ELECTRONIC SUPPLEMENTARY INFORMATION

Development of a generic sample preparation by dispersive liquid-liquid micro-extractions for the monitoring of leachable compounds in hospital pharmacy-prepared prefilled drug products

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Table S1. Physical-chemical properties and mass parameters of all standards used in the development of DLLME

N°	Name of Compound	CAS	Log P	pKa	Retention time (minutes)	Polarity	Monoisotopic mass (Da)	m/z	Adduct	Category	Functional group
1	Diphenyl hydrogen phosphate	838-85-7	1.34	0.87	0.43	Negative	250.03949	249.03222	-H	Degradant of plasticizer and flame retardants	phosphate
2	4,4'-Sulfonyldiphenol	80-09-1	1.83	7.42	0.77	Negative	250.029984	249.0227	-H	Monomer and epoxy degradant	Phenol
3	4,4'-Methylenediphenol	620-92-8	2.73	9.84	1.27	Negative	200.083725	199.07645	-H	Monomer and epoxy degradant	Phenol
4	4-Methoxy-2-(2-methyl-2-propanyl)phenol - 4-methoxy-3-(2-methyl-2-propanyl)phenol (1:1)	121-00-6 / 88-32-4	3	10.57/10.01	2.24	Negative	180.115036	179.10775	-H	Antioxidant	Phenol
5	4,4'-(1,1-Ethanediyl)diphenol	05.08.2081	3.08	9.81	1.63	Negative	214.09938	213.0921	-H	Monomer and epoxy degradant	Phenol
6	4,4'-(2,2-Propanediyl)diphenol	80-05-7	3.43	9.78	1.85	Negative	228.115036	227.10775	-H	Monomer and epoxy degradant	Phenol
7	4,4'-(2,2-Butanediyl)diphenol	77-40-7	3.96	9.77	2.46	Negative	241.1234	242.130676	-H	Monomer and epoxy degradant	Phenol
8	Phenyl phosphate	115-86-6	4.1	-	4	Positive	326.070801	327.07807	+H	Flame retardant / plasticizer	Phosphate
9	4-(2-Phenyl-2-propanyl)phenol	599-64-4	4.17	10.08	3.16	Negative	212.120117	211.11284	-H	Degradant of Bisphenol A	Phenol

10	3-[4-Hydroxy-3,5-bis(2-methyl-2-propanyl)phenyl]propanoic acid	20170-32-5	4.48	4.79	3.34	Negative	278.188202	277.18092	-H	Monomer of complex antioxidants	Carboxylic acid
11	4-Methoxy-2,6-bis(2-methyl-2-propanyl)phenol	489-01-0	4.69	11.21	4.04	Negative	236.177628	235.17035	-H	Antioxidant	Phenol
12	B4-Hydroxy-3,5-bis(2-methyl-2-propanyl)benzoic acid	1421-49-4	4.8	4.36	2.9	Negative	250.156891	249.14962	-H	Oxidation of Bisphenol A	Carboxylic acid
13	4-Methyl-2,6-bis(2-methyl-2-propanyl)phenol	128-37-0	5.32	11.6	4.72	Negative	220.182709	219.17544	-H	Antioxidant	Phenol
14	4,4'-(1,3-Phenylenedi-2,2-propanediyl)diphenol	13595-25-0	6.12	9.78	4.37	Negative	346.193268	345.186	-H	Monomer and epoxy degradant	Phenol
15	2,4,6-Tris(2-methyl-2-propanyl)phenol	732-26-3	6.55	11.49	5.4	Negative	262.229675	261.22239	-H	Antioxidant	Phenol
16	2-(5-Chloro-2H-benzotriazol-2-yl)-4-methyl-6-(2-methyl-2-propanyl)phenol	05.11.3896	6.58	10.08	6.3	Negative	315.113831	314.10656	-H	UV absorber	Phenol
17	2,2'-Methylenebis[4-methyl-6-(2-methyl-2-propanyl)phenol]	119-47-1	7.03	8.92	5.8	Negative	340.240234	339.23295	-H	Antioxidant	Phenol
18	(9Z)-9-Octadecenamide	301-02-0	7.07	-	6.47	Positive	281.271851	282.27914	+H	Lubricant	Amide

19	[2-Hydroxy-4-(octyloxy)phenyl](phenyl)methanone	1843-05-6	7.36	7.07	6.14	Negative	326.188202	325.18092	-H	UV absorber	Phenol
20	4,4'-Sulfanediylbis[5-methyl-2-(2-methyl-2-propanyl)phenol]	96-69-5	7.63	9.69	5.04	Negative	358.196655	357.18937	-H	Antioxidant	Phenol
21	2,2'-Methylenebis[4-ethyl-6-(2-methyl-2-propanyl)phenol]	88-24-4	8.09	8.88	6.16	Negative	368.271515	367.26425	-H	Antioxidant	Phenol
22	2-(2H-Benzotriazol-2-yl)-4,6-bis(2-methyl-2-butanyl)phenol	25973-55-1	8.28	9.94	6.69	Negative	351.231049	350.22379	-H	UV absorber	Phenol
23	3-[4-Hydroxy-3,5-bis(2-methyl-2-propanyl)phenyl]-N'-{3-[4-hydroxy-3,5-bis(2-methyl-2-propanyl)phenyl]propanoyl}propanehydrazide	32687-78-8	8.37	10.37	6.5	Negative	552.3927	551.38543	-H	Antioxidant	Amide
24	Octyl 3-[4-hydroxy-3,5-bis(2-methyl-2-propanyl)phenyl]propanoate	125643-61-0	8.62	10.75	6.38	Negative	390.313385	389.30612	-H	Antioxidant	Ester
25	1,3,5-Tris[4-hydroxy-3,5-bis(2-methyl-2-propanyl)benzyl]-1,3,5-triazinane-2,4,6-trione	27676-62-6	10.34	-	12	Positive	783.518616	801.55246	+NH4	Antioxidant	Phenol

26	1,2-Ethanediyl bis{3,3-bis[4-hydroxy-3-(2-methyl-2-propanyl)phenyl]butanoate}	32509-66-3	11.62	9.52	6.07	Negative	794.475769	793.46849	-H	Antioxidant	Ester
27	(2R)-2,5,7,8-Tetramethyl-2-[(4R,8R)-4,8,12-trimethyltridecyl]-6-chromanol	59-02-9	11.9	10.8	7.31	Negative	430.381073	429.3738	-H	Antioxidant	Phenol
28	Didodecyl 3,3'-sulfanediyldipropanoate	123-28-4	12.88	-	12	Positive	514.405579	515.41286	+H	Antioxidant	Thiol
29	4,4',4''-[(2,4,6-Trimethylbenzene-1,3,5-triyl)tris(methylene)]tris[2,6-bis(2-methyl-2-propanyl)phenol]	1709-70-2	17.49	-	13	Positive	774.595093	792.62892	+NH4	Antioxidant	Phenol

