

SUPPORTING INFORMATION

Mantonico and Pecorello grape seed extracts: chemical characterization and evaluation of *in vitro* wound-healing and anti-inflammatory activities

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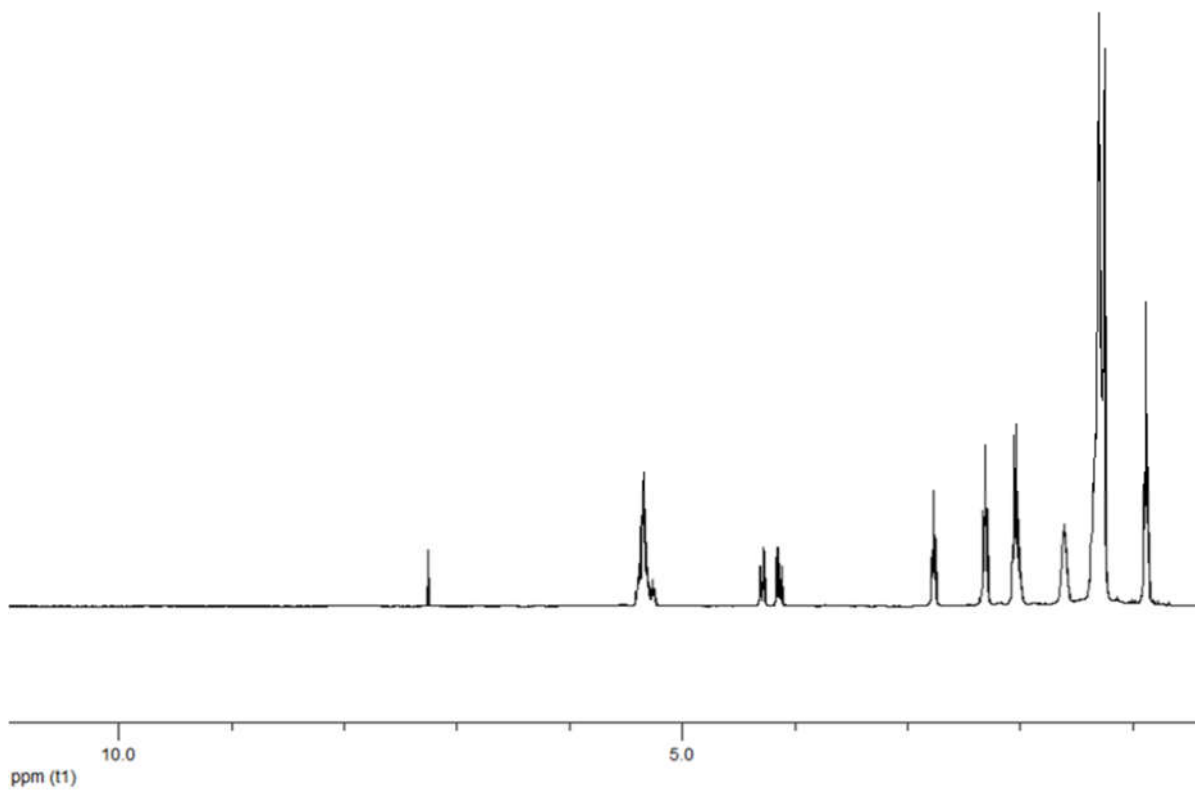


