134.70 (0.36)	0.27	3.05
2-Hydroxybenzothiazole*	2OH-BTH	C ₇ H ₅ NOS	150.0019	[M-H] ⁻	123.75 (0.02)	0.02	1.81
2-Aminobenzothiazole*	2NH ₂ -BTH	C ₇ H ₆ N ₂ S	151.0324 149.0179	[M+H] ⁺ [M-H] ⁻	128.60 (0.03) 122.71 (0.07)	0.02 0.05	3.01 1.70
2-(Methylthio)benzothiazole*	2-MeSBTH	C ₈ H ₇ NS ₂	182.0093	[M+H] ⁺	131.32 (0.06)	0.05	3.54
Tris(2-butoxyethyl) phosphate	TBOEP	C ₁₈ H ₃₉ O ₇ P	399.2506 421.2326	[M+H] ⁺ [M+Na] ⁺	194.44 (0.18) 199.36 (0.11)	0.09 0.06	1.33 0.50
Tri-iso-butyl phosphate*	TiBP	C ₁₂ H ₂₇ O ₄ P	267.1720 289.1539 533.3367 555.3186	[M+H] ⁺ [M+Na] ⁺ [2M+H] ⁺ [2M+Na] ⁺	165.44 (0.23) 183.19 (0.08) 234.54 (0.09) 248.38 (0.12)	0.14 0.04 0.04 0.05	0.61 3.65 0.44 0.85
Tri- <i>n</i> -butyl phosphate*	TnBP	C ₁₂ H ₂₇ O ₄ P	267.1720 289.1539 533.3367 555.3186	[M+H] ⁺ [M+Na] ⁺ [2M+H] ⁺ [2M+Na] ⁺	166.73 (0.06) 184.54 (0.10) 236.49 (0.09) 250.03 (0.12)	0.03 0.05 0.04 0.05	2.44 3.72 0.88 0.74
Triphenyl phosphate	TPhP	C ₁₈ H ₁₅ O ₄ P	327.0781 349.0600 675.1308	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	174.74 (0.03) 184.96 (0.06) 249.80 (0.06)	0.01 0.03 0.03	2.47 1.97 1.94
Tris(2-ethylhexyl) phosphate*	TEHP	C ₂₄ H ₅₁ O ₄ P	435.3598 457.3417 869.7123 891.6942	[M+H] ⁺ [M+Na] ⁺ [2M+H] ⁺ [2M+Na] ⁺	219.15 (0.13) 231.80 (0.12) 315.91 (0.47) 327.65 (0.19)	0.06 0.05 0.15 0.06	1.30 1.56 2.10 0.41
Triethyl phosphate*	TEP	C ₆ H ₁₅ O ₄ P	183.0781 205.0600 387.1308	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	132.63 (0.06) 150.93 (0.11) 192.65 (0.22)	0.05 0.07 0.11	1.55 0.22 1.16
Tri- <i>m</i> -tolyl phosphate*	TMTP	C ₂₁ H ₂₁ O ₄ P	369.1250 391.1070 759.2247	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	188.56 (0.10) 198.56 (0.12) 272.51 (0.16)	0.06 0.06 0.06	0.93 1.08 0.29
Tri- <i>o</i> -tolyl phosphate*	TOTP	C ₂₁ H ₂₁ O ₄ P	369.1250 391.1070 759.2247	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	182.39 (0.08) 192.43 (0.16) 263.75 (0.20)	0.04 0.08 0.08	1.31 0.73 0.82
Tri- <i>p</i> -tolyl phosphate	TPTP	C ₂₁ H ₂₁ O ₄ P	369.1250 391.1070 759.2247	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	190.02 (0.06) 200.02 (0.08) 273.74 (0.13)	0.03 0.04 0.05	1.41 1.65 0.51

