Supplement of

Characterization of Organic Matter of the Laptev Sea Eroded Coastal Sediments: A Case Study from the Cape Muostakh, Bykovsky Peninsula

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Table S1. Characteristics of the samples from the Cape Muostakh, Bykovsky Peninsula.

Sample	Above sea level, m	Age[1]	Short description	TOC[2], %	$\delta^{13}C$[3], ‰
21.5	21.5	Holocene	Holocene peat formation (color brown-brown, odorless).	34.15	−28.1
20	20.0	Upper Pleistocene	Ice complex deposits with plant residues.	5.35	−28.0
15	15.0	Upper Pleistocene	Ice Complex deposits (silt from sand and gravel admixture).	2.02	−24.4
11	11.0	Upper Pleistocene	Ice Complex deposits. The bulk of aleurite lithological size. There is the presence of sand and gravel debris.	1.72	−24.4
5	5.0	Upper Pleistocene	Ice Complex deposits. (Sample selected piece is likely to preserve the natural stratification).	0.96	−23.9
VP1	1.0	Upper Pleistocene	Deposits of aleurite lithology with an admixture of sand material. The sample selected in the wave-cut niche. Organic residues are not observed.	2.75	−26.1
KV1	1.0	Holocene, Upper Pleistocene	Ice Complex deposits. It is noted the presence of plant residues (most likely "slipped" deposits with more upper horizons, because the shore is exposed to thermoabrasive processes).	2.96	−27.1

[1] Data from [39].
[2] TOC is the total organic carbon content determined by Rock-Eval pyrolitic method.
[3] $\delta^{13}C$ is the carbon isotopic composition.

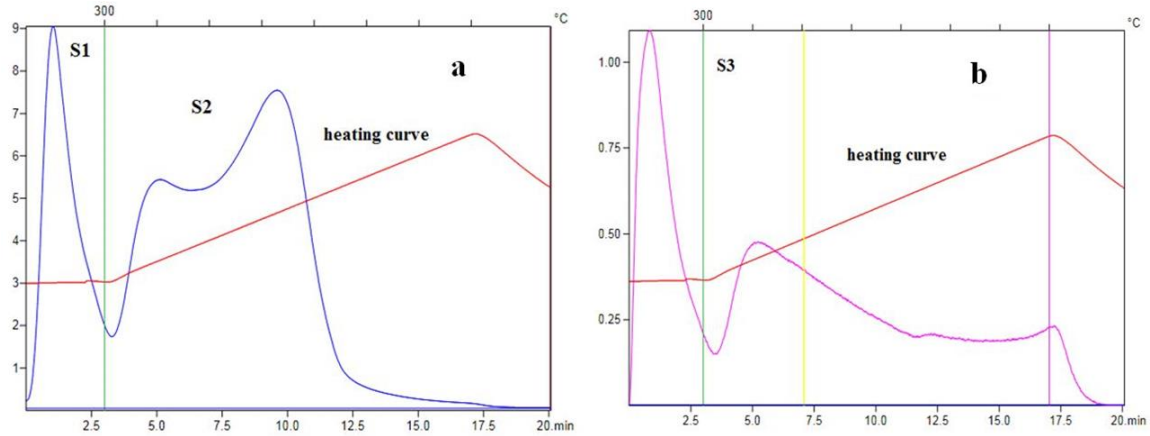
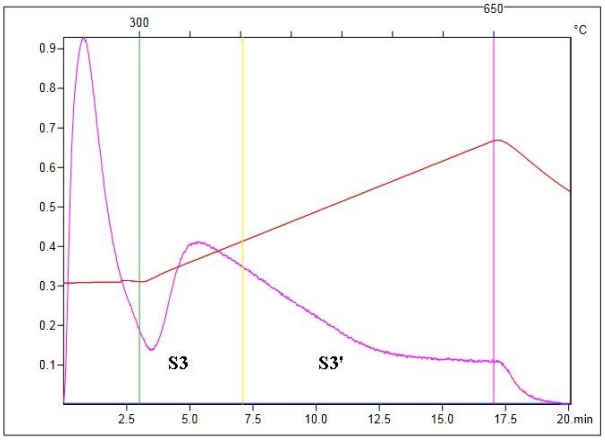
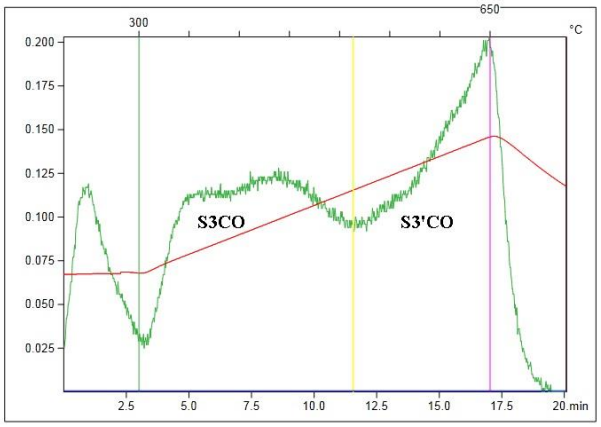


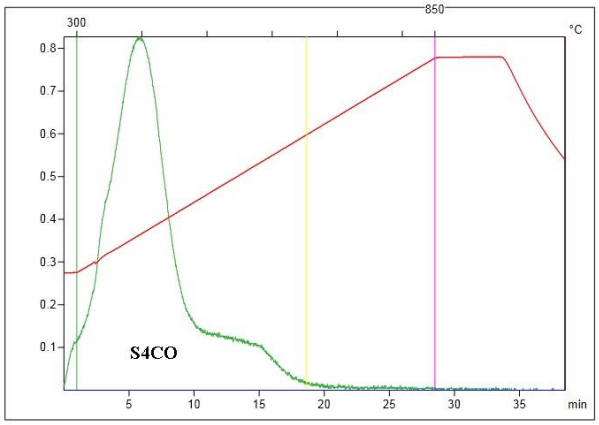
Figure S1. Rock-Eval pyrograms of the sample «20». The red line corresponds to the oven heating curve. The blue line (**a**) is the flame ionization detector signal (mV) in the analysis process. The pink line (**b**) is the signal from the infrared cell that detects the amount of CO and CO_2.



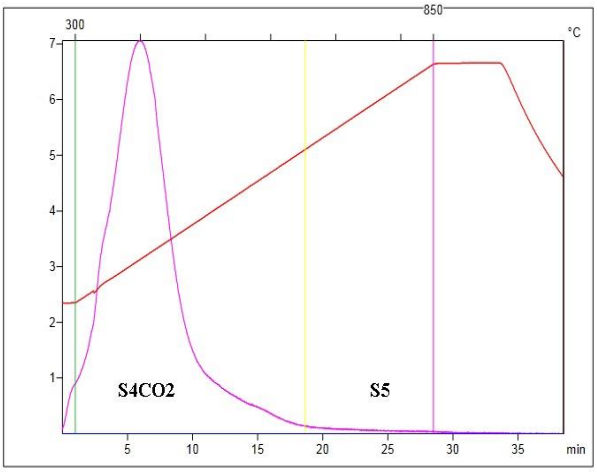
(**a**)



(**b**)



(**c**)



(**d**)

Figure S2. Rock-Eval pyrograms of the sample «20». The red line on pyrograms corresponds to the oven heating curve. The green and pink lines are the signals from the infrared cell that detects the amount of CO and CO_2.

Table S2. The results of X-ray diffraction analysis of bulk sediment.

Sample ID	Mass fraction of the minerals, % wt.						Total, %
	Quartz	Plagioclase	Potassium feldspar	Illite/Muscovite	Kaolinite	Chlorite	
20	47.9	29.4	5.4	11.5	2.1	3.7	100.0
15	54.9	23.3	2.4	14.0	0.0	5.4	100.0
11	41.2	26.3	9.3	16.4	4.1	2.7	100.0
5	43.9	24.5	11.5	12.1	3.2	4.8	100.0
VP1	47.6	28.0	3.3	13.3	1.0	6.8	100.0
KV1	45.0	25.7	2.0	18.0	1.9	7.4	100.0

Table S3. The results of X-ray diffraction analysis. (Clay component analysis).

Sample ID	Mass fraction of the clay minerals, % wt					Total, %
	Illite	I/S[1]	Kaolinite	Smectite	Chlorite	
20	54.4	2.6	5.1	0.0	37.9	100.0
15	64.4	0.0	3.0	0.0	32.6	100.0
11	72.0	6.0	9.0	0.0	13.0	100.0
5	64.1	0.0	3.7	0.0	32.2	100.0
VP1	59.9	3.1	3.9	0.0	33.1	100.0
KV1	59.0	6.0	4.0	0.0	31.0	100.0

[1] I/S — mixed layered Illite/Smectite.

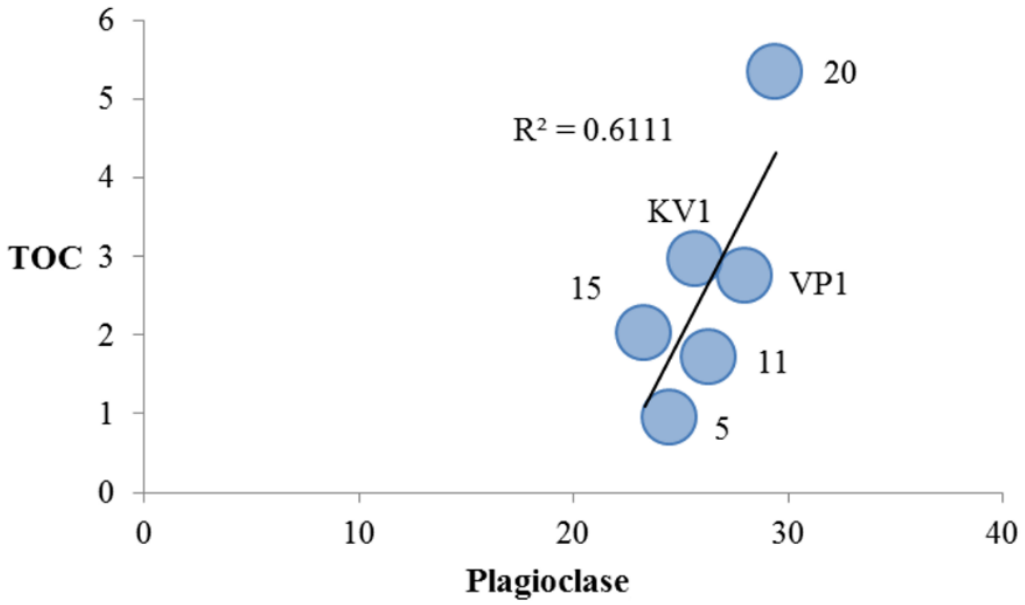


Figure S3. Relationship between TOC and plagioclase content in mineralogical composition.

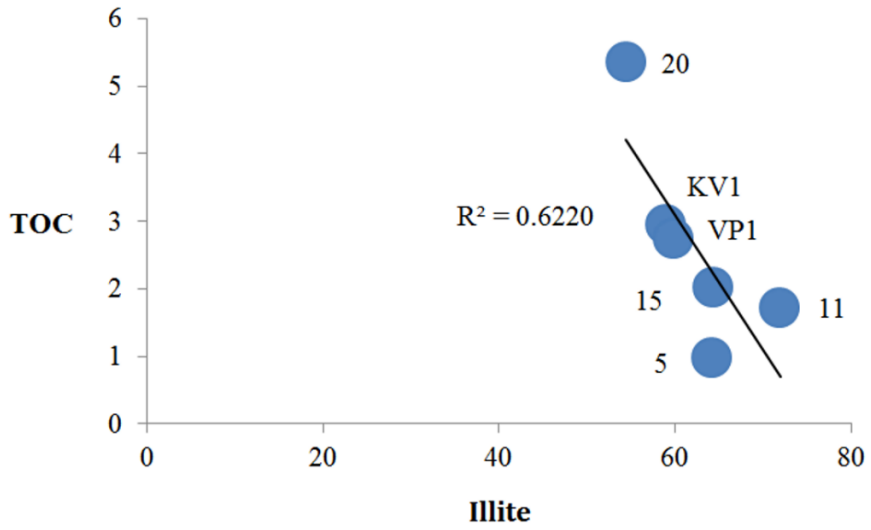


Figure S4. Relationship between TOC and Illite content in the clay (size) fraction.

