Method for identification - Agilent LC/MS QTOF

Table S1. LC (liquid chromatography) conditions

Analytical column	**Agilent Zorbax SB-Aq, 4.6×150 mm, 3.5 μm**	
Column temperature	40 °C	
Flow rate	0.4 mL/min	
Injection volume	5 μL	
Mobile phase	A) Water (LC/MS) + 0.1% acetic acid+ 1mM ammonium acetate (v/v/v) B) Acetonitrile (LC/MS) + 0.1 % acetic acid (v/v)	
Step gradient	Time (min)	Mobile phase
	0	100% A
	2	100% A
	14	2% A
	16	2% A
	19	100% A
	19.5	100% A
	20	100% A
Run time	20 min	
Post time	5 min	

Table S2. MS (mass spectrometry) conditions

ESI		
Ionization source	Dual AJS ESI	
Sheath gas temperature	350 °C	
Sheath gas flow rate	12 L/min	
Drying gas temperature	160 °C	
Drying gas flow rate	12 L/min	
Nebulizer pressure	30 psi	
Fragmentor	100 V	
Skimmer	65 V	
OCT 1 RF Vpp	750 V	
Mode	**Negative**	**Positive**
Nozzle voltage	3500 V	4500 V
Capillary voltage	1000 V	500 V
MS1 additional conditions		
Collision energy	10 V	10 V
MS2 additional conditions		
Collision energy	0-10-20-40 V	0-10-20-40 V

Detailed results –LC/MS QTOF analysis

Table S3. Plasticizers reported in TWP **[1]**

Compound	CAS	Base peak	Fragment peaks (obtained from PubChem)	
			CE 10V	CE 40 V
Dibutyl phthalate	84-74-2	279.1591	149.0239, 205.0855, 150.0268, 279.1593, 206.0891	149.0236, 121.0285, 93.0329, 121.0388, 150.0271
diethyl phthalate	84-66-2	223.0965	177.055, 149.0229, 178.0574, 150.0263, 223.0961	149.0233, 121.0283, 93.0326, 121.0386, 111.0437
di(2-ethylhexyl)phthalate	117-81-7	391.2843	149.0232, 71.0856, 57.0702, 167.0339	149.0233, 121.0285, 57.0703, 93.0337, 65.0391
diisobutyl phthalate	84-69-5	279.1591	149.0235, 57.0699, 109.0649, 223.0758	109.0649, 149.0235, 57.0699, 167.0855
dimethyl phtalate	131-11-3	195.065	163.0395, 164.0419, 195.0648	77.0392, 92.025, 95.0485, 105.0442, 105.0332

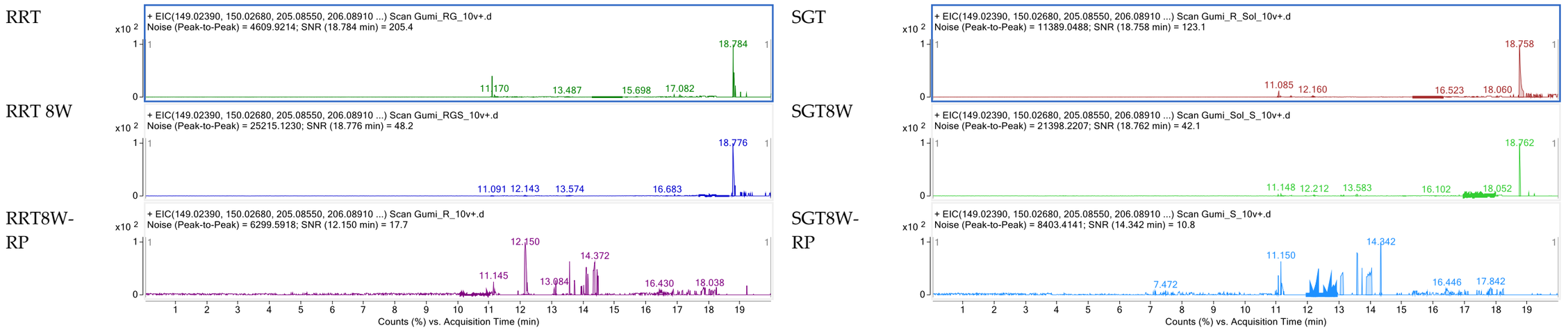

Figure S1. Dibutyl phthalate - EIC (extracted ion chromatograph) at retention time 18.78 min

