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Supplementary material

SUPPLEMENTARY MATERIAL TO

Preliminary organic geochemical study of lignite from the Smederevsko Pomoravlje field (Kostolac Basin, Serbia) – reconstruction of geological evolution and potential for rational utilization

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GEOLOGICAL SETTINGS

The Kostolac Coal Basin, covering an area of 145 km^2, is located about 90 km east of Belgrade. It is divided into three coal fields: the Drmno field in the eastern, the Ćirikovac field in the central and the Smederevsko Podunavlje field in the western part of the Basin (Fig. S-1). The Drmno field is exploited, while the Smederevsko Podunavlje field is still under preliminary exploration. Exploitation in the Ćirikovac field was ceased a few years ago.

The basement of the Kostolac Basin is formed of Devonian crystalline rocks overlain by Neogene sediments. The total thickness of the Neogene sediments ranges from 300 to 5000 m in the central part of the depression.[1] The complete Neogene generally dips towards the north–west at a low angle of 5–15° with the coal seams following the same dip. The Neogene complex consists of several units, which were explained in detail in a previous paper.[2]

The Upper Pontian coal-bearing series in the Smederevsko Pomoravlje field were studied in detail by Životić[3] and were found to consist of sand, clayey sand, siltstone, clay, sandy clay, carbonaceous clay and five coal seams, named from bottom to top III, II-a, II, I-a, and I, respectively. Coal seams III, II and I are considered to be important for rational exploitation, whereas coal seams II-a and

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I-a are only locally developed. About 100 exploration boreholes were drilled in the Smederevsko Pomoravlje field.

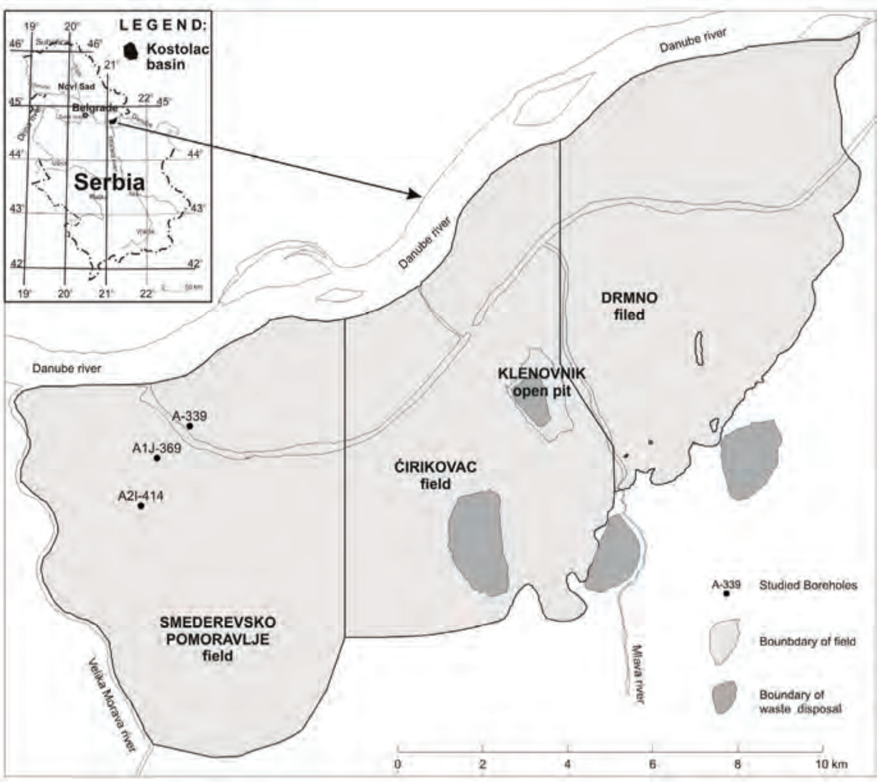


Fig. S-1. Location and coal fields of the Kostolac Basin.

