CLAP RRF from LCMS (Negative Ion Detection Mode)

RST Name: **Chemicals List for Analytical Performance (CLAP)**

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Contact: **RST_CDRH@fda.hhs.gov**

Code	Trivial Name	CAS #	RRF from LCMS (EIC) (Negative Ion Detection Mode)		
			5 µg/mL	10 µg/mL	20 µg/mL
RM2	Irganox 1076	2082-79-3	n.d.	n.d.	n.d.
RM4	Butylated hydroxytoluene	128-37-0	below DL	below DL	below DL
RM5	2,4-di-tert-butylphenol	96-76-4	below DL	below DL	below DL
RM8	Di-(2-ethylhexyl)phthalate	117-81-7	n.d.	n.d.	n.d.
RM13	Caprolactam	105-60-2	n.d.	n.d.	n.d.
RM14	Bisphenol A	80-05-7	n.d.	n.d.	n.d.
RM15	Erucamide	112-84-5	n.d.	n.d.	n.d.
RM16	Oleamide	301-02-0	n.d.	n.d.	n.d.
RM25	Dibenzylamine	103-49-1	n.d.	n.d.	n.d.
RM26	Benzoic acid	65-85-0	n.d.	n.d.	n.d.
RM27	2-Ethylhexanoic acid	149-57-5	n.d.	n.d.	n.d.
RM28	Bis(4-chlorophenyl) sulfone	80-07-9	n.d.	n.d.	n.d.
RM29	3,5-Di-tert-butyl-4-hydroxybenzyl alcohol	88-26-6	0.002	0.003	0.003
RM30	1,3-Di-tert-butylbenzene	1014-60-4	n.d.	n.d.	n.d.
RM31	tris(2,4-ditert-butylphenyl) phosphate	95906-11-9	n.d.	n.d.	n.d.
RM32	Palmitic acid	57-10-3	n.d.	n.d.	n.d.
RM37	5-Chloro-2-(2,4-dichlorophenoxy)phenol	3380-34-5	0.314	0.323	0.389

U.S. Food & Drug Administration
10903 New Hampshire Avenue
Silver Spring, MD 20993
FDA.GOV

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Code	Trivial Name	CAS #	RRF from LCMS (EIC) (Negative Ion Detection Mode)		
			5 µg/mL	10 µg/mL	20 µg/mL
RM46	Irganox 3125	34137-09-2	0.020	0.017	0.016
RM56	2-Mercaptobenzothiazole	149-30-4	0.384	0.448	0.448
RM57	Stearic Acid	57-11-4	n.d.	n.d.	n.d.
RM62	Sodium bis(2,2-methylene-bis(4,6-di-tert-butylphenyl)phosphate)	85209-91-2	0.869	0.951	0.997
RM70	DEHS	7313-54-4	0.005	0.007	0.010
RM82	Triisooctyl trimellitate	27251-75-8	n.d.	n.d.	n.d.
RM84	Tri(n-octyl, n-decyl) trimellitate	67989-23-5	n.d.	n.d.	n.d.
RM92	**Benzophenone-1**	131-56-6	**1.000**	**1.000**	**1.000**
RM93	Tinuvin P	2440-22-4	n.d.	n.d.	n.d.
RM97	PFDA	335-76-2	0.979	1.072	1.143
RM104	Dodecylbenzene sulfonic acid	27176-87-0	0.246	0.261	0.268

Note: the relative response factor (RRF) for each chemical in LCMS is established by comparing its signal intensity to that of the internal standard at same concentration. The signal intensity of each chemical was determined by calculating the normalized peak area obtained from the extracted ion chromatogram (EIC). The fragment ions selected for EIC were determined from the reference mass spectrum or, when it is unavailable, the major fragment ions with intensities above 10% of the base peak in full MS were chosen.

Chemicals highlighted in bold serve as internal standards in their corresponding ion detection modes.

In this test, commercial RM84 is comprised of a blend of tri-n-octyl (CAS# 89-04-3, MW 546.8) and tri-n-dodecyl trimellitate (CAS# 4130-35-2, MW 630.9). For LCMS data analysis, we could monitor only tri-n-octyl trimellitate in this experimental condition and its signal intensity was employed to calculate RRF value.

n.d.: not detected

below DL: below the detection limit, where the peak may be discernible but the signal-to-noise ratio of the sample peak in the EIC was less than 3.