Legend to the supplementary figures

Figure 1S. Scattergrams depicting the distribution of sebum excretion rates (SER) in the study participants according to their clinical severity grade. The red line and cross represent the median and mean values, respectively. *p≤0.05 indicated statistically significant differences towards clear participants calculated by analysis of variance (ANOVA) following post-hoc HSD Tukey's test.

Figure 2S. Eulero-Venn's diagram depicting the number of entities that were commonly modified in the respective severity grades compared to unaffected sebum with a FC≥2.

Figure 3S. MS spectra of diglycerides (DGs) differently regulated in acne sebum according to the severity grade.

Table 1S Demographic characteristics of study participants

GRADING	SIZE	%	[1]AGE (MEAN ± SD)	[2]SER (MEAN ± SD)
CLEAR	17	27.9	14.1 ± 1.2	4.1 ± 2.2
MILD	13	21.3	13.5 ± 1.1	4.6 ± 1.7
MODERATE	19	31.1	14.2 ± 1.8	5.7 ± 3.0
SEVERE	12	19.7	15.2 ± 1.8	7.2 ± 2.5*
TOTAL	61	100	14.2 ± 1.6	5.3 ± 2.7

GRADING	F	%	[1]AGE (MEAN ± SD)	[2]SER (MEAN ± SD)
CLEAR	10	16.4	14.2 ± 1.3	4.3 ± 2.6
MILD	8	13.1	13.5 ± 1.4	4.6 ± 1.7
MODERATE	12	19.7	14.3 ± 2.2	4.3 ± 1.5
SEVERE	2	3.3	14.0 ± 1.4	7.3 ± 1.7*
TOTAL	32	52.5	14.1 ± 1.7	4.8 ± 2.2

GRADING	M	%	[1]AGE (MEAN ± SD)	[2]SER (MEAN ± SD)
CLEAR	7	11.5	14.0 ± 1.0	3.9 ± 1.6
MILD	5	8.2	13.6 ± 0.5	4.6 ± 1.7
MODERATE	7	11.5	13.9 ± 0.9	5.2 ± 2.0
SEVERE	10	16.4	15.4 ± 1.8	7.2 ± 2.7*
TOTAL	29	47.5	14.4 ± 1.4	5.9 ± 3.0

[1]In years
[2]SER= Sebum excretion rate (μg/cm^2/minute)
*$p<0.05$, significance of difference between clear and acne grade calculated with ANOVA with post-hoc HSD Tukey's test.
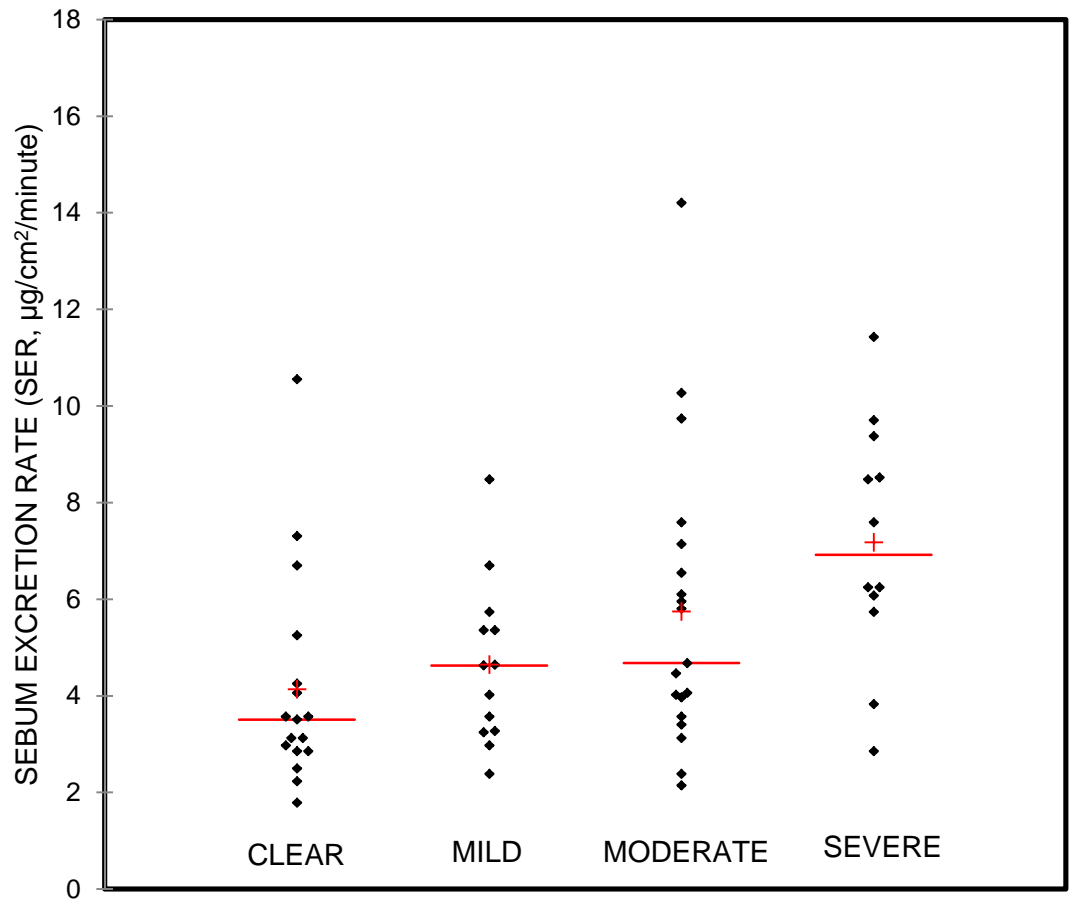
Table 2S. List of the shared lipid species in the Eulero-Venn's diagram (Supplementary Figure 2S)

