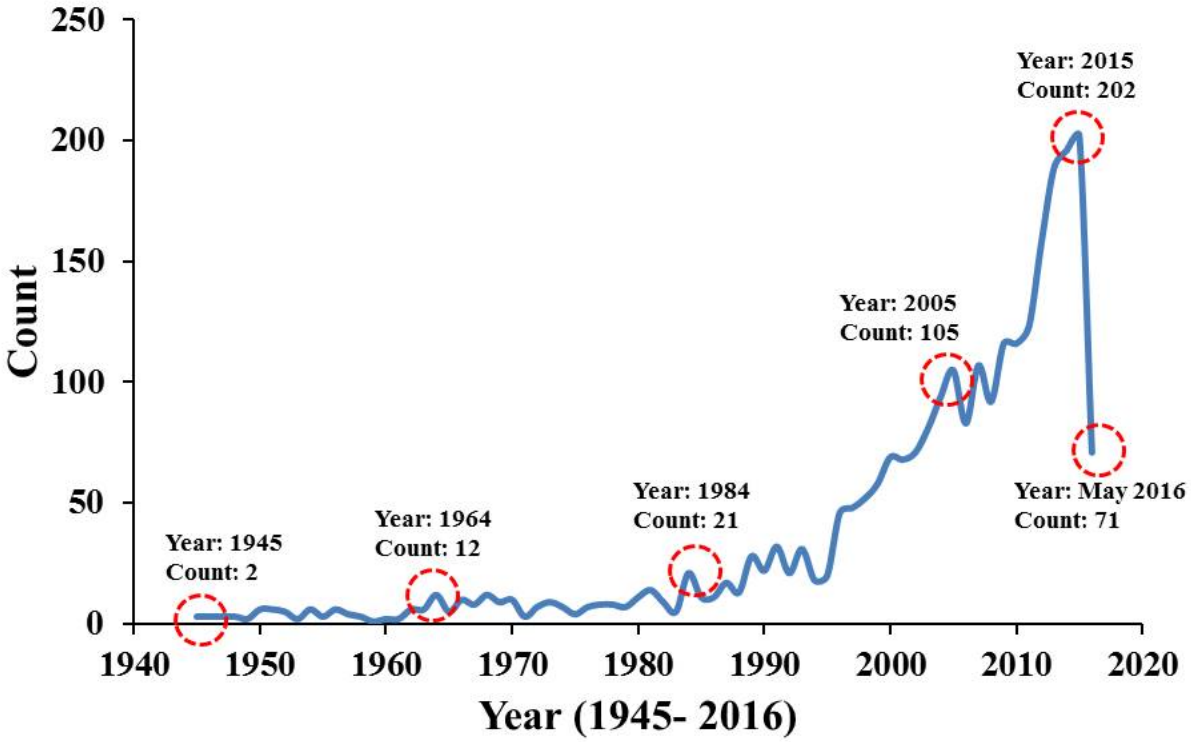
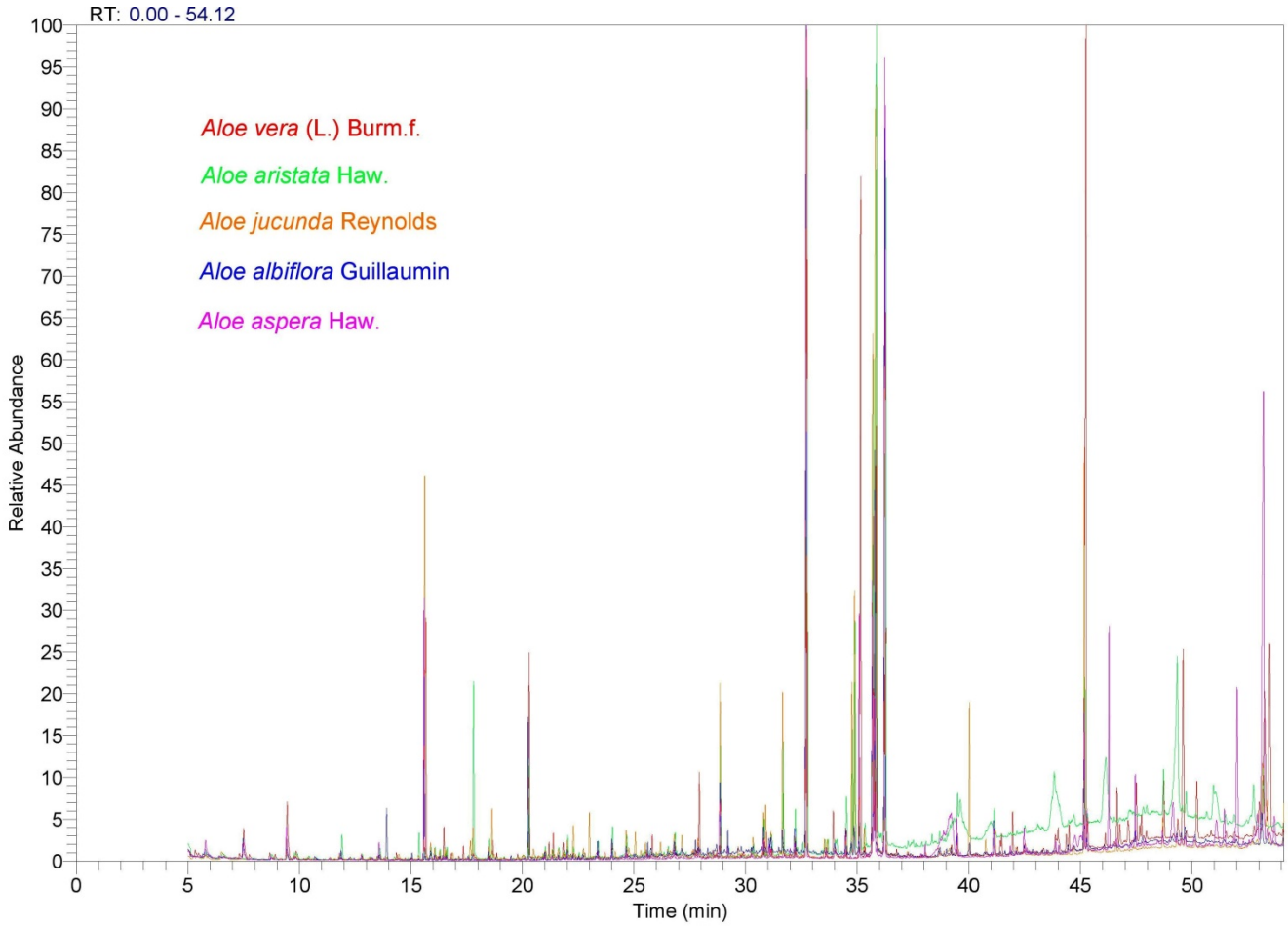
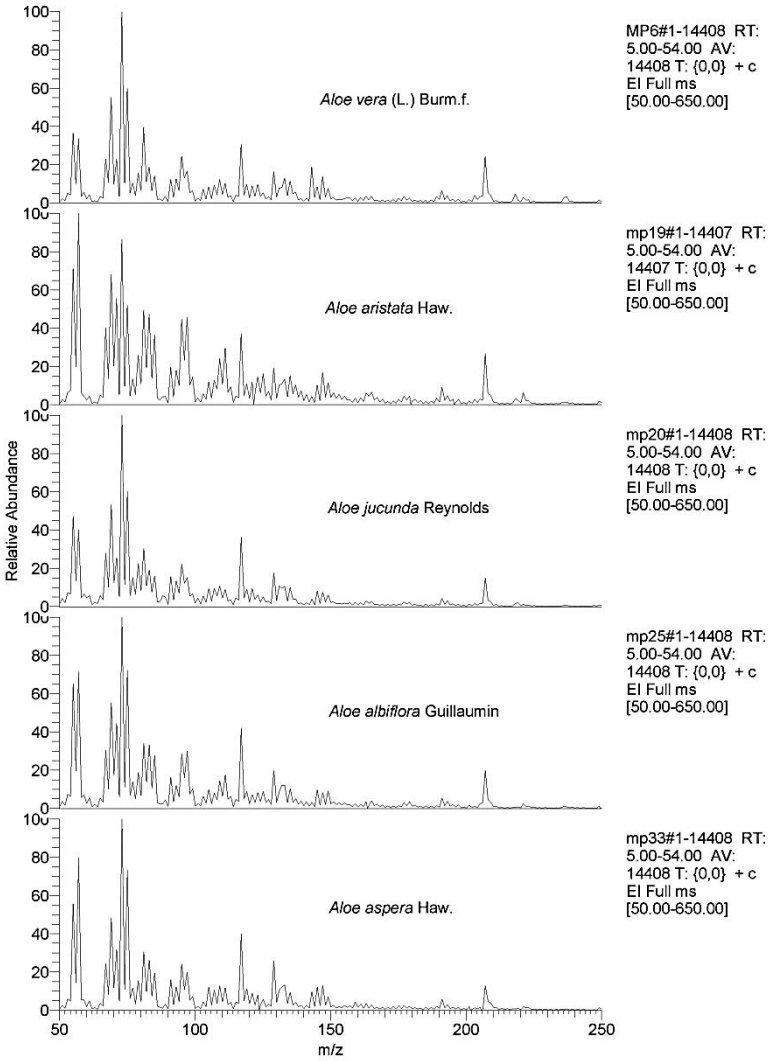
Supplementary Data



