

Supplementary materials

Identification of molecules from tomato plant residues using sustainable green chemicals

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Table S1: Mean compound table for solvents. RT retention time, 2-MTHF 2-methyltetrahydrofuran, NEQ naphthalene equivalent, kg_{dw} kilogram dry weight

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
Fatty acid / ester	6.731	Isopropyl acetate	C5H10O2	102.13				6.35 ± 1.89	
	7.732	Butylformate	C5H10O2	102.13		105.49 ± 3.04			
	8.234	Ethyl propionate	C5H10O2	102.13	0.92 ± 0.16	8.47 ± 1.18		519.57 ± 59.5	8.88 ± 2.24
	10.818	Ethyl butyrate	C6H12O2	116.16	683.17 ± 39.29	140.52 ± 16.24	5.22 ± 3.15	93 ± 12.77	6.14 ± 0.13
	11.743	Butanoic acid, 2-ethyl-2-methyl-	C7H14O2	130.18		1985.9 ± 417.08			
	12.616	Ethyl lactate	C5H10O3	118.13		1.39 ± 0*			2.1 ± 0.05
	12.981	Isopropyl formate	C4H8O2	88.12		1.95 ± 0*		3.87 ± 0.84	
	13.736	Butyric Acid	C4H8O2	88.11	0.91 ± 0*		0.9 ± 0.24	13.07 ± 0*	3.72 ± 0.06
	14.553	Amyl acetate	C7H14O2	130.18		4.01 ± 0.67			

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
Fatty acid / ester	16.015	1,2-Ethanediol, monoacetate	C4H8O3	104.1				2.21 ± 0.35	
	18.919	Isopropyl caproate	C9H18O2	158.27		68.97 ± 46.2			
	19.583	Butyrolactone	C4H6O2	86.09					2.96 ± 0*
	20.924	(E)-3-Hexenoic acid	C6H10O2	114.16					5.42 ± 0*
	21.516	2-Hexenoic acid	C6H10O2	114.16					8.04 ± 0*
	23.8	Pantolactone	C6H10O3	130.16		2.19 ± 0*			
	23.842	Octyl acetate	C10H20O2	172.26				4.34 ± 0.79	
	23.88	β-Hydroxybutyric acid	C4H8O3	104.1		11.36 ± 1.39			
	27.725	Sulfurous acid, isohexyl hexyl ester	C12H26O3S	250.4		9.03 ± 0*			
	28.78	1,5-Diacetoxypentane	C9H16O4	188.25		4.55 ± 0.73			
	29.096	Monoacetin	C5H10O4	134.13		10.88 ± 1.49	0.93 ± 0.15	12.21 ± 7.09	
	29.367	Glycerol diacetat	C7H12O5	176.17		0.67 ± 0*		2.42 ± 0*	
	31.898	Acetic acid, 2-methyl-6-oxo-heptyl ester	C10H18O3	186.28		6.13 ± 0.67			
	32.144	Methyl dodecanoate	C13H26O2	214.34			0.84 ± 0*	5.4 ± 0.83	
	34.170	Isopropyl dodecanoate	C15H30O2	242.4	0.81 ± 0*			1.76 ± 0.03	
	35.469	Carbonic acid, decyl undecyl ester	C22H44O3	356.6		1.53 ± 0*	1.2 ± 0*	8.62 ± 0*	
	36.223	Trihexadecyl borate	C48H99BO3	735.1				17.12 ± 0*	
	36.606	Acetic acid, 3,7,11,15-tetramethyl-hexadecyl ester	C22H44O2	340.6			0.59 ± 0*	3.49 ± 0.71	
	36.804	Methyl tetradecanoate	C15H30O2	242.4	3.93 ± 0*		2.96 ± 1.44	9.93 ± 0*	
	37.3	Tridecanal	C13H26O	198.39		2.29 ± 0.3			
	38.519	3,4-dimethyl valeric acid	C7H14O2	130.21					5.55 ± 0.12