Triamyl phosphate*	TAP	C ₁₅ H ₃₃ O ₄ P	309.2189 331.2009 617.4306 639.4125	[M+H] ⁺ [M+Na] ⁺ [2M+H] ⁺ [2M+Na] ⁺	183.21 (0.05) 199.96 (0.09) 262.51 (0.35) 275.71 (0.08)	0.03 0.05 0.13 0.03	1.50 2.13 0.58 0.68
Tris(2-chloroethyl) phosphate	TCEP	C ₆ H ₁₂ Cl ₃ O ₄ P	284.9612 306.9431	[M+H] ⁺ [M+Na] ⁺	151.31 (0.05) 161.39 (0.08)	0.03 0.05	1.46 2.14
Tris(2-chloroisopropyl) phosphate	TCIPP	C ₉ H ₁₈ Cl ₃ O ₄ P	327.0081 348.9900	[M+H] ⁺ [M+Na] ⁺	161.66 (0.10) 171.33 (0.05)	0.06 0.03	0.87 1.28
Tris(2,3-dibromopropyl) phosphate*	TDBPP	C ₉ H ₁₅ Br ₆ O ₄ P	692.5881 714.5700 716.5680	[M+H] ⁺ [M+Na] ⁺ [M+Na] ⁺	197.25 (0.20) 206.37 (0.78) 206.90 (0.07)	0.10 0.38 0.03	1.06 1.82 0.75
Tris(1,3-dichloro-2-propyl) phosphate	TDCIPP	C ₉ H ₁₅ Cl ₆ O ₄ P	428.8912 450.8731	[M+H] ⁺ [M+Na] ⁺	178.56 (0.02) 191.22 (0.06)	0.01 0.03	2.97 3.26
Tris(tert-butylphenyl) phosphate*	TTBPP	C ₃₀ H ₃₉ O ₄ P	495.2659 517.2478	[M+H] ⁺ [M+Na] ⁺	237.14 (0.17) 243.95 (0.10)	0.07 0.04	1.24 2.18
Resorcinol bis(diphenyl phosphate)*	Fyrolflex RDP	C ₃₀ H ₂₄ O ₈ P ₂	575.1019 597.0839	[M+H] ⁺ [M+Na] ⁺	228.77 (0.06) 231.58 (0.03)	0.02 0.01	1.22 1.27
Bisphenol A bis(diphenyl phosphate)*	Fyrolflex BDP	C ₃₉ H ₃₄ O ₈ P ₂	693.1802 715.1621	[M+H] ⁺ [M+Na] ⁺	246.33 (0.16) 256.61 (0.12)	0.06 0.05	0.41 0.29
Isodecyl diphenyl phosphate	iDPP	C ₂₂ H ₃₁ O ₄ P	391.2033 413.1852 803.3812	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	200.20 (0.09) 207.30 (0.03) 290.51 (0.05)	0.05 0.01 0.02	0.95 1.73 0.91
2-Ethylhexyl diphenyl phosphate	EHDPP	C ₂₀ H ₂₇ O ₄ P	385.1539 725.3367 747.3186	[M+Na] ⁺ [2M+H] ⁺ [2M+Na] ⁺	202.70 (0.05) 269.03 (0.17) 278.58 (0.08)	0.02 0.06 0.03	3.75 4.48 3.28
Antiblaze V6	V6	C ₁₃ H ₂₄ Cl ₆ O ₈ P ₂	580.9150 602.8970 1182.8047	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	211.37 (0.04) 216.57 (0.08) 304.65 (0.16)	0.02 0.04 0.05	2.73 2.93 2.32
Bis(3,5,5-trimethylhexyl) phosphate*		C ₁₈ H ₃₉ O ₄ P	351.2659 373.2478	[M+H] ⁺ [M+Na] ⁺	202.09 (0.05) 210.41 (0.09)	0.03 0.04	5.14 3.66
Diphenylcresyl phosphate	CDPHP	C ₁₉ H ₁₇ O ₄ P	341.0937 363.0757 681.1802 703.1621	[M+H] ⁺ [M+Na] ⁺ [2M+H] ⁺ [2M+Na] ⁺	180.48 (0.02) 190.53 (0.05) 250.72 (0.42) 257.29 (0.04)	0.01 0.03 0.17 0.02	3.45 3.35 4.16 2.66
Di-o-cresyl phosphate*	DOCP	C ₁₄ H ₁₅ O ₄ P	279.0781 301.0600 557.1489 579.1308	[M+H] ⁺ [M+Na] ⁺ [2M+H] ⁺ [2M+Na] ⁺	163.59 (0.07) 169.40 (0.07) 218.36 (0.35) 225.36 (0.15)	0.04 0.04 0.16 0.07	2.94 2.19 3.55 2.28
Di-n-butyl phosphate*	DnBP	C ₈ H ₁₉ PO ₄	233.0913 209.0948	[M+Na] ⁺ [M-H] ⁻	167.54 (0.04) 150.89 (0.02)	0.02 0.01	1.40 3.92
Diphenyl hydrogen phosphate*	DPhP	C ₁₂ H ₁₁ O ₄ P	251.0468 273.0287 249.0322	[M+H] ⁺ [M+Na] ⁺ [M-H] ⁻	157.41 (0.07) 164.38 (0.15) 152.82 (0.02)	0.04 0.09 0.01	2.37 0.87 1.22
Bis(2-chloropropyl) hydrogen phosphate*	BCIPP	C ₆ H ₁₃ Cl ₂ O ₄ P	272.9821 498.9784	[M+Na] ⁺ [2M-H] ⁻	156.45 (0.02) 203.44 (0.11)	0.01 0.05	0.77 1.41
Bis(2-chloroethyl) phosphate*	BCEP	C ₄ H ₉ Cl ₂ O ₄ P	222.9688 244.9508 442.9158	[M+H] ⁺ [M+Na] ⁺ [2M-H] ⁻	138.08 (0.08) 149.04 (0.09) 189.12 (0.14)	0.06 0.06 0.07	0.78 2.09 0.68
Bis(1,3-dichloro-2-propyl) phosphate*	BDCIPP	C ₆ H ₁₁ Cl ₄ O ₄ P	318.9222 316.9076 634.8225	[M+H] ⁺ [M-H] ⁻ [2M-H] ⁻	178.72 (0.04) 157.71 (0.01) 220.13 (0.10)	0.02 0.01 0.05	1.56 0.90 1.13
bis(1-chloro-2-propyl) 1-hydroxy-2-propyl phosphate*	BCIPHIPP	C ₉ H ₁₉ Cl ₂ O ₅ P	309.0420 331.0239	[M+H] ⁺ [M+Na] ⁺	160.61 (0.03) 168.89 (0.03)	0.02 0.02	0.49 3.84
2-ethylhexyl phenyl phosphate*	EHPHP	C ₁₄ H ₂₃ O ₄ P	309.1226 573.2741 285.1261 571.2595	[M+Na] ⁺ [2M+H] ⁺ [M-H] ⁻ [2M-H] ⁻	183.41 (0.28) 240.74 (0.09) 170.46 (0.03) 236.38 (0.03)	0.15 0.04 0.02 0.01	0.91 2.52 3.21 1.41
Bis(2-butoxyethyl) phosphate*	BBOEP	C ₁₂ H ₂₇ O ₆ P	299.1618 321.1437 297.1472	[M+H] ⁺ [M+Na] ⁺ [M-H] ⁻	171.77 (0.04) 175.66 (0.04) 175.92 (0.02)	0.02 0.02 0.01	1.15 1.81 1.79
5-Hydroxy-2-ethylhexyl diphenyl phosphate*	5OH-EHDPP	C ₂₀ H ₂₇ O ₅ P	379.1669 401.1488 779.3084	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	186.66 (0.06) 194.97 (0.06) 268.40 (0.08)	0.03 0.03 0.03	3.44 3.69 2.62

