

Supplementary material

Lipid biomarker and stable isotopic profiles through Later carboniferous – Early Triassic of the deepest Well MS-1 in the Junggar Basin, northwest China

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The following supplementary material is available for this article online:

Table S1 TOC and rock pyrolysis parameters of the Late Carboniferous-Early Triassic rocks in MS-1 well

Table S2 Parameters of $\delta^{13}\text{C}$ values of n-alkanes, Pr, Ph, β -carotene and chloroform extracts from MS1 wells of the Late Carboniferous-Early

Table S3 Parameters of hopane and sterane in Late Carboniferous-Early Triassic of MS1 well

Table S1 TOC and rock pyrolysis parameters of the Late Carboniferous-Early Triassic rocks in MS-1 well

Strata	Sample No.	Depth (m)	Lithology	TOC (%)	S ₁ +S ₂ (mg/g)	T _{max} °C
T _{1b}	JM-1	5951.00	Gray mudstone	0.64	1.26	439
	JM-2	5982.67	Brown siltstone mudstone	0.17	0.15	507
	JM-3	5983.15	Brown siltstone mudstone	0.15	0.12	482
	JM-4	5990.00	Gray mudstone	0.6	1.51	439
	JM-5	6011.00	Gray mudstone	0.62	1.7	441
	JM-6	6046.00	Gray mudstone	0.5	1.27	439
	JM-7	6078.00	Gray mudstone	0.63	1.56	438
	JM-8	6114.00	Gray mudstone	0.77	2.47	446
	JM-9	6169.00	Gray mudstone	0.62	2.83	437
P _{3w}	JM-10	6193.00	Gray-brown mudstone	0.64	2.34	436
	JM-11	6227.00	Gray-brown mudstone	0.46	0.99	440
	JM-12	6246.00	Gray-brown mudstone	0.44	0.54	442
	JM-13	6274.00	Gray mudstone	0.92	3.41	440
	JM-14	6301.00	Brown siltstone mudstone	0.63	1.52	443
	JM-15	6322.00	Brown siltstone mudstone	0.62	1.84	433
	JM-16	6333.00	Brown siltstone mudstone	0.46	0.79	428

P _{2w}	JM-17	6379.00	Brown siltstone mudstone	0.37	0.57	453
	JM-18	6393.00	Gray mudstone	0.38	1.03	431
	JM-19	6407.00	Gray mudstone	1.21	1.74	434
	JM-20	6435.00	Brown siltstone mudstone	0.72	1.04	436
	JM-21	6459.00	Gray mudstone	0.94	1.59	432
	JM-22	6476.00	Gray mudstone	0.91	3.16	407
	JM-23	6486.00	Gray mudstone	0.75	1.36	
	JM-24	6492.00	Gray mudstone	0.18	1.25	425
	JM-25	6513.00	Gray mudstone	0.61	0.86	423
	JM-26	6531.00	Gray mudstone	0.73	0.96	413
	JM-27	6543.86	Gray mudstone	0.69	0.38	471
	JM-28	6545.1	Brown siltstone mudstone	0.64	0.29	483
	JM-29	6553.00	Gray mudstone	0.74	0.63	424
	JM-30	6568.00	Gray mudstone	0.55	0.54	396
	JM-31	6591.00	Gray mudstone	0.64	0.7	463
	JM-32	6632.00	Gray mudstone	0.33	1.01	411
P _{2x}	JM-33	6642.00	Gray mudstone	0.59	0.63	425
	JM-34	6668.00	Gray mudstone	0.05	0.26	445
	JM-35	6680.00	Brown siltstone mudstone	0.55	0.19	