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
Fatty acid / ester	38.71	Isopropyl myristate	C17H34O2	270.5		19.21 ± 2.39		26.8 ± 0*	14.95 ± 7.41
	40.766	Octadecanol	C18H38O	270.5		1.24 ± 0.11		4.34 ± 0*	3.04 ± 0*
	40.992	Methyl 4-methyloctanoate	C10H20O2	172.3		4.8 ± 0.15		3.56 ± 2.7	4.09 ± 0.16
	41.575	Methyl (Z)-5,11,14,17-eicosatetraenoate	C21H34O2	318.5			5.27 ± 0*	6.52 ± 0*	
	41.688	Glyceryl diacetate 1-linolenate	C25H40O6	436.6			10.73 ± 0*		
	42.188	Ethyl palmitate	C18H36O2	284.5	3.94 ± 0.97		10.41 ± 3.05	6.02 ± 2.23	
	42.239	Ethyl palmitate	C18H36O2	284.5		1.3 ± 0.42			8.12 ± 1.31
	43.408	Acetic acid, 3,7,11,15-tetramethyl-hexadecyl ester	C22H44O2	340.6			2.63 ± 0.95		
	43.648	Palmitic Acid	C16H32O2	256.42	1.75 ± 0.6		2.54 ± 0.45	3.49 ± 0.95	27.74 ± 2.02
	44.885	Methyl elaidate	C19H36O2	296.5	1.39 ± 0*				
	44.954	Methyl henicosanoate	C22H44O2	340.6				10.77 ± 0.07	
	44.999	Methyl α-linolenate	C19H32O2	292.5			2.2 ± 0.23		
	45.747	Mandenol	C20H36O2	308.5	4.23 ± 1.18		10.65 ± 4.38	13.21 ± 0.63	9.03 ± 0.19
	45.918	Ethyl stearate	C20H40O2	312.5			2.88 ± 1.23	8.76 ± 0*	
	45.951	4-Oxazolecarboxylic acid, 4,5-dihydro-2-phenyl-, 1-methylethyl ester	C13H15NO3	233.26	0.96 ± 0.29		1.2 ± 0*	4.05 ± 0*	
	46.035	Ethyl linolenate	C20H34O2	306.5	5.08 ± 1.2	1.9 ± 0*	7.16 ± 1.47	10.3 ± 5.82	3.89 ± 0.69
	47.092	Linoleic acid	C18H32O2	280.4	83 ± 20.09			99.6 ± 15.22	
	47.192	Cerasynt	C22H44O4	372.66			77.32 ± 23.79		
	47.773	Dimethylaminoethyl palmitate	C20H41NO2	327.5	112.91 ± 5.36	9.73 ± 0.87		20.41 ± 17.73	37.51 ± 4.18
	48.255	Dimethylaminoethyl palmitate	C20H41NO2	327.5			7.46 ± 6.15		

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
Fatty acid / ester	48.292	Arachidonoyl-N-methyl amide	C21H35NO	317.5			3.86 ± 1.42		
	48.575	Glycol palmitate	C18H36O3	300.54		1.78 ± 0.51	3.99 ± 0.42		
	48.756	Vinyl palmitate	C18H34O2	282.5			6.83 ± 0.63	4.64 ± 0.12	
	48.931	Glycidyl palmitate	C19H36O3	312.5		13.51 ± 1.5	6.17 ± 0.74	4.98 ± 0.84	4.09 ± 1.04
	49.258	Ethyl arachidate	C22H44O2	340.6		1.02 ± 0*	3.18 ± 0*		12.74 ± 8.54
	50.945	Vinyl palmitate	C18H34O2	282.5			1.24 ± 0*		
	52.059	Glyceryl monolinoleate	C21H38O4	354.5		2.67 ± 0.89			
	52.475	Palmitoleamide	C16H31NO	253.48		8.14 ± 0.88			
	52.535	trans-Oxiraneundecanoic acid, 3-pentyl-, methyl ester	C19H36O3	312.55		12.66 ± 0.57			7.64 ± 1.26
	52.576	Diethyl adipate	C22H42O4	370.64				3.19 ± 0*	
	52.91	Linolenic acid	C18H30O2	278.4		3.2 ± 0.73			15.31 ± 1.18
	53.057	Methyl (Z)-5,11,14,17-eicosatetraenoate	C21H34O2	318.5					5.5 ± 0*
	54.042	Bis(2-ethylhexyl) phthalate	C24H38O4	390.6		2.34 ± 0*			5.89 ± 1.07
	55.914	2-Monopalmitin	C19H38O4	330.5		23.45 ± 5.4	27.88 ± 3.71		115.05 ± 1.39
	56.242	Linolenic acid	C18H30O2	278.4					9.84 ± 3.51
	57.553	Methyl melissate	C31H62O2	466.8				2.48 ± 0*	
	57.608	Glyceryl monolinoleate	C21H38O4	354.5			3.13 ± 1.33		
	57.696	Glyceryl linolenate	C21H36O4	352.5			7.15 ± 1.66	4.23 ± 0.65	

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
Fatty acid / ester	57.803	Trilinolein	C57H98O6	879.4			3.52 ± 0.8	4.53 ± 1.02	
	57.862	Erucylamide	C22H43NO	337.6			1.16 ± 0*	14.26 ± 0*	
	57.921	Glyceryl linolenate	C21H36O4	352.5			4.73 ± 1.41	7.22 ± 0.69	
Hydrocarbon	9.609	Toluene	C7H8	92.14				4.44 ± 0	
	13.907	4-Methylnonane	C10H22	142.28				1.75 ± 0.34	
	15.200	Decane	C10H22	142.28	3.04 ± 0*			15.82 ± 2.64	
	15.869	Heptane, 5-ethyl-2-methyl-	C10H22	142.28				2.61 ± 0.44	
	18.424	Undecane	C11H24	156.31	0.75 ± 0*			3.23 ± 0.72	
	21.584	Octane, 2,3,3-trimethyl-	C11H24	156.35	0.82 ± 0.02		0.53 ± 0*	2.41 ± 0.22	
	21.637	1-Dodecene	C12H24	168.32			0.63 ± 0*	3.22 ± 0.49	2.1 ± 0.7
	23.46	Dodecane, 4,6-dimethyl-	C14H30	198.39		7.65 ± 1.74	0.4 ± 0*		
	27.214	Tetradecane	C14H30	198.39	1.43 ± 0*		1.75 ± 0*	4.06 ± 0.19	
	27.289	<i>α</i> -Ionene	C13H18	174.28			0.94 ± 0.34	5.15 ± 0.65	
	27.339	1-Tridecene	C13H26	182.35					4.14 ± 1.42
	27.546	<i>A</i> -Ionene	C13H18	174.28		10.35 ± 6.2		5.03 ± 0*	
	28.333	Naphthalene, 1,2-dihydro-1,1,6-trimethyl-	C13H16	172.27		4.25 ± 0.19	3.22 ± 1.33	1.75 ± 0*	
	29.217	Eicosane	C20H42	282.5		1.72 ± 0*			
	29.315	Pentadecane	C15H32	212.41				2.38 ± 0.2	
	29.684	Hexadecane	C16H34	226.44			0.84 ± 0*		
	29.817	Pentadecane	C15H32	212.41					