30	3-({3-[4-Hydroxy-3,5-bis(2-methyl-2-propanyl)phenyl]propanoyl}oxy)-2,2-bis[({3-[4-hydroxy-3,5-bis(2-methyl-2-propanyl)phenyl]propanoyl}oxy)methyl]propyl 3-[4-hydroxy-3,5-bis(2-methyl-2-propanyl)phenyl]propanoate	6683-19-8	18.89	-	13	Positive	1176.784058	1194.8179	+NH4	Antioxidant	Ester
31	Bis(2-ethylhexyl)phthalate-3,4,5,6-d4	93951-87-2	8.71	-	8.68	Positive	394.3021167	395.30939	+H	Plasticizer	Ester
32	Tinuvin® 327	3864-99-1	6.49	10.07	9.69	Negative	357.1607901	356.15351	-H	UV Stabilizer	Benzotriazole
33	Bisphenol A-d16	96210-87-6	4.04	9.78	2.39	Negative	244.2154577	241.19563	-H	Monomer and epoxy degradant	Phenol

Table S2. Compilation of all information obtained after DLLME application on all products in the in-house database (DELTA). Information include some physical chemical properties, mass spectral information and DLLME recovery and relative standard deviation (RSD).

N°	Name of Compounds	CAS	Product Code	Retention time (mins)	Log P	Polarity	M/Z	DLLME Recovery (%)	RSD
1	N-methylformamide	123-39-7	RA7	2	-0.855	positive	60.04439	0.00	2.62%
2	N,N-Dimethylformamide	68-12-2	RA5	1.99	-0.632	positive	74.06004	0.00	7.02%
3	Caprolactam	105-60-2	O1	2.2	0.31	positive	114.09134	63.10	3.45%
4	Methylbutanedioic acid, dimethyl ester	1604-11-1	PZ108	2.21	0.436	positive	161.08084	60.70	6.02%
5	Diethyl hydrogen phosphate	598-02-7	PZ45	1.22	0.449	positive	155.04677	63.70	6.87%
6	Hydroxyphenylacetamide	17194-82-0	RA2	1.98	0.5	positive	152.0706	69.10	6.87%
7	N-butylacetamide	1119-49-9	RA3	2.02	0.517	positive	116.10699	67.20	5.74%
8	Dimethyl adipate	627-93-0	PZ8	2.2	0.782	positive	175.09648	73.80	2.30%
9	methacrylic acid	79-41-4	AD10	2.09	0.928	negative	85.0295	76.10	2.31%
10	2-Hydroxyethyl terephthalate	1137-99-1	PZ117	1.66	0.944	negative	209.04555	75.20	5.87%
11	N-cyclohexylformamide	766-93-8	RA8	2.24	0.944	positive	128.10699	76.80	4.60%
12	2-hydroxypropyl methacrylate	27813-02-1	AD11	2.24	1.034	positive	145.08592	76.20	6.92%

13	Vinyl caprolacam	2235-00-9	O4	2.45	1.038	positive	140.10699	84.90	5.89%
14	Caprolactone	502-44-3	O3	2.21	1.039	positive	115.07536	86.49	4.62%
15	3-ethyl-3-methylpentanedioic acid	5345-01-7	PZ25	2.234	1.078	positive	175.0965	96.10	3.93%
16	Bisphenol F Bis(2,3-dihydroxypropyl) Ether	72406-26-9	BP28	2.08	1.109	positive	366.19111	92.10	7.26%
17	N-butylformamide	111-36-4	RA9	2.018	1.281	positive	102.09134	81.00	3.70%
18	Benzotriazole	95-14-7	UV25	2.08	1.301	positive	120.05562	89.00	2.57%
19	Dimethyl-1,4-cyclohexanedicarboxylate	94-60-0	PZ19	2.478	1.405	positive	201.11214	86.23	6.96%
20	Phthalic anhydride	85-44-9	PZ90	2.94	1.423	positive	149.02332	79.56	2.51%
21	Diethyl adipate	141-28-6	PZ3	2.581	1.496	positive	203.12779	85.78	5.83%
22	Phthalide	87-41-2	PZ92	2.11	1.528	positive	135.04406	86.65	4.62%
23	pentaerythritol triacrylate	3524-68-3	AD4	2.21	1.554	positive	299.11253	84.57	7.09%
24	4 , 4'-diaminobenzophenone	611-98-3	UV16	1.97	1.66	positive	213.10224	86.61	6.93%
25	Methylparaben	99-76-3	AM1	2.29	1.673	negative	151.04007	87.12	3.44%
26	Bisphenol A bis(2,3-dihydroxypropyl) ether	5581-32-8	BP17	2.92	1.696	positive	394.22241	82.42	3.64%
27	tetrahydrofurfuryl methacrylate	2455-24-5	AD9	2.52	1.726	positive	171.10157	87.40	4.58%

28	Bis(4-hydroxybutyl) terephthalate	23358-95-4	PZ113	2.23	1.755	positive	311.14891	82.05	4.88%
29	4,4'-bis(Diethylamino)benzophenone	90-93-7	UV39	5.92	1.775	positive	325.22744	87.32	5.73%
30	Azelaic acid	123-99-9	PZ13	2.59	1.824	positive	189.11214	87.39	4.58%
31	Bis(2-methoxyethyl) phthalate	117-82-8	PZ68	2.35	1.886	positive	283.11761	85.66	3.50%
32	Dimethyl isophthalate	1459-93-4	PZ97	2.5	1.98	positive	195.06519	87.40	6.87%
33	Dimethyl phthalate	131-11-3	PZ69	2.29	1.98	positive	195.06519	81.38	7.37%
34	Monoethyl terephthalate	713-57-5	PZ112	2.54	1.991	positive	195.06519	66.50	9.02%
35	2-Methyl-5-methylenehexanoic acid, dimethyl ester	4513-62-6	PZ9	2.53	2.01	positive	201.11214	77.59	2.58%
36	N,N-Dibutylformamide	761-65-9	RA6	2.85	2.016	positive	158.15394	85.75	7.00%
37	Ethylparaben	120-47-8	AM2	2.41	2.03	negative	165.05572	78.89	5.07%
38	Tris (2-chloroethyl) phosphate	115-96-8	PZ40	2.467	2.107	positive	284.96116	75.12	5.32%
39	Nonanedioic acid, dimethyl ester	1732-10-1	PZ31	2.859	2.116	positive	217.14344	82.68	7.26%
40	tetraethyleneglycol dimethacrylate	109-17-1	AD17	2.91	2.303	positive	348.20168	82.76	7.25%
41	bisphenol S	80-09-1	BP36	1.974	2.32	negative	249.0227	81.28	3.69%
42	triethyleneglycol dimethacrylate	109-16-0	AD16	2.91	2.35	positive	304.17546	83.04	3.61%