	JM-36	6703.00	Gray mudstone	0.46	0.29	458
	JM-37	6728.00	Gray mudstone	1.16	0.65	439
	JM-38	6750.00	Brown siltstone mudstone	0.24	0.15	463
	JM-39	6766.00	Brown siltstone mudstone	0.21	0.14	458
	JM-40	6790.00	Gray mudstone	0.88	0.96	437
	JM-41	6800.00	Gray mudstone	0.42	0.27	468
C _{2t}	JM-42	6820.00	Gray-brown mudstone	0.39	0.22	472
	JM-43	6840.00	Gray-brown mudstone	0.59	0.22	476
	JM-44	6873.00	Gray-brown mudstone	0.39	0.16	479
	JM-45	6886.00	Gray mudstone	0.4	0.27	438
	JM-46	6932.00	Gray mudstone	0.43	0.29	459
	JM-47	6996.58	Gray tuff	0.04	0.04	468
	JM-48	6998.32	Gray tuff	0.06	0.05	357
	JM-49	7000.74	Gray tuff	0.06	0.07	480
	JM-50	7001.00	Gray tuff	0.17	0.1	502
	JM-51	7014.00	Gray tuff	0.34	0.26	437
	JM-52	7030.00	Gray tuff	0.26	0.26	437
	JM-53	7048.00	Coal	32.53	28.85	435
	JM-54	7070.00	Coal	27.26	20.49	435

JM-55	7090.00	Gray tuff	0.24	0.17	449
JM-56	7114.00	Gray tuff	0.14	0.19	456
JM-57	7153.00	Gray tuff	0.62	0.28	436
JM-58	7168.00	Gray-black tuff	0.61	0.25	453
JM-59	7180.00	Gray-black tuff	0.83	0.42	441
JM-60	7201.00	Gray-black tuff	0.64	0.25	447
JM-61	7206.00	Gray-black tuff	1.18	0.53	444
JM-62	7216.00	Gray tuff	0.43	0.58	430
JM-63	7245.00	Gray tuffaceous mudstone	0.29	0.63	427
JM-64	7298.00	Gray tuff	0.2	0.22	450
JM-65	7323.00	Gray tuff	0.35	1.15	427
JM-66	7361.00	Gray-black tuffaceous mudstone	4.64	10.18	430
JM-67	7410.00	Gray tuff	0.41	0.35	437
JM-68	7419.00	Gray tuff	0.2	0.16	460
JM-69	7439.00	Gray-black tuffaceous mudstone	2.88	0.63	431
JM-70	7468.00	Gray-black tuffaceous mudstone	0.61	0.23	446
JM-71	7480.00	Gray-black tuffaceous mudstone	0.44	0.36	436
JM-72	7489.00	Gray tuff	0.18	0.12	460
JM-73	7493.00	Gray tuff	0.36	0.13	458

Table S2 Parameters of $\delta^{13}\text{C}$ values of n-alkanes, Pr, Ph, β -carotene and chloroform extracts from MS1 wells of the Late Carboniferous-Early

