Supplementary materials

Table S1. Chemical compounds identified by GC-MS as constituents of lipidome in Hass avocado pulp.

#	Compound	Common name	Formula	m/z	RT	Exact mass	BP °C	Exp KI	Theo KI	SI	Average area	%Error KI	Pubchem CID	HMDB	Adduct	S/N
1	Octanal	Octanal	$C_8H_{16}O$	41	3.160	128.120115	171	704.1	982	94	41040507.33	28.3032693	454	HMDB0001140	[M + H]	115.46
2	|E|-2-Octenal	(E)-2-Octenal	$C_8H_{14}O$	41	3.840	126.104465	-	730.4	1034	99	13034595.67	29.3648448	5283324	-	[M + H]	2.27
3	n-Nonanal	Nonanal	$C_9H_{18}O$	41	4.470	142.135765	195	754.7	1081	100	107168039.7	30.1814174	31289	HMDB0059835	[M + H]	154.55
4	2-Nonenal, (E)-	(E)-2-Nonenal	$C_9H_{16}O$	41	5.415	140.120115	-	791.3	1133,3	98	15996088.67	30.1777166	5283335	-	[M+H]	0.35
5	RT6.065	-	-	41	6.065	-	-	813.6	-	-	9019774.333	-	-	-	[M+H]	4.86
6	Decanal	Decanal	$C_{10}H_{20}O$	41	6.210	156.151415	212	818.2	1183	100	26530258	30.8383924	8175	HMDB0011623	[M+H]	234.02
7	RT6.485	-	-	81	6.485	-	-	827.0	-	-	8021946.667	-	-	-	[M+H]	45.16
8	RT7.095	-	-	43	7.095	-	-	846.4	-	-	9241240.667	-	-	-	[M+H]	7.7
9	2-Decenal, (Z)-	(Z)-2-Decenal	$C_{10}H_{18}O$	41	7.400	154.135765	-	856.1	1227	100	50426087.67	30.2249103	5354834	-	[M+H]	1111.95
10	2,4-Undecadien-1-ol	(2E,4E)-undeca-2,4-dien-1-ol	$C_{11}H_{20}O$	41	8.072	168.151415	-	877.6	1373	100	10781646.67	36.0833389	5362760	-	[M+H]	3.48
11	2,4-Decadienal, (E,E)-	(2E, 4E)-Decadienal	$C_{10}H_{16}O$	81	8.595	152.120115	-	894.3	1288	100	8753318.333	30.5700021	5283349	-	[M+H]	7.91
12	RT9.355	-	-	164	9.355	-	-	913.8	-	-	11319076	-	-	-	[M+H]	767.06
13	Eugenol	Eugenol	$C_{10}H_{12}O_2$	164	9.364	164.083730	225	914.1	1337	100	44894786.33	31.6337114	3314	HMDB0005809	[M+H]	556.9
14	2-Undecenal, E-	(2E)-Undecenal	$C_{11}H_{20}O$	41	9.485	168.151415	115	916.9	1350	100	31346595.67	32.0781402	5283356	HMDB0040247	[M+H]	9670.71
15	Tridecane	Tridecane	$C_{13}H_{28}$	57	10.106	184.219101	235	931.8	1300	99	242317.3333	28.3256839	12388	HMDB0034284	[M+H]	34.03
16	RT10.250	-	-	91	10.250	-	-	935.2	-	-	754733	-	-	-	[M+H]	14.6
17	RT10.820	-	-	133	10.820	-	-	948.8	-	-	473502	-	-	-	[M+H]	25.85
18	RT10.995	-	-	55	10.995	-	-	953.0	-	-	855303.6667	-	-	-	[M+H]	39.49
19	RT11.245	-	-	73	11.245	-	-	958.9	-	-	122234	-	-	-	[M+H]	110.64
20	Isoeugenol, (Z)-	(Z)-Isoeugenol	$C_{10}H_{12}O_2$	164	11.446	164.083730	-	963.7	1379	99	2005706.667	30.1126166	1549041	-	[M+H]	142.4
21	RT12.085	-	-	41	12.085	-	-	979.0	-	-	117578.3333	-	-	-	[M+H]	4.98