43	ethyleneglycol dimethacrylate	97-90-5	AD15	2.78	2.444	positive	216.12303	84.41	2.37%
44	2-hydroxybenzophenone	117-99-7	UV15	3.24	2.486	negative	197.0608	84.69	7.08%
45	Propylparaben	94-13-3	AM3	2.6	2.552	negative	179.07137	85.80	5.83%
46	4-aminobenzophenone	1137-41-3	UV19	2.31	2.604	positive	198.09134	78.51	2.55%
47	Neopentyl glycol diacrylate	2223-82-7	AD21	2.8	2.684	positive	213.11214	80.18	2.49%
48	Diethyl phthalate	84-66-2	PZ55	2.61	2.694	positive	223.09649	83.43	4.79%
49	Tripropylene glycol diacrylate	42978-66-5	AD2	2.98	2.809	positive	318.19111	87.07	4.59%
50	4-hydroxy-2' , 4'-dimethyloxybenzophenone	41351-30-8	UV17	2.35	2.814	negative	257.08193	84.58	4.73%
51	4,4'-Dihydoxy-benzophenone	611-99-4	UV8	2	2.825	negative	213.05572	85.93	3.49%
52	Nonanedioic acid, diethyl ester	624-17-9	PZ33	3.55	2.83	positive	245.17474	83.25	3.60%
53	Bisphenol A (2,3-dihydroxypropyl) glycidyl ether	76002-91-0	BP15	2.98	2.858	positive	376.21185	84.58	4.73%
54	2 , 3 , 4 , 4'-tetrahydroxybenzophenone	31127-54-5	UV13	2.93	2.868	negative	245.04555	86.85	3.45%
55	Monoisobutyl phthalate	30833-53-5	PZ96	1.99	2.879	positive	223.09649	82.11	4.87%
56	1,3-butanediol dimethacrylate	1189-08-8	AD18	3.16	2.92	positive	227.12779	83.63	2.39%
57	Diphenyl sulfone	127-63-9	BP51	2.44	2.928	positive	219.04743	80.70	7.44%

58	2,4'-Dihydroxydiphenyl sulfone	5397-34-2	BP4	2.12	2.971	negative	249.0227	76.26	3.93%
59	Laurolactam	947-04-6	O2	2.93	2.977	positive	198.18524	86.07	2.32%
60	3-(4-{2-[4-(3-chloro-2-hydroxypropoxy)phenyl]propan-2-yl}phenoxy)propane-1,2-diol	227947-06-0	BP20	3.047	3.05	positive	412.18853	67.67	2.96%
61	Phosphoric acid, diphenyl ester	838-85-7	PZ42	1.22	3.052	negative	249.03222	75.42	2.65%
62	3-tert-butyl-4-methoxyphenol	88-32-4	AO118	2.7	3.057	negative	179.10775	71.52	2.80%
63	2-tert-butyl-4-methoxyphenol	121-00-6	AO117	2.7	3.057	negative	179.10775	81.05	3.70%
64	Tributyl citrate	77-94-1	PZ16	4.609	3.087	positive	361.22208	84.90	4.71%
65	1,6 hexanediol diacrylate	13048-33-4	AD20	3.16	3.119	positive	227.12779	85.81	5.83%
66	4-Hydroxybenzophenone	1137-42-4	UV6	2.45	3.129	negative	197.0608	83.53	3.59%
67	3-hydroxybenzophenone	13020-57-0	UV18	2.45	3.129	negative	197.0608	87.37	6.87%
68	Drometrizole	2440-22-4	UV31	4.28	3.186	negative	224.08294	85.45	3.51%
69	3-(3-5-di-tert-butyl-1-hydroxy-4-oxo-2,5-cyclohexadiene-1-yl)propanoic acid	83237-15-4	AO45	2.636	3.191	negative	293.17583	87.18	4.59%
70	4-tert-butylphenyl glycidyl ether	3101-60-8	O9	3.67	3.202	positive	224.16451	87.37	6.87%
71	Bisphenol S-monoisopropyl ether	95235-30-6	BP37	2.57	3.24	negative	291.06965	86.98	4.60%

72	Diisobutyl adipate	141-04-8	PZ5	4.125	3.271	positive	259.19039	85.78	2.33%
73	4-Fluoro-4'-hydroxybenzophenone	25913-05-7	UV5	2.52	3.272	negative	215.05138	87.21	5.73%
74	trimethylol propane triacrylate	15625-89-5	AD3	2.99	3.279	positive	314.15981	86.50	4.62%
75	Tris (2-chloro-1-methylethyl) phosphate	13674-84-5	PZ39	3.16	3.357	positive	327.00811	87.14	4.59%
76	Monobenzyl phthalate	2528-16-7	PZ80	2.03	3.359	positive	257.08084	86.58	3.47%
77	Diphenylamine	122-39-4	PZ12	3.184	3.413	positive	170.09643	86.26	4.64%
78	Dibutyl adipate	105-99-7	PZ4	4.27	3.43	positive	259.19039	86.60	3.46%
79	Bisphenol F Diglycidyl ether	2095-03-6	BP30	3.54	3.43	positive	330.16998	85.83	3.50%
80	Benzophenone	119-61-9	UV7	3.03	3.433	positive	183.08044	86.90	6.90%
81	Diallyl phthalate	131-17-9	PZ74	2.98	3.443	positive	247.09649	86.25	4.64%
82	2,2'-bisphenol F	2467-02-9	BP57	2.5	3.458	negative	199.07645	85.97	3.49%
83	bisphenol F	620-92-8	BP27	2.2	3.458	negative	199.07645	84.89	3.53%
84	2,4’dihydroxydiphenylmethane	2467-03-0	BP58	2.26	3.458	negative	199.07645	86.60	3.46%
85	Benzoresorcinol	131-56-6	UV1	2.6	3.475	negative	213.05572	87.02	3.45%
86	2,2',4,4'-Tetrahydroxybenzophenone	131-55-5	UV2	2.1	3.518	negative	245.04555	84.97	4.71%

87	Acetyl tributyl citrate	77-90-7	PZ17	5.384	3.528	positive	403.23264	87.28	5.73%
88	2,6-di-tert-butyl-4-hydroxy-4-methylcyclohexa-2,5-dien-1-one	10396-80-2	AO120	3.508	3.544	negative	235.17035	87.38	6.87%
89	4 , 4'-thiobisphenol	2664-63-3	BP9	2.27	3.55	negative	217.03287	87.25	5.73%
90	Oxybenzone	131-57-7	UV4	3.53	3.621	positive	229.08592	81.88	7.33%
91	2-tert-butyl-5-methylphenol	88-60-8	AO30	3.22	3.728	negative	163.11284	85.83	2.33%
92	2-tert-Butyl-4-methylphenol	2409-55-4	AO29	3.22	3.728	negative	163.11284	86.80	5.76%
93	Dipropyl phthalate	131-16-8	PZ76	3.35	3.739	positive	251.12779	80.03	5.00%
94	Bisphenol E	2081-08-5	BP26	2.29	3.75	negative	213.0921	84.75	7.08%
95	p-Benzylphenol	101-53-1	BP41	2.8	3.76	negative	183.08154	86.07	4.65%
96	Bisphenol F bis(3-chloro-2-hydroxypropyl) ether	235741-59-0	BP29	3.62	3.81	positive	402.12334	86.88	3.45%
97	Benzophenone-6	131-54-4	UV10	3.27	3.81	negative	273.07685	86.78	4.61%
98	7,9-di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione	82304-66-3	AO36	3.85	3.855	positive	277.17982	86.33	5.79%
99	Tris (2-butoxyethyl) phosphate	78-51-3	PZ38	4.881	3.945	positive	399.25062	85.13	5.87%
100	2 , 2'-dihydroxy-4-methoxybenzophenone	131-53-3	UV11	2.94	3.968	negative	243.06628	86.96	5.75%
101	Isopentyl p-methoxycinnamate	71617-10-2	UV40	4.62	3.969	positive	249.14852	86.22	3.48%