Triassic

Strata	Sample No.	β - carotene / ΣC_{12-35}	C_{max}	CPI_1^{a}	CPI_2^{b}	$\text{Alk}_{\text{terr}}^{\text{c}}$	$\text{LMW}/\text{HMW}^{\text{d}}$	Pr/C17	Ph/C18	Pr/Ph	$\delta^{13}\text{C}$
<i>T_{1b}</i>	JM-1	0.05	C17	1.05	1.17	0.01	6.08	0.26	0.37	0.67	-29.58
	JM-2	0.04	C17	1.05	1.17	0.01	6.09	0.27	0.38	0.74	
	JM-3	0.55	C19	1.06	1.15	0.06	1.39	0.28	0.34	0.72	-30.62
	JM-4	0.51	C19	1.05	1.15	0.05	1.74	0.28	0.36	0.72	-30.81
	JM-5	0.04	C17	1.06	1.14	0.01	8.26	0.25	0.38	0.68	-29.65
	JM-6	0.60	C19	1.05	1.19	0.06	1.61	0.27	0.34	0.70	
	JM-7		C17	1.06	1.17	0.01	8.69	0.25	0.41	0.70	-29.28
	JM-8	0.67	C19	1.06	1.16	0.05	1.59	0.28	0.33	0.72	-30.52
	JM-9	0.90	C19	1.05	1.19	0.06	1.49	0.28	0.35	0.72	
	JM-10	0.79	C19	1.06	1.19	0.04	2.25	0.24	0.38	0.62	-29.50
	JM-11	0.05	C17	1.05	1.15	0.01	8.47	0.25	0.41	0.66	
	JM-12	0.04	C17	1.05	1.16	0.01	8.15	0.26	0.39	0.68	
	JM-13	1.17	C19	1.06	1.15	0.06	1.64	0.26	0.37	0.62	
	JM-14	0.03	C17	1.06	1.11	0.01	11.43	0.27	0.45	0.69	-29.58
	JM-15	0.93	C19	1.06	1.18	0.05	1.75	0.25	0.37	0.63	-30.11
	JM-16	0.47	C19	1.06	1.18	0.04	2.01	0.23	0.34	0.59	-29.28
	JM-17		C25	1.03	1.15	0.21	0.37	0.19	0.26	0.57	-32.17
	JM-18	1.46	C19	1.05	1.12	0.07	1.44	0.35	0.43	0.80	
	JM-19		C17	1.03	1.65	0.00	4.65	0.23	0.35	0.56	-29.15
<i>P_{3w}</i>	JM-20	0.80	C19	1.04	1.20	0.06	1.56	0.26	0.35	0.63	-29.66
<i>P_{2w}</i>	JM-21	1.12	C19	1.07	1.19	0.07	1.18	0.21	0.32	0.49	-29.61

			JM-22	C19	1.03	1.25	0.01	2.02	0.23	0.35	0.50	-28.47
		0.73	JM-23	C17	1.06	1.18	0.04	2.17	0.28	0.44	0.65	
		0.67	JM-24	C19	1.06	1.16	0.04	2.01	0.26	0.40	0.64	-29.90
		0.28	JM-25	C17	1.07	1.22	0.04	2.29	0.28	0.45	0.64	
		0.49	JM-26	C17	1.08	1.15	0.03	3.54	0.29	0.51	0.70	-30.14
		0.33	JM-27	C17	1.07	1.16	0.03	2.73	0.28	0.43	0.66	
			JM-28	C17	1.08	1.19	0.01	11.64	0.29	0.51	0.74	-30.05
		0.40	JM-29	C19	1.07	1.21	0.03	2.27	0.27	0.40	0.62	-29.30
			JM-30	C17	1.06	1.22	0.01	8.87	0.30	0.53	0.66	
			JM-31	C17	1.06	1.13	0.03	2.90	0.25	0.44	0.57	-29.80
			JM-32	C17	1.07	1.19	0.02	4.19	0.28	0.44	0.69	-29.13
			JM-33	C19	1.02	0.98	0.07	1.26				-25.22
			JM-34	C19	1.02	1.07	0.07	1.15				-23.93
		0.54	JM-35	C19	1.07	1.14	0.03	2.82	0.26	0.42	0.60	-28.44
		0.31	JM-36	C17	1.08	1.16	0.01	7.80	0.31	0.54	0.74	-29.54
		0.28	JM-37	C17	1.05	1.12	0.05	2.09	0.32	0.42	0.83	-29.00
			JM-38	C19	1.10	0.82	0.06	1.57	0.29	0.43	0.67	-28.44
		3.85	JM-39	C17	1.01	1.21	0.10	1.79	0.21	0.39	0.57	
			JM-40	C17	1.03	1.09	0.08	1.32	0.27	0.43	0.67	-28.32
			JM-41	C19	1.05	1.08	0.06	1.29	0.27	0.33	0.67	-28.97
P _{2x}		1.00	JM-42	C19	1.06	1.16	0.04	1.81	0.29	0.43	0.67	-29.76
		0.65	JM-43	C17	1.05	1.18	0.03	2.36	0.25	0.40	0.64	-28.77
			JM-44	C19	1.04	1.12	0.06	1.24	0.21	0.30	0.56	
C _{2t}			JM-45	C19	0.95	1.21	0.14	0.63				