22	Nonadecane	Nonadecane	$C_{19}H_{40}$	57	12.235	268.313001	330	982.6	1900	100	2646582	48.2853913	12401	HMDB0034289	[M+H]	36.14

23	Butylated Hydroxytoluene	2,6-Di-t-butyl-4-methylphenol	$C_{15}H_{24}O$	205	12.380	220.182715	265	986.0	1503.9	96	2495555	34.434591	31404	HMDB0033826	[M+H]	460.69
24	2-n-Octylfuran	2-Octylfuran	$C_{12}H_{20}O$	81	12.590	180.151415	-	991.1	1281	100	15776316.67	22.6346511	77845	-	[M+H]	2106.34
25	RT12.730	-	-	119	12.730	-	-	994.4	-	-	2208223	-	-	-	[M+H]	14.81
26	RT14.210	-	-	107	14.210	-	-	1026.7	-	-	1022251.333	-	-	-	[M+H]	83.43
27	RT14.345	-	-	81	14.345	-	-	1029.6	-	-	715618.6667	-	-	-	[M+H]	1.97
28	Hexadecanal	palmitaldehyde	$C_{16}H_{32}O$	43	14.691	240.245316	-	1037.0	1795	99	1077423.667	42.2306788	984	HMDB0001551	[M+H]	9.27
29	Tetradecanal	Myristaldehyde	$C_{14}H_{28}O$	43	14.695	212.214016		1037.0	1592	99	2076373.333	34.8589844	31291	HMDB34283	[M+H]	6.44
30	RT14.875	-	-	81	14.875	-	-	1040.9	-	-	1238549.667	-	-	-	[M+H]	16.19
31	1,E-11,Z-13-Octadecatriene	(11E,13Z)-1,11,13-Octadecatriene	$C_{18}H_{32}$	67	15.595	248.250401	-	-	1685	100	1583018.667	37.3105688	5365585	-	[M+H]	53.37
32	1,6,11-Dodecatriene, (Z)-	(6Z)-1,6,11-Dodecatriene	$C_{12}H_{20}$	67	15.595	164.156501	-	1056.3	1202	100	511240	12.1200569	5365569	-	[M+H]	14.12
33	7-Hexadecyne	7-Hexadecyne	$C_{16}H_{30}$	67	15.720	222.234751	-	1059.0	1629	100	2975003.333	34.9911862	549042	-	[M+H]	10.69
34	7-Tetradecyne	7-Tetradecyne	$C_{14}H_{26}$	67	15.730	194.203451	-	1059.2	1416	100	806713	25.1971957	141979	-	[M+H]	30.16
35	9-Hexadecyn-1-ol	9-Hexadecyne-1-ol	$C_{16}H_{30}O$	55	15.855	238.229666	-	1061.9	1872	100	1539590.667	43.2754077	145155	-	[M+H]	9.81
36	Bicyclo[10.1.0]tridec-1-ene	Bicyclo[10.1.0]tridec-1-ene	$C_{13}H_{22}$	67	15.860	178.172151	-	1062.0	-	100	1634894.667	-	548879	-	[M+H]	11.86
37	1-Nonadecene	1-Nonadecene	$C_{19}H_{38}$	55	15.870	266.297351	-	1062.2	1891	100	4747704.333	43.8283677	29075	-	[M+H]	9.85
38	RT15.985	-	-	55	15.985	-	-	1064.7	-	-	884834	-	-	-	[M+H]	1.37
39	RT16.180	-	-	97	16.180	-	-	1068.8	-	-	2383562.333	-	-	-	[M+H]	113.76
40	RT16.305	-	-	41	16.305	-	-	1071.5	-	-	2039631.667	-	-	-	[M+H]	11.24
41	RT16.610	-	-	105	16.610	-	-	1078.1	-	-	243370	-	-	-	[M+H]	76.53
42	RT17.480	-	-	183	17.480	-	-	1096.7	-	-	614889	-	-	-	[M+H]	165.51
43	RT18.220	-	-	43	18.220	-	-	1112.3	-	-	3683428	-	-	-	[M+H]	21.31
44	RT18.320	-	-	43	18.320	-	-	1114.4	-	-	339376.6667	-	-	-	[M+H]	1.89
45	1-Octadecyne	1-Octadecyne	$C_{18}H_{34}$	81	18.335	250.266051	-	1114.7	1808	96	308255	38.3442012	69425	-	[M+H]	6.77
