Table S-I. The maceral composition based on mineral matter-free, vol. %

Lithotype	Sample ID	*T*[a]	*U*[b]	*A*[c]	*D*[d]	*G*[e]	*Ch*[f]	*HUM*[g]	*Sp*[h]	*Cu*[i]	*R*[j]	*Su*[k]
MC	2/79	23.0	14.2	4.0	40.2	5.4	2.0	88.8	1.8	0.2	0.2	0.2
MXC	3/79	24.0	6.6	16.6	31.4	2.8	2.2	83.6	1.8	0.3	0.0	0.3
XC	4/79	52.7	17.2	4.2	10.2	3.4	2.3	90.0	1.5	0.0	0.2	0.0
MXC	5/79	17.4	12.9	15.8	33.6	3.2	5.3	88.2	2.2	0.4	0.4	1.0
MMiC	6/79	19.1	17.2	8.9	34.8	3.6	6.0	89.6	1.6	0.2	0.2	0.2
MXC	8/79	15.2	28.4	7.0	34.4	3.2	6.8	95.0	0.6	0.0	0.4	0.2
MMiC	11/79	9.5	9.0	12.5	53.5	3.3	2.8	90.6	0.9	0.0	0.3	0.0
XC	14/79	18.0	37.2	2.6	22.4	4.6	7.2	92.0	0.7	0.0	0.5	0.4
XC	16/79	12.0	40.9	0.6	18.0	7.7	5.0	84.2	1.1	0.0	0.2	1.0
MMiC	17/79	2.6	17.2	8.4	40.6	4.2	1.6	74.6	0.6	0.0	0.0	0.0
MXC	18/79	11.2	25.8	6.8	30.6	5.4	1.4	81.2	1.8	0.4	0.2	0.2
MMiC	19/79	5.8	23.8	4.2	35.0	8.6	1.6	79.0	1.2	0.6	0.6	0.0
MMiC	20/79	4.0	16.8	5.2	50.8	4.4	2.3	83.5	1.0	0.0	0.8	0.3
MC	26/91	16.6	19.8	3.0	40.0	6.0	6.9	92.3	0.7	0.2	0.4	0.4
XC	27/91	18.4	38.0	2.2	24.9	6.2	2.0	91.7	0.8	1.0	0.4	0.4
MC	28/91	8.8	25.4	3.6	41.4	2.4	2.6	84.2	1.8	0.4	1.2	0.0
XC	29/91	23.8	36.1	3.9	18.2	2.9	4.6	89.5	1.2	0.2	0.8	0.8
MC	30/91	4.0	25.1	2.4	39.8	7.2	3.1	81.6	1.1	0.8	0.2	0.6
MMiC	31/91	3.0	17.3	7.7	58.4	3.4	2.3	92.1	1.0	0.6	0.8	0.0
MXC	33/91	6.3	29.1	2.2	39.6	4.0	5.9	87.1	0.5	0.2	1.3	0.2
XC	34/91	14.6	47.4	1.6	23.6	2.2	4.4	93.8	0.7	0.2	0.2	0.4
MMiC	36/91	8.0	29.4	3.6	32.6	8.4	4.2	86.2	1.0	0.2	0.3	0.0
XC	38/91	24.2	47.8	1.7	14.1	3.0	2.8	93.6	0.7	0.2	1.2	0.5
MMiC	39/91	7.2	22.9	1.3	41.9	6.1	2.3	81.7	1.3	0.5	0.7	0.0
MC	40/91	8.2	28.8	3.0	46.0	4.6	3.0	93.6	0.6	0.4	0.2	0.4
XC	42/601	22.0	39.1	3.2	23.7	5.6	1.4	95.0	1.0	0.6	0.5	0.2
MC	43/601	8.4	25.1	2.2	52.1	4.0	2.6	94.4	1.6	0.0	0.2	0.2
MXC	45/601	7.9	27.3	2.2	47.5	4.6	2.5	92.0	0.7	0.2	0.7	0.2
MC	46/601	5.4	27.5	0.8	47.6	1.9	1.6	84.8	1.8	0.8	0.2	0.2
MMiC	48/601	10.4	26.8	4.7	42.8	4.9	3.9	93.5	0.8	0.2	1.1	0.2
MC	49/601	9.8	28.2	3.7	39.5	4.1	5.6	90.9	0.2	0.2	0.4	1.0
XC	50/603	13.2	44.7	0.4	16.8	7.4	4.3	86.8	1.2	0.2	0.4	0.4
MC	51/603	20.0	45.6	0.2	17.8	2.6	3.4	89.6	1.4	0.4	0.6	0.2
XC	52/603	13.0	47.4	0.2	22.6	7.5	1.9	92.6	1.9	0.2	0.2	0.2
MXC	53/603	5.3	37.2	2.1	34.5	3.8	3.5	86.4	1.7	0.2	0.2	0.7
XC	54/603	22.7	44.3	0.2	20.2	1.5	3.0	91.9	1.2	0.2	2.0	0.2
MXC	55/603	15.8	32.0	1.3	37.6	1.3	1.4	89.4	1.7	0.2	1.6	0.2
MMiC	56/603	5.8	32.2	3.3	36.1	3.8	4.2	85.4	1.7	1.0	1.0	0.7