3-Hydroxyphenyl diphenyl phosphate*	3OH-TPHP	C ₁₈ H ₁₅ O ₅ P	343.0730 365.0549 685.1387 707.1206 341.0584 683.1241	[M+H] ⁺ [M+Na] ⁺ [2M+H] ⁺ [2M+Na] ⁺ [M-H] ⁻ [2M-H] ⁻	180.35 (0.01) 189.06 (0.07) 246.58 (0.21) 252.85 (0.09) 180.46 (0.10) 241.97 (0.05)	0.01 0.04 0.09 0.04 0.06 0.02	4.09 4.11 4.73 3.14 2.87 1.55
Bis(2-butoxyethyl) 2-hydroxyethyl phosphate*	BBOEHP	C ₁₈ H ₁₅ O ₅ P	343.1880 365.1700 707.3507	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	179.27 (0.01) 182.29 (0.03) 259.02 (0.08)	0.01 0.02 0.03	4.36 1.16 1.59
Bis(2-butoxyethyl) 3'-hydroxy-2-butoxyethyl phosphate*	3OH-TBOEP	C ₁₈ H ₃₉ O ₈ P	415.2456 437.2275 851.4658	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	195.45 (0.04) 200.38 (0.05) 286.24 (0.10)	0.02 0.02 0.03	3.19 3.24 2.61
4-Hydroxyphenyl diphenyl phosphate*	4OH-TPHP	C ₁₈ H ₁₅ O ₅ P	341.0584 683.1241 343.0730 365.0549 685.1387 707.1206	[M-H] ⁻ [2M-H] ⁻ [M+H] ⁺ [M+Na] ⁺ [2M+H] ⁺ [2M+Na] ⁺	181.90 (0.05) 251.30 (0.24) 178.12 (0.01) 188.50 (0.04) 248.96 (0.08) 254.81 (0.03)	0.03 0.09 0.01 0.02 0.03 0.01	2.97 3.48 3.77 0.26 0.59 0.20
4-Hydroxyphenyl phenyl phosphate*	4OH-PhP	C ₁₂ H ₁₁ O ₅ P	267.0417 289.0236 265.0271	[M+H] ⁺ [M+Na] ⁺ [M-H] ⁻	162.44 (0.02) 169.02 (0.11) 157.56 (0.07)	0.01 0.07 0.04	1.51 0.63 0.78
Di(2-ethylhexyl) phthalate	DEHP	C ₂₄ H ₃₈ O ₄	391.2843 413.2662 803.5432	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	211.00 (0.08) 215.33 (0.05) 299.81 (0.12)	0.04 0.02 0.04	0.88 1.76 0.60
Diisononyl phthalate*	DiNP	C ₂₆ H ₄₂ O ₄	419.3156 441.2975 859.6058	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	220.60 (0.10) 220.94 (0.09) 313.44 (0.39)	0.05 0.04 0.12	1.11 1.20 0.90
Diisodecyl phthalate*	DiDP	C ₂₈ H ₄₆ O ₄	447.3469 469.3288 915.6684	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	227.85 (0.11) 226.42 (0.11) 325.43 (0.35)	0.05 0.05 0.11	1.91 1.64 0.57
Diphenyl phthalate*	DPP	C ₂₀ H ₁₄ O ₄	341.0784 659.1676	[M+H] ⁺ [M+Na] ⁺	181.27 (0.04) 238.24 (0.05)	0.02 0.02	1.72 0.92
Diisononyl hexahydrophthalate ^{2,*}	DINCH	C ₂₆ H ₄₈ O ₄	425.3625 447.3445 871.6997	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	224.82 (0.37) 222.03 (0.12) 316.74 (0.38)	0.17 0.05 0.12	0.85 1.16 0.81
Mono(2-ethylhexyl) phthalate*	MEHP	C ₁₆ H ₂₂ O ₄	301.1410 277.1445	[M+Na] ⁺ [M-H] ⁻	182.27 (0.04) 168.91 (0.06)	0.02 0.03	2.20 1.21
Monoisobutyl phthalate*	MiBP	C ₁₂ H ₁₄ O ₄	245.0784 221.0819	[M+Na] ⁺ [M-H] ⁻	163.43 (0.06) 151.83 (0.05)	0.03 0.03	1.69 1.18
Mono-n-butyl phthalate*	MnBP	C ₁₂ H ₁₄ O ₄	245.0784 221.0819	[M+Na] ⁺ [M-H] ⁻	163.94 (0.03) 151.11 (0.04)	0.02 0.03	1.77 0.76
Monocyclohexyl phthalate*	MCHP	C ₁₄ H ₁₆ O ₄	247.0976	[M-H] ⁻	159.72 (0.07)	0.04	1.25
Monoethyl phthalate*	MEP	C ₁₀ H ₁₀ O ₄	193.0506	[M-H] ⁻	141.67 (0.04)	0.03	0.52
Monomethyl phthalate*	MMP	C ₉ H ₈ O ₄	203.0315 179.0350	[M+Na] ⁺ [M-H] ⁻	146.13 (0.12) 137.01 (0.06)	0.09 0.04	2.87 0.42
6-Hydroxy monopropylheptyl phthalate*	6OH-MPHP	C ₁₈ H ₂₆ O ₅	345.1672 321.1707	[M+Na] ⁺ [M-H] ⁻	181.90 (0.07) 178.62 (0.03)	0.04 0.02	1.33 0.91
Mono-2-(propyl-6-oxoheptyl) phthalate*	6-oxo-MPHP	C ₁₈ H ₂₄ O ₅	343.1516 319.1551	[M+Na] ⁺ [M-H] ⁻	180.20 (0.07) 177.70 (0.05)	0.04 0.03	0.26 2.74
Mono(2-propyl-6-carboxyhexyl) phthalate*	6-cx-MPHxP	C ₁₈ H ₂₄ O ₆	359.1465 335.1500	[M+Na] ⁺ [M-H] ⁻	183.65 (0.06) 179.64 (0.02)	0.03 0.01	0.38 0.31
Mono(2-ethyl-5-hydroxyhexyl) phthalate*	5OH-MEHP	C ₁₆ H ₂₂ O ₅	317.1359 293.1394	[M+Na] ⁺ [M-H] ⁻	172.92 (0.05) 168.99 (0.03)	0.03 0.02	0.88 0.72
Mono(2-ethyl-5-oxohexyl)phthalate*	5-oxo-MEHP	C ₁₆ H ₂₀ O ₅	315.1203 291.1238	[M+Na] ⁺ [M-H] ⁻	170.18 (0.03) 168.35 (0.03)	0.02 0.02	1.91 1.28
Mono-(3-carboxypropyl) phthalate*	3-cx-MCPP	C ₁₂ H ₁₂ O ₆	275.0526	[M+Na] ⁺	156.95 (0.09)	0.05	3.13
Mono-(2-ethyl-5-carboxypentyl) phthalate*	5-cx-MEPP	C ₁₆ H ₂₀ O ₆	331.1152 307.1187	[M+Na] ⁺ [M-H] ⁻	174.45 (0.07) 169.87 (0.06)	0.04 0.03	1.19 0.56
Mono-hydroxy-isononyl phthalate*	7OH-MiNP	C ₁₇ H ₂₄ O ₅	331.1516 307.1551	[M+Na] ⁺ [M-H] ⁻	176.60 (0.02) 172.50 (0.03)	0.01 0.02	1.23 2.68
Mono-carboxy-isononyl phthalate*	7-cx-MiNP	C ₁₈ H ₂₄ O ₆	359.1465 335.1500	[M+Na] ⁺ [M-H] ⁻	182.64 (0.10) 177.47 (0.04)	0.06 0.02	0.59 1.17