Figure S1. Monodimensional ^1H spectrum of CM

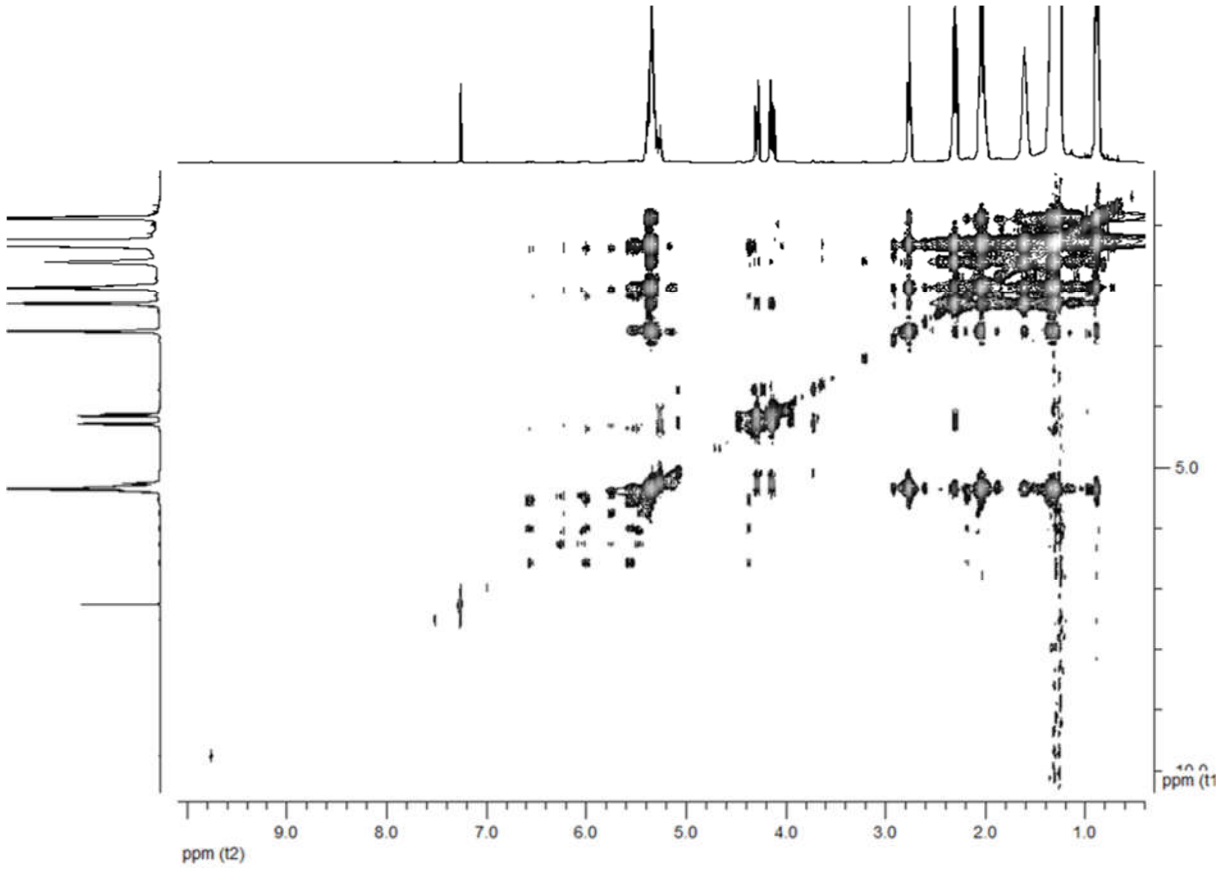


Figure S2. Bidimensional ^1H - ^1H TOCSY spectrum of CM

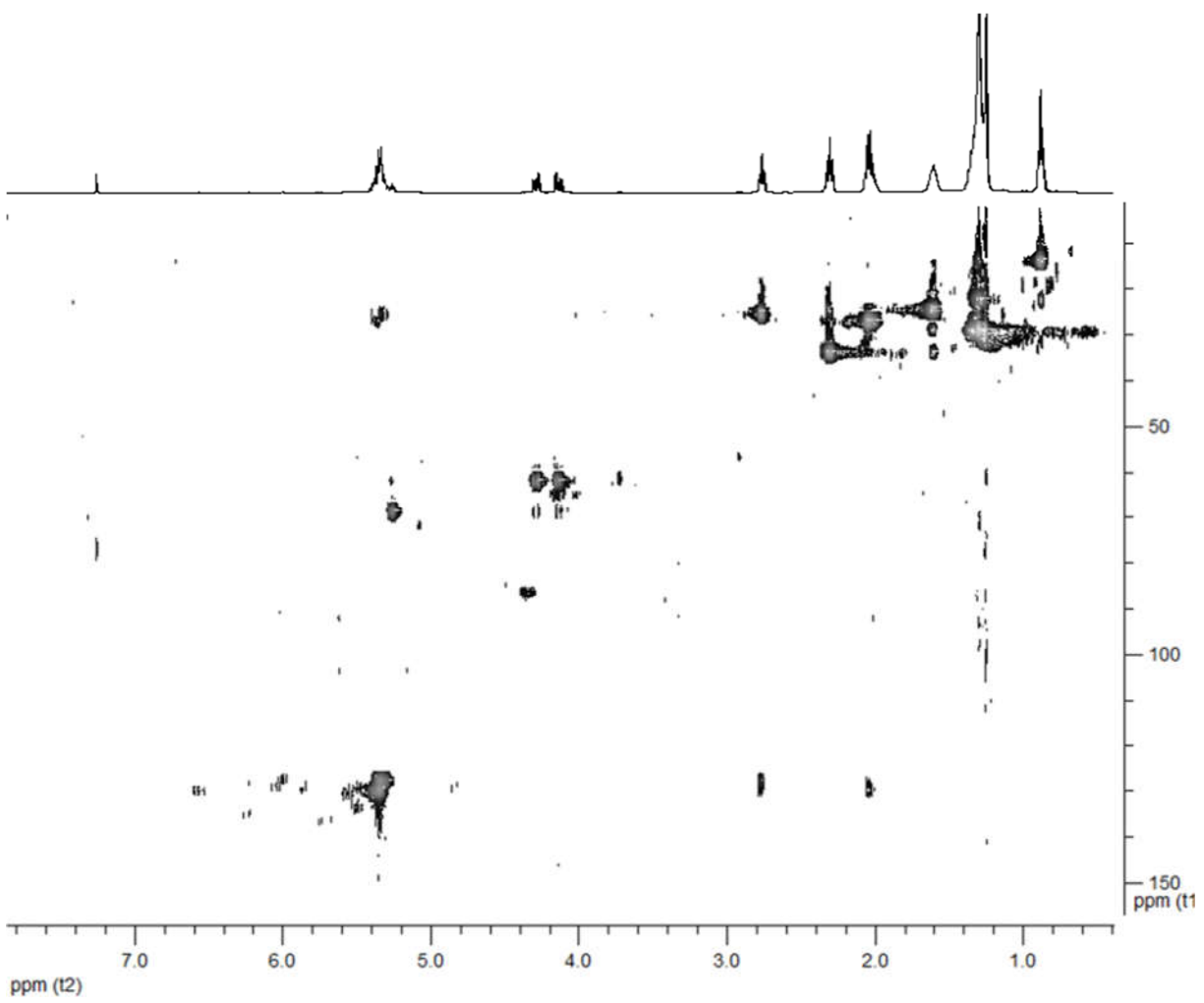


Figure S3. Bidimensional ^1H - ^{13}C HSQC spectrum of CM

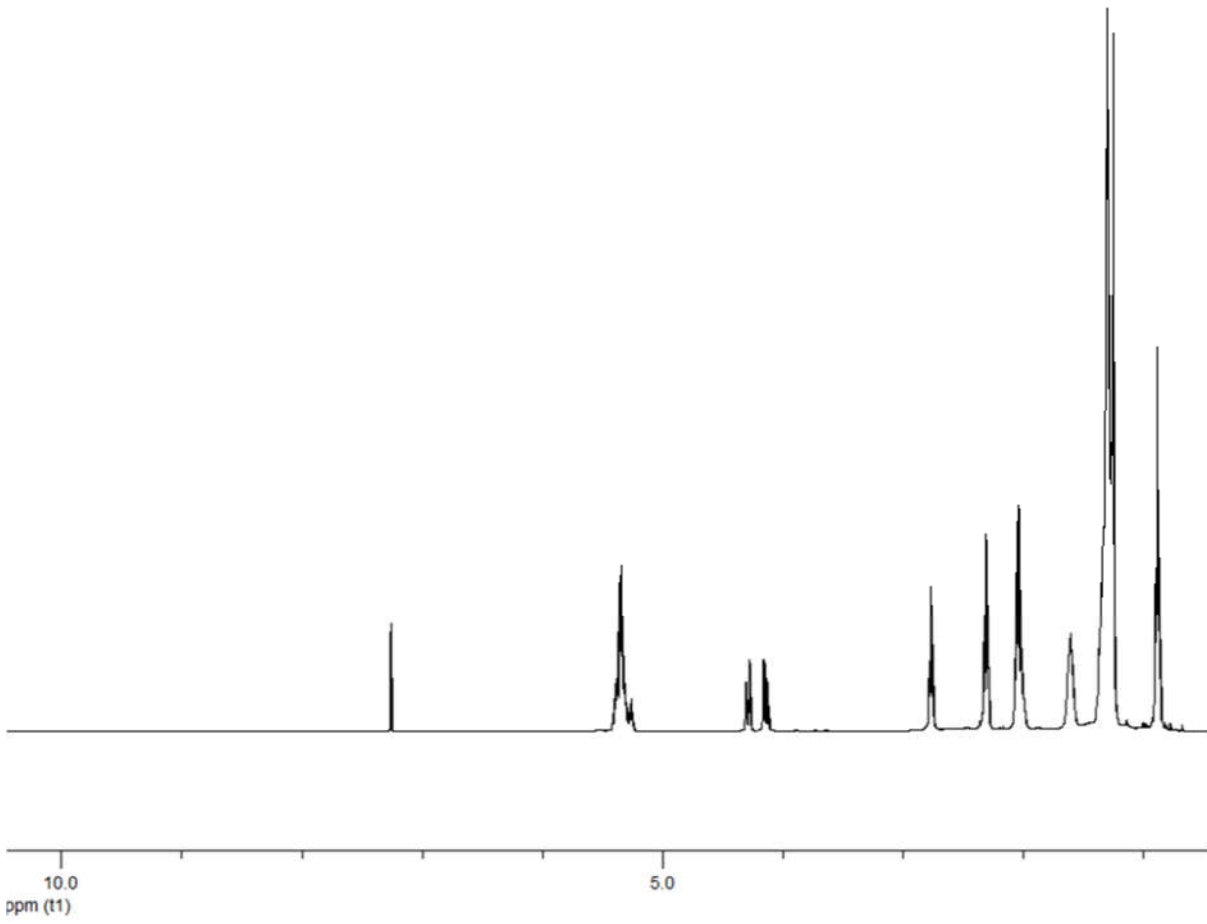


Figure S4. Monodimensional ¹H spectrum of CP

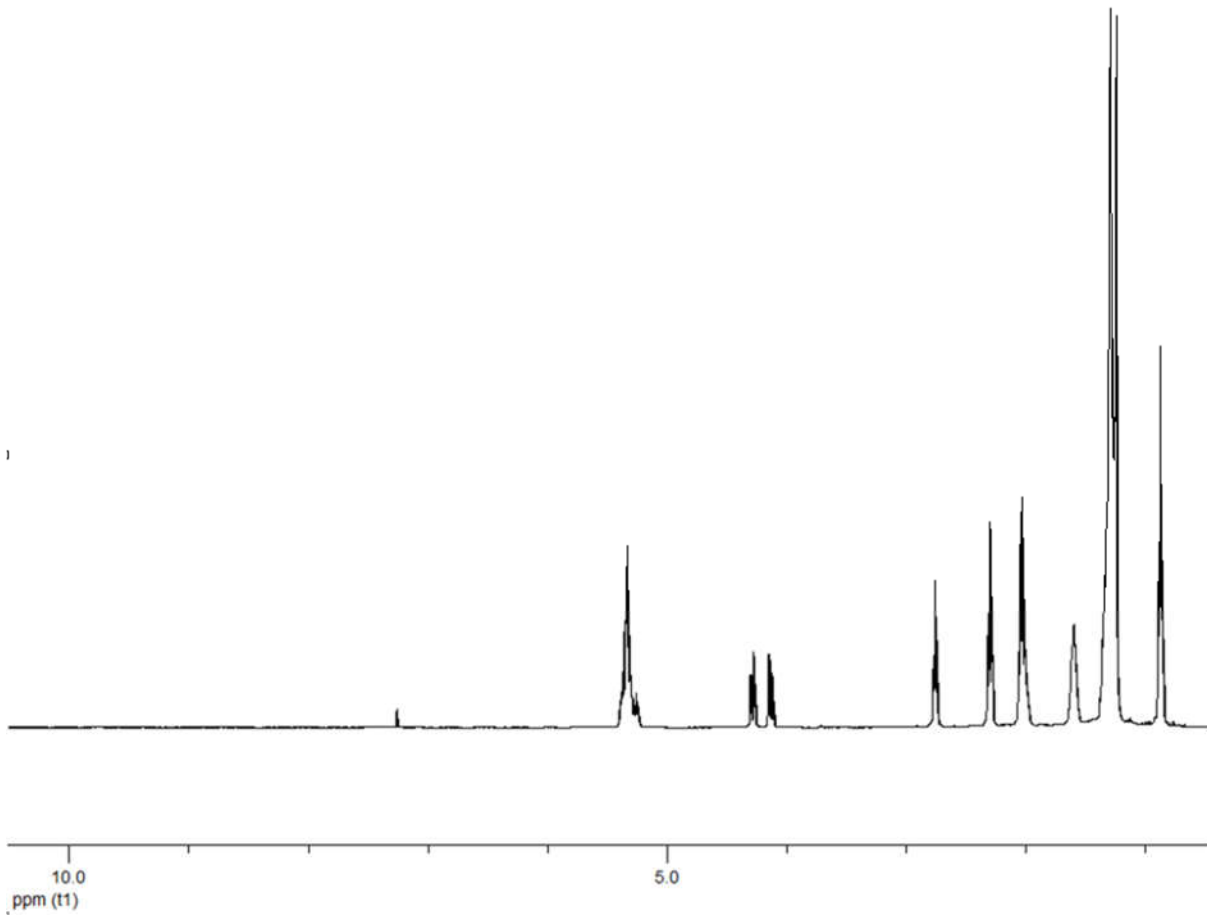


Figure S5. Monodimensional ^1H spectrum of HM

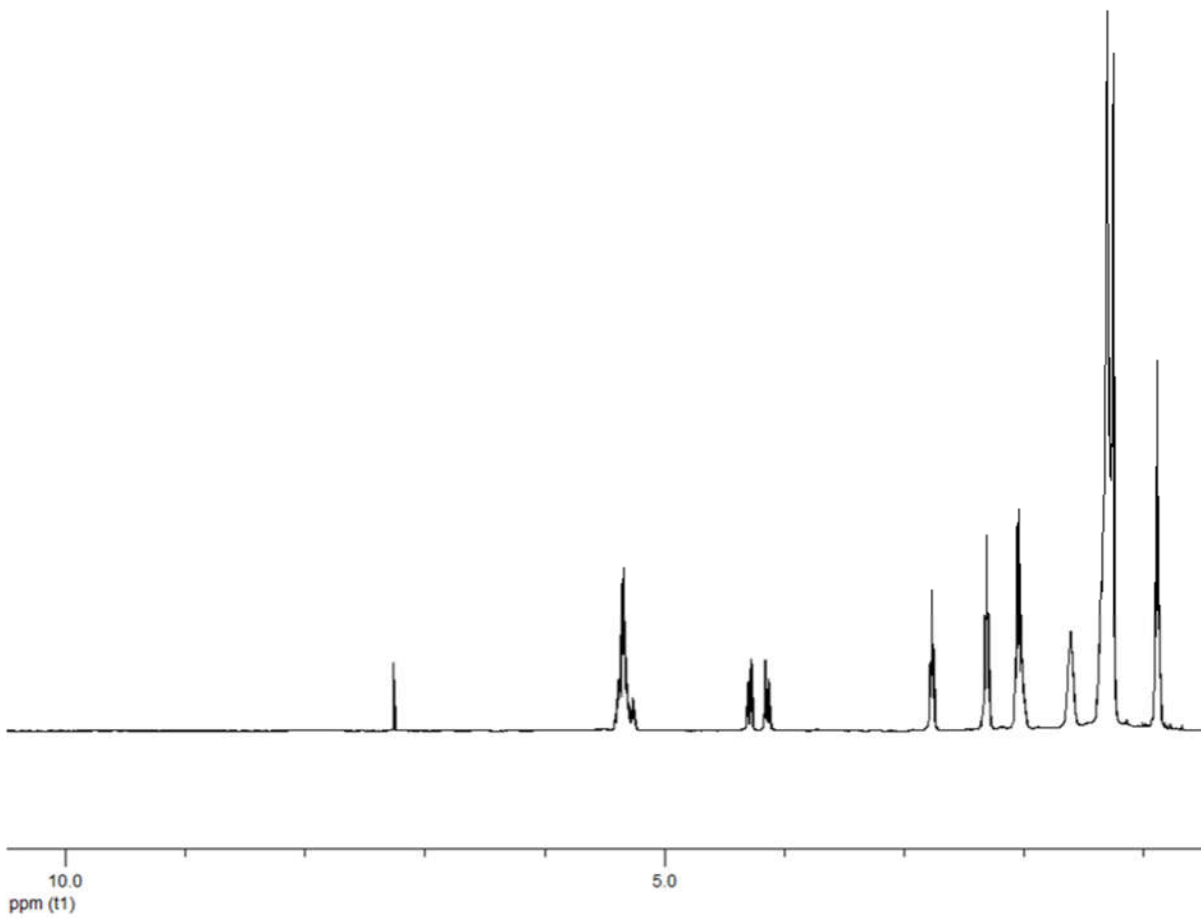


Figure S6. Monodimensional ¹H spectrum of HP

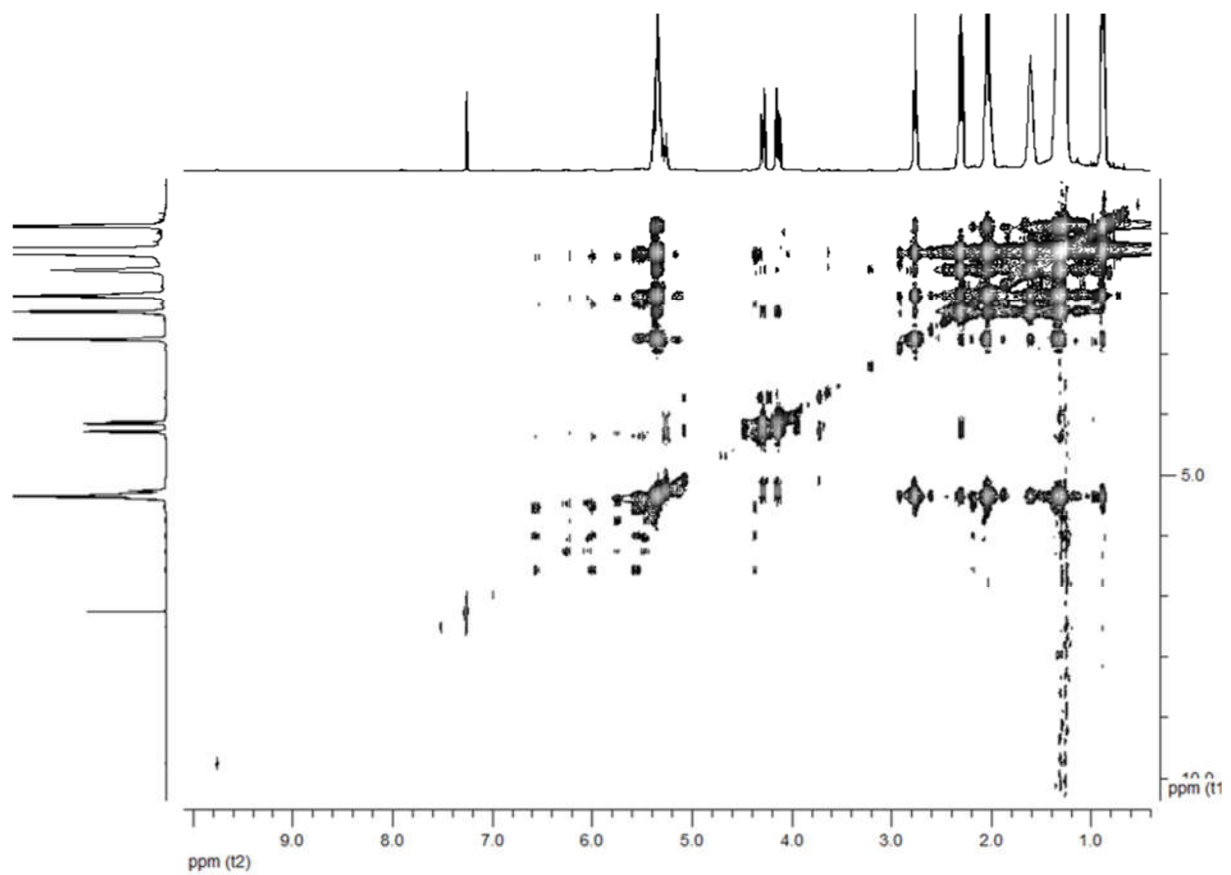


Figure S7. Bidimensional ^1H - ^1H TOCSY spectrum of HP

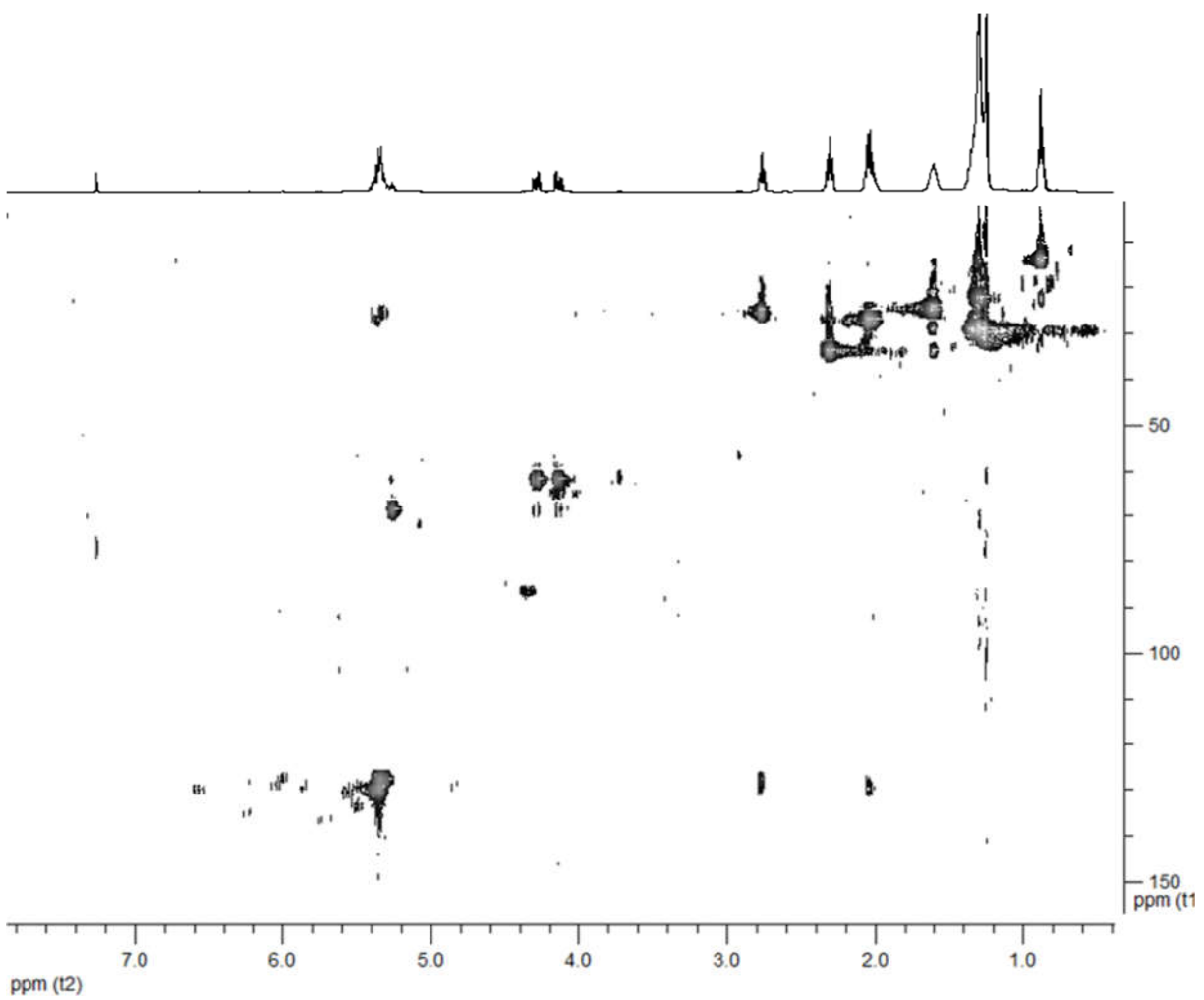