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
Hydrocarbon	30.045	Naphthalene, 2,6-dimethyl-	C12H12	165.22				3.38 ± 0*	
	30.150	Heptadecane	C17H36	240.5			0.55 ± 0*		
	32.413	1-Pentadecene	C15H30	210.4	9.04 ± 0*			4.54 ± 0.8	4.22 ± 0*
	32.471	Cetene	C16H32	224.42				15.14 ± 9.93	
	34.353	Eicosane	C20H42	282.5			0.76 ± 0*	7.1 ± 0*	
	34.466	Hexadecane	C16H34	226.44				5.57 ± 3.67	
	35.841	Tetradecane, 5-methyl-	C15H32	212.41				4.41 ± 0*	
	35.968	Heptadecane, 4-methyl-	C18H38	254.5				5.42 ± 0*	
	36.096	Tetracosane	C24H50	338.7			1.42 ± 0*		
	36.351	5-Undecene, 5-methyl-	C12H24	168.32				6.2 ± 0*	
	36.478	1-Pentadecene, 2-methyl-	C16H32	224.42				5.14 ± 0*	
	36.971	1-Octadecene	C18H36	252.54					3.06 ± 0*
	38.959	Nonadecane	C19H40	268.5	0.49 ± 0*		0.68 ± 0.24		
	41.101	Hexatriacontane	C36H74	507	10.15 ± 3.28	2.19 ± 0.27	5.53 ± 1.55	16.58 ± 0*	
	41.395	1-Nonadecene	C19H38	266.5				6.4 ± 0*	
	41.418	Eicosane	C20H42	282.5			5.39 ± 0*		
	41.440	Phenanthrene	C14H10	178.23				8.31 ± 0.61	
	42.010	Heneicosane	C21H44	296.6			2.03 ± 0*		
	42.290	Hexatriacontane	C36H74	507	50.72 ± 3.16		13.16 ± 0*	91.8 ± 48.98	
	42.429	Dotriacontane, 2-methyl-	C33H68	464.9	26.61 ± 6.93		10.47 ± 0*	106.03 ± 0*	
	42.569	Hexatriacontane	C36H74	507			217.94 ± 13.89		
	43.129	Anthracene, 2-methyl-	C15H12	192.25				5.22 ± 0*	

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
Hydrocarbon	43.268	Tetracosane	C24H50	338.7			0.88 ± 0*	3.48 ± 0*	
	43.548	7-Tetradecene	C14H28	196.42				2.15 ± 0*	
	44.708	Heneicosane	C21H44	296.6		1.12 ± 0*		3.54 ± 0*	
	44.862	Heneicosane	C21H44	296.6				12.86 ± 0*	
	44.908	Heneicosane	C21H44	296.6	6.16 ± 0*		5.1 ± 1.67		
	45.022	Isononacosane	C29H60	408.8	2.57 ± 0.84		1.27 ± 0*	6.81 ± 0*	
	45.619	4-Methyl-4-nonadecene	C20H40	280.6		1.52 ± 0.14			
	46.449	Docosane	C22H46	310.6		1.91 ± 0.08		3.89 ± 1.55	
	48.111	Tetratriacontane	C34H70	478.9			36.07 ± 35.22	110.49 ± 0*	
	49.802	3-Ethyl-2,6,10-trimethylundecane	C16H34	226.44		3.18 ± 0.5		5.76 ± 0*	5.65 ± 0.39
	51.572	Heneicosane	C21H44	296.6		7.73 ± 1.78			9.16 ± 0.23
	51.734	Nonacosane, 3-methyl-	C30H62	422.8	4.53 ± 0.92		5 ± 2.77	13.9 ± 0*	
	53.586	Tetracosane	C24H50	338.7	56.81 ± 11.32	42.14 ± 3.94			30.33 ± 2.64
	53.790	Tetratriacontane	C34H70	478.9	54.81 ± 1.91			11.92 ± 6.95	
	55.844	Nonacosane	C29H60	408.8			15.48 ± 10.16	2.22 ± 0*	
	56.301	1,3,5-tris(cyclohexyl)pent-1-ene	C23H40	316.6				2.05 ± 0*	
	57.503	Tetratriacontane	C34H70	478.9			25.21 ± 12.35	29.67 ± 12.58	
	57.528	Isononacosane	C29H60	408.8		13.91 ± 3.59	17.29 ± 0*		
	58.097	Tetracosane	C24H50	338.7	26.37 ± 1.18		19.74 ± 2.49	47.92 ± 10.76	
	58.723	Tetratetracontane	C44H90	619.2		152.68 ± 37.05			35.76 ± 2.09
Phenolic compounds	29.557	4-Vinylguaiacol	C9H10O2	150.17					4.18 ± 0.5

