

## CLAP RRF from LCMS (Positive Ion Detection Mode)

RST Name: [Chemicals List for Analytical Performance \(CLAP\)](#)

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Code	Trivial Name	CAS #	RRF from LCMS (EIC) <b>(Positive Ion Detection Mode)</b>		
			5 µg/mL	10 µg/mL	20 µg/mL
RM1	Irganox 1010	6683-19-8	0.557	0.537	0.521
RM2	Irganox 1076	2082-79-3	0.012	0.019	0.017
RM4	Butylated hydroxytoluene	128-37-0	0.320	0.390	0.435
RM5	2,4-Di-t-butyl phenol	96-76-4	n.d.	n.d.	n.d.
RM8	Di-(2-ethylhexyl)phthalate	117-81-7	0.650	0.552	0.635
RM13	Caprolactam	105-60-2	12.128	10.499	13.718
RM14	Bisphenol A	80-05-7	n.d.	n.d.	n.d.
RM15	Erucamide	112-84-5	3.895	4.691	5.387
RM16	Oleamide	301-02-0	8.755	6.478	6.468
RM17	Butyl stearate	123-95-5	0.003	0.003	0.003
RM22	Diisooctyl azelate	26544-17-2	1.780	1.840	1.879
RM25	Dibenzylamine	103-49-1	10.305	9.543	10.708
RM26	Benzoic acid	65-85-0	below DL	0.039	0.055
RM27	2-Ethylhexanoic acid	149-57-5	0.034	0.040	0.054
RM28	Bis(4-chlorophenyl) sulfone	80-07-9	0.398	0.455	0.571
RM29	3,5-Di-tert-butyl-4-hydroxybenzyl alcohol	88-26-6	n.d.	n.d.	n.d.

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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	0.779	0.556	0.423
RM32	Palmitic acid	57-10-3	n.d.	n.d.	n.d.
RM34	Ditolylguanidine	97-39-2	2.239	2.468	2.778
RM35	IPPD	101-72-4	1.558	1.817	2.111
RM36	Iragnox 3114	27676-62-6	0.033	0.029	0.024
RM38	Zinc pyrithione	13463-41-7	below DL	below DL	below DL
RM39	AEM 5772	199111-50-7	n.d.	n.d.	n.d.
RM40	Vitamin E	10191-41-0	0.149	0.172	0.190
RM42	DUSTANTOX 80	60160-25-0	0.881	1.073	1.408
RM43	Tetrone A	120-54-7	n.d.	n.d.	n.d.
RM45	Antioxidant 852	154862-43-8	n.d.	n.d.	n.d.
RM46	Irganox 3125	34137-09-2	1.140	0.947	0.846
RM47	Lauramide DEA	120-40-1	0.661	0.764	0.869
RM48	Monostearin	123-94-4	0.028	0.031	0.038
RM49	Benzothiazole	95-16-9	0.293	0.396	0.533
RM54	6-(Dibutylamino)-1,3,5-triazine-2,4-dithiol	29529-99-5	0.099	0.162	0.247
RM56	2-Mercaptobenzothiazole	149-30-4	0.702	0.604	0.734
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	1.380	1.337	1.531
RM63	Triethyl phosphate	78-40-0	1.914	2.272	2.599
RM64	Triacetin	102-76-1	0.280	0.343	0.400

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RM65	Triethyl citrate	77-93-0	1.360	1.443	1.506
RM72	Diisooctyl phthalate	27554-26-3	0.496	0.481	0.518
RM74	Acetyltributyl citrate	77-90-7	0.903	1.014	1.085
RM77	Diisononyl phthalate	28553-12-0	0.768	0.775	0.754
RM78	Diisononyl hexahydrophthalate	166412-78-8	1.000	1.091	1.129
RM79	Diisodecyl adipate	27178-16-1	0.992	1.076	1.197
<b>RM81</b>	<b>Butyryl trihexyl citrate</b>	82469-79-2	<b>1.000</b>	<b>1.000</b>	<b>1.000</b>
RM82	Triisooctyl trimellitate	27251-75-8	n.d.	n.d.	n.d.
RM84	Tri(n-octyl, n-decyl) trimellitate	67989-23-5	0.834	0.676	0.736
RM85	Phthalic anhydride	85-44-9	0.004	0.004	0.005
RM86	Benzotriazole	95-14-7	0.551	0.686	0.884
RM89	Octabenzone	1843-05-6	0.249	0.321	0.458
RM93	2-(2-Hydroxy-5-methylphenyl)benzotriazole	2440-22-4	0.660	0.713	0.843
RM94	Octrizole	3147-75-9	0.238	0.305	0.423
RM96	Ethylene thiourea	96-45-7	0.091	0.154	0.249
RM99	Laurolactam	947-04-6	1.291	1.578	1.871
RM104	Dodecylbenzene sulfonic acid	27176-87-0	n.d.	n.d.	n.d.
RM105	Dilauryl thiodipropionate	123-28-4	0.313	0.321	0.327
RM106	Ethyl carbitol	111-90-0	0.489	0.602	0.713

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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.