

Bioinformatics strategies for lipidomics analysis: characterization of obesity related hepatic steatosis

Laxman Yetukuri¹, Mikko Katajamaa², Gema Medina-Gomez³, Tuulikki Seppänen-Laakso¹, Antonio Vidal Puig³ and Matej Orešič^{1,*}

¹VTT Technical Research Centre of Finland, Tietotie 2, FIN-02044, Espoo, Finland,

²Turku Centre for Biotechnology, Tykistökatu 6, FIN-20521, Turku, Finland and

³University of Cambridge Department of Clinical Biochemistry, Addenbrooke's Hospital, Hills Road, CB2 2QR, Cambridge, UK

Additional file 2

Title of data: Table of seed fatty acids

Description of data: The table lists the fatty acids utilized for the lipid scaffold generation

Seed number	Systematic Name (LIPID MAPS nomenclature)	SMILES representation	Score	Total No of Carbons
1	decanoyl	<chem>OC(=O)CCCCCCCCC</chem>	1	10
2	undecanoyl	<chem>OC(=O)CCCCCCCCCCC</chem>	4	11
3	dodecanoyl	<chem>OC(=O)CCCCCCCCCCCC</chem>	1	12
4	tridecanoyl	<chem>OC(=O)CCCCCCCCCCCCC</chem>	4	13
5	tetradecanoyl	<chem>OC(=O)CCCCCCCCCCCCC</chem>	1	14
6	(5-tetradecenoyl)	<chem>OC(=O)CCCC=CCCCCCCCC</chem>	2	14
7	pentadecanoyl	<chem>OC(=O)CCCCCCCCCCCCC</chem>	4	15
8	(6-pentadecenoyl)	<chem>OC(=O)CCCC=CCCCCCCCC</chem>	4	15
9	hexadecanoyl	<chem>OC(=O)CCCCCCCCCCCCC</chem>	1	16
10	(9-hexadecenoyl)	<chem>OC(=O)CCCCCCCC=CCCCCCC</chem>	1	16
11	(7-hexadecenoyl)	<chem>OC(=O)CCCCCC=CCCCCCCCC</chem>	2	16
12	heptadecanoyl	<chem>OC(=O)CCCCCCCCCCCCC</chem>	4	17
13	(10-heptadecenoyl)	<chem>OC(=O)CCCCCCCC=CCCCC C</chem>	4	17
14	(8-heptadecenoyl)	<chem>OC(=O)CCCCCCC=CCCCCCC C</chem>	4	17
15	octadecanoyl	<chem>OC(=O)CCCCCCCCCCCCC C</chem>	1	18
16	(9-octadecenoyl)	<chem>OC(=O)CCCCCCCC=CCCCC CC</chem>	1	18

17	(11-octadecenoyl)	OC(=O)CCCCCCCCC=CCCCC CC	1	18
18	(9,12-octadecadienoyl)	OC(=O)CCCCCCCC=CCC=CCC CCC	1	18
19	(9,12,15-octadecatrienoyl)	OC(=O)CCCCCCCC=CCC=CCC =CCC	1	18
20	(6,9,12,15-octadecatetraenoyl)	OC(=O)CCCCC=CCC=CCC=CC C=CCC	1	18
21	nondecenoyl	OC(=O)CCCCCCCCCCCCCCCC CC	4	19
22	(10-nondecenoyl)	OC(=O)CCCCCCCCC=CCCCC CCC	4	19
23	(12-nondecenoyl)	OC(=O)CCCCCCCCCCCC=CCCC CCC	4	19
24	(10,13-nondecadienoyl)	OC(=O)CCCCCCCCC=CCC=CC CCCC	4	19
25	(10,13,16-nondecatrienoyl)	OC(=O)CCCCCCCCC=CCC=CC C=CCC	4	19
26	(7,10,13,16-nondecetetraenoyl)	OC(=O)CCCCCC=CCC=CCC=C CC=CCC	4	19
27	eicosanoyl	OC(=O)CCCCCCCCCCCCCCCC CCC	1	20
28	(11-eicosenoyl)	OC(=O)CCCCCCCCC=CCCCC CCCC	1	20
29	(13-eicosenoyl)	OC(=O)CCCCCCCCCCCC=CCC CCCC	2	20
30	(11,14-eicosadienoyl)	OC(=O)CCCCCCCCC=CCC=C CCCCC	2	20
31	(8,11,14-eicosetrienoyl)	OC(=O)CCCCC=CCC=CCC= CCCCC	1	20
32	(5,8,11,14-eicosetetraenoyl)	OC(=O)CCCC=CCC=CCC=CCC =CCCCC	1	20
33	(5,8,11,14,17-eicosepentaenoyl)	OC(=O)CCCC=CCC=CCC=CCC =CCC=CCC	1	20
34	heneicosanoyl	OC(=O)CCCCCCCCCCCCCCCC CCCC	4	21
35	(12-heneicosenoyl)	OC(=O)CCCCCCCCCCCC=CCCC CCCCC	4	21
36	(14-heneicosenoyl)	OC(=O)CCCCCCCCCCCC=CC	4	21

