Table S1

TAG detected in sebum by RR-RP-HPLC/ESI TOF-MS

	No.	Species	RT (min)	SD	$[M+NH_4]^+$formula	calculated *m/z*	average *m/z*	SD	ppm
DB:0	1	TAG 36:0	22.7	0.06	C39 H78 N O6	656.5824	656.5822	0.0016	2.4
	2	TAG 37:0	23.1	0.04	C40 H80 N O6	670.5989	670.5969	0.0017	2.6
	3	TAG 38:0	23.3	0.04	C41 H82 N O6	684.6142	684.6129	0.0016	2.4
	4	TAG 39:0	23.6	0.05	C42 H84 N O6	698.6293	698.6280	0.0017	2.4
	6	TAG 40:0	24.0	0.13	C43 H86 N O6	712.6455	712.6444	0.0017	2.4
	7	TAG 41:0	24.3	0.04	C44 H88 N O6	726.6606	726.6603	0.0016	2.2
	8	TAG 42:0	24.7	0.05	C45 H90 N O6	740.6763	740.6761	0.0017	2.3
	9	TAG 43:0	25.1	0.05	C46 H92 N O6	754.6919	754.6907	0.0019	2.5
	10	TAG 44:0	25.6	0.06	C47 H94 N O6	768.7076	768.7075	0.0016	2.1
	11	TAG 45:0	26.0	0.08	C48 H96 N O6	782.7232	782.7232	0.0017	2.2
	12	TAG 46:0	26.6	0.08	C49 H98 N O6	796.7389	796.7389	0.0018	2.2
	13	TAG 47:0	27.0	0.10	C50 H100 N O6	810.7545	810.7540	0.0019	2.3
	14	TAG 48:0	27.7	0.12	C51 H102 N O6	824.7702	824.7698	0.0020	2.4
	15	TAG 49:0	28.2	0.10	C52 H104 N O6	838.7858	838.7853	0.0020	2.4
	16	TAG 50:0	29.2	0.15	C53 H106 N O6	852.8015	852.8005	0.0021	2.5
	17	TAG 51:0	29.9	0.20	C54 H108 N O6	866.8171	866.8164	0.0019	2.1
	18	TAG 52:0	31.0	0.17	C55 H110 N O6	880.8328	880.8339	0.0012	1.4
	19	TAG 53:0	32.0	0.20	C56 H112 N O6	894.8484	894.8464	0.0018	2.1
	20	TAG 54:0	33.2	0.26	C57 H114 N O6	908.8641	908.8644	0.0020	2.2
	21	TAG 55:0	34.4	0.29	C58 H116 N O6	922.8797	922.8781	0.0029	3.1
DB:1	1	TAG 36:1	22.4	0.04	C39 H76 N O6	654.5667	654.5660	0.0014	2.1
	2	TAG 37:1	22.7	0.04	C40 H78 N O6	668.5824	668.5824	0.0006	0.9
	3	TAG 38:1	23.0	0.05	C41 H80 N O6	682.5980	682.5980	0.0016	2.4
	4	TAG 39:1	23.2	0.04	C42 H82 N O6	696.6137	696.6132	0.0017	2.4
	5	TAG 40:1	23.5	0.04	C43 H84 N O6	710.6363	710.6322	0.0012	1.7
	6	TAG 41:1	23.8	0.04	C44 H86 N O6	724.6450	724.6448	0.0016	2.2
	7	TAG 42:1	24.2	0.04	C45 H88 N O6	738.6606	738.6601	0.0014	1.9
	8	TAG 43:1	24.5	0.05	C46 H90 N O6	752.6763	752.6755	0.0015	2.0
	9	TAG 44:1	25.0	0.05	C47 H92 N O6	766.6919	766.6921	0.0014	1.9
	10	TAG 45:1	25.4	0.06	C48 H94 N O6	780.7076	780.7082	0.0013	1.6
	11	TAG 46:1	25.9	0.06	C49 H96 N O6	794.7232	794.7233	0.0018	2.3