The thickness of coal seam III varies over a wide range due to interbedding, from 18.50 m to 76.00 m (average 38.47 m). Coal seam III splits into three coal layers, the thicknesses of which, from bottom to top, are 0.15–9.00 m (average 2.81 m), 1.00–15.70 m (average 6.93 m) and 0.80–12.40 m (average 4.35 m), respectively. The interbedded waste rocks consist of sand, clay, carbonaceous clay, marly clay, silt and thin coal layers. Their thicknesses between the third and second, and, second and first coal layers vary from a few to 32 m and 36 m, respectively. The coal seam II-a was formed locally in the southern part of the field. The seam thickness varies from 0.15 to 1.00 m. The coal seam II occurs across the entire Smederevsko Pomoravlje field. Typical features of this coal seam are stratification followed by a high content of clayey–sandy sediments. The seam thickness varies from 0.20 to 16.20 m (average 5.69 m). The coal seam I-a is developed in the central, north, north–east, north–west and west parts of the field. The seam thickness varies from 0.10 to 6.00 m (average 2.11 m). The coal seam I occurs in the central, north, north–east and north–west parts of the field, and it is stratified across the entire area. The thickness of coal seam I varies from 1.40 to 47.50 m (average 28.30 m). Coal seam I splits into two coal layers with thickness from bottom to top of 0.20–12.70 m (average 5.74 m) and 5.65–20.90 m (average 15.70 m), respectively. The interbedded waste sediments between the second and first coal layers comprise sand, carbonaceous-, sandy- and marly-clays, and silt. The thickness of this package varies from 1.72 to 24.50 m (average 8.95 m).

The youngest Upper Pontian sediments, overlying coal seam I, include sand, clayey sand and clays with thin layers of carbonaceous clays, coal and limestone. The thickness of this package varies from 0.80 m to 76.50 m (average 26.92 m).

Quaternary series of Pleistocene age is made of gravel and sand, occasionally with clay and loess. The thickness of the Quaternary sediments varies from 16.70 to 42.40 m (average 22.59 m).

ORGANIC AND OTHER GEOCHEMICAL PARAMETERS

TABLE S-I. Values of group organic geochemical parameters

Borehole	Coal seam	Sample	c_{Ash}[a] %, db[b]	C_{org}[c] %, db	S %, db	N %, db	C/N[d]	Q_g[e] MJ kg^{-1}, db	Q_d[f] MJ kg^{-1}, db	Bitumen, ppm, db	c_{Asp}[g] %	$c_{Sat\ HC}$[h] %	$c_{Arom\ HC}$[i] %	c_{NSO}[j] %
A-339	I	1	9.7	55.3	1.5	0.8	80.6	21.5	21.1	29228	53.2	5.2	4.9	36.7
	I	2	12.1	53.2	1.0	0.7	88.7	20.2	19.3	32872	49.1	5.9	4.8	40.3
	I	3	18.3	50.9	1.0	0.6	99.0	18.4	17.6	27302	43.4	5.7	5.6	45.2
	I	4	25.5	44.1	1.4	0.8	64.3	17.1	16.4	34673	40.4	6.0	6.5	47.1
	I	5	28.1	47.3	1.3	0.6	92.0	14.6	14.0	24641	42.8	6.0	5.3	45.9
	II	6	36.2	40.0	1.0	0.7	66.7	13.2	12.6	31312	47.0	5.6	5.4	42.0
A2I-414	I	7	11.2	55.2	1.3	0.9	71.6	21.0	20.1	31034	52.8	5.3	4.3	37.6
	I	8	34.8	44.1	1.2	0.7	73.5	14.2	13.5	27608	48.3	4.7	5.0	42.0
	I	9	16.8	51.0	1.3	0.7	85.0	19.1	18.4	34698	42.6	5.6	5.8	46.0
	I	10	43.5	36.0	0.7	0.6	70.0	9.9	9.4	15662	50.3	4.7	3.8	41.2
	I	11	46.7	29.9	0.8	0.5	69.8	10.0	9.5	20828	47.1	5.4	5.0	42.5
	I	12	31.5	44.3	1.3	0.7	73.8	13.4	12.7	33387	46.2	5.0	5.4	43.3
	II	13	26.8	45.2	1.7	0.6	87.9	15.2	14.4	21443	42.1	5.4	6.2	46.3
A1J-369	I	14	11.3	54.5	0.9	0.9	70.6	25.3	24.5	23841	41.9	5.4	6.6	46.1
	I	15	47.4	30.0	0.6	0.3	116.7	11.6	11.4	29638	47.9	5.4	4.3	42.4
	I	16	15.2	51.5	2.2	0.6	100.1	23.1	22.3	36409	49.3	4.7	4.3	41.8
	I	17	11.1	53.8	1.0	0.8	78.5	22.9	22.1	27510	52.4	3.4	3.7	40.5
	I	18	41.8	40.5	1.0	0.6	78.8	15.1	14.6	19315	52.5	4.0	3.9	39.7
	I	19	30.8	43.5	0.9	0.6	84.6	16.9	16.4	24335	48.5	4.4	4.7	42.4
	II	20	45.7	29.7	1.0	0.5	69.3	9.0	8.5	16870	40.1	6.6	6.3	47.0
	II	21	45.3	33.4	1.4	0.6	64.9	10.2	9.7	12754	43.4	5.3	5.0	46.3
Drmno field[2]	II, III	Range	8.7–47.0	30.7–58.1	0.6–3.4	N.D.[k]	N.D.	N.D.	N.D.	6642–79400	41.4–70.9	2.2–13.2	2.2–5.5	13.7–50.3
"A" field[4]	I, II	Range	12.6–82.6	8.9–60.9	0.2–1.7	0.3–1.2	55.2–97.1	N.D.	N.D.	3326–28145	N.D.	1.2–5.2	2.0–2.8	N.D.