Mono-isononyl-cyclohexane-1,2-dicarboxylate*	cis-MINCH	C ₁₇ H ₃₀ O ₄	321.2036 297.2071	[M+Na] ⁺ [M-H] ⁻	185.87 (0.05) 175.48 (0.03)	0.03 0.02	1.06 1.43
Cyclohexane-1,2-dicarboxylic mono carboxyisooctyl ester*	cis-cx-MINCH	C ₁₇ H ₂₈ O ₆	351.1778 327.1813	[M+Na] ⁺ [M-H] ⁻	179.93 (0.06) 176.73 (0.02)	0.03 0.01	0.44 0.90
Cyclohexane-1,2-dicarboxylic mono hydroxyisononyl ester*	cis-OH-MINCH	C ₁₇ H ₃₀ O ₅	337.1985 313.2020	[M+Na] ⁺ [M-H] ⁻	178.57 (0.08) 175.32 (0.02)	0.05 0.01	0.41 0.79
Mono(2-ethylhexyl) terephthalate*	MEHTP	C ₁₆ H ₂₂ O ₄	277.1445	[M-H] ⁻	183.54 (0.03)	0.02	1.86
Mono(2-ethyl-5-hydroxyhexyl) terephthalate*	5OH-MEHTP	C ₁₆ H ₂₂ O ₅	293.1394	[M-H] ⁻	185.08 (0.09)	0.05	1.90
Mono(2-ethyl-5-carboxypentyl) terephthalate*	5-cx-MEPTP	C ₁₆ H ₂₀ O ₆	307.1187	[M-H] ⁻	168.42 (0.05)	0.03	0.63
Di(2-ethylhexyl) adipate*	DEHA	C ₂₂ H ₄₂ O ₄	371.3156 393.2975 763.6058	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	209.38 (0.03) 218.46 (0.07) 294.67 (0.03)	0.01 0.03 0.01	3.00 2.36 3.01
Diisobutyl adipate*	DIBA	C ₁₄ H ₂₆ O ₄	259.1904 281.1723 539.3554	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	167.82 (0.13) 180.16 (0.04) 235.89 (0.12)	0.08 0.02 0.05	1.82 1.80 0.34
Di(2-ethylhexyl) terephthalate*	DEHT	C ₂₄ H ₃₈ O ₄	413.2662	[M+Na] ⁺	215.81 (0.12)	0.05	1.08
Isooctyl-2-phenoxyethylterephthalate*	IOPhEt	C ₂₄ H ₃₀ O ₅	399.2166 421.1985	[M+H] ⁺ [M+Na] ⁺	218.61 (0.09) 227.37 (0.09)	0.04 0.04	0.40 0.57
Mono(2-ethyl-5-oxohexyl) adipate*	5-oxo-MEHA	C ₁₄ H ₂₄ O ₅	295.1516 271.1551	[M+Na] ⁺ [M-H] ⁻	165.91 (0.05) 165.29 (0.05)	0.03 0.03	0.50 0.38
Mono(2-ethylhexyl) adipate*	MEHA	C ₁₄ H ₂₆ O ₄	281.1723 257.1758	[M+Na] ⁺ [M-H] ⁻	177.32 (0.11) 166.76 (0.03)	0.06 0.02	0.69 1.59
Mono(2-ethyl-5-hydroxyhexyl) adipate*	5OH-MEHA	C ₁₄ H ₂₆ O ₅	297.1672 273.1708	[M+Na] ⁺ [M-H] ⁻	168.70 (0.03) 165.79 (0.04)	0.02 0.02	0.30 2.75
Mono(2-ethyl-5-carboxypentyl) adipate*	5-cx-MEPA	C ₁₄ H ₂₄ O ₆	311.1465 287.1500	[M+Na] ⁺ [M-H] ⁻	170.01 (0.05) 167.03 (0.03)	0.03 0.02	4.16 0.23
Tris(2-ethylhexyl)trimellitate*	TOTM	C ₃₃ H ₅₄ O ₆	569.3813	[M+Na] ⁺	264.41 (0.39)	0.15	2.06
2,4-Di-(2-ethylhexyl) trimellitate*	2,4-DEHTM	C ₂₅ H ₃₈ O ₆	435.2741 457.2561 433.2596	[M+H] ⁺ [M+Na] ⁺ [M-H] ⁻	218.39 (0.07) 233.33 (0.12) 222.86 (0.04)	0.03 0.05 0.02	1.44 1.28 2.99
Mono-1-(2-ethyl-5-carboxyhexyl)trimellitate*		C ₁₇ H ₂₀ O ₈	375.1050 351.1085	[M+Na] ⁺ [M-H] ⁻	187.56 (0.09) 180.56 (0.03)	0.05 0.02	0.69 2.96
Mono-1-[2(carboxymethyl)hexyl] trimellitate*		C ₁₇ H ₂₀ O ₈	375.1050 351.1085	[M+Na] ⁺ [M-H] ⁻	189.84 (0.05) 182.23 (0.10)	0.03 0.05	0.40 3.25
Mono-1-(2-ethyl-5-oxo-hexyl) trimellitate*		C ₁₇ H ₂₀ O ₇	335.1136	[M-H] ⁻	178.84 (0.01)	0.01	1.70
Dibutylsebacate*	DBS	C ₁₈ H ₃₄ O ₄	315.2530 337.2349	[M+H] ⁺ [M+Na] ⁺	183.89 (0.02) 193.48 (0.03)	0.01 0.02	1.19 1.46
Dimethylsebacate*	DMS	C ₁₂ H ₂₂ O ₄	253.1410	[M+Na] ⁺	159.71 (0.04)	0.02	1.63
Butyryl trihexyl citrate*	BTHC	C ₂₈ H ₅₀ O ₈	515.3578 537.3398 105.6904	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	240.45 (0.18) 245.25 (0.07) 348.02 (0.20)	0.07 0.03 0.06	1.21 1.20 0.37
Tributyl acetylcitrate*	ATBC	C ₂₀ H ₃₄ O ₈	403.2326 425.2146 827.4400	[M+H] ⁺ [M+Na] ⁺ [2M+Na] ⁺	199.82 (0.23) 205.77 (0.06) 291.52 (0.14)	0.12 0.03 0.05	1.60 0.72 0.64
Acetyltriethyl citrate*	ATEC	C ₁₄ H ₂₂ O ₈	341.1207 659.2522	[M+Na] ⁺ [2M+Na] ⁺	174.36 (0.06) 244.35 (0.24)	0.03 0.10	2.60 0.62
Tri-n-hexyltrimellitate*	THTM	C ₂₇ H ₄₂ O ₆	463.3054 485.2874	[M+H] ⁺ [M+Na] ⁺	236.57 (0.26) 247.49 (0.39)	0.11 0.16	0.49 1.41
Dimethyl azelate*	DMA	C ₁₁ H ₂₀ O ₄	239.1254	[M+Na] ⁺	155.54 (0.03)	0.02	2.16
Atrazine		C ₈ H ₁₄ ClN ₅	216.1010	[M+H] ⁺	149.53 (0.01)	0.01	1.72
Diazinon*		C ₁₂ H ₂₁ N ₂ O ₃ PS	305.1083 327.0903	[M+H] ⁺ [M+Na] ⁺	173.15 (0.05) 177.72 (0.06)	0.03 0.03	0.09 1.93
p-Nitrophenol*		C ₆ H ₅ NO ₃	138.0197	[M-H] ⁻	119.78 (0.03)	0.03	3.38
3,5,6-Trichloro-2-pyridinol*	TCPy	C ₅ H ₂ Cl ₃ NO	197.9275	[M+H] ⁺	130.45 (0.04)	0.03	0.54
3-Phenoxybenzoic acid*	3-PBA	C ₁₃ H ₁₀ O ₃	213.0557	[M-H] ⁻	155.84 (0.07)	0.04	0.30
3,5-ditert-butyl-4-hydroxybenzaldehyde*		C ₁₅ H ₂₂ O ₂	235.1693 257.1512 ²	[M+H] ⁺ [M+Na] ⁺	165.21 (0.04) 185.31 (0.10)	0.02 0.06	4.69 6.70
Dipropyleneglycol dibenzoate*		C ₂₀ H ₂₂ O ₅	365.1359	[M+Na] ⁺	186.32 (1.35)	0.73	3.50
4-((4-Isopropoxyphenyl)	D-8	C ₁₅ H ₁₆ O ₄ S	291.0697	[M-H] ⁻	174.81 (0.02)	0.01	4.69