	12	TAG 47:1	26.3	0.08	C50 H98 N O6	808.7389	808.7380	0.0016	2.0
	13	TAG 48:1	26.9	0.08	C51 H100 N O6	822.7545	822.7553	0.0017	2.1
	14	TAG 49:1	27.4	0.09	C52 H102 N O6	836.7702	836.7700	0.0017	2.0
	15	TAG 50:1	28.1	0.11	C53 H104 N O6	850.7858	850.7858	0.0020	2.3
	16	TAG 51:1	28.8	0.12	C54 H106 N O6	864.8015	864.8022	0.0018	2.1
	17	TAG 52:1	29.5	0.13	C55 H108 N O6	878.8171	878.8179	0.0012	1.4
	18	TAG 53:1	30.4	0.16	C56 H110 N O6	892.8328	892.8329	0.0021	2.3
	19	TAG 54:1	31.4	0.25	C57 H112 N O6	906.8484	906.8472	0.0010	1.1
	20	TAG 55:1	32.7	0.24	C58 H114 N O6	920.8671	920.8627	0.0020	2.2
	21	TAG 56:1	34.0	0.24	C59 H116 N O6	934.8797	934.8775	0.0016	1.7
	22	TAG 57:1	35.1	0.26	C60 H118 N O6	948.8954	948.8940	0.0007	0.7
DB:2	1	TAG 38:2	22.6	0.04	C41 H78 N O6	680.5824	680.5812	0.0014	2.1
	2	TAG 39:2	22.9	0.04	C42 H80 N O6	694.5981	694.5980	0.0015	2.2
	3	TAG 40:2	23.2	0.04	C43 H82 N O6	708.6137	708.6122	0.0008	1.1
	4	TAG 41:2	23.4	0.03	C44 H84 N O6	722.6285	722.6284	0.0016	2.2
	5	TAG 42:2	23.7	0.03	C45 H86 N O6	736.6450	736.6441	0.0019	2.6
	6	TAG 43:2	24.1	0.04	C46 H88 N O6	750.6606	750.6602	0.0019	2.6
	7	TAG 44:2	24.5	0.04	C47 H90 N O6	764.6763	764.6753	0.0015	1.9
	8	TAG 45:2	24.8	0.05	C48 H92 N O6	778.6919	778.6913	0.0016	2.1
	9	TAG 46:2	25.2	0.05	C49 H94 N O6	792.7076	792.7076	0.0017	2.2
	10	TAG 47:2	25.7	0.06	C50 H96 N O6	806.7232	806.7235	0.0017	2.2
	11	TAG 48:2	26.2	0.07	C51 H98 N O6	820.7389	820.7384	0.0015	1.8
	12	TAG 49:2	26.6	0.07	C52 H100 N O6	834.7545	834.7540	0.0019	2.3
	13	TAG 50:2	27.2	0.09	C53 H102 N O6	848.7702	848.7701	0.0016	1.9
	14	TAG 51:2	27.8	0.09	C54 H104 N O6	862.7858	862.7865	0.0016	1.9
	15	TAG 52:2	28.4	0.10	C55 H106 N O6	876.8015	876.8016	0.0015	1.7
	16	TAG 53:2	29.2	0.17	C56 H108 N O6	890.8171	890.8182	0.0021	2.3
	17	TAG 54:2	29.9	0.14	C57 H110 N O6	904.8328	904.8326	0.0021	2.3
	18	TAG 55:2	31.0	0.25	C58 H112 N O6	918.8484	918.8481	0.0011	1.2
	19	TAG 56:2	32.2	0.34	C59 H114 N O6	932.8641	932.8621	0.0019	2.0
	20	TAG 57:2	33.4	0.22	C60 H116 N O6	946.8797	946.8759	0.0011	1.2
DB:3	1	TAG 42:3	23.3	0.04	C45 H84 N O6	734.6293	734.6282	0.0006	0.8
	2	TAG 43:3	23.6	0.03	C46 H86 N O6	748.6450	748.6448	0.0014	1.8