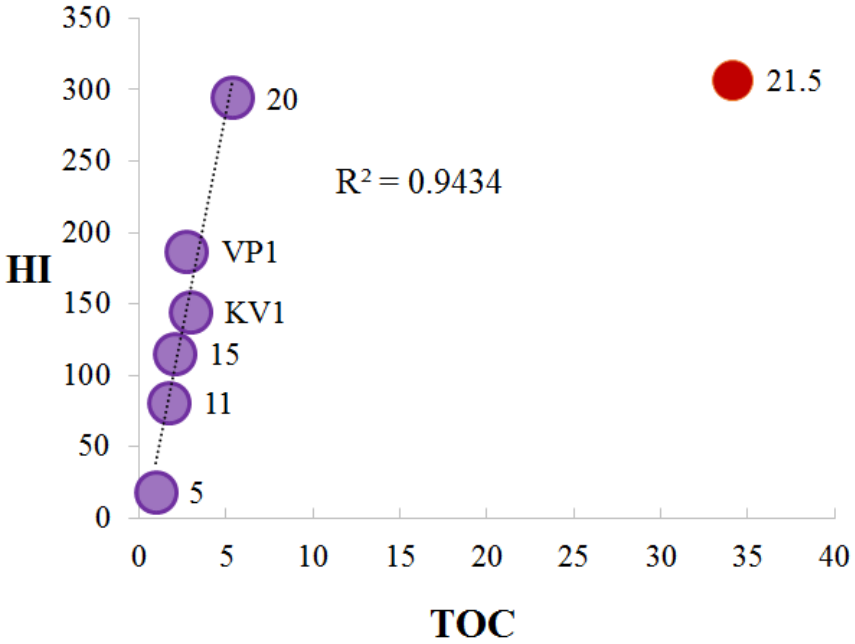


Figure S5. Relationship between hydrogen index (HI) and TOC. Sample "21.5" falls out from the trend.

Table S4. The yields of fractions obtained by column liquid-adsorption chromatography (CLAC).

Sample	Aliphatic fraction, % dw.	Aromatic fraction, % dw.	Polar fraction, % dw.	Insoluble residue, % dw.
21.5	5.76	1.54	58.20	34.50
20	14.11	3.21	82.63	0.05
15	12.78	2.07	75.86	9.29
11	17.26	2.64	62.58	17.51
5	23.86	0.00	45.10	31.05
VP1	12.51	2.03	76.24	9.22
KV1	15.61	1.35	80.83	2.21

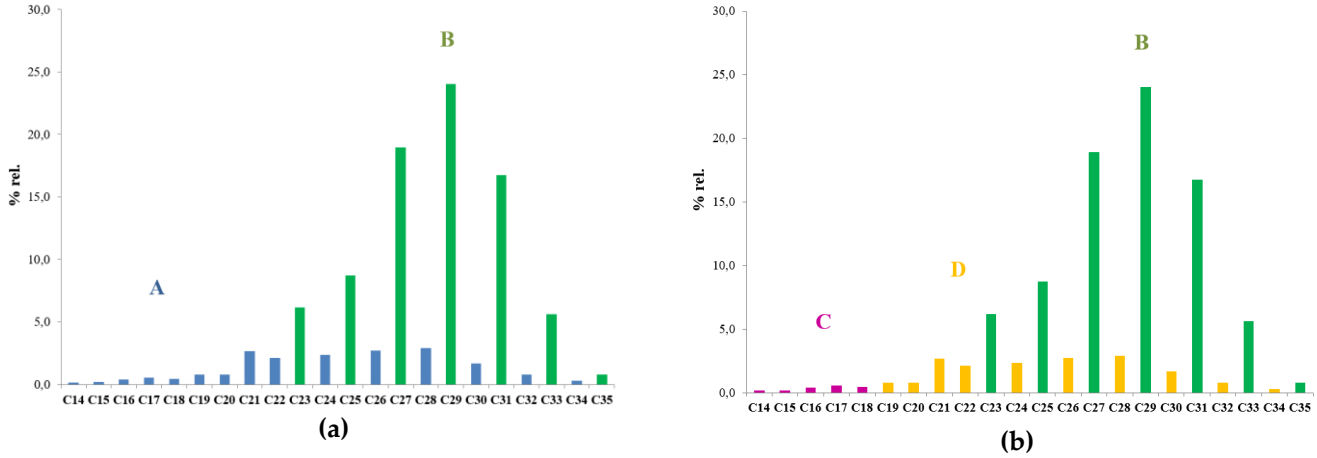


Figure S6. Molecular weight distribution of n-alkanes (sample "KV1"). Scheme for calculating A/B and C/D parameters is shown. a) ***A***, the sum of n-alkane peaks on the even envelope (highlighted in blue); ***B***, the sum of the peaks of high-molecular n-alkanes, which are markers of land plants, on the odd envelope – C_{23}, C_{25}, C_{27}, C_{29}, C_{31}, C_{33}, C_{35} (highlighted in green). b) ***C***, the sum of the peaks of low-molecular n-alkanes on the even envelope C_{14}–C_{18} (highlighted in purple); ***D***, the sum of the peaks of high-molecular n-alkanes on the even envelope C_{19}–C_{34} (highlighted in yellow).

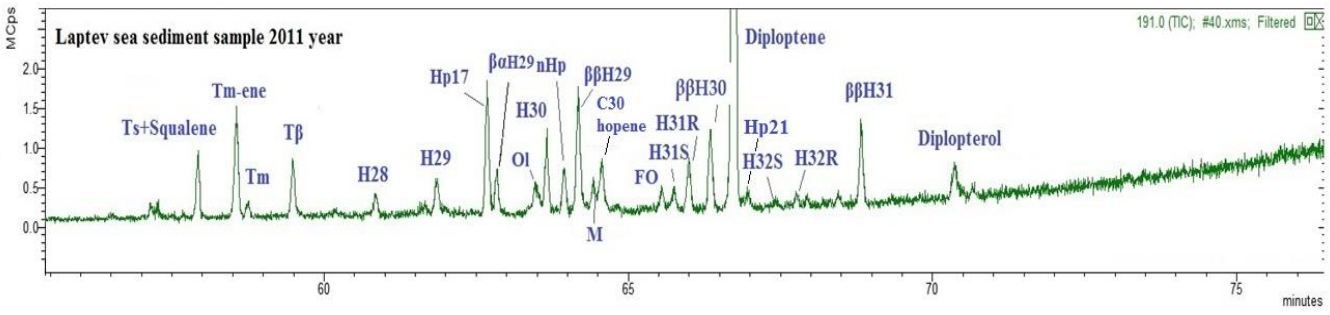


Figure S7. Chromatogram m/z 191 of the Laptev Sea sediments collected in 2011 year expedition (non-polar fraction of the total lipid extract). Ts – 18α(H)-22, 29, 30-trisnorneohopane; Tm-ene – 17α(H)-22, 29, 30-trisnorhop-(17,21)-ene; Tm – 17α(H)-22, 29, 30-trisnorhopane; Tβ – 17β(H)-22, 29, 30-trisnorhopane; H29 – 17α(H), 21β(H)-30-norhopane; Hp17 – C_{30} hop-17(21)-ene; Hp21 – hop-21(22)-ene; βαH29 – 17β(H), 21α(H)-30-norhopane (normoretane); Ol – oleanane; H30 – 17α(H), 21β(H) C_{30} hopane; nHp – C30 neohop-13(18)-ene; βββH29 – 17β(H),21β(H)-30-norhopane; M – 17β(H), 21α(H)-hopane (moretane); C_{30} hopene – unknown C_{30} hopene; FO – D:A-friedolean-6-ene; αβH31S и αβH31R – C_{31} 17α(H), 21β(H) homohopanes 22S and 22R epimers respectively; βββH30 – C_{30} 17β(H), 21β(H)-hopane; Diploptene – (C_{30} hop-22(29)-ene); Hp21 – C_{30} hop-21(22)-ene; αβH32S and αβH32R – C_{32} 17α(H), 21β(H) bishomohopanes 22S and 22R epimers respectively; βββH31 – C_{31} 17β(H), 21β(H)-homohopane, Diplopterol – hopane-22-ol.

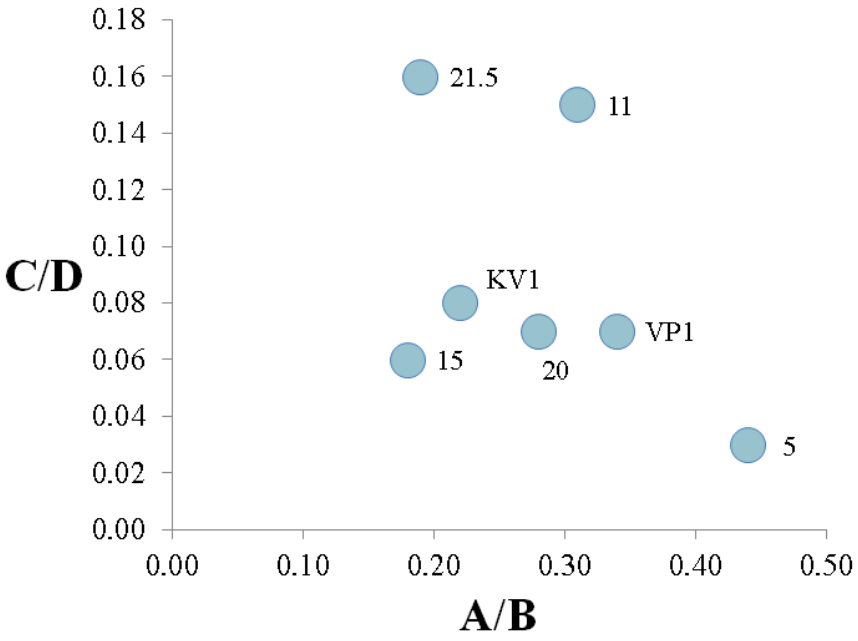


Figure S8. Absence of correlation between A/B and C/D parameters for the studied sediments.

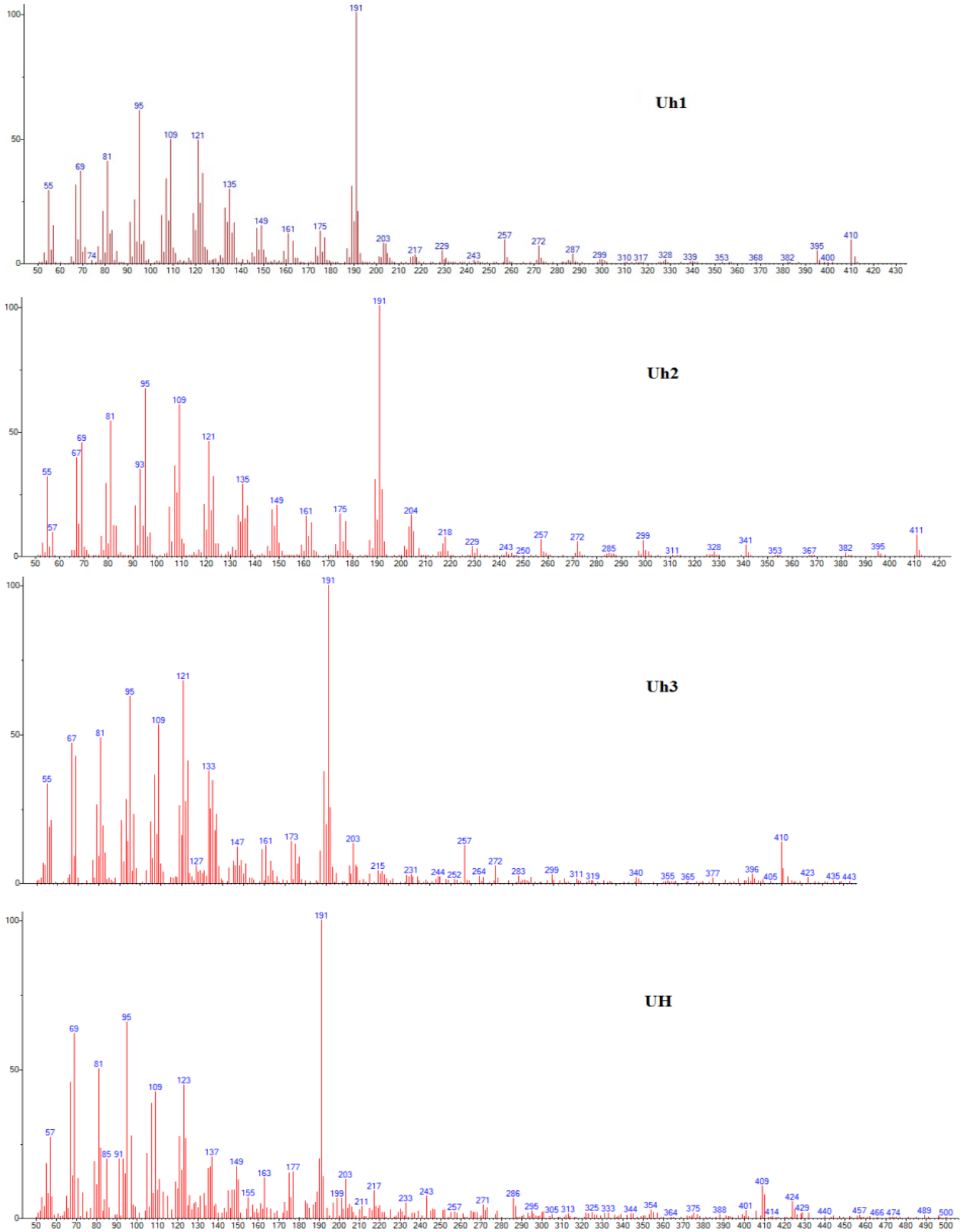


Figure S9. Mass spectra of the unidentified triterpenoids.