46	Myristic acid, TMS derivative	Trimethylsilyl myristate	$C_{17}H_{36}O_2Si$	117	18.560	300.248457	-	1119.5	1842	98	980454.5	39.2250986	519592	-	[M+H]	170.93

47	RT18.650	-	-	41	18.650	-	-	1121.4	-	-	143796	-	-	-	[M+H]	1.8
48	RT18.958	-	-	118	18.958	-	-	1127.9	-	-	1063334.333	-	-	-	[M+H]	11.21
49	9-Octadecenal, (Z)-	9Z-Octadecenal	$C_{18}H_{34}O$	41	19.074	266.260966	-	1130.3	2007	97	1742697.333	43.6823748	5364492	-	[M+H]	2.92
50	RT19.515	-	-	69	19.515	-	-	1139.6	-	-	1112094.333	-	-	-	[M+H]	11.53
51	Tetradec-(7Z)-en-2-one	7Z-Tetradecen-2-one	$C_{14}H_{26}O$	43	19.705	210.198365	-	1143.6	-	99	1774629	-	11344862	-	[M+H]	10.54
52	RT19.940	-	-	81	19.940	-	-	1148.5	-	-	4338112.667	-	-	-	[M+H]	61.31
53	9,17-Octadecadienal, (Z)-	(z)-9,17-octadecadienal	$C_{18}H_{32}O$	67	19.960	264.245316	-	1148.9	2297	96	4213849	49.9805238	5365667	-	[M+H]	14.98
54	Tetradec-(11Z)-enal	11Z-Tetradecenal	$C_{14}H_{26}O$	41	20.076	210.198365	-	1151.4	-	99	1443309.333	-	6427099	-	[M+H]	0.91
55	(E)-13-Docosenoic acid	(E)-13-Docosenoic acid	$C_{22}H_{42}O_2$	41	20.084	338.318481	-	1151.6	2572	99	31813462	55.2271425	5282772	-	[M+H]	0.33
56	Palmitoleic acid methyl ester	Methyl Palmitoleate	$C_{17}H_{32}O_2$	55	20.195	268.240230	-	1153.9	1885.8	99	14735073.33	38.8133405	643801	-	[M+H]	72.86
57	Tridecanoic acid, methyl ester	Methyl Tridecanoate	$C_{14}H_{28}O_2$	74	20.557	228.208930	-	1161.5	1606	98	4110368,667	27.6764764	15608	-	[M+H]	1007.05
58	Hexadecanoic acid, methyl ester	Methyl Palmitate	$C_{17}H_{34}O_2$	74	20.600	270.255880	417	1162.4	1908	100	28219121	39.0764647	8181	HMDB0061859	[M+H]	1087.57
59	RT20.685	-	-	41	20.685	-	-	1164.2	-	-	858583,6667	-	-	-	[M+H]	0.12
60	RT20.720	-	-	118	20.720	-	-	1164.9	-	-	603163	-	-	-	[M+H]	30.75
61	RT20.850	-	-	41	20.850	-	-	1167.7	-	-	191525	-	-	-	[M+H]	1.05
62	2-Tridecylfuran	2-tridecylfuran	$C_{17}H_{30}O$	81	21.078	250.229666	-	1172.5	-	100	17895597,33	-	6857795	-	[M+H]	138.49
63	RT21.080	-	-	43	21.080	-	-	1172.5	-	-	1810679,333	-	-	-	[M+H]	0.06
64	RT21.150	-	-	149	21.150	-	-	1174.0	-	-	703279,6667	-	-	-	[M+H]	297.76
65	RT21.400	-	-	79	21.400	-	-	1179.3	-	-	191625,6667	-	-	-	[M+H]	1.42
66	RT21.520	-	-	79	21.520	-	-	1181.8	-	-	2202286,333	-	-	-	[M+H]	3.76
67	RT21.650	-	-	81	21.650	-	-	1184.5	-	-	11982672,33	-	-	-	[M+H]	19.04
68	Pentadecane	Pentadecane	$C_{15}H_{32}$	57	21.805	212.250401	271	1187.8	1500	98	2551395,667	20.8140351	12391	HMDB0059886	[M+H]	15.98
69	RT21.900	-	-	81	21.900	-	-	1189.8	-	-	30412676	-	-	-	[M+H]	25.56
