Non-invasive characterization of the adipogenic differentiation of human bone marrow-derived mesenchymal stem cells by HS-SPME/GC-MS

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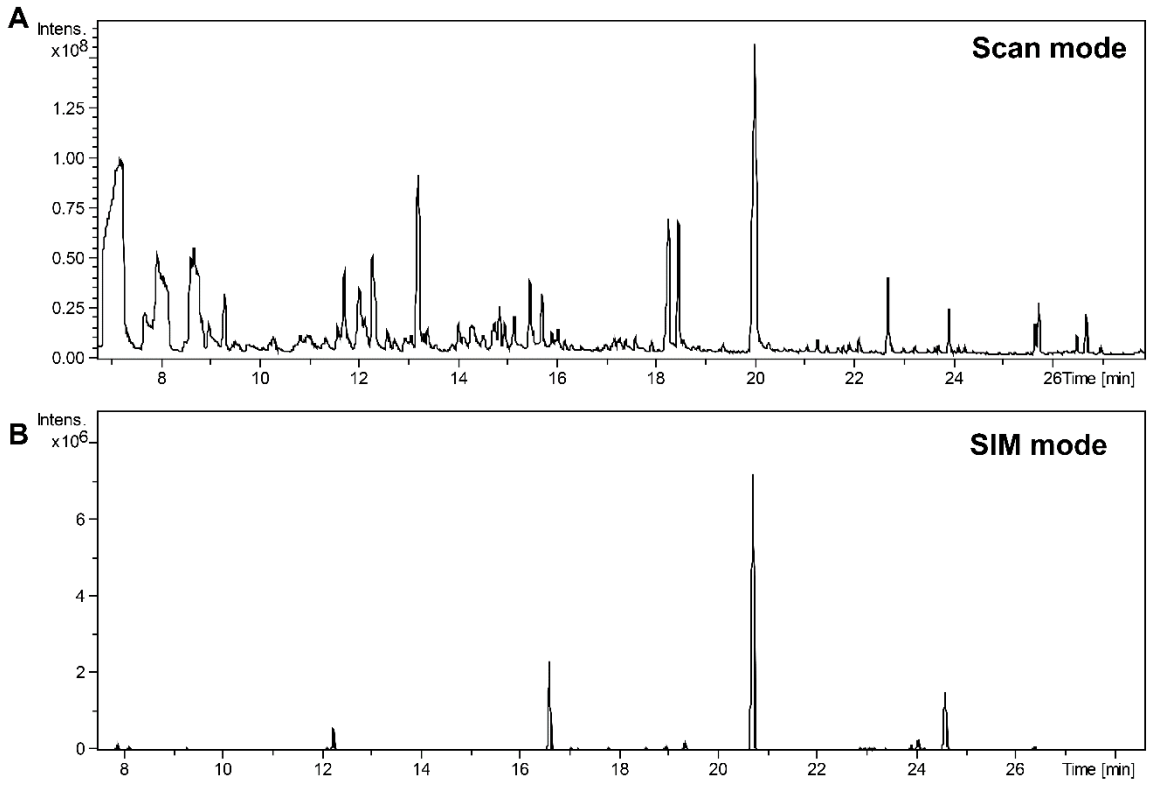
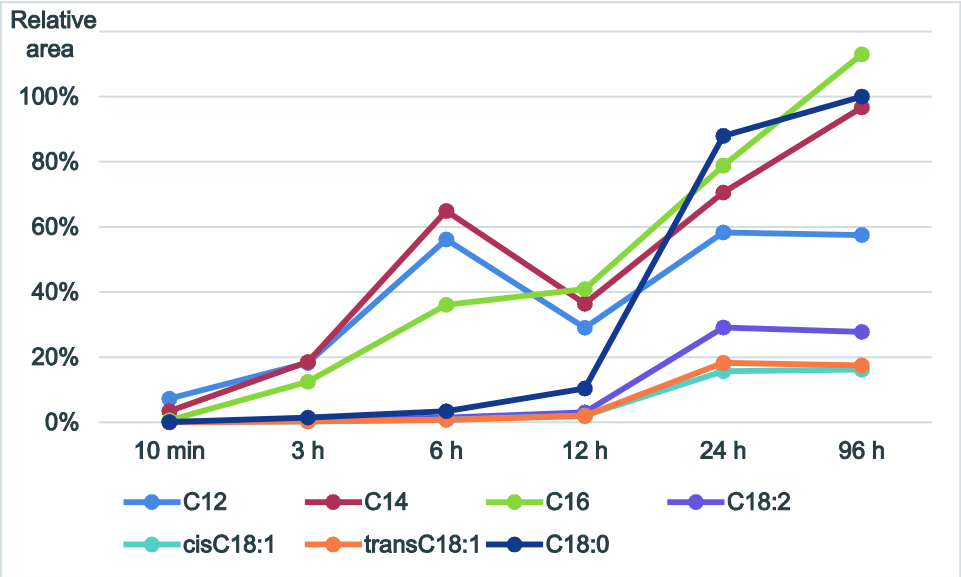
Supplementary Figure S1 Chromatograms in scan mode (A) and SIM mode (B) for the analyzed hMSCs. There were the other VOCs observed when using scan mode, but only FAMEs were detected in SIM mode.