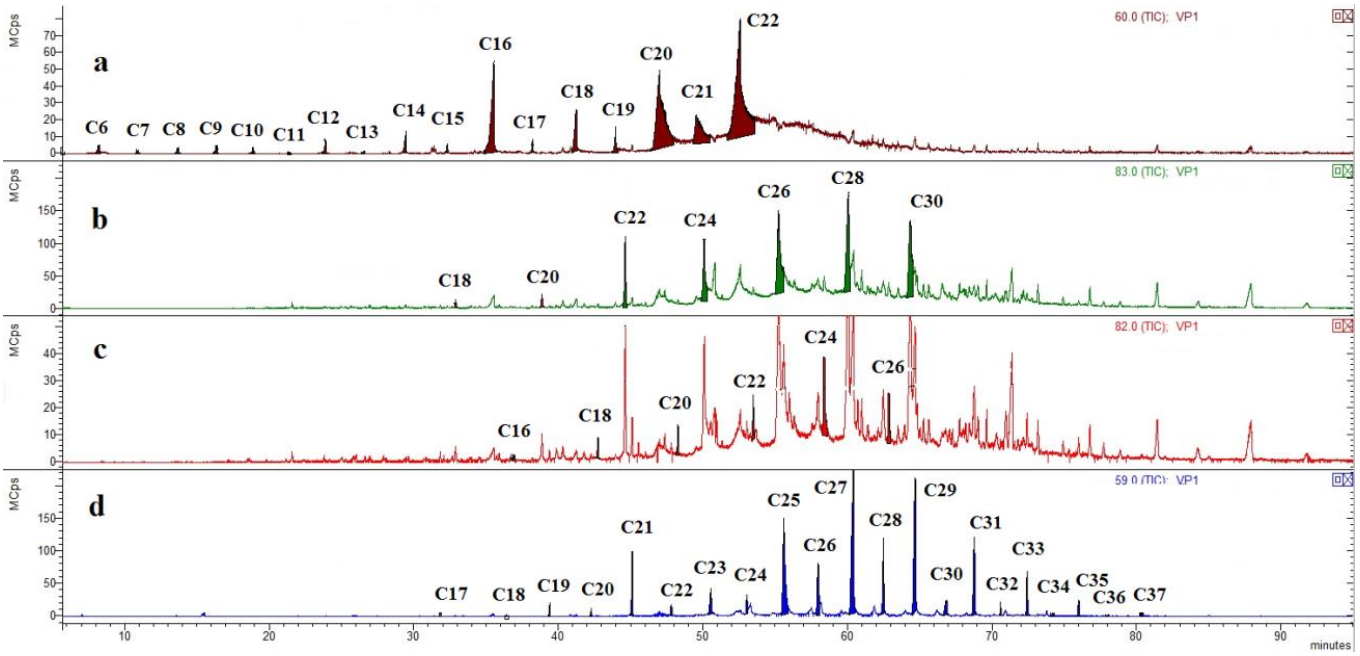


Figure S10. Distribution of the various biomarkers in the polar fraction of the sample collected in the zone of the wave-cut niche (VP1): (**a**) distribution of the fatty acids (m/z 60); (**b**) distribution of the alcohols (m/z 83); (**c**) distribution of the aldehydes (m/z 82); (**d**) distribution of the methylketones (m/z 59).

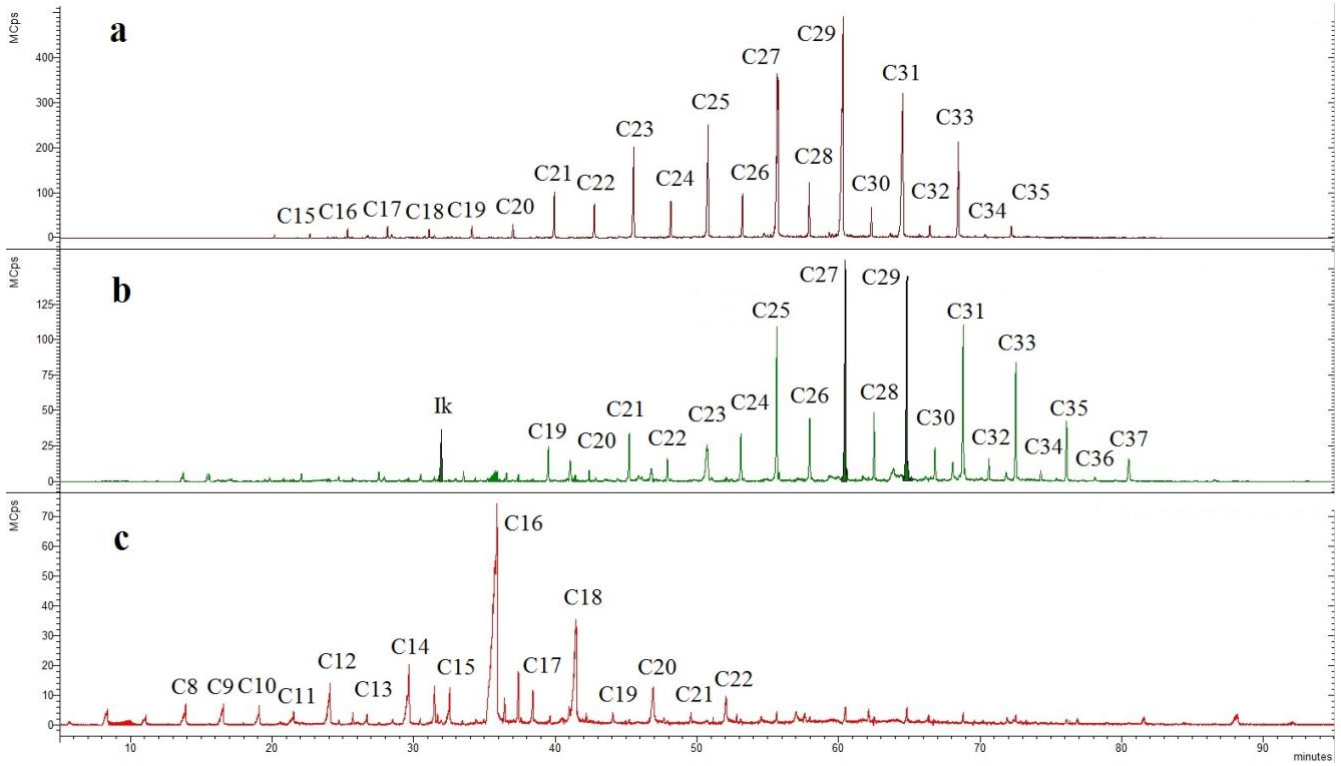


Figure S11. Comparison of the distributions of n-alkanes (**a**, m/z 57), methylketones (**b**, m/z 59) and fatty acids (**c**, m/z 60) for the "KV1" sample. Here we can observe the certain similarities between distributions of n-alkanes and the methylketones (slight shift to the high-molecular area in the methylketones distribution), but there is no resemblance between fatty acids distribution and the methylketones distribution.

Ik is the 6,10,14-trimethylpentadecan-2-one.

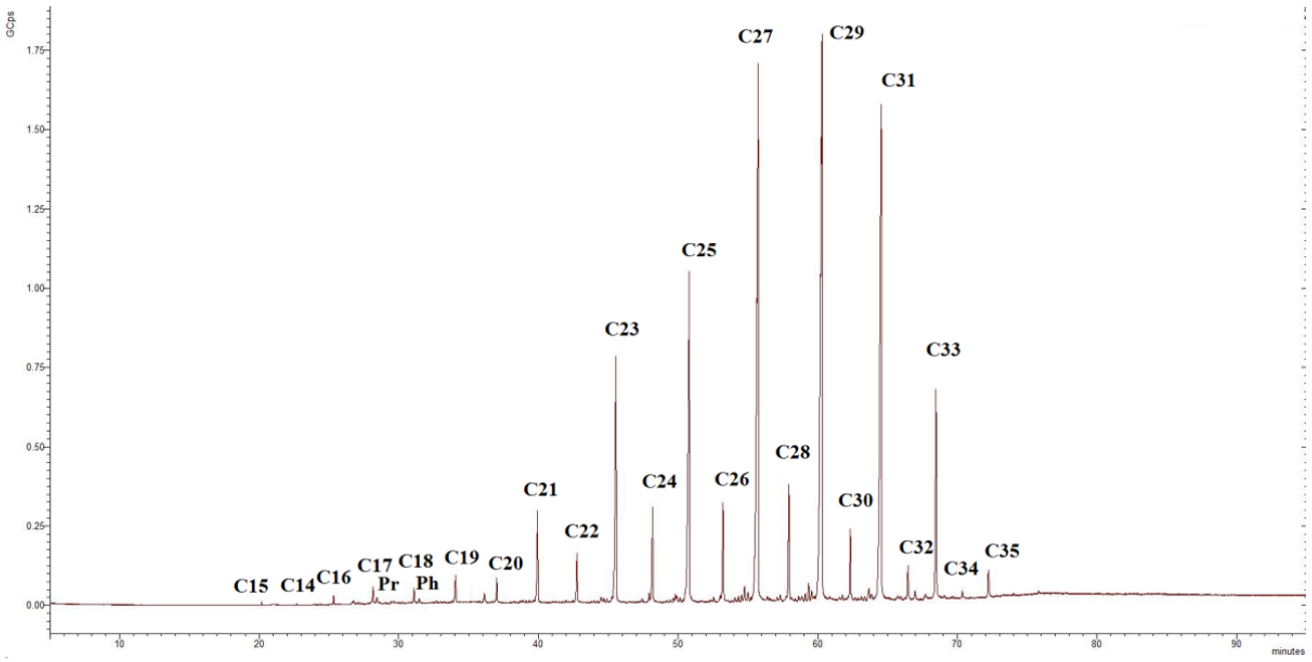


Figure S12. TIC chromatogram of the aliphatic fraction of the sample «15». n-Alkanes are labeled according to the number of carbon atoms in the molecule. Pr − pristane, Ph − phytane.