			C27	0.99	1.08	0.18	0.40				
			C21	1.06	1.10	0.08	0.83	0.22	0.29	0.61	-28.14
			C19	1.03	1.25	0.04	1.52	0.16	0.25	0.44	
			C23	1.09	1.29	0.11	0.65	0.20	0.38	0.33	-28.62
			C19	1.03	1.14	0.06	1.67	0.11	0.22	0.29	
			C21	1.13	1.38	0.10	0.74	0.25	0.29	0.50	
			C19	1.03	1.24	0.12	1.08	0.20	0.18	0.50	
			C23	1.06	1.30	0.14	0.63	0.18	0.27	0.49	-28.38
			C23	1.08	1.36	0.11	0.89	0.20	0.36	0.50	-28.37
			C23	1.08	1.41	0.12	0.92	0.22	0.43	0.53	-27.00
			C19	1.07	1.30	0.02	1.68	0.17	0.27	0.43	-29.52
			C19	1.06	1.22	0.07	1.22	0.21	0.31	0.50	
	0.56		C25	1.04	1.12	0.18	0.63	0.24	0.39	0.57	-28.46
			C19	1.33	2.00	0.06	0.80				
			C16	1.07	1.11	0.06	2.27	0.21	0.42	0.60	-29.05
			C17	1.04	1.04	0.13	1.02	0.17	0.29	0.63	-28.41
	1.75		C25	1.03	1.07	0.14	0.50	0.25	0.27	0.67	-28.06
			C19	1.05	1.35	0.05	0.81				-28.40
	2.70		C27	0.97	1.12	0.19	0.43	0.21	0.35	0.43	

^a CPI₁: $1/2[\Sigma C_{15-21}(\text{odd carbon})/\Sigma C_{14-20}(\text{even carbon}) + \Sigma C_{15-21}(\text{odd carbon})/$

$\Sigma C_{16-22}(\text{even carbon})]$

^b CPI₂: $1/2[\Sigma C_{25-35}(\text{odd carbon})/\Sigma C_{24-34}(\text{even carbon}) + \Sigma C_{25-35}(\text{odd carbon})/$

$\Sigma C_{26-36}(\text{even carbon})]$

^c Alkterr: $(C_{27} + C_{29} + C_{31} + C_{33})/\Sigma C_{14-38}$

^d LMW/HMW: $\Sigma nC_{21-}/\Sigma nC_{22+}$

^e $\delta^{13}C = \delta^{13}C$ of chloroform extracts

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Table S3 Parameters of hopane and sterane in Late Carboniferous-Early Triassic of MS1 well