70	RT21.995	-	-	81	21.995	-	-	1191.8	-	-	12774583,67	-	-	-	[M+H]	49.23
71	RT22.110	-	-	81	22.110	-	-	1194.2	-	-	4791474,333	-	-	-	[M+H]	1.37
72	RT22.530	-	-	79	22.530	-	-	1204.9	-	-	18121023.67	-	-	-	[M+H]	4.31

73	RT22.640	-	-	94	22.640	-	-	1208.6	-	-	2284799.333	-	-	-	[M+H]	4.51
74	RT22.735	-	-	94	22.735	-	-	1211.8	-	-	15718368.67	-	-	-	[M+H]	3.59
75	RT22.875	-	-	41	22.875	-	-	1216.5	-	-	14899574.67	-	-	-	[M+H]	1.15
76	RT23.045	-	-	41	23.045	-	-	1222.2	-	-	6380726	-	-	-	[M+H]	0.37
	Oleic Acid	Oleic Acid	$C_{18}H_{34}O_2$	55	23.097	282,255880	286	1224.0	2113	99	102369447	42.0741569	445639	HMDB0000207	[M+H]	4.28
77	RT23.100	-	-	43	23.100	-	-	1224.1	-	-	19817073.67	-	-	-	[M+H]	1.37
78	RT23.280	-	-	94	23.280	-	-	1230.1	-	-	23958198.67	-	-	-	[M+H]	18.76
79	RT23.305	-	-	94	23.305	-	-	1231.0	-	-	16168745	-	-	-	[M+H]	75.72
80	9,12-Octadecadienoic acid, methyl ester, (E,E)-	Methyl linolelaidate	$C_{19}H_{34}O_2$	67	23.463	294.255880	-	1236.3	2078	99	21250900	40.5054718	5362793	-	[M+H]	22.3
81	9-Octadecenoic acid, methyl ester, (E)-	Methyl elaidate	$C_{19}H_{34}O_2$	55	23.465	296.271530	-	1236.4	2084	98	106096829	40.6735299	5280590	-	[M+H]	37.47
82	9-Octadecenoic acid (Z)-, methyl ester	Methyl oleate	$C_{19}H_{36}O_2$	55	23.566	296.271530	219	1239.8	2082	99	9919157,667	40.4532032	5364509	-	[M+H]	12.04
83	RT23.835	-	-	43	23.835	-	-	1248.8	-	-	2142927	-	-	-	[M+H]	1.08
84	RT23.950	-	-	74	23.950	-	-	1252.7	-	-	4411043	-	-	-	[M+H]	16.67
85	2-Cyclopenten-1-one, 2-pentyl-	2-Pentyl-2-cyclopenten-1-one	$C_{10}H_{16}O$	97	24.048	152.120115	-	1256.0	1259	93	11830965.33	0.23881922	117549	-	[M+H]	12.51
86	13-Octadecenoic acid, (E)-, TMS derivative	13-Octadecenoic acid, (E)-, TMS derivative	$C_{21}H_{42}O_2Si$	73	24.190	354.295407	-	1260.8	-	38	9548583	-	91696380	-	[M+H]	3.31
87	RT24.295	-	-	67	24.295	-	-	1264.3	-	-	1148683	-	-	-	[M+H]	0.21
88	,delta,-Dodecalactone	delta-Dodecanolactone	$C_{12}H_{22}O_2$	99	24.316	198.161980	-	1265.0	1670	96	9520027.667	24.2504889	12844	HMDB0037742	[M+H]	35.41
89	RT24.450	-	-	43	24.450	-	-	1269.5	-	-	14337499.33	-	-	-	[M+H]	0.93
90	RT24.620	-	-	97	24.620	-	-	1275.3	-	-	7239736.333	-	-	-	[M+H]	8.35
91	1-Heptadec-1-ynyl-cyclopentanol	1-Heptadec-1-ynyl-cyclopentanol	$C_{22}H_{40}O$	41	24.705	320.307916	-	1278.1	2419	98	11443840.67	47.1635189	536340	-	[M+H]	7.46
92	RT24.870	-	-	81	24.870	-	-	1283.7	-	-	47730361.67	-	-	-	[M+H]	975.48
93	RT24.930	-	-	259	24.930	-	-	1285.7	-	-	293360168.3	-	-	-	[M+H]	4.43