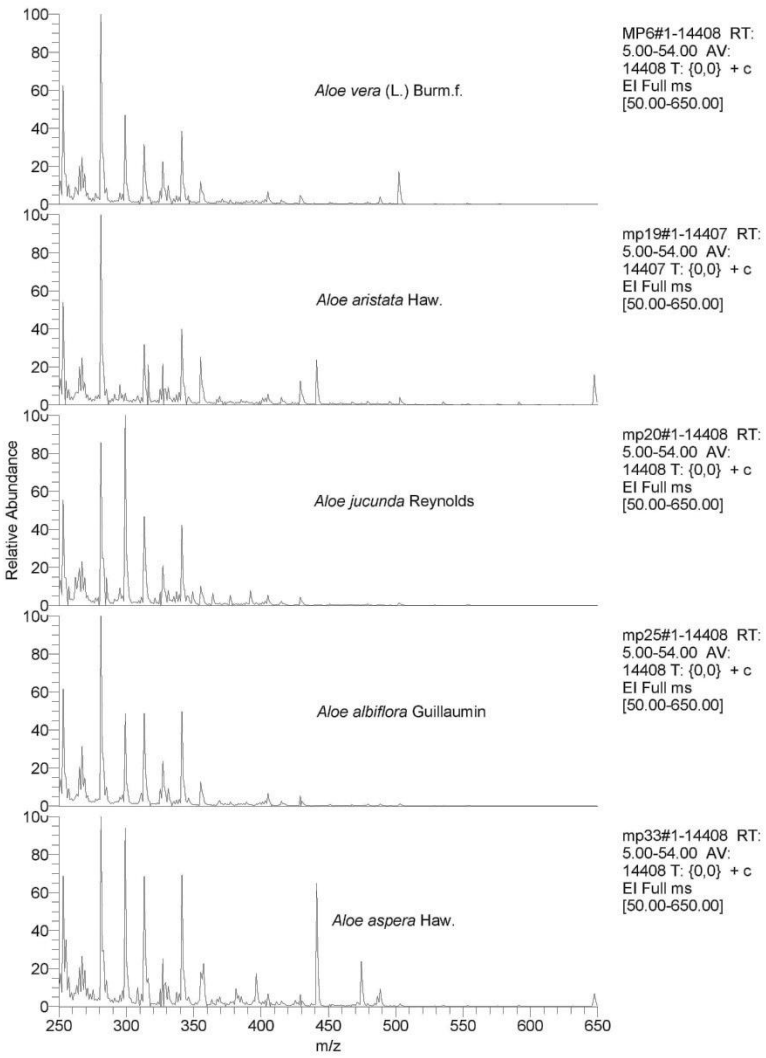
Supplementary figure 1: The global trend of increased count in research on *Aloe vera*. The graphical representation is based on data collected from 'results by year' option of the PubMed database with the keyword '*Aloe vera*'.



Supplementary figure 2: All GC chromatograms merged.



Supplementary figure 3: Total mass fragment details (50-250 amu)



Supplementary figure 4: Total mass fragment details (250-650 amu)

Phytochemicals identified in *Aloe vera* (L.) Burm.f.

Compound name	**Formula**	**[M-H]$^-$**	**Identifying mass fragments**	**Retention time**	**Relative abundance[#]**
Ethylene glycol, di-TMS	$C_8H_{22}O_2Si_2$	205	191 ($C_7H_{19}O_2Si_2$), 147* ($C4H_{11}O_2Si_2$), 103 ($C4H_{11}OSi$)	7.31	0.94 ± 0.16
Propylene glycol, di-TMS	$C_9H_{24}O_2Si_2$	219	147 ($C_6H_{15}O_2Si$), 117* ($C_5H_{13}OSi$)	7.76	0.88 ± 0.12
Butane, 2,3-bis(trimethylsiloxy)-	$C_{10}H_{26}O_2Si_2$	233	147 ($C_6H_{15}O_2Si$), 117* ($C_5H_{13}OSi$)	8.68	1.06 ± 0.22
Glycolic acid, di-TMS	$C_8H_{20}O_3Si_2$	219	147* ($C_5H_{11}O_3Si$)	9.85	1.48 ± 0.35
Octadecane, 6-methyl-	$C_{19}H_{40}$	267	98* (C_7H_{14})	13.16	0.55 ± 0.08
4-Ethylbenzaldehyde	$C_9H_{10}O$	133*	119 (C_8H_7O), 105 (C_8H_9)	13.62	0.86 ± 0.18
4-Hydroxybutyric acid, diTMS	$C_{10}H_{24}O_3Si_2$	247	147* ($C_3H_7O_3Si_2$), 117 ($C_4H_9O_2Si$)	14.35	1.38 ± 0.35
Benzoic acid, TMS	$C_{10}H_{14}O_2Si$	193	179 ($C_9H_{11}O_2Si$), 105* (C_7H_5O)	14.50	0.48 ± 0.07
(±)-2-Hydroxyoctanoic acid, trimethylsilyl ester	$C_{11}H_{24}O_3Si$	231	117 ($C_4H_9O_2Si$), 97 (C_7H_{13}), 73* (C_3H_9Si)	14.74	0.51 ± 0.12
Octanoic acid, TMS ester	$C_{11}H_{24}O_2Si$	215	201* ($C_{10}H_{21}O_2Si$), 145 ($C_8H_{17}O_2$)	15.01	0.52 ± 0.06
Phosphoric acid, triTMS	$C_9H_{27}O_4PSi_3$	313	299* ($C_8H_{24}O_4PSi_3$), 211 ($C_5H_{16}O_3PSi$)	15.67	29.34 ± 2.29
Succinate, bis-TMS	$C_{10}H_{22}O_4Si_2$	261	147* ($C_6H_{15}O_2Si$)	16.48	5.02 ± 0.84
Methyl succinic acid, bis-TMS	$C_{11}H_{24}O_4Si_2$	275	147* ($C_6H_{15}O2Si$)	16.82	0.94 ± 0.25
Glyceric acid, (3TMS)	$C_{12}H_{30}O_4Si_3$	321	189 ($C_7H_{17}O_2Si_2$), 147 ($C_5H_{11}O_3Si$), 73* (C_3H_9Si)	17.15	0.74 ± 0.28
Fumaric acid, bis-TMS ester	$C_{10}H_{20}O_4Si_2$	259	245* ($C_9H_{17}O_4Si_2$), 147 ($C_6H_{13}O2Si_2$)	17.35	1.85 ± 0.49