Figure S8. Bidimensional ^1H - ^{13}C HSQC spectrum of HP

Table S1. Table of resonance assignments

Compound ¹	Assignment ²	¹ H δ (ppm)	Multiplicity ³	¹³ C δ (ppm)
Stearic acid	CH ₃	0.87	t	14.05
	n-CH ₂	1.26	m	29.32
	<u>CH</u> ₂ -CH ₂ -CO ₂ ⁻	1.62	m	24.61
	CH ₂ -CO ₂ ⁻	2.30	t	33.52
Oleic acid	CH ₃	0.88	t	14.07
	n-CH ₂	1.27	m	29.35
	CH ₂ -CH=CH	2.03	m	27.14
	CH=CH	5.35	m	129.84; 127.43
	<u>CH</u> ₂ -CH ₂ -CO ₂ ⁻	1.62	m	24.61
	CH ₂ -CO ₂ ⁻	2.31	t	33.96
Linoleic acid	CH ₃	0.86	t	14.06
	n-CH ₂	1.36	m	29.37
	<u>CH</u> ₂ -CH=CH	2.04	m	29.45
	CH=CH	5.37	m	130.29; 128.45
	=CH- <u>CH</u> ₂ -CH=	2.76	t	25.68
	<u>CH</u> ₂ -CH ₂ -CO ₂ ⁻	2.06	m	24.75