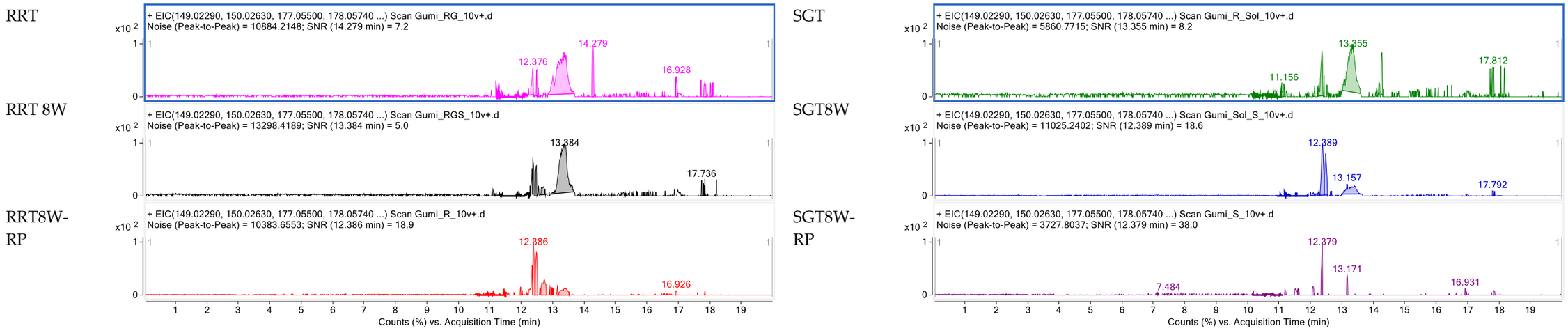

Figure S2. Diethyl phthalate - EIC (extracted ion chromatograph) at retention time 13.35 min

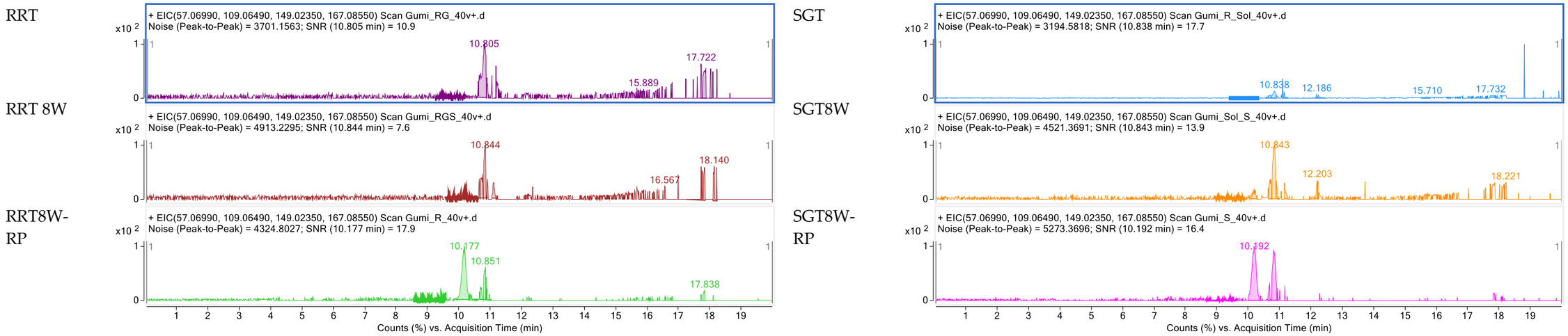

Figure S3. Diisobutyl phthalate - EIC (extracted ion chromatograph) at retention time 10.83 min

Table S4. Detailed results – database search (combined table with graphical representation – showing compound abundance at given retention time)