Nonanoic acid, TMS ester	$C_{12}H_{26}O_2Si$	229	215* ($C_{11}H_{23}O_2Si$), 117 ($C_4H_9O_2Si$)	17.60	0.51 ± 0.12
Phenol, 2-methoxy-3-(2-propenyl)-	$C_{10}H_{12}O_2$	163*	149 ($C_9H_9O_2$), 131 (C_9H_7O)	17.82	0.98 ± 0.24
Tetradecane	$C_{14}H_{30}$	197	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	18.54	0.82 ± 0.35
Methyleugenol	$C_{11}H_{14}O_2$	177*	163 ($C_{10}H_{11}O_2$), 147 ($C_{10}H_{11}O$)	18.67	2.59 ± 0.52
Glutarate, bis-TMS	$C_{11}H_{24}O_4Si_2$	275	204 ($C_8H_{16}O_4Si$), 158 ($C_7H_{14}O_2Si$), 147* ($C_6H_{15}OSi$)	18.85	0.96 ± 0.27
1-Dodecanol, O-TMS	$C_{15}H_{34}OSi$	257	243* ($C_{14}H_{31}OSi$)	19.78	0.88 ± 0.24
4-Allyl-2-methoxyphenoxy-TMS	$C_{13}H_{20}O_2Si$	235	206* ($C_{11}H_{14}O_2Si$), 179 ($C_9H_{11}O_2Si$)	20.30	25.26 ± 2.29
β-copaene	$C_{15}H_{24}$	203	161* ($C_{12}H_{17}$), 119 (C_6H_{13}), 105 (C_7H_{15})	20.59	0.47 ± 0.05
Malic acid, tris-TMS	$C_{13}H_{30}O_5Si_3$	349	245 ($C_9H_{17}O_4Si_2$), 233 ($C_9H_{21}O_3Si_2$), 147 ($C_8H_{22}O_2Si_2$), 73* (C_3H_9Si)	21.20	2.53 ± 0.34
Adipic acid, (2TMS)	$C_{12}H_{26}O_4Si_2$	289	141 ($C_7H_{13}OSi$), 111 ($C_6H_7O_2$), 73* (C_3H_9Si)	21.38	3.36 ± 0.68
2-methyl-1-Hexadecanol	$C_{17}H_{36}O$	255	69 (C_5H_9), 57* (C_4H_9)	21.64	0.98 ± 0.20
Pyroglutamic acid, bis(trimethylsilyl)-	$C_{11}H_{23}NO_3Si_2$	272	156* ($C_7H_{14}NOSi$)	21.82	2.28 ± 0.47
m-Hydroxybenzoic acid, (TMS)	$C_{13}H_{22}O_3Si_2$	281	267* ($C_{12}H_{19}O_3Si_2$), 193 ($C_{10}H_{13}O_2Si$)	22.78	1.01 ± 0.12
Pimelic acid, bis-TMS	$C_{13}H_{28}O_4Si_2$	303	155 ($C_8H_{15}OSi$), 125 ($C_7H_9O_2Si$), 73* (C_3H_9Si)	23.69	1.14 ± 0.18
Dodecanoic acid, 1-methylethyl ester	$C_{15}H_{30}O_2$	241	102 ($C_5H_{10}O_2$), 60* (C_3H_8O)	24.04	2.24 ± 0.56
4-Hydroxybenzoic acid (2TMS)	$C_{13}H_{22}O_3Si_2$	281	267* ($C_{12}H_{19}O_3Si_2$), 193 ($C_{10}H_{13}O_2Si$)	24.20	0.58 ± 0.33

Lauric acid (TMS)	$C_{15}H_{32}O_2Si$	271	257 ($C_{14}H_{29}O_2Si$), 117* ($C_4H_9O_2Si$)	24.68	2.16 ± 0.69
1-[(Trimethylsilyl)oxy]-2-methylanthraquinone	$C_{18}H_{18}O_3Si$	309	295* ($C_{17}H_{15}O_3Si$), 265 ($C_{16}H_{13}O_2Si$)	25.55	1.32 ± 0.43
Suberic acid (2TMS)	$C_{14}H_{30}O_4Si_2$	317	169 ($C_9H_{17}O_4Si$), 129 ($C_5H_9O_2Si$), 73* (C_3H_9Si)	25.81	3.36 ± 0.48
Geranyl isovalerate	$C_{15}H_{26}O_2$	237	121 (C_9H_{13}), 103 ($C_5H_{11}O_2$), 85* (C_5H_9O)	25.90	0.61 ± 0.15
Tetradecane, 2,6,10-trimethyl-	$C_{17}H_{36}$	239	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	26.85	2.12 ± 0.62
1,3-Benzenedicarboxylic acid, bis(trimethylsilyl) ester	$C_{14}H_{22}O_4Si_2$	309	295* ($C_{13}H_{19}O_4Si_2$), 221 ($C_{11}H_{13}O_3Si$)	27.79	2.38 ± 0.68
Azelaic acid, diTMS	$C_{15}H_{32}O_4Si_2$	331	201 ($C_{10}H_{21}O_2Si$), 129 ($C_5H_9O_2Si$), 73* (C_3H_9Si)	27.92	2.06 ± 0.41
Protocatechuic acid (TMS)	$C_{16}H_{30}O_4Si_3$	369	281 ($C_{13}H_{21}O_2Si_3$), 193 ($C_9H_{10}OSi$), 73* (C_3H_9Si)	28.53	1.49 ± 0.37
Tetradecanoic acid, TMS	$C_{17}H_{36}O_2Si$	299	285 ($C_{16}H_{33}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	28.89	8.36 ± 0.96
Sebacic acid (bis-TMS)	$C_{16}H_{34}O_4Si_2$	245	129 ($C_5H_9O_2Si$), 215 ($C_{12}H_{23}O_2Si$), 73* (C_3H_9Si)	29.90	13.63 ± 3.53
Pentadecanoic acid, TMS ester	$C_{18}H_{38}O_2Si$	313	299 ($C_{17}H_{35}O_2Si$), 117* (C4H9O2Si)	30.84	1.94 ± 0.42
Phenol, 2,4,6-tris(1,1-dimethylethyl)-	$C_{18}H_{30}O$	261	247* ($C_{17}H_{27}O$)	30.93	2.31 ± 0.45
Undecandioic acid di-TMS	$C_{17}H_{36}O_4Si_2$	359	345 ($C_{16}H_{33}O_4Si_2$), 229 ($C_{12}H_{25}O_2Si$), 73* (C_3H_9Si)	31.78	1.54 ± 0.28
Palmitelaidic acid, trimethylsilyl ester	$C_{19}H_{38}O_2Si$	325	311 ($C_{18}H_{35}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	32.24	1.36 ± 0.44
Palmitic acid, TMS	$C_{19}H_{40}O_2Si$	327	313 ($C_{18}H_{37}O_2Si$), 117 ($C_4H_9O_2Si$), 73*	32.76	71.74 ± 2.26