(Table S-I footnote) [a]c_{Ash} – ash content; [b]db – dry basis; [c]C_{org} – organic carbon content; [d]C/N – carbon to nitrogen ratio is given as the molar ratio; [e]Q_g – gross calorific value; [f]Q_d – net calorific value; [g]c_{Asp} – asphaltene content; [h]$c_{Sat\ HC}$ – content of saturated hydrocarbons; [i]$c_{Arom\ HC}$ – content of aromatic hydrocarbons; [j]c_{NSO} – content of NSO fraction (polar fraction, which contains nitrogen-, sulphur- and oxygen--containing compounds); [k]N.D. – not determined

TABLE S-II. Results of the Rock Eval pyrolysis

Bore-hole	Coal seam	Sam-ple	*TOC*[a] %	S_1[b] mg HC (g sample)$^{-1}$	S_2[d] mg HC (g sample)$^{-1}$	S_3[e] mg CO_2 (g sample)$^{-1}$	T_{max}[f] °C	*PI*[g]	S_2/S_3	*HI*[h] mg HC (g TOC)$^{-1}$	*OI*[i] mg CO_2 (g TOC)$^{-1}$
A-339	I	1	51.06	4.66	86.89	32.44	349	0.05	2.68	170	64
	I	2	49.51	5.62	93.86	28.79	348	0.06	3.26	190	58
	I	3	43.81	4.86	85.93	27.89	349	0.05	3.08	196	64
	I	4	39.94	4.11	79.57	31.53	350	0.05	2.52	162	64
	I	5	37.42	4.41	67.59	26.21	366	0.06	2.58	169	66
	II	6	33.41	4.65	68.22	23.19	352	0.06	2.94	182	62
A2I-414	I	7	49.15	5.21	83.17	31.72	347	0.06	2.62	169	65
	I	8	35.85	3.59	70.33	21.89	347	0.05	3.21	196	61
	I	9	46.54	6.60	91.97	27.15	347	0.07	3.39	198	58
	I	10	26.55	1.07	43.20	19.86	350	0.02	2.18	163	75
	I	11	26.72	1.88	44.12	17.15	347	0.04	2.57	165	64
	I	12	36.83	4.91	72.59	23.26	371	0.06	3.12	197	63
	II	13	38.11	3.46	76.33	22.89	346	0.04	3.33	200	60
A1J-369	I	14	52.31	5.27	90.73	33.02	346	0.05	2.75	173	63
	I	15	24.12	1.61	44.77	15.05	346	0.03	2.97	186	62
	I	16	47.48	6.66	89.16	27.45	346	0.07	3.25	188	58
	I	17	50.66	4.27	84.75	30.94	346	0.05	2.74	167	61
	I	18	32.61	2.34	53.24	21.17	349	0.04	2.51	163	65
	I	19	37.85	3.23	70.21	22.72	349	0.04	3.09	185	60
	II	20	25.35	1.10	44.69	13.96	354	0.02	3.20	176	55
	II	21	26.93	1.20	42.37	20.34	387	0.03	2.08	157	76

[a]*TOC* – total organic carbon obtained from Rock–Eval pyrolysis; [b]S_1 – free hydrocarbons; [c]HC – hydrocarbons; [d]S_2 – pyrolysate hydrocarbons; [e]S_3 – amount of CO_2 generated from oxygenated functional groups; [f]T_{max} – temperature corresponding to the S_2 peak maximum; [g]*PI* – production Index = $S_1/(S_1+S_2)$; [h]*HI* – hydrogen index = (S_2×100/*TOC*); [i]*OI* – oxygen index = (S_3×100/*TOC*); note: Rock–Eval pyrolysis was not performed on samples from the Drmno and "A" fields; therefore, data could not be compared