	CH ₂ -CO ₂ ⁻	2.31	t	34.05
Monoacylglycerol	CH ₂	3.65-3.55	dd	65.45
	CH ₂	4.05-4.15	dd	70.32
	CH	3.82	m	75.12
Triglyceride	CH	5.13-5.21	m	77.45
	2CH ₂	4.15-4.29	dd	68.23
Oleanoic acid	CH ₂ -1	0.85	t	45.4
	CH ₂ -2	1.44	m	24.5
	CH-3	3.60	m	76.7
	CH-5	0.66	m	54.6
	CH ₂ -6	1.30	m	28.8
	CH ₂ -7	1.63	m	28.9
	CH-9	1.44	m	46.8
	CH ₂ -11	1.82	d	22.6
	CH-12	5.16	bs	121.4

	CH2-16	1.63	m	24.5
	CH2-17	1.44	m	24.5
	CH-18	2.76	m	34.2
	CH-19	1.63	m	45.8
	CH2-21	1.30	m	13.8
	CH2-22	1.44	m	29.3
	CH3-23,24	0,87	t	11.4
	CH3-25,26	0.66	m	13.8
	CH3-27	1.10	m	25.4
	CH3-29	0.87	t	31.8
	CH3-30	0.87	t	22.5
Carotenoids	CH ₂ -2,2'	1.47	m	39.62
	CH ₂ -3,3'	1.62	m	19.27
	CH ₂ -4,4'	2.02	m	33.18
	CH-7,7'	6.15	d	126.68
	CH-8,8'	6.14	d	137.78
	CH-10,10'	6.14	d	130.88
	CH-11,11'	6.68	m	125.04
	CH-12,12'	6.35	d	137.26
	CH-14,14'	6.25	d	132.45
	CH-15,15'	6.63	m	130.02
	CH ₃ -16,16',17,17'	1.03	s	29.01
	CH ₃ -18,18'	1.72	s	21.77
CH ₃ -19,19'	1.97	s	12.81	
Phenols	Aromatic moieties	6.8-7.0	m	130-140
Aldehydes	CHO	9.76	bs	204.01

¹Metabolites identified in the ¹H NMR spectrum of the chloroform (C) and hexane (H) extracts of marcs; ²In bold are evidenced the resonances chosen for metabolite quantification; ³ s: singlet, bs: broad singlet, d: doublet, t: triplet, dd: doublet of doublets, m: multiplet.