		CCCCC		
37	(12,15-heneicosadienoyl)	OC(=O)CCCCCCCCCCC=CCC=CCCCC	4	21
38	(9,12,15-heneicosatrienoyl)	OC(=O)CCCCCCCC=CCC=CCC=CCCCC	4	21
39	(6,9,12,15-heneicosetetraenoyl)	OC(=O)CCCCC=CCC=CCC=CC=CCCCC	4	21
40	(6,9,12,15,18-heneicosapentaenoyl)	OC(=O)CCCCC=CCC=CCC=CC=CCC=CCC	4	21
41	docosanoyl	OC(=O)CCCCCCCCCCCCCCCCCCCCCCCC	1	22
42	(13-docosenoyl)	OC(=O)CCCCCCCCCCCCC=CCCCCCCC	1	22
43	(13,16-docosadienoyl)	OC(=O)CCCCCCCCCCCCC=CCC=CCCCCCC	2	22
44	(13,16,19-docosatrienoyl)	OC(=O)CCCCCCCCCCCCC=CCC=CCC=CCC	2	22
45	(10,13,16,19-docosatetraenoyl)	OC(=O)CCCCCCCCC=CCC=CC=CCC=CCC	2	22
46	(7,10,13,16,19-docosapentaenoyl)	OC(=O)CCCCC=CCC=CCC=C=CC=CCC=CCC	1	22
47	(4,7,10,13,16,19-docosahexaenoyl)	OC(=O)CCC=CCC=CCC=CCC=CCC=CCC=CCC	1	22
48	tricosanoyl	OC(=O)CCCCCCCCCCCCCCCCCCCCCCCC	4	23
49	(14-tricosenoyl)	OC(=O)CCCCCCCCCCCCC=CCCCCCCC	4	23
50	(14,17-tricosadienoyl)	OC(=O)CCCCCCCCCCCCC=CC=CCCCCCC	4	23
51	(14,17,20-tricosatrienoyl)	OC(=O)CCCCCCCCCCCCC=CC=CCC=CCC	4	23
52	(11,14,17,20-tricosatetraenoyl)	OC(=O)CCCCCCCCC=CCC=C=CC=CCC=CCC	4	23
53	(8,11,14,17,20-tricosapentaenoyl)	OC(=O)CCCCC=CCC=CCC=CCC=CCC=CCC=CCC	4	23
54	(5,8,11,14,17,20-tricosahexaenoyl)	OC(=O)CCCC=CCC=CCC=CCC=CCC=CCC=CCC=CCC	4	23
55	tetracosanoyl	OC(=O)CCCCCCCCCCCCCCCCCCCCCCCC	1	24

