

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-Ethanediy)ldiphenol	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-Propanediy)ldiphenol	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-Butanediy)ldiphenol	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'-Sulfanediybis[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-EthanediyI 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