Figure S9. GC-MS qualitative analysis for CM extract

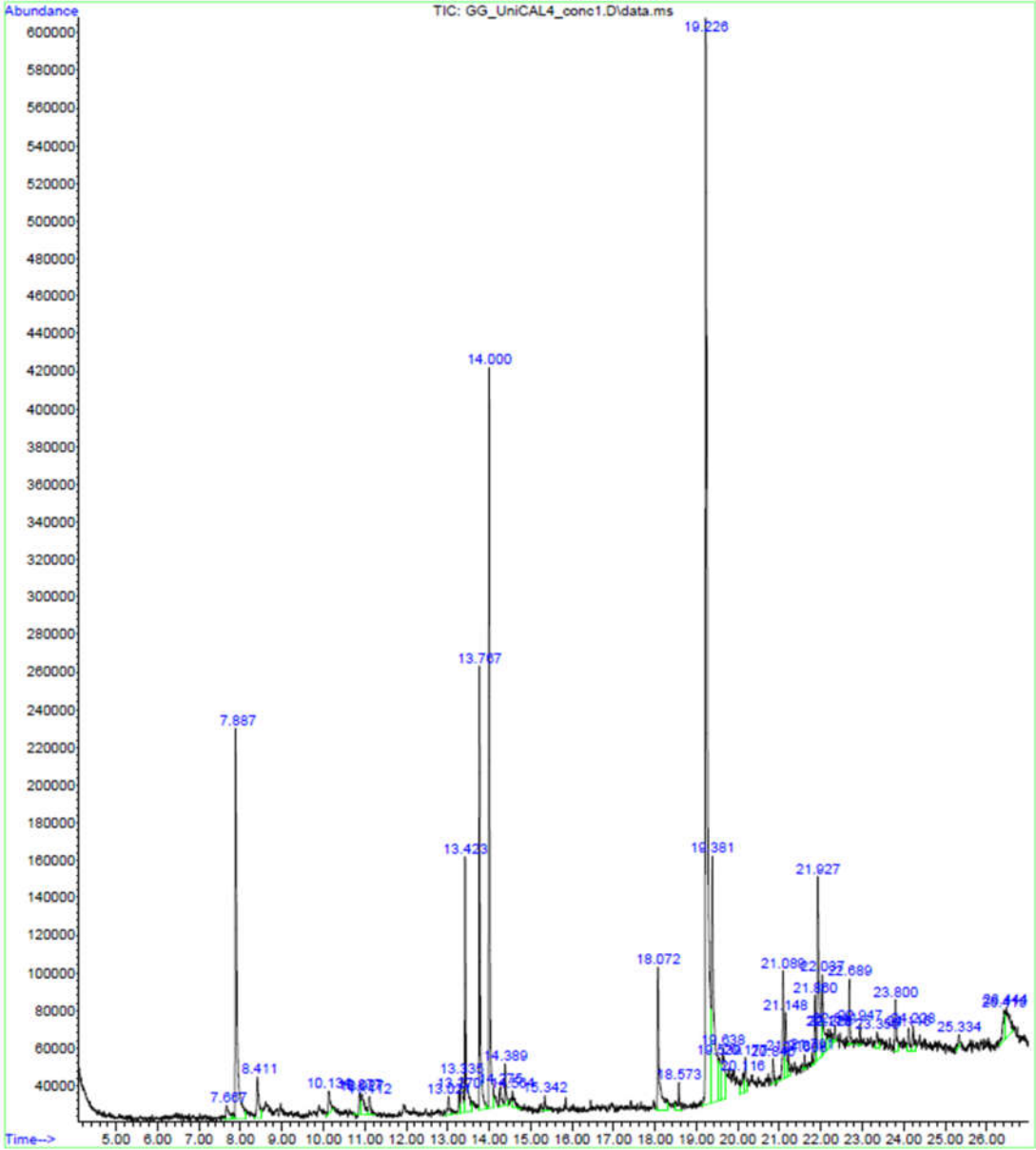


Table S2. Identification of CM peaks

RT	Area%	Library/ID	Quality
7.890	12,45	2-Heptenal, (E)-	83
13.769	9,17	2,4-Decadienal, (E,E)-	91
13.997	13,43	2,4 DECADIENAL	97
18.071	5,10	Hexadecanoic acid	96
18.570	0,86	Hexadecanoic acid	90
19.227	42,50	9,12-Octadecadienoic acid (Z,Z)-	99
19.385	11,22	Octadecanoic acid	91
19.543	2,38	9,12-Octadecadienoic acid (Z,Z)-	90
21.085	2,91	LINOLEIC ACID, BUTYL ESTER	80
<u>Total Identification:</u>		73,32%	