	3	TAG 44:3	24.0	0.03	C47 H88 N O6	762.6606	762.6603	0.0017	2.2
	4	TAG 45:3	24.3	0.04	C48 H90 N O6	776.6763	776.6768	0.0013	1.6
	5	TAG 46:3	24.7	0.04	C49 H92 N O6	790.6919	790.6913	0.0017	2.1
	6	TAG 47:3	25.1	0.05	C50 H94 N O6	804.7076	804.7070	0.0014	1.8
	7	TAG 48:3	25.5	0.06	C51 H96 N O6	818.7232	818.7232	0.0017	2.1
	8	TAG 49:3	26.0	0.07	C52 H98 N O6	832.7389	832.7370	0.0020	2.4
	9	TAG 50:3	26.3	0.27	C53 H100 N O6	846.7545	846.7545	0.0020	2.4
	10	TAG 51:3	26.9	0.08	C54 H102 N O6	860.7702	860.7701	0.0018	2.1
	11	TAG 52:3	27.5	0.09	C55 H104 N O6	874.7858	874.7855	0.0014	1.6
	12	TAG 53:3	28.1	0.10	C56 H106 N O6	888.8015	888.8019	0.0018	2.1
	13	TAG 54:3	28.7	0.11	C57 H108 N O6	902.8171	902.8175	0.0020	2.3
	14	TAG 55:3	29.5	0.13	C58 H110 N O6	916.8328	916.8305	0.0015	1.6
	15	TAG 56:3	30.3	0.15	C59 H112 N O6	930.8484	930.8491	0.0017	1.8
	16	TAG 57:3	31.4	0.20	C60 H114 N O6	944.8641	944.8669	0.0005	0.6
DB:4	1	TAG 46:4	24.2	0.05	C49 H90 N O6	788.6763	788.6759	0.0005	0.6
	2	TAG 47:4	24.5	0.04	C50 H92 N O6	802.6919	802.6904	0.0010	1.3
	3	TAG 48:4	24.9	0.05	C51 H94 N O6	816.7076	816.7063	0.0012	1.5
	4	TAG 49:3	25.3	0.06	C52 H96 N O6	830.7232	830.7237	0.0015	1.8
	5	TAG 50:4	25.8	0.07	C53 H98 N O6	844.7389	844.7398	0.0008	0.9
	6	TAG 51:4	26.3	0.06	C54 H100 N O6	858.7545	858.7554	0.0008	0.9
	7	TAG 52:4	26.7	0.07	C55 H102 N O6	872.7702	872.7708	0.0011	1.2
	8	TAG 53:4	27.3	0.09	C56 H104 N O6	886.7858	886.7869	0.0007	0.7
	9	TAG 54:4	27.7	0.09	C57 H106 N O6	900.8015	900.8025	0.0007	0.7
	10	TAG 55:4	28.5	0.11	C58 H108 N O6	914.8171	914.8174	0.0002	0.2
	11	TAG 56:4	29.2	0.12	C59 H110 N O6	928.8328	928.8369	0.0002	0.2
	12	TAG 57:4	29.4	0.45	C60 H112 N O6	942.8484	942.8504	0.0011	1.1
DB:5	1	TAG 54:5	26.9	0.07	C57 H104 N O6	898.7858	898.7869	0.0010	1.1
	2	TAG 55:5	27.6	0.10	C58 H106 N O6	912.8021	912.8031	0.0010	1.1
	3	TAG 56:5	28.2	0.10	C59 H108 N O6	926.8171	926.8199	0.0024	2.5
	4	TAG 57:5	28.9	0.15	C60 H110 N O6	940.8328	940.8355	0.0024	2.4

Table S2
DAG detected in sebum by RR-RP-HPLC/ESI TOF-MS and MS/MS

	Species	RT (min)	SD	$[M+NH_4]^+$ formula	calculated m/z	$[M+NH_4\text{-}R1COONH_4]^+$ formula	calculated m/z	$[M+NH_4\text{-}R2COONH_4]^+$ formula	calculated m/z	NL (QqQ)	substituent FA