102	3,5-Di-tert-butyl-4-hydroxybenzyl alcohol	88-26-6	AO48	3.13	3.99	negative	235.17035	85.14	2.35%
103	Bisphenol A diglycidyl ether	1675-54-3	BP19	4.11	4.019	positive	358.20128	87.20	6.88%
104	Bisphenol A	80-05-7	BP14	2.38	4.04	negative	227.10775	87.39	3.43%
105	Bisphenol A-d16	96210-87-6	IS5	2.39	4.045	negative	241.19563	86.55	
106	4-(1-phenylethyl)phenol	1988-89-2	BP55	3.08	4.05	negative	197.09719	77.64	3.86%
107	Tributyl phosphate	126-73-8	PZ35	4.12	4.085	positive	267.17197	77.68	6.44%
108	Bisphenol A (3-chloro-2-hydroxypropyl) glycidyl ether	13836-48-1	BP16	4.21	4.212	positive	394.17796	83.85	7.16%
109	2-(1,1-dimethylethyl)-4,6-dimethylphenol	1879-09-0	AO31	3.52	4.242	negative	177.12849	74.46	4.03%
110	Butyl glycolyl butyl phthalate	85-70-1	PZ67	4.38	4.252	positive	337.16456	72.87	8.23%
111	Tris (1 , 3-dichloro-2-propyl) phosphate	13674-87-8	PZ37	4.26	4.28	positive	428.89119	75.30	19.64%
112	2-hydroxy-5-methylbenzophenone	1470-57-1	UV14	3.63	4.292	negative	211.07645	87.30	5.92%
113	3',5'-Bis(tert-butyl)-4'-hydroxyacetophenone	14035-33-7	AO38	3.903	4.317	positive	249.18491	94.40	3.10%
114	p-cumylphenol	599-64-4	BP42	3.35	4.34	negative	211.11284	78.00	21.71%
115	1-chloro-3-(4-{2-[4-(3-chloro-2-hydroxypropoxy)phenyl]propan-2-yl}phenoxy)propan-2-ol	4809-35-2	BP18	4.26	4.405	positive	430.15464	80.15	3.74%
116	3,5-Di-tert-butyl-4-hydroxybenzoic acid	1421-49-4	AO22	3.05	4.417	negative	249.14962	86.22	3.48%

117	trimethylopropane trimethacrylate	3290-92-4	AD8	4.22	4.466	positive	356.20676	86.81	5.76%
118	Diisobutyl phthalate	84-69-5	PZ52	4.33	4.469	positive	279.15909	85.14	5.87%
119	3,5-di-tert-butyl-4-hydroxybenzaldehyde	1620-98-0	AO25	3.82	4.472	negative	233.1547	87.20	2.29%
120	bisphenol B	77-40-7	BP24	2.62	4.49	negative	241.1234	87.39	5.72%
121	Tetradecanamide	638-58-4	LB3	4.82	4.561	positive	228.23219	87.01	4.60%
122	3,5-di-tert-butyl-4-hydroxyanisole	489-01-0	AO21	4.25	4.602	negative	235.17035	87.11	4.59%
123	Dibutyl phthalate	84-74-2	PZ50	4.15	4.628	positive	279.15909	85.48	5.85%
124	Mono(2-ethylhexyl) terephthalate	155603-50-2	PZ110	3.42	4.657	negative	277.14453	87.14	5.74%
125	Mono-(2-ethylhexyl)phthalate	4376-20-9	PZ60	2.53	4.657	positive	279.15909	86.62	4.62%
126	3,5-(1,1-Dimethylethyl)-4-hydroxy-benzenepropanol	36294-23-2	AO56	3.726	4.726	negative	263.20165	87.31	4.58%
127	3,5-ditert-butylphenol	1138-52-9	AO32	3.83	4.76	negative	205.15979	87.40	6.87%
128	2,4-di-tert-butylphenol	96-76-4	AO17	4.22	4.76	negative	205.15979	85.71	5.83%
129	2,6-Di-tert-butylphenol	128-39-2	AO37	4.84	4.76	negative	205.15979	85.55	5.84%
130	bisphenol AF	1478-61-1	BP22	2.67	4.77	negative	335.05122	83.96	7.15%
131	3-(3,5-di-tert-butyl-4-hydroxyphenyl)propanoic acid	20170-32-5	AO26	3.52	4.842	negative	277.18092	84.77	2.36%

132	Di-trimethylol propane tetraacrylate	94108-97-1	AD7	4.7	4.858	positive	484.25411	80.73	2.48%
133	bisphenol Z	843-55-0	BP38	3.13	4.915	negative	267.13905	87.20	3.44%
134	Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	6386-38-5	AO27	4.8	4.988	negative	291.19657	87.39	2.29%
135	2,6-Di-tert-butyl-4-(ethoxymethyl)phenol	3080-84-0	AO119	4.785	4.992	negative	263.20165	63.36	3.16%
136	Benzyl butyl phthalate	85-68-7	PZ48	4.53	5.029	positive	313.14344	87.38	2.29%
137	Triphenyl phosphate	115-86-6	PZ36	3.95	5.088	positive	327.07807	86.38	3.47%
138	p-Octylacetophenone	10541-56-7	AO109	5.91	5.156	positive	233.18999	86.88	5.76%
139	Bisphenol AP	1571-75-1	BP23	2.95	5.179	negative	289.1234	86.67	6.92%
140	Diisopentyl phthalate	605-50-5	PZ66	5.31	5.202	positive	307.19039	83.67	5.98%
141	4,4'-(4-Methylpentane-2,2-diyl)diphenol	6807-17-6	BP10	3.24	5.22	negative	269.1547	93.20	3.44%
142	Di-tert-butyl-m-cresol	497-39-2	AO39	4.63	5.273	negative	219.17544	87.36	2.29%
143	4,6-di-tert-butyl-o-cresol	616-55-7	AO34	4.63	5.273	negative	219.17544	77.03	5.19%
144	2,6-di-tert-butyl-p-cresol	128-37-0	AO95	5.26	5.273	negative	219.17544	87.31	6.87%
145	Diphenyl phthalate	84-62-8	PZ75	4	5.296	positive	319.09649	85.96	3.49%
146	bumetrizole	3896-11-5	UV27	8.7	5.331	negative	314.10656	86.29	3.48%

