Supplementary material

Miniaturized Matrix Solid-Phase Dispersion for the Analysis of Ultraviolet Filters and Other Cosmetic Ingredients in Personal Care Products

Maria Celeiro, Lua Vazquez, J. Pablo Lamas, Marlene Vila, Carmen Garcia-Jares and Maria Llompart *

Laboratory of Research and Development of Analytical Solutions (LIDSA), Department of Analytical Chemistry, Nutrition and Food Science, Faculty of Chemistry, University of Santiago de Compostela, E-15782, Santiago de Compostela, Spain

* Correspondence: maria.llompart@usc.es; Tel.: +34-881-814-225

Table S1. Retention time and MS/MS transitions for the fragrance allergens, preservatives, plasticizers and synthetic musks.

Compounds	Ret. time (min)	MS/MS transition			CE [a]
Fragrance allergens					
Pinene	4.30	77.1	→	50.8	15
		92.8	→	39.0	35
		92.8	→	77.0	10
Limonene	5.85	67.9	→	53.0	10
		92.8	→	77.0	15
		92.8	→	91.0	10
Benzyl alcohol	5.93	79.0	→	50.9	20
		107.1	→	79.1	10
		108.2	→	79.1	15
Linalool	6.94	71.0	→	43.0	10
		92.9	→	77.0	10
		92.9	→	91.0	10
Methyl-2-octynoate	8.14	79.0	→	77.0	10
		94.9	→	67.0	10
		122.9	→	67.1	10
Citronellol	8.42	67.1	→	41.0	15
		95.0	→	67.1	10
		123.1	→	81.1	10
Citral	8.82	68.9	→	41.0	10
		94.0	→	79.0	10
		108.9	→	81.0	10
Geraniol	8.65	92.9	→	51.0	25
		92.9	→	77.1	10
		110.9	→	93.1	5
Cinnamaldehyde	8.9	103.1	→	77.0	10
		131.1	→	51.0	40
		131.1	→	77.0	25
Hydroxycitronellal	8.99	59.0	→	31.0	10
		71.0	→	43.0	10
		95.1	→	67.1	10
Anise alcohol	8.99	109.1	→	77.0	15
		109.1	→	94.0	10
		137.0	→	77.0	20
Cinnamyl alcohol	9.18	92.1	→	91.0	10
		134.1	→	78.0	15
		134.1	→	91.2	20
Eugenol	9.53	131.1	→	103.0	10

		164.2	→	103.0	20
		147.0	→	91.1	10
Methyleugenol	9.86	163.0	→	107.1	10
		178.1	→	147.1	10
		77.0	→	50.9	15
Isoeugenol	10.19	103.0	→	77.0	10
		164.1	→	149.1	10
		118.0	→	89.0	20
Coumarin	10.16	118.0	→	90.1	10
		146.1	→	118.1	10
		107.0	→	91.0	10
α-isomethylionone	10.39	150.1	→	91.0	20
		150.1	→	135.1	10
		189.2	→	131.1	10
Lilial®	10.72	204.2	→	147.2	10
		204.2	→	189.2	10
		116.8	→	115.1	10
Amylcinnamaldehyde	11.5	128.9	→	128.0	20
		202.0	→	129.1	10
		92.9	→	77.0	10
Lyral®	11.65	136.1	→	79.0	10
		136.1	→	93.1	10
		91.1	→	65.0	15
Amylcinnamyl alcohol	11.77	133.1	→	55.0	10
		133.1	→	115.1	10
Farnesol	11.95	69.0	→	39.0	15
		69.0	→	41.0	10
		116.8	→	91.0	15
Hexylcinnamaldehyde	12.3	129.0	→	127.0	20
		216.3	→	129.1	10
		90.9	→	65.0	15
Benzyl benzoate	12.56	105.1	→	77.0	10
		194.1	→	165.1	20
		131.1	→	77.0	20
Benzyl cinnamate	17.39	131.1	→	103.0	10
		192.0	→	191.2	15
		90.9	→	65.0	15
Benzyl benzoate	12.56	105.1	→	77.0	10
		194.1	→	165.1	20
Preservatives					
		134.9	→	107.0	5
Bronidox	8.30	13.0	→	109.0	5
		94.0	→	65.1	15
Phenoxyethanol (PhEtOH)	8.36	94.0	→	65.8	10
		138.0	→	94.1	10
		94.0	→	65.8	10
Methyl paraben (MeP)	10.22	138.0	→	94.1	10
		121.0	→	65.1	15
		121.0	→	93.1	10
Butylhydroxyanisole (BHA)	10.30	152.0	→	121.1	10
		137.1	→	77.1	20
		165.2	→	137.1	10
Butylhydroxytoluene (BHT)	10.55	180.1	→	165.1	10
		205.1	→	145.1	15
		205.1	→	177.2	10
Ethyl paraben (EtP)	10.64	220.2	→	205.2	10
		121.0	→	65.1	15