Supplementary Figure S2 Optimization of extraction time of 7 FAMEs using PDMS/DVB fiber



Supplementary Table S1 Assigned VOCs from adipogenic medium (blank medium of adipogenic cell) and growth medium (blank medium of MSCs)

Retention time (min)	Compound name	Molecular weight	Formula	Similarity index	Adipogenic medium	Growth medium
4.76	Spiro[2.4]hepta-4,6-diene	92	C_7H_8	95	o	o
6.53	Dimethylsulfoxonium formylmethylide	120	$C_4H_8O_2S$	95	o	
6.86	2,4-Dimethyl-1-heptene	126	C_9H_{18}	89		o
7.43	Ethylbenzene	106	C_8H_{10}	94	o	o
7.68	Benzene, 1,3-dimethyl-	106	C_8H_{10}	97	o	o
8.11	Cyclohexanol	100	$C_6H_{12}O$	95		o
8.33	Styrene	104	C_8H_8	92		o
8.41	Benzene, 1,2-dimethyl-	106	C_8H_{10}	96	o	o
10.50	Benzaldehyde	106	C_7H_6O	92	o	o
11.26	Phosphonic acid, (p-hydroxyphenyl)-	174	$C_6H_7O_4P$	93	o	o
11.66	Benzene, 1-ethenyl-3-methyl-	118	C_9H_{10}	94	o	o
11.76	Benzene, 1,1'-(1-ethenyl-1,3-propanediyl)bis-	222	$C_{17}H_{18}$	93	o	o
11.91	Octane, 2,5-dimethyl-	142	$C_{10}H_{22}$	88		o
12.69	Decane, 2,2-dimethyl-	170	$C_{12}H_{26}$	92	o	o
12.78	2-Propyl-1-pentanol	130	$C_8H_{18}O$	94	o	o
13.00	Nonane, 3-methyl-5-propyl-	184	$C_{13}H_{28}$	90	o	o
13.62	Octane, 2,6-dimethyl-	142	$C_{10}H_{22}$	89	o	
13.84	Acetophenone	120	C_8H_8O	89	o	o
13.91	Undecane, 2,5-dimethyl-	184	$C_{13}H_{28}$	82	o	o
14.30	Benzaldehyde, 4-methyl-	120	C_8H_8O	85	o	
14.47	Benzenemethanol, .alpha.-methyl-.alpha.-(1-methyl-2-propenyl)-	176	$C_{12}H_{16}O$	84		o

15.01	Undecane	156	$C_{11}H_{24}$	84	o	o
15.07	Nonanal	142	$C_9H_{18}O$	93	o	
15.21	Maltol	126	$C_6H_6O_3$	94	o	o
17.22	Benzeneacetic acid, methyl ester	150	$C_9H_{10}O_2$	91	o	
17.72	Methyl salicylate	152	$C_8H_8O_3$	94	o	
17.94	Dodecane	170	$C_{12}H_{26}$	97	o	o
18.05	Decanal	156	$C_{10}H_{20}O$	92	o	o
18.76	2-Propenoic acid, 2-ethylhexyl ester	184	$C_{11}H_{20}O_2$	89	o	
19.44	Benzene, 1,3-bis(1,1-dimethylethyl)-	190	$C_{14}H_{22}$	85		o
19.88	1-Dodecanol	186	$C_{12}H_{26}O$	89		o
20.17	Nonane, 5-methyl-5-propyl-	184	$C_{13}H_{28}$	90	o	o
20.67	Decane, 5-propyl-	184	$C_{13}H_{28}$	89	o	o
21.43	Ethyl-4-chlorobenzoate	184	$C_9H_9C_lO_2$	88	o	
22.07	Propanoic acid, 2-methyl-, 2,2-dimethyl-1-(2-hydroxy-1-methylethyl)propyl ester	216	$C_{12}H_{24}O_3$	90	o	
22.09	Tridecane, 5-methyl-	198	$C_{14}H_{30}$	88		o
22.36	2,4,4,6,6,8,8-Heptamethyl-2-nonene	224	$C_{16}H_{32}$	87	o	o
22.51	2-Bromo dodecane	248	$C_{12}H_{25}Br$	89		o
22.59	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	216	$C_{12}H_{24}O_3$	90	o	o
23.05	1-Tetradecene	196	$C_{14}H_{28}$	96	o	o
23.27	Tetradecane	198	$C_{14}H_{30}$	92	o	o
24.00	Ethanone, 1,1'-(1,4-phenylene)bis-	162	$C_{10}H_{10}O_2$	94	o	o
24.81	Tetradecane, 2-methyl-	212	$C_{15}H_{32}$	89	o	o
24.95	2,6-Di-tert-butyl-1,4-benzoquinone	220	$C_{14}H_{20}O_2$	91	o	
25.41	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	192	$C_{13}H_{20}O$	92	o	o

