Supplementary Material

Article

Upgrading/Deacidification of organic liquid phase by liquid-liquid extraction using methanol/water as solvente

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Table S1 – Copper corrosivity values of raffinate streams for different water contents in methanol.

Water content (%)	Copper corrosivity		
	Raffinate$_1$	**Raffinate$_2$**	**Raffinate$_4$**
5	1A	1A	1A
10	1A	1A	1A
15	1A	1A	1A
20	1A	1A	1A
25	1A	1A	1A

Table S2 - Mass balance and the respective distribution coefficient values for BO_1, BO_2, and BO_4 deacidification using different water contents in methanol.

Acid values of the original BOs	Water content in methanol	Acid value (Raffinate)	Input streams		Output streams		Distribution coefficient
(mg KOH/g)	(%)	(mg KOH/g)	BOs (g)	Aqueous methanol (g)	Raffinate (g)	Extract (g)	
BO_1 = 24.38	5	6.67	105.03	105.08	89.93	120.18	2.4468
	10	9.53	100.77	100.79	98.48	96.59	1.6481
	15	11.50	100.00	100.02	101.82	93.91	1.1730
	20	13.47	100.11	100.56	143.04	53.24	0.7171
	25	15.73	100.17	100.56	100.65	98.59	0.5535
BO_2 = 33.21	5	10.86	100.10	100.14	82.75	97.80	2.2838
	10	15.75	100.63	100.65	97.00	101.35	1.1365
	15	16.98	100.11	100.2	98.38	99.75	0.9766
	20	17.78	100.05	100.04	95.65	102.31	0.8917
	25	18.53	100.11	100.12	101.31	96.67	0.8080
BO_4 = 73.77	5	45.07	105.61	105.14	115.35	90.68	0.6342
	10	40.27	100.07	100.75	92.10	101.28	0.9006
	15	37.59	100.03	100.17	100.89	95.15	1.0028
	20	34.88	100.17	100.07	100.8	96.7	1.1485
	25	34.30	100.08	100.87	102.66	95.88	1.1742

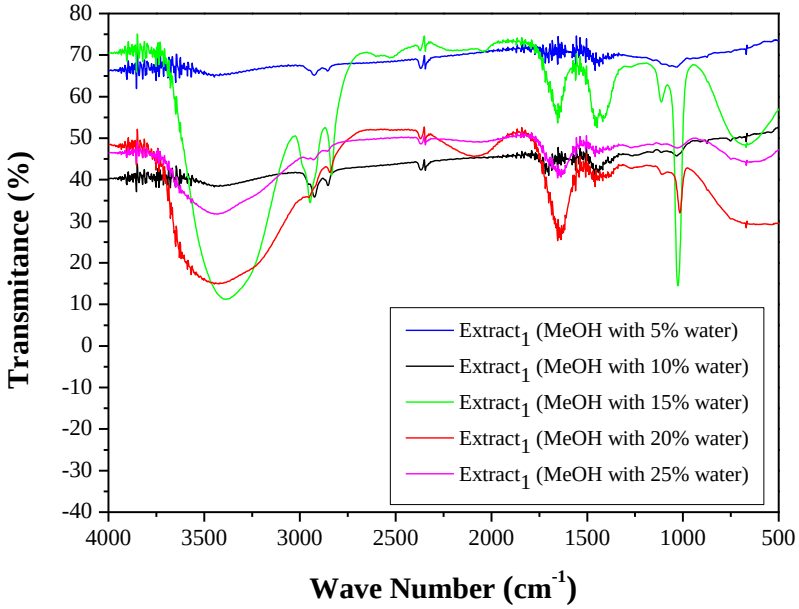

Figure S1 – FTIR spectrum of extract streams referring to BO_1 deacidification using different water contents in methanol.

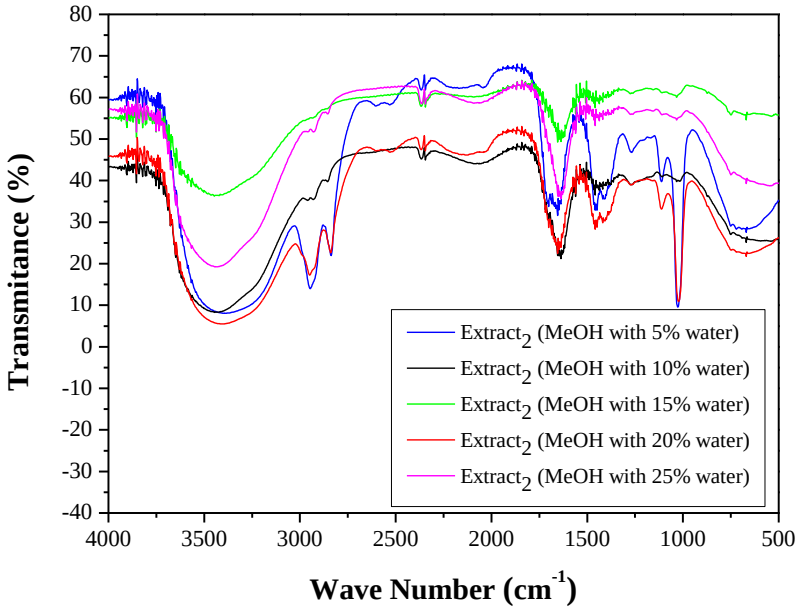

Figure S2 – FTIR spectrum of extract streams referring to BO_2 deacidification using different water contents in methanol.

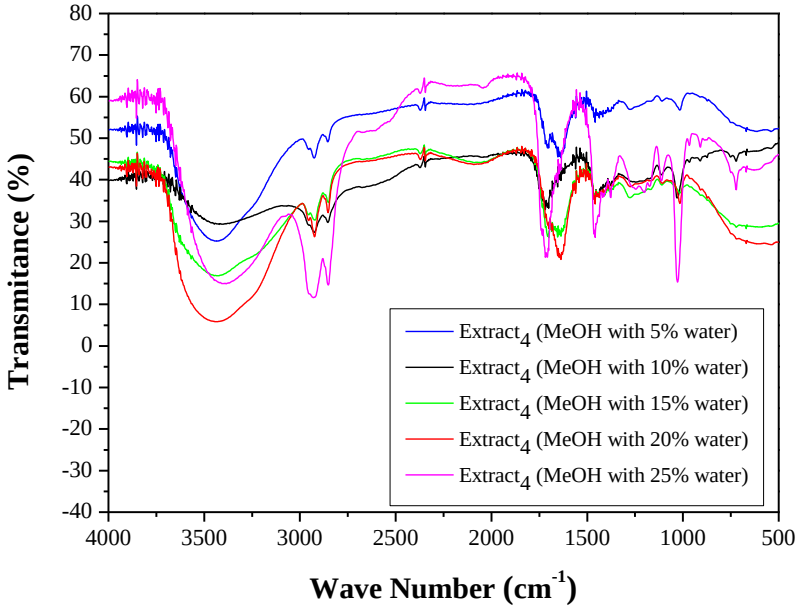

Figure S3 – FTIR spectrum of extract streams referring to BO_4 deacidification using different water contents in methanol.

Table S3 – Copper corrosivity values of raffinate streams referring to BO_3 deacidification using different water contents in methanol at 25 °C and 35 °C.

Teor de água (%)	**Corrosividade ao cobre**	
	25 °C	**35 °C**
5	1A	1A
10	1A	1A
15	1A	1A
20	1A	1A
25	1A	1A

Table S4 – Mass balance and the respective distribution coefficient values for BO_3 deacidification using different water contents in methanol at 25 °C and 35 °C.

Temperature	Water content in methanol	Acid value (Raffinate)	Input streams		Output streams		Distribution coefficient
(°C)	(%)	(mg KOH/g)	BO_3 (g)	Aqueous methanol (g)	Raffinate (g)	Extract (g)	
T = 25	5	30,16	100	100	91,0593	95,7442	0,8345
	10	33,79	100	100	95,72	94,24	0,6035
	15	37,42	100	100	98,15	96,49	0,4108
	20	37,93	100	100	98,95	94,89	0,3898
	25	38,44	100	100	98,94	93,92	0,3747
T = 35	5	25,46	100,1	100,14	86,51	101,03	1,1500
	10	28,91	100,63	100,65	94,57	92,82	0,9149
	15	30,97	100,11	100,2	96,76	92,91	0,7525
	20	31,65	100,05	100,04	97,84	92,81	0,7022
	25	35,21	100,11	100,12	89,42	98,52	0,5805

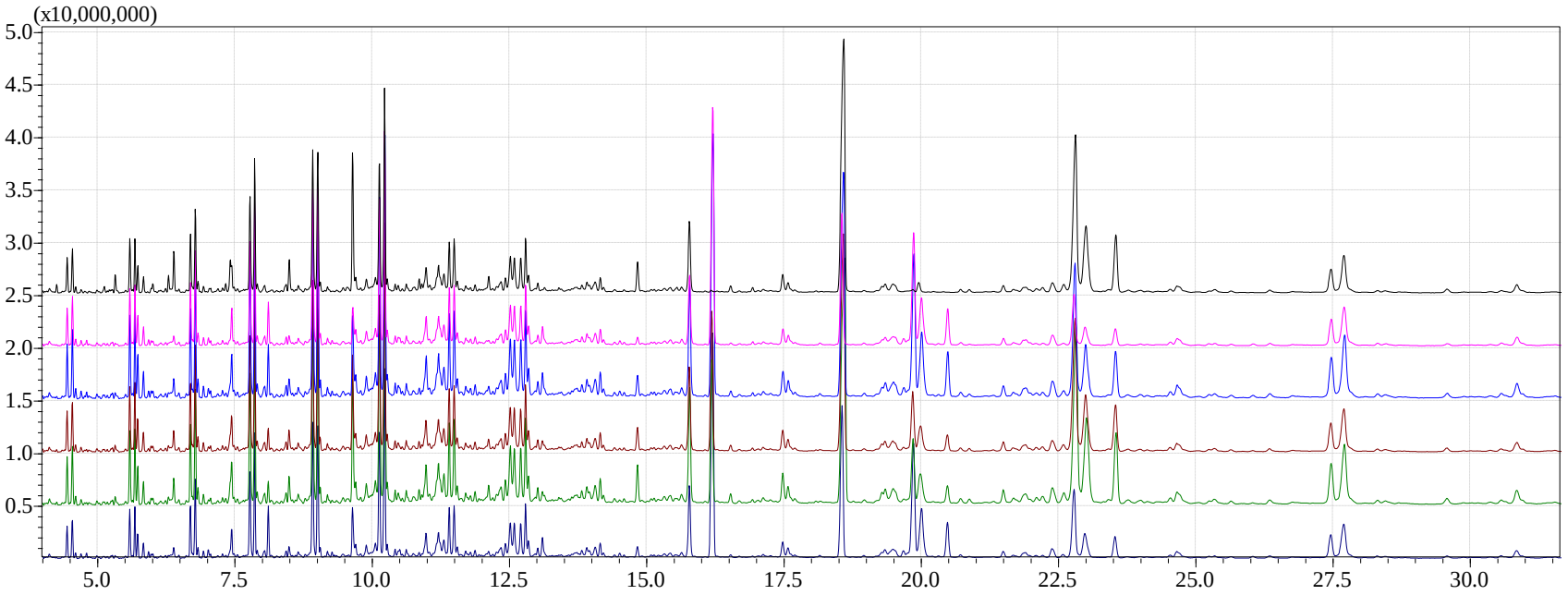

Figure S4 - Chromatograms of the raffinate streams obtained after liquid-liquid extraction at 25 °C and with different water contents in methanol: ▬ BO_3; ▬ Raffinate 3 (MeOH with 5% water); ▬ Raffinate 3 (MeOH with 10% water); ▬ Raffinate 3 (MeOH with 15% water); ▬ Raffinate 3 (MeOH with 20% water); ▬ Raffinate 3 (MeOH with 25% water).