Figure S10. GC-MS qualitative analysis for CP extract

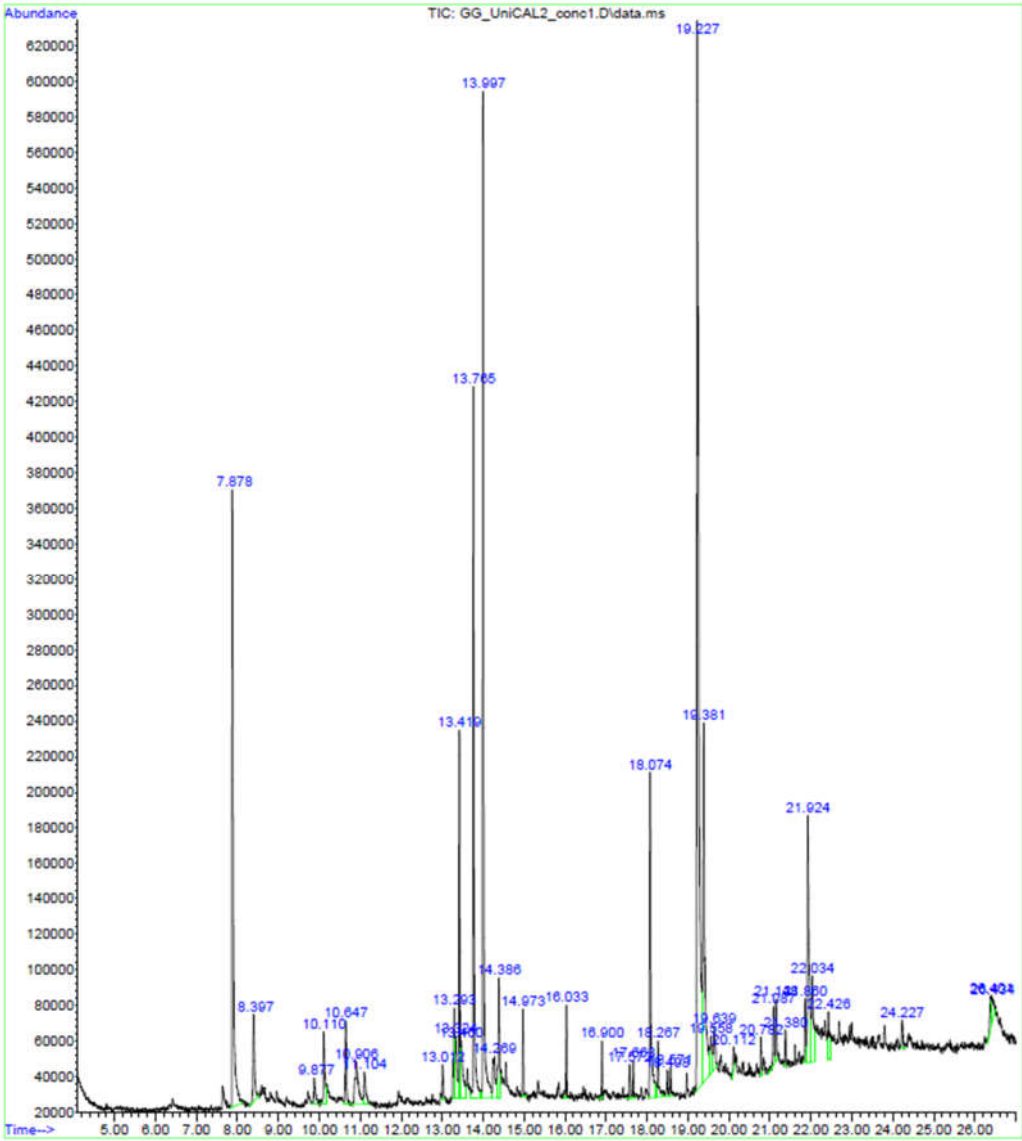


Table S3. Identification of CP peaks

RT	Area%	Library/ID	Quality
7.881	12,59	2-Heptenal, (E)-	96
8.398	2,09	1 OCTEN 3 OL	90
10.106	1,58	2 OCTENAL	90
10.650	1,58	Hexane, 1,1-diethoxy-	90
13.419	5,01	2-Decenal, (E)- (CAS) \$\$ trans-2-D	87
13.769	10,21	2,4-Decadienal, (E,E)-	91
13.997	15,59	2,4-Decadienal, (E,E)-	94
14.969	0,90	Cycloheptasiloxane, tetradecamethyl-	86
17.572	0,51	Phthalic acid, isobutyl nonyl ester	86
17.659	0,53	Eicosamethylcyclodecasiloxane	90
18.071	5,58	Hexadecanoic acid	98
18.264	0,98	Tetradecanoic acid, ethyl ester	90
18.571	0,50	Hexadecanoic acid	90
19.228	31,19	9,12-Octadecadienoic acid (Z,Z)-	97
19.385	9,87	Linoleic acid ethyl ester	99
19.561	1,31	9,12-Octadecadienoic acid (Z,Z)-	97
Total Identification:		74,26 %	

Figure S11. GC-MS qualitative analysis for HM extract

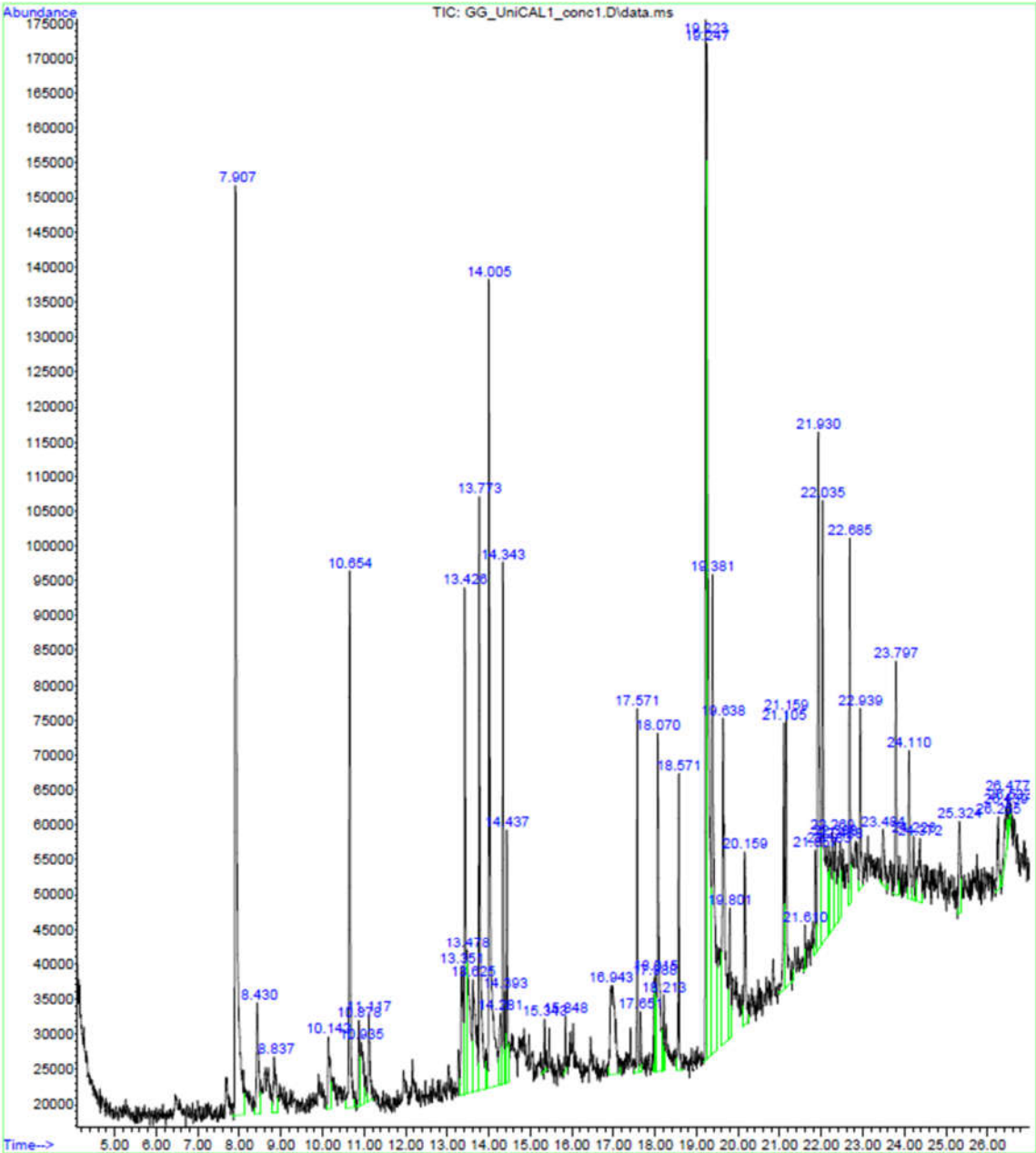


Table S4. Identification of HM peaks

RT	Area%	Library/ID	Quality
7.907	12,45	2-Heptenal, (E)-	96
10.650	5,27	Hexane, 1,1-diethoxy-	91
13.427	4,02	2-Decenal, (Z)-	86
13.769	5,95	2,4-Decadienal	91
14.005	9,76	2,4 DECADIENAL	97
16.941	3,31	1-Octanamine, N-methyl-N-octyl-	80
17.572	2,19	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	90
18.071	3,96	Hexadecanoic acid	91
18.570	2,07	Hexadecanoic acid	93
19.219	6,59	9,12-Octadecadienoic acid (Z,Z)-	98
19.245	14,09	9-Octadecenoic acid (Z)-	95
19.385	7,58	Octadecanoic acid	92
19.639	5,92	9,12-Octadecadienoic acid (Z,Z)-	98
19.797	1,69	Octadecanoic acid	81
20.156	2,13	1-Octanamine, N,N-dioctyl-	86
21.103	2,50	7,12-dioxobenzo[k]fluoranthene	86
21.155	2,53	Octadecane	97
22.031	5,57	Eicosane	95
22.689	2,41	13-Hexacosyne	80
Total Identification:		70,73 %	