DB:0	**DAG 28:0**	19.50	0.025	C31 H64 NO5	530.4784	C17 H33 O3	285.2431	R1=R2	285.2431	245	14:0; 14:0
	DAG 29:0	19.87	0.034	C32 H66 N O5	544.4941	C17 H33 O3	285.2431	C18 H35 O3	299.2586	245; 259	14:0; 15:0
	DAG 30:0	20.47	0.032	C33 H68 N O5	558.5097	C17 H33 O3	285.2431	C19 H37 O3	313.2743	245; 273	14:0; 16:0
	DAG 31:0	20.85	0.047	C34 H70 NO5	572.5254	C18 H35 O3	299.2586	C19 H37 O3	313.2743	259; 273	15:0; 16:0
	DAG 31:0	"	"	"	"	C17 H33 O3	285.2431	C20 H39 O3	327.2899	245; 287	14:0; 17:0
	DAG 32:0	21.33	0.037	C35 H72 N O5	586.5411	C19 H37 O3	313.2743	R1=R2	313.2743	273	16:0; 16:0
	DAG 32:0	"	"	"	"	C17 H33 O3	285.2431	C21 H41 O3	341.3056	245; 301	14:0; 18:0
	DAG 32:0	"	"	"	"	C18 H35 O3	299.2586	C20 H39 O3	327.2899	259; 287	15:0; 17:0
	DAG 33:0	21.64	0.034	C36 H74 NO5	600.5567	C19 H37 O3	313.2743	C20 H39 O3	327.2899	273; 287	16:0; 17:0
	DAG 34:0	22.11	0.036	C37 H76 NO5	614.5723	C19 H37 O3	313.2743	C21 H41 O3	341.3056	273; 301	16:0; 18:0
	DAG 34:0	"	"	"	"	C20 H39 O3	327.2899	R1=R2	327.2899	287	17:0; 17:0
	DAG 35:0	22.18	0.035	C38 H78 NO5	628.5881	C20 H39 O3	327.2899	C21 H41 O3	341.3056	287; 301	17:0; 18:0
	DAG 36:0	22.50	0.020	C39 H80 NO5	642.6036	C21 H41 O3	341.3056	R1=R2	341.3056	301	18:0; 18:0
DB:1	**DAG 28:1**	18.83	0.048	C31 H62 NO5	528.4628	C17 H33 O3	285.2431	C17 H31 O3	283.2273	243; 245	14:1; 14:0
	DAG 29:1	19.24	0.046	C32 H64 NO5	542.4784	C17 H31 O3	283.2273	C18 H35 O3	299.2586	243; 259	14:1; 15:0
	DAG 30:1	19.88	0.044	C33 H66 N O5	556.4941	C17 H31 O3	283.2273	C19 H37 O3	313.2743	243; 273	14:1; 16:0
	DAG 30:1	"	"	"	"	C17 H33 O3	285.2431	C19 H35 O3	311.2586	245; 271	14:0; 16:1
	DAG 31:1	20.31	0.077	C34 H68 NO5	570.5097	C18 H33 O3	297.2431	C19 H37 O3	313.2743	257; 273	15:1; 16:0
	DAG 31:1	"	"	"	"	C16 H29 O3	269.2117	C21 H41 O3	341.3056	229; 301	13:1; 18:0
	DAG 31:1	"	"	"	"	C18 H35 O3	299.2586	C19 H35 O3	311.2586	259; 271	15:0; 16:1
	DAG 32:1	20.80	0.040	C35 H70 NO5	584.5254	C17 H33 O3	285.2431	C21 H39 O3	339.2899	245; 299	14:0; 18:1
	DAG 32:1	"	"	"	"	C19 H35 O3	311.2586	C19 H37 O3	313.2743	271; 273	16:1; 16:0
	DAG 33:1	21.15	0.037	C36 H72 N O5	598.5411	C18 H33 O3	297.2431	C21 H41 O3	341.3056	257; 301	15:1; 18:0