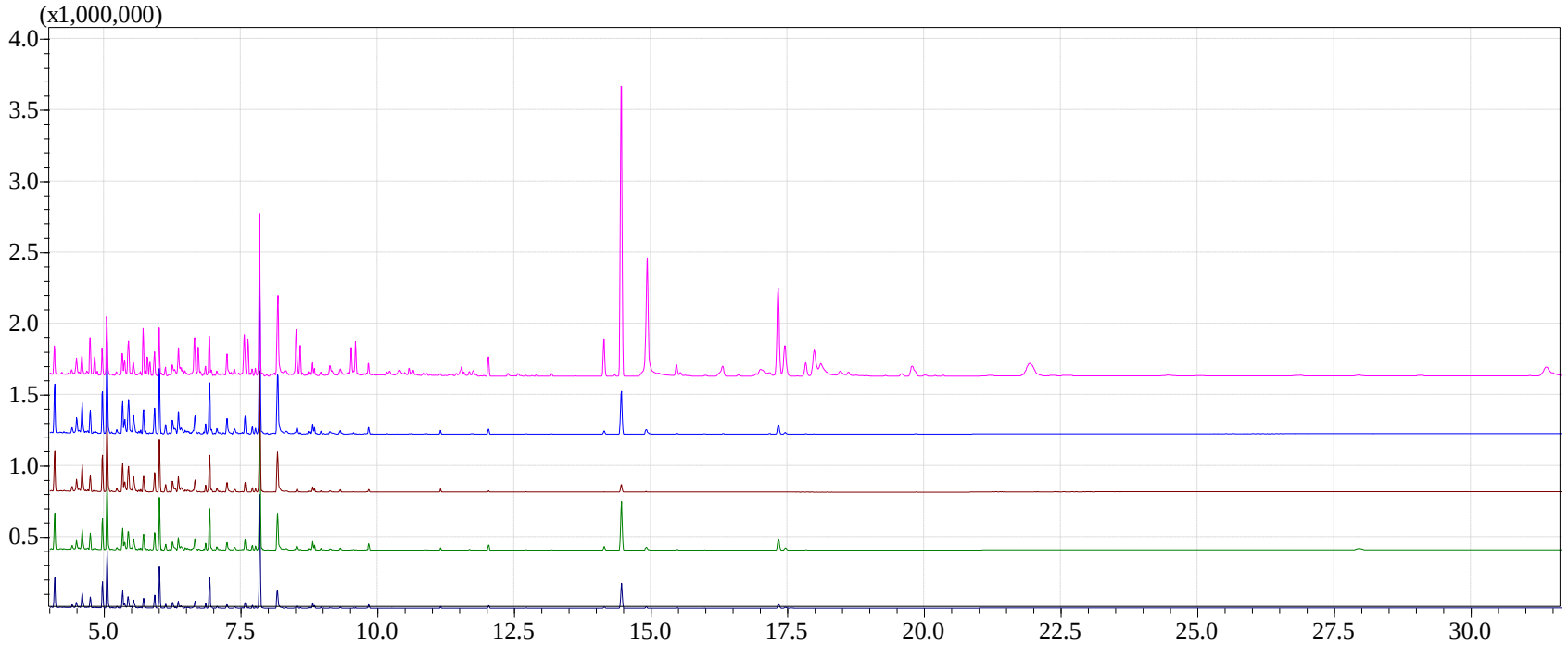

Figure S5 - Chromatograms of the extract streams obtained after liquid-liquid extraction at 25 °C and with different water contents in methanol: Extract 3 (MeOH with 5% water); Extract 3 (MeOH with 10% water); Extract 3 (MeOH with 15% water); Extract 3 (MeOH with 20% water); Extract 3 (MeOH with 25% water).

Table S5 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of BO_3.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.442	0.70	C10H20	1-Decene
4.540	0.86	C10H22	Decane
5.275	0.23	C10H18	Cyclohexene, 1-butyl-
5.321	0.36	C6H12O2	Hexanoic acid
5.584	1.14	C11H22	1-Undecene
5.678	1.19	C11H24	Undecane
5.731	0.56	C11H22	2-Undecene, (E)-
6.387	1.02	C11H22	2-Undecene, (Z)-
6.690	1.4	C12H24	1-Dodecene
6.777	1.84	C13H28	Tridecane
7.437	1.37	C3H8O3	Glycerol
7.772	2.25	C13H26	1-Tridecene
7.859	2.95	C13H28	Tridecane
8.430	0.27	C13H26	Cyclotridecane
8.489	0.82	C9H18O2	Nonanoic acid
8.916	3.68	C14H28	1-Tetradecene
9.006	3.41	C14H30	Tetradecane
9.058	0.23	C9H18	Cyclooctane, methyl-
9.644	3.77	C10H20O2	Decanoic acid
9.699	0.35	C11H20	Cyclopentene,1-hexyl-
9.894	0.50	C14H26	Cyclohexene, 1-octyl-
10.059	0.84	C18H36	9-Octadecene, (E)-
10.130	3.58	C15H30	1-Pentadecene
10.225	5.40	C15H32	Pentadecane
10.274	0.29	C16H32	7-Hexadecene, (Z)-
10.620	0.25	C10H18	Cyclohexene, 3-(2-methylpropyl)-
10.979	0.94	C15H30	n-Nonylcyclohexane
11.206	1.56	C15H28	Cyclohexene, 1-nonyl-
11.305	0.68	C16H32	3-Hexadecene, (Z)-
11.401	1.47	C16H32	1-Hexadecene
11.492	1.49	C16H34	Hexadecane
11.547	0.28	C14H28	Cyclotetradecane
11.703	0.42	C16H32	Cyclohexadecane
12.121	0.32	C12H24O2	Dodecanoic acid
12.344	0.37	C15H30	Cyclopentadecane
12.428	0.38	C18H36O	Oleyl Alcohol
12.515	1.39	C18H36	9-Octadecene, (E)-
12.587	1.31	C20H40	9-Eicosene, (E)-
12.705	1.09	C17H34	1-Heptadecene
12.794	1.59	C18H38	Octadecane
12.847	0.42	C15H30	Cyclopentadecane
14.060	0.39	C17H34	1-Heptadecene
14.152	0.42	C18H38	Octadecane
14.833	0.93	C14H28O2	Tetradecanoic acid

15.778	2.75	C19H38O	2-Nonadecanone
17.475	0.64	C18H36O2	Hexadecanoic acid, ethyl ester
17.574	0.25	C18H36O	Octadecan-4-one
18.588	16.66	C16H32O2	Hexadecanoic acid
19.344	0.24	C20H38O2	Z-10-Octadecen-1-ol acetate
19.482	0.46	C20H42O	1-Eicosanol
19.954	0.42	C19H38O	2-Nonadecanone
21.494	0.28	C20H38O2	Oleic acid, ethyl ester
22.595	0.31	C18H32O2	9,12-Octadecadienoic acid (Z,Z)-
22.806	10.68	C18H34O2	Oleic acid
22.998	5.39	C18H34O2	Oleic acid
23.544	3.11	C18H36O2	Octadecanoic acid
27.462	1.33	C23H46	9-Tricosene, (Z)-
27.697	2.46	C23H46	9-Tricosene, (Z)-
30.846	0.31	C18H36O	8-Octadecanone

Table S6 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Raffinate 3 (MeOH with 5% water) obtained at 25 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.443	0.80	C10H20	1-Decene
4.540	1.04	C10H22	Decane
5.584	1.29	C11H22	1-Dodecene
5.678	1.47	C11H24	Undecane
5.731	0.67	C11H22	2-Undecene, (E)-
5.832	0.40	C11H22	2-Undecene, (Z)-
6.690	1.43	C12H24	1-Dodecene
6.777	2.28	C12H26	Dodecane
6.825	0.25	C12H24	2-Dodecene, (E)-
6.928	0.19	C12H24	Cyclododecane
7.015	0.21	C10H20O2	Nonanoic acid, methyl ester
7.439	0.77	C3H8O3	Glycerol
7.772	2.64	C13H26	1-Tridecene
7.860	3.54	C13H28	Tridecane
8.109	0.99	C11H22O2	Decanoic acid, methyl ester
8.432	0.17	C13H26	Cyclotridecane
8.917	4.33	C14H28	1-Tridecene
9.006	4.18	C14H30	Tetradecane
9.058	0.23	C14H28	7-Tetradecene, (Z)-
9.183	0.18	C14H28	Cyclotetradecane
9.699	0.31	C12H22	Cyclohexene,1-heptyl-
9.894	0.34	C14H26	Cyclohexene,1-octyl-
10.059	0.74	C18H36	9-Octadecene, (E)-
10.131	4.17	C15H30	1-Pentadecene
10.226	6.24	C15H32	Pentadecane
10.275	0.28	C15H30	Cyclopentadecane
10.418	0.21	C16H32	7-Hexadecene, (Z)-
10.508	0.27	C13H26O2	Dodecanoic acid, methyl ester
10.621	0.17	C9H16	Cyclohexene,1-propyl-
10.980	0.94	C15H30	n-Nonylcyclohexane
11.207	1.74	C15H28	Cyclohexene, 1-nonyl-
11.305	0.70	C16H32	3-Hexadecene, (Z)-
11.402	1.66	C16H32	1-Hexadecene
11.493	1.71	C16H34	Hexadecane
11.550	0.27	C14H28	Cyclotetradecane
11.700	0.41	C16H32	Cyclohexadecane
11.875	0.19	C16H30	Cyclohexene, 1-decyl-
12.429	0.44	C18H36O	Oleyl Alcohol
12.515	1.64	C17H34	8-Heptadecene
12.588	1.60	C17H34	8-Heptadecene
12.706	1.33	C17H34	1-Heptadecene
12.795	1.93	C18H38	Octadecane
12.848	0.53	C15H30	Cyclopentadecane
13.018	0.19	C20H40	Cycloeicosane