Figure S12. GC-MS qualitative analyses for HP extract

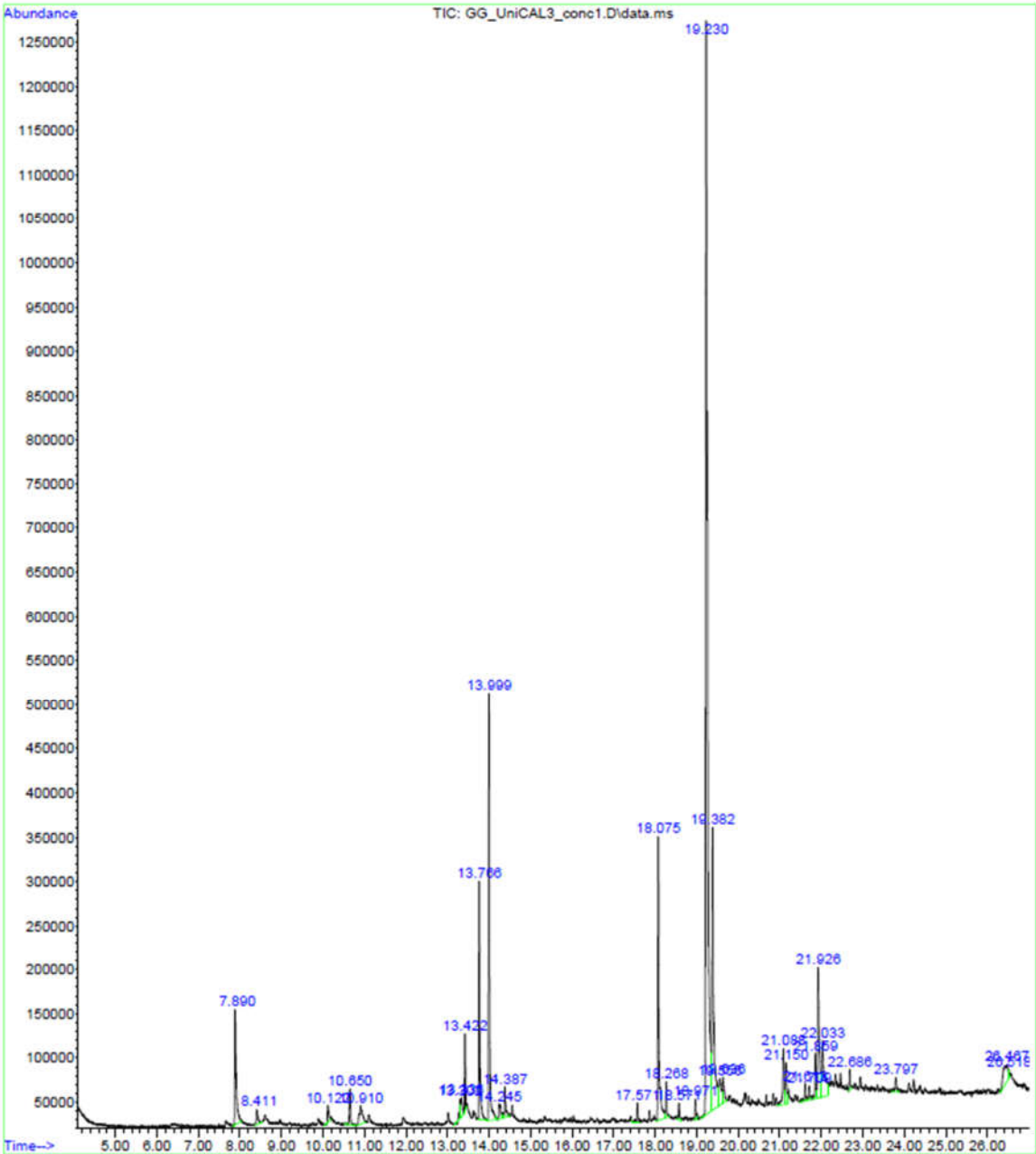


Table S5. Identification of HP peaks

RT	Area%	Library/ID	Quality
7.890	4,53	2-Heptenal, (E)-	90
10.124	0,59	2-Octenal, (E)-	90
10.650	1,18	Hexane, 1,1-diethoxy-	91
13.418	1,48	2-Decenal, (E)-	80
13.769	5,83	2,4-Decadienal, (E,E)-	91
13.997	10,37	2,4 DECADIENAL	97
14.382	0,93	E-2-dodecenal	80
17.572	0,53	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	86
18.071	8,03	Hexadecanoic acid	99
18.264	0,89	Hexadecanoic acid, ethyl ester	99
18.570	0,52	Hexadecanoic acid	93
19.228	49,60	9,12-Octadecadienoic acid (Z,Z)-	99
19.385	12,30	9,12-Octadecadienoic acid, ethyl ester	97
19.552	1,54	9,12-Octadecadienoic acid (Z,Z)-	93
19.639	1,20	9,12-Octadecadienoic acid (Z,Z)-	86
21.611	0,48	Eicosane	93
Total Identification:		81,07%	

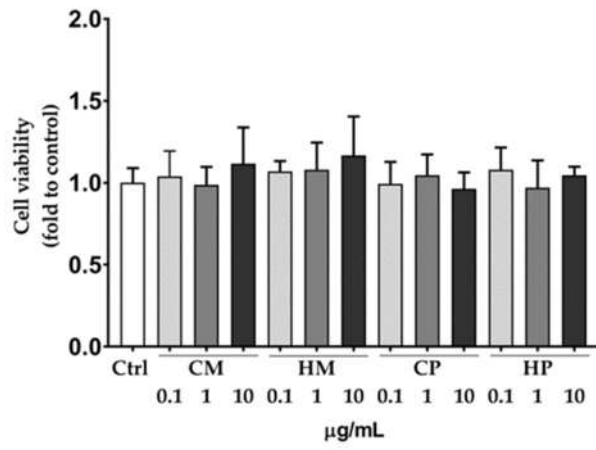


Figure S13. HaCaT cell viability assay