147	Ethyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propanoate	36294-24-3	AO28	5.26	5.345	negative	305.21222	84.68	4.72%
148	2-Ethylhexyl trans-4-methoxycinnamate	83834-59-7	UV38	6.42	5.38	negative	291.19547	84.77	3.54%
149	Dipentyl phthalate	131-18-0	PZ54	5.6	5.517	positive	307.19039	84.66	2.36%
150	Dicyclohexyl phthalate	84-61-7	PZ51	5.855	5.579	positive	331.19039	87.40	3.43%
151	Nonylphenol	26543-97-5	O10	5.01	5.582	positive	219.17544	87.24	6.88%
152	2,6-di-tert-butyl-4-ethylphenol	4130-42-1	AO35	5.758	5.718	negative	233.19109	87.39	4.58%
153	Bisphenol TMC	129188-99-4	BP47	4.13	5.79	negative	309.186	87.33	5.73%
154	Octrizole	123307-21-1	UV30	7.95	5.903	negative	322.19249	86.80	6.91%
155	Oleamide	301-02-0	LB1	6.6	5.977	positive	282.27914	91.20	4.61%
156	4,4'-Isopropylidenedi-2,6-xylol	5613-46-7	BP12	3.54	6.099	negative	283.17035	80.67	2.48%
157	4-benzoyl-4-methyldiphenyl sulfide	83846-85-9	UV23	6.39	6.135	positive	305.09946	85.79	2.33%
158	2 , 2'-diallyl bisphenol A	1745-89-7	BP2	3.75	6.242	negative	307.17035	85.27	3.52%
159	2, 4 ,6-tri-t-butylphenol	732-26-3	AO101	6.35	6.305	negative	261.22239	86.86	5.76%
160	Bisphenol BP	1844-01-5	BP44	3.74	6.31	negative	351.13905	85.85	5.82%
161	Dihexyl phthalate	84-75-3	PZ65	6.82	6.406	positive	335.22169	85.37	7.03%

162	Butyl octyl phthalate	84-78-6	PZ93	6.89	6.406	positive	335.22169	86.07	5.81%
163	2,4-Di-tert-butyl-6-(5-chlorobenzotriazol-2-yl) phenol	3864-99-1	UV29/IS4	9.69	6.491	negative	356.15351	86.52	4.62%
164	Bisphenol G	127-54-8	BP45	4.01	6.53	negative	311.20165	85.92	3.49%
165	Tri-p-cresyl phosphate	1330-78-5	PZ44	5.628	6.628	positive	369.12502	86.52	4.62%
166	Bisphenol A dimethacrylate	3253-39-2	BP21	6.04	6.637	positive	382.20128	82.11	7.31%
167	Bisphenol P	2167-51-3	BP35	4.5	6.724	negative	345.186	82.09	4.87%
168	Octabenzone	1843-05-6	UV20	8.15	6.724	negative	325.18092	87.80	3.45%
169	bis(2-ethylhexyl) fumarate	141-02-6	PZ21	7.71	6.763	positive	341.26864	91.30	5.83%
170	2-(2H-Benzotriazol-2-yl)-4,6-bis(2-methyl-2-butanyl)phenol	25973-55-1	UV28	9.54	6.766	negative	350.22379	85.52	3.51%
171	Di-(2-ethylhexyl) adipate	103-23-1	PZ2	8.69	6.828	positive	371.31559	86.33	2.32%
172	Bisphenol M	13595-25-0	BP34/IS2	4.28	7.01	negative	345.186	85.27	2.35%
173	Bisphenol PH	24038-68-4	BP46	3.98	7.339	negative	379.17035	84.21	2.37%
174	butyryl trihexyl citrate	82469-79-2	PZ124	9.656	7.34	positive	515.35785	77.83	3.85%
175	2 , 2-methylenebis (6-t-butyl-p-cresol)	119-47-1	AO102	7.05	7.575	negative	339.23295	84.10	7.13%
176	2,5-Bis(5-tert-butyl-benzoxazol-2-yl)thiophene	7128-64-5	UV32	9.82	7.58	positive	431.17878	84.99	7.06%

177	6,6'-di-tert-butyl-4,4'-thiodi-m-cresol	96-69-5	AO97/IS3	5.22	7.672	negative	357.18937	84.39	7.11%
178	Bis(2-ethylhexyl) phthalate	117-81-7	PZ49	8.676	8.025	positive	391.28429	83.85	2.39%
179	DEHP-3,4,5,6-d4	93951-87-2	PZ123/IS1	8.68	8.025	positive	395.30939	87.40	6.87%
180	Octyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propanoate	125643-61-0	AO23	8.59	8.09	negative	389.30612	79.10	5.85%
181	Diisononyl hexahydrophthalate	166412-78-8	PZ56	10.24	8.183	positive	425.36254	74.80	4.71%
182	Dioctyl phthalate	117-84-0	PZ71	9.035	8.185	positive	391.28429	67.80	3.44%
183	2 , 2-methylenebis (4-ethyl-6-t-butylphenol)	88-24-4	AO100	8	8.464	negative	367.26425	73.60	4.78%
184	1,2-Bis(3,5-di-tert-butyl-4-hydroxyhydrocinnamoyl)hydrazine	32687-78-8	AO5	6.43	8.511	negative	551.38543	75.90	5.56%
185	1,10-bis(2-ethylhexyl) decanedioate	122-62-3	PZ104	10.24	8.606	positive	444.40474	72.99	2.74%
186	Diisononyl phthalate	68515-48-0	PZ63	9.46	8.759	positive	419.31559	67.90	3.92%
187	Tris (2-ethylhexyl) phosphate	78-42-2	PZ41	9.984	9.182	positive	435.35977	69.10	2.59%
188	Bis[2,4-bis(2-methyl-2-propanyl)phenyl] hydrogen phosphate	69284-93-1	AO41	1.87	9.232	negative	473.2826	63.10	2.52%
189	2,2’,6,6’-Tetra-tert-butyl-4,4’-methylenediphenol	118-82-1	AO94	9.1	9.638	negative	423.32685	59.10	2.51%
190	Diisodecyl phthalate	26761-40-0	PZ62	10.35	9.648	positive	447.34569	69.20	5.01%
191	Bis(2-propylheptyl) phthalate	53306-54-0	PZ53	10.34	9.804	positive	447.34689	61.20	2.44%