sulfonyl) phenol*			583.1466	[2M-H]-	226.14 (0.08)	0.03	0.85
4-(4-hydroxy-3-prop-2-enylphenyl)sulfonyl-2-prop-2-enyl phenol*	TGSA	C ₁₈ H ₁₈ O ₄ S	329.0853 659.1779	[M-H]- [2M-H]-	180.00 (0.15) 240.99 (0.05)	0.08 0.02	0.96 0.33
4-((4-(Benzyloxy)phenyl)-sulfonyl) phenol*	BPS-MAE	C ₁₅ H ₁₄ O ₄ S	289.0540	[M-H]-	172.68 (0.02)	0.01	1.40
4-Nonylphenol*		C ₁₅ H ₂₄ O	219.1754	[M-H]-	161.07 (0.07)	0.05	1.13
4-t-Octylphenol*		C ₁₄ H ₂₂ O	205.1598	[M-H]-	156.73 (0.04)	0.02	0.46
4-n-Octylphenol*		C ₁₄ H ₂₂ O	205.1598	[M-H]-	160.03 (0.04)	0.02	0.81
Triclosan*	TCS	C ₁₂ H ₇ Cl ₃ O ₂	286.9439	[M-H]-	158.94 (0.09)	0.06	1.14
Perfluoro-n-butanoic acid	PFBA	C ₄ HF ₇ O ₂	168.9894	[M-H-CO ₂]-	109.53 (0.10)	0.09	0.60
Perfluoropentanoic acid	PFPeA	C ₅ HF ₉ O ₂	218.9862 526.9593	[M-H-CO ₂]- [2M-H]-	116.78 (0.06) 179.96 (0.10)	0.05 0.05	2.85 1.04
Perfluoro-n-hexanoic acid	PFHxA	C ₆ HF ₁₁ O ₂	268.9830 626.9529	[M-H-CO ₂]- [2M-H]-	124.47 (0.03) 195.94 (0.07)	0.04 0.03	4.03 0.25
Perfluoro-n-heptanoic acid	PFHpA	C ₇ HF ₁₃ O ₂	362.9696 318.9798 726.9465	[M-H]- [M-H-CO ₂]- [2M-H]-	147.61 (0.14) 132.30 (0.07) 211.59 (0.15)	0.10 0.06 0.07	1.34 2.99 0.53
Perfluoro-n-octanoic acid	PFOA	C ₈ HF ₁₅ O ₂	412.9664 368.9766 826.9401	[M-H]- [M-H-CO ₂]- [2M-H]-	156.37 (0.09) 139.44 (0.07) 226.58 (0.08)	0.06 0.05 0.04	1.90 2.18 0.30
Perfluoro-n-nonanoic acid	PFNA	C ₉ HF ₁₇ O ₂	462.9632 418.9734 926.9337	[M-H]- [M-H-CO ₂]- [2M-H]-	165.06 (0.11) 147.05 (0.04) 240.71 (0.15)	0.07 0.03 0.06	0.90 4.10 0.12
Perfluoro-n-decanoic acid	PFDA	C ₁₀ HF ₁₉ O ₂	512.9600 468.9702 102.,9273	[M-H]- [M-H-CO ₂]- [2M-H]-	174.29 (0.08) 155.63 (0.07) 254.24 (0.14)	0.05 0.05 0.05	4.34 4.11 0.52
Perfluoro-n-undecanoic acid	PFUDa	C ₁₁ HF ₂₁ O ₂	562.9568 518.9670 1126.9209	[M-H]- [M-H-CO ₂]- [2M-H]-	182.86 (0.06) 163.84 (0.08) 266.81 (0.12)	0.03 0.05 0.04	0.61 3.19 0.21
Perfluoro-n-dodecanoic acid	PFDaA	C ₁₂ HF ₂₃ O ₂	612.9536 568.9638 1226.9145	[M-H]- [M-H-CO ₂]- [2M-H]-	192.16 (0.09) 172.25 (0.08) 278.80 (0.19)	0.05 0.05 0.07	1.69 0.99 0.48
Perfluoro-n-tridecanoic acid	PFTDA	C ₁₃ HF ₂₅ O ₂	662.9504 618.9606 1326.9081	[M-H]- [M-H-CO ₂]- [2M-H]-	201.05 (0.04) 180.30 (0.04) 290.64 (0.06)	0.02 0.02 0.02	4.38 0.29 0.45
Perfluoro-n-tetradecanoic acid	PFTeDA	C ₁₄ HF ₂₇ O ₂	712.9472 668.95739 1426.9017	[M-H]- [M-H-CO ₂]- [2M-H]-	209.91 (0.06) 188.43 (0.05) 302.02 (0.14)	0.03 0.03 0.05	0.40 1.28 0.66
Perfluoro-n-hexadecanoic acid	PFHxDA	C ₁₆ HF ₃₁ O ₂	812.9409 1626.8891 768.9511	[M-H]- [M-H-CO ₂]- [2M-H]-	227.34 (0.05) 204.50 (0.08) 325.43 (0.18)	0.02 0.04 0.06	0.82 0.29 0.27
Perfluoro-n-octadecanoic acid*	PFODA	C ₁₈ HF ₃₅ O ₂	912.9345 868.9447	[M-H]- [M-H-CO ₂]-	243.53 (0.05) 220.15 (0.05)	0.02 0.02	2.67 3.73
Perfluorobutanesulfonic acid	PFBS	C ₄ HF ₉ O ₃ S	298.9430 598.8933	[M-H]- [2M-H]-	133.28 (0.03) 196.88 (0.14)	0.02 0.07	0.74 1.07
Perfluorohexanesulfonic acid	PFHxS	C ₆ HF ₁₃ O ₃ S	398.9366 798.8805	[M-H]- [2M-H]-	150.81 (0.06) 228.66 (0.10)	0.04 0.04	2.27 0.77
Perfluorooctylsulfonic acid	PFOS	C ₈ HF ₁₇ O ₃ S	498.9302 998.8677	[M-H]- [2M-H]-	168.89 (0.07) 257.72 (0.12)	0.04 0.05	0.75 1.24
Perfluorodecane sulfonic acid	PFDS	C ₁₀ HF ₂₁ O ₃ S	598.9238	[M-H]-	186.91 (0.07)	0.04	2.10
Sodium 1H,1H,2H,2H-perfluorooctane sulfonate	6:2 FTS	C ₈ H ₅ F ₁₃ O ₃ S	426.9679 854.9431	[M-H]- [2M-H]-	168.47 (0.06) 236.24 (0.11)	0.04 0.05	0.56 2.28
8:2 Fluorotelomer sulfonic acid	8:2 FTS	C ₁₀ H ₅ F ₁₇ O ₃ S	526.9617 1054.9307	[M-H]- [2M-H]-	186.39 (0.07) 263.38 (0.25)	0.04 0.10	3.14 0.39
1H,1H,2H,2H-Perfluoro-dodecanesulfonic acid	10:2 FTS	C ₁₂ H ₅ F ₂₁ O ₃ S	626.9551 1254.9175	[M-H]- [2M-H]-	204.21 (0.03) 288.72 (0.09)	0.02 0.03	1.51 1.04
6:2 chlorinated polyfluorinated ether sulfonate	F-53B	C ₈ ClF ₁₆ O ₄ SK	530.89558	[M-H]-	170.98 (0.01)	0.01	3.65
8:2 Fluorotelomer unsaturated carboxylate*	8:2 FTUCA	C ₁₀ H ₂ F ₁₆ O ₂	456.9727 914.9526	[M-H]- [2M-H]-	172.63 (0.04) 239.96 (0.09)	0.02 0.04	1.08 0.51
10:2 Fluorotelomer unsaturated carboxylate*	10:2 FTUCA	C ₁₂ H ₂ F ₂₀ O ₂	556.9663 1114.9398	[M-H]- [2M-H]-	189.84 (0.04) 265.53 (0.08)	0.02 0.03	0.43 0.30