	DAG 33:1	"	"	"	"	C18 H35 O3	299.2586	C21 H39 O3	339.2899	259; 299	15:0; 18:1
	DAG 33:1	"	"	"	"	C19 H35 O3	311.2586	C20 H39 O3	327.2899	271; 287	16:1; 17:0
	DAG 33:1	"	"	"	"	C19 H37 O3	313.2743	C20 H37 O3	325.2743	273; 285	16:0; 17:1
	DAG 34:1	21.55	0.035	C37 H74 N O5	612.5567	C19 H37 O3	313.2743	C21 H39 O3	339.2899	273; 299	16:0; 18:1
	DAG 34:1	"	"	"	"	C19 H35 O3	311.2586	C21 H41 O3	341.3056	271; 301	16:1; 18:0
	DAG 35:1	21.73	0.154	C38 H76 NO5	626.5723	C19 H37 O3	313.2743	C22 H41 O3	353.3056	273; 313	16:0; 19:1
	DAG 35:1	"	"	"	"	C19 H35 O3	311.2586	C22 H43 O3	355.3212	271; 315	16:1; 19:0
	DAG 35:1	"	"	"	"	C20 H39 O3	327.2899	C21 H39 O3	339.2899	287; 299	17:0; 18:1
	DAG 36:1	22.29	0.043	C39 H78 NO5	640.5881	C19 H37 O3	313.2743	C23 H43 O3	367.3212	273; 327	16:0; 20:1
	DAG 36:1	"	"	"	"	C21 H39 O3	339.2899	C21 H41 O3	341.3056	299; 301	18:1; 18:0
DB:2	**DAG 28:2**	18.48	0.058	C31 H60 NO5	526.4471	C17 H31 O3	283.2273	R1=R2	283.2273	243	14:1; 14:1
	DAG 30:2	19.25	0.045	C33 H64 NO5	554.4784	C17 H31 O3	283.2273	C19 H35 O3	311.2586	243; 271	14:1; 16:1
	DAG 31:2	19.77	0.045	C34 H66 NO5	568.4941	C18 H33 O3	297.2431	C19 H35 O3	311.2586	257; 271	15:1; 16:1
	DAG 32:2	20.24	0.038	C35 H68 NO5	582.5097	C19 H35 O3	311.2586	R1=R2	311.2586	271	16:1; 16:1
	DAG 32:2	"	"	"	"	C17 H31 O3	283.2273	C21 H39 O3	339.2899	243; 299	14:1; 18:1
	DAG 32:2	"	"	"	"	C17 H33 O3	285.2431	C21 H37 O3	337.2743	245; 297	14:0; 18:2
	DAG 33:2	20.63	0.037	C36 H70 N O5	596.5254	C19 H35 O3	311.2586	C20 H37 O3	325.2743	271; 285	16:1; 17:1
	DAG 33:2	"	"	"	"	C18 H33 O3	297.2431	C21 H39 O3	339.2899	257; 299	15:1; 18:1
	DAG 33:2	"	"	"	"	C18 H35 O3	299.2586	C21 H37 O3	337.2743	259; 297	15:0; 18:2
	DAG 34:2	21.04	0.044	C37 H72 NO5	610.5411	C19 H35 O3	311.2586	C21 H39 O3	339.2899	271; 299	16:1; 18:1
	DAG 34:2	"	"	"	"	C19 H37 O3	313.2743	C21 H37 O3	337.2743	273; 297	16:0; 18:2
	DAG 35:2	21.25	0.184	C38 H74 NO5	624.5567	C20 H39 O3	327.2899	C21 H37 O3	337.2743	287; 297	17:0; 18:2
	DAG 35:2	"	"	"	"	C19 H35 O3	311.2586	C22 H41 O3	353.3056	271; 313	16:1; 19:1
	DAG 35:2	"	"	"	"	C20 H37 O3	325.2743	C21 H39 O3	339.2899	285, 299	17:1; 18:1
	DAG 36:2	21.75	0.032	C39 H76 NO5	638.5723	C21 H39 O3	339.2899	R1=R2	339.2899	299	18:1; 18:1
