

APPENDIX 3

Extraction yields, *n*-alkane distribution type and values of aliphatic biomarker ratios of the extracts

Sample code	extract yield [mg/g]	<i>n</i> -alkane distribution type	CPI 1)	$\Sigma 2/\Sigma 1$ 2)	C_{23}/C_{31} 3)	Pr/Ph 4)	Pr/ <i>n</i> -C ₁₇ 5)	Ph/ <i>n</i> -C ₁₈ 6)	$C_{31}S/(S+R)$ 7)	Ts/(Ts+Tm) 8)	$C_{30}\beta\alpha/(\alpha\beta+\beta\alpha)$ 9)	$C_{29}S/(S+R)$ 10)	$C_{29}\alpha\beta\beta/(\alpha\alpha\alpha+\alpha\beta\beta)$ 11)	C_{29}/C_{27} 12)	C_{27} dia/ C_{27} reg 13)
E1	0.20	3 ¹⁾	1.21	1.80	1.73	0.98	1.00	0.64	0.56	0.26	0.16	0.42	0.45	1.10	0.34
E2	0.03	3	1.42	6.36	0.61	0.11	0.66	0.86	0.54	0.75	0.22	0.38	0.44	0.85	0.81
E3	0.17	2	1.48	3.10	1.24	0.60	0.59	0.33	0.56	0.36	0.22	0.33	0.55	0.84	0.45
E4	0.08	3	1.54	7.11	1.09	0.44	1.25	0.88	0.42	0.69	0.31	0.23	0.32	0.99	0.59
E5	0.12	2	1.31	5.46	1.16	0.49	1.18	0.61	0.48	0.88	0.30	–	–	–	–
E6	0.42	3	1.55	3.83	0.81	2.11	2.50	1.10	–	–	–	–	–	–	–
E7	0.94	1	1.01	2.24	1.51	0.61	0.80	1.10	0.58	0.77	0.07	0.51	0.51	1.40	–
E8	7.74	2	3.16	10.22	0.90	5.54	5.83	1.45	–	–	–	–	–	–	–
E9	0.05	3	1.27	4.53	0.55	0.48	1.07	0.79	0.55	0.76	0.11	0.40	0.37	0.81	0.17
E10	2.51	3	1.13	1.98	1.75	2.82	2.40	0.89	0.57	0.28	0.10	0.40	0.38	1.00	–
E11	1.47	1	1.04	1.30	4.19	2.27	2.00	0.79	0.52	0.70	0.16	–	–	–	–
E12	0.03	3	1.24	2.59	2.08	0.33	0.75	0.39	0.58	0.84	0.24	0.61	0.42	0.68	0.51
E13	0.22	3	1.29	3.66	2.00	0.37	1.04	0.78	0.56	0.87	0.21	–	–	–	–
E14	0.35	3	1.76	4.90	0.47	1.51	2.46	1.00	0.57	–	–	–	–	–	–
E15	0.09	1	1.09	2.22	3.68	0.80	0.43	0.22	0.30	0.85	0.04	0.41	0.42	0.80	0.82
E16	0.05	2	1.12	15.47	0.59	0.32	0.66	0.45	0.33	0.50	0.47	0.57	0.38	0.87	0.63
EG1	0.05	2	1.25	7.47	0.65	0.10	0.62	0.88	0.55	0.21	0.21	0.27	0.22	1.15	0.32
EG2	0.30	1	1.07	2.57	2.56	1.17	0.36	0.23	0.51	0.57	0.13	0.34	0.50	0.63	0.82
EG3	2.74	3	1.34	1.54	2.21	5.28	2.99	0.65	0.58	0.91	0.26	–	–	–	–
EG4	0.26	1	0.98	1.87	2.72	1.12	0.33	0.24	–	–	–	0.47	0.50	0.51	0.85