Lithotype	Sample ID	*Al*[l]	*Ld*[m]	*LIP*[n]	*F*[o]	*Sf*[p]	*Ma*[q]	*Fg*[r]	*Id*[s]	*IN*[t]	*MM*[u]
MC	2/79	0.7	2.7	5.8	2.0	0.4	0.0	1.6	1.4	5.4	8.0
MXC	3/79	0.7	3.9	7.0	2.8	1.2	0.3	0.4	4.7	9.4	23.9
XC	4/79	0.0	1.9	3.6	3.0	0.4	0.2	0.2	2.6	6.4	9.9
MXC	5/79	0.0	3.4	7.4	0.5	0.4	0.0	1.8	1.7	4.4	8.6
MMiC	6/79	0.2	2.4	4.8	0.6	0.3	0.2	1.0	3.5	5.6	13.0
MXC	8/79	0.0	1.8	3.0	0.4	0.0	0.0	0.8	0.8	2.0	9.4
MMiC	11/79	0.3	1.4	2.9	1.3	0.7	0.4	0.9	3.2	6.5	29.7
XC	14/79	0.0	1.8	3.4	1.2	0.4	0.5	0.8	1.7	4.6	8.8
XC	16/79	0.0	0.3	2.6	4.2	3.9	0.2	0.4	4.5	13.2	3.3
MMiC	17/79	0.0	0.6	1.2	9.4	1.2	0.2	0.2	13.2	24.2	11.4
MXC	18/79	0.0	1.6	4.2	2.8	0.8	1.6	0.6	8.8	14.6	14.4
MMiC	19/79	0.3	2.2	4.9	2.8	1.8	1.2	0.8	9.5	16.1	13.5

Table S-I continued

Lithotype	Sample ID	*Al*[l]	*Ld*[m]	*LIP*[n]	*F*[o]	*Sf*[p]	*Ma*[q]	*Fg*[r]	*Id*[s]	*IN*[t]	*MM*[u]
MMiC	20/79	0.0	0.7	2.8	2.0	3.0	0.4	0.3	8.0	13.7	20.4
MC	26/91	0.0	0.4	2.1	1.0	0.4	0.4	1.2	2.6	5.6	16.8
XC	27/91	0.0	1.4	4.0	0.8	0.2	0.2	0.2	2.9	4.3	4.2
MC	28/91	0.2	3.2	6.8	2.2	0.2	0.2	1.0	5.4	9.0	5.5
XC	29/91	0.0	2.0	5.0	1.0	0.4	0.4	0.5	3.2	5.5	8.8
MC	30/91	0.0	1.0	3.7	2.4	0.5	1.2	0.2	10.4	14.7	15.0
MMiC	31/91	0.0	1.6	4.0	1.4	0.0	0.3	0.6	1.6	3.9	22.9
MXC	33/91	0.2	2.5	4.9	1.8	0.2	0.2	0.8	5.0	8.0	14.8
XC	34/91	0.0	1.7	3.2	0.2	0.4	0.0	1.7	0.7	3.0	8.1
MMiC	36/91	0.0	1.7	3.2	2.6	0.8	0.2	0.6	6.4	10.6	13.9
XC	38/91	0.0	1.4	4.0	0.7	0.3	0.0	0.7	0.7	2.4	11.4
MMiC	39/91	0.0	1.8	4.3	1.0	1.5	0.0	1.4	10.1	14.0	15.9
MC	40/91	0.0	2.4	4.0	0.2	0.2	0.2	1.2	0.6	2.4	9.3
XC	42/601	0.0	0.7	3.0	0.5	0.2	0.0	0.2	1.1	2.0	11.2
MC	43/601	0.0	1.5	3.5	0.2	0.4	0.0	0.2	1.3	2.1	7.4
MXC	45/601	0.5	1.7	4.0	0.2	0.7	0.2	0.9	2.0	4.0	12.4
MC	46/601	0.6	1.0	4.6	2.7	2.5	0.6	0.6	4.2	10.6	11.5
MMiC	48/601	0.2	1.4	3.9	0.2	0.5	0.2	0.2	1.5	2.6	15.0
MC	49/601	0.4	2.1	4.3	1.0	0.4	0.4	0.8	2.2	4.8	9.9
XC	50/603	0.0	1.4	3.6	3.2	1.0	0.4	0.6	4.4	9.6	4.6
MC	51/603	0.0	2.2	4.8	2.0	0.4	0.2	0.4	2.6	5.6	4.3
XC	52/603	0.0	0.9	3.4	0.2	0.8	0.4	0.8	1.8	4.0	5.5
MXC	53/603	0.2	3.9	6.9	0.9	0.2	0.9	1.2	3.5	6.7	19.3
XC	54/603	0.0	2.2	5.8	0.2	0.2	0.0	0.9	1.0	2.3	7.8
MXC	55/603	0.0	2.3	6.0	0.5	1.1	0.5	0.2	2.3	4.6	17.8
MMiC	56/603	0.0	2.9	7.3	1.7	0.7	0.4	0.4	4.1	7.3	19.2

[a]*T* – Textinite; [b]*U* – Ulminite; [c]*A* – Attrinite; [d]*D* – Densinite; [e]*G* – Gelinite; [f]*Ch* – Corpohuminite; [g]*HUM* – Total huminite; [h]*Sp* – Sporinite; [i]*Cu* – Cutinite; [j]*R* – Resinite; [k]*Su* – Suberinite; [l]*Al* – Alginite; [m]*Ld* – Liptodetrinite; [n]*LIP* – Total liptinite; [o]*F* – Fusinite; [p]*Sf* – Semifusinite; [q]*Ma* – Macrinite; [r]*Fg* – Funginite; [s]*Id* – Inertodetrinite; [t]*IN* – Total inertinite; [u]*MM* – Total mineral matter.