TABLE S-III. Values of parameters calculated from distributions and abundances of *n*-alkanes and isoprenoids

Borehole	Coal seam	Sample	*n*-Al-kane C range	*n*-Alkane maximum	$CPI_{16\text{-}34}$[a]	$CPI_{16\text{-}20}$[b]	*OEP* 1[c]	*OEP* 2[d]	Pristane/ phytane
A-339	I	1	16–35	*n*-C_{29}	4.30	1.09	1.24	3.34	0.75
	I	2	16–35	*n*-C_{29}	5.12	0.98	1.74	3.65	0.95
	I	3	15–35	*n*-C_{29}	4.37	1.33	1.68	3.20	1.14
	I	4	15–35	*n*-C_{29}	6.14	2.11	2.53	4.08	1.42
	I	5	15–35	*n*-C_{29}	4.31	1.71	2.17	3.19	1.50
	II	6	15–35	*n*-C_{29}	4.95	1.60	2.33	3.75	1.27

TABLE S-III. Continued

Borehole	Coal seam	Sample	*n*-Alkane C range	*n*-Alkane maximum	$CPI_{16\text{-}34}$[a]	$CPI_{16\text{-}20}$[b]	*OEP* 1[c]	*OEP* 2[d]	Pristane/ phytane
A2I-414	I	7	16–35	n-C_{29}	3.67	0.91	1.46	2.99	1.07
	I	8	16–35	n-C_{29}	4.90	0.75	2.01	3.64	0.72
	I	9	15–35	n-C_{29}	7.91	2.53	1.80	3.12	1.15
	I	10	16–35	n-C_{29}	4.00	1.41	1.58	2.83	1.09
	I	11	16–35	n-C_{29}	3.35	1.71	1.42	3.42	0.67
	I	12	16–35	n-C_{29}	4.15	2.58	1.94	2.77	1.05
	II	13	15–35	n-C_{29}	3.46	2.14	3.25	3.78	1.65
A1J-369	I	14	15–35	n-C_{29}	4.59	0.41	2.80	3.67	1.13
	I	15	15–35	n-C_{29}	4.07	0.81	1.26	3.13	1.06
	I	16	16–35	n-C_{29}	3.85	0.45	1.66	3.39	1.12
	I	17	15–35	n-C_{29}	3.62	0.59	1.33	3.42	1.05
	I	18	15–35	n-C_{29}	3.80	0.63	1.27	3.35	1.40
	I	19	16–35	n-C_{29}	3.01	1.01	1.65	2.96	0.66
	II	20	15–35	n-C_{29}	3.82	1.56	2.00	3.08	1.07
	II	21	15–35	n-C_{29}	3.78	0.64	1.77	3.19	0.97
Drmno field[2]	II, III	Range	16–33	n-C_{29}	2.87–5.30	0.50–2.34	0.92–5.50	3.24–5.13	0.08–1.26
“A” field[4]	I, II	Range	15–33	n-C_{27} or n-C_{29}	1.23–5.94	0.65–1.61	1.14–1.80	1.68–5.14	0.74–1.16

[a]$CPI_{16\text{-}34}$ – Carbon Preference Index determined for the full distribution of *n*-alkanes C_{16}–C_{34} (mass chromatogram *m/z* 71), $CPI_{16\text{-}34}$ = 1/2 [Σodd(n-C_{17} – n-C_{33})/Σeven(n-C_{16} – n-C_{32}) + Σodd(n-C_{17} – n-C_{33})/Σeven(n-C_{18} – n-C_{34})]; [b]$CPI_{16\text{-}20}$ – Carbon Preference Index determined for the distribution of *n*-alkanes C_{16}–C_{20} (mass chromatogram *m/z* 71), $CPI_{16\text{-}20}$ = 1/2 [Σodd(n-C_{17} – n-C_{19})/Σeven(n-C_{16} – n-C_{18}) + Σodd(n-C_{17} – n-C_{19})/Σeven(n-C_{18} – n-C_{20})]; [c]*OEP* 1 = 1/4 [(n-C_{21} + 6 n-C_{23} + n-C_{25})/(n-C_{22} + n-C_{24})], *OEP* – odd–even predominance; [d]*OEP* 2 = 1/4 [(n-C_{25} + 6 n-C_{27} + n-C_{29})/(n-C_{26} + n-C_{28})]

TABLE S-IV. Values of parameters calculated from the distributions and abundances of diterpenoids and non-hopanoid triterpenoids