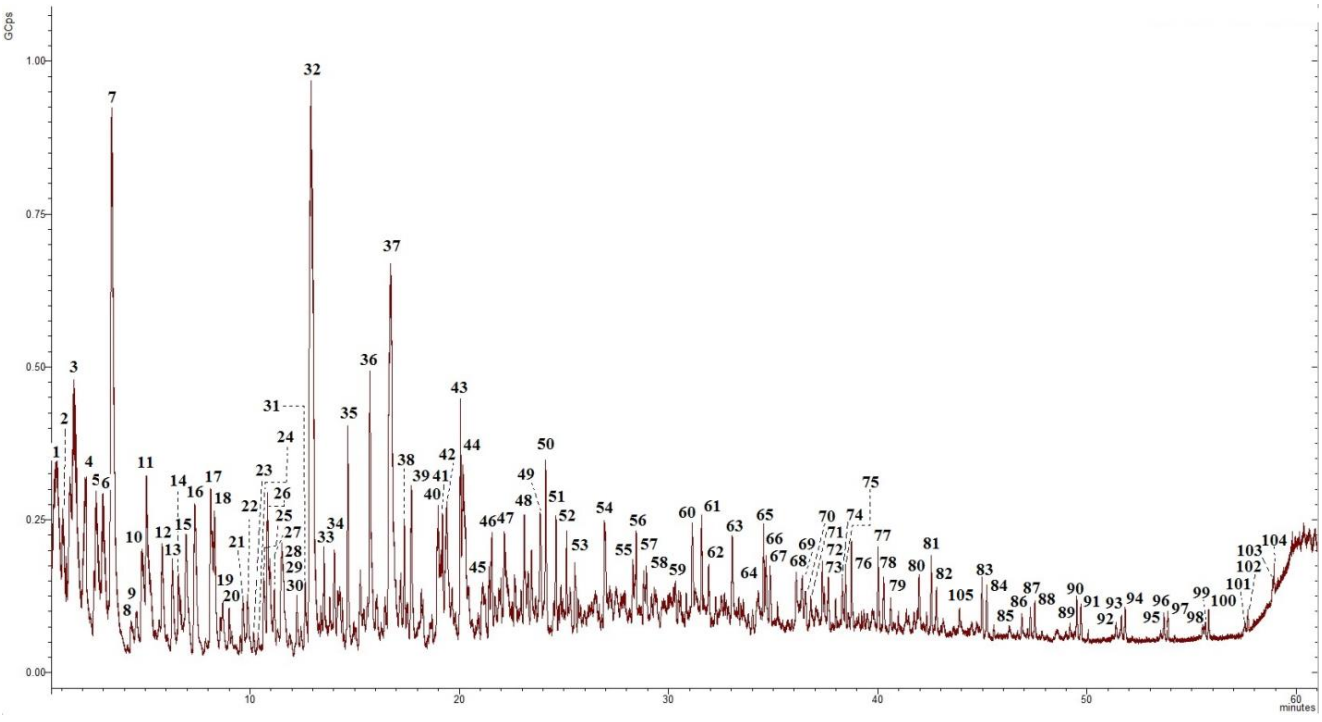


Figure S13. Pyrogram of the total ion current (TIC) of the "KV1" sample. The numbers indicate the component peaks. (Identification is given in Table S5).

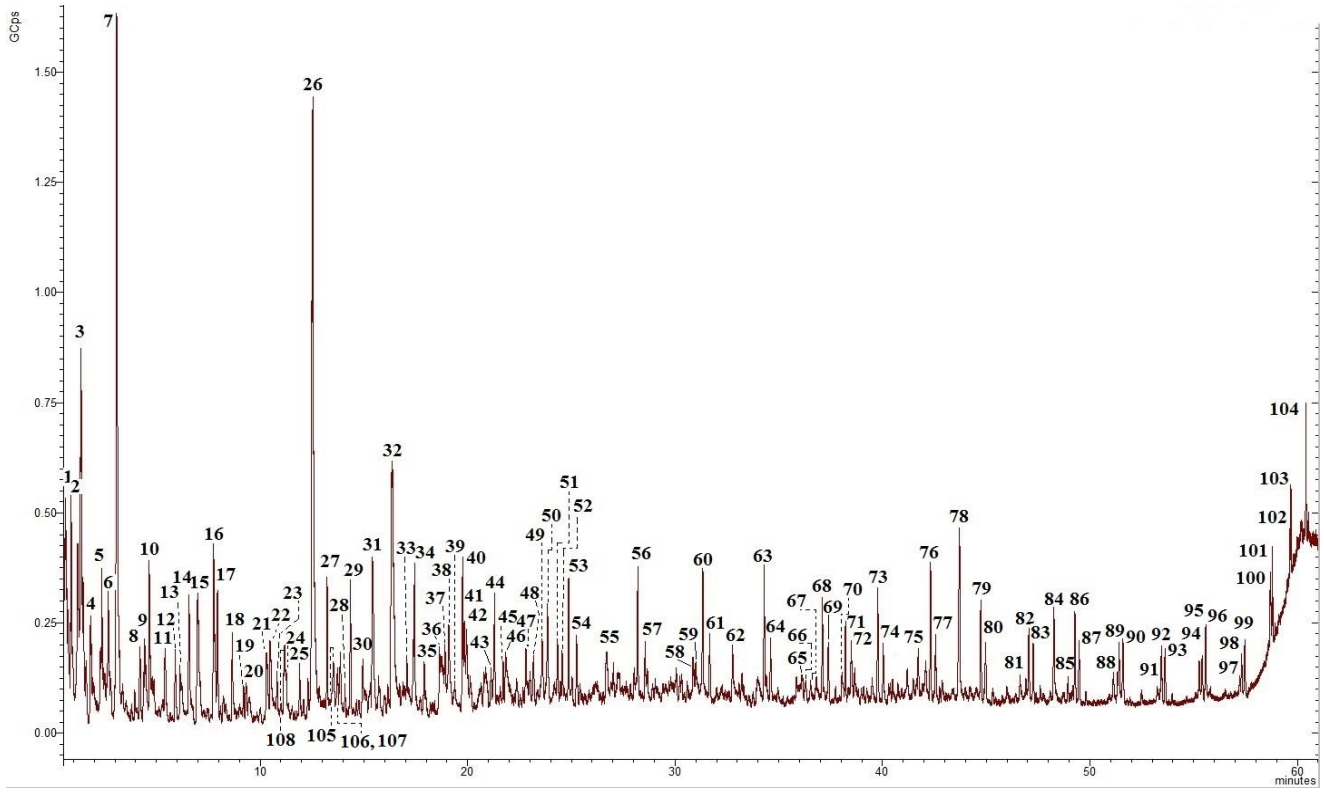


Figure S14. Pyrogram of the total ion current (TIC) of the "VP1" sample. The numbers indicate the component peaks. (Identification is given in Table S5).

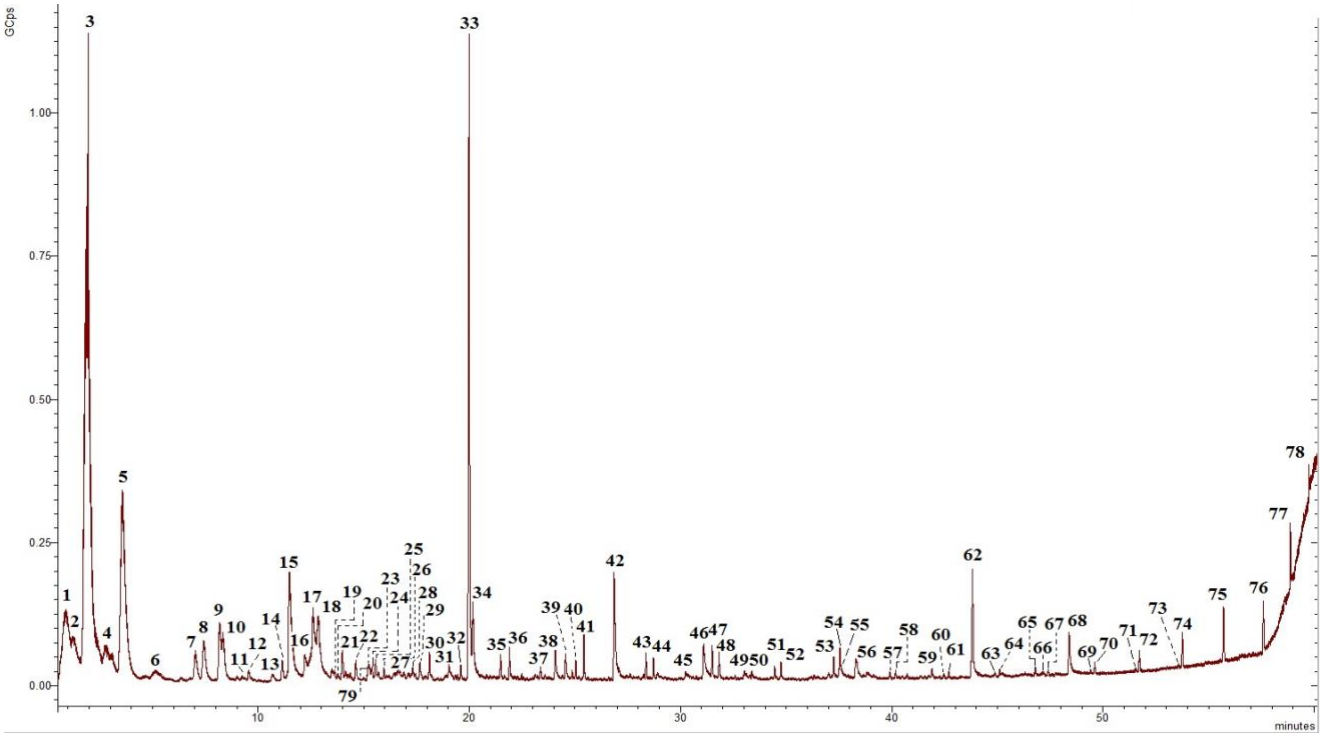


Figure S15. Pyrogram of the total ion current (TIC) of the "5" sample. The numbers indicate the component peaks. (Identification is given in Table S6).

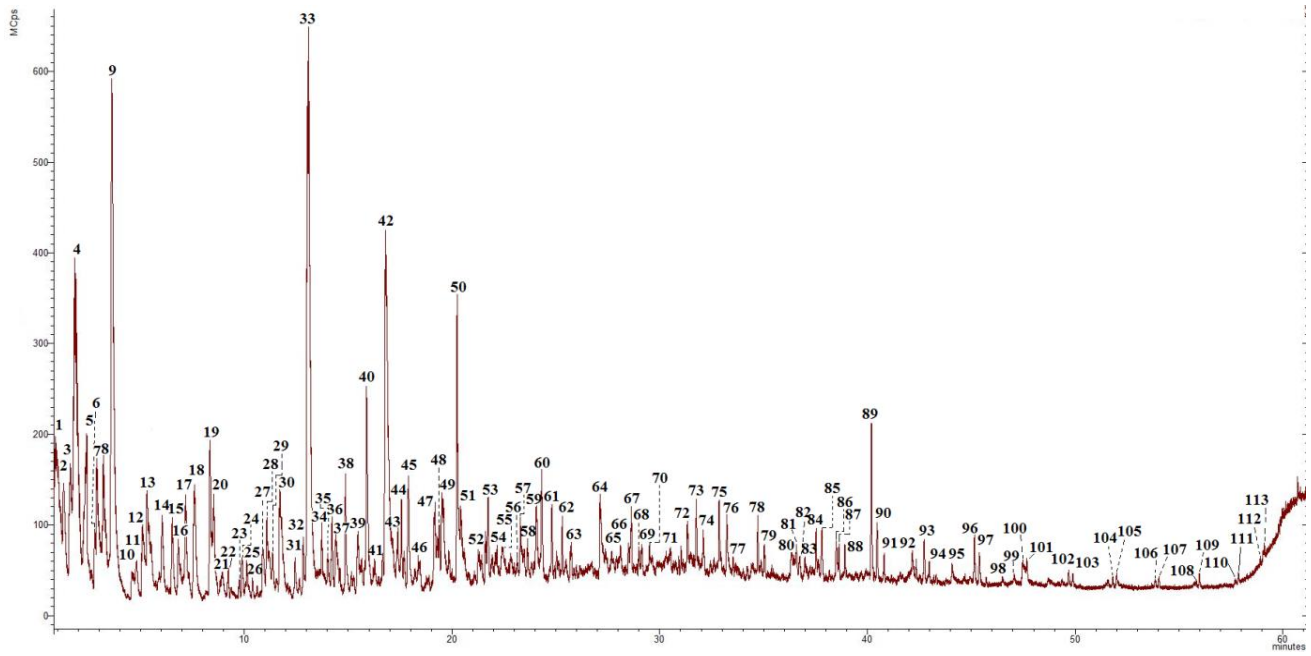


Figure S16. Pyrogram of the total ion current (TIC) of the "11" sample. The numbers indicate the component peaks. (Identification is given in Table S7).