13.101	0.58	C15H30O2	Methyl tetradecanoate
13.908	0.63	C18H36	9-Octadecene, (E)-
14.062	0.35	C18H36	3-Octadecene, (E)-
14.153	0.44	C18H38	Octadecane
14.834	0.21	C14H28O2	Tetradecanoic acid
15.781	2.99	C19H38O	2-Nonadecanone
16.203	11.56	C17H34O2	Hexadecanoic acid, methyl ester
17.479	0.59	C18H36O2	Hexadecanoic acid, ethyl ester
17.579	0.23	C18H36O	Octadecan-4-one
18.555	6.73	C16H32O2	Hexadecanoic acid
19.859	6.08	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
20.003	3.14	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
20.479	1.82	C19H38O2	Octadecanoic acid, methyl ester
22.782	3.01	C18H34O2	Oleic acid
22.982	1.30	C18H34O2	Oleic acid
23.535	0.87	C18H36O2	Octadecanoic acid
27.468	1.52	C23H46	9-Tricosene, (Z)-
27.701	2.88	C23H46	9-Tricosene, (Z)-

Table S7 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Raffinate 3 (MeOH with 10% water) obtained at 25 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.442	0.73	C10H20	1-Decene
4.540	0.92	C10H22	Decane
5.317	0.27	C6H12O2	Hexanoic acid
5.584	1.22	C11H22	1-Undecene
5.677	1.35	C11H24	Undecane
5.730	0.63	C11H22	2-Undecene, (E)-
5.831	0.41	C11H22	Cyclopropane, octyl-
5.973	0.20	C11H20	1,4-Undecadiene, (E)-
6.690	1.30	C12H24	1-Dodecene
6.777	2.01	C12H26	Dodecane
6.825	0.23	C12H24	2-Dodecene, (E)-
7.438	0.79	C3H8O3	Glycerol
7.773	2.33	C13H26	1-Tridecene
7.861	2.98	C13H28	Tridecane
8.108	0.75	C11H22O2	Decanoic acid, methyl ester
8.918	3.46	C14H28	1-Tetradecene
9.008	3.41	C14H30	Tetradecane
9.058	0.20	C14H28	7-Tetradecene, (E)-
9.644	1.69	C10H20O2	Decanoic acid
9.699	0.34	C11H20	Cyclopentene,1-hexyl-
9.893	0.50	C14H26	Cyclohexene, 1-octyl-
10.060	0.88	C18H36	9-Octadecene, (E)-
10.133	3.71	C15H30	1-Pentadecene
10.230	5.28	C15H32	Pentadecane
10.508	0.22	C13H26O2	Dodecanoic acid, methyl ester
10.981	1.07	C15H30	n-Nonylcyclohexane
11.207	1.79	C15H28	Cyclohexene, 1-nonyl-
11.305	0.73	C16H32	3-Hexadecene, (Z)-
11.401	1.61	C16H32	1-Hexadecene
11.493	1.61	C16H34	Hexadecane
11.548	0.29	C14H28	Cyclotetradecane
11.704	0.42	C16H32	Cyclohexadecane
12.258	0.20	C18H36O	Oleyl Alcohol
12.345	0.43	C15H30	Cyclopentadecane
12.428	0.44	C18H36O	Oleyl Alcohol
12.514	1.56	C17H34	8-Heptadecene
12.588	1.49	C18H36	9-Octadecene, (E)-
12.706	1.24	C17H34	1-Heptadecene
12.795	1.77	C17H36	Heptadecane
12.848	0.49	C15H30	Cyclopentadecane
13.100	0.53	C15H30O2	Tetradecanoic acid, methyl ester
13.909	0.27	C20H40	9-Eicosene, (E)-
14.062	0.62	C20H40	3-Eicosene, (E)-
14.152	0.43	C18H38	Octadecane

14.832	0.46	C14H28O2	Tetradecanoic acid
15.783	3.08	C19H38O	2-Nonadecanone
16.208	8.66	C17H34O2	Hexadecanoic acid, methyl ester
17.479	0.64	C18H36O2	Hexadecanoic acid, ethyl ester
17.579	0.26	C18H36O	Octadecan-4-one
18.585	9.57	C16H32O2	Hexadecanoic acid
19.864	4.97	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
20.007	2.70	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
20.481	1.48	C19H38O2	Octadecanoic acid, methyl ester
21.495	0.30	C20H38O2	Oleic acid, ethyl ester
22.387	0.64	C21H36	Benzene, pentadecyl-
22.798	5.51	C18H34O2	Oleic acid
22.993	2.76	C18H34O2	Oleic acid
23.538	1.67	C18H36O2	Octadecanoic acid
27.468	1.59	C23H46	9-Tricosene, (Z)-
27.711	2.91	C23H46	9-Tricosene, (Z)-

Table S8 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Raffinate 3 (MeOH with 15% water) obtained at 25 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.441	0.72	C10H20	1-Decene
4.538	0.91	C10H22	Decane
5.317	0.29	C6H12O2	Hexanoic acid
5.583	1.26	C11H22	1-Dodecene
5.676	1.35	C11H24	Undecane
5.728	0.64	C11H22	Cyclopropane, 1-pentyl-2-propyl-
5.830	0.40	C11H22	Cyclopropane, octyl-
6.688	1.44	C12H24	1-Dodecene
6.775	1.97	C12H26	Dodecane
6.824	0.25	C12H24	5-Dodecene, (E)-
7.058	0.21	C13H24	5-Tridecene
7.436	0.94	C3H8O3	Glycerol
7.770	2.46	C13H26	1-Tridecene
7.859	3.20	C13H28	Tridecane
8.106	0.43	C11H22O2	Decanoic acid, methyl ester
8.486	0.45	C9H18O2	Nonanoic acid
8.915	3.97	C14H28	1-Tetradecene
9.006	3.72	C14H30	Tetradecane
9.052	0.26	C14H28	Cyclotetradecane
9.642	2.41	C10H20O2	Decanoic acid
9.700	0.34	C11H20	Cyclopentene,1-hexyl-
9.891	0.69	C14H26	Cyclohexene, 1-octyl-
10.058	0.91	C18H36	9-Octadecene, (E)-
10.130	3.99	C15H30	1-Pentadecene
10.225	5.68	C15H32	Pentadecane
10.273	0.31	C16H32	7-Hexadecene, (Z)-
10.415	0.56	C16H32	7-Hexadecene, (Z)-
10.617	0.49	C10H18	Cyclohexene, 3-(2-methylpropyl)-
10.977	1.15	C15H30	n-Nonylcyclohexane
11.204	1.85	C15H28	Cyclohexene, 1-nonyl-
11.303	0.72	C16H32	3-Hexadecene, (Z)-
11.399	1.64	C16H32	1-Hexadecene
11.492	1.62	C16H34	Hexadecane
11.546	0.30	C14H28	Cyclotetradecane
11.692	0.49	C16H32	1-Hexadecene
12.427	0.40	C18H36O	Oleyl Alcohol
12.513	1.49	C18H36	9-Octadecene, (E)-
12.585	1.39	C20H40	9-Eicosene, (E)-
12.703	1.17	C17H34	1-Heptadecene
12.793	1.73	C18H38	Octadecane
12.846	0.45	C20H40	5-Eicosene, (E)-
13.908	0.26	C16H34O	1-Hexadecanol
14.060	0.57	C20H40	3-Eicosene, (E)-
14.150	0.40	C19H40	Nonadecano

14.831	0.65	C14H28O2	Tetradecanoic acid
15.776	2.87	C19H38O	2-Nonadecanone
16.184	4.91	C17H34O2	Hexadecanoic acid, methyl ester
17.475	0.67	C18H36O2	Hexadecanoic acid, ethyl ester
17.574	0.25	C18H36O	Octadecan-4-one
18.583	12.39	C16H32O2	Hexadecanoic acid
19.842	2.42	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
19.987	1.43	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
20.473	0.64	C19H38O2	Octadecanoic acid, methyl ester
21.495	0.23	C20H38O2	Oleic acid, ethyl ester
22.799	7.78	C18H34O2	Oleic acid
22.991	3.9	C18H34O2	Oleic acid
23.538	2.27	C18H36O2	Octadecanoic acid
27.460	1.36	C23H46	9-Tricosene, (Z)-
27.697	2.35	C23H46	9-Tricosene, (Z)-

Table S9 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Raffinate 3 (MeOH with 20% water) obtained at 25 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.442	0.66	C10H20	1-Decene
4.540	0.82	C10H22	Decane
5.317	0.27	C6H12O2	Hexanoic acid
5.584	1.13	C11H22	1-Undecene
5.677	1.21	C11H24	Undecane
5.730	0.57	C11H22	2-Undecene, (E)-
5.831	0.36	C11H22	Cyclopropane, octyl-
5.973	0.22	C11H20	1,4-Undecadiene, (E)-
6.690	1.28	C12H24	1-Dodecene
6.776	1.73	C12H26	Dodecane
7.437	0.93	C3H8O3	Glycerol
7.772	2.21	C13H26	1-Tridecene
7.860	2.83	C13H28	Tridecane
8.107	0.32	C11H22O2	Decanoic acid, methyl ester
8.487	0.46	C9H18O2	Nonanoic acid
8.917	3.36	C14H28	1-Tetradecene
9.008	3.33	C14H30	Tetradecane
9.644	2.50	C10H20O2	Decanoic acid
9.698	0.33	C11H20	Cyclopentene,1-hexyl-
9.893	0.52	C14H26	Cyclohexene, 1-octyl-
10.058	0.91	C12H24	Cyclododecane
10.132	3.69	C15H30	1-Pentadecene
10.229	5.16	C15H32	Pentadecane
10.275	0.32	C15H30	Cyclopentadecane
10.417	0.22	C16H32	7-Hexadecene, (Z)-
10.619	0.31	C9H14O	Bicyclo[3.1.0]hexan-2-one, 3,3,6-
10.979	1.04	C15H30	n-Nonylcyclohexane
11.205	1.72	C15H28	Cyclohexene, 1-nonyl-
11.306	0.68	C16H32	3-Hexadecene, (Z)-
11.401	1.60	C16H32	1-Hexadecene
11.493	1.59	C16H34	Hexadecane
11.546	0.28	C14H28	Cyclotetradecane
11.702	0.37	C16H32	Cyclohexadecane
12.120	0.22	C12H24O2	Dodecanoic acid
12.345	0.61	C18H36	Cyclodecane, octyl-
12.427	0.44	C18H36O	Oleyl Alcohol
12.515	1.55	C17H34	8-Heptadecene
12.587	1.47	C20H40	9-Eicosene, (E)-
12.704	1.24	C17H34	1-Heptadecene
12.794	1.79	C17H36	Heptadecane
12.846	0.48	C20H40	5-Eicosene, (E)-
13.907	0.28	C20H40	9-Eicosene, (E)-
14.060	0.35	C18H36	1-Octadecene
14.150	0.49	C18H38	Octadecane