8:2 Fluorotelomer phosphate diester*	8:2 diPAP	C ₂₀ H ₉ F ₃₄ O ₄ P	988.9623	[M-H]-	261.61 (0.06)	0.02	0.58
Perfluorodecylphosphonic acid*	PFDPA	C ₁₀ H ₂ F ₂₁ O ₃ P	598.9333	[M-H]-	188.25 (0.01)	0.01	0.74
8-Chloroperfluorooctylphosphonic acid*	CI-PFOPA	C ₈ H ₂ ClF ₁₆ O ₃ P	514.9102	[M-H]-	175.27 (0.01)	0.01	0.34
6-Chloroperfluorohexylphosphonic acid*	CI-PFHxPA	C ₆ H ₂ ClF ₁₂ O ₃ P	414.9166	[M-H]-	157.41 (0.01)	0.01	1.33
Hexafluoropropylene oxide dimer acid*	HFPO-DA	C ₆ H ₂ F ₁₁ O ₃	284.9779 658.9427	[M-H-CO ₂]- [2M-H]-	126.89 (0.09) 198.61 (0.09)	0.07 0.05	1.33 1.14
Perfluorooctane sulfonamide*	FOSA	C ₈ H ₂ F ₁₇ NO ₂ S	497.9462	[M-H]-	170.13 (0.02)	0.01	0.93
N-ethylperfluorooctane sulfonamide*	N-EtFOSA	C ₁₀ H ₆ F ₁₇ NO ₂ S	525.9775	[M-H]-	178.42 (0.03)	0.01	3.69
N-ethylperfluorooctane sulfonamido acetic acid	N-EtFOSAA	C ₁₂ H ₈ F ₁₇ NO ₄ S	583.9830 1168.9732	[M-H]- [2M-H]-	196.81 (0.06) 283.56 (0.06)	0.03 0.02	1.64 0.28
N-Methylperfluorooctane sulfonamide*	N-MeFOSA	C ₉ H ₄ F ₁₇ NO ₂ S	511.9619	[M-H]-	173.97 (0.03)	0.02	1.08
N-methylperfluorooctane sulfonamido acetic acid	N-MeFOSAA	C ₁₁ H ₆ F ₁₇ NO ₄ S	569.9673 1140.9419	[M-H]- [2M-H]-	193.17 (0.03) 275.84 (0.10)	0.02 0.04	2.40 0.28

¹Compounds were detected showing high abundances at used concentration. Detector saturation is assumed to negatively influence mass accuracy.

²The diisononyl hexahydrophthalate (DINCH) standard used here represents a mixture of approximately 10% trans and 90% cis-isomers similar to industrially used DINCH (National Industrial Chemicals Notification and Assessment Scheme 2008). Within the acquisition of ^{DT}CCS_{N2} values a distinguishment between isomers was not possible as only one signal was visible for which the ^{DT}CCS_{N2} value is reported.

Table S6: ^{DT}CCS_{N2} database compiled within this study. The compound name, abbreviation, SMILES, molecular formula, mass-to-charge ratio (*m/z*), adduct species, average observed ^{DT}CCS_{N2} values, standard deviation (SD), relative standard deviation (RSD), InChI, InChI Key and compound class are reported.

(available as separate CSV and XLSX files)

Table S9: Comparison of experimentally determined $^{DT}CCS_{N_2}$ values ($^{DT}CCS_{N_2exp.}$) and data available from literature ($CCS_{N_2lit.}$). For each compound, the absolute percentage of error was calculated. $^{DT}CCS_{N_2}$ derived from reference [35] for PFAS and reference [42] for di(2-ethylhexyl) phthalate. $^{TW}CCS_{N_2}$ for OPs derived from reference [38].

Compound name	<i>m/z</i>	Ion	$^{DT}CCS_{N_2exp.}$ ($\pm SD$) [\AA^2]	$CCS_{N_2lit.}$ [\AA^2]	Error [%]
tris(2-butoxyethyl) phosphate (TBOEP)	399.2506	[M+H] ⁺	196.44 (0.18)	198.34	0.96
triphenyl phosphate (TPhP)	327.0781	[M+H] ⁺	174.74 (0.03)	169.9	2.85
Tri-p-tolyl phosphate (TPTP)	369.1250	[M+H] ⁺	190.02 (0.06)	187.0	1.62
2-Ethylhexyl diphenyl phosphate (EHDPHP)	385.1539	[M+Na] ⁺	202.70 (0.05)	201.6	0.55
Isodecyl diphenyl phosphate (iDPP)	391.2033	[M+H] ⁺	200.20 (0.09)	202.4	1.08
Diphenylcresyl phosphate (CDPHP)	341.0937	[M+H] ⁺	180.48 (0.02)	177.1	1.92
Antiblaze V6	580.9150	[M+H] ⁺	211.37 (0.04)	212.1	0.34
tris(2-chloroethyl) phosphate (TCEP)	284.9612	[M+H] ⁺	151.31 (0.05)	150.4	0.59
Tris(2-chloroisopropyl)-phosphate (TCIPP)	327.0081	[M+H] ⁺	161.66 (0.10)	161.9	0.13
tris(1,3-dichloro-2-propyl)phosphate (TDCIPP)	428.8912	[M+H] ⁺	178.56 (0.02)	176.5	1.19
Perfluoro-n-butanoic acid (PFBA)	168.9894	[M-H-CO ₂] ⁻	109.53 (0.10)	110.8	1.15
Perfluoro-n-pentanoic acid (PFPeA)	218.9862	[M-H-CO ₂] ⁻	116.78 (0.06)	117.4	0.53
Perfluoro-n-hexanoic acid (PFHxA)	268.9830	[M-H-CO ₂] ⁻	124.47 (0.03)	125.1	0.50
Perfluoro-n-heptanoic acid (PFHpA)	318.9798	[M-H-CO ₂] ⁻	132.30 (0.07)	132.4	0.08
Perfluoro-n-octanoic acid (PFOA)	368.9766	[M-H-CO ₂] ⁻	139.44 (0.07)	139.5	0.04
Perfluoro-n-nonanoic acid (PFNA)	462.9632	[M-H] ⁻	165.06 (0.11)	165.2	0.08
	418.9734	[M-H-CO ₂] ⁻	147.05 (0.04)	147.0	0.04
Perfluoro-n-decanoic acid (PFDA)	512.9600	[M-H] ⁻	174.29 (0.08)	174.2	0.05
	468.9702	[M-H-CO ₂] ⁻	155.63 (0.07)	155.3	0.21
Perfluoro-n-undecanoic acid (PFUdA)	562.9568	[M-H] ⁻	182.86 (0.06)	182.9	0.02
	518.9670	[M-H-CO ₂] ⁻	163.84 (0.08)	163.4	0.27
Perfluoro-n-dodecanoic acid (PFDoA)	612.9536	[M-H] ⁻	192.16 (0.09)	191.4	0.40
	568.9638	[M-H-CO ₂] ⁻	172.25 (0.08)	171.5	0.44
Perfluoro-n-tridecanoic acid (PFTTrDA)	662.9504	[M-H] ⁻	201.05 (0.04)	200.8	0.13
	618.9606	[M-H-CO ₂] ⁻	180.30 (0.04)	179.6	0.39
Perfluoro-n-tetradecanoic acid (PFTeDA)	712.9472	[M-H] ⁻	209.91 (0.06)	209.2	0.34
	668.9574	[M-H-CO ₂] ⁻	188.43 (0.05)	187.6	0.44
Perfluoro-n-hexadecanoic acid (PFHxDA)	812.9409	[M-H] ⁻	227.34 (0.05)	226.1	0.55
	768.9511	[M-H-CO ₂] ⁻	204.50 (0.08)	203.7	0.39
Perfluorobutanesulfonic acid (PFBS)	298.9430	[M-H] ⁻	133.28 (0.03)	133.6	0.24
Perfluorohexanesulfonic acid (PFHxS)	398.9366	[M-H] ⁻	150.81 (0.06)	150.5	0.20
Perfluorooctylsulfonic acid (PFOS)	498.9302	[M-H] ⁻	168.89 (0.07)	168.3	0.35
Perfluorodecane sulfonic acid (PFDS)	598.9238	[M-H] ⁻	186.91 (0.07)	186.2	0.38
Sodium 1H,1H,2H,2H-perfluorooctane sulfonate (6:2 FTS)	426.9679	[M-H] ⁻	168.47 (0.06)	168.1	0.22
8:2 Fluorotelomer sulfonic acid (8:2 FTS)	526.9617	[M-H] ⁻	186.39 (0.07)	185.8	0.32
1H,1H,2H,2H-Perfluoro-dodecanesulfonic acid (10:2 FTS)	626.9551	[M-H] ⁻	204.21 (0.03)	203.6	0.30
6:2 chlorinated polyfluorinated ether sulfonate (F-53B)	530.8956	[M-H] ⁻	170.98 (0.01)	170.2	0.46
N-ethylperfluorooctane sulfonamido acetic acid (N-EtFOSAA)	583.9830	[M-H] ⁻	196.81 (0.06)	196.3	0.26
N-methylperfluorooctane sulfonamido acetic acid (N-MeFOSAA)	569.9673	[M-H] ⁻	193.17 (0.03)	192.7	0.24
Di(2-ethylhexyl) phthalate	391.2843	[M+H] ⁺	211.00 (0.08)	212.2	0.57
	413.2662	[M+Na] ⁺	215.33 (0.05)	215.9	0.26