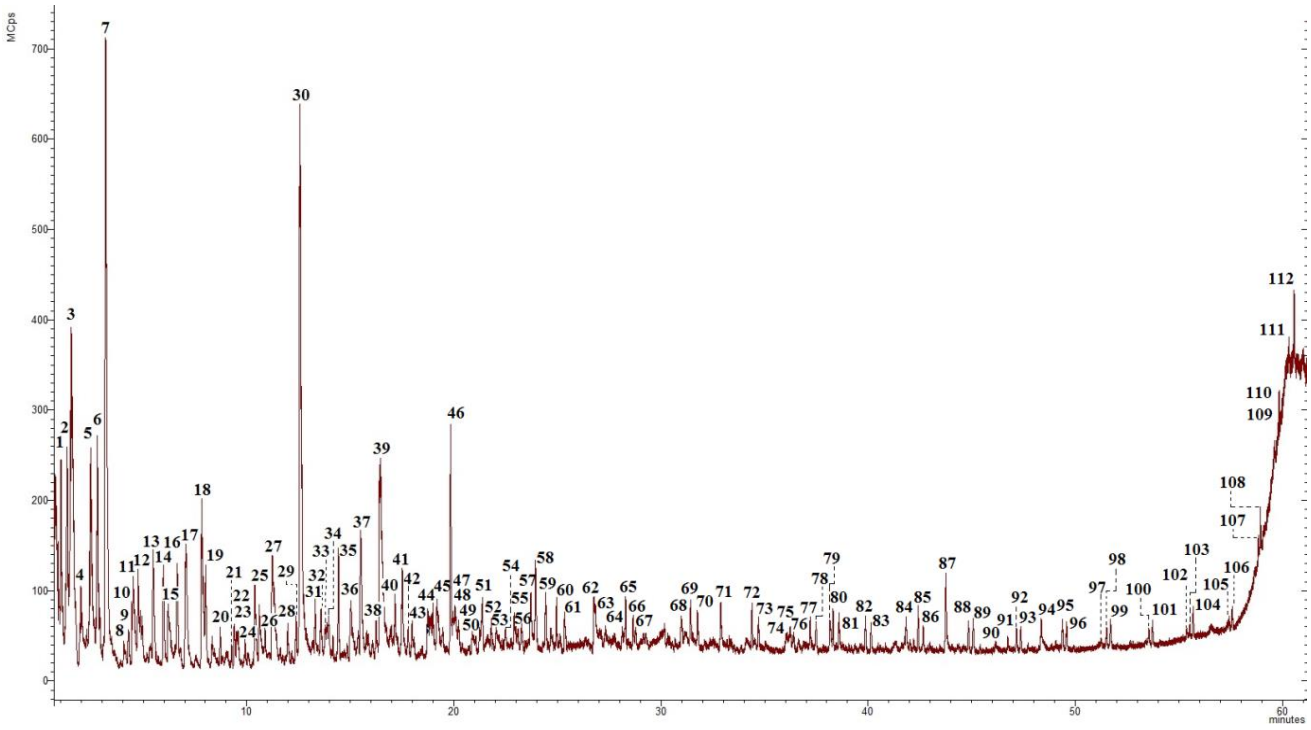


Figure S17. Pyrogram of the total ion current (TIC) of the "15" sample. The numbers indicate the component peaks. (Identification is given in Table S8).

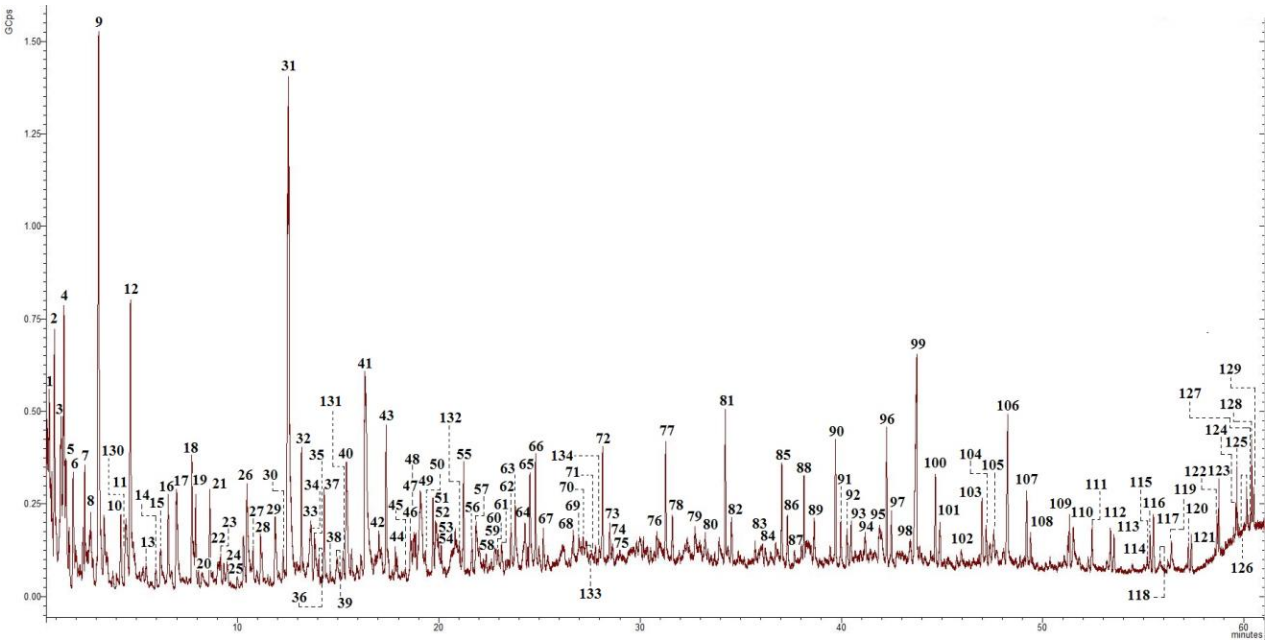


Figure S18. Pyrogram of the total ion current (TIC) of the "20" sample. The numbers indicate the component peaks. (Identification is given in Table S9).

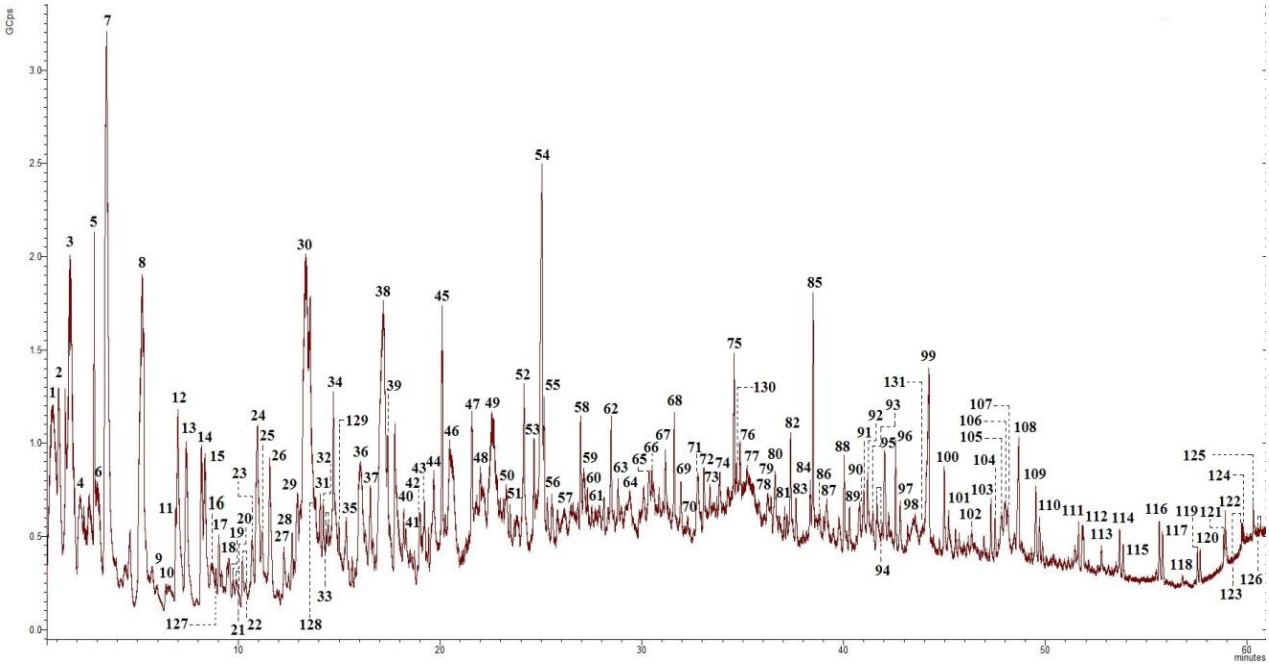


Figure S19. Pyrogram of the total ion current (TIC) of the "21.5" sample. The numbers indicate the component peaks. (Identification is given in Table 10).

Table S5. Components identified by the Py-GC-MS in samples "KV1" and "VP1".

Sample					
KV1			VP1		
ID	**Component**	**m/z**	**ID**	**Component**	**m/z**
1	1,4-pentadiene	68	1	1,4-pentadiene	68
2	Methylfuran	53, 82	2	Methylfuran	53, 82
3	Benzene	78	3	Benzene	78
4	4-Cyclohexene-1,2-diol	60, 96	4	Heptene	60, 96
5	Pyridine	52, 79	5	Pyridine	52, 79
6	3-(2-propenyl)-cyclopentene	67, 79	6	3-(2-propenyl)-cyclopentene	67, 79
7	Toluene	91, 92	7	Toluene	91, 92
8	Furfural	67, 95	8	3-methylheptene-1	55,83
9	5-methylundecene-4	55, 69	9	2-Cyclopenten-1-one	54, 82
10	Methylpyridine	66, 93	10	Furfural	95, 96
11	3-Furaldehyde	95, 96	11	2-methyl-1H-pyrrole	80, 81
12	2-methyl-1H-pyrrole	80, 81	12	3-methyl-1H-pyrrole	78, 80, 81
13	3-methyl-1H-pyrrole	78, 80, 81	13	Methylpyridine	92, 93
14	Methylpyridine	92, 93	14	Ethylbenzene	91, 106
15	Ethylbenzene	91, 106	15	p-Xylene	91, 105, 106
16	p-Xylene	91, 105, 106	16	Styrene	103, 104
17	Styrene	78, 104	17	o-Xylene	91, 106
18	o-Xylene	91, 106	18	Nonene	55, 97
19	Acetylfuran	95, 110	19	Nonane	57, 75
20	Nonene	55, 97	20	2,3-dimethyl-1H-pyrrole	80, 94, 95
21	2,3-dimethyl-, 1H-pyrrole	80, 94, 95	21	Benzaldehyde	77, 105, 106
22	3,5-dimethylpyridine	79, 106, 107	22	5-Methylfurfural	53, 109, 110
23	2,5-dimethyl-, 1H-pyrrole	79, 106, 107	23	n-Propylbenzene	91, 120
24	3,4-dimethylpyridine	79, 106, 107	24	(1-methylethyl)benzene	105, 120
25	Benzaldehyde	75, 105, 106	25	1-ethyl-4-methyl-benzene	105, 120
26	5-methyl-2-furanecarboxyaldehyde	53, 109, 110	26	Phenol	66, 94
27	n-Propylbenzene	91, 120	27	Decene	55, 97
28	Benzonitrile	76, 103	28	Indane	117, 118
29	1-ethyl, 2-methylbenzene	105, 120	29	Indene	115, 116
30	1-methylethylbenzene	105, 120	30	Acetophenone	77, 105
31	Benzofuran	89, 90, 118	31	o-Cresol	107, 108
32	Phenol	66,94	32	p-Cresol	107, 108
33	Decene	55,83	33	2-methylbenzofuran	131, 132
34	1,2,4-trimethylbenzene	105, 120	34	Undecene	55, 97
35	Indene	89, 115, 116	35	Undecane	57, 71
36	2-methylphenol	77, 107, 108	36	1H-Indene, 1-methyl-	129, 130
37	3-methylphenol	77, 107, 108	37	1H-Indene, 3-methyl-	129, 130
38	2-methylbenzofurane	131, 132	38	Dimethylphenol	122, 130
39	Benzyl nitrile	90, 117	39	n-Pentylbenzene	91, 92, 148
40	1,2-Dihydronaphthalene	115, 129, 130	40	Naphthalene	128
41	3-methyl-1H-Indene	115, 130	41	Ethylphenol	107, 122
42	2,5-dimethylphenol	107, 122	42	Ethylphenol	107, 122
43	Naphtalene	128	43	Pentenylbenzene	91, 146
44	4-ethylphenol	107, 122	44	Dodecene	55, 97
45	3,5-dimethylphenol	107, 121, 122	45	Dodecane	57, 71
46	4,7-dimethylbenzofuran	145, 146	46	2,3-Dihydrobenzofuran	94, 120
47	2,3-dihydrobenzofuran	91, 120	47	1,2-Dihydro-3-methylnaphthalene	129, 144
48	2,3-dihydro-1H-Indenone-1	104, 132	48	Unknown compound	91, 121, 129, 144, 162
49	Indole	89, 90, 117	49	Indole	90, 117
50	2-methylnaphtalene	115, 141, 142	50	2-Methylnaphthalene	141, 142
51	1-methylnaphtalene	115, 141, 142	51	1-Methylnaphthalene	141, 142
52	Tridecene	55,97	52	3-tert-butylphenol	135, 150
53	Tridecane	57, 85	53	Tridecene	55, 97
54	Biphenyl	130, 154	54	Tridecane	57, 71
55	Dimethylnaphtalene	141, 156	55	Unknown compound	130, 154
56	Tetradecene	55, 97	56	Tetradecene	55, 97
57	Tetradecane	57, 71	57	Tetradecane	57, 71
58	Dimethylnaphtalene	141, 156	58	Dibenzofuran	139, 168
59	Methylbiphenyl	152, 168	59	α-Naphthol	115, 144
60	Dibenzofuran	139, 168	60	Pentadecene	55, 97