14.831	0.82	C14H28O2	Tetradecanoic acid
15.781	3.19	C19H38O	2-Nonadecanone
16.185	3.96	C17H34O2	Hexadecanoic acid, methyl ester
16.525	0.22	C15H30O2	n-Pentadecanoic acid
17.476	0.75	C18H36O2	Hexadecanoic acid, ethyl ester
17.574	0.30	C18H36O	Octadecan-4-one
18.604	12.77	C16H32O2	Hexadecanoic acid
19.344	0.49	C14H26O	Ethanone, 1-cyclododecyl-
19.849	2.09	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
19.983	1.38	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
20.474	0.50	C19H38O2	Octadecanoic acid, methyl ester
21.493	0.39	C20H38O2	Oleic acid, ethyl ester
22.817	9.13	C18H34O2	Oleic acid
23.007	4.86	C18H34O2	Oleic acid
23.547	2.79	C18H36O2	Octadecanoic acid
27.465	1.59	C23H46	9-Tricosene, (Z)-
27.706	2.92	C23H46	9-Tricosene, (Z)-

Table S10 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Raffinate 3 (MeOH with 25% water) obtained at 25 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.441	0.70	C10H20	1-Decene
4.538	0.87	C10H22	Decane
5.583	1.14	C11H22	1-Undecene
5.676	1.20	C11H24	Undecane
5.729	0.59	C11H22	Cyclopropane, 1-pentyl-2-propyl-
5.830	0.34	C11H22	Cyclopropane, octyl-
5.927	0.13	C9H18O2	Octanoic acid, methyl ester
6.689	1.25	C12H24	1-Dodecene
6.776	1.87	C13H28	Tridecane
6.824	0.22	C12H24	5-Dodecene, (E)-
6.926	0.16	C12H24	Cyclododecane
7.012	0.16	C10H20O2	Nonanoic acid, methyl ester
7.437	0.72	C3H8O3	Glycerol
7.771	2.30	C13H26	1-Tridecene
7.859	3.02	C13H28	Tridecane
8.107	1.23	C11H22O2	Decanoic acid, methyl ester
8.915	3.62	C14H28	1-Tetradecene
9.006	3.52	C14H30	Tetradecane
9.058	0.21	C14H28	5-Tetradecene, (E)-
9.642	1.64	C10H20O2	Decanoic acid
9.700	0.26	C11H20	Cyclopentene,1-hexyl-
9.892	0.29	C13H24	Cyclohexene,1-heptyl-
10.058	0.59	C18H36	9-Octadecene, (E)-
10.129	3.78	C15H30	1-Pentadecene
10.224	5.62	C15H32	Pentadecane
10.274	0.24	C16H32	7-Hexadecene, (Z)-
10.416	0.20	C18H36	5-Octadecene, (E)-
10.501	0.33	C13H26O2	Dodecanoic acid, methyl ester
10.619	0.55	C9H14O	Bicyclo[3.1.0]hexan-2-one, 3,3,6-
10.978	1.07	C15H30	n-Nonylcyclohexane
11.205	1.96	C15H28	Cyclohexene, 1-nonyl-
11.304	0.71	C16H32	3-Hexadecene, (Z)-
11.400	1.62	C16H32	1-Hexadecene
11.491	1.63	C16H34	Hexadecane
11.547	0.29	C14H28	Cyclotetradecane
11.700	0.51	C16H32	Cyclohexadecane
11.873	0.17	C16H30	Cyclohexene, 1-decyl-
12.427	0.41	C18H36O	Oleyl Alcohol
12.513	1.50	C18H36	9-Octadecene, (E)-
12.586	1.41	C20H40	9-Eicosene, (E)-
12.704	1.18	C17H34	1-Heptadecene
12.792	1.74	C18H38	Octadecane
12.845	0.45	C15H30	Cyclopentadecane
13.015	0.19	C16H32	1-Hexadecene

13.099	0.66	C15H30O2	Tetradecanoic acid, methyl ester
13.906	0.25	C20H40	9-Eicosene, (E)-
14.061	0.56	C20H40	3-Eicosene, (E)-
14.150	0.40	C18H38	Octadecane
14.830	0.35	C14H28O2	Tetradecanoic acid
15.777	3.02	C17H34O	2-Heptadecanone
16.201	11.13	C17H34O2	Hexadecanoic acid, methyl ester
17.474	0.58	C18H36O2	Hexadecanoic acid, ethyl ester
17.573	0.25	C18H36O	Octadecan-4-one
18.557	8.15	C16H32O2	Hexadecanoic acid
19.856	6.50	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
20.004	3.33	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
20.475	1.84	C19H38O2	Octadecanoic acid, methyl ester
22.782	4.33	C18H34O2	Oleic acid
22.976	1.96	C18H34O2	Oleic acid
23.529	1.17	C18H36O2	Octadecanoic acid
27.458	1.36	C23H46	9-Tricosene, (Z)-
27.694	2.57	C23H46	9-Tricosene, (Z)-

Table S11 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Extract 3 (MeOH with 5% water) obtained at 25 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.085	1.26	C7H14O2	Hexanoic acid, methyl ester
4.490	0.96	C6H12O2	Hexanoic acid
4.587	1.10	C6H6O	Phenol
4.737	1.93	C10H22O	1-Octanol, 2,7-dimethyl-
4.821	0.97	C11H24	Undecane
4.958	1.10	C8H14O2	6-Heptenoic acid, methyl ester
5.043	2.65	C8H16O2	Heptanoic acid, methyl ester
5.326	1.00	C7H8O	Phenol, 2-methyl-
5.440	1.96	C7H14O2	Heptanoic acid
5.527	0.86	C7H8O	Phenol, 3-methyl-
5.709	1.87	C10H22O	1-Octanol, 2,7-dimethyl-
5.786	0.96	C11H24	Undecane
5.832	0.59	C11H22	Cyclopropane, octyl-
6.002	1.93	C9H18O2	Octanoic acid, methyl ester
6.242	0.57	C8H10O	Phenol, 2,5-dimethyl-
6.355	1.51	C8H16O2	Octanoic Acid
6.648	2.28	C10H22O	1-Octanol, 2,7-dimethyl-
6.717	1.19	C13H28	Tridecane
6.848	0.46	C10H18O2	8-Nonenoic acid, methyl ester
6.919	1.80	C10H20O2	Nonanoic acid, methyl ester
7.241	1.46	C9H18O2	Nonanoic acid
7.559	2.73	C14H28	1-Tetradecene
7.627	1.49	C13H28	Tridecane
7.837	7.35	C11H22O2	Decanoic acid, methyl ester
8.173	4.57	C10H20O2	n-Decanoic acid
8.508	2.18	C15H30	1-Pentadecene
8.581	1.19	C14H30	Tetradecane
8.806	0.50	C12H24O2	Undecanoic acid, methyl ester
9.515	1.46	C14H28	1-Tetradecene
9.591	1.53	C14H30	Tetradecane
9.830	0.42	C13H26O2	Dodecanoic acid, methyl ester
10.217	0.38	C14H28	Cyclohexane, octyl-
10.572	0.32	C14H28	1-Tetradecene
10.650	0.26	C13H28	Undecane, 3,8-dimethyl-
12.023	0.96	C15H30O2	Tetradecanoic acid, methyl ester
14.138	2.27	C19H38O	2-Nonadecanone
14.454	19.74	C17H34O2	Hexadecanoic acid, methyl ester
14.930	9.68	C15H30O2	Pentadecanoic acid
15.465	0.68	C17H34O2	Pentadecanoic acid, ethyl ester
17.323	7.50	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
17.446	2.98	C19H36O2	7-Octadecenoic acid, methyl ester
17.828	1.10	C19H38O2	Octadecanoic acid, methyl ester
17.985	2.30	C18H34O2	Oleic Acid

Table S12 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Extract 3 (MeOH with 10% water) obtained at 25 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.090	4.73	C7H14O2	Hexanoic acid, methyl ester
4.217	0.19	C5H8O	3-Penten-2-one
4.493	1.98	C6H12O2	Hexanoic acid
4.592	3.47	C6H6O	Phenol
4.741	2.13	C8H16O	2-Octanone
4.963	4.12	C8H14O2	6-Heptenoic acid, methyl ester
5.048	9.28	C8H16O2	Heptanoic acid, methyl ester
5.331	3.21	C7H8O	o-Cresol
5.442	4.42	C7H14O2	Heptanoic acid
5.533	2.75	C7H8O	m-Cresol
5.714	2.43	C9H18O	2-Nonanone
6.006	6.15	C9H18O2	Octanoic acid, methyl ester
6.245	1.86	C8H10O	p-Xylenol
6.355	2.76	C8H16O2	Octanoic Acid
6.656	2.58	C10H20O	2-Decanone
6.851	0.84	C10H18O2	8-Nonenoic acid, methyl ester
6.924	5.59	C10H20O2	Nonanoic acid, methyl ester
7.242	2.05	C9H18O2	Nonanoic acid
7.573	2.23	C11H22O	2-Undecanone
7.841	17.81	C11H22O2	Decanoic acid, methyl ester
8.170	8.79	C10H20O2	n-Decanoic acid
8.483	0.37	C3H8N2	Formaldehyde, dimethylhydrazone
8.809	0.99	C12H24O2	Undecanoic acid, methyl ester
9.313	0.64	C10H18O3	2-Methylbutanoic anhydride
9.833	0.63	C13H26O2	Dodecanoic acid, methyl ester
14.141	0.41	C7H14O	Hexanal, 2-methyl-
14.456	6.09	C17H34O2	Hexadecanoic acid, methyl ester
17.328	1.50	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester

Table S13 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Extract 3 (MeOH with 15% water) obtained at 25 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.090	5.93	C7H14O2	Hexanoic acid, methyl ester
4.492	2.17	C6H12O2	Hexanoic acid
4.593	4.81	C6H6O	Phenol
4.699	0.37	C9H18O	2,2,5-Trimethylhexan-4-one
4.741	2.28	C8H16O	2-Octanone
4.964	5.35	C8H14O2	6-Heptenoic acid, methyl ester
5.049	11.8	C8H16O2	Heptanoic acid, methyl ester
5.332	4.31	C7H8O	Phenol, 2-methyl-
5.440	4.93	C7H14O2	Heptanoic acid
5.533	3.46	C7H8O	m-Cresol
5.716	2.17	C9H18O	2-Nonanone
6.007	7.47	C9H18O2	Octanoic acid, methyl ester
6.246	2.20	C8H10O	p-Xylenol
6.353	2.82	C8H16O2	Octanoic Acid
6.404	1.32	C13H20O	(2S,6R,7S,8E)-(+)-2,7-Epoxy-4,8-
6.657	2.50	C10H20O	2-Decanone
6.925	6.06	C10H20O2	Nonanoic acid, methyl ester
7.242	1.97	C9H18O2	Nonanoic acid
7.842	17.98	C11H22O2	Decanoic acid, methyl ester
8.167	7.86	C10H20O2	n-Decanoic acid
8.809	0.69	C10H20O2	Nonanoic acid, methyl ester
14.456	1.55	C17H34O2	Hexadecanoic acid, methyl ester