Borehole	Coal seam	Sample	Bicyclic diterpe-noids[a] %	Tricyclic diterpe-noids[b] %	Tetracyc-lic diter-penoids[c] %	Tricyclic diterpenoids/ tetracyclic diterpenoids	Pimarane/ 16α(*H*)-phyllo-cladane	ΣDiterpenoids/(ΣDi-terpe-noids + ΣTriter-penoids)[d]
A-339	I	1	0.07	36.01	63.93	0.56	0.52	0.9983
	I	2	0.04	36.05	63.90	0.56	0.48	0.9990
	I	3	0.39	33.44	66.17	0.51	0.47	0.9958
	I	4	0.29	8.20	91.51	0.09	0.07	0.9765
	I	5	0.47	24.38	75.16	0.32	0.27	0.9879
	II	6	0.90	27.47	71.64	0.38	0.32	0.9746
A2I-414	I	7	0.07	42.74	57.19	0.75	0.65	0.9975
	I	8	0.10	46.94	52.96	0.89	0.84	0.9899
	I	9	0.05	30.50	69.45	0.44	0.25	0.9896
	I	10	0.19	31.58	68.23	0.46	0.44	0.9936
	I	11	0.03	46.87	53.10	0.88	0.89	0.9945

TABLE S-IV. Continued

Borehole	Coal seam	Sample	Bicyclic diterpe-noids[a] %	Tricyclic diterpe-noids[b] %	Tetracyc-lic diter-penoids[c] %	Tricyclic diterpenoids/ tetracyclic diterpenoids	Pimarane/ 16α(*H*)- -phyllo-cladane	ΣDiterpen oids/(ΣDi-terpe-noids + ΣTriter-penoids)[d]
A2I-414	I	12	0.13	5.61	94.27	0.06	0.05	0.9915
	II	13	0.25	35.31	64.44	0.55	0.51	0.9933
A1J-369	I	14	0.29	44.75	54.96	0.81	0.79	0.9975
	I	15	0.05	42.25	57.69	0.73	0.69	0.9980
	I	16	0.04	48.90	51.06	0.96	0.90	0.9996
	I	17	0.09	31.66	68.25	0.46	0.43	0.9958
	I	18	0.15	52.92	46.94	1.13	1.11	0.9972
	I	19	0.20	48.28	51.52	0.94	0.93	0.9938
	II	20	0.58	25.89	73.54	0.35	0.31	0.9923
	II	21	0.47	36.09	63.44	0.57	0.41	0.9331
Drmno field[2]	II, III	Range	N.D.[e]	4.39–75.19	24.81–25.60	0.05–3.03	0.03–3.22	0.8096–1.0000
"A" field[4]	I, II	Range	N.D.	12.97–57.37	42.63–87.03	0.15–1.35	0.06–0.69	0.9441–1.0000

[a]Bicyclic diterpenoids = (α-labdane + β-labdane)×100 / ΣDiterpenoids, ΣDiterpenoids = α-labdane + β-labdane + isopimaradienes + norisopimarane + pimaradiene + atisene + norpimarane + beyerane + isophyllocladene + isopimarane + fichtelite + pimarane + 16β(*H*)-phyllocladane + 16α(*H*)-phyllocladane + 16α(*H*)-kaurane, calculated from the *TIC* of the saturated fraction; [b]tricyclic diterpenoids = (isopimaradienes + norisopimarane + pimaradiene + norpimarane + isopimarane + fichtelite + pimarane)×100 / ΣDiterpenoids, calculated from the *TIC* of the saturated fraction; [c]tetracyclic diterpenoids = (atisene + beyerane + isophyllocladene + 16β(*H*)-phyllocladane + 16α(*H*)-phyllocladane + 16α(*H*)-kaurane)×100 / ΣDiterpenoids, calculated from the *TIC* of the saturated fraction; [d]ΣDiterpenoids = α-labdane + β-labdane + isopimaradienes + norisopimarane + pimaradiene + atisene + norpimarane + beyerane + isophyllocladene + isopimarane + fichtelite + pimarane + 16β(*H*)-phyllocladane + 16α(*H*)-phyllocladane + 16α(*H*)-kaurane, ΣTriterpenoids = (des-A-olean-13(18)-ene + des-A-olean-12-ene + des-A-olean-18-ene + des-A-urs-13(18)-ene + des-A-oleanadiene + des-A-urs-12-ene + des-A-lupane + des-A-triterpene + des-A-oleanane), calculated from the *TIC* of the saturated fraction; [e]N.D. – not determined

TABLE S-V. Values of parameters calculated from the distributions and abundances of steroids and hopanoids