Table S10: $^{DT}CCS_{N_2}$ values of 15 organophosphate metabolites acquired in spiked human urine. Pooled urine spiked at two concentration levels (20 ng/mL and 50 ng/mL) was analyzed in triplicate. Average measured m/z ratios and $^{DT}CCS_{N_2}$ values are reported. Also, the calculated mass error and absolute percent error of the experimental $^{DT}CCS_{N_2}$ values in comparison with database values are given. Bis(2-chloropropyl) hydrogen phosphate and bis(2-chloroethyl) phosphate were spiked in urine but not detected after sample preparation. Therefore, no data is reported for these compounds. n.d. = not detected

Concentration level		20 ng/mL				50 ng/mL			
Compound	Ion	Measured m/z	$\Delta m/z$ [ppm]	$^{DT}CCS_{N_2}$ [Å ²]	$\Delta ^{DT}CCS_{N_2}$ [abs%]	Measured m/z	$\Delta m/z$ [ppm]	$^{DT}CCS_{N_2}$ [Å ²]	$\Delta ^{DT}CCS_{N_2}$ [abs%]
Di-n-butyl phosphate	[M-H]-	209.0937	5.36	150.70	0.13	209.0936	5.38	150.79	0.07
Diphenyl hydrogen phosphate	[M-H]-	249.0314	3.31	152.93	0.03	249.0315	2.91	152.96	0.01
4-Hydroxyphenyl phenyl phosphate	[M-H]-	265.0256	5.75	157.79	0.15	265.0261	3.86	157.63	0.04
Bis(2-chloropropyl) hydrogen phosphate	n.d.	n.d.		n.d.		n.d.		n.d.	
Bis(2-chloroethyl) phosphate	n.d.	n.d.		n.d.		n.d.		n.d.	
Bis(1,3-dichloro-2-propyl) phosphate	[M-H]-	n.d.		n.d.		301.9038	2.95	157.80	0.03
bis(1-chloro-2-propyl) 1-hydroxy-2-propyl phosphate	[M+H]+ [M+Na]+	n.d. n.d.		n.d. n.d.		309.0418 331.0247	0.57 2.36	160.80 168.92	0.12 0.02
tris(2-chloroethyl) phosphate	[M+H]+	284.9627	5.35	151.48	0.12	284.9613	0.44	151.62	0.20
Bis(2-butoxyethyl) phosphate	[M+H]+ [M+Na]+	299.1623 n.d.	1.75	171.34 n.d.	0.25	299.1616 321.1436	0.59 0.37	171.69 175.99	0.05 0.19
bis(2-butoxyethyl) 2-hydroxyethyl phosphate	[M+H]+ [M+Na]+	343.1890 365.1703	2.87 0.94	179.29 182.04	0.01 0.14	343.1884 365.1703	1.12 0.94	179.48 182.29	0.12 0.03
2-ethylhexyl phenyl phosphate	[M-H]-	285.1254	2.54	170.21	0.15	285.1252	3.24	170.08	0.22
5-Hydroxy-2-ethylhexyl diphenyl phosphate	[M+H]+ [M+Na]+	379.1676 401.1501	1.91 3.20	186.59 193.52	0.04 0.74	379.1664 401.1489	1.26 0.20	186.88 193.61	0.12 0.70
Bis(2-butoxyethyl) 3'-hydroxy-2-butoxyethyl phosphate	[M+H]+ [M+Na]+	415.2468 437.2282	2.95 1.56	195.36 199.70	0.04 0.34	415.2465 437.2272	2.23 0.73	195.79 200.16	0.18 0.11
3-Hydroxyphenyl phenyl phosphate	[M-H]-	341.0567	5.05	180.44	0.01	341.0570	4.18	180.46	0.01
4-Hydroxyphenyl phenyl phosphate	[M-H]-	341.0569	4.47	182.04	0.02	341.0573	3.30	182.06	0.03
		Average				0.15			
						0.12			

Table S9: $^{DT}CCS_{N_2}$ values of 15 alternative plasticizers metabolites acquired in spiked human urine. Pooled urine spiked at two concentration levels (20 ng/mL and 50 ng/mL) were analyzed in triplicate. Average measured m/z ratios and $^{DT}CCS_{N_2}$ values are reported. Also, the calculated mass error and absolute percent error of the experimental $^{DT}CCS_{N_2}$ values in comparison with database values are given. Mono-hydroxy-isononyl phthalate, mono-carboxy-isononyl phthalate and mono(2-ethyl-5-carboxypentyl) adipate were spiked in urine but not detected after sample preparation. Therefore, no data is reported for these compounds. n.d. = not detected