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
	33.392	Phenol, 4,6-di(1,1-dimethylethyl)-2-methyl-	C15H24O	220.35				9.19 ± 0*	
	33.993	2,4-Di-tert-butylphenol	C14H22O	206.32				5.36 ± 0.59	
	41.800	2,4-Dimethyl-6-(1-phenylethyl)phenol	C16H18O	226.31			3.39 ± 0*		
	43.785	2-Bromo-4-fluorophenol	C6H4BrFO	191				5.98 ± 0*	
	48.364	DL-α-tocopherol	C29H50O2	430.7			3.5 ± 1.37	15.46 ± 2.64	3.67 ± 0*
Terpene / Terpenoid	16.995	α-Terpinene	C10H16	136.32	0.56 ± 0.04	5.88 ± 1.77			
	17.201	D-Limonene	C10H16	136.23	69.76 ± 5.09	18.36 ± 7.92	1.85 ± 0.22	2.52 ± 0.11	1.57 ± 0.62
	17.592	Sabinene	C10H16	136.23	1.37 ± 0.04	77.88 ± 0.78			
	17.768	p-Cymene	C10H14	134.24	34.55 ± 2.37	68.77 ± 82.21	2.72 ± 1.99	3.6 ± 0.93	2.78 ± 0.13
	29.304	Caryophyllene	C15H24	204.35	1.26 ± 0.17	2.44 ± 0.81		2.38 ± 0.22	1.76 ± 0*
	32.861	trans-β-Ionone	C13H20O2	192.3	1.54 ± 0.06	3.44 ± 0.42	0.9 ± 0.34	3.34 ± 0.64	2.19 ± 0.76
	33.613	β-Ionone 5,6-epoxide	C13H20O2	208.3	0.49 ± 0*			1.88 ± 0*	
	37.431	Megastigmatrienone	C13H18O3	192.28					3.25 ± 0*
	37.567	Iolollide	C11H16O2	180.24		2.8 ± 0.4			
	37.896	Phytene-2	C20H40	280.5	2.64 ± 0.77	47.82 ± 3.88	8.38 ± 1.8	66.66 ± 11.7	18.05 ± 2.14
	38.136	Neophytadiene	C20H38	278.5	26.75 ± 12.15	718.25 ± 54.89	472.53 ± 96.88	781.2 ± 112.66	523.98 ± 43.17
	38.61	Phytol	C20H40O	296.5	1.8 ± 0.74	127.57 ± 1.25	227.38 ± 51.66	107.51 ± 15.68	181.49 ± 30.08
	39.124	Phytol	C20H40O	296.5	9.1 ± 1.56	226.72 ± 13.68	339.6 ± 74.21	213.63 ± 3.65	284.87 ± 32.71
	39.482	Menthyl acetate	C12H22O2	198.34			1.1 ± 0*	7.36 ± 0.07	

Type	RT	Name	Molecular formula	Molecular weight	Hexane	2-MTHF	Hexane / Ethanol	Ethyl acetate	Ethanol
	[min]			[g mol ⁻¹]			[mgNEQ kg _{dw} ⁻¹]		
Terpene / Terpenoid	39.854	3-Oxo- α -ionol	C13H20O2	208.33			4.6 $\pm$ 0.4	6.95 $\pm$ 0.84	
	39.954	Phytone	C18H36O3	268.5	2.51 $\pm$ 0.24	8.75 $\pm$ 1.31			7.16 $\pm$ 0.66
	40.115	β -Springene	C20H32	275.5		3.64 $\pm$ 0.5	1.75 $\pm$ 0.36	3.5 $\pm$ 0.34	2.83 $\pm$ 0*
	40.499	3-Hydroxy-5,6-epoxy- β -ionone	C13H20O3	224.3		4.02 $\pm$ 1.16		8.15 $\pm$ 0*	3.29 $\pm$ 0*
	41.211	α -Springene	C20H362	272.5			3.12 $\pm$ 1.12	11.83 $\pm$ 1.4	
	41.481	Isophytol	C20H40O	296.5			2.52 $\pm$ 0.78	2.1 $\pm$ 0*	
	44.369	Dehydrovomifoliol	C13H18O3	222.28		3.37 $\pm$ 0.44			8.65 $\pm$ 1.54
	44.622	Phytol	C20H40O	296.5		4.76 $\pm$ 0.47		7.64 $\pm$ 0*	28.83 $\pm$ 8.95
	45.124	Phytol	C20H40O	296.5		94.21 $\pm$ 7.18	7.85 $\pm$ 5.31	32.04 $\pm$ 2.53	237.15 $\pm$ 20.24
	45.160	Dehydrovomifoliol	C13H18O3	222.28			1.12 $\pm$ 0*	9.72 $\pm$ 0*	
	46.386	Phytyl acetate	C22H42O2	338.6	4.5 $\pm$ 0*	2.63 $\pm$ 0.14	2.89 $\pm$ 0.73	3.18 $\pm$ 0.35	2.85 $\pm$ 0.37
	46.747	Linalyl isovalerate	C15H26O2	238.37		5.13 $\pm$ 0.73	1.83 $\pm$ 0.41		5.74 $\pm$ 0.71
	46.783	Geranyllinalool	C20H34O	290.5				4 $\pm$ 0*	
	47.5	Lanostan-3 β -ol, 11 β ,19-epoxy-	C30H52O2	444.82		2.35 $\pm$ 0*	3.45 $\pm$ 0*		
	47.533	β -Sitosterol	C29H50O	414.79		7.05 $\pm$ 0*			
	48.219	β -Ocimene	C10H16	136.32			1.15 $\pm$ 0*	45.1 $\pm$ 30.42	
	48.781	cis-(Z)- α -Bisabolene epoxide	C15H24O	220.35			3.82 $\pm$ 1.38		