Table S-II. Petrographic indices and bulk organic geochemical parameters

Lithotype	Sample ID	ΣG[a] /vol. %	GI[b]	TPI[c]	VI[d]	GWI[e]	TOC[f] /%	S[g] /%
MC	2/79	43.85	1.86	0.93	0.86	1.35	56.06	1.88
MXC	3/79	30.44	0.84	0.74	0.65	1.28	24.23	1.67
XC	4/79	24.03	0.48	5.15	3.97	0.35	52.90	2.87
MXC	5/79	39.69	1.46	0.73	0.65	1.10	44.67	0.78
MMiC	6/79	44.43	1.81	0.98	0.79	1.27	20.21	0.51
MXC	8/79	52.12	2.97	1.23	1.03	1.06	45.79	3.34
MMiC	11/79	47.96	2.48	0.34	0.31	2.88	8.31	0.21
XC	14/79	51.73	2.86	2.49	2.05	0.74	51.64	1.53
XC	16/79	52.11	3.01	3.30	2.71	0.64	57.01	1.33
MMiC	17/79	44.47	1.77	0.63	0.49	2.05	27.16	0.82
MXC	18/79	44.58	2.01	1.06	0.90	1.18	43.97	1.45
MMiC	19/79	49.60	2.76	0.84	0.71	1.74	48.90	1.70
MMiC	20/79	51.94	3.66	0.45	0.43	3.00	27.52	2.13
MC	26/91	52.96	2.89	1.02	0.86	1.77	37.36	1.80
XC	27/91	50.31	2.68	2.17	1.91	0.64	50.80	1.98
MC	28/91	49.82	3.48	0.86	0.74	1.37	29.97	1.73
XC	29/91	43.82	1.86	2.91	2.36	0.54	49.29	1.41
MC	30/91	53.67	3.60	0.80	0.65	2.07	29.58	3.33
MMiC	31/91	56.37	5.72	0.36	0.35	3.11	26.10	4.40
MXC	33/91	55.86	4.89	1.03	0.80	1.71	39.65	1.46
XC	34/91	54.14	4.41	2.64	2.32	0.60	48.67	1.65
MMiC	36/91	54.10	3.22	1.21	0.95	1.44	26.22	1.35
XC	38/91	47.38	2.37	4.78	4.22	0.42	51.58	0.80
MMiC	39/91	51.74	3.42	0.77	0.64	2.11	39.27	1.00
MC	40/91	57.69	6.50	0.82	0.75	1.57	33.71	0.92
XC	42/601	49.16	2.40	2.34	2.23	0.65	40.44	2.28
MC	43/601	58.25	6.60	0.67	0.63	1.85	39.93	2.85
MXC	45/601	57.17	6.30	0.76	0.70	1.79	40.72	1.86
MC	46/601	53.77	5.90	0.76	0.76	1.86	41.38	1.69
MMiC	48/601	55.49	4.39	0.87	0.79	1.59	23.70	2.94
MC	49/601	55.02	4.41	1.02	0.86	1.42	41.01	0.97
XC	50/603	52.91	3.12	3.72	2.80	0.57	53.16	1.67
MC	51/603	48.49	2.70	3.90	3.10	0.43	57.97	0.82
XC	52/603	56.28	4.76	2.69	2.51	0.62	56.69	1.68
MXC	53/603	55.17	6.45	1.25	1.05	1.37	27.12	1.63
XC	54/603	47.72	2.80	3.44	3.01	0.48	56.06	1.67
MXC	55/603	49.30	3.59	1.26	1.22	1.18	17.14	1.07
MMiC	56/603	53.73	4.86	1.10	0.97	1.53	8.04	0.22

Lithotype	Sample ID	Q_g[h] / MJ kg^{-1}	Q_d[i] / MJ kg^{-1}	Ash, %	Bitumen, mg (g TOC)$^{-1}$	Saturated hydrocar-bons, %	Aromatic hydrocar-bons, %	Asphaltenes+ NSO[j] compounds, %
MC	2/79	25.9	24.8	19.00	65.99	1.04	3.39	95.56
MXC	3/79	18.9	17.8	59.84	87.97	1.94	2.26	95.81
XC	4/79	26.1	25.1	20.63	59.63	2.11	3.01	94.88
MXC	5/79	24.8	23.7	28.02	62.07	1.25	4.74	94.01
MMiC	6/79	17.9	17.0	63.83	44.25	0.91	2.13	96.96
MXC	8/79	25.1	23.9	25.70	36.78	3.21	2.75	94.04
MMiC	11/79	15.7	14.3	78.20	39.66	2.05	3.22	94.74
XC	14/79	26.3	25.3	12.62	52.62	1.08	2.16	96.76
XC	16/79	25.6	24.6	8.66	22.65	1.45	2.54	96.01
MMiC	17/79	23.5	22.5	56.29	39.40	1.75	0.70	97.54
MXC	18/79	24.2	23.3	27.62	51.75	1.49	1.19	97.32