			(C_3H_9Si)		
Phytol	$C_{20}H_{40}O$	295	123 (C_9H_{15}), 71* (C_4H_7O)	33.93	5.27 ± 0.97
(2E)-3,7,11,15-Tetramethyl-2-hexadecenyl trimethylsilyl ether #	$C_{23}H_{48}OSi$	367	143* ($C_7H_{15}OSi$), 123 (C_9H_{15})	35.16	81.92 ± 1.52
Dodecanedioic acid di-TMS	$C_{18}H_{38}O_4Si_2$	373	359* ($C_{17}H_{35}O_4Si_2$), 243 ($C_{13}H_{27}O_2Si$), 129 ($C_5H_9O_2Si$)	35.35	1.55 ± 0.30
Linoleic acid, TMS	$C_{21}H_{40}O_2Si$	351	262 ($C_{18}H_{30}O$), 129 ($C_5H_9O_2Si$), 73* (C_3H_9Si)	35.72	40.06 ± 3.54
α-Linolenic acid, TMS	$C_{21}H_{38}O_2Si$	349	129 ($C_5H_9O_2Si$), 95 (C_7H_{11}), 73* (C_3H_9Si)	35.85	55.28 ± 1.72
Octadecanoic acid, TMS	$C_{21}H_{44}O_2Si$	355	341 ($C_{20}H_{41}O_2Si$), 117* ($C_4H_9O_2Si$)	36.28	63.51 ± 1.26
Eicosanoic acid, TMS ester	$C_{23}H_{48}O_2Si$	383	145 ($C_6H_{13}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	39.51	1.04 ± 0.20
2-Monopalmitoylglycerol trimethylsilyl ether	$C_{25}H_{54}O_4Si_2$	473	239 ($C_{16}H_{31}O$), 218 ($C_9H_{22}O_2Si_2$), 129* ($C_6H_{13}OSi$)	41.48	1.29 ± 0.42
1-Monopalmitin trimethylsilyl ether	$C_{25}H_{54}O_4Si_2$	473	313 ($C_{17}H_{33}O_3Si$), 218 ($C_9H_{22}O_2Si2$), 129* ($C_6H_{13}O$)	41.97	4.76 ± 0.74
Docosanoic acid, TMS ester	$C_{25}H_{52}O_2Si$	411	397 ($C_{24}H_{49}O_2Si$), 117* ($C_4H_9O_2Si$)	42.53	0.89 ± 0.26
9-Octadecenoic acid, 1,3-bis-(OTMS)-2-propyl ester	$C_{27}H_{56}O_4Si_2$	499	221 ($C_{16}H_{29}$), 203 ($C_8H_{19}O_2Si_2$), 73* (C_3H_9Si)	44.50	2.57 ± 0.54
Squalene	$C_{30}H_{50}$	409	81 (C_6H_9), 69* (C_5H_9)	45.25	98.26 ± 2.83
Tetracosanoic acid, trimethylsilyl ester	$C_{27}H_{56}O_2Si$	439	145 ($C_6H_{13}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	45.33	6.53 ± 0.44
Heptacosane	$C_{27}H_{56}$	379	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	48.74	8.76 ± 0.43
(+)-α-Tocopherol, O-	$C_{32}H_{58}O_2Si$	501*	277 ($C_{16}H_{25}O_2Si$), 237 ($C_{17}H_{33}$)	49.61	19.25 ± 1.06

trimethylsilyl-					
β-Sitosterol TMS	$C_{32}H_{58}OSi$	485	396 ($C_{29}H_{48}$), 255 ($C_{19}H_{27}$), 129* ($C_6H_{13}OSi$)	53.25	16.87 ± 0.82
β-Amyrin, TMS	$C_{33}H_{58}OSi$	487	218* ($C_{16}H_{26}$), 203 ($C_{15}H_{23}$)	53.49	23.48 ± 2.57

* = Base peak; # = Relative abundance after baseline normalization.

Phytochemicals identified in *Aloe aristata* Haw.

Compound name	Formula	$[M-H]^-$	Identifying mass fragments	Retention time	Relative abundance
Benzeneacetaldehyde	C_8H_8O	119	91* (C_7H_7)	8.77	0.46 ± 0.13
Lactic acid, bis-TMS	$C_9H_{22}O_3Si_2$	233	147 ($C_5H_{11}O_3Si$), 117 ($C_5H_{13}OSi$), 73* (C_3H_9Si)	9.46	0.38 ± 0.54
2-Undecanethiol, 2-methyl-	$C_{12}H_{26}S$	201	83 (C_6H_{11}), 69 (C_5H_9), 55* (C_4H_7)	9.79	0.94 ± 0.17
Benzaldehyde, 2,5-dimethyl-	$C_9H_{10}O$	133*	105 (C_8H_9)	13.62	1.12 ± 0.28
Phenol, 2-ethyl, TMS	$C_{11}H_{18}OSi$	193	179 ($C_{10}H_{15}OSi$), 103 ($C_4H_{11}OSi$), 73* (C_3H_9Si)	13.95	0.31 ± 0.06
3-Ethylphenol, trimethylsilyl ether	$C_{11}H_{18}OSi$	193	179* ($C_{10}H_{15}OSi$)	14.27	0.55 ± 0.12
p-Ethylguaiacol	$C_9H_{12}O_2$	151	137* ($C_8H_9O_2$), 122 ($C_7H_6O_2$)	15.37	1.58 ± 0.32
Phosphoric acid, triTMS	$C_9H_{27}O_4PSi_3$	313	299* ($C_8H_{24}O_4PSi_3$), 211 ($C_5H_{16}O_3PSi$)	15.62	1.27 ± 0.47
Tridecane	$C_{13}H_{28}$	183	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	15.90	1.31 ± 0.29
3-Eicosene, (E)-	$C_{20}H_{40}$	279	83 (C_6H_{11}), 69 (C_5H_9), 57* (C_4H_9)	16.08	1.26 ± 0.25
2-methyl-1-Hexadecanol	$C_{17}H_{36}O$	255	69 (C_5H_9), 57* (C_4H_9)	16.31	1.45 ± 0.61
Dodecane, 2,6,11-trimethyl-	$C_{15}H_{32}$	211	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	16.61	1.38 ± 0.34
Eugenol	$C_{10}H_{12}O_2$	163*	149 ($C_9H_9O_2$), 131 ($C_9H_7O_2$), 103	17.81	20.53 ± 1.55

			(C_7H_3O)		
Vanillin, TMS	$C_{11}H_{16}O_3Si$	223	209 ($C_{10}H_{13}O_3Si$), 194* ($C_9H_{10}O_3Si$)	18.53	2.29 ± 0.86
Methyleugenol	$C_{11}H_{14}O_2$	177*	163 ($C_{10}H_{11}O_2$), 147 ($C_{10}H_{11}O$)	18.66	1.01 ± 0.27
4-Allyl-2-methoxyphenoxy-TMS	$C_{13}H_{20}O_2Si$	235	206* ($C_{11}H_{14}O_2Si$), 179 ($C_9H_{11}O_2Si$)	20.28	10.14 ± 0.89
Hexadecane	$C_{16}H_{34}$	225	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	21.03	1.22 ± 0.42
Phenol, 2,4-bis(1,1-dimethylethyl)- (Antioxidant No. 33)	$C_{14}H_{22}O$	205	191* ($C_{13}H_{19}O$), 57 (C_4H_9)	21.36	1.26 ± 0.36
Nonadecane	$C_{19}H_{40}$	267	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	23.40	1.87 ± 0.28
Dodecanoic acid, 1-methylethyl ester	$C_{15}H_{30}O_2$	241	102 ($C_5H_{10}O_2$), 60* (C_3H_8O)	24.04	4.06 ± 0.69
Lauric acid (TMS)	$C_{15}H_{32}O_2Si$	271	257 ($C_{14}H_{29}O_2Si$), 117* ($C_4H_9O_2Si$)	24.68	3.12 ± 0.53
Tetradecane, 2,6,10-trimethyl-	$C_{17}H_{36}$	239	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	25.65	0.96 ± 0.08
Heptadecane, 2,6,10,15-tetramethyl-	$C_{21}H_{44}$	295	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	26.84	1.59 ± 0.26
Myristic acid, trimethylsilyl ester	$C_{17}H_{36}O_2Si$	299	285 ($C_{16}H_{33}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	28.88	13.72 ± 2.04
Pentadecanoic acid, TMS ester	$C_{18}H_{38}O_2Si$	313	299 ($C_{17}H_{35}O_2Si$), 117* ($C4H_9O_2Si$)	30.84	4.28 ± 0.59
Ethyl palmitate	$C_{18}H_{36}O_2$	283	157 ($C_9H_{17}O_2$), 101 ($C_5H_9O_2$), 88* ($C_4H_8O_2$)	31.69	14.23 ± 1.74
cis-9-Hexadecenoic acid, trimethylsilyl ester	$C_{19}H_{38}O_2Si$	325	311 ($C_{18}H_{35}O_2Si$), 145 ($C_6H_{13}O_2Si$), 117* ($C_4H_9O_2Si$)	32.24	6.58 ± 1.33