56	(15-tetracosenoyl)	OC(=O)CCCCCCCCCCCCCCC=C CCCCCCCC	1	24
57	(15,18-tetracosadienoyl)	OC(=O)CCCCCCCCCCCCCCC=C CC=CCCCC	2	24
58	(15,18,21-tetracosatrienoyl)	OC(=O)CCCCCCCCCCCCCCC=C CC=CCC=CCC	2	24
59	(12,15,18,21-tetracosatetraenoyl)	OC(=O)CCCCCCCCCCC=CCC= CCC=CCC=CCC	2	24
60	(9,12,15,18,21-tetracosapentaenoyl)	OC(=O)CCCCCCCC=CCC=CCC =CCC=CCC=CCC	2	24
61	(6,9,12,15,18,21-tetracosahexaenoyl)	OC(=O)CCCCC=CCC=CCC=CC C=CCC=CCC=CCC	2	24
62	pentacosanoyl	OC(=O)CCCCCCCCCCCCCCCC CCCCCCCC	4	25
63	(16-pentacosenoyl)	OC(=O)CCCCCCCCCCCCCCCC=C CCCCCCCC	4	25
64	(16,19-pentacosadienoyl)	OC(=O)CCCCCCCCCCCCCCCC=C CCC=CCCCC	4	25
65	(16,19,22-pentacosatrienoyl)	OC(=O)CCCCCCCCCCCCCCCC=C CCC=CCC=CCC	4	25
66	(13,16,19,22-pentacosatetraenoyl)	OC(=O)CCCCCCCCCCC=CCC =CCC=CCC=CCC	4	25
67	(10,13,16,19,22-pentacosapentaenoyl)	OC(=O)CCCCCCCC=CCC=CC C=CCC=CCC=CCC	4	25
68	(7,10,13,16,19,22-pentacosahexaenoyl)	OC(=O)CCCCCC=CCC=CCC=C CC=CCC=CCC=CCC	4	25
69	hexacosanoyl	OC(=O)CCCCCCCCCCCCCCCC CCCCCCCC	2	26
70	(17-hexacosenoyl)	OC(=O)CCCCCCCCCCCCCCCC =CCCCCCCC	2	26
71	(17,20-hexacosadienoyl)	OC(=O)CCCCCCCCCCCCCCCC =CCC=CCCCC	2	26
72	(17,20,23-hexacosatrienoyl)	OC(=O)CCCCCCCCCCCCCCCC =CCC=CCC=CCC	2	26
73	(14,17,20,23-hexacosatetraenoyl)	OC(=O)CCCCCCCCCCCCC=CC C=CCC=CCC=CCC	2	26
74	(11,14,17,20,23-hexacosapentaenoyl)	OC(=O)CCCCCCCCC=CCC=C CC=CCC=CCC=CCC	2	26
75	(8,11,14,17,20,23-	OC(=O)CCCCCCC=CCC=CCC= CCCCCCCC	2	26

	hexacosahexaenoyl)	CCC=CCC=CCC=CCC		
76	heptacosanoyl	OC(=O)CCCCCCCCCCCCCCCCC CCCCCCCCC	4	27
77	(18-heptaacosenoyl)	OC(=O)CCCCCCCCCCCCCCCCC C=CCCCCCCCC	4	27
78	(18,21-heptacosadienoyl)	OC(=O)CCCCCCCCCCCCCCCCC C=CCC=CCCCCC	4	27
79	(18,21,24-heptacosatrienoyl)	OC(=O)CCCCCCCCCCCCCCCCC C=CCC=CCC=CCC	4	27
80	(15,18,21,24-heptacosatetraenoyl)	OC(=O)CCCCCCCCCCCCCCC=C CC=CCC=CCC=CCC	4	27
81	(12,15,18,21,24- heptacosapentaenoyl)	OC(=O)CCCCCCCCCCC=CCC= CCC=CCC=CCC=CCC	4	27
82	(9,12,15,18,21,24- heptacosahexaenoyl)	OC(=O)CCCCCCCC=CCC=CCC =CCC=CCC=CCC=CCC	4	27