Table S-II continued

Lithotype	Sample ID	Q_g[h] / MJ kg^{-1}	Q_d[i] / MJ kg^{-1}	Ash, %	Bitumen, mg (g *TOC*)$^{-1}$	Saturated hydrocarbons, %	Aromatic hydrocarbons, %	Asphaltenes+ *NSO*[j] compounds, %
MMiC	19/79	25.8	24.8	25.51	81.28	1.94	3.23	94.84
MMiC	20/79	21.3	20.3	58.27	34.78	2.27	1.70	96.02
MC	26/91	23.3	22.1	42.91	72.18	4.27	3.73	92.00
XC	27/91	25.1	24.1	17.90	48.64	2.50	2.19	95.31
MC	28/91	23.0	21.7	50.85	64.37	1.13	3.38	95.49
XC	29/91	25.3	24.2	20.08	54.20	0.97	2.27	96.75
MC	30/91	22.8	22.1	40.76	38.13	1.24	3.72	95.04
MMiC	31/91	21.0	20.1	52.56	60.52	1.30	3.26	95.44
MXC	33/91	24.3	23.3	35.95	75.09	1.28	1.92	96.81
XC	34/91	25.9	24.8	21.74	54.29	1.57	1.89	96.54
MMiC	36/91	21.2	19.9	56.11	131.69	0.60	1.79	97.62
XC	38/91	25.5	24.4	16.38	46.25	1.09	1.09	97.83
MMiC	39/91	24.4	23.3	37.05	73.43	2.10	3.89	94.01
MC	40/91	23.9	22.6	37.92	58.30	0.65	2.28	97.07
XC	42/601	24.2	23.2	31.36	57.62	10.57	4.38	85.05
MC	43/601	24.3	23.3	34.23	43.43	8.58	4.48	86.94
MXC	45/601	23.8	22.7	35.43	47.30	2.24	3.19	94.57
MC	46/601	23.4	22.5	24.40	55.28	1.75	1.75	96.49
MMiC	48/601	20.2	19.1	57.75	100.17	0.91	1.52	97.56
MC	49/601	24.2	23.1	34.11	105.33	2.93	2.05	95.01
XC	50/603	26.0	24.9	18.69	52.94	1.18	2.35	96.47
MC	51/603	28.3	27.2	16.86	36.89	1.24	2.17	96.59
XC	52/603	26.4	25.5	12.58	28.77	1.42	1.98	96.60
MXC	53/603	22.3	21.1	52.90	75.55	1.75	2.05	96.20
XC	54/603	27.8	26.7	13.85	64.38	1.42	2.49	96.09
MXC	55/603	21.7	20.9	54.98	52.94	2.92	2.50	94.58
MMiC	56/603	16.9	16.3	68.60	41.36	5.24	2.80	91.96

[a]ΣG = Gelinite + Corpohuminite + 0.67 (Ulminite + Densinite), (mineral matter-free basis); [b]*GI* – Gelification Index = (Ulminite + Corpohuminite + Densinite + Macrinite)/(Textinite + Attrinite + Fusinite + Inertodetrinite); [c]*TPI* – Tissue Preservation Index = (Textinite + Ulminite + Corpohuminite + Fusinite)/(Attrinite + Densinite + Macrinite); [d]*VI* – Vegetation Index = (Telohuminite + Fusinite + Semifusinite + Cutinite + Sporinite + Suberinite + Resinite)/(Detrohuminite + Inertodetrinite + Alginite + Liptodetrinite + Other liptinites); [e]*GWI* – Groundwater Index = (Gelohuminite + Densinite + Mineral Matter)/(Telohuminite + Attrinite); [f]*TOC* – Total organic carbon content, dry basis; [g]*S* – Total sulphur content, dry basis; [h]Q_g – Gross calorific value; [i]Q_d – Net calorific value; [j]*NSO* – Polar fraction, which contains nitrogen, sulphur and oxygen compounds.