Lipid class	Elemental formula or annotation	RT*	MILD	MODERATE	SEVERE
Fatty acyls	C21H36O5	8.4710		#	#
Fatty acyls	C27H36O	16.418	#	#	#
Fatty acyls	C21H36O5	8.4710		#	#
Fatty acyls	C40H56O	21.803		#	#
Glycerolipids	DG 30:1	22.999		#	#
Glycerolipids	MG 16:0**	23.699		#	#
Glycerolipids	DG 31:1	23.889		#	#
Glycerolipids	DG 32:1	24.602		#	#
Glycerolipids	DG 34:1	25.799		#	#

*RT= retention time in minutes
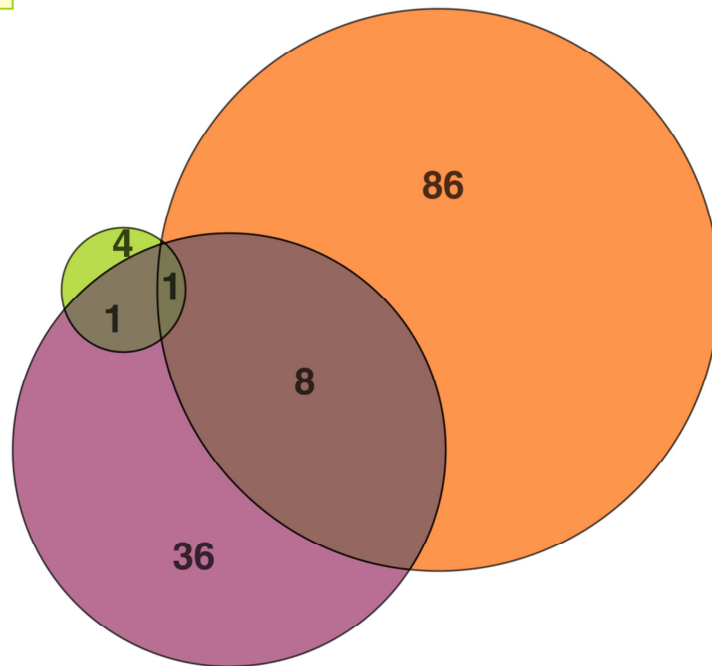**Interpreted as a fragment of FA 16:0-bearing DGs
#Fold change > 2