DB:3	**DAG 34:3**	20.62	0.037	C37 H70 NO5	608.5254	C19 H35 O3	311.2586	C21 H37 O3	337.2743	271; 297	16:1; 18:2
	DAG 34:3	"	"	"	"	C17 H31 O3	283.2273	C23 H41 O3	365.3056	243; 325	14:1; 20:2
	DAG 36:3	21.35	0.077	C39 H74 NO5	636.5567	C21 H37 O3	337.2743	C21 H39 O3	339.2899	297; 299	18:2; 18:1
DB:4	**DAG 36:4**	20.68	0.038	C39 H72 NO5	634.5411	C21 H37 O3	337.2743	R1=R2	337.2743	297	18:2; 18:2

Table S3

WE tentatively identified in sebum by RR-RP-HPLC/ESI TOF-MS and MS/MS

	No.	FA 16:1-WE	FOH	RT (min)	SD	$[M+H]^+$ formula	calculated m/z	average m/z	SD	ppm
DB:1	1	WE 28:1	12:0	21.6	0.04	C28 H55 O2	423.4202	423.4199	0.0012	2.41
	2	WE 29:1	13:0	22.0	0.04	C29 H57 O2	437.4359	437.4363	0.0017	3.56
	3	WE 30:1	14:0	22.4	0.04	C30 H59 O2	451.4515	451.4520	0.0015	3.33
	4	WE 31:1	15:0	22.8	0.04	C31 H61 O2	465.4672	465.4675	0.0015	2.90
	5	WE 32:1	16:0	23.2	0.04	C32 H63 O2	479.4828	479.4834	0.0016	3.11
	6	WE 33:1	17:0	23.6	0.04	C33 H65 O2	493.4985	493.4990	0.0015	3.02
	7	WE 34:1	18:0	24.0	0.05	C34 H67 O2	507.5141	507.5146	0.0017	3.14
	8	WE 35:1	19:0	24.4	0.06	C35 H69 O2	521.5298	521.5297	0.0018	2.83
	9	WE 36:1	20:0	24.9	0.07	C36 H71 O2	535.5454	535.5447	0.0017	2.72
	10	WE 37:1	21:0	25.3	0.07	C37 H73 O2	549.5611	549.5612	0.0015	2.05
	11	WE 38:1	22:0	25.8	0.12	C38 H75 O2	563.5767	563.5775	0.0021	3.60
	12	WE 39:1	23:0	26.4	0.09	C39 H77 O2	577.5924	577.5928	0.0027	3.84
	13	WE 40:1	24:0	27.0	0.13	C40 H79 O2	591.6081	591.6084	0.0021	3.20
	14	WE 41:1	25:0	27.6	0.11	C41 H81 O2	605.6231	605.6219	0.0027	4.44
	15	WE 42:1	26:0	28.2	0.12	C42 H83 O2	619.6393	619.6393	0.0021	2.52
DB:2	1	WE 30:2	14:1	21.9	0.03	C30 H57 O2	449.4353	449.4344	0.0016	2.10
	2	WE 31:2	15:1	22.3	0.03	C31 H59 O2	463.4509	463.4511	0.0014	1.17
	3	WE 32:2	16:1	22.7	0.03	C32 H61 O2	477.4666	477.4668	0.0013	1.65
	4	WE 33:2	17:1	23.0	0.05	C33 H63 O2	491.4823	491.4824	0.0016	2.50
	5	WE 34:2	18:1	23.4	0.04	C34 H65 O2	505.4979	505.4986	0.0015	2.44
	6	WE 35:2	19:1	23.7	0.04	C35 H67 O2	519.5136	519.5145	0.0016	3.17
	7	WE 36:2	20:1	24.1	0.05	C36 H69 O2	533.5292	533.5311	0.0009	2.80
	8	WE 37:2	21:1	24.6	0.05	C37 H71 O2	547.5449	547.5455	0.0015	2.03