		121.0	→	93.1	10
Isopropyl paraben (iPrP)	10.82	138.0	→	121.0	10
		121.0	→	65.1	15
		121.0	→	93.0	10
Propyl paraben (PrP)	11.28	138.1	→	121.1	10
		121.0	→	65.0	15
		121.0	→	93.1	10
Iodopropynylbutyl carbamate (IPBC)	11.62	138.1	→	121.0	10
		164.9	→	126.9	35
		181.9	→	153.9	10
Isobutyl paraben (iBuP)	11.70	121.1	→	65.1	15
		121.1	→	93.1	10
		138.0	→	121.1	10
Butyl paraben (BuP)	12.06	121.1	→	65.1	15
		121.1	→	93.1	10
		138.0	→	121.1	10
Triclosan (TCS)	17.44	218.0	→	126.9	30
		288.0	→	218.0	15
		121.0	→	65.1	20
Benzyl paraben (BzP)	17.99	121.0	→	93.1	10
		228.2	→	121.1	10
Plasticizers					
		111.0	→	83.0	10
Dimethyl adipate (DMA)	8.55	114.0	→	71.0	15
		114.0	→	113.0	10
		128.3	→	99.0	10
Diethyl adipate (DEA)	9.72	157.0	→	83.0	15
		157.0	→	111.0	5
		149.0	→	121.1	10
Diethyl phthalate (DEP)	11.07	176.7	→	149.1	10
		149.0	→	65.0	25
Diisobutyl phthalate (DIBP)	13.41	149.0	→	121.0	15
		223.1	→	149.0	10
		149.0	→	65.1	20
Dibutyl phthalate (DBP)	14.76	149.0	→	93.0	15
		149.0	→	121.0	10
		104.2	→	76.0	10
Dimethoxyethyl phthalate (DMEP)	15.36	148.9	→	65.0	20
		148.9	→	121.0	10
		149.0	→	93.0	15
Diisopentyl phthalate (DIPP)	16.57	149.0	→	121.0	15
		237.1	→	149.0	10
		149.0	→	65.0	25
Dipentyl phthalate (DPP)	18.02	149.0	→	93.0	15
		149.0	→	121.0	15
		149.0	→	65.1	20
Benzylbuty phthalate (BBP)	19.86	149.0	→	93.0	15
		205.9	→	149.1	10
		129.0	→	83.0	10
Diethylhexyl adipate (DEHA)	20.11	129.0	→	101.0	5
		146.9	→	101.0	10
		149.0	→	65.0	25
Diisohetpty phthalate (DIHP)	20.45	149.0	→	121.0	15
		265.1	→	149.0	10
		149.0	→	65.0	25
Dicyclohexyl phthalate (DCHP)	20.78	149.0	→	93.0	15
		249.1	→	149.1	15
Diethylhexyl phthalate (DEHP)	20.84	149.0	→	93.0	15

		149.0	→	121.0	15
		279.1	→	149.1	10
		225.0	→	77.0	20
Diphenyl phthalate (DPhP)	20.92	225.0	→	115.0	30
		225.0	→	152.8	10
		149.0	→	93.0	15
Di-n-octyl phthalate (DnOP)	21.9	149.0	→	121.0	15
Synthetic musks					
		163.1	→	107.1	10
Cashmeran	10.58	191.1	→	135.1	10
		206.2	→	191.2	10
		229.3	→	173.1	10
Celestolide	11.94	244.2	→	173.1	15
		244.2	→	229.2	10
		187.0	→	145.2	10
Phantolide	12.35	229.2	→	187.0	10
		244.2	→	229.2	10
		253.1	→	105.9	10
Ambrette	13.06	253.1	→	119.9	10
		268.1	→	253.1	5
		173.0	→	131.1	10
Trasolide	13.25	215.2	→	173.1	10
		258.2	→	215.2	10
		213.2	→	171.2	10
Galaxolide	13.35	243.2	→	198.2	20
		243.2	→	213.2	10
		187.1	→	43.0	15
Tonalide	13.42	243.2	→	159.2	10
		258.2	→	187.2	10
		263.1	→	127.8	40
Musk Moskene	13.69	263.1	→	200.9	10
		263.1	→	221.1	10
Musk Tibetene	14.28	251.1	→	159.9	10
		266.3	→	251.2	5
Ambrettolide	14.46	95.9	→	81.1	10
		108.9	→	67.1	10
		108.9	→	81.0	10
Musk Ketone	15.02	279.1	→	117.9	20
		279.1	→	191.0	10