Strata	Sample No.	C31 $\alpha\beta$ -22S/ (S+R)	C32 $\alpha\beta$ -22S/ (S+R)	Gama.	C29/C30	C35/C34	Ts/Tm	C29 $\alpha\alpha\alpha$ -20S/ 20(S+R)	C29 $\alpha\beta\beta$ / ($\alpha\beta\beta + \alpha\alpha\alpha$)	C27 $\alpha\alpha\alpha$ 20R	C28 $\alpha\alpha\alpha$ 20R	C29 $\alpha\alpha\alpha$ 20R
T _{1b}	JM-1	0.60	0.59	0.32	0.67	0.55	0.48	0.44	0.51	25.61	21.15	53.24
	JM-2	0.61	0.60	0.31	0.59	0.57	0.79	0.44	0.53	27.50	19.33	53.17
	JM-3	0.59	0.58	0.42	0.78	0.83	0.52	0.46	0.56	32.89	19.82	47.29
	JM-4	0.57	0.62	0.43	0.56	0.90	0.49	0.50	0.57	34.27	20.55	45.19
	JM-5	0.59	0.39	0.35	0.80	0.71	0.65	0.45	0.53	29.76	19.67	50.57
	JM-6	0.60	0.61	0.83	0.82	0.94	0.22	0.43	0.47	11.37	33.16	55.47
	JM-7	0.65	0.66	0.21	0.42	0.33	0.74	0.48	0.56	21.16	25.40	53.45
	JM-8	0.59	0.62	0.41	0.63	0.89	0.54	0.50	0.55	30.10	26.86	43.04
	JM-9	0.58	0.58	0.45	0.60	0.81	0.54	0.49	0.52	24.51	26.80	48.70
P _{3w}	JM-10	0.57	0.58	0.67	0.56	0.83	0.42	0.46	0.47	16.74	32.35	50.91
	JM-11	0.59	0.41	0.36	0.57	0.55	0.69	0.45	0.51	24.88	25.81	49.32
	JM-12	0.54	0.56	0.32	0.59	0.52	0.50	0.47	0.52	22.76	25.70	51.54
	JM-13	0.57	0.61	0.56	0.54	0.57	0.58	0.46	0.48	23.30	26.57	50.14

	JM-14	0.60	0.61	0.21	0.89	0.50	0.28	0.45	0.48	20.69	24.04	55.28
	JM-15	0.58	0.57	0.55	0.57	0.97	0.54	0.48	0.51	20.92	30.51	48.57
	JM-16	0.57	0.57	0.56	0.62	0.86	0.51	0.46	0.47	22.16	28.49	49.36
	JM-17	0.59	0.57	0.58	0.55	0.87	0.45	0.42	0.47	21.76	26.70	51.54
	JM-18	0.58	0.55	0.65	0.60	0.95	0.46	0.44	0.48	20.76	29.00	50.25
	JM-19	0.53	0.57	0.60	0.63	0.76	0.49	0.49	0.53	27.40	29.50	43.11
	JM-20	0.60	0.57	0.67	0.60	0.93	0.44	0.47	0.49	20.81	30.63	48.56
	JM-21	0.56	0.55	0.59	0.55	0.99	0.49	0.48	0.50	22.47	29.76	47.77
	JM-22	0.57	0.56	0.46	0.48	0.56	0.64	0.42	0.44	24.09	26.52	49.39
	JM-23	0.57	0.59	0.55	0.75	0.80	0.41	0.45	0.50	24.25	26.57	49.18
	JM-24	0.57	0.60	0.74	0.78	0.77	0.41	0.46	0.50	22.51	30.62	46.87
	JM-25	0.58	0.68	0.44	0.78	0.71	0.47	0.47	0.52	30.47	25.26	44.27
	JM-26	0.57	0.57	0.74	0.72	0.78	0.35	0.52	0.53	22.63	32.94	44.43
	JM-27	0.58	0.57	0.51	0.68	0.79	0.43	0.47	0.48	22.66	27.56	49.78
	JM-28	0.57	0.57	0.42	0.58	0.79	0.57	0.45	0.52	28.57	23.25	48.18
	JM-29	0.64	0.60	0.47	0.68	1.28	0.64	0.50	0.50	29.70	24.84	45.46
	JM-30	0.51	0.59	0.60	0.61	0.00	0.58	0.46	0.53	31.34	27.88	40.79
	JM-31	0.60	0.60	0.52	0.65	0.81	0.53	0.44	0.51	27.32	24.73	47.95
	JM-32	0.57	0.55	0.49	0.72	0.90	0.55	0.48	0.51	29.53	25.86	44.61
	JM-33	0.59	0.56	0.94	0.66	0.83	0.55	0.45	0.52	25.62	26.72	47.66
	JM-34	0.57	0.56	1.30	0.70	0.64	0.35	0.49	0.50	27.44	27.41	45.15
	JM-35	0.57	0.58	0.47	0.70	0.75	0.48	0.46	0.49	27.63	24.57	47.79
	JM-36	0.60	0.60	0.51	0.51	0.73	0.70	0.46	0.52	27.48	25.79	46.73
P _{2w}	JM-37	0.59	0.56	0.50	0.62	0.87	0.60	0.44	0.53	30.41	24.14	45.45