Palmitic acid, TMS	$C_{19}H_{40}O_2Si$	327	313 ($C_{18}H_{37}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	32.77	92.25 ± 3.52
cis-10-Heptadecenoic acid, trimethylsilyl ester	$C_{20}H_{40}O_2Si$	339	325* ($C_{19}H_{37}O_2Si$), 145 ($C_6H_{13}O_2Si$), 117 ($C_4H_9O_2Si$)	34.09	2.02 ± 0.46
Heptadecanoic acid, TMS	$C_{20}H_{42}O_2Si$	341	327 ($C_{19}H_{39}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	34.52	5.69 ± 0.85
9,12-Octadecadienoic acid, ethyl ester	$C_{20}H_{36}O_2$	307	95 (C_7H_{11}), 81 (C_6H_9), 67* (C_5H_7)	34.79	15.18 ± 0.78
Ethyl 9,12,15-octadecatrienoate	$C_{20}H_{34}O_2$	305	108 (C_8H_{12}), 95 (C_7H_{11}), 79* (C_6H_7)	34.91	28.66 ± 1.16
Linoleic acid, TMS	$C_{21}H_{40}O_2Si$	351	262 ($C_{18}H_{30}O$), 129 ($C_5H_9O_2Si$), 73* (C_3H_9Si)	35.72	58.24 ± 3.59
α-Linolenic acid, TMS	$C_{21}H_{38}O_2Si$	349	129 ($C_5H_9O_2Si$), 95 (C_7H_{11}), 73* (C_3H_9Si)	35.87	93.22 ± 2.48
Octadecanoic acid, TMS	$C_{21}H_{44}O_2Si$	355	341 ($C_{20}H_{41}O_2Si$), 117* ($C_4H_9O_2Si$)	36.28	81.87 ± 1.36
α-Amyrin	$C_{30}H_{50}O$	425	218* ($C_{16}H_{26}$), 203 ($C_{15}H_{23}$)	43.82	7.04 ± 0.92
Squalene	$C_{30}H_{50}$	409	81 (C_6H_9), 69* (C_5H_9)	45.20	18.48 ± 1.63
Ethyl iso-allocholate	$C_{26}H_{44}O_5$	435	253 ($C_{15}H_{25}O_3$), 129 ($C_7H_{13}O_2$), 107 (C_8H_{11}), 55* (C_3H_3O)	49.74	2.25 ± 0.55
β-Sitosterol TMS	$C_{32}H_{58}OSi$	485	396 ($C_{29}H_{48}$), 255 ($C_{19}H_{27}$), 129* ($C_6H_{13}OSi$)	53.19	7.21 ± 0.34

* = Base peak; # = Relative abundance after baseline normalization.

Phytochemicals identified in *Aloe jucunda* Reynolds

Compound name	Formula	$[M-H]^-$	Identifying mass fragments	Retention time	Relative abundance
Benzaldehyde	C_7H_6O	105	77* (C_6H_5)	6.52	0.48 ± 0.16
Lactic acid, bis-TMS	$C_9H_{22}O_3Si_2$	233	147 ($C_5H_{11}O_3Si$), 117 ($C_5H_{13}OSi$), 73* (C_3H_9Si)	9.42	0.96 ± 0.22
Phenol, 2-ethyl, TMS	$C_{11}H_{18}OSi$	193	179 ($C_{10}H_{15}OSi$), 103 ($C_4H_{11}OSi$), 73* (C_3H_9Si)	13.92	0.24 ± 0.07
Benzoic acid, TMS	$C_{10}H_{14}O_2Si$	193	179 ($C_9H_{11}O_2Si$), 105* (C_7H_5O)	14.46	0.39 ± 0.04
Octanoic acid, TMS ester	$C_{11}H_{24}O_2Si$	315	201* ($C_{10}H_{21}O_2Si$), 145 ($C_8H_{17}O_2$)	14.98	0.53 ± 0.08
Phosphoric acid, triTMS	$C_9H_{27}O_4PSi_3$	313	299* ($C_8H_{24}O_4PSi_3$), 211 ($C_5H_{16}O_3PSi$)	15.62	45.22 ± 2.58
Phenylacetic acid, monoTMS	$C_{11}H_{16}O_2Si$	208	193 ($C_{10}H_{13}O_2Si$), 91 (C_7H_7), 73* (C_3H_9Si)	15.88	1.68 ± 0.43
Benzene, 4-ethyl-1,2-dimethoxy-	$C_{10}H_{14}O_2$	165	151* ($C_9H_{11}O_2$), 135 ($C_9H_{11}O$), 95 (C_7H_{11})	16.52	1.27 ± 0.57
Benzaldehyde, 2-[(trimethylsilyl)oxy]-	$C_{10}H_{14}O_2Si$	193	179* ($C_9H_{11}O_2Si$), 161 ($C_9H_9O_2Si$), 149 ($C_8H_9O_2Si$)	16.88	0.79 ± 0.21
4-Vinylveratrole	$C_{10}H_{12}O_2$	163*	149 ($C_9H_9O_2$), 91 (C_7H_7)	17.67	1.37 ± 0.24
Eugenol	$C_{10}H_{12}O_2$	163*	149 ($C_9H_9O_2$), 131 ($C_9H_7O_2$), 103 (C_7H_3O)	17.78	1.85 ± 0.54
Tetradecane	$C_{14}H_{30}$	197	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	18.50	0.98 ± 0.16
Methyleugenol	$C_{11}H_{14}O_2$	177*	163 ($C_{10}H_{11}O_2$), 147 ($C_{10}H_{11}O$)	18.64	6.21 ± 0.78

2-Allyl-1,4-dimethoxy-3-methyl-benzene	$C_{12}H_{16}O_2$	191*	177 ($C_{11}H_{13}O_2$), 149 ($C_9H_9O_2$), 91 (C_7H_7)	19.49	0.34 ± 0.25
4-Allyl-2-methoxyphenoxy-TMS	$C_{13}H_{20}O_2Si$	235	206* ($C_{11}H_{14}O_2Si$), 179 ($C_9H_{11}O_2Si$)	20.26	14.89 ± 0.69
Nonadecane	$C_{19}H_{40}$	267	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	21.00	0.66 ± 0.16
Phenol, 3,5-bis(1,1-dimethylethyl)-	$C_{14}H_{22}O$	205	191* ($C_{13}H_{19}O$), 57 (C_4H_9)	21.33	0.58 ± 0.08
1,2-Dimethoxy-4-(2-methoxyethenyl)benzene	$C_{11}H_{14}O_3$	193*	179 ($C_{10}H_{11}O_3$), 151 ($C_9H_{11}O_2$), 91 (C_7H_7)	21.43	0.52 ± 0.12
1-Dodecanol, O-TMS	$C_{15}H_{34}OSi$	257	243* ($C_{14}H_{31}OSi$)	22.73	3.38 ± 0.75
Estragole	$C_{10}H_{12}O$	147*	133 (C_9H_9O), 121 (C_8H_9O), 77 (C_6H_5)	23.00	4.26 ± 0.59
Dodecanoic acid, 1-methylethyl ester	$C_{15}H_{30}O_2$	241	102 ($C_5H_{10}O_2$), 60* (C_3H_8O)	24.01	1.04 ± 0.18
4-Hydroxybenzoic acid (2TMS)	$C_{13}H_{22}O_3Si_2$	281	267* ($C_{12}H_{19}O_3Si_2$), 223 ($C_{11}H_3O2Si$), 193 ($C_{10}H_{13}O_2Si$)	24.16	0.65 ± 0.22
Lauric acid (TMS)	$C_{15}H_{32}O_2Si$	271	257 ($C_{14}H_{29}O_2Si$), 117* ($C_4H_9O_2Si$)	24.65	2.10 ± 0.46
β-bisabolol	$C_{15}H_{26}O$	221	204 ($C_{15}H_{24}$), 119 (C_9H_{11}), 93 (C_7H_9), 81* (C_6H_9)	25.06	1.87 ± 0.48
Tetradecane, 2,6,10-trimethyl-	$C_{17}H_{36}$	239	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	26.81	1.75 ± 0.27
Geranyl isovalerate	$C_{15}H_{26}O_2$	237	121 (C_9H_{13}), 103 ($C_5H_{11}O_2$), 85* (C_5H_9O)	27.14	2.04 ± 0.52
Tetradecanoic acid, (TMS)	$C_{17}H_{36}O_2Si$	299	285 ($C_{16}H_{33}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	28.85	21.22 ± 3.63
Benzoic acid, 3,5-bis(1,1-dimethylethyl)-	$C_{16}H_{24}O_3$	263	249* ($C_{15}H_{21}O_3$), 233 ($C_{15}H_{21}O_2$)	29.67	0.94 ± 0.20