94	Eicosane	Eicosane	$C_{20}H_{42}$	57	25.114	282.328651	344	1291.9	2000	100	16230369	35.4057239	8222	HMDB0059909	[M+H]	111.8
95	RT25.325	-	-	79	25.325	-	-	1299.0	-	-	15441647.67	-	-	-	[M+H]	1.67
96	RT25.535	-	-	79	25.535	-	-	1309.0	-	-	46719004.67	-	-	-	[M+H]	0.55
97	RT25.670	-	-	69	25.670	-	-	1315.7	-	-	9321805	-	-	-	[M+H]	5.65
98	RT26.045	-	-	79	26.045	-	-	1334.4	-	-	129971600.7	-	-	-	[M+H]	26.525
99	RT26.270	-	-	94	26.270	-	-	1345.6	-	-	4138178.333	-	-	-	[M+H]	8.13
100	RT26.560	-	-	94	26.560	-	-	1360.1	-	-	2631527	-	-	-	[M+H]	2.61
101	Docosane	Docosane	$C_{22}H_{46}$	57	26.654	310.359951	369	1364.8	2200	96	1234143.333	37.9641805	12405	HMDB0061865	[M+H]	6.05
102	Heneicosane	Heneicosane	$C_{21}H_{44}$	57	26.662	296.344301	359	1365.2	2100	100	14788082.33	34.9910937	12403	HMDB0061782	[M+H]	756.29
103	RT26.820	-	-	69	26.820	-	-	1373.1	-	-	784085	-	-	-	[M+H]	5.17
104	RT26.950	-	-	94	26.950	-	-	1379.6	-	-	3863362	-	-	-	[M+H]	5.09
105	RT27.260	-	-	81	27.260	-	-	1395.0	-	-	3925883	-	-	-	[M+H]	5.69
106	RT27.705	-	-	52	27.705	-	-	1421.6	-	-	4647838.333	-	-	-	[M+H]	2.17
107	RT27.880	-	-	69	27.880	-	-	1432.5	-	-	513568.6667	-	-	-	[M+H]	6.59
108	RT27.905	-	-	81	27.905	-	-	1434.1	-	-	5235480.667	-	-	-	[M+H]	6.28
109	RT28.000	-	-	57	28.000	-	-	1440.0	-	-	688701	-	-	-	[M+H]	12.38
110	Cyclopropanecarboxyllic acid, tridec-2-ynyl ester	Cyclopropanecarboxyllic acid, tridec-2-ynyl ester	$C_{17}H_{28}O_2$	69	28.202	264.208930	-	1452.6	1898	99	5758378.667	23.46549	531185	-	[M+H]	3.11
111	RT28.405	-	-	67	28.405	-	-	1465.3	-	-	2421785	-	-	-	[M+H]	13.55
112	3-Methyl-1-dodecyn-3-ol	3-methyldodec-1-yn-3-ol	$C_{13}H_{24}O$	69	28.615	196.182715	-	1478.4	1403	98	11145212.67	5.37687099	21908640	-	[M+H]	3.7
113	RT28.800	-	-	69	28.800	-	-	1490.0	-	-	4257823.333	-	-	-	[M+H]	8.57
114	2-Methyltetracosane	2-Methyltetracosane	$C_{25}H_{52}$	57	29.010	352.406902	381	1503.6	2463	92	6838477.667	38.9510206	527459	HMDB0031069	[M+H]	1.95
115	RT29.020	-	-	41	29.020	-	-	1504.4	-	-	2430089.333	-	-	-	[M+H]	2.73
116	Undecane, 2,9-dimethyl-	2,9-Dimethylundecane	$C_{13}H_{28}$	57	29.165	184.219101	-	1514.9	1233	97	4189671.333	22.8636732	519385	-	[M+H]	2.84
117	RT29.430	-	-	149	29.430	-	-	1534.2	-	-	4398279.667	-	-	-	[M+H]	43.16
118	RT29.865	-	-	43	29.865	-	-	1565.8	-	-	1569176.667	-	-	-	[M+H]	4.08
119	RT30.295	-	-	81	30.295	-	-	1597.1	-	-	5083808	-	-	-	[M+H]	48.96
120	RT30.430	-	-	67	30.430	-	-	1607.7	-	-	7196255.667	-	-	-	[M+H]	8.6
121	Heptadecane, 3-methyl-	3-Methylheptadecane	$C_{18}H_{38}$	43	30.585	254.297351	-	1620.2	1774	96	3410595.667	8.66725395	94321	-	[M+H]	0.1