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Terpene / Terpenoid	49.175	Phytyl acetate	C22H42O2	338.6	2.94 ± 1.05	3.33 ± 0.23	3.15 ± 0.68	8.02 ± 2.66	4.17 ± 0.16
	49.95	Tetrahydropyranyl ether of citronellol	C15H28O2	240.43		5.02 ± 0*		6.36 ± 1.21	
	51.211	Lupeol	C30H50O	426.7					3.06 ± 0*
	51.395	Lupeol	C30H50O	426.7		7.54 ± 1.4			35.56 ± 8.88
	51.917	(3.α.)-12-Oleanen-3-yl acetate	C32H52O2	468.84		9.66 ± 0*			
	52.407	Aplotaxene	C17H28	232.4		1.55 ± 0.12			
	52.715	DL-Isopulegol	C10H18O2	170.28		16.04 ± 0.73			
	56.517	Phytol	C20H40O	296.5					
	57.325	Squalene	C30H50	410.7		8.85 ± 0*			19.07 ± 14.14
Uncategorized	6.004	2-Butanone	C4H8O	72.11				3.32 ± 0.31	
	7.668	Isovaleral	C5H10O2	102.13					6.72 ± 0*
	7.79	Butanal, 2-methyl-	C5H10O	86.15					4.18 ± 0*
	8.306	Allyl acetate	C5H8O2	100.12		18.96 ± 3.96			
	8.313	Allyl acetate	C5H8O2	100.12		3.41 ± 0.95			
	8.627	Silane, diethoxydimethyl-	C6H16O2Si	148.28		6.54 ± 0.3	2.98 ± 0*	32.3 ± 0*	
	9.434	Acetol	C3H6O2	74.08					1.26 ± 0*
	10.327	Isoamyl alcohol	C5H12O	88.17					1.55 ± 0*
	10.978	Silane, dimethoxydimethyl-	C4H12O2Si	120.25		6.26 ± 0.96			
	11.371	Acetic acid, butyl ester	C6H12O2	116.16		6.89 ± 0.76			
	11.639	Hexanal	C6H12O	100.16		1.52 ± 0.5	1.57 ± 0*	2.36 ± 0.27	

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
Uncategorized	11.979	Dihydroxyacetone	C3H6O3	90.09		7.08 ± 0*		3.2 ± 0*	2.39 ± 0.57
	12.630	Phenelzine	C8H12N2	136.19	1.25 ± 0*		18.56 ± 0*	1.5 ± 0*	
	13.854	Disiloxane, 1,3-diethoxy-1,1,3,3-tetramethyl-	C8H22O3Si2	222.43				3.92 ± 0*	
	14.027	[S-(R*,R*)]-2,3-Butanediol	C4H10O2	90.14				1.72 ± 0.04	1.03 ± 0*
	14.161	2-Hexenal	C6H10O	98.16	0.88 ± 0.19	1.29 ± 0*		2.89 ± 0.32	
	14.25	Leaf alcohol	C6H12O	100.18				1.44 ± 0*	
	14.363	[R-(R*,R*)]-2,3-Butanediol	C4H10O2	90.14					1.52 ± 0*
	14.464	1-Hexanol	C6H14O	102.2		2.85 ± 0.35			
	14.482	2-Nonen-1-ol	C9H18O	142.27					
	14.699	Butane, 1,1-diethoxy-3-methyl-	C9H20O2	160.25					
	14.851	Diacetone alcohol	C6H12O2	116.16	0.66 ± 0*			2.07 ± 0.08	
	15.655	Furfuryl alcohol	C5H6O2	98.11					1.35 ± 0.13
	15.786	Oxetane, 2,4-dimethyl-, trans-	C5H10O	86.15		1.55 ± 0			
	16.17	Pentane, 1,1-diethoxy-	C9H20O2	160.29					
	16.308	2-Butanone	C4H8O	72.11		8.35 ± 0.6			
	16.562	2-Butanol, 3-methyl-	C5H12O	88.15		5.14 ± 4.23		2.06 ± 0*	
	16.873	Cyclohexane, isobutyl-	C10H20	140.24		6.11 ± 0*		1.9 ± 0.16	
	17.968	Isocitric lactone	C6H6O6	174.12		108.09 ± 74.4			
	18.075	AMG-C16	C20H42O3	330.62		24.8 ± 15.64			
	18.292	1,3-Butanediol, (S)-	C4H10O2	90.14		394.59 ± 17.19			
	18.492	Pentanal, 2-methyl-	C6H12O	100.18		208.3 ± 58.41			
	18.843	2H-Pyran-2-methanol, tetrahydro-	C6H12O2	116.16		146.51 ± 61.62			