25.63	Hexadecane, 7,9-dimethyl-	254	$C_{18}H_{38}$	89	o	o
25.69	Pentadecane	212	$C_{15}H_{32}$	95	o	o
25.95	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	$C_{14}H_{22}O$	90	o	
26.26	Methyl laurate	214	$C_{13}H_{26}O_2$	92	o	o
27.84	Diethyl Phthalate	222	$C_{12}H_{14}O_4$	94		o
27.82	n-Pentadecanol	228	$C_{15}H_{32}O$	92	o	
27.99	Hexadecane	226	$C_{16}H_{34}$	94		o
28.25	Tetradecanal	212	$C_{14}H_{28}O$	96	o	o
28.64	Benzophenone	182	$C_{13}H_{10}O$	91	o	o
28.87	Phenol, 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-	262	$C_{18}H_{30}O$	88	o	o
29.38	2-Bromotetradecane	276	$C_{14}H_{29}Br$	83	o	o
29.86	Bis(2-ethylhexyl) methylphosphonate	320	$C_{17}H_{37}O_3P$	85		o
29.97	Phenol, 2,4-di-t-butyl-6-nitro-	251	$C_{14}H_{21}NO_3$	90	o	o
30.17	Heptadecane	240	$C_{17}H_{36}$	94	o	o
30.67	Methyl myristate	240	$C_{15}H_{30}O_2$	92	o	o
32.24	Octadecane	254	$C_{18}H_{38}$	94	o	
32.56	Pentadecanal-	226	$C_{15}H_{30}O$	95		o
32.74	Pentadecanoic acid, methyl ester	256	$C_{16}H_{32}O_2$	85	o	o
34.30	Methyl palmitoleate	268	$C_{17}H_{32}O_2$	95	o	o
34.32	1-Hexadecanamine, N,N-dimethyl-	269	$C_{18}H_{39}N$	92		o
34.60	5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl-, (E,E)-	262	$C_{18}H_{30}O$	86		o
34.72	Methyl palmitate	270	$C_{17}H_{34}O_2$	88	o	o
35.32	n-Hexadecanoic acid	214	$C_{13}H_{26}O_2$	84		o
35.35	Pentadecanoic acid	242	$C_{15}H_{30}O_2$	91	o	
37.81	Methyl linoleate	294	$C_{19}H_{34}O_2$	94	o	o
37.92	Methyl oleate	296	$C_{19}H_{36}O_2$	94	o	o

38.03	Methyl elaidate	296	$C_{19}H_{36}O_2$	93	o	
38.38	Methyl stearate	298	$C_{19}H_{38}O_2$	95	o	o
39.18	Phenol, 4,4'-(1-methylethylidene)bis-	228	$C_{15}H_{16}O_2$	92	o	

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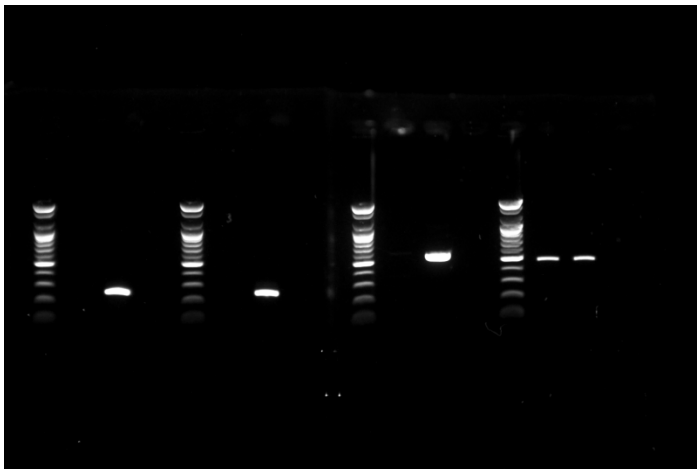
Supplementary Table S2 VOCs released from the adipogenic differentiated MSCs (relatively high quantity on the cells compared to blank medium)