	9	WE 38:2	22:1	25.0	0.06	C38 H73 O2	561.5605	561.5613	0.0015	2.27
	10	WE 39:2	23:1	25.5	0.05	C39 H75 O2	575.5762	575.5761	0.0016	1.08
	11	WE 40:2	24:1	26.1	0.08	C40 H77 O2	589.5918	589.5922	0.0017	1.92
	12	WE 41:2	25:1	26.5	0.12	C41 H79 O2	603.6075	603.6071	0.0018	2.03
	13	WE 42:2	26:1	27.1	0.10	C42 H81 O2	617.6231	617.6227	0.0018	2.13

Table S4
CE tentatively identified in sebum with RR-RP-HPLC/ESI TOF-MS and MS/MS

No.	Species	RT	SD	$[M+Na]^+$ formula	calculated m/z	detected m/z	SD	ppm	PI (QqQ) $[RCOOH+Na]^+$
1	CE 14:1	26.7	0.05	C41 H70 Na O2	617.5274	617.5295	0.0031	3.4	249.2
2	CE 15:1	27.4	0.05	C42 H72 Na O2	631.5431	631.5447	0.0056	2.5	263.1
3	CE 16:0	29.5	0.16	C43 H76 Na O2	647.5738	647.5759	0.0017	3.2	279.3
4	CE 16:1	28.1	0.06	C43 H74 Na O2	645.5581	645.5591	0.0018	1.6	277.4
5	CE 16:2	27.1	0.05	C43 H72 Na O2	643.5431	643.5432	0.0058	0.2	275.2
6	CE 17:1	28.8	0.07	C44 H76 Na O2	659.5743	659.5755	0.0037	1.9	291.1
7	CE 18:0	31.4	0.10	C45 H80 Na O2	675.6056	675.6034	0.0021	3.3	307.3
8	CE 18:1	29.8	0.08	C45 H78 Na O2	673.5911	673.5897	0.0028	2.1	305.3
9	CE 18:2	28.5	0.06	C45 H76 Na O2	671.5738	671.5745	0.0045	1.0	303.2

Tabe S5
FFA tentatively identified in sebum by RR-RP-HPLC/ESI TOF-MS

	No.	Species	RT (min)	SD	$[M-H]^-$ formula	calculated m/z	average m/z	SD	ppm
DB:0	1	FFA 12:0	4.8	0.06	C12 H23 O2	199.1704	199.1702	0.0006	2.03
	2	FFA 13:0	5.9	0.16	C13 H25 O2	213.1861	213.1855	0.0005	2.73
	3	FFA 14:0	7.5	0.08	C14 H27 O2	227.2017	227.2022	0.0007	2.46
	4	FFA 15:0	9.0	0.08	C15 H29 O2	241.2173	241.2175	0.0004	1.25
	5	FFA 16:0	10.4	0.08	C16 H31 O2	255.2331	255.2337	0.0002	2.18
	6	FFA 17:0	11.7	0.21	C17 H33 O2	269.2486	269.2489	0.0002	1.23
	7	FFA 18:0	13.2	0.07	C18 H35 O2	283.2643	283.2651	0.0003	3.00
	8	FFA 19:0	14.4	0.08	C19 H37 O2	297.2799	297.2821	0.0042	1.94
	9	FFA 20:0	15.5	0.09	C20 H39 O2	311.2956	311.2961	0.0004	1.89
	10	FFA 21:0	16.4	0.07	C21 H41 O2	325.3112	325.3124	0.0010	3.78
	11	FFA 22:0	17.3	0.08	C22 H43 O2	339.3269	339.3276	0.0006	3.04
	12	FFA 23:0	18.1	0.08	C23 H45 O2	353.3425	353.3430	0.0003	1.43
	13	FFA 24:0	18.8	0.10	C24 H47 O2	367.3576	367.3474	0.0081	2.63
	14	FFA 25:0	19.4	0.07	C25 H49 O2	381.3733	381.3754	0.0003	4.05