Table S14 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Extract 3 (MeOH with 20% water) obtained at 25 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.091	4.89	C7H14O2	Hexanoic acid, methyl ester
4.490	1.52	C6H12O2	Hexanoic acid
4.593	3.43	C6H6O	Phenol
4.742	2.39	C8H16O	2-Octanone
4.965	4.07	C8H14O2	6-Heptenoic acid, methyl ester
5.049	9.78	C8H16O2	Heptanoic acid, methyl ester
5.332	2.89	C7H8O	o-Cresol
5.437	3.27	C7H14O2	Heptanoic acid
5.533	2.30	C7H8O	m-Cresol
5.715	1.90	C9H18O	2-Nonanone
6.008	6.66	C9H18O2	Octanoic acid, methyl ester
6.246	1.87	C8H10O	Phenol, 2,5-dimethyl-
6.352	2.00	C8H16O2	Octanoic Acid
6.656	1.33	C10H20O	2-Decanone
6.925	5.75	C10H20O2	Nonanoic acid, methyl ester
7.241	1.49	C9H18O2	Nonanoic acid
7.574	1.63	C10H20O	2-Decanone
7.842	21.39	C11H22O2	Decanoic acid, methyl ester
8.167	6.35	C10H20O2	n-Decanoic acid
8.810	1.78	C12H24O2	Undecanoic acid, methyl ester
9.834	0.81	C13H26O2	Dodecanoic acid, methyl ester
14.144	0.58	C7H14O	Hexanal, 2-methyl-
14.458	9.40	C17H34O2	Hexadecanoic acid, methyl ester
17.330	2.52	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester

Table 15 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Extract 3 (MeOH with 25% water) obtained at 25 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.091	6.22	C7H14O2	Hexanoic acid, methyl ester
4.410	0.60	C5H8O2	2(3H)-Furanone, dihydro-5-methyl-
4.487	1.46	C6H12O2	Hexanoic acid
4.594	3.82	C6H6O	Phenol
4.743	2.09	C8H16O	2-Octanone
4.965	5.27	C8H14O2	6-Heptenoic acid, methyl ester
5.050	12.39	C8H16O2	Heptanoic acid, methyl ester
5.333	3.69	C7H8O	o-Cresol
5.434	3.07	C7H14O2	Heptanoic acid
5.533	2.23	C7H8O	p-Cresol
5.717	1.98	C9H18O	2-Nonanone
6.008	8.04	C9H18O2	Octanoic acid, methyl ester
6.351	1.61	C8H16O2	Octanoic Acid
6.657	1.65	C10H20O	2-Decanone
6.925	6.59	C10H20O2	Nonanoic acid, methyl ester
7.575	1.11	C10H20O	2-Decanone
7.842	23.71	C11H22O2	Decanoic acid, methyl ester
8.164	5.36	C10H20O2	n-Decanoic acid
8.810	1.58	C14H28O2	Tetradecanoic acid, methyl ester
14.145	0.35	C4H10N2	Butanimidamide
14.459	7.18	C17H34O2	Hexadecanoic acid, methyl ester

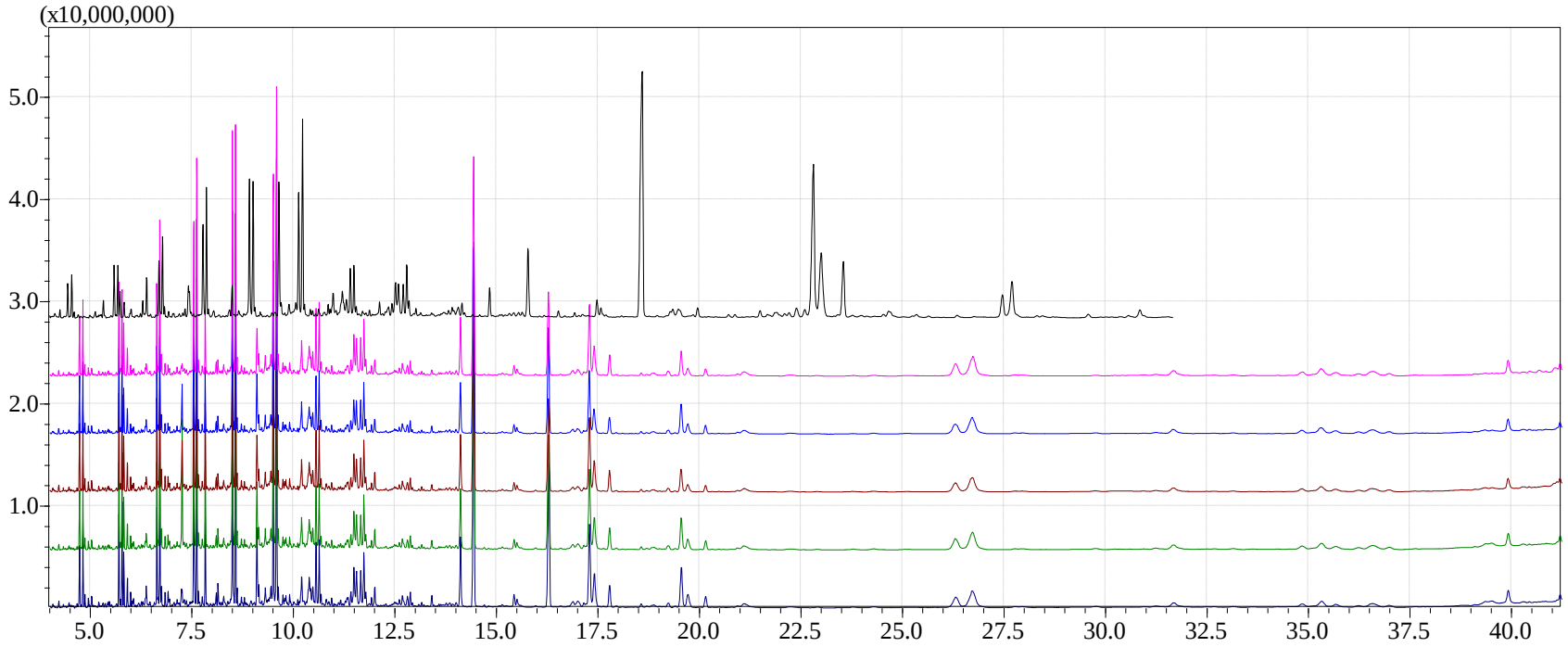

Figure S6 - Chromatograms of the raffinate streams obtained after liquid-liquid extraction at 35 °C and with different water contents in methanol: ——— BO_3; ——— Raffinate 3 (MeOH with 5% water); ——— Raffinate 3 (MeOH with 10% water); ——— Raffinate 3 (MeOH with 15% water); ——— Raffinate 3 (MeOH with 20% water); ——— Raffinate 3 (MeOH with 25% water).

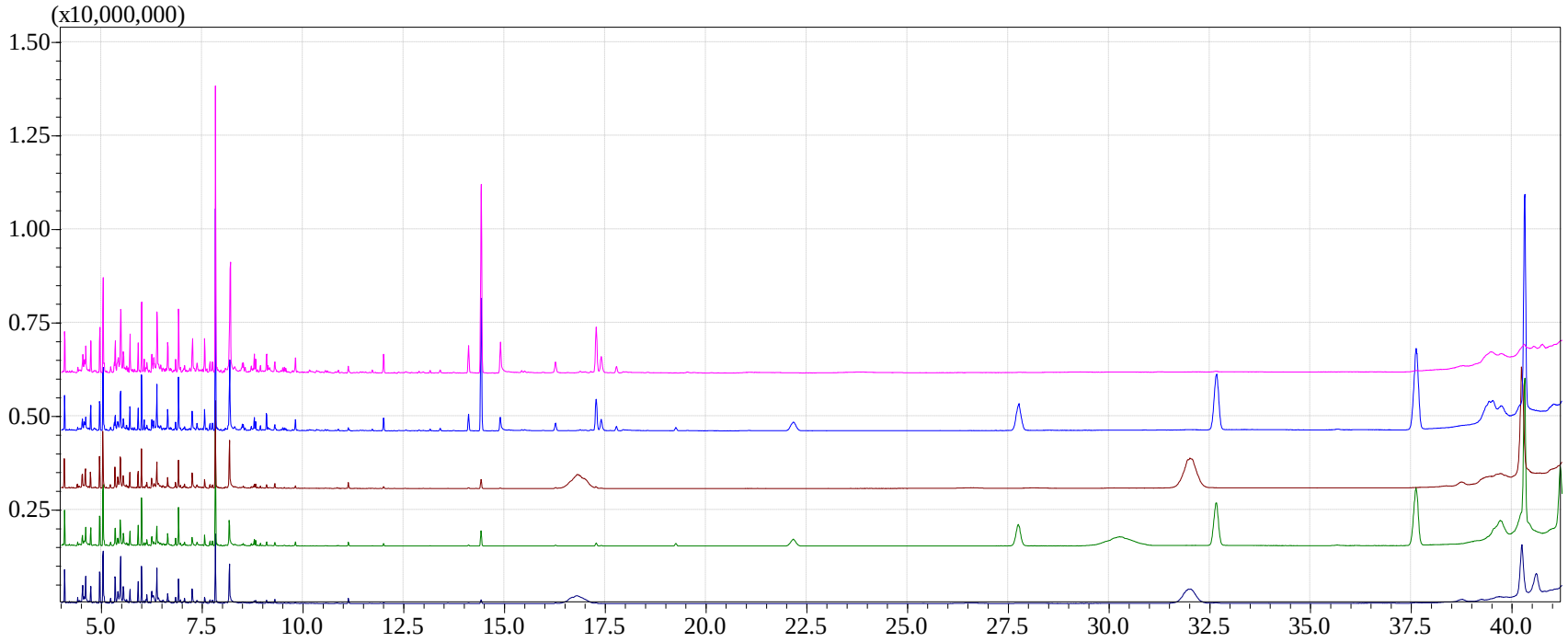

Figure S7 - Chromatograms of the extract streams obtained after liquid-liquid extraction at 35 °C and with different water contents in methanol: Extract 3 (MeOH with 5% water); Extract 3 (MeOH with 10% water); Extract 3 (MeOH with 15% water); Extract 3 (MeOH with 20% water); Extract 3 (MeOH with 25% water).