Table S-III. Contents of biomarkers, μg (g *TOC*)$^{-1}$ and values of biomarker ratios

Lithotype	Sample ID	*Di*[a]	*Tri*[b]	*n*-Alkanes	Hopanoids	Steroids
MC	2/79	1139.31	84.63	590.43	259.21	25.84
MXC	3/79	1108.06	318.22	1483.32	322.86	13.82
XC	4/79	1626.55	131.93	300.02	499.94	18.87
MXC	5/79	2934.05	203.75	275.28	228.14	20.05
MMiC	6/79	613.16	130.70	373.30	176.00	33.36
MXC	8/79	390.34	155.99	598.21	312.20	35.09
MMiC	11/79	741.27	118.40	578.86	128.63	17.27
XC	14/79	981.63	55.91	111.70	243.18	54.84
XC	16/79	321.58	49.55	178.48	111.41	10.54
MMiC	17/79	235.91	40.32	195.62	53.71	3.45
MXC	18/79	667.59	30.43	296.06	162.14	20.43
MMiC	19/79	1030.30	15.60	507.78	263.41	15.13
MMiC	20/79	691.39	111.94	292.94	220.98	27.81
MC	26/91	3463.61	84.66	567.22	417.51	45.51
XC	27/91	1544.68	77.73	179.78	135.10	23.63
MC	30/91	1152.86	206.61	149.17	213.27	25.20
MMiC	36/91	1973.07	187.79	255.32	143.52	15.22
XC	38/91	361.40	92.68	251.35	93.81	14.46
MMiC	39/91	1228.42	277.47	493.94	355.86	28.80
MC	40/91	439.23	196.65	529.10	152.65	27.95
MXC	45/601	1297.23	63.75	248.43	148.95	25.00
MC	46/601	401.86	90.64	639.55	187.27	9.21
MMiC	48/601	1154.87	133.22	104.93	59.10	17.27
MC	49/601	2603.85	59.40	708.22	239.95	22.39
MC	51/603	343.12	64.56	239.35	139.64	10.04
XC	52/603	286.72	65.96	263.16	156.83	33.57
MXC	53/603	1176.59	149.07	458.98	288.81	21.11
XC	54/603	1986.93	52.67	62.40	93.62	12.36
MXC	55/603	1842.38	124.73	388.71	117.31	8.78
MMiC	56/603	1278.70	130.57	1076.70	301.19	8.56

Lithotype	Sample ID	Proportion of *Di*	Diterpenoids/ *n*-Alkanes	*Di/(Di+Tri)*	Aromatic *Di*	Perylene
MC	2/79	0.54	1.93	0.931	215.68	7.36
MXC	3/79	0.34	0.75	0.777	182.78	23.16
XC	4/79	0.63	5.42	0.925	481.57	18.16
MXC	5/79	0.80	10.66	0.935	408.89	21.42
MMiC	6/79	0.46	1.64	0.824	192.67	14.50
MXC	8/79	0.26	0.65	0.714	157.46	3.60
MMiC	11/79	0.47	1.28	0.862	139.40	9.44
XC	14/79	0.68	8.79	0.946	148.89	7.03
XC	16/79	0.48	1.80	0.866	43.90	1.94
MMiC	17/79	0.45	1.21	0.854	97.99	3.65
MXC	18/79	0.57	2.25	0.956	135.81	7.40
MMiC	19/79	0.56	2.03	0.985	117.19	0.57
MMiC	20/79	0.51	2.36	0.861	384.65	19.87
MC	26/91	0.76	6.11	0.976	213.45	2.36
XC	27/91	0.79	8.59	0.952	165.34	4.26
MC	30/91	0.66	7.73	0.848	383.88	15.68
MMiC	36/91	0.77	7.73	0.913	280.98	24.99
XC	38/91	0.44	1.44	0.796	48.69	4.41

Table S-III continued

Lithotype	Sample ID	Proportion of *Di*	Diterpenoids/ *n*-Alkanes	*Di/(Di+Tri)*	Aromatic *Di*	Perylene
MMiC	39/91	0.52	2.49	0.816	122.27	20.92
MC	40/91	0.33	0.83	0.691	97.65	16.64
MXC	45/601	0.73	5.22	0.953	173.16	8.19
MC	46/601	0.30	0.63	0.816	56.51	3.69
MMiC	48/601	0.79	11.01	0.897	366.77	N.D.[c]
MC	49/601	0.72	3.68	0.978	100.47	8.49
MC	51/603	0.43	1.43	0.842	71.38	5.26
XC	52/603	0.36	1.09	0.813	35.67	2.06
MXC	53/603	0.56	2.56	0.888	147.25	15.51
XC	54/603	0.90	31.84	0.974	377.30	7.12
MXC	55/603	0.74	4.74	0.937	139.48	11.63
MMiC	56/603	0.46	1.19	0.907	135.59	20.04

[a]*Di* – Diterpenoids; [b]*Tri* – Non-hopanoid triterpenoids; [c]N.D. – Not determined.
Note: Biomarkers in the samples 28/91, 29/91, 31/91, 33/91, 34/91, 42/601, 43/601 and 50/603 have not been analysed.