Bore-hole	Coal seam	Sample	C_{27} Stere-nes[a] %	C_{28} Stere-nes[b] %	C_{29} Sterenes[c] %	ΣSte-roids/ ΣHop-ano-ids[d]	Hopane maximum[e]	$C_{27}β$-Hop-ane[f] %	$C_{29}ββ$-Hop-ane[f] %	$C_{30}ββ$-Hop-ane[f] %	$C_{31}ββ$-Hop-ane[f] %	$C_{30}ββ$-Hopane to C_{30} (ββ+αβ) -Hop-anes
A-339	I	1	2.02	8.74	89.24	0.15	$C_{27}β$	39.81	27.91	20.52	11.76	0.80
	I	2	1.82	6.18	92.01	0.18	$C_{27}β$	38.79	28.43	20.28	12.50	0.80
	I	3	1.35	7.47	91.17	0.09	$C_{31}αβ(R)$	36.15	25.41	20.46	17.98	0.78
	I	4	1.73	6.41	91.86	0.08	$C_{27}β$	40.55	26.25	20.83	12.37	0.78
	I	5	1.79	4.89	93.31	0.09	$C_{27}β$	44.06	28.39	17.73	9.82	0.77
	II	6	3.54	7.96	88.50	0.06	$C_{27}β$	42.87	25.73	20.19	11.21	0.78

TABLE S-V. Continued

Bore-hole	Coal seam	Sample	C_{27} Sterenes[a] %	C_{28} Sterenes[b] %	C_{29} Sterenes[c] %	ΣSteroids/ ΣHopanoids[d]	Hopane maximum[e]	$C_{27}\beta$-Hopane[f] %	$C_{29}\beta\beta$-Hopane[f] %	$C_{30}\beta\beta$-Hopane[f] %	$C_{31}\beta\beta$-Hopane[f] %	$C_{30}\beta\beta$-Hopane to C_{30} ($\beta\beta$+$\alpha\beta$)-Hopanes
A2I-414	I	7	2.26	8.49	89.24	0.02	$C_{31}\alpha\beta(R)$	43.20	31.79	9.30	15.71	0.62
	I	8	4.22	10.91	84.86	0.03	$C_{31}\alpha\beta(R)$	48.43	23.34	15.59	12.65	0.57
	I	9	2.17	9.82	88.01	0.04	$C_{31}\alpha\beta(R)$	41.25	27.69	17.15	13.91	0.71
	I	10	3.46	6.57	89.97	0.11	$C_{27}\beta$	43.35	27.12	19.35	10.18	0.74
	I	11	4.02	4.49	91.50	0.24	$C_{31}\alpha\beta(R)$	56.97	24.18	11.64	7.21	0.52
	I	12	3.06	7.11	89.83	0.08	$C_{27}\beta$	51.36	25.33	14.49	8.81	0.65
	II	13	1.11	5.75	93.14	0.26	$C_{27}\beta$	43.85	25.36	19.69	11.10	0.63
A1J-369	I	14	2.53	8.65	88.82	0.12	$C_{27}\beta$	45.47	25.46	18.15	10.93	0.64
	I	15	3.96	10.85	85.20	0.09	$C_{27}\beta$	53.88	24.25	13.99	7.88	0.57
	I	16	1.02	7.25	91.73	0.02	$C_{31}\alpha\beta(R)$	45.54	23.59	18.21	12.67	0.59
	I	17	1.62	9.07	89.31	0.06	$C_{31}\alpha\beta(R)$	45.12	26.19	18.06	10.64	0.67
	I	18	2.13	10.04	87.83	0.03	$C_{27}\beta$	43.59	26.20	18.47	11.74	0.59
	I	19	3.10	7.46	89.43	0.17	$C_{27}\beta$	58.56	25.91	10.44	5.10	0.61
	II	20	3.07	6.14	90.78	0.02	$C_{27}\beta$	51.90	24.04	15.57	8.48	0.58
	II	21	4.45	7.88	87.67	0.04	$C_{27}\beta$	43.57	25.31	19.68	11.44	0.68
Drmno field[4]	II, III	Range	0.00–4.55	0.00–15.94	84.06–100.00	0.07–0.25	$C_{27}\beta$ or $C_{31}\alpha\beta(R)$	26.93–50.24	23.98–36.78	11.52–31.17	8.38–13.93	0.53–0.90
"A" field[5]	I, II	Range	1.20–4.16	2.88–10.64	86.95–95.40	0.04–0.20	$C_{27}\beta$ or $C_{31}\alpha\beta(R)$	24.93–46.13	23.38–39.11	15.16–23.93	8.91–25.35	0.52–0.82