192	N,N'-(Hexane-1,6-diyl)bis(3-(3,5-di-tert-butyl-4-hydroxyphenyl)propanamide)	23128-74-7	AO12	7.269	9.813	negative	635.47933	62.70	4.83%
193	Naugard DLTDP	123-28-4	AO4	11.96	10.499	positive	515.41286	57.80	3.62%
194	Alpha tocopherol	59-02-9	AO108	10.78	10.508	negative	429.3738	33.20	6.10%
195	Dioctyldiphenylamine	101-67-7	AO111	10.54	10.664	positive	394.34683	59.10	7.04%
196	Diundecyl phthalate	3648-20-2	PZ72	11.4	10.852	positive	475.37819	54.80	4.59%
197	Tris(2-ethylhexyl) benzene-1,2,4-tricarboxylate	3319-31-1	PZ122	11.8	11.051	positive	547.39932	53.10	2.34%
198	Irganox 259	35074-77-2	AO8	10.48	11.271	negative	637.44736	43.20	2.36%
199	tris isocyanuric acid	40601-76-1	AO116	10.05	11.615	positive	717.45856	47.90	7.18%
200	Ditridecyl phthalate	119-06-2	PZ78	12.41	12.63	positive	531.44079	39.10	4.60%
201	Hostanox O3	32509-66-3	AO6	7.39	12.639	negative	793.46849	33.70	6.88%
202	irganox 3114	27676-62-6	AO3	11.97	13.169	positive	801.55246	29.70	3.85%
203	2,4-Bis(octylthio)-6-(4-hydroxy-3,5-ditert-butylanilino)-1,3,5-triazine	991-84-4	AO16	12.198	13.372	negative	587.3823	33.90	2.48%
204	irganox 1330	1709-70-2	AO2	12.8	18.149	positive	792.62892	14.90	3.68%
205	irganox 1010	6683-19-8	AO1	13.2	19.288	positive	1194.8179	13.70	3.76%

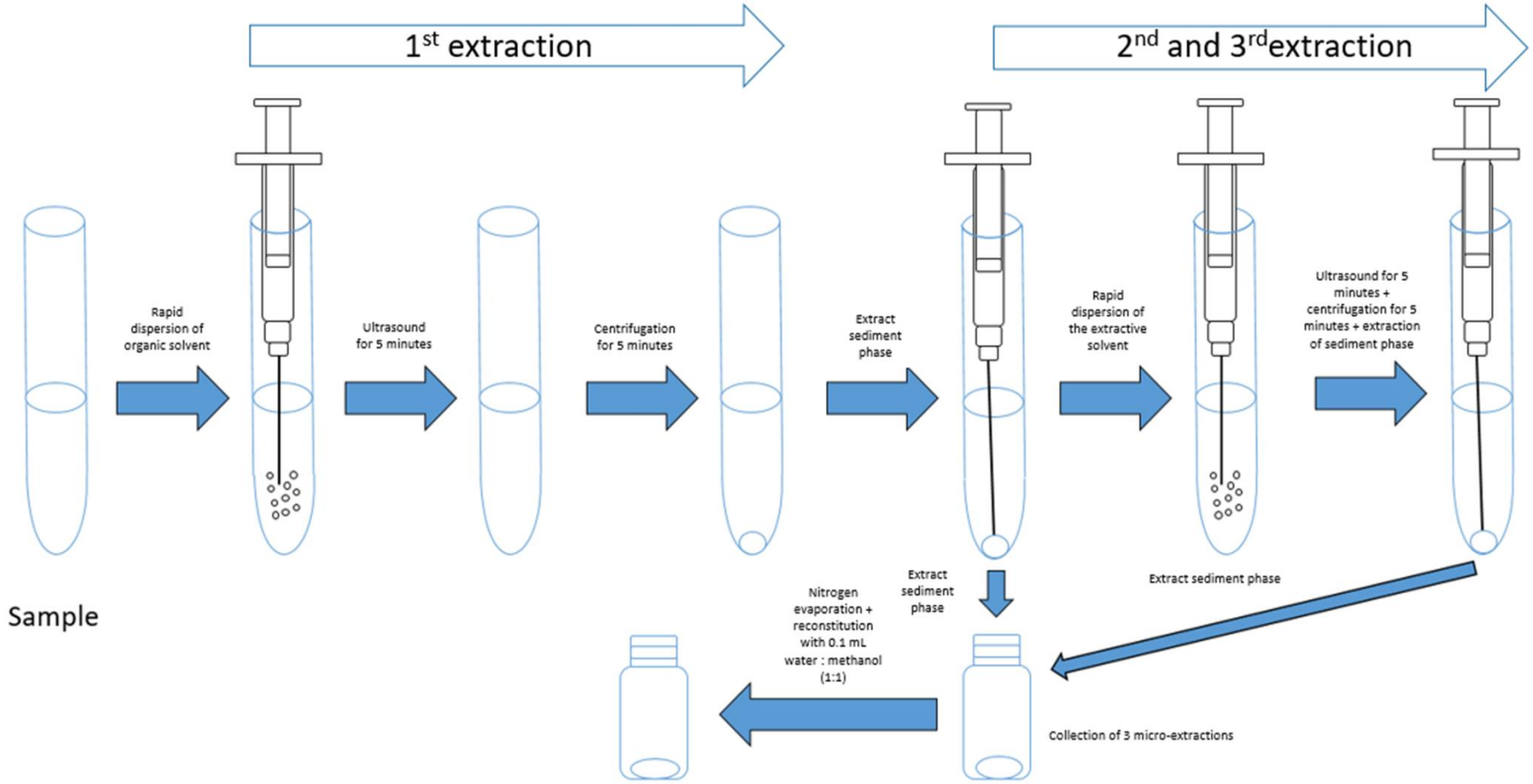

Figure S1: A demonstration of ultrasound-assisted and multiple extraction points dispersive liquid-liquid microextraction (UA-DLLME)