Compound	Found	Score (Tgt, max)	Mass (avg)	RT (avg)	RSD (Mass, ppm)		RRT	RRT8W	RRT8W -RP	SGT	SGT8W	SGT8W -RP	Additional confirmation mode
NEG - CE 0 V													
HOBT / 2-Hydroxybenzothia	6	98	151.01	14.62	1.59	Score (Tgt)	95.59	87.69	92.72	98.01	96.86	91.61	NEG - CE 10 V
BIT / Benzisothiazolinone	6	98	151.01	14.62	1.59	Area	497267	80766	882497	1038412	763514	638011	NEG - CE 40 V
2-Mercaptobenzoxazole	6	98	151.01	14.62	1.59	Diff (Tgt, ppm)	5.69	6.3	7.28	3.44	4.59	7.58	NEG MS2
						Ions	4	3	3	4	4	3	
NPE / 4-Nonylphenoxyacetic	6	96.7	278.189	17.61	1.57	Score (Tgt)	81.43	94.58	94.43	94.91	96.69	84.05	NEG - CE 10 V
						Area	246257	275579	278236	219229	252757	296067	NEG - CE 40 V
						Diff (Tgt, ppm)	1.4	2.09	2.25	-1.83	0.91	2.31	
						Ions	2	3	3	3	4	3	
Benzothiazole-2-sulfonic acid	6	96.4	214.972	12.51	2.52	Score (Tgt)	90.81	74.9	90.16	96.44	96.27	61.31	NEG - CE 10 V
						Area	269077	94535	441325	506368	1092945	1410123	NEG - CE 40 V
						Diff (Tgt, ppm)	4.65	9.33	4.76	1.72	3.68	5.58	NEG MS2
						Ions	3	3	3	3	4	2	
4-Hydroxybenzoic acid	3	95.6	138.033	12.58	2.58	Score (Tgt)				85.5	95.64	90.76	NEG - CE 10 V
						Area				402910	429367	886489	
						Diff (Tgt, ppm)				3.84	6.1	8.98	NEG MS2
						Ions				3	4	3	
Camphor	5	95.4	152.121	17.12	1.46	Score (Tgt)	77.78		71.88	95.43	82.52	66.89	NEG - CE 10 V
						Area	60912		68329	104120	75418	69148	
						Diff (Tgt, ppm)	2.4		4.05	0.07	1.73	2.81	
						Ions	2		2	3	2	2	
Isoborneol	6	95.1	154.136	16.25	5.03	Score (Tgt)	85.12	47.62	80.82	70.39	95.09	89.27	NEG - CE 10 V
						Area	44952	14510	142365	75624	309814	742027	NEG - CE 40 V
						Diff (Tgt, ppm)	-2.29	-7.62	4.38	2.67	3.81	5.39	
						Ions	2	2	2	2	3	3	
Dibutyl adipate	6	94.9	258.184	16.58	2.38	Score (Tgt)	66.62	71.67	84.41	71.05	85.51	94.92	NEG - CE 10 V
						Area	12200	14533	18321	10570	87374	766977	NEG - CE 40 V
						Diff (Tgt, ppm)	7.51	2.69	2.37	1.08	1.42	4.27	NEG MS2
						Ions	3	2	2	2	3	3	
Methylsalicylate	6	93.1	152.048	13.84	1.45	Score (Tgt)	88.59	70.04	70.89	93.14	78.37	88.51	NEG - CE 10 V
						Area	178015	201231	216099	169120	193713	379543	
						Diff (Tgt, ppm)	5.91	7.76	8.43	4.88	5.99	8.11	NEG MS2
						Ions	3	2	2	3	2	3	
2-tert-Butyl-4-methoxyphenc	6	92.2	180.116	17.13	5.6	Score (Tgt)	68.64	88.12	88.38	92.19	81.51	50.16	NEG - CE 10 V
						Area	140822	142722	133314	143592	141631	126493	
						Diff (Tgt, ppm)	3.34	1.12	2.48	1.24	0.77	15.02	
						Ions	3	3	3	4	2	2	
Ionone	4	85.7	192.152	16.79	5.3	Score (Tgt)	63.99		85.25		85.71	85.11	NEG - CE 10 V
						Area	12237		206245		105395	356474	
						Diff (Tgt, ppm)	12.4		2.93		0.22	3.37	
						Ions	2		2		2	2	
N4-Acetylsulfaguanidin (Ace	6	85	256.064	17.67	1.94	Score (Tgt)	83.92	83.08	82.35	85.02	83.89	79.64	NEG - CE 10 V
						Area	613533	419623	277487	580462	716669	212297	
						Diff (Tgt, ppm)	2.36	3.14	3.97	0.55	1.43	5.16	
						Ions	4	4	5	4	5	4	

Compound	Found	Score (Tgt, max)	Mass (avg)	RT (avg)	RSD (Mass, ppm)		RRT	RRT8W	RRT8W -RP	SGT	SGT8W	SGT8W -RP	Additional confirmation mode
NEG - CE 10 V													
4-tert-Octylphenol (4-(1,1,3,3-T	6	99.5	206.168	18.59	5.27	**Score (Tgt)**	98.3	94.75	78.57	99.51	99.27	73.97	
2-Octylphenol	6	99.5	206.168	18.59	5.27	**Area**	4714466	4815228	5048462	3938955	4347205	5368873	NEG - CE 40 V
						Diff (Tgt, ppm)	2.82	5.19	11.77	1.31	1.73	13.55	NEG MS2
						Ions	4	4	4	4	4	3	
Ethylsulfate (Ethyl sulfate)	3	97.9	125.999	5.377	1.84	**Score (Tgt)**	71.85			97.89	97.23		
						Area	37282			133607	67305		NEG - CE 40 V
						Diff (Tgt, ppm)	5.92			2.94	2.55		NEG MS2
						Ions	3			4	3		
4-tert-Butylbenzoic acid	4	95.5	178.097	16.5	2.82	**Score (Tgt)**	75.77	95.47		81.24	88.79		
						Area	115154	113272		119036	101878		NEG - CE 40 V
						Diff (Tgt, ppm)	-12.22	-13.9		-16.23	-9.47		
						Ions	4	5		5	5		
NEG - CE 40 V													
Benzothiazole	3	87.5	135.016	12.8	1.44	**Score (Tgt)**		50.63			81.21	87.5	
						Area		30522			91811	204294	
						Diff (Tgt, ppm)		8.62			7.71	10.53	
						Ions		2			3	4	
NEG MS2													
MBT / 2-Mercaptobenzothiazo	2	98.5	166.987	15.41	1.56	**Score (Tgt)**	98.15			98.54			
						Area	4000265			3180092			
						Diff (Tgt, ppm)	-0.08			2.12			
						Ions	5			3			