[a] CE: Collision Energy, eV. Underlined MS/MS transitions: quantification transitions.

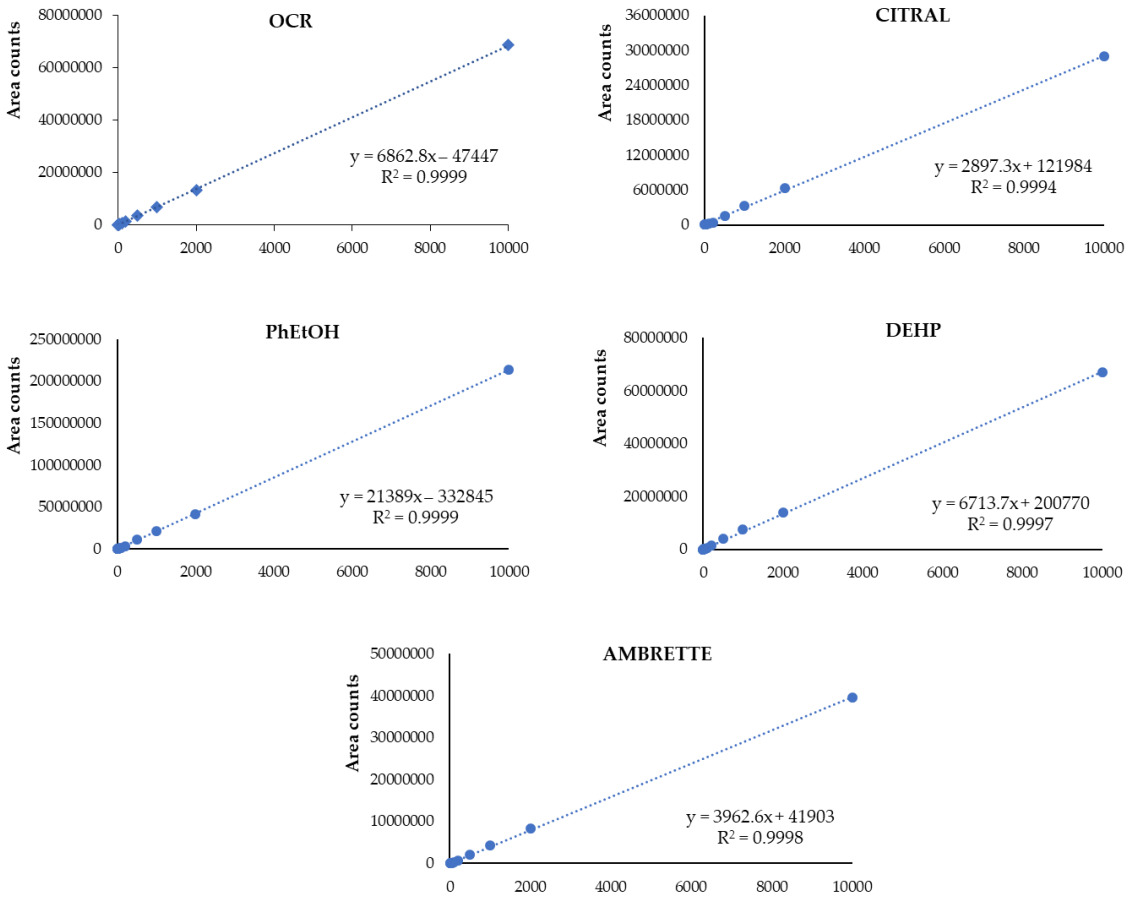

Figure S1. Calibration plots for some representatives compounds of each studied family.