122	RT30.785	-	-	69	30.785	-	-	1636.4	-	-	414270.6667	-	-	-	[M+H]	1.67
123	RT31.060	-	-	69	31.060	-	-	1658.7	-	-	10023380.67	-	-	-	[M+H]	27.34
124	RT31.280	-	-	55	31.280	-	-	1676.5	-	-	2934111	-	-	-	[M+H]	1.66
125	RT31.410	-	-	69	31.410	-	-	1687.0	-	-	1239008	-	-	-	[M+H]	3.74
126	Nonadecane, 2-methyl-	2-Methylnonadecane	$C_{20}H_{42}$	43	31.750	282.328651	-	1715.7	1964	98	869757.3333	12.6415212	137081	-	[M+H]	0.97
127	RT31.835	-	-	43	31.835	-	-	1723.1	-	-	1923780.333	-	-	-	[M+H]	4.51
128	RT31.920	-	-	57	31.920	-	-	1730.6	-	-	3000473	-	-	-	[M+H]	11.32
129	RT32.075	-	-	43	32.075	-	-	1744.1	-	-	6269129.333	-	-	-	[M+H]	13.05
130	Octadecane	Octadecane	$C_{18}H_{38}$	57	32.240	254.297351	316	1758.5	1800	100	9084739.667	2.30470645	11635	HMDB0033721	[M+H]	49.63
131	Tricosane, 2-methyl-	2-Methyltricosane	$C_{24}H_{50}$	43	33.030	338.391252	372	1829.2	2363	98	614086.3333	22.5913387	283510	HMDB0031071	[M+H]	0.09
132	Hexatriacontane	Hexatriacontane	$C_{36}H_{74}$	57	33.165	506.579052	298	1841.7	3600	99	1325963	48.8425926	12412	-	[M+H]	7.4
133	Octadecane, 2-methyl	2-methyloctadecane	$C_{19}H_{40}$	57	34.274	268.313001	-	1947.0	1864	98	248417.6667	4.45068585	15264	-	[M+H]	0.06
134	Eicosane, 3-methyl-	3-Methyleicosane	$C_{21}H_{44}$	57	34.403	296.344301	-	1959.6	2074	98	278895.6667	5.51553312	98417	-	[M+H]	4.6
135	Octacosane	Octacosane	$C_{28}H_{58}$	57	34.645	394.453852	432	1993.1	2800	100	8265109.667	28.8165266	12408	HMDB0061868	[M+H]	130.89
136	Hexacosane	Hexacosane	$C_{26}H_{54}$	57	34.745	366.422552	415	1993.1	2600	100	20796036.67	23.3408748	12407	HMDB0061867	[M+H]	71.66
137	RT35.250	-	-	164	35.250	-	-	2044.6	-	-	725361.6667	-	-	-	[M+H]	115.55
138	RT35.480	-	-	57	35.480	-	-	2068.2	-	-	307188.3333	-	-	-	[M+H]	0.11
139	RT36.100	-	-	43	36.100	-	-	2133.5	-	-	2068023	-	-	-	[M+H]	0.95
140	RT36.390	-	-	105	36.390	-	-	2164.9	-	-	2045314.667	-	-	-	[M+H]	16.49
141	RT36.785	-	-	43	36.785	-	-	2207.8	-	-	1211222.667	-	-	-	[M+H]	3.33
142	RT37.315	-	-	43	37.315	-	-	2267.0	-	-	31401787.33	-	-	-	[M+H]	93.68
143	RT37.650	-	-	164	37.650	-	-	2304.7	-	-	1820868	-	-	-	[M+H]	165.97

m/z: mass-to-charge ratio; RT: retention time; BP: boiling point; KI exp: experimental Kovats index; KI theo: theoretical Kovats index; SI: similarity index; % error KI: percent error in Kovats index; pubchem CID: PubChem Compound ID; HMDB: Human Metabolome Database code; Adudct: ionized form of the analyte; S/N: signal-to-noise ratio.