Table S16 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Raffinate 3 (MeOH with 5% water) obtained at 35 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.733	1.10	C10H20	1-Decene
4.816	1.43	C10H22	Decane
5.701	1.71	C11H22	1-Undecene
5.779	1.83	C11H24	Undecane
5.824	0.93	C11H22	Cyclopropane, 1,2-dibutyl-
5.911	0.60	C11H22	Cyclopropane, 1-pentyl-2-propyl-
6.636	2.13	C12H24	Cyclopropane, nonyl-
6.710	3.01	C12H26	Dodecane
6.750	0.38	C12H24	2-Dodecene, (E)-
6.911	0.29	C10H20O2	Nonanoic acid, methyl ester
7.546	3.66	C13H26	1-Tridecene
7.620	4.91	C13H28	Tridecane
7.750	0.29	C12H24	Cyclododecane
7.828	1.36	C11H22O2	Decanoic acid, methyl ester
8.098	0.27	C12H24	Cyclopentane, 1-hexyl-3-methyl-
8.383	0.29	C13H26O	Cyclododecanemethanol
8.499	5.97	C14H28	1-Tetradecene
8.574	5.70	C16H34	Hexadecane
8.617	0.37	C14H28	7-Tetradecene
8.720	0.39	C14H28	Cyclotetradecane
8.957	0.39	C16H30	Cyclopentene, 3-undecyl-
9.149	0.47	C12H22	Cyclopentene,1-heptyl-
9.307	0.78	C14H26	Cyclohexene, 1-octyl-
9.446	1.27	C18H36	9-Octadecene, (E)-
9.506	5.41	C15H30	1-Pentadecene
9.585	8.02	C15H32	Pentadecane
9.625	0.52	C12H24	Cyclododecane
9.741	0.34	C18H36	5-Octadecene, (E)-
9.817	0.40	C13H26O2	Dodecanoic acid, methyl ester
9.908	0.44	C9H14O	Bicyclo[3.1.0]hexan-2-one, 3,3,6-
10.202	1.12	C15H30	n-Nonylcyclohexane
10.390	1.36	C11H20	Cyclohexene, 1-pentyl-
10.425	0.28	C18H36	9-Octadecene, (E)-
10.476	0.60	C14H28	1-Tetradecene
10.556	1.61	C17H34	1-Heptadecene
10.633	1.72	C17H36	Heptadecane
10.679	0.28	C16H32	Cyclohexadecane
10.809	0.26	C18H36	1-Octadecene
11.346	0.48	C19H38	1-Nonadecene
11.415	0.45	C18H36O	Oleyl Alcohol
11.492	1.82	C20H40	9-Eicosene, (E)-
11.555	1.33	C17H34	1-Heptadecene
11.658	1.26	C17H34	1-Heptadecene

11.736	1.91	C17H36	Heptadecane
11.783	0.39	C16H32	1-Hexadecene
11.926	0.35	C17H34	1-Heptadecene
12.005	0.44	C15H30O2	Tetradecanoic acid, methyl ester
12.683	0.45	C23H46	9-Tricosene, (Z)-
12.809	0.37	C17H34	1-Heptadecene
12.879	0.44	C21H44	Heneicosane
14.116	2.28	C15H30O	2-Pentadecanone
14.440	9.54	C17H34O2	Hexadecanoic acid, methyl ester
15.433	0.38	C18H36O2	Hexadecanoic acid, ethyl ester
16.280	4.51	C16H32O2	Hexadecanoic acid
17.291	4.02	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
17.408	1.96	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
17.790	1.17	C19H38O2	Octadecanoic acid, methyl ester
19.551	1.45	C18H34O2	Oleic acid
20.150	0.37	C18H36O2	Octadecanoic acid
26.315	0.71	C23H46	9-Tricosene, (Z)-
26.734	2.03	C23H46	9-Tricosene, (Z)-

Table S17 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Raffinate 3 (MeOH with 10% water) obtained at 35 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.733	1.12	C10H20	1-Decene
4.816	1.43	C10H22	Decane
5.700	1.67	C11H22	1-Undecene
5.780	1.76	C11H24	Undecane
5.824	0.91	C11H22	Cyclopropane, 1,2-dibutyl-
5.910	0.57	C11H22	Cyclopropane, 1-pentyl-2-propyl-
6.635	2.00	C12H24	Cyclopropane, nonyl-
6.709	2.80	C12H26	Dodecane
6.750	0.35	C12H24	2-Dodecene, (E)-
7.258	1.43	C10H20O2	Glycerol
7.545	4.21	C13H26	1-Tetradecene
7.618	4.75	C13H28	Tridecane
7.657	0.30	C12H24	Cyclopropane, nonyl-
7.826	1.39	C11H22O2	Decanoic acid, methyl ester
8.098	0.25	C12H24	Cyclopentane, 1-hexyl-3-methyl-
8.383	0.28	C13H26O	Cyclododecanemethanol
8.498	5.64	C14H28	1-Tetradecene
8.573	5.33	C16H34	Hexadecane
8.617	0.35	C14H28	7-Tetradecene
8.719	0.29	C14H28	7-Tetradecene
8.955	0.37	C16H30	Cyclopentene, 3-undecyl-
9.147	0.44	C12H22	Cyclopentene,1-heptyl-
9.307	0.74	C14H26	Cyclohexene, 1-octyl-
9.445	1.17	C18H36	9-Octadecene, (E)-
9.505	5.07	C15H30	1-Pentadecene
9.583	7.65	C15H32	Pentadecane
9.623	0.46	C14H28	Cyclotetradecane
9.741	0.31	C18H36	5-Octadecene, (E)-
9.907	0.39	C9H14O	Bicyclo[3.1.0]hexan-2-one, 3,3,6-trimethyl-
10.201	1.20	C15H30	n-Nonylcyclohexane
10.389	1.61	C11H20	Cyclohexene, 1-pentyl-
10.422	0.52	C14H28	1-Tetradecene
10.475	0.76	C14H28	1-Tetradecene
10.555	1.83	C17H34	1-Heptadecene
10.633	1.73	C16H34	Hexadecane
10.676	0.33	C16H32	Cyclohexadecane
10.807	0.41	C16H32	1-Hexadecene
11.346	0.49	C19H38	1-Nonadecene
11.413	0.44	C18H36O	Oleyl Alcohol
11.488	1.63	C20H40	9-Eicosene, (E)-
11.553	1.31	C17H34	1-Heptadecene

11.657	1.16	C17H34	1-Heptadecene
11.734	1.70	C17H36	Heptadecane
11.781	0.42	C14H28	Cyclotetradecane
11.925	0.33	C17H34	1-Heptadecene
12.003	0.42	C15H30O2	Tetradecanoic acid, methyl ester
12.682	0.40	C23H46	9-Tricosene, (Z)-
12.807	0.33	C18H36	1-Octadecene
12.878	0.39	C21H44	Heneicosane
14.113	2.13	C15H30O	2-Pentadecanone
14.438	8.72	C17H34O2	Hexadecanoic acid, methyl ester
15.432	0.37	C18H36O2	Hexadecanoic acid, ethyl ester
16.282	5.91	C16H32O2	Hexadecanoic acid
17.287	3.56	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
17.403	1.74	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
17.783	0.98	C19H38O2	Octadecanoic acid, methyl ester
19.548	2.11	C18H34O2	Oleic acid
19.716	0.89	C18H34O2	Oleic acid
20.150	0.54	C18H36O2	Octadecanoic acid
26.719	2.21	C23H46	9-Tricosene, (Z)-

Table S18 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Raffinate 3 (MeOH with 15% water) obtained at 35 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.734	1.30	C10H20	1-Decene
4.816	1.55	C10H22	Decane
5.034	0.24	C8H16O2	Heptanoic acid, methyl ester
5.446	0.28	C10H18	Cyclohexene, 1-butyl-
5.701	1.84	C11H22	1-Undecene
5.781	1.86	C11H24	Undecane
5.825	0.98	C11H22	Cyclopropane, 1,2-dibutyl-
5.912	0.61	C11H22	Cyclopropane, 1-pentyl-2-propyl-
5.993	0.28	C9H18O2	Octanoic acid, methyl ester
6.637	2.11	C12H24	Cyclopropane, nonyl-
6.710	2.88	C12H26	Dodecane
6.751	0.37	C12H24	2-Dodecene, (E)-
6.840	0.29	C12H24	Cyclododecane
6.912	0.38	C10H20O2	Nonanoic acid, methyl ester
7.133	0.27	C12H24	Cyclohexane, (4-methylpentyl)-
7.258	1.25	C10H20O2	Glycerol
7.547	3.51	C13H26	1-Tridecene
7.620	4.60	C13H28	Tridecane
7.658	0.25	C12H24	Cyclopropane, nonyl-
7.828	1.83	C11H22O2	Decanoic acid, methyl ester
8.099	0.25	C13H26	Decanoic acid, methyl ester
8.383	0.27	C13H26O	Cyclododecanemethanol
8.500	5.44	C14H28	1-Tetradecene
8.575	5.12	C16H34	Hexadecane
8.613	0.35	C14H28	7-Tetradecene
8.720	0.31	C14H28	Cyclotetradecane
8.954	0.43	C16H30	Cyclopentene, 3-undecyl-
9.149	0.49	C12H22	Cyclopentene,1-heptyl-
9.225	0.24	C15H30	Cyclopentadecane
9.307	0.77	C14H26	Cyclohexene, 1-octyl-
9.446	1.19	C18H36	9-Octadecene, (E)-
9.506	4.86	C15H30	9-Octadecene, (E)-
9.585	7.14	C15H32	Pentadecane
9.624	0.51	C12H24	Cyclododecane
9.742	0.36	C18H36	5-Octadecene, (E)-
9.816	0.24	C13H26O2	Dodecanoic acid, methyl ester
9.908	0.50	C9H14O	Bicyclo[3.1.0]hexan-2-one, 3,3,6-trimethyl-
10.202	1.16	C15H30	n-Nonylcyclohexane
10.390	1.68	C11H20	Cyclohexene, 1-pentyl-
10.425	0.37	C18H36	3-Octadecene, (E)-
10.476	0.81	C14H28	1-Tetradecene

10.557	1.65	C17H34	1-Heptadecene
10.633	1.61	C17H36	Heptadecane
10.679	0.31	C16H32	Cyclohexadecane
10.809	0.40	C15H30	1-Pentadecene
11.162	0.39	C12H24O2	Dodecanoic acid
11.347	0.47	C22H44O2	1-Nonadecene
11.415	0.42	C18H36O	Oleyl Alcohol
11.492	1.58	C20H40	9-Eicosene, (E)-
11.558	1.15	C20H40	9-Eicosene, (E)-
11.658	1.08	C20H40	1-Heptadecene
11.736	1.56	C17H36	Heptadecane
11.782	0.40	C14H28	Cyclotetradecane
11.926	0.33	C17H34	1-Heptadecene
12.005	0.63	C15H30O2	Tetradecanoic acid, methyl ester
12.684	0.37	C23H46	9-Tricosene, (Z)-
12.808	0.30	C18H36	1-Octadecene
12.880	0.36	C21H44	Heneicosane
14.116	2.01	C17H34O	2-Heptadecanone
14.446	10.45	C17H34O2	Hexadecanoic acid, methyl ester
15.433	0.35	C18H36O2	Hexadecanoic acid, ethyl ester
15.504	0.24	C18H36O	Octadecan-4-one
16.283	4.63	C16H32O2	Hexadecanoic acid
17.291	3.94	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
17.408	1.90	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
17.784	1.10	C19H38O2	Octadecanoic acid, methyl ester
19.546	1.37	C18H34O2	Oleic acid
19.710	0.54	C18H34O2	Oleic acid
20.151	0.35	C18H36O2	Octadecanoic acid
26.729	0.94	C23H46	9-Tricosene, (Z)-