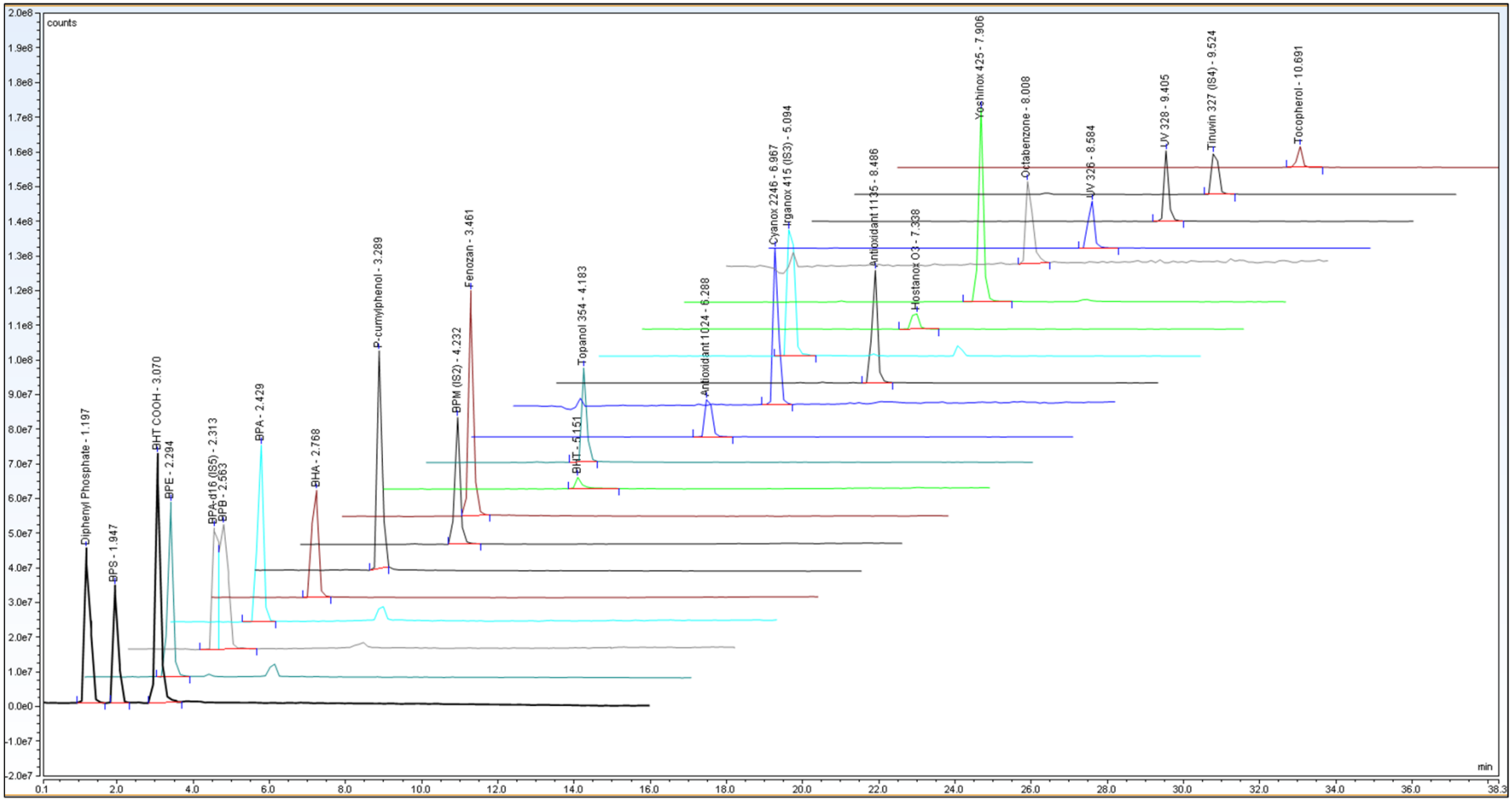

Figure S2: Chromatogram compiling negative mode compounds after DLLME sample preparation procedure

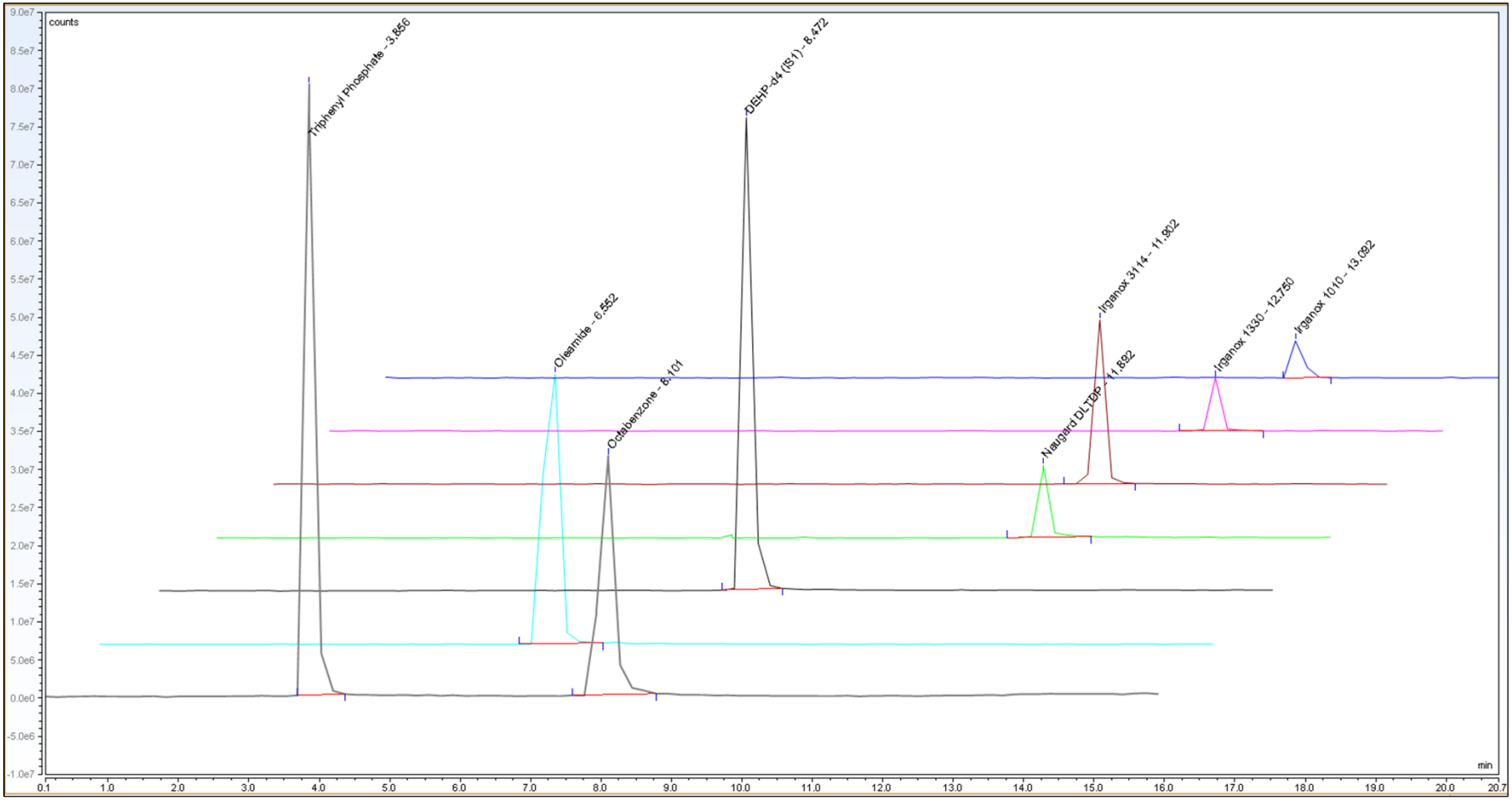

Figure S3: Chromatogram compiling positive mode compounds after DLLME sample preparation procedure