	15	FFA 26:0	20.1	0.17	C26 H51 O2	395.3889	395.3914	0.0011	4.65
	16	FFA 27:0	20.7	0.05	C27 H53 O2	409.4046	409.4065	0.0003	3.44
	17	FFA 28:0	21.2	0.05	C28 H55 O2	423.4202	423.4223	0.0004	3.68
	18	FFA 29:0	21.6	0.10	C29 H57 O2	437.4359	437.3869	0.0999	1.57
	19	FFA 30:0	22.0	0.06	C30 H59 O2	451.4515	451.4525	0.0012	2.16
DB:1									
	1	FFA 14:1	5.8	0.07	C14 H25 O2	225.1861	225.1864	0.0004	1.77
	2	FFA 15:1	7.2	0.20	C15 H27 O2	239.2017	239.2018	0.0003	2.18
	3	FFA 16:1	8.6	0.08	C16 H29 O2	253.2173	253.2177	0.0005	1.83
	4	FFA 17:1	10.1	0.08	C17 H31 O2	267.2331	267.2334	0.0005	2.27
	5	FFA 18:1	11.3	0.08	C18 H33 O2	281.2486	281.2493	0.0004	2.44
	6	FFA 19:1	12.6	0.07	C19 H35 O2	295.2637	295.2644	0.0009	2.42
	7	FFA 20:1	13.8	0.07	C20 H37 O2	309.2799	309.2808	0.0006	2.73
	8	FFA 21:1	14.9	0.09	C21 H39 O2	323.2951	323.2954	0.0011	2.48
	9	FFA 22:1	15.9	0.08	C22 H41 O2	337.3107	337.3109	0.0006	1.14
	10	FFA 23:1	16.8	0.07	C23 H43 O2	351.3263	351.3278	0.0012	3.64
	11	FFA 24:1	17.6	0.08	C24 H45 O2	365.3421	365.4175	0.1507	2.22
	12	FFA 25:1	18.3	0.08	C25 H47 O2	379.3576	379.3587	0.0013	3.37
	13	FFA 26:1	19.0	0.09	C26 H49 O2	393.3733	393.3741	0.0020	4.64
	14	FFA 27:1	19.7	0.13	C27 H51 O2	407.3889	407.3897	0.0011	1.69
	15	FFA 28:1	20.3	0.11	C28 H53 O2	421.4046	421.4056	0.0008	3.34
	16	FFA 29:1	20.7	0.08	C29 H55 O2	435.4202	435.4204	0.0018	1.05
	17	FFA 30:1	21.2	0.05	C30 H57 O2	449.4359	449.4371	0.0009	2.36
DB:2	1	FFA 16:2	6.9	0.08	C16 H27 O2	251.2017	251.2014	0.0002	0.67
	2	FFA 17:2	8.4	0.14	C17 H29 O2	265.2173	265.2169	0.0005	3.50
	3	FFA 18:2	9.8	0.09	C18 H31 O2	279.2331	279.2336	0.0004	2.40
	4	FFA 19:2	11.3	0.08	C19 H33 O2	293.2486	293.2492	0.0008	2.48
	5	FFA 20:2	12.4	0.08	C20 H35 O2	307.2643	307.2649	0.0002	2.00
	6	FFA 21:2	13.5	0.10	C21 H37 O2	321.2794	321.2795	0.0012	2.83
	7	FFA 22:2	14.6	0.08	C22 H39 O2	335.2951	335.2959	0.0012	2.87
DB:3	1	FFA 18:3	8.2	0.09	C18 H29 O2	277.2168	277.2167	0.0009	2.79
	2	FFA 20:3	11.0	0.08	C20 H33 O2	305.2481	305.2484	0.0008	2.02
	3	FFA 22:3	13.4	0.07	C22 H37 O2	333.2794	333.2802	0.0004	1.07
DB:4	1	FFA 20:4	9.7	0.32	C20 H31 O2	303.2324	303.2329	0.0008	2.06
	2	FFA 22:4	11.9	0.09	C22 H35 O2	331.2637	331.2650	0.0018	3.81