Table S-IV. The $\delta^{13}C$ values of individual diterpenoids and non-hopanoid triterpenoids of selected samples

Lithotype	Sample ID	Beyerane	Pimarane	16α(H)-Phyllocladane	Dehydroabietane	Simonellite	Retene	24,25-Dinorlupa-1,3,5(10)-triene	2,2,4a,9-Tetramethyl-1,2,3,4,4a,5,6,14b-octahydropicene
MC	2/79	-25.33	-25.86	-26.95	-25.53	-25.89	-27.62	-28.08	N.D.[a]
MXC	3/79	N.D.	N.D.		-26.40	-26.77	-28.27	-28.92	-30.72
XC	4/79	-25.32	-25.86	-26.31	-26.43	-26.87	N.D.	-29.27	N.D.
MXC	5/79	N.D.	N.D.	N.D.	-26.96	-27.43	N.D.	N.D.	N.D.
MMiC	6/79	N.D.	N.D.	N.D.	-26.77	-26.74	N.D.	N.D.	N.D.
MXC	8/79	-25.99	-25.42	-26.95	N.D.	N.D.	N.D.	N.D.	N.D.
MMiC	11/79	-26.91	-27.43	-27.35	-25.16	-25.17	N.D.	-29.31	-30.48
XC	16/79	-27.27	-27.04	-26.71	-26.59	-27.27	-28.08	-28.23	-30.00
MXC	18/79	N.D.	N.D.	N.D.	-27.05	-27.48	N.D.	-28.90	N.D.
XC	27/91	-25.80	-26.42	-26.43	-27.36	-28.24	N.D.	-30.33	N.D.
MC	30/91	-25.07	-25.85	-25.95	-27.20	-28.13	-29.33	N.D.	-30.33
MXC	33/91	-25.99	-26.06	-26.19	-25.81	-26.20	N.D.	-29.60	N.D.
XC	34/91	-25.83	-26.07	-26.61	-26.79	-26.83	-28.12	-29.17	-29.63
XC	38/91	-26.33	-27.54	-27.75	-26.35	-26.58	-29.64	-28.96	-29.98
MC	40/91	-25.53	-26.22	-26.93	-26.73	-26.90	-27.90	-29.18	-29.80
MXC	45/601	-25.74	-26.50	-26.75	-27.02	-26.46	-28.94	-27.40	-27.81
MC	46/601	-26.11	-25.71	-26.38	-27.14	-27.26	N.D.	-28.61	-29.11
MMiC	48/601	-25.64	-25.60	-27.14	-27.21	-28.39	-28.51	-27.91	-27.94
MC	49/601	-27.04	-27.03	-27.44	-27.06	-27.71	N.D.	-27.60	-28.51
XC	50/603	-26.07	-27.09	-26.25	-27.51	-27.81	N.D.	-28.64	-28.65
MC	51/603	-25.60	-25.95	-26.89	-26.66	-25.93	-28.03	N.D.	-28.47
XC	52/603	N.D.	N.D.	N.D.	-27.15	-26.74	-30.75	-28.64	-29.95
MXC	53/603	N.D.	N.D.	N.D.	-26.21	-26.44	N.D.	-29.74	-29.82
XC	54/603	-26.93	-26.74	-27.34	-27.00	-28.09	-27.45	-28.05	-28.65
MMiC	56/603	-25.76	-26.64	-26.73	-25.47	-25.77	-28.25	N.D.	N.D.

[a]N.D. – Not determined.

Table S-V. Parameters calculated from distributions and abundances of *n*-alkanes and sterenes, and contents of main individual hopanoids, μg (g *TOC*)$^{-1}$

Lithotype	Sample ID	*CPI*[a]	Proportion of C_{15}-C_{20} *n*-alkanes	Proportion of C_{21}-C_{25} *n*-alkanes	Proportion of C_{26}-C_{35} *n*-alkanes	C_{30} Hop-17(21)-ene	C_{27} 17β(H)-Hopane
MC	2/79	5.47	0.08	0.16	0.76	87.09	9.95
MXC	3/79	4.88	0.04	0.35	0.62	102.17	27.56
XC	4/79	1.67	0.03	0.23	0.73	72.31	13.73
MXC	5/79	2.59	0.04	0.16	0.80	57.75	6.36
MMiC	6/79	2.44	0.10	0.20	0.70	68.37	9.81
MXC	8/79	4.05	0.07	0.24	0.69	112.92	21.39
MMiC	11/79	4.38	0.13	0.33	0.54	35.55	10.63
XC	14/79	3.51	0.12	0.23	0.65	66.89	8.43
XC	16/79	1.24	0.06	0.28	0.66	40.77	7.38
MMiC	17/79	2.78	0.20	0.32	0.47	9.01	6.39
MXC	18/79	2.97	0.11	0.25	0.64	48.38	11.50
MMiC	19/79	3.35	0.07	0.35	0.58	81.34	19.30
MMiC	20/79	3.25	0.09	0.32	0.59	22.68	7.06
MC	26/91	N.D.[e]	0.09	0.25	0.66	129.77	45.38
XC	27/91	5.72	0.12	0.18	0.70	21.81	5.00
MC	30/91	1.23	0.14	0.23	0.62	17.20	7.98
MMiC	36/91	2.39	0.13	0.51	0.36	29.33	2.36
XC	38/91	2.86	0.07	0.27	0.66	24.16	4.76
MMiC	39/91	6.89	0.19	0.20	0.61	78.48	107.53
MC	40/91	3.06	0.08	0.18	0.73	70.82	10.01
MXC	45/601	3.26	0.14	0.19	0.66	46.45	10.83
MC	46/601	6.95	0.08	0.26	0.66	66.28	25.61
MMiC	48/601	2.45	0.18	0.28	0.53	16.72	5.49
MC	49/601	5.73	0.20	0.22	0.57	129.99	19.34
MC	51/603	1.26	0.11	0.24	0.65	31.22	9.13
XC	52/603	3.71	0.07	0.35	0.58	33.40	11.80
MXC	53/603	3.37	0.11	0.23	0.66	82.76	18.60
XC	54/603	4.85	0.18	0.26	0.56	15.71	3.96
MXC	55/603	4.67	0.31	0.23	0.46	21.10	9.51
MMiC	56/603	2.87	0.20	0.25	0.54	0.00	43.84