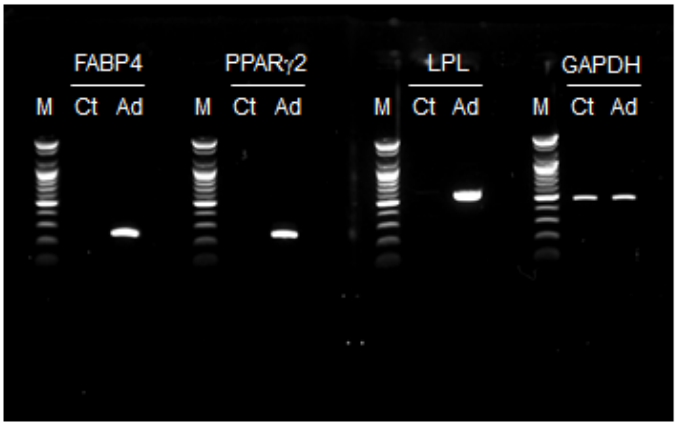
Retention time (min)	Compound name	Molecular weight	Formula	Similarity index
25.69	heptadecane	240	$C_{17}H_{36}$	95
26.25	Methyl laurate	214	$C_{13}H_{26}O_2$	92
29.86	Cyclopentadecanone	224	$C_{15}H_{28}O$	86
30.12	2-pentadecanone	226	$C_{15}H_{30}O$	96
30.67	Methyl myristate	240	$C_{15}H_{30}O_2$	92
33.31	Arachidonic acid	304	$C_{20}H_{32}O_2$	88
33.57	Z-5,17-Octadecadien-1-ol acetate	308	$C_{20}H_{36}O_2$	85
33.78	Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate	268	$C_{16}H_{28}O_3$	85
33.91	4-Octadecylmorpholine	339	$C_{22}H_{45}NO$	92
34.22	9-Hexadecenoic acid, methyl ester	268	$C_{17}H_{32}O_2$	89
34.27	2-Nonadecanone	282	$C_{19}H_{38}O$	88
34.31	Methyl palmitoleate	268	$C_{17}H_{32}O_2$	95
34.70	Methyl palmitate	270	$C_{17}H_{34}O_2$	91
36.58	Methyl margarate	284	$C_{18}H_{36}O_2$	95
37.27	cis,cis,cis-7,10,13-Hexadecatrienal	234	$C_{16}H_{26}O$	85
37.82	Methyl linoleate	294	$C_{19}H_{34}O_2$	96
37.93	Methyl oleate	296	$C_{19}H_{36}O_2$	92
38.03	Methyl elaidate	296	$C_{19}H_{36}O_2$	93
38.41	Methyl stearate	298	$C_{19}H_{38}O_2$	94
40.42	cis-4,7,10,13,16,19-Docosahexanoic acid	328	$C_{22}H_{32}O_2$	86
40.65	Methyl arachidonate	318	$C_{21}H_{34}O_2$	91

Supplementary Table S3 VOCs released from the non-differentiated MSCs (relatively high quantity on the cells compared to blank medium)

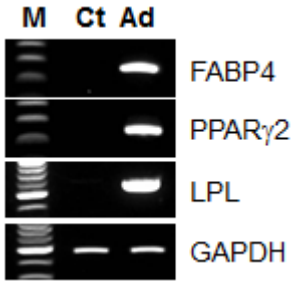
Retention time	Compound name	Molecular weight	Formula	Similarity index
12.79	1-Decene, 2,4-dimethyl-	168	$C_{12}H_{24}$	91
13.98	2-Octen-1-ol	128	$C_8H_{16}O$	93
14.07	1-Octanol	130	$C_8H_{18}O$	89
20.01	(3Z)-3-Octenyl acetate	170	$C_{10}H_{18}O_2$	84
20.13	(2E)-2-Decenyl acetate	198	$C_{12}H_{22}O_2$	85
22.24	3-Cyclohexene-1-ethanol	126	$C_8H_{14}O$	85
22.73	2-Ethyl-1,6-dioxaspiro[4.4]nonane	156	$C_9H_{16}O_2$	86
30.13	2-Pentadecanone	226	$C_{15}H_{30}O$	94

Full-length blots for Figure 3D





Regarding Figure 3D, we found original RNA samples and performed re-analysis including cDNA synthesis, RT-PCR and electrophoresis. Our results were reproducible when RT-PCR figure was compared with previous one. Old Figure 3D was replaced with new Figure 3D as follows.



Regarding Figure 1C, we could not find RNA as well as full-length blots.