Concentration level		20 ng/mL					50 ng/mL			
Compound	Ion	Measured m/z	$\Delta m/z$ [ppm]	$^{DT}CCS_{N_2}$ [\AA^2]	$\Delta ^{DT}CCS_{N_2}$ [abs%]		Measured m/z	$\Delta m/z$ [ppm]	$^{DT}CCS_{N_2}$ [\AA^2]	$\Delta ^{DT}CCS_{N_2}$ [abs%]
Mono(2-ethylhexyl) terephthalate	[M-H]-	277.1446	0.38	183.55	0.01		277.1450	1.98	183.61	0.04
Mono(2-ethyl-5-hydroxyhexyl) terephthalate	[M-H]-	293.1405	3.44	185.22	0.08		293.1403	3.06	185.31	0.12
Mono(2-ethylhexyl) adipate	[M-H]-	257.1765	2.87	166.62	0.09		257.1760	0.75	166.69	0.05
Mono(2-ethyl-5-hydroxyhexyl) adipate	[M-H]-	273.1718	4.29	165.79	<0.01		273.1713	2.18	165.75	0.02
Mono(2-ethyl-5-oxohexyl) adipate	[M-H]-	271.1624	2.62	165.17	0.07		271.1556	1.79	165.09	0.12
Mono-isononyl-cyclo-hexane-1,2-dicarboxylate	[M-H]-	297.2071	0.16	174.82	0.38		297.2072	0.99	174.75	0.42
Cyclohexane-1,2-dicarboxylic mono carboxyisooctyl ester	[M-H]-	327.1813	0.28	176.50	0.13		327.1811	0.58	176.61	0.07
Cyclohexane-1,2-dicarboxylic mono hydroxyisononyl ester	[M-H]-	313.2026	2.32	175.22	0.06		313.2021	0.09	175.26	0.03
6-Hydroxy monopropylheptyl phthalate	[M-H]-	321.1714	2.13	178.73	0.06		321.1719	2.02	178.63	<0.01
Mono-2-(propyl-6-oxoheptyl)-phthalate	[M-H]-	319.1551	0.19	177.77	0.04		321.1713	1.08	177.83	0.08
Mono(2-propyl-6-carboxyhexyl) phthalate	[M-H]-	335.1513	4.71	179.80	0.09		335.1551	3.37	179.83	0.10
Mono(2-ethyl-5-carboxypentyl) terephthalate	[M-H]-	n.d.	n.d.	n.d.	n.d.		307.1201	4.39	168.61	0.11
Mono-hydroxy-isononyl phthalate	n.d.	n.d.	n.d.	n.d.	n.d.		n.d.	n.d.	n.d.	n.d.
Mono-carboxy-isononyl phthalate	n.d.	n.d.	n.d.	n.d.	n.d.		n.d.	n.d.	n.d.	n.d.
Mono(2-ethyl-5-carboxypentyl) adipate	n.d.	n.d.	n.d.	n.d.	n.d.		n.d.	n.d.	n.d.	n.d.
Average					0.09		0.10			

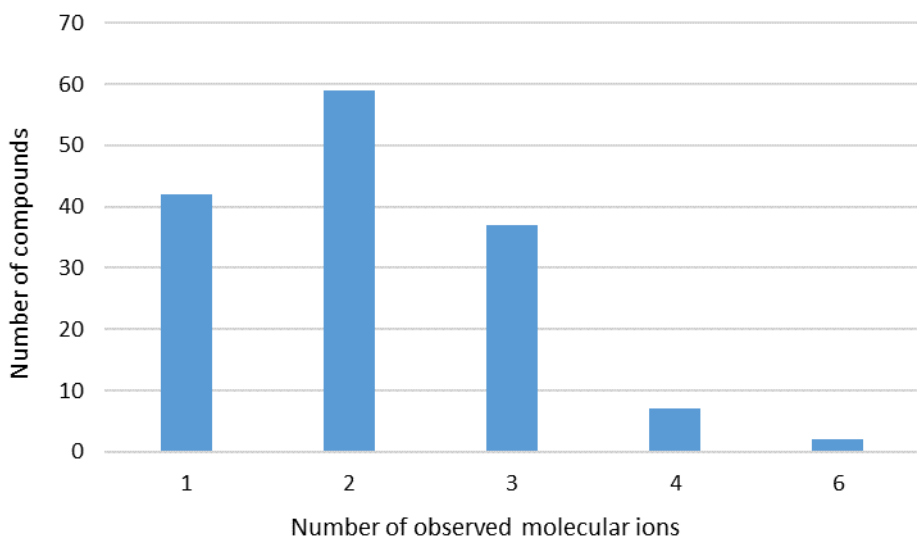


Figure S2: Number of observed ions for the studied compounds.

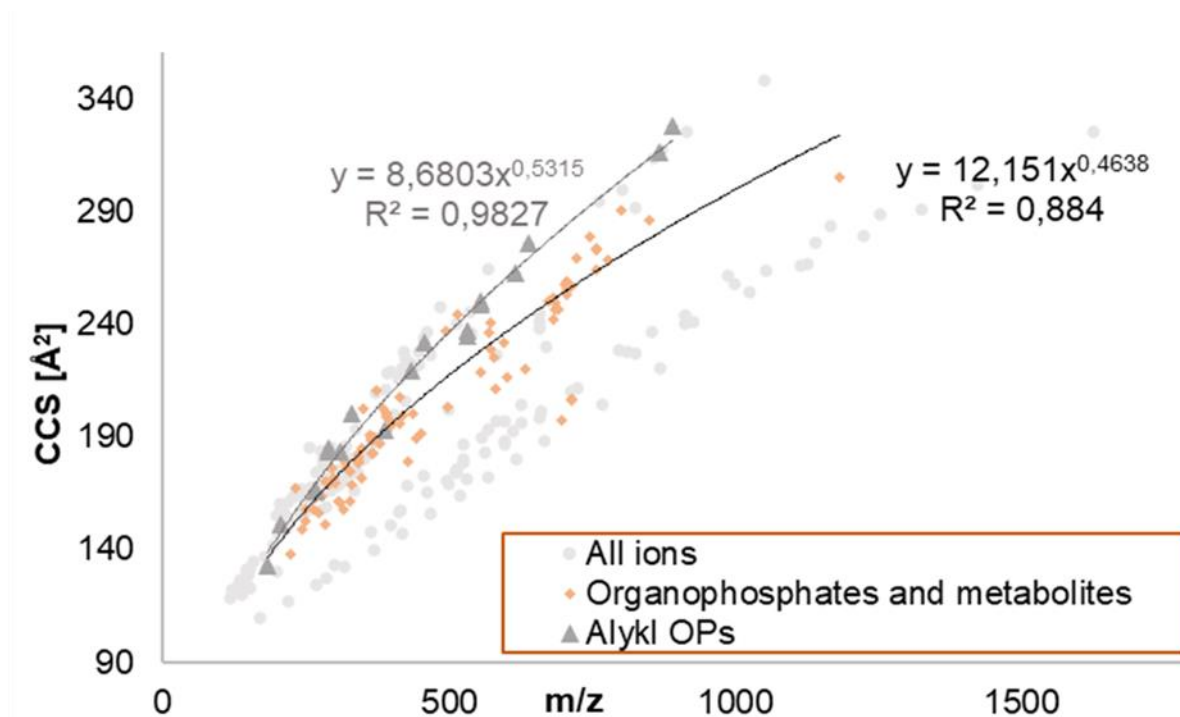


Figure S2: Depiction of $DTCCS_{N2}$ vs. m/z for organophosphates (OPs) and metabolites. The trendline calculated for all OPs and their metabolites ($n = 37$) is indicated. The subclass of alkyl OPs is marked separately with the corresponding trendline indicated in grey. For comparison, all acquired $DTCCS_{N2}$ values are also displayed in grey.