Supplementary Figure 1S
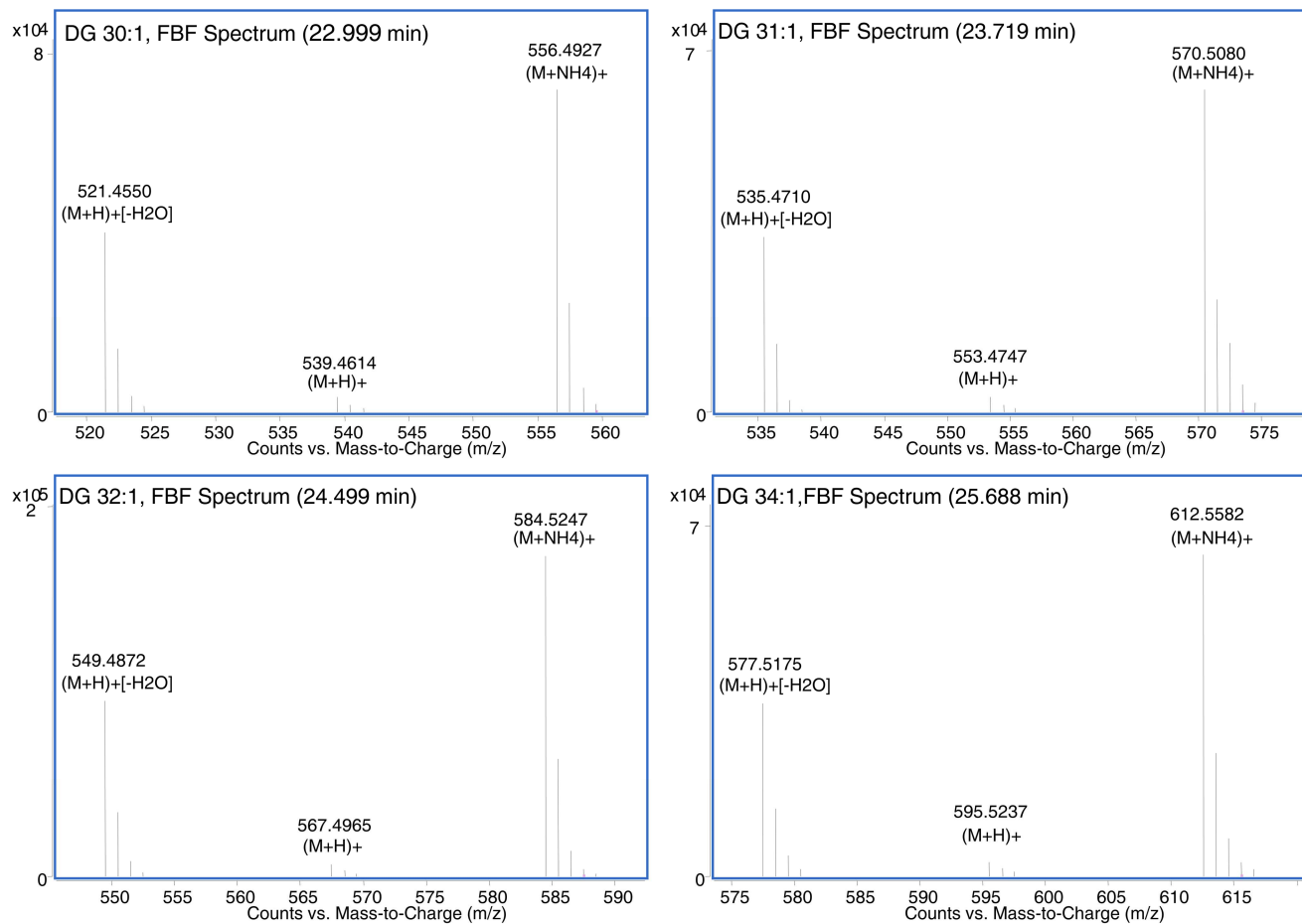
Entity List 1 : (6) T Test unpaired [MILD] Vs [CLEAR] P <= 0.05 FC >=2.0
6 entities

Entity List 2 : (95) T Test unpaired [MODERATE] Vs [CLEAR] P <= 0.05 FC >=2.0
95 entities

Entity List 3 : (46) T Test unpaired [SEVERE] Vs [CLEAR] P <= 0.05 FC >=2.0
46 entities

Supplementary Figure 2S

DG 30:1, FBF Spectrum (22.999 min)

×10⁴

556.4927
(M+NH4)+

521.4550
(M+H)+[-H2O]

539.4614
(M+H)+

Counts vs. Mass-to-Charge (m/z)

DG 31:1, FBF Spectrum (23.719 min)

×10⁴

570.5080
(M+NH4)+

535.4710
(M+H)+[-H2O]

553.4747
(M+H)+

Counts vs. Mass-to-Charge (m/z)

DG 32:1, FBF Spectrum (24.499 min)

×10⁵

584.5247
(M+NH4)+

549.4872
(M+H)+[-H2O]

567.4965
(M+H)+

Counts vs. Mass-to-Charge (m/z)

DG 34:1,FBF Spectrum (25.688 min)

×10⁴

612.5582
(M+NH4)+

577.5175
(M+H)+[-H2O]

595.5237
(M+H)+

Counts vs. Mass-to-Charge (m/z)

Supplementary Figure 3S