Table S19 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Raffinate 3 (MeOH with 20% water) obtained at 35 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.734	1.10	C10H20	1-Decene
4.817	1.31	C10H22	Decane
5.035	0.22	C8H16O2	Heptanoic acid, methyl ester
5.702	1.57	C11H22	1-Undecene
5.781	1.62	C11H24	Undecane
5.825	0.85	C11H22	Cyclopropane, 1,2-dibutyl-
5.912	0.54	C11H22	Cyclopropane, 1-pentyl-2-propyl-
5.993	0.24	C9H18O2	Octanoic acid, methyl ester
6.638	2.02	C12H24	Cyclopropane, nonyl-
6.711	2.65	C12H26	Dodecane
6.751	0.37	C12H24	2-Dodecene, (E)-
6.840	0.25	C12H24	Cyclododecane
6.912	0.31	C10H20O2	Nonanoic acid, methyl ester
7.259	2.64	C10H20O2	Glycerol
7.548	3.28	C14H28	1-Tetradecene
7.621	4.29	C13H28	Tridecane
7.659	0.24	C12H24	Cyclopropane, nonyl-
7.830	1.76	C11H22O2	Decanoic acid, methyl ester
8.099	0.29	C15H30	Cyclopentane, decyl-
8.500	5.18	C14H28	1-Tetradecene
8.575	4.82	C16H34	Hexadecane
8.614	0.33	C14H28	7-Tetradecene
8.721	0.31	C14H28	Cyclotetradecane
9.103	2.07	C10H20O2	Decanoic acid
9.149	0.46	C12H22	Cyclopentene,1-heptyl-
9.225	0.23	C16H32	Cyclohexadecane
9.308	0.74	C14H26	Cyclohexene, 1-octyl-
9.447	1.14	C18H36	9-Octadecene, (E)-
9.507	4.61	C15H30	1-Pentadecene
9.587	6.88	C15H32	Pentadecane
9.625	0.50	C12H24	Cyclododecane
9.742	0.34	C18H36	5-Octadecene, (E)-
9.816	0.24	C13H26O2	Dodecanoic acid, methyl ester
9.908	0.48	C9H14O	Bicyclo[3.1.0]hexan-2-one, 3,3,6-
10.202	1.23	C15H30	n-Nonylcyclohexane
10.391	1.62	C11H20	Cyclohexene, 1-pentyl-
10.425	0.36	C14H28	1-Tetradecene
10.477	0.81	C14H28	1-Tetradecene
10.557	1.57	C17H34	1-Heptadecene
10.633	1.56	C16H34	Hexadecane
10.679	0.30	C16H32	Cyclohexadecane
10.809	0.39	C17H34	1-Heptadecene

11.347	0.40	C21H44O	1-Heneicosanol
11.415	0.38	C18H36O	Oleyl Alcohol
11.492	1.50	C20H40	9-Eicosene, (E)-
11.555	1.10	C20H40	9-Eicosene, (E)-
11.658	1.03	C17H34	1-Heptadecene
11.735	1.55	C17H36	Heptadecane
11.783	0.32	C15H30	1-Pentadecene
11.927	0.28	C17H34	1-Heptadecene
12.005	0.50	C15H30O2	Tetradecanoic acid, methyl ester
12.683	0.36	C23H46	9-Tricosene, (Z)-
12.809	0.30	C18H36	1-Octadecene
12.880	0.36	C21H44	Heneicosane
13.408	0.22	C14H28O2	Tetradecanoic acid
14.116	2.08	C17H34O	2-Heptadecanone
14.445	10.07	C17H34O2	Hexadecanoic acid, methyl ester
15.435	0.34	C18H36O2	Hexadecanoic acid, ethyl ester
16.286	5.67	C18H36O2	Hexadecanoic acid
17.291	3.96	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
17.411	1.91	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
17.788	1.10	C19H38O2	Octadecanoic acid, methyl ester
19.550	1.89	C18H34O2	Oleic acid
19.710	0.79	C18H34O2	Oleic acid
20.155	0.48	C18H36O2	Octadecanoic acid
26.720	1.69	C23H46	9-Tricosene, (Z)-

Table S20 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Raffinate 3 (MeOH with 25% water) obtained at 35 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.735	1.10	C10H20	1-Decene
4.817	1.39	C10H22	Decane
5.033	0.27	C8H16O2	Heptanoic acid, methyl ester
5.208	0.65	C10H20	Cyclohexane, butyl-
5.475	0.38	C6H12O2	Hexanoic acid
5.703	1.83	C11H22	1-Undecene
5.782	1.84	C11H24	Undecane
5.825	0.97	C11H22	Cyclopropane, 1,2-dibutyl-
5.913	0.62	C11H22	Cyclopropane, 1-pentyl-2-propyl-
5.993	0.29	C9H18O2	Octanoic acid, methyl ester
6.639	2.10	C12H24	Cyclopropane, nonyl-
6.712	2.84	C12H26	Dodecane
6.752	0.36	C12H24	2-Dodecene, (E)-
6.841	0.27	C12H24	Cyclododecane
6.917	0.40	C10H20O2	Nonanoic acid, methyl ester
7.549	3.49	C13H26	1-Tridecene
7.622	4.46	C13H28	Tridecane
7.659	0.23	C12H24	Cyclopropane, nonyl-
7.830	1.81	C11H22O2	Decanoic acid, methyl ester
8.500	5.23	C14H28	1-Tetradecene
8.575	4.87	C16H34	Hexadecane
8.615	0.32	C14H28	7-Tetradecene
9.103	2.16	C10H20O2	Decanoic acid
9.150	0.44	C12H22	Cyclopentene,1-heptyl-
9.309	0.61	C14H26	Cyclohexene, 1-octyl-
9.447	0.97	C18H36	9-Octadecene, (E)-
9.507	4.64	C15H30	1-Pentadecene
9.587	6.91	C15H32	Pentadecane
9.626	0.36	C12H24	Cyclododecane
9.817	0.29	C13H26O2	Dodecanoic acid, methyl ester
10.204	0.91	C15H30	n-Nonylcyclohexane
10.392	1.39	C11H20	Cyclohexene, 1-pentyl-
10.425	0.30	C14H28	1-Tetradecene
10.478	0.60	C14H28	1-Tetradecene
10.558	1.57	C17H34	1-Heptadecene
10.635	1.55	C16H34	Hexadecane
10.679	0.25	C16H32	Cyclohexadecane
10.808	0.36	C16H32	1-Hexadecene
11.346	0.30	C21H44O	1-Heneicosanol
11.416	0.41	C18H36O	Oleyl Alcohol
11.492	1.63	C20H40	9-Eicosene, (E)-
11.556	1.19	C17H34	1-Heptadecene

11.659	1.12	C17H34	1-Heptadecene
11.736	1.71	C17H36	Heptadecane
11.783	0.35	C15H30	1-Pentadecene
11.926	0.31	C17H34	1-Heptadecene
12.005	0.48	C15H30O2	Tetradecanoic acid, methyl ester
12.684	0.39	C23H46	9-Tricosene, (Z)-
12.809	0.31	C17H34	1-Heptadecene
12.880	0.39	C21H44	Heneicosane
13.410	0.31	C14H28O2	Tetradecanoic acid
14.117	2.43	C15H30O	2-Pentadecanone
14.446	10.43	C17H34O2	Hexadecanoic acid, methyl ester
15.434	0.46	C18H36O2	Hexadecanoic acid, ethyl ester
16.291	7.39	C16H32O2	Hexadecanoic acid
17.294	4.21	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
17.413	2.03	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
17.788	1.12	C19H38O2	Octadecanoic acid, methyl ester
19.554	2.44	C18H34O2	Oleic acid
19.720	1.02	C18H34O2	Oleic acid
20.154	0.54	C18H36O2	Octadecanoic acid

Table S21 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Extract 3 (MeOH with 5% water) obtained at 35 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.085	1.93	C7H14O2	Hexanoic acid, methyl ester
4.408	0.69	C5H8O2	2(3H)-Furanone, dihydro-5-methyl-
4.533	1.45	C6H12O2	Hexanoic acid
4.576	0.93	C5H10O2	Pentanoic acid
4.609	1.60	C6H6O	Phenol
4.735	1.91	C8H16O	2-Octanone
4.957	2.10	C8H14O2	6-Heptenoic acid, methyl ester
5.040	4.87	C8H16O2	Heptanoic acid, methyl ester
5.340	2.18	C7H8O	Phenol, 2-methyl-
5.415	1.66	C7H12O2	3-Heptenoic acid
5.543	1.44	C7H8O	Phenol, 3-methyl-
5.657	0.2	C9H18O	3-Nonanone
5.707	1.86	C9H18O	2-Nonanone
5.996	3.53	C9H18O2	Octanoic acid, methyl ester
6.059	0.59	C7H8	Toluene
6.126	0.76	C8H10O	Phenol, 2-ethyl-
6.249	1.22	C8H10O	Phenol, 2,4-dimethyl-
6.644	1.84	C10H20O	2-Decanone
6.840	0.47	C10H18O2	8-Nonenoic acid, methyl ester
6.911	3.55	C10H20O2	Nonanoic acid, methyl ester
7.258	2.29	C9H18O2	Nonanoic acid
7.559	1.78	C11H22O	2-Undecanone
7.691	0.69	C11H20O2	4-Decenoic acid, methyl ester
7.826	12.91	C11H22O2	4-Decenoic acid, methyl ester
8.196	9.37	C10H20O2	n-Decanoic acid
8.492	0.63	C13H26	1-Tridecene
8.716	0.37	C12H22O2	10-Undecenoic acid, methyl ester
8.792	1.03	C12H24O2	Undecanoic acid, methyl ester
8.825	0.60	C12H22O2	10-Undecenoic acid, methyl ester
8.942	0.28	C12H22O2	10-Undecenoic acid, methyl ester
9.097	0.90	C10H20O2	Decanoic acid
9.134	0.27	C11H22O2	Undecanoic acid
9.300	0.69	C11H20O2	2(3H)-Furanone, 5-heptyldihydro-
9.812	0.73	C13H26O2	Dodecanoic acid, methyl ester
11.125	0.34	C12H22O4	Decanedioic acid, dimethyl ester
12.000	1.20	C15H30O2	Tetradecanoic acid, methyl ester
13.403	0.19	C14H28O2	Tetradecanoic acid
14.108	2.14	C17H34O	2-Heptadecanone
14.422	16.27	C17H34O2	Hexadecanoic acid, methyl ester
14.900	2.99	C15H30O2	Pentadecanoic acid
16.263	1.12	C16H32O2	Hexadecanoic acid
17.275	5.53	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester

17.400	2.22	C19H36O2	8-Octadecenoic acid, methyl ester
17.776	0.68	C19H38O2	Octadecanoic acid, methyl ester