[a]C_{27}-Sterenes = 100 × $C_{27}(\Delta^2 + \Delta^4 + \Delta^5)$-sterenes / [$\Sigma(C_{27}–C_{29})(\Delta^2 + \Delta^4 + \Delta^5)$-sterenes + $C_{29}\Delta^{22}$-sterene + C_{29}-sterene]; [b]C_{28}-Sterenes = 100 × $C_{28}(\Delta^2 + \Delta^4 + \Delta^5)$-sterenes / [$\Sigma(C_{27}–C_{29})(\Delta^2 + \Delta^4 + \Delta^5)$-sterenes + $C_{29}\Delta^{22}$-Sterene + C_{29}-sterene]; [c]C_{29}-Sterenes = 100 × [$C_{29}(\Delta^2 + \Delta^4 + \Delta^5 + \Delta^{22})$-sterenes + C_{29}-sterene] / [$\Sigma(C_{27}–C_{29})(\Delta^2 + \Delta^4 + \Delta^5)$-sterenes + $C_{29}\Delta^{22}$-sterene + C_{29}-sterene]; [d]ΣSteroids / ΣHopanoids = [$\Sigma(C_{27}–C_{29})(\Delta^2 + \Delta^4 + \Delta^5)$-sterenes + $C_{29}\Delta^{22}$-sterene + C_{29}-sterene] / [$\Sigma(C_{29}–C_{32})17\alpha(H)21\beta(H)$-hopanes + $\Sigma(C_{29}–C_{32})17\beta(H)21\alpha(H)$-hopanes + $\Sigma(C_{29}–C_{32})17\beta(H)21\beta(H)$-hopanes + $C_{27}17\alpha$(H)-Hopane + $C_{27}17\beta$(H)-Hopane + C_{30}-Hop-17(21)-ene + C_{27}-Hop-17(21)-ene +C_{27}-Hop-13(18)-ene]; [e]Hopane maximum – The most abundant hopanoid in the *m*/*z* 191 mass chromatogram, $\beta\beta$ and $\alpha\beta$ designate the configurations at C_{17} and C_{21} in hopanes, (*R*) designates the configuration at C_{22} in the hopanes; Sterenes were quantified from the *m*/*z* 215 mass chromatogram, hopenes and hopanes were quantified from the *m*/*z* 191 mass chromatogram; [f]against (C_{27}+ΣC_{29}–C_{31})-$\beta\beta$-hopanes

CHROMATOGRAPHIC AND SPECTROMETRY DATA

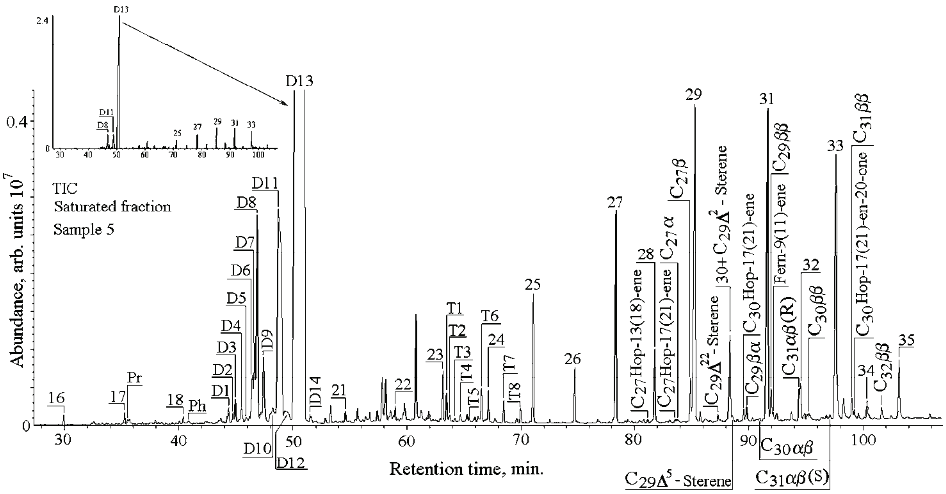
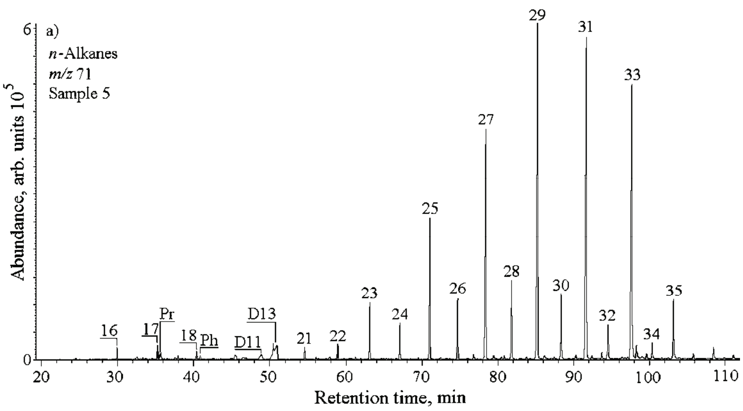
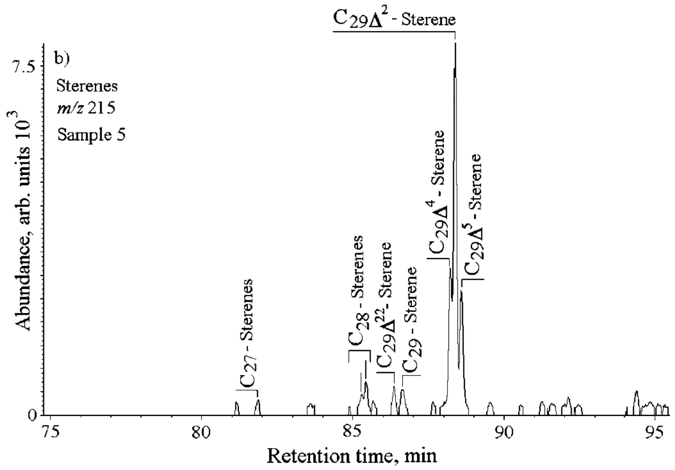