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
Uncategorized	18.925	Dianhydrogalactitol	C6H10O4	146.16				3.11 ± 0*	3.16 ± 0*
	19.017	Diisobutyl cellosolve	C10H22O2	174.32		289.21 ± 0*			
	19.171	Tetrahydro-2H-pyran-2-carboxylic acid	C6H10O3	130.139		441.83 ± 62.1			
	19.206	Hexane, 1,1-diethoxy-	C10H22O2	174.32					1.16 ± 0*
	19.425	(E,E)-2,4-Heptadienal	C7H10O	110.17		11.45 ± 0*			
	19.658	Trimethylene acetate	C7H12O4	160.17		113.09 ± 20.69	0.88 ± 0*		
	20.428	3-Hexanone, 5-hydroxy-2-methyl-	C7H14O2	130.21		1.34 ± 0.16			
	20.447	2-Methyliminoperhydro-1,3-oxazine	C5H10N2O	114.17					4.78 ± 0.01
	20.569	Citraconic anhydride	C5H4O3	112.09					5.44 ± 0*
	20.708	Dihydroxyacetone	C3H6O3	90.09		1.23 ± 0*			
	20.848	2-Pentanone, 4-hydroxy-	C5H10O2	102.13		1.33 ± 0.28			
	20.903	Acetic acid, heptyl ester	C9H18O2	158.24		8.98 ± 0.42			
	21.128	3,3-Dimethoxy-2-butanone	C6H12O3	132.18		3.45 ± 0*			
	21.282	Benzeneacetaldehyde	C8H8O	120.16		2.25 ± 0*			
	21.386	1,2-Dichlorooctane	C8H16Cl2	183.14					
	21.74	Butane, 1-cyclopropylidene-5-(tetrahydro-2H-pyran-2-yloxy)-	C12H20O2	196.32		3.05 ± 0*			
	21.814	Benzyl alcohol	C7H8O	108.15					
	21.847	Diallyl methyl carbinol	C8H14O	126.22		1.16 ± 0*			
	22.045	Diallyl methyl carbinol	C8H14O	126.22		1.26 ± 0*			
	22.472	Bioxane	C10H18O2	170.28		2.29 ± 0*			
	22.598	Furaneol	C6H8O3	128.14					3.4 ± 0*
	22.793	Cyclohexanol, 2,6-dimethyl-	C8H16O	128.21	1.13 ± 0*	1.92 ± 0.12		3.72 ± 0*	

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
Uncategorized	22.817	1-Methylcycloheptanol	C8H16O	128.21					
	23.115	2-Pentanone, 5-(acetyloxy)-	C7H14O3	144.17		1.66 ± 0.31			
	23.297	Glycerin	C3H8O3	92.09		46.92 ± 11.01			39.84 ± 8.52
	23.398	Diallyl methyl carbinol	C8H14O	126.22		3.03 ± 0*			
	23.548	Glycerin	C3H8O3	92.09				7.57 ± 5.35	
	24.058	Aldol	C4H8O2	88.12		5.84 ± 1.62			
	24.130	Violet leaf aldehyde	C9H14O	138.21			2.37 ± 1.69		
	24.462	1-Ethyl-2-pyrrolidinone	C6H11NO	113.16	2.52 ± 0.33	4.78 ± 0.28	3.35 ± 0.83	2.63 ± 0.62	
	24.817	γ-Lactam	C4H7NO	85.1			2.16 ± 0*		7.53 ± 0.6
	24.95	2-Propanol, 1-propoxy-	C6H14O2	118.2		1.21 ± 0*			
	25.394	3'-Methylacetophenone	C9H10O	134.17				1.56 ± 0*	
	25.912	1,4-Butanediol, diacetate	C8H14O4	174.19		3.98 ± 0.81			
	26.245	5-Hydroxypentyl acetate	C7H14O3	146.21		1.66 ± 0.41		8.53 ± 2.2	
	26.395	Acetylacetone	C5H8O2	100.13		9.42 ± 0.33			
	28.171	Isovalerylcyanid	C6H9NO	111.14		2.9 ± 0.51	10.93 ± 6.97		15.63 ± 0.68
	28.274	Diallyl methyl carbinol	C8H14O	126.22		23.82 ± 19.49			
	28.57	2-Ethyl-3-methylmaleimide	C7H9NO2	139.15		2.16 ± 0.26			
	29.175	3,7-Dimethyloct-6-ene-1,2,3-triol	C10H20O3	188.26				9.34 ± 0*	
	29.217	Butoxyethoxyethyl acetate	C10H20O4	204.26		1.72 ± 0*			
	29.527	3-Octyn-2-ol	C8H14O	126.22		2.98 ± 0.39			
	30.454	Isoamyl nitrite	C5H11NO2	117.17					