Table S22 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Extract 3 (MeOH with 10% water) obtained at 35 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.083	1.49	C7H14O2	Hexanoic acid, methyl ester
4.524	1.02	C6H12O2	Hexanoic acid
4.569	0.68	C5H10O2	Pentanoic acid
4.608	0.89	C6H6O	Phenol
4.732	1.15	C8H16O	2-Octanone
4.953	1.44	C8H14O2	6-Heptenoic acid, methyl ester
5.038	3.39	C8H16O2	Heptanoic acid, methyl ester
5.339	1.22	C7H8O	Phenol, 2-methyl-
5.401	0.89	C7H12O2	3-Heptenoic acid
5.542	0.99	C7H8O	Phenol, 3-methyl-
5.703	1.19	C9H18O	2-Nonanone
5.994	2.44	C9H18O2	Octanoic acid, methyl ester
6.058	0.51	C7H8	Toluene
6.125	0.50	C8H10O	Phenol, 2-ethyl-
6.642	1.43	C10H20O	2-Decanone
6.838	0.51	C10H18O2	8-Nonenoic acid, methyl ester
6.909	2.54	C10H20O2	Nonanoic acid, methyl ester
7.249	1.48	C9H18O2	Nonanoic acid
7.558	1.19	C11H22O	2-Undecanone
7.690	0.57	C11H20O2	4-Decenoic acid, methyl ester
7.825	9.58	C11H22O2	Decanoic acid, methyl ester
8.181	5.55	C10H20O2	n-Decanoic acid
8.492	1.10	C14H28	1-Tetradecene
8.716	0.45	C12H22O2	10-Undecenoic acid, methyl ester
8.791	0.78	C12H24O2	Undecanoic acid, methyl ester
8.825	0.44	C12H22O2	10-Undecenoic acid, methyl ester
8.941	0.37	C12H22O2	10-Undecenoic acid, methyl ester
9.095	1.19	C10H20O2	Decanoic acid
9.299	0.57	C11H20O2	2(3H)-Furanone, 5-heptyldihydro-
9.496	0.36	C14H30O	1-Tetradecanol
9.811	0.66	C13H26O2	Dodecanoic acid, methyl ester
11.999	0.86	C15H30O2	Hexadecanoic acid, methyl ester
14.107	1.36	C15H30O	2-Pentadecanone
14.420	11.57	C15H30O2	Hexadecanoic acid, methyl ester
14.894	1.42	C15H30O2	Pentadecanoic acid
16.265	0.81	C16H32O2	Hexadecanoic acid
17.272	4.06	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
17.398	1.56	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
17.776	0.49	C19H38O2	Octadecanoic acid, methyl ester
19.251	0.39	C21H44	Heneicosane
22.171	2.81	C21H44	Heneicosane
27.765	9.27	C21H44	Heneicosane

32.672	18.83	C21H44	Heneicosane

Table S23 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Extract 3 (MeOH with 15% water) obtained at 35 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.076	1.65	C7H14O2	Hexanoic acid, methyl ester
4.399	0.29	C5H8O2	2(3H)-Furanone, dihydro-5-methyl-
4.442	0.32	C6H10O2	5-Hexenoic acid
4.522	1.44	C6H12O2	Hexanoic acid
4.598	1.70	C6H6O	Phenol
4.683	0.16	C8H16O	3-Heptanone, 5-methyl-
4.725	0.93	C8H16O	2-Octanone
4.950	1.75	C8H14O2	2-Octanone
5.034	3.50	C8H16O2	Heptanoic acid, methyl ester
5.217	0.30	C7H10O	2-Cyclopenten-1-one, 2,3-dimethyl-
5.332	1.48	C7H8O	Phenol, 2-methyl-
5.402	1.15	C7H12O2	3-Heptenoic acid
5.469	3.18	C7H14O2	Heptanoic acid
5.538	1.48	C7H8O	Phenol, 3-methyl-
5.700	1.01	C9H18O	2-Nonanone
5.992	2.05	C9H18O2	Octanoic acid, methyl ester
6.123	0.58	C8H10O	Phenol, 2-ethyl-
6.244	0.97	C8H10O	Phenol, 2,4-dimethyl-
6.309	0.56	C8H14O2	7-Octenoic acid
6.373	1.87	C8H16O2	7-Octenoic acid
6.407	0.66	C8H10O	Phenol, 3-ethyl-
6.641	0.98	C10H20O	2-Decanone
6.836	0.52	C10H18O2	8-Nonenoic acid, methyl ester
6.909	1.72	C10H20O2	Nonanoic acid, methyl ester
6.957	0.19	C9H12O	Phenol, 2-ethyl-4-methyl-
7.059	0.48	C9H12O	Phenol, 3-(1-methylethyl)-
7.250	1.45	C9H18O2	Nonanoic acid
7.559	0.66	C11H22O	2-Undecanone
7.689	0.29	C11H20O2	4-Decenoic acid, methyl ester
7.824	5.35	C11H22O2	Decanoic acid, methyl ester
8.174	4.53	C10H20O2	n-Decanoic acid
8.790	0.25	C12H24O2	Undecanoic acid, methyl ester
8.824	0.23	C12H22O2	10-Undecenoic acid, methyl ester
9.300	0.35	C10H18O2	2(3H)-Furanone, 5-hexyldihydro-
9.811	0.16	C13H26O2	Dodecanoic acid, methyl ester
11.125	0.44	C12H22O4	Decanedioic acid, dimethyl ester
14.418	0.98	C17H34O2	Hexadecanoic acid, methyl ester
16.800	14.72	C40H82	Tetracontane
16.992	4.40	C40H82	Tetracontane
32.006	35.27	C44H90	Tetratetracontane

Table S24 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Extract 3 (MeOH with 20% water) obtained at 35 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.083	2.69	C7H14O2	Hexanoic acid, methyl ester
4.524	1.44	C6H12O2	Hexanoic acid
4.607	2.15	C6H6O	Phenol
4.692	0.17	C8H16O	3-Octanone
4.733	1.37	C8H16O	2-Octanone
4.954	2.65	C8H14O2	6-Heptenoic acid, methyl ester
5.039	5.78	C8H16O2	Heptanoic acid, methyl ester
5.338	1.92	C7H8O	Phenol, 2-methyl-
5.400	0.99	C7H12O2	3-Heptenoic acid
5.467	3.22	C7H14O2	Heptanoic acid
5.542	1.69	C7H8O	Phenol, 3-methyl-
5.705	1.24	C9H18O	2-Nonanone
5.994	3.71	C9H18O2	Octanoic acid, methyl ester
6.125	0.68	C8H10O	Phenol, 2-ethyl-
6.248	1.67	C8H10O	Phenol, 2,4-dimethyl-
6.642	1.16	C10H20O	2-Decanone
6.839	0.48	C10H18O2	8-Nonenoic acid, methyl ester
6.910	2.98	C10H20O2	Nonanoic acid, methyl ester
6.958	0.19	C10H20O2	Nonanoic acid, methyl ester
7.559	0.93	C11H22O	2-Undecanone
7.690	0.46	C11H20O2	4-Decenoic acid, methyl ester
7.825	10.75	C11H22O2	Decanoic acid, methyl ester
8.168	3.40	C10H20O2	Decanoic acid, methyl ester
8.716	0.20	C12H22O2	10-Undecenoic acid, methyl ester
8.791	0.71	C12H24O2	Undecanoic acid, methyl ester
8.825	0.42	C12H22O2	10-Undecenoic acid, methyl ester
8.942	0.32	C12H22O2	10-Undecenoic acid, methyl ester
9.098	0.37	C10H20O2	Decanoic acid
9.300	0.33	C10H18O2	2(3H)-Furanone, 5-hexyldihydro-
9.812	0.42	C13H26O2	2(3H)-Furanone, 5-hexyldihydro-
11.126	0.38	C12H22O4	Decanedioic acid, dimethyl ester
12.000	0.26	C14H28O2	Tridecanoic acid, methyl ester
14.417	2.16	C17H34O2	Hexadecanoic acid, methyl ester
17.274	0.61	C19H36O2	9-Octadecenoic acid (Z)-, methyl ester
19.251	0.50	C21H44	Heneicosane
22.166	3.88	C21H44	Heneicosane
27.747	12.53	C21H44	Heneicosane
32.664	25.19	C21H44	Heneicosane

Table S25 - Retention times, relative contents and identification of the prominent peaks obtained by GC-MS analysis of Extract 3 (MeOH with 25% water) obtained at 35 C.

Retention time (min)	Area (%)	Molecular Formula	Compund name
4.034	0.27	C4H8O3	Butanoic acid, 4-hydroxy-
4.083	4.14	C7H14O2	Hexanoic acid, methyl ester
4.409	0.69	C5H8O2	2(3H)-Furanone, dihydro-5-methyl-
4.532	3.17	C6H12O2	Hexanoic acid
4.567	1.19	C5H10O2	Pentanoic acid
4.606	5.00	C6H6O	Phenol
4.692	0.32	C8H16O	3-Octanone
4.733	2.20	C8H16O	2-Octanone
4.954	4.48	C8H14O2	6-Heptenoic acid, methyl ester
5.038	8.60	C8H16O2	Heptanoic acid, methyl ester
5.224	0.81	C7H10O	2-Cyclopenten-1-one, 2,3-dimethyl-
5.337	4.24	C7H8O	Phenol, 2-methyl-
5.406	3.05	C7H12O2	3-Heptenoic acid
5.474	8.33	C7H14O2	Heptanoic acid
5.542	3.66	C7H8O	Phenol, 3-methyl-
5.656	0.22	C9H18O	3-Nonanone
5.705	2.19	C9H18O	2-Nonanone
5.994	4.70	C9H18O2	Octanoic acid, methyl ester
6.125	1.60	C8H10O	Phenol, 2-ethyl-
6.247	2.32	C8H10O	Phenol, 2,4-dimethyl-
6.374	4.84	C8H16O2	Octanoic Acid
6.411	1.55	C8H10O	Phenol, 4-ethyl-
6.642	2.30	C12H24O	2-Dodecanone
6.839	1.12	C10H18O2	8-Nonenoic acid, methyl ester
6.909	3.31	C10H20O2	Nonanoic acid, methyl ester
6.958	0.45	C9H12O	Phenol, 2-ethyl-4-methyl-
7.058	1.14	C9H12O	Phenol, 3-(1-methylethyl)-
7.250	2.85	C9H18O2	Nonanoic acid
7.560	1.67	C11H22O	2-Undecanone
7.689	0.58	C11H20O2	4-Decenoic acid, methyl ester
7.825	8.49	C11H22O2	Decanoic acid, methyl ester
8.173	7.55	C10H20O2	n-Decanoic acid
8.792	0.33	C12H24O2	Undecanoic acid, methyl ester
8.824	0.36	C12H22O2	10-Undecenoic acid, methyl ester
9.300	0.61	C10H18O2	2(3H)-Furanone, 5-hexyldihydro-
11.126	0.81	C12H22O4	Decanedioic acid, dimethyl ester
14.419	0.86	C17H34O2	Hexadecanoic acid, methyl ester