4-hydroxy-, methyl ester					
Hexadecanoic acid, methyl ester	$C_{17}H_{34}O_2$	269	143 ($C_8H_{15}O_2$), 87 ($C_4H_7O_2$), 74* ($C_3H_6O_2$)	30.33	1.68 ± 0.56
Phenol, 2,4,6-tris(1,1-dimethylethyl)-	$C_{18}H_{30}O$	261	247* ($C_{17}H_{27}O$)	30.90	6.24 ± 0.21
Ethyl palmitate	$C_{18}H_{36}O_2$	283	157 ($C_9H_{17}O_2$), 101 ($C_5H_9O_2$), 88* ($C_4H_8O_2$)	31.66	19.08 ± 2.57
Palmitelaidic acid, trimethylsilyl ester	$C_{19}H_{38}O_2Si$	325	311 ($C_{18}H_{35}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	32.20	2.48 ± 0.85
Palmitic acid, TMS	$C_{19}H_{40}O_2Si$	327	313 ($C_{18}H_{37}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	32.73	98.51 ± 1.03
Linolenic acid, methyl ester	$C_{19}H_{32}O_2$	291	236 ($C_{15}H_{24}O_2$), 95 (C_7H_{11}), 79* (C6H7)	33.66	2.43 ± 0.34
Heptadecanoic acid, TMS	$C_{20}H_{42}O_2Si$	341	327 ($C_{19}H_{39}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	34.49	3.65 ± 0.61
9,12-Octadecadienoic acid, ethyl ester	$C_{20}H_{36}O_2$	307	95 (C_7H_{11}), 81 (C_6H_9), 67* (C_5H_7)	34.76	20.08 ± 2.11
Ethyl 9,12,15-octadecatrienoate	$C_{20}H_{34}O_2$	305	108 (C_8H_{12}), 95 (C_7H_{11}), 79* (C_6H_7)	34.88	31.25 ± 1.63
Stearic acid, ethyl ester	$C_{20}H_{40}O_2$	311	157 ($C_9H_{17}O_2$), 101 ($C_5H_9O_2$), 88* ($C_4H_8O_2$)	35.32	3.78 ± 0.28
Linoleic acid, TMS	$C_{21}H_{40}O_2Si$	351	262 ($C_{18}H_{30}O$), 129 ($C_5H_9O_2Si$), 73* (C_3H_9Si)	35.69	61.22 ± 2.94
α-Linolenic acid, TMS	$C_{21}H_{38}O_2Si$	349	129 ($C_5H_9O_2Si$), 95 (C_7H_{11}), 73* (C_3H_9Si)	35.83	91.69 ± 2.53
Octadecanoic acid, TMS	$C_{21}H_{44}O_2Si$	355	341 ($C_{20}H_{41}O_2Si$), 117* ($C_4H_9O_2Si$)	36.25	78.22 ± 3.78

Eicosanoic acid, TMS ester	$C_{23}H_{48}O_2Si$	383	145 ($C_6H_{13}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	39.47	2.04 ± 0.32
Bumetrizole	$C_{17}H_{18}ClN_3O$	314	300* ($C_{16}H_{15}ClN_3O$), 272 ($C_{15}H_{15}ClN_3$), 147 ($C_{10}H_{11}O$)	41.19	3.26 ± 0.58
cis-13-Docosenoic acid, trimethylsilyl ester	$C_{25}H_{50}O_2Si$	409	395 ($C_{24}H_{47}O_2Si$), 129 ($C_5H_9O_2Si$), 73* (C_3H_9Si)	42.13	0.75 ± 0.39
Docosanoic acid, TMS ester	$C_{25}H_{52}O_2Si$	411	397 ($C_{24}H_{49}O_2Si$), 117* ($C_4H_9O_2Si$)	42.48	1.18 ± 0.06
Squalene	$C_{30}H_{50}$	409	81 (C_6H_9), 69* (C_5H_9)	45.18	48.67 ± 1.63
Heptacosane	$C_{27}H_{56}$	379	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	48.70	3.95 ± 0.87
Ethyl iso-allocholate	$C_{26}H_{44}O_5$	435	253 ($C_{15}H_{25}O_3$), 129 ($C_7H_{13}O_2$), 107 (C_8H_{11}), 55* (C_3H_3O)	49.33	0.63 ± 0.12
β-Amyrin, TMS	$C_{33}H_{58}OSi$	497	218* ($C_{16}H_{26}$), 203 ($C_{15}H_{23}$)	53.38	2.58 ± 0.93

* = Base peak; # = Relative abundance after baseline normalization.

Phytochemicals identified in *Aloe albiflora* Guillaumin

Compound name	Formula	$[M-H]^-$	Identifying mass fragments	Retention time	Relative abundance
2-Hexanol, trimethylsilyl ether	$C_9H_{22}OSi$	173	159 ($C_8H_{19}OSi$), 117* ($C_5H_{13}OSi$)	5.78	0.45 ± 0.06
Benzeneacetaldehyde	C_8H_8O	119	91* (C_7H_7)	8.72	0.22 ± 0.08
Lactic acid, bis-TMS	$C_9H_{22}O_3Si_2$	233	147 ($C_5H_{11}O_3Si$), 117 ($C_5H_{13}OSi$), 73* (C_3H_9Si)	9.41	1.02 ± 0.13
Hydrocinnamic acid, benzyldimethylsilyl ester	$C_{18}H_{22}O_2Si$	297	207* ($C_{11}H_{15}O_2Si$), 91 (C_7H_7), 75 (C_6H_3)	10.70	0.28 ± 0.08
Benzaldehyde, 2,4-dimethyl-	$C_9H_{10}O$	133*	105 (C_8H_9)	13.57	0.53 ± 0.11
Phenol, 2-ethyl, TMS	$C_{11}H_{18}OSi$	193	179 ($C_{10}H_{15}OSi$), 103 ($C_4H_{11}OSi$), 73* (C_3H_9Si)	13.91	6.08 ± 0.24
9-Decen-1-ol, trimethylsilyl ether	$C_{13}H_{28}OSi$	227	213 ($C_{12}H_{25}OSi$), 103 (C_4H_1OSi), 75* (C_2H_7OSi)	15.05	0.84 ± 0.09
Phosphoric acid, triTMS	$C_9H_{27}O_4PSi_3$	313	299* ($C_8H_{24}O_4PSi_3$), 211 ($C_5H_{16}O_3PSi$)	15.59	22.15 ± 1.65
Benzeneacetic acid, trimethylsilyl ester	$C_{11}H_{16}O_2Si$	207	164 ($C_{10}H_{12}O_2Si$), 91 (C_7H_7), 73* (C_3H_9Si)	15.87	1.24 ± 0.47
Nonanoic acid, trimethylsilyl ester	$C_{12}H_{26}O_2Si$	229	215* ($C_{11}H_{23}O_2Si$), 129 ($C_5H_9O_2Si$), 117 ($C_4H_9O_2Si$)	17.56	0.37 ± 0.06
Phenol, 2-methoxy-3-(2-propenyl)-	$C_{10}H_{12}O_2$	163*	149 ($C_9H_9O_2$), 131 (C_9H_7O)	17.76	0.68 ± 0.12