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
Uncategorized	30.546	<i>trans</i> -2-Heptenyl acetate	C9H16O2	156.22		11.26 ± 1.24			
	30.677	3-Methyl-4-nonanone	C10H20O	156.3					
	30.896	3-Hexenoic acid, 5-hydroxy-2-methyl-, [<i>R</i> *, <i>R</i> *-(<i>E</i>)]-	C8H14O3	158.19		19.38 ± 0*			
	30.997	Laurylalkohol	C12H26O	186.33	81.67 ± 0*	20.55 ± 1.07	2.04 ± 1.02		
	31.248	Dodecyl propyl ether	C15H32O	228.47		1.63 ± 0.36			
	31.369	Celestolide	C13H16O	188.26					
	31.403	Hexylene glycol diacetate	C10H18O4	202.28		280.19 ± 33.59			
	32.359	3-Heptanol	C7H16O	116.23					3.51 ± 0.94
	32.827	Glycidyl isobutyl ether	C7H14O2	130.21					9.37 ± 0.36
	33.035	Diallyl methyl carbinol	C8H14O	126.22		1.34 ± 0*		1.72 ± 0*	
	34.865	1[5'-(Hydroxymethyl)furfuryl]pyrrolidine	C10H15NO2	181.26				11.91 ± 0*	4.8 ± 0*
	34.976	Silane, triethyl-1-pentenyl-	C11H24Si	184.39			2.63 ± 0.84	10.69 ± 0*	4.91 ± 0*
	35.459	Hexahydrofarnesol	C15H32O	228.41		6.16 ± 0.54	1.73 ± 0.66	4.71 ± 0.27	3.47 ± 0.3
	35.757	D-Allose	C6H12O6	180.16				3.09 ± 0.25	8.37 ± 0.21
	36.648	Hexahydrofarnesol	C15H32O	228.41		6.2 ± 1.61			1.71 ± 0*
	36.712	Diethyl Phthalate	C12H14O4	222.24			0.69 ± 0*	7.29 ± 0*	
	36.717	2-Heptanone, 3-propylidene-	C10H18O	138.28		1.85 ± 0*			
	36.925	Lauryl glycidyl ether	C15H30O2	242.4			0.72 ± 0.09	9.78 ± 1.09	
	37.345	Hexadecanal	C16H32O	240.42			5.29 ± 3.1	5.31 ± 2.7	
	37.498	Myristaldehyde	C14H28O	212.37				3.5 ± 0.94	2.33 ± 0.77
	37.649	Phytene-2	C20H40	280.5	1.37 ± 0.46	22.68 ± 1.49	3.94 ± 0.97	35.68 ± 5.58	8.4 ± 0.88
	37.690	1,7-Di-iso-propylnaphthalene	C16H20	212.33				3.78 ± 0*	

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
Uncategorized	38.475	α-Lactose	C12H22O11	342.34		9.05 ± 0.23			
	38.887	Levoglucosan	C6H10O5	162.14		6.63 ± 0.75		4.78 ± 0*	
	38.98	D-Allose	C6H12O6	180.16		2.53 ± 0*		10.26 ± 0*	63.71 ± 4.41
	39.225	2 <i>H</i> -Indeno[1,2- <i>b</i>]furan-2-one, 3,3a,4,5,6,7,8,8b-octahydro-8,8-dimethyl	C13H18O2	206.31	1.21 ± 0*		1.91 ± 0.7	5.59 ± 0.66	3.84 ± 0*
	39.344	1,2,3,4,5,6,7,8-Octahydro-2-naphthol, 4-methylene-2,5,5-trimethyl-	C14H22O	206.36		3.04 ± 1.02	4.61 ± 0*		3.72 ± 0*
	40.26	Ethanol, 2-(1-methylethoxy)-, acetate	C7H14O3	146.21				4 ± 0.39	2.2 ± 0*
	41.87	Uracil	C4H4N2O2	112.09	1.02 ± 0.1	2.97 ± 0.54		2.25 ± 0.06	9.83 ± 1.5
	41.913	Diisobutyl phthalate	C16H22O4	278.34	1.01 ± 0.37		1.96 ± 1.15	4.1 ± 1.51	
	42.179	1,6-Anhydro-β-D-glucofuranose	C6H10O5	162.16					1.72 ± 0*
	42.49	1,6-Anhydro-α-D-galactofuranose	C6H10O5	162.16				83.09 ± 0*	4 ± 0*
	42.644	1,4-Benzodioxin-6-methanamine, 2,3-dihydro-N-(3-methoxypropyl)-	C13H19NO3	237.33					
	42.709	Hexacosane, 1-iodo-	C26H53I	492.6				216.3 ± 0*	
	42.795	β-D-Glucopyranoside, methyl	C7H14O6	194.21	438.26 ± 86.31	2.9 ± 0.47		124.98 ± 70.64	7.52 ± 0.84
	42.989	Anthracene, 9-methyl-	C15H12	192.27				2.71 ± 0*	
	43.629	5,7-Octadien-2-one, 3-acetyl-	C10H14O2	166.24		1.47 ± 0.07			
	43.828	<i>cis,cis,cis</i> -7,10,13-Hexadecatrienal	C16H26O	234.42					
	43.891	Oleyl alcohol	C18H36O	268.5		1.77 ± 0.24			
	43.92	Hexahydrofarnesol	C15H32O	228.41					7.82 ± 0.44