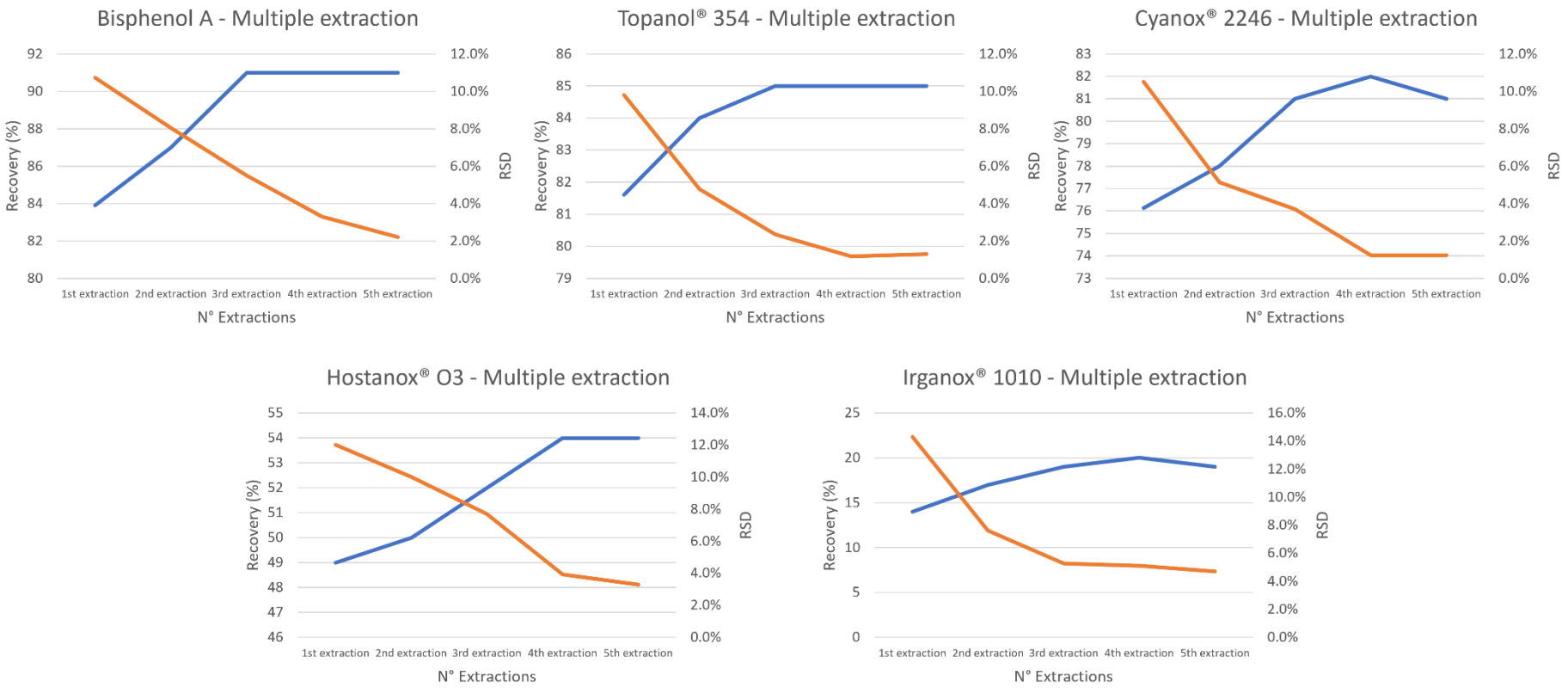

Figure S4: Description of results obtained from multiple extractions and the appearance of the asymptotic curve for all 5 representative sets of compounds, and vice versa, the decrease of the RSD in the form of a reverse asymptotic curve.

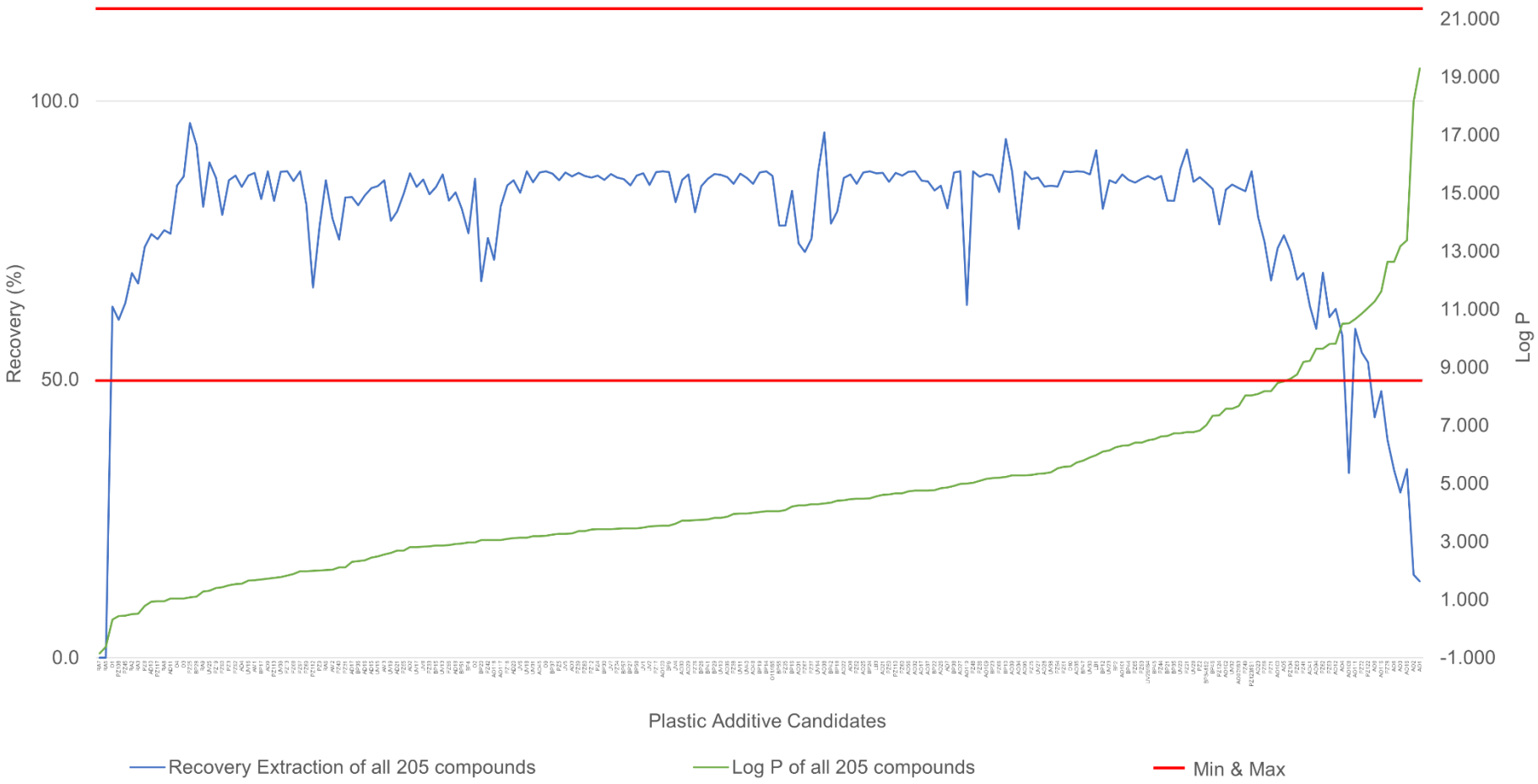

Figure S5: Graphic diagram describing the extraction recovery of all 205 compounds (%) via UA-DLLME in terms of their log P.