- 1) $CPI = 0.5 \left\{ \frac{(n-C_{25} + n-C_{27} + n-C_{29} + n-C_{31} + n-C_{33})}{(n-C_{24} + n-C_{26} + n-C_{28} + n-C_{30} + n-C_{32})} + \frac{(n-C_{25} + n-C_{27} + n-C_{29} + n-C_{31} + n-C_{33})}{(n-C_{26} + n-C_{28} + n-C_{30} + n-C_{32} + n-C_{34})} \right\}$; Carbon Preference Index; $m/z = 71$; thermal maturity parameter (Bray and Evans, 1963).
 - 2) $\Sigma 2/\Sigma 1 = \left[\frac{\Sigma (\text{from } n-C_{23} \text{ to } n-C_{37})}{\Sigma (\text{from } n-C_{11} \text{ to } n-C_{22})} \right]$; $m/z = 71$, source indicator (Tissot and Welte, 1984).
 - 3) $C_{23}/C_{31} = n\text{-tricosane}/n\text{-hentriacontane}$ (Pankost et al., 2002).
 - 4) Pr/Ph = pristane/phytane; parameter of environment oxicity (with exception of coals); $m/z = 71$ (Didyk et al., 1978).
 - 5) Pr/*n*-C₁₇ = pristane/*n*-heptadecane; $m/z = 71$ (Leythauser and Schwartzkopf, 1985).
 - 6) Ph/*n*-C₁₈ = phytane/*n*-octadecane; $m/z = 71$ (Leythauser and Schwartzkopf, 1985).
 - 7) $C_{31}S/(S+R) = 17\alpha(H), 21\beta(H)\text{-}29\text{-homohopane } 22S / (17\alpha(H), 21\beta(H)\text{-}29\text{-homohopane } 22S + 17\alpha(H), 21\beta(H)\text{-}29\text{-homohopane } 22R)$; $m/z = 191$; thermal maturity parameter (Seifert and Moldowan 1986).
 - 8) $Ts/(Ts+Tm) = 18\alpha(H)\text{-}22, 29, 30\text{-trisorneohopane} / (18\alpha(H)\text{-}22, 29, 30\text{-trisorneohopane} + 17\alpha(H)\text{-}22, 29, 30\text{-trisorhopane})$; $m/z = 191$; thermal maturity parameter (Seifert and Moldowan 1986).
 - 9) $C_{30}\beta\alpha/(\alpha\beta+\beta\alpha) = 17\beta(H), 21\alpha(H)\text{-}29\text{-hopane } C_{30} / (17\alpha(H), 21\beta(H)\text{-}29\text{-hopane } C_{30} + 17\beta(H), 21\alpha(H)\text{-}29\text{-hopane } C_{30})$; $m/z = 191$ (Seifert and Moldowan 1986).
 - 10) $C_{29}\alpha\alpha\alpha/(S+R) = \text{ratio of } C_{29}\text{-}5<, 14<, 17< \text{ (H)-stigmastane } 20S \text{ to a sum of its diastereomers } 20S \text{ and } 20R$; $m/z = 217$. (Seifert and Moldowan 1986).
 - 11) $C_{29}\alpha\alpha\alpha/(C_{29}\alpha\alpha\alpha + C_{29}\alpha\beta\beta) = \text{ratio of } C_{29}\text{-}5<, 14\alpha, 17\alpha(H)\text{-stigmastane } (20S + 20R) \text{ to a sum of its distereomers } C_{29}\text{-}5<, 14<, 17< \text{ (H)-stigmastane } (20S+20R) + C_{29}\text{-}5<, 14<, 17< \text{ (H)-stigmastane } (20S + 20R)$, $m/z = 217$ (Seifert and Moldowan 1986).
 - 12) $C_{29}/C_{27} = \text{sum of } C_{29} \text{ sterane diastereomers} / \text{sum of } C_{27} \text{ sterane diastereomers}$, $m/z = 217$ (Huang and Meinschein 1979)
- * number denotes a distribution type described in the text “
 “–” compounds not detected or in concentrations too low to calculate a parameter value