Lithotype	Sample ID	C_{29} 17β(H)21β(H)-Hopane	C_{31} 17α(H)21β(H) 22(R)-Hopane	C_{28} 28.30-Bisnorneohop-13(18)-ene	C_{27} S[b] /%	C_{28} S[c] /%	C_{29} S[d] /%
MC	2/79	8.87	0.00	14.60	1.43	4.03	94.54
MXC	3/79	15.47	8.73	12.04	2.64	2.76	94.6
XC	4/79	8.25	172.00	6.15	5.67	11.20	83.13
MXC	5/79	4.52	10.40	2.84	2.76	12.50	84.74
MMiC	6/79	5.32	21.21	3.90	1.69	6.23	92.08
MXC	8/79	9.41	41.01	19.40	0.69	7.48	91.83
MMiC	11/79	8.18	7.33	11.45	8.24	11.04	80.73
XC	14/79	4.02	41.11	16.67	0.71	6.29	93.00
XC	16/79	3.02	2.85	23.08	0.59	2.08	97.33
MMiC	17/79	0.00	10.22	0.00	1.53	8.34	90.13
MXC	18/79	8.25	4.53	10.45	1.84	9.66	88.5
MMiC	19/79	10.24	22.54	15.31	1.00	7.03	91.98
MMiC	20/79	4.84	6.87	6.78	0.69	9.55	89.76
MC	26/91	27.89	43.79	30.55	N.D.	N.D.	N.D.
XC	27/91	3.47	5.31	7.93	1.33	7.40	91.26

Table S-V continued

Lithotype	Sample ID	C_{29} 17β(H)21β(H)-Hopane	C_{31} 17α(H)21β(H) 22(R)-Hopane	C_{28} 28.30-Bisnorneohop-13(18)-ene	*C_{27} S*[b] /%	*C_{28} S*[c] /%	*C_{29} S*[d] /%
MC	30/91	4.83	4.26	3.48	3.35	10.05	86.60
MMiC	36/91	6.02	3.88	12.94	2.56	8.92	88.52
XC	38/91	4.31	5.41	7.34	1.43	9.99	88.58
MMiC	39/91	16.22	18.66	16.31	0.58	4.01	95.41
MC	40/91	6.57	7.52	24.58	0.85	6.52	92.63
MXC	45/601	6.40	1.47	6.38	1.45	4.85	93.70
MC	46/601	15.85	2.94	9.69	0.95	5.65	93.40
MMiC	48/601	1.96	0.79	0.81	3.39	6.63	89.98
MC	49/601	10.32	5.48	11.28	1.25	6.50	92.25
MC	51/603	4.83	31.38	4.55	1.63	7.91	90.46
XC	52/603	7.05	2.46	27.33	1.72	2.88	95.40
MXC	53/603	11.08	8.88	13.87	1.84	7.41	90.76
XC	54/603	1.97	11.65	1.24	1.61	10.64	87.75
MXC	55/603	5.94	4.49	5.19	2.99	7.57	89.44
MMiC	56/603	24.49	47.94	38.34	2.68	5.52	91.80

[a]*CPI* – Carbon Preference Index determined for distribution of *n*-alkanes C_{23}-C_{33}, $CPI = 1/2\ [\Sigma odd(n\text{-}C_{23} - n\text{-}C_{33})/\Sigma even(n\text{-}C_{22} - n\text{-}C_{32}) + \Sigma odd(n\text{-}C_{23} - n\text{-}C_{33})/\Sigma even(n\text{-}C_{24} - n\text{-}C_{34})]$; [b]$C_{27}\ S = 100xC_{27}(\Delta^2 + \Delta^4 + \Delta^5)$-Sterenes/$\Sigma(C_{27}\text{-}C_{29})(\Delta^2 + \Delta^4 + \Delta^5)$-Sterenes; [c]$C_{28}\ S = 100xC_{28}(\Delta^2 + \Delta^4 + \Delta^5)$-Sterenes/$\Sigma(C_{27}\text{-}C_{29})(\Delta^2 + \Delta^4 + \Delta^5)$-Sterenes; [d]$C_{29}\ S = 100xC_{29}(\Delta^2 + \Delta^4 + \Delta^5)$-Sterenes/$\Sigma(C_{27}\text{-}C_{29})(\Delta^2 + \Delta^4 + \Delta^5)$-Sterenes; [e]N.D. – Not determined.