61	9-Heptadecanol	69, 97	61	Pentadecane	57, 71
62	Pentadecane	57, 71	62	Fluorene	165, 166
63	Fluorene	165, 166	63	Hexadecene	55, 97
64	Dimethylbiphenyl	167, 182	64	Hexadecane	57, 71
65	Hexadecene	55, 97	65	Methylfluorene	165, 180
66	6H-Dibenzo[b,d]-pyran	152, 181, 182	66	Methylfluorene	165, 180
67	Hexadecane	55, 97	67	Methylfluorene	165, 180
68	3-Phenoxyphenol	158, 186	68	Heptadecene	55, 97
69	Methylfluorene	165, 180	69	Heptadecane	57, 71
70	Methylfluorene	165, 180	70	Phenanthrene	152, 178
71	Methylfluorene	165, 180	71	Unknown compound (O-containing compound)	69, 126
72	Heptadecene	55, 97	72	2-methylhexadecan-1-ol	69, 111
73	Heptadecane	57, 71	73	Octadecene	55, 97
74	Phenanthrene	178	74	Octadecane	57, 71
75	2-methylhexadecanol-1	69, 111	75	Hexadecanenitrile	97, 110
76	Cis-2-methyl-octadecene-7	69, 111	76	Nonadecene	55, 97
77	Octadecene	55, 97	77	Nonadecane	57, 71
78	Octadecane	57, 71	78	n-Hexadecanoic acid	73, 129
79	1,2,3-trimethyl-4-propenylnaphthalene	195, 210	79	Eicosene	55, 97
80	Hexadecanenitrile	97, 110	80	Eicosane	57, 71
81	Nonadecene	55, 97	81	Octadecanenitrile	97, 110
82	Nonadecane	57, 71	82	Heneicosene	55, 97
83	Eicosene	55, 97	83	Heneicosane	57, 71
84	Eicosane	57, 71	84	n-Octadecanoic acid	73, 129
85	Pyrene	101, 202	85	Nonadecanenitrile	97, 110
86	Octadecanenitrile	97, 110	86	Docosene	55, 97
87	Heneicosene	55, 97	87	Docosane	57, 71
88	Heneicosane	57, 71	88	Eicosanenitrile	97, 110
89	Nonadecanenitrile	97, 110	89	Tricosene	55, 97
90	Docosene	55, 97	90	Tricosane	57, 71
91	Docosane	57, 71	91	Heneicosanenenitrile	97, 110
92	Eicosanenitrile	97, 110	92	Tetracosene	55, 97
93	Tricosene	55, 97	93	Tetracosane	57, 71
94	Tricosane	57, 71	94	Docosanenitrile	97, 110
95	Heneicosanenitrile	97, 110	95	Pentacosene	55, 97
96	Tetracosene	55, 97	96	Pentacosane	57, 71
97	Tetracosane	57, 71	97	Tricosanenitrile	97, 110
98	Docosanenitrile	97, 110	98	Hexacosene	55, 97
99	Pentacosene	55, 97	99	Hexacosane	57, 71
100	Pentacosane	57, 71	100	Heptacosene	55, 97
101	Hexacosene	55, 97	101	Heptacosane	57, 71
102	Hexacosane	57, 71	102	Octacosene	55, 97
103	Heptacosene	55, 97	103	Octacosane	57, 71
104	Heptacosane	57, 71	104	Nonacosane	57, 71
105	Hexadecanoic acid	73, 129	105	2,5-dimethylcyclopentanone	69, 112
—	—	—	106	1-methyl-2-ethylbenzene	105, 120
—	—	—	107	Decane	57, 71
—	—	—	108	Benzonitrile	76, 103

Table S6. Components identified by the Py-GC-MS in sample "5".

ID	Component	m/z
1	1,4-pentadiene	68
2	Methylfuran	53, 82
3	Benzene	77, 78
4	Pyridine	52, 79
5	Toluene	91, 92
6	Hexane, 3-ethyl-	84, 85
7	Ethylbenzene	91, 106
8	p-Xylene	91, 105, 106
9	Styrene	78, 104
10	o-Xylene	91, 105, 106
11	Nonene	55, 97
12	Nonane	57, 71
13	Benzaldehyde	77, 105, 106
14	n-Propylbenzene	91, 120
15	Benzonitrile	76, 103
16	(1-methylethyl)benzene	105, 120
17	Benzofuran	89, 90, 118
18	Phenol	66, 94
19	Decene	55, 97
20	Decane	57, 71
21	Trimethylbenzene	105, 120
22	Indene	115, 116
23	Acetophenone	77, 105
24	Methylpropylbenzene	105, 134
25	n-Butylbenzene	91, 105, 134
26	Methylpropylbenzene	105, 134
27	o-Cresol	107, 108
28	Methylbenzofuran	131, 132
29	Undecene	55, 97
30	Undecane	57, 71
31	1H-Indene, 1-methylene-	102, 128
32	n-Pentylbenzene	91, 105, 148
33	Naphthalene	128
34	Benzothiophene	89, 134
35	Dodecene	55, 97
36	Dodecane	57, 71
37	n-Hexylbenzene	91, 105, 162
38	2-Methylnaphthalene	115, 141, 142
39	1-Methylnaphthalene	115, 141, 142
40	Tridecene	55, 97
41	Tridecane	57, 71
42	Biphenyl	130, 154
43	Tetradecene	55, 97
44	Tetradecane	57, 71
45	n-Octylbenzene	91, 92, 190
46	Dibenzofuran	139, 168
47	Pentadecene	55, 97
48	Pentadecane	57, 71
49	Fluorene	165, 166
50	n-Nonylbenzene	91, 92, 204
51	Hexadecene	55, 97
52	Hexadecane	57, 71
53	Heptadecene	55, 97
54	Heptadecane	57, 71
55	Dibenzothiophene	184
56	Phenanthrene	178
57	Octadecene	55, 97
58	Octadecane	57, 71
59	Hexadecanenitrile	97, 110
60	Nonadecene	55, 97
61	Nonadecane	57, 71
62	n-Hexadecanoic acid	73, 129
63	Eicosene	55, 97

64	Eicosane	57, 71
65	Octadecanenitrile	97, 110
66	Heneicosene	55, 97
67	Heneicosane	57, 71
68	n-Octadecanoic acid	73, 129
69	Docosene	55, 97
70	Docosane	57, 71
71	Tricosene	55, 97
72	Tricosane	57, 71
73	Tetracosene	55, 97
74	Tetracosane	57, 71
75	Pentacosane	57, 71
76	Hexacosane	57, 71
77	Heptacosane	57, 71
78	Octacosane	57, 71
79	Methylbenzonitrile	90, 117

Table S7. Components identified by the Py-GC-MS in sample "11".

ID	Component	m/z
1	1,4-pentadiene	68
2	Methylfuran	53, 82
3	1,4-Cyclohexadiene	52, 79
4	Benzene	78
5	Acetic acid	60
6	N-Methylpyrrole	53, 80, 81
7	Pyridine	52, 79
8	Pyrrole	67
9	Toluene	91, 92
10	Furfural	67, 95
11	Methylpyridine	66, 93
12	2-Cyclopenten-1-one	54, 82
13	3-Furaldehyde	95, 96
14	2-methyl-1H-pyrrole	80, 81
15	3-methyl-1H-pyrrole	78, 80, 81
16	Methylpyridine	66, 93
17	Ethylbenzene	91, 106
18	p-Xylene	91, 105, 106
19	Styrene	103, 104
20	o-Xylene	91, 106
21	Acetylfuran	95, 110
22	Nonene	55, 97
23	Nonane	57, 71
24	Dimethylpyrrole	94, 95
25	Dimethylpyridine	106, 107
26	Dimethylpyrrole	94, 95
27	Benzaldehyde	75, 105, 106
28	5-Methylfurfural	53, 109, 110
29	n-Propylbenzene	91, 120
30	Benzonitrile	76, 103
31	(Methylethyl)benzene	105, 120
32	Benzofuran	90, 118
33	Phenol	66, 94
34	Decene	55, 97
35	Dimethylphenol	107, 122
36	Trimethylbenzene	105, 120
37	Propenylbenzene	91, 117, 118
38	Indene	115, 116
39	Acetophenone	77, 105
40	o-Cresol	107, 108
41	Methylbenzonitrile	90, 117
42	p-Cresol	107, 108
43	Methylbenzofuran	131, 132
44	Methylbenzofuran	131, 132
45	Benzyl nitrile	90, 117

46	Undecane	57, 71
47	Methylindene	129, 130
48	1,2-Dihydronaphthalene	115, 129, 130
49	Dimethylphenol	107, 122
50	Naphthalene	128
51	Ethylphenol	107, 122
52	Unknown compound ((O-containing))	122, 131, 146
53	Dimethylbenzofuran	131, 145, 146
54	Dodecane	57, 71
55	1-Hydroxytetralin	91, 120, 130
56	2-Ethyl-1-H-indene	129, 144
57	Methyldihydronaphthalene	129, 144
58	1-Naphthol, 1,2,3,4-tetrahydro-3-methyl-	120, 129, 144
59	Indole	117, 90
60	2-Methylnaphthalene	141, 142
61	1-Methylnaphthalene	141, 142
62	Tridecene	55, 97
63	Tridecane	57, 71
64	Biphenyl	130, 154
65	Ethylnaphthalene	141, 156
66	Dimethylnaphthalene	141, 156
67	Tetradecene	55, 97
68	Tetradecane	57, 71
69	Dimethylnaphthalene	141, 156
70	Dimethylnaphthalene	141, 156
71	Methylbiphenyl	152, 168
72	Dibenzofuran	139, 168
73	Pentadecene	55, 97
74	Pentadecane	57, 71
75	Trimethylnaphthalene	155, 170
76	Fluorene	165, 166
77	Trimethylnaphthalene	155, 170
78	Hexadecene	55, 97
79	Hexadecane	57, 71
80	Unknown compound (O-containing)	93, 186
81	Methylfluorene	165, 180
82	Methylfluorene	165, 180
83	Tetramethylnaphthalene	184, 169
84	Heptadecene	55, 97
85	Heptadecane	57, 71
86	Phenanthrene	178
87	2-methylhexadecan-1-ol	69, 111
88	methylhexadecanol	69, 111
89	Octadecene	55, 97
90	Octadecane	57, 71
91	Hexadecanol	83, 97, 111
92	Hexadecanenitrile	97, 110
93	Nonadecene	55, 97
94	Nonadecane	57, 71
95	n-Hexadecanoic acid	73, 129
96	Eicosene	55, 97
97	Eicosane	57, 71
98	Pyrene	101, 202
99	Octadecanenitrile	97, 110
100	Heneicosene	55, 97
101	Heneicosane	57, 71
102	Docosene	55, 97
103	Docosane	57, 71
104	Tricosene	55, 97
105	Tricosane	57, 71
106	Tetracosene	55, 97
107	Tetracosane	57, 71
108	Pentacosene	55, 97
109	Pentacosane	57, 71
110	Hexacosene	55, 97
111	Hexacosane	57, 71

112	Heptacosene	55, 97
113	Heptacosane	57, 71

Table S8. Components identified by the Py-GC-MS in sample "15".