	JM-38	0.59	0.61	0.56	0.64	0.81	0.56	0.45	0.51	26.60	24.16	49.24
	JM-39	0.64	0.60	0.61	0.43	0.31	0.65	0.42	0.47	34.92	24.01	41.07
	JM-40	0.59	0.59	0.51	0.59	0.69	0.91	0.49	0.50	31.43	22.70	45.87
	JM-41	0.58	0.61	0.61	0.76	0.89	0.49	0.49	0.50	21.92	30.91	47.16
P_{2x}	JM-42	0.59	0.56	0.73	0.58	0.86	0.33	0.43	0.51	17.95	29.30	52.75
	JM-43	0.58	0.56	0.53	0.58	0.76	0.60	0.45	0.49	29.60	26.91	43.50
	JM-44	0.58	0.59	0.58	0.59	0.68	0.80	0.49	0.49	32.31	26.54	41.15
	JM-45	0.61	0.63	0.63	0.64	0.54	0.80	0.48	0.46	28.11	25.12	46.77
	JM-46	0.60	0.58	0.64	0.61	0.77	0.74	0.48	0.44	28.24	26.66	45.10
	JM-47	0.57	0.56	0.63	0.57	0.78	0.71	0.47	0.51	32.39	24.66	42.95
	JM-48	0.55	0.55	0.57	0.54	0.75	0.76	0.44	0.47	30.51	23.05	46.44
	JM-49	0.61	0.60	0.73	0.51	0.66	1.03	0.48	0.46	33.50	25.57	40.93
	JM-50	0.60	0.59	0.95	0.50	0.60	0.88	0.41	0.41	37.70	22.84	39.46
	JM-51	0.61	0.61	0.69	0.61	0.56	0.88	0.45	0.43	36.57	23.34	40.09
	JM-52	0.55	0.56	0.86	0.43	0.52	0.78	0.42	0.46	25.81	25.75	48.43
	JM-53	0.50	0.49	0.38	0.54	0.84	0.43	0.36	0.44	26.47	23.68	49.85
	JM-54	0.38	0.46	0.29	0.52	0.76	0.27	0.19	0.35	18.25	18.21	63.54
	JM-55	0.41	0.45	0.28	0.56	0.66	0.30	0.20	0.37	20.00	17.76	62.24
	JM-56	0.59	0.57	0.50	0.68	0.92	0.54	0.41	0.50	30.30	21.00	48.70
	JM-57	0.61	0.55	0.56	0.70	0.75	0.55	0.42	0.44	39.27	23.58	37.14
	JM-58	0.56	0.57	0.65	0.41	0.59	0.90	0.32	0.36	38.39	22.77	38.84
	JM-60	0.56	0.57	2.47	0.34		1.18	0.32	0.23	25.63	27.67	46.70
	JM-62	0.61	0.61	0.71	0.71	0.56	0.58	0.48	0.47	34.84	25.40	39.76
C_{2t}	JM-67	0.62	0.62	0.62	0.57	0.97	0.70	0.42	0.39	24.43	21.27	54.30

	JM-69	0.54	0.50	0.90	0.50	0.55	0.58	0.41	0.46	27.41	23.30	49.28
	JM-71	0.64	0.63	0.68	0.66	0.65	0.78	0.46	0.46	22.29	24.32	53.39
	JM-73	0.67	0.62	0.69	0.72	0.68	0.57	0.44	0.44	18.56	23.46	57.98