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
Uncategorized	44.436	Hexahydrofarnesol	C15H32O	228.41			1.46 ± 0*		19.73 ± 3.49
	44.444	Adenine	C5H5N5	135.15		3.92 ± 0.78		4.98 ± 0*	11.7 ± 0.36
	44.976	5,9,13,17-Tetramethyl 4,8,12,16-octadecatetraenoic acid	C22H36O2	332.5	3.98 ± 0*		2.68 ± 1.13	4.32 ± 0*	
	45.027	1-Methyl-1-(3-methylbutyl)oxy-1-silacyclobutane	C9H20OSi	172.38		1.17 ± 0*			4.39 ± 0*
	45.33	Oxazole, 4,5-dihydro-2-pentadecyl-	C18H35NO	281.54		1.79 ± 0*	4.65 ± 0*	10.99 ± 3.41	
	45.411	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	C17H24O3	276.4			2.74 ± 0*	3.84 ± 0*	
	45.507	6-Hydroxy-4,4,7a-trimethyl-5,6,7,7a-tetrahydrobenzofuran-2(4H)-one	C11H16O3	196.24			5.65 ± 0.07	10.63 ± 0*	
	46.231	Trioctylamine	C24H51N	353.7	0.85 ± 0.04		0.98 ± 0*		
	46.505	Cyclopentanone, 2-octadecyl-	C23H44O	336.6			2.05 ± 0*	4.48 ± 0.1	
	47.025	3-(4-Hydroxy-5,7-dimethyl-3-methylene-2-oxo-3,3a,4,5,8,8a-hexahydro-2H-cyclohepta[b]furan-6-yl)propyl acetate	N.A.	N.A.-					
	47.413	Dihomo-linolenic acid	C20H34O2	306.54					
	47.872	2-(Dimethylamino)ethyl vaccenoate	N.A.	N.A.-		9.12 ± 7.5			22.98 ± 2.7
	48.083	Clionasterol	C29H50O	414.79		7.06 ± 0*			40.47 ± 8.01
	48.162	Behenic alcohol	C22H46O	326.68		15.22 ± 1.25			19.64 ± 2.45
	48.344	(-)-Neoclovene-(I), dihydro-	C15H22	202.37	7.39 ± 6.81		9.72 ± 0.23	8.59 ± 0*	
	48.509	Gleenol	C15H26O	222.37			2.74 ± 0.07		
	48.715	((8Z,11Z)-2-Heptadeca-8,11-dienyl)-4,5-dihydro-oxazole	C20H35NO	305.5	0.8 ± 0*	2.95 ± 0.83		11.92 ± 0*	6.7 ± 1.2
	48.95	Stearamide	C18H37NO	283.56		2.17 ± 0.41	1.93 ± 0.02	4.24 ± 0*	13.46 ± 0*

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
Uncategorized	49.092	1,5-Naphthalenediol, decahydro-	C10H18O2	170.28					
	49.351	E-11-Hexadecenal	C16H30O	238.46		23.71 ± 2.13			16.16 ± 1.55
	49.683	cis-9-Hexadecenal	C16H30O	238.41	66.62 ± 12.38	3.82 ± 0.63	29.79 ± 1.72	94.18 ± 9.33	4.05 ± 0.34
	50.118	Fucosterol	C29H48O	412.77	1.85 ± 0.12	9.51 ± 0*	7.92 ± 1.26	5.94 ± 2.76	14.29 ± 0*
	50.294	(Z)-9-Octadecenal	C18H34O	266.5		9.74 ± 0*	3.82 ± 1.5	7.65 ± 0.55	
	50.426	Fucosterol	C29H48O	412.77		2.39 ± 0*		1.1 ± 0*	15.94 ± 5.65
	51.062	Icosanal	C20H40O	296.5		2.46 ± 0.33			6.97 ± 1.28
	51.314	1-Methoxy-3-(trimethylsilyloxymethyl)nonane	C14H32O2Si	260.49		7.33 ± 0*		5.22 ± 0*	
	51.676	Behenic alcohol	C22H46O	326.68		10.05 ± 1.24			24.07 ± 9.79
	52.155	Nonadecanenitrile	C19H37N	279.57	1.21 ± 0*				
	52.955	2-(Dimethylamino)ethyl vaccenoate	N.A.	N.A.-					
	53.378	[1,2,4]Triazolo[3,4-b][1,3,4]thiadiazole, 3-methyl-6-tricyclo[3.3.1.1(3,7)]dec-1-yl-	C14H18N4S	274.39			1 ± 0.03	21.75 ± 0*	
	53.379	Heptacosyl acetate	C29H58O2	438.8					7.01 ± 0*
	53.745	1-Heptacosanol	C27H56O	396.67	14.84 ± 0*				
	53.931	Palmitoyl chloride	C16H31ClO	274.9					
	54.777	Henicosanal	C21H42O	310.6		1.32 ± 0.04		22.75 ± 15.11	
	55.558	Cycloheptadecanol	C17H34O	254.51					
	56.128	1-Tricosanol	C23H48O	340.71		3.55 ± 0.3			
	56.168	1-Heptacosanol	C27H56O	396.67		3.02 ± 0*			6.49 ± 0.12

Type	RT [min]	Name	Molecular formula	Molecular weight [g mol ⁻¹]	Hexane	2-MTHF	Hexane / Ethanol [mgNEQ kg _{dw} ⁻¹]	Ethyl acetate	Ethanol
Uncategorized	57.175	Stigmasterol	C29H48O	412.77		4.03 ± 1.48			15.16 ± 0*
	57.276	Stigmasterol	C29H48O	412.77		12.2 ± 3.16			21.62 ± 0*
	57.416	Hexacosanal	C26H52O	380.7		4.73 ± 1.33			15.14 ± 0*
	57.578	1-Hydroxy-2-(2,3,4,6-tetra-O-acetyl-β-d-glucopyranosyl)-9H-xanthene-3,6,7-triyl triacetate	C33H34O18	718.6			5.49 ± 0*		9.82 ± 2.29