Phenol, 3-(2-trimethylsilyloxyethyl)-	$C_{11}H_{18}O_2Si$	209	195 ($C_{10}H_{15}O_2Si$), 103 ($C_4H_{11}O_2Si$), 73* (C_3H_9Si)	18.46	0.92 ± 0.35
Methyleugenol	$C_{11}H_{14}O_2$	177*	163 ($C_{10}H_{11}O_2$), 147 ($C_{10}H_{11}O$)	18.63	0.30 ± 0.04
1,2-Ethanediol, phenyl, bis-TMS	$C_{14}H_{26}O_2Si_2$	281	179* ($C_{10}H_{15}OSi$), 147 ($C_9H_7O_2$)	19.49	0.87 ± 0.15
4-Allyl-2-methoxyphenoxy-TMS	$C_{13}H_{20}O_2Si$	235	206* ($C_{11}H_{14}O_2Si$), 179 ($C_9H_{11}O_2Si$)	20.25	16.34 ± 0.73
Phenol, 2,4-bis(1,1-dimethylethyl)- (Antioxidant No. 33)	$C_{14}H_{22}O$	205	206* ($C_{11}H_{14}O_2Si$), 179 ($C_9H_{11}O_2Si$)	21.32	0.52 ± 0.08
2-methyl-1-Hexadecanol	$C_{17}H_{36}O$	255	69 (C_5H_9), 57* (C_4H_9)	22.25	0.31 ± 0.02
Nonadecane	$C_{19}H_{40}$	267	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	23.37	2.03 ± 0.68
Dodecanoic acid, 1-methylethyl ester	$C_{15}H_{30}O_2$	241	102 ($C_5H_{10}O_2$), 60* (C_3H_8O)	24.00	3.65 ± 0.33
Lauric acid (TMS)	$C_{15}H_{32}O_2Si$	271	257 ($C_{14}H_{29}O_2Si$), 117* ($C_4H_9O_2Si$)	24.64	1.19 ± 0.21
β-bisabolol	$C_{15}H_{26}O$	221	204 ($C_{15}H_{24}$), 119 (C_9H_{11}), 93 (C_7H_9), 81* (C_6H_9)	25.05	0.24 ±
Tetradecane, 2,6,10-trimethyl-	$C_{17}H_{36}$	239	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	25.75	1.62 ± 0.56
tert-Hexadecanethiol	$C_{16}H_{34}S$	257	83 (C_6H_{11}), 69 (C_5H_9), 57* (C_4H_9)	26.50	0.25 ± 0.22
Tetradecanoic acid, (TMS)	$C_{17}H_{36}O_2Si$	299	285 ($C_{16}H_{33}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	28.84	9.05 ± 0.89
Pentadecanoic acid, TMS ester	$C_{18}H_{38}O_2Si$	313	299 ($C_{17}H_{35}O_2Si$), 117* (C4H9O2Si)	30.80	1.38 ± 0.53

Hexadecanoic acid, ethyl ester	$C_{18}H_{36}O_2$	283	239 ($C_{16}H_{31}O$), 101 ($C_5H_9O_2$), 88* ($C_4H_8O_2$)	31.65	1.88 ± 0.38
cis-9-Hexadecenoic acid, trimethylsilyl ester	$C_{19}H_{38}O_2Si$	325	311 ($C_{18}H_{35}O_2Si$), 145 ($C_6H_{13}O_2Si$), 117* ($C_4H_9O_2Si$)	32.20	2.26 ± 0.52
Palmitic acid, TMS	$C_{19}H_{40}O_2Si$	327	313 ($C_{18}H_{37}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	32.71	97.63 ± 2.48
cis-13-Eicosenoic acid	$C_{20}H_{38}O_2$	309	292 ($C_{20}H_{36}O$), 69 (C_5H_9), 55* (C_4H_7)	33.05	0.18 ± 0.05
Heptadecanoic acid, TMS	$C_{20}H_{42}O_2Si$	341	327 ($C_{19}H_{39}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	34.48	2.47 ± 0.29
Ethyl 9,12,15-octadecatrienoate	$C_{20}H_{34}O_2$	305	108 (C_8H_{12}), 95 (C_7H_{11}), 79* (C_6H_7)	34.87	2.53 ± 0.48
Linoleic acid, TMS	$C_{21}H_{40}O_2Si$	351	262 ($C_{18}H_{30}O$), 129 ($C_5H_9O_2Si$), 73* (C_3H_9Si)	35.66	21.67 ± 2.24
α-Linolenic acid, TMS	$C_{21}H_{38}O_2Si$	349	129 ($C_5H_9O_2Si$), 95 (C_7H_{11}), 73* (C_3H_9Si)	35.80	48.05 ± 1.09
Octadecanoic acid, TMS	$C_{21}H_{44}O_2Si$	355	341 ($C_{20}H_{41}O_2Si$), 117* ($C_4H_9O_2Si$)	36.24	86.46 ± 2.65
Eicosanoic acid, TMS ester	$C_{23}H_{48}O_2Si$	383	145 ($C_6H_{13}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	39.46	2.24 ± 0.35
Squalene	$C_{30}H_{50}$	409	81 (C_6H_9), 69* (C_5H_9)	45.16	11.85 ± 1.17
β-Sitosterol TMS	$C_{32}H_{58}OSi$	485	396 ($C_{29}H_{48}$), 255 ($C_{19}H_{27}$), 129* ($C_6H_{13}OSi$)	53.13	3.16 ± 0.46

* = Base peak; # = Relative abundance after baseline normalization.

Phytochemicals identified in *Aloe aspera* Haw.

Compound name	Formula	[M-H]$^-$	Identifying mass fragments	Retention time	Relative abundance
2-Pentanol, trimethylsilyl ether	$C_8H_{20}OSi$	159	145 ($C_7H_{17}OSi$), 117 ($C_5H_{13}OSi$)	5.80	1.45 ± 0.25
M-Pyrol	C_5H_9NO	98*	71 (C_3H_5NO)	8.73	0.32 ± 0.04
Lactic acid, (2TMS)	$C_9H_{22}O_3Si_2$	233	147 ($C_5H_{11}O_3Si$), 117 ($C_5H_{13}OSi$), 73* (C_3H_9i)	9.42	3.86 ± .38
Benzaldehyde, 3,5-dimethyl-	$C_9H_{10}O$	133*	177 (C_8H_9)	13.57	1.54 ± 0.51
Benzoic acid, TMS	$C_{10}H_{14}O_2Si$	193	179 ($C_9H_{11}O_2Si$), 105* (C_7H_5O)	14.45	0.29 ± 0.02
Phosphoric acid, triTMS	$C_9H_{27}O_4PSi_3$	313	299* ($C_8H_{24}O_4PSi_3$), 211 ($C_5H_{16}O_3PSi$)	15.59	32.18 ± 0.94
Succinic acid (2TMS)	$C_{10}H_{22}O_4Si_2$	261	247 ($C_9H_{19}O_4Si_2$), 147* ($C_6H_{15}O_2Si$)	16.42	0.69 ± 0.18
Fumaric acid (2TMS)	$C_{10}H_{20}O_4Si_2$	259	245* ($C_9H_{17}O_4Si_2$), 147 ($C_4H_1O_2Si$)	17.31	0.36 ± 0.07
Nonanoic acid, TMS ester	$C_{12}H_{26}O_2Si$	229	215* ($C_{11}H_{23}O_2Si$), 117 ($C_4H_9O_2Si$)	17.55	0.48 ± 0.12
Tetradecane	$C_{14}H_{30}$	197	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	18.49	0.33 ± 0.04
Decanoic acid, trimethylsilyl ester	$C_{13}H_{28}O_2Si$	243	299* ($C_{12}H_{25}O_2Si$), 117 ($C_4H_9O_2Si$)	20.03	0.24 ± 0.02
Phenol, 2,4-bis(1,1-dimethylethyl)- (Antioxidant No. 33)	$C_{14}H_{22}O$	205	191* ($C_{13}H_{19}O$), 57 (C_4H_9)	21.32	0.39 ± 0.10
Decane, 2,3,5,8-tetramethyl-	$C_{14}H_{30}$	197	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	22.00	0.67 ± 0.14
2-methyl-1-	$C_{17}H_{36}O$	255	69 (C_5H_9), 57* (C_4H_9)	22.24	0.20 ± 0.03