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132 Table S-VI. The δ^{13}C values of individual *n*-alkanes and hopanoids of selected samples

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Lithotype	Sample ID	*n*-C_{25}	*n*-C_{27}	*n*-C_{29}	*n*-C_{31}	*n*-C_{33}	C_{30} Hop-17(21)-ene
MC	2/79	-30.19	-31.51	-31.67	-31.80	-30.23	-44.86
MXC	3/79	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
XC	4/79	-29.71	-31.36	-31.23	-31.74	-30.51	-39.00
MXC	5/79	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
MMiC	6/79	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
MXC	8/79	-30.22	-30.91	-31.06	-31.52	-31.35	-41.65
MMiC	11/79	-29.66	-30.62	-30.89	-29.24	-31.01	-45.83
XC	16/79	-27.24	-29.08	-28.86	-29.69	-29.04	-39.92
MXC	18/79	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
XC	27/91	-29.09	-30.69	-30.57	-31.44	-30.21	-39.13
MC	30/91	-29.70	-30.72	-30.02	-30.21	-29.36	-41.59
MXC	33/91	-30.48	-31.01	-31.68	N.D. [a]	-30.67	-46.05
XC	34/91	-30.22	-31.03	-30.92	-31.58	-29.48	-47.43
XC	38/91	-28.76	-30.11	-30.58	-30.80	-30.44	-40.26
MMiC	39/91	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
MC	40/91	-30.19	-31.59	-31.98	N.D.	-31.42	-46.46
MXC	45/601	-28.94	-30.51	-31.14	-31.32	-30.32	-45.48
MC	46/601	-28.20	-29.38	-29.37	-29.54	-30.63	-45.51
MMiC	48/601	-29.79	-31.45	-31.04	-31.33	-30.35	-44.50
MC	49/601	-29.31	-31.46	-31.60	-31.67	-30.62	-44.75
XC	50/603	-29.04	-30.15	-29.24	-29.74	-29.03	-42.36
MC	51/603	-29.66	-30.94	-30.78	-31.28	-31.45	-43.96
XC	52/603	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
MXC	53/603	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
XC	54/603	N.D.	-31.95	-31.80	-31.76	-30.92	-51.35
MMiC	56/603	-28.86	-30.78	-30.76	-31.32	-31.12	N.D.

Lithotype	Sample ID	C_{27} 17β(H)-Hopane	C_{29} 17β(H)21β(H)-Hopane	C_{31} 17α(H)21β(H) 22(R)-Hopane	C_{28} 28,30-Bisnorneohop-13(18)-ene	D-ring monoaromatic hopane	ABCD-ring tetraaromatic hopane
MC	2/79	-41.32	-44.29	N.D.[a]	-34.96	N.D.	-34.13
MXC	3/79	N.D.	N.D.	N.D.	N.D.	-34.41	N.D.
XC	4/79	-36.79	-38.02	-25.94	-33.59	-32.35	N.D.
MXC	5/79	N.D.	N.D.	N.D.	N.D.	-37.46	N.D.
MMiC	6/79	N.D.	N.D.	N.D.	N.D.	-32.49	N.D.
MXC	8/79	-36.97	-38.32	-27.54	-33.97	N.D.	N.D.
MMiC	11/79	-43.89	-44.04	N.D.	-36.07	N.D.	-31.26
XC	16/79	-38.37	-39.05	N.D.	-34.32	-35.98	-33.27
MXC	18/79	N.D.	N.D.	N.D.	N.D.	-34.94	-33.33
XC	27/91	N.D.	N.D.	N.D.	N.D.	-33.28	-31.34
MC	30/91	-38.74	-40.69	-25.65	-36.33	-33.22	N.D.
MXC	33/91	-41.98	-45.20	N.D.	-35.33	-33.38	N.D.
XC	34/91	-38.41	-45.08	N.D.	-34.12	-35.03	-31.07
XC	38/91	-38.19	-39.79	-26.05	-34.08	-33.14	-30.07
MMiC	39/91	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
MC	40/91	-41.35	-46.00	N.D.	-36.48	N.D.	-32.03
MXC	45/601	-38.96	-40.46	N.D.	-33.82	-32.69	-30.29
MC	46/601	-37.74	-38.44	N.D.	-33.58	-32.90	-30.88
MMiC	48/601	-42.01	-43.75	N.D.	N.D.	N.D.	N.D.
MC	49/601	-41.69	-42.62	N.D.	-36.60	-33.74	-30.97
XC	50/603	-39.57	-40.43	-25.15	-35.79	-32.82	N.D.
MC	51/603	-38.90	-40.84	-27.28	N.D.	-36.47	-31.31

Table S-VI continued

Lithotype	Sample ID	C_{27} 17β(H)-Hopane	C_{29} 17β(H)21β(H)-Hopane	C_{31} 17α(H)21β(H) 22(R)-Hopane	C_{28} 28,30-Bisnorneohop-13(18)-ene	D-ring monoaromatic hopane	ABCD-ring tetraaromatic hopane
XC	52/603	N.D.	N.D.	N.D.	N.D.	-38.04	-32.66
MXC	53/603	N.D.	N.D.	N.D.	N.D.	-35.81	-32.29
XC	54/603	N.D.	N.D.	-24.15	N.D.	-35.94	-34.36
MMiC	56/603	-38.42	-41.42	-26.09	N.D.	N.D.	-34.51

[a]N.D. – Not determined.