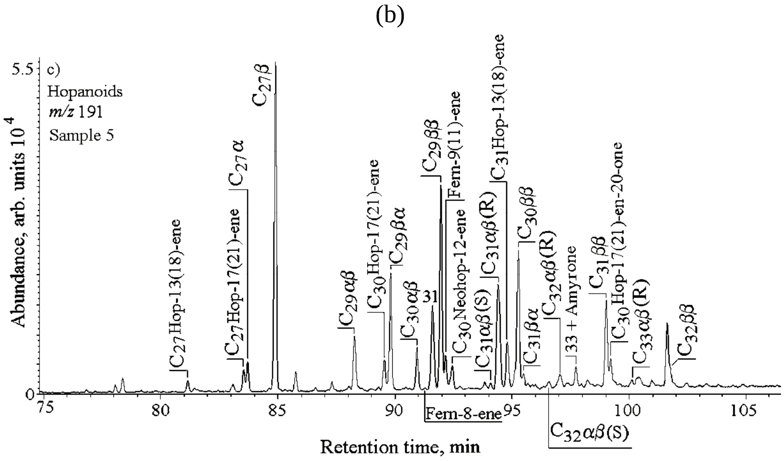
Fig. S-2. Total ion current (*TIC*) of the saturated fraction typical for the investigated samples. Peak assignments: *n*-alkanes are labelled according to their carbon number; Pr – pristane; Ph – phytane; D1 – isopimaradiene; D2 – 8*β*(*H*)-Labdane; D3 – isopimaradiene; D4 – norisopimarane; D5 – 8*α*(*H*) – labdane; D6 – atisene; D7 – norpimarane; D8 – beyerane; D9 – isophyllocladene; D10 – fichtelite; D11 – pimarane; D12 – 16*β*(*H*)-phyllocladane; D13 –16*α*(*H*)-phyllocladane; D14 – 16*α*(*H*)-kaurane; T1 – des-A-olean-13(18)-ene; T2 – des-A-olean-12-ene; T3 – des-A-olean-18-ene + Des-A-urs-13(18)-ene; T4 – des-A-oleanadiene; T5 – des-A-urs-12-ene; T6 – des-A-lupane; T7 – des-A-triterpene;[5] T8 – des-A-oleanane;[6] *ββ*, *βα* and *αβ* designate configurations at C_{17} and C_{21} in hopanes; (*S*) and (*R*) designate configuration at C_{22} in hopanes.



(a)



(b)



(c)

Fig. S-3. GC–MS mass chromatograms of: a) *n*-alkanes, *m/z* 71, b) sterenes, *m/z* 215 and c) hopanoids, *m/z* 191, typical for the investigated samples. For peak assignments, see the legend to Fig. S-2.

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