Hexadecanol					
Hexadecane	$C_{16}H_{34}$	225	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	23.36	0.45 ± 0.06
Dodecanoic acid, 1-methylethyl ester	$C_{15}H_{30}O_2$	241	102 ($C_5H_{10}O_2$), 60* (C_3H_8O)	24.00	0.53 ± 0.15
Lauric acid (TMS)	$C_{15}H_{32}O_2Si$	271	257 ($C_{14}H_{29}O_2Si$), 117* ($C_4H_9O_2Si$)	24.63	0.44 ± 0.09
Nonadecane	$C_{19}H_{40}$	267	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	25.61	0.35 ± 0.11
Heptadecane, 2,6,10,15-tetramethyl-	$C_{21}H_{44}$	295	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	26.80	0.71 ± 0.36
Tetradecane, 2,6,10-trimethyl-	$C_{17}H_{36}$	239	85 (C_6H_{13}), 71 (C_5H_{11}), 57* (C_4H_9)	27.76	0.58 ± 0.24
Azelaic acid, diTMS	$C_{15}H_{32}O_4Si_2$	331	201 ($C_{10}H_{21}O_2Si$), 129 ($C_5H_9O_2Si$), 73* (C_3H_9Si)	27.88	0.48 ± 0.18
Myristic acid, isopropyl ester	$C_{17}H_{34}O_2$	269	228 ($C_{14}H_{28}O_2$), 102* (C_5H_{10O2})	28.31	0.24 ± 0.03
Tetradecanoic acid (TMS)	$C_{17}H_{36}O_2Si$	299	285 ($C_{16}H_{33}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	28.84	6.63 ± 0.27
Pentadecanoic acid, TMS ester	$C_{18}H_{38}O_2Si$	313	299 ($C_{17}H_{35}O_2Si$), 117* ($C4H_9O_2Si$)	30.80	1.74 ± 0.14
cis-9-Hexadecenoic acid, trimethylsilyl ester	$C_{19}H_{38}O_2Si$	325	311 ($C_{18}H_{35}O_2Si$), 145 ($C_6H_{13}O_2Si$), 117* ($C_4H_9O_2Si$)	32.19	0.59 ± 0.08
Palmitic acid, TMS	$C_{19}H_{40}O_2Si$	327	313 ($C_{18}H_{37}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	32.72	98.15 ± 2.56
Heneicosane	$C_{21}H_{44}$	295	85 (C_6H_{13}), 71 (C_6H_{11}), 57* (C_4H_9)	33.61	0.46 ± 0.09
Heptadecanoic acid, TMS	$C_{20}H_{42}O_2Si$	341	327 ($C_{19}H_{39}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	34.48	1.97 ± 0.24
Linoleic acid, TMS	$C_{21}H_{40}O_2Si$	351	262 ($C_{18}H_{30}O$), 129 ($C_5H_9O_2Si$), 73* (C_3H_9Si)	35.67	31.86 ± 1.09
Oleic acid,	$C_{21}H_{42}O_2Si$	353	339 ($C_{20}H_{39}O_2Si$), 117 ($C_4H_9O_2Si$), 73*	35.77	19.38 ± 0.68

trimethylsilyl ester			(C_3H_9Si)		
Octadecanoic acid, TMS	$C_{21}H_{44}O_2Si$	355	341 ($C_{20}H_{41}O_2Si$), 117* ($C_4H_9O_2Si$)	36.24	96.45 ± 1.62
Eicosanoic acid, TMS ester	$C_{23}H_{48}O_2Si$	383	145 ($C_6H_{13}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	39.46	5.22 ± 0.43
1-Docosanol, trimethylsilyl ether	$C_{25}H_{54}OSi$	397	383* ($C_{24}H_{51}OSi$), 103 (C_4H_1OSi)	41.15	3.43 ± 0.31
Docosanoic acid, TMS ester	$C_{25}H_{52}O_2Si$	411	397 ($C_{24}H_{49}O_2Si$), 117* ($C_4H_9O_2Si$)	42.48	3.19 ± 0.78
Squalene	$C_{30}H_{50}$	409	81 (C_6H_9), 69* (C_5H_9)	45.16	18.72 ± 0.63
Tetracosanoic acid, trimethylsilyl ester	$C_{27}H_{56}O_2Si$	439	145 ($C_6H_{13}O_2Si$), 117 ($C_4H_9O_2Si$), 73* (C_3H_9Si)	45.29	26.34 ± 0.68
Tocopherol-γ-tms-derivative	$C_{31}H_{56}O_2Si$	487*	263 ($C_{15}H_{23}O_2Si$), 223 ($C_{16}H_{31}$), 73*	47.46	8.37 ± 0.52
Ethyl iso-allocholate	$C_{26}H_{44}O_5$	435	253 ($C_{15}H_{25}O_3$), 129 ($C_7H_{13}O_2$), 107 (C_8H_{11}), 55* (C_3H_3O)	49.69	0.48 ± 0.08
1-Heptatriacotanol	$C_{37}H_{76}O$	535	69 (C_5H_9), 55* (C_4H_7)	50.10	0.41 ± 0.05
Campesterol, TMS	$C_{31}H_{56}OSi$	471	382 ($C_{28}H_{46}$), 343 ($C_{25}H_{43}$), 129* ($C_6H_{13}OSi$)	51.45	3.66 ± 0.08
Stigmasterol, TMS	$C_{32}H_{56}OSi$	483	394 ($C_{29}H_{46}$), 255 ($C_{19}H_{27}$), 129 (C_6H_{13} OSi), 83* (C_6H_{11})	52.03	19.02 ± 1.43
β-Sitosterol TMS	$C_{32}H_{58}OSi$	485	396 ($C_{29}H_{48}$), 255 ($C_{19}H_{27}$), 129* ($C_6H_{13}OSi$)	53.21	53.48 ± 2.36

* = Base peak; # = Relative abundance after baseline normalization.

Additional Statistical Data

Correlation Matrix						
		A. vera	*A. aristata*	*A. jukunda*	*A. albiflora*	*A. aspera*
Correlation	*A. vera*	1.000	-.626	-.420	-.578	-.446
	A. aristata	-.626	1.000	.790	.708	.899
	A. jukunda	-.420	.790	1.000	.503	.881
	A. albiflora	-.578	.708	.503	1.000	.536
	A. asparata	-.446	.899	.881	.536	1.000
Sig. (1-tailed)	*A. vera*		.000	.000	.000	.000
	A. aristata	.000		.000	.000	.000
	A. jukunda	.000	.000		.000	.000
	A. albiflora	.000	.000	.000		.000
	A. aspera	.000	.000	.000	.000	

Total Variance Explained

Component	Initial Eigenvalues			Extraction Sums of Squared Loadings			Rotation Sums of Squared Loadings		
	Total	% of Variance	Cumulative %	Total	% of Variance	Cumulative %	Total	% of Variance	Cumulative %
1	3.591	71.817	71.817	3.591	71.817	71.817	2.520	50.403	50.403
2	.778	15.550	87.367	.778	15.550	87.367	1.848	36.965	87.367
3	.412	8.233	95.601						
4	.169	3.375	98.976						
5	.051	1.024	100.000						

Extraction Method: Principal Component Analysis.

Component Matrix[a]		
	Component	
	1	2
A. vera	-.702	.584
A. aristata	.960	.050
A. jukunda	.866	.392
A. albiflora	.775	-.390
A. asparata	.909	.358
Extraction Method: Principal Component Analysis.		
a. 2 components extracted.		

Proximity Matrix					
Case	Matrix File Input				
	A. vera	*A. aristata*	*A. jukunda*	*A. albiflora*	*A. aspera*
A. vera	.000	195.082	170.410	189.330	173.536
A. aristata	195.082	.000	25.258	35.064	12.139
A. jukunda	170.410	25.258	.000	59.619	14.279
A. albiflora	189.330	35.064	59.619	.000	55.678
A. asparata	173.536	12.139	14.279	55.678	.000

Agglomeration Schedule

Stage	Cluster Combined		Coefficients	Stage Cluster First Appears		Next Stage
	Cluster 1	Cluster 2		Cluster 1	Cluster 2	
1	2	5	12.139	0	0	2
2	2	3	19.769	1	0	3
3	2	4	50.120	2	0	4
4	1	2	182.090	0	3	0