ID	Component	m/z
1	Methylfuran	53, 82
2	Cyclohexadiene	79
3	Benzene	78
4	2-Methylbutyronitrile	54, 55
5	Pyridine	52, 79
6	Pyrrole	67
7	Toluene	91, 92
8	Furfural	67, 95
9	Octene	55, 97
10	Methylpyridine	66, 93
11	2-Cyclopenten-1-one	54, 82
12	3-Furaldehyde	95, 96
13	2-methyl-1H-pyrrole	80, 81
14	3-methyl-1H-pyrrole	78, 80, 81
15	Methylpyridine	66, 93
16	Ethylbenzene	91, 106
17	p-Xylene	91, 105, 106
18	Styrene	103, 104
19	o-Xylene	91, 106
20	Nonene	55, 97
21	Nonane	57, 71
22	Dimethylpyrrole	94, 95
23	Dimethylpyridine	106, 107
24	Dimethylpyrrole	94, 95
25	5-Methylfurfural	53, 109, 110
26	n-Propylbenzene	91, 120
27	Benzonitrile	76, 103
28	Methylethylbenzene	105, 120
29	Benzofuran	90, 118
30	Phenol	66, 94
31	Decene	55, 97
32	Trimethylpyrrole	94, 108
33	Decane	57, 71
34	Propenylbenzene	91, 117, 118
35	Indene	115, 116
36	Acetophenone	77, 105
37	o-Cresol	107, 108
38	Methoxyphenol	81, 109, 124
39	p-Cresol	107, 108
40	Methylbenzofuran	131, 132
41	Undecene	55, 97
42	Benzyl nitrile	90, 117
43	Undecane	57, 71
44	Methylindene	129, 130
45	Dimethylphenol	107, 122
46	Naphthalene	128
47	Ethylphenol	107, 122
48	Ethylphenol	107, 122
49	Ethylphenol	107, 122
50	Dimethylphenol	107, 122
51	Dodecene	55, 97
52	Dodecane	57, 71
53	1-Hydroxytetralin	91, 120, 130
54	Trimethylphenol	121, 136
55	1-Indanone	104, 132
56	Hexylbenzene	91, 162
57	Indole	117, 90
58	2-Methylnaphthalene	141, 142
59	1-Methylnaphthalene	141, 142

60	Tridecene	55, 97
61	Tridecane	57, 71
62	Biphenyl	130, 154
63	Methylindole	130, 131
64	Dimethylnaphthalene	141, 156
65	Tetradecene	55, 97
66	Tetradecane	57, 71
67	Dimethylnaphthalene	141, 156
68	Dibenzofuran	139, 168
69	Pentadecene	55, 97
70	Pentadecane	57, 71
71	Fluorene	165, 166
72	Hexadecene	55, 97
73	Hexadecane	57, 71
74	Unknown compound (O-containing)	93, 186
75	Methylfluorene	165, 180
76	Methylfluorene	165, 180
77	Heptadecene	55, 97
78	Heptadecane	57, 71
79	Phenanthrene	178
80	2-methylhexadecan-1-ol	69, 111
81	methylhexadecanol	69, 111
82	Octadecene	55, 97
83	Octadecane	57, 71
84	Hexadecanenitrile	97, 110
85	Nonadecene	55, 97
86	Nonadecane	57, 71
87	n-Hexadecanoic acid	73, 129
88	Eicosene	55, 97
89	Eicosane	57, 71
90	Pyrene	101, 202
91	Octadecanenitrile	97, 110
92	Heneicosene	55, 97
93	Heneicosane	57, 71
94	n-Octadecanoic acid	73, 129
95	Docosene	55, 97
96	Docosane	57, 71
97	Eicosanenitrile	97, 110
98	Tricosene	55, 97
99	Tricosane	57, 71
100	Tetracosene	55, 97
101	Tetracosane	57, 71
102	Docosanenitrile	97, 110
103	Pentacosene	55, 97
104	Pentacosane	57, 71
105	Hexacosene	55, 97
106	Hexacosane	57, 71
107	Heptacosene	55, 97
108	Heptacosane	57, 71
109	Octacosene	55, 97
110	Octacosane	57, 71
111	Nonacosene	55, 97
112	Nonacosane	57, 71

Table S9. Components identified by the Py-GC-MS in sample "20".

ID	Component	m/z
1	1,4-pentadiene	68
2	Methylfuran	53, 82
3	1,3-Cyclohexadiene	79
4	Benzene	78
5	1,4-Cyclohexadiene	79
6	Heptene	56, 70
7	Pyridine	52, 79
8	Pyrrole	67
9	Toluene	91, 92
10	Octene	55, 97
11	2-Cyclopenten-1-one	54, 82
12	3-Furaldehyde	95, 96
13	2-methyl-1H-pyrrole	80, 81
14	3-methyl-1H-pyrrole	78, 80, 81
15	Methylpyridine	66, 93
16	Ethylbenzene	91, 106
17	p-Xylene	91, 105, 106
18	Styrene	103, 104
19	o-Xylene	91, 106
20	Acetylfuran	95, 110
21	Nonene	55, 97
22	Cyclohexanone	55, 98
23	Nonane	57, 71
24	Dimethylpyridine	106, 107
25	Dimethylpyridine	106, 107
26	5-Methylfurfural	53, 109, 110
27	n-Propylbenzene	91, 120
28	Methylethylbenzene	105, 120
29	Methylethylbenzene	105, 120
30	Benzofuran	90, 118
31	Phenol	66, 94
32	Decene	55, 97
33	Trimethylbenzene	105, 120
34	Decane	57, 71
35	Propenylbenzene	91, 117, 118
36	Indane	117, 118
37	Indene	115, 116
38	3-Butenylbenzene	91, 132
39	Acetophenone	77, 105
40	o-Cresol	107, 108
41	p-Cresol	107, 108
42	Methylbenzofuran	131, 132
43	Undecene	55, 97
44	Undecane	57, 71
45	Methylindane	117,132
46	Methylindene	129, 130
47	Methylindene	129, 130
48	Methylindene	129, 130
49	Dimethylphenol	107, 122
50	n-Pentylbenzene	91, 105, 148
51	Naphthalene	128
52	Ethylphenol	107, 122
53	Ethylphenol	107, 122
54	Dimethylphenol	107, 122
55	Dodecene	55, 97
56	Dodecane	57, 71
57	Dihydrobenzofuran	91, 120
58	4-Ethyl-o-cresol	121, 136
59	Dihydromethylnaphthalene	129, 144
60	Dihydromethylnaphthalene	129, 144
61	Dihydromethylnaphthalene	129, 144
62	Indole	117, 90
63	2-Methylnaphthalene	141, 142

64	1-Methylnaphthalene	141, 142
65	3-tert-Butylphenol	107, 135, 150
66	Tridecene	55, 97
67	Tridecane	57, 71
68	Methylindole	130, 131
69	Methylindole	130, 131
70	Ethylnaphthalene	141, 156
71	Dimethylnaphthalene	141, 156
72	Tetradecene	55, 97
73	Tetradecane	57, 71
74	Dimethylnaphthalene	141, 156
75	Dimethylnaphthalene	141, 156
76	Dibenzofuran	139, 168
77	Pentadecene	55, 97
78	Pentadecane	57, 71
79	Fluorene	165, 166
80	Dodecanoic acid	60, 73
81	Hexadecene	55, 97
82	Hexadecane	57, 71
83	Methylfluorene	165, 180
84	Methylfluorene	165, 180
85	Heptadecene	55, 97
86	Heptadecane	57, 71
87	Phenanthrene	178
88	2-methylhexadecan-1-ol	69, 111
89	Tetradecanoic acid	60, 73
90	Octadecene	55, 97
91	Octadecane	57, 71
92	Pentadecanoic acid	60, 73
93	Unknown compound (ester?)	69, 129, 185
94	Unknown compound (ester?)	73, 129, 192
95	Hexadecanol-1	69, 83
96	Nonadecene	55, 97
97	Nonadecane	57, 71
98	Hexadecenoic acid	55, 69
99	n-Hexadecanoic acid	73, 129
100	Eicosene	55, 97
101	Eicosane	57, 71
102	Pyrene	101, 202
103	Heneicosene	55, 97
104	Heneicosane	57, 71
105	Oleic acid	55, 83
106	n-Octadecanoic acid	73, 129
107	Docosene	55, 97
108	Docosane	57, 71
109	Tricosene	55, 97
110	Tricosane	57, 71
111	Eicosanoic acid	73, 129
112	Tetracosene	55, 97
113	Tetracosane	57, 71
114	Heneicosanoic acid	73, 129, 326
115	Docosanenitrile	97, 110
116	Pentacosene	55, 97
117	Pentacosane	57, 71
118	Tricosanol	69, 83
119	Docosanoic acid	73, 129, 340
120	Hexacosene	55, 97
121	Hexacosane	57, 71
122	Heptacosene	55, 97
123	Heptacosane	57, 71
124	Octacosene	55, 97
125	Octacosane	57, 71
126	C_{27} hopene	191, 231, 368
127	Nonacosene	55, 97
128	Nonacosane	57, 71
129	ββ-C_{28} hopane	191, 384

130	Methylpyridine	66, 93
131	n-Butylbenzene	91, 134
132	Octanoic acid	60, 73
133	Decanoic acid	60, 73
134	Dimethylnaphthalene	141, 156

Table S10. Components identified by the Py-GC-MS in sample "21.5".

ID	Component	m/z
1	1,4-pentadiene	68
2	Methylfuran	53, 82
3	Benzene	78
4	Heptene	56, 70
5	Pyridine	52, 79
6	Pyrrole	67
7	Toluene	91, 92
8	Furfural	67, 95
9	2-methyl-1H-pyrrole	80, 81
10	3-methyl-1H-pyrrole	78, 80, 81
11	Methylpyridine	66, 93
12	Ethylbenzene	91, 106
13	p-Xylene	91, 105, 106
14	Styrene	103, 104
15	o-Xylene	91, 106
16	Acetylfuran	95, 110
17	Nonene	55, 97
18	3-Ethyl-2-methylheptane	57, 98
19	Nonane	57, 71
20	Dimethylpyrrole	94, 95
21	Vinylpyridine	79, 105
22	Dimethylpyridine	106, 107
23	Benzaldehyde	77, 105, 106
24	5-Methylfurfural	53, 109, 110
25	n-Propylbenzene	91, 120
26	Benzonitrile	76, 103
27	Methylethylbenzene	105, 120
28	Benzofuran	90, 118
29	Trimethylbenzene	105, 120
30	Phenol	66, 94
31	Trimethylbenzene	105, 120
32	Propenylbenzene	91, 117, 118
33	Indane	117, 118
34	Indene	115, 116
35	Acetophenone	77, 105
36	o-Cresol	107, 108
37	2-Methoxyphenol	109, 124
38	p-Cresol	107, 108
39	Methylbenzofuran	131, 132
40	Undecene	55, 97
41	Undecane	57, 71
42	Methylindene	129, 130
43	Methylindene	129, 130
44	Dimethylphenol	107, 122
45	Naphthalene	128
46	Ethylphenol	107, 122
47	Dodecene	55, 97
48	Dodecane	57, 71
49	Dihydrobenzofuran	91, 120
50	1-Indanone	104, 132
51	Phenol, 4-ethyl-2-methoxy-	137, 152
52	2-Methylnaphthalene	141, 142
53	1-Methylnaphthalene	141, 142
54	3-tert-Butylphenol	107, 135, 150
55	Tridecene	55, 97
56	Tridecane	57, 71

57	Syringol (2,6-Dimethoxyphenol)	139, 154
58	Biphenyl	130, 154
59	Methylindole	130, 131
60	2-Dodecanol	83, 97
61	Ethylnaphthalene	141, 156
62	Tetradecene	55, 97
63	Tetradecane	57, 71
64	Phenol, 2-allyl-6-methoxy-	131, 149, 164
65	Methylbiphenyl	167, 168
66	p-tert-Butylcatechol	123, 151, 166
67	Dibenzofuran	139, 168
68	Pentadecene	55, 97
69	Pentadecane	57, 71
70	Trimethylnaphthalene	155, 170
71	Dimethoxyacetophenone	165, 180
72	Fluorene	165, 166
73	Trimethylnaphthalene	155, 170
74	Dimethoxyallylphenol	91, 119, 194
75	Hexadecene	55, 97
76	Hexadecane	57, 71
77	Dimethoxyallylphenol	91, 119, 194
78	Phenoxyphenol	129, 186
79	Methylfluorene	165, 180
80	Dimethoxypropenylphenol (Methoxyeugenol)	91, 119, 194
81	2-Pentadecanone	58, 85
82	Heptadecene	55, 97
83	Heptadecane	57, 71
84	Phenanthrene	178
85	2-methylhexadecan-1-ol	69, 111
86	2-Hexadecanone	58, 85
87	Tetradecanoic acid	60, 73
88	Octadecene	55, 97
89	Octadecane	57, 71
90	i-Propyl 13-methyltetradecanoate	129, 199, 242
91	i-Propyl 12-methyltetradecanoate	60, 185, 242
92	Neophytadiene	68, 95, 123
93	2-Heptadecanol	69, 83, 111
94	Pentadecanoic acid	60, 73
95	1-Hexadecanol	69, 83, 97
96	Nonadecene	55, 97
97	Nonadecane	57, 71
98	Phenylnaphthalene	202, 204
99	n-Hexadecanoic acid	73, 129
100	Eicosene	55, 97
101	Eicosane	57, 71
102	n-Heptadecanoic acid	73, 129
103	Heneicosene	55, 97
104	Heneicosane	57, 71
105	Linoleic acid	67, 81, 280
106	cis-Vaccenic acid	69, 83, 264
107	Oleic Acid	69, 83, 264
108	n-Octadecanoic acid	73, 129
109	Docosene	55, 97
110	Docosane	57, 71
111	Tricosene	55, 97
112	Tricosane	57, 71
113	Eicosanoic acid	73, 129
114	Tetracosene	55, 97
115	Tetracosane	57, 71
116	Pentacosene	55, 97
117	Pentacosane	57, 71
118	Unknown β-hopane	177, 191
119	Hexacosene	55, 97
120	Hexacosane	57, 71
121	Heptacosene	55, 97
122	Heptacosane	57, 71

123	Octacosene	55, 97
124	Octacosane	57, 71
125	Nonacosene	55, 97
126	Nonacosane	57, 71
127	Ethylpyridine	79, 106
128	Ethoxybenzene	94, 122
129	3-Butenylbenzene	91, 132
130	6H-Dibenzo[b,d]-pyran	152, 181, 182
131	Hexadecenoic acid	55, 69

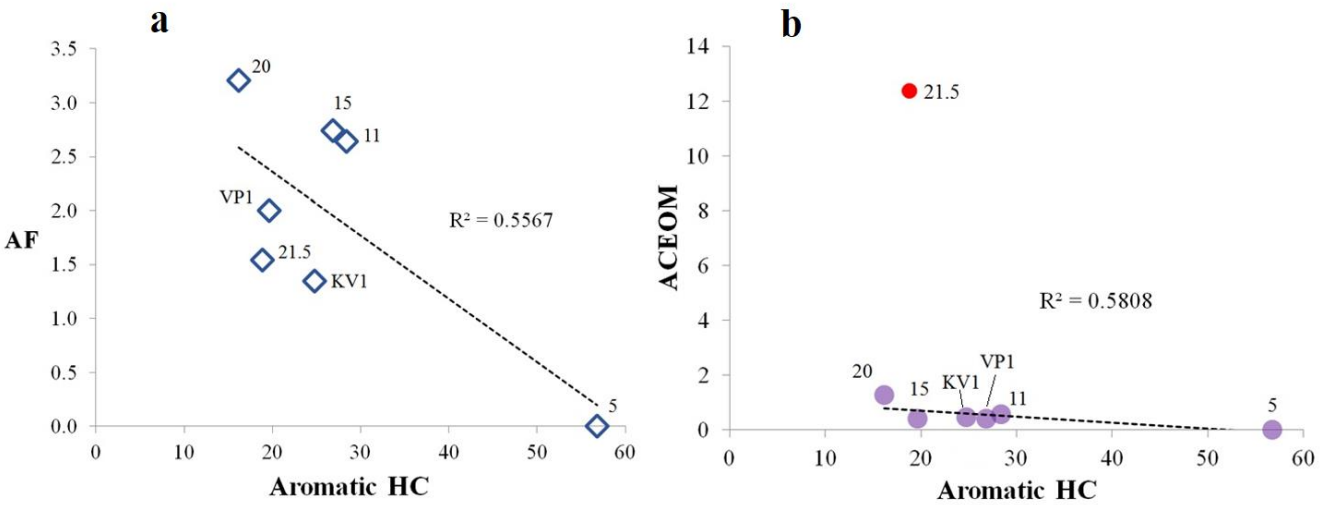


Figure S20. Relationship between different parameters which characterize aromatic hydrocarbons distribution in sediments: (**a**) Relationship between relative content of the aromatic hydrocarbons (Aromatic HC) determined by Py-GC-MS analysis and yield of the aromatic fraction, determined by CLAC (AF); (**b**) interrelation between Aromatic HC and the sum of the identified aromatic compounds in the extractable OM (ACEOM). Peat sample (21.5) falls out from the general trend.

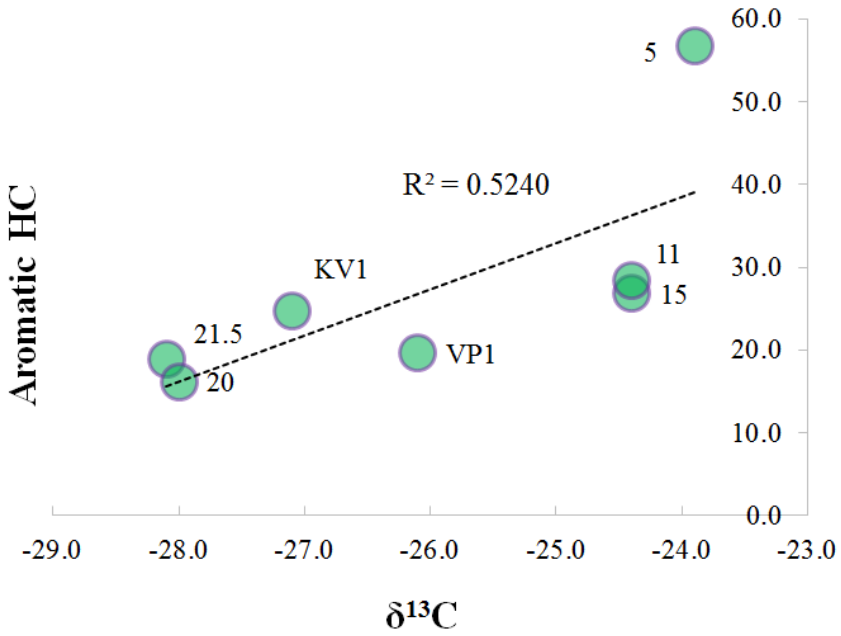


Figure S21. Relationship between relative content of the aromatic hydrocarbons (Aromatic HC) determined by Py-GC-MS and isotopic composition ($\delta^{13}C$) of the samples.

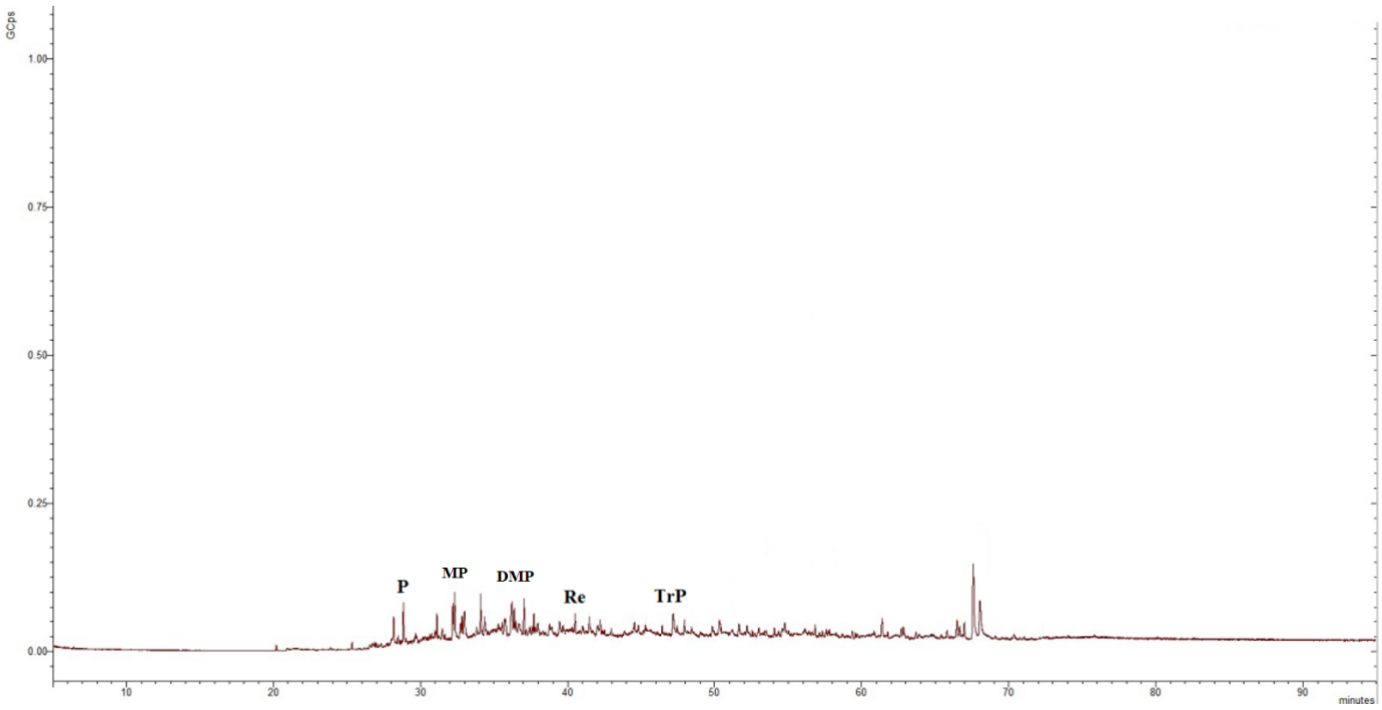


Figure S22. TIC chromatogram of the aromatic fraction of the sample «15». P − phenanthrene, MP − methylphenanthrene, DMP− dimethylphenanthrene; Re − retene; TrP − triphenylene.

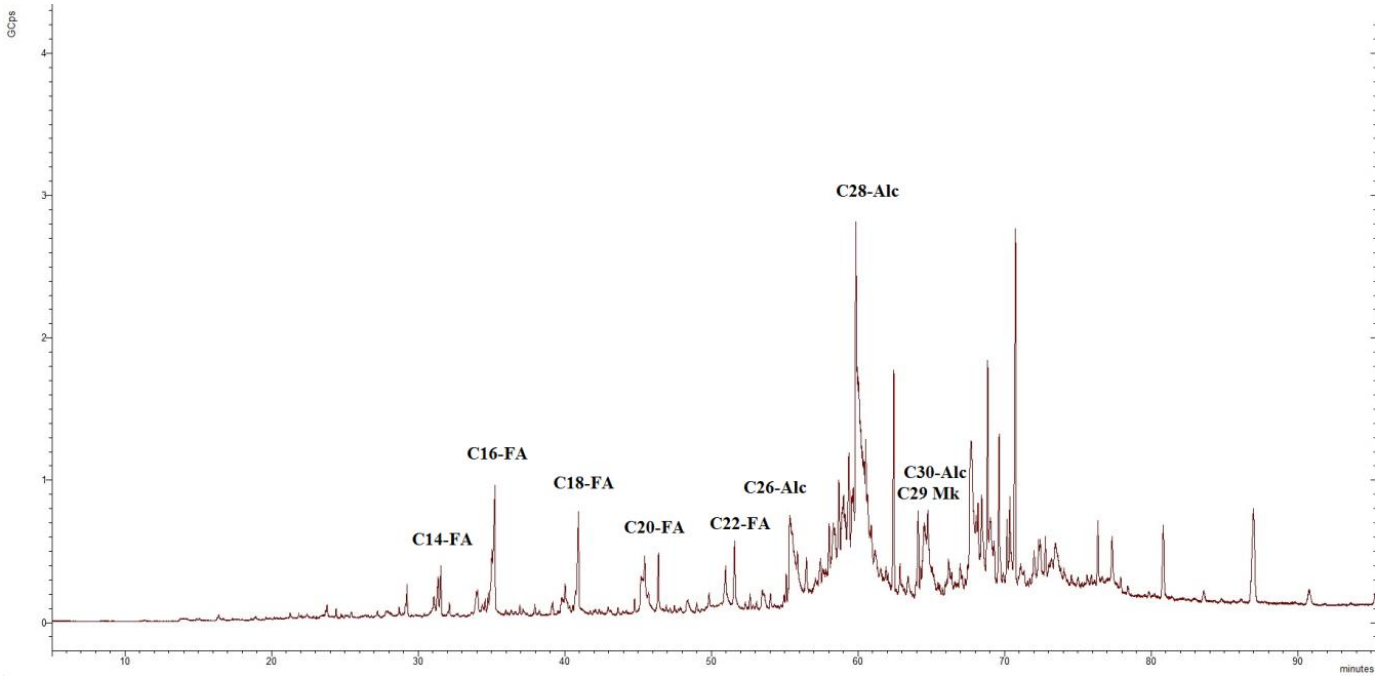


Figure S23. TIC chromatogram of the «polar» fraction of the sample «15». «C16» (for example) means number of the carbon atoms in the molecule: FA − fatty acid; Alc − alcohol; Mk − methylketone.