Table S1. Statistical data of contour maps of coal seam thickness and burial depth (Well information is from Research Institute of Exploration and Development, Petro China Tuha Oilfield Company, and the data are statistics for this study).

Well ID	Coal seam thickness(m)	Coal seam burial depth(m)
Tiao 15	13.08	877.5
Tiao 11	42.3	1420
Tiao 18	30.5	1670
Tiao 26	13.3	1650
Ma 76	44.66	1861
Ma 18	20	1177
Ma 37	52	988
Ma 19	24.6	1247
Ma 51	61.3	1520
Ma 53	41	1450
Tang 1	46.9	1034.4
Ma 20	20	1200
Bei 2	38.8	1964
L5-2	6.5	280
310-1	4.2	380
340-3	3.7	270
Tangqican 1	40.03	723

Table S2. Maceral compositions of the coals in the Xishanyao Formation of the Santanghu Basin (Data from Research Institute of Exploration and Development, Petro China Tuha Oilfield Company, the data with * in Well ID are the results of this study).

Well ID	Depth（m）	Maceral compositions（%）			$R_{o, ran}$
		Vitrinite	Inertinite	Liptinite	
Tangqican1	**722.4**	**41**	**59**	**0**	
Tangqican1	723.91	34	52	14	0.59
Tangqican1	724.73	22	78	0	
Tangqican1	726.54	33	67	0	
Tangqican1	728.28	46	54	0	0.66
Tangqican1	728.6	40	60	0	
Tangqican1	728.79	49	51	0	
Tangqican1	729.18	36	50	14	
Tangqican1	729.88	52	48	0	
Tangqican1	729.98	25	63	12	
Tangqican1	730.16	32	55	13	
Tangqican1	730.75	63	37	0	
Tangqican1	731.6	57	43	0	
Tangqican1	735.83	43	57	0	
Tangqican1	737.53	27	58	15	
Tangqican1	738.22	46	54	0	
Tangqican1	738.78	42	58	0	
Tangqican1	739.35	52	48	0	
Tangqican1	740.7	65	35	0	0.57
Tangqican1	740.88	58	42	0	

Tangqican1	741.06	51	49	0	
Tangqican1	741.25	63	37	0	0.56
Tangqican1	741.42	60	40	0	
Tangqican1	741.83	57	43	0	
Tangqican1	741.99	53	47	0	
Tangqican1	742.4	68	32	0	
Tangqican1	742.75	58	42	0	
Tangqican1	742.92	51	49	0	
Tangqican1	743.19	55	45	0	
Tangqican1	743.36	30	59	11	0.53
Tangqican1	743.7	66	34	0	
Tangqican1	745.75	71	29	0	
Tangqican1	746.39	65	35	0	
Tangqican1	746.75	57	43	0	
Tangqican1	746.98	30	62	8	0.61
Tangqican1	747.28	60	40	0	
Tangqican1	747.43	73	27	0	
Tangqican1	748.26	54	46	0	
Tangqican1	749.79	26	46	28	
Tangqican1	757.06	39	61	0	0.74
Tang 1*	991.57-992.31	36.4	59	4.6	0.51
Tang1	994.00-994.35	12.6	87.4	0.0	0.48
Tang1	998.10-998.45	27.2	72.8	0.0	0.48
Tang1	1002.2	38.4	58.4	3.2	
Tang1	1004.00-1004.35	15.1	84.9	0.0	0.49
Tang 1*	1008.01-1009.63	44.2	53.9	1.9	0.36
Tang1	1012.43-1012.45	33.0	62.0	5.0	
Tang 1*	1017.74-1019.46	45.3	52.9	1.8	0.24
Tang 1	1020.8	38.4	56.3	5.3	0.54
Tang 1	1024.5	35	63.7	1.3	0.55
Tang1	1026.78-1027.13	71.0	28.5	0.5	0.42
Tang3	1186.3	90	8	2	0.57
Bei2	1966.2	30	64	6	0.61
Tiao15	843.72--844.01	43.9	54.6	1.5	0.39
Tiao15	844.73--845.00	41	58.5	0.5	0.44
Tiao15	846.56-846.58	46	47	7	
Tiao15	846.80--847.10	42.3	55.1	2.6	0.46
Tiao15	847.10--847.40	42.1	57.3	0.5	0.45
Tiao15	847.40--847.70	39.3	60.3	0.4	0.44
Tiao15	847.70--848.00	38.1	61.2	0.7	0.45
Tiao15	848.00--848.26	30.2	68.7	1.1	0.45
Tiao15	848.41--848.69	26	73	1	0.46
Tiao15	848.69--848.86	32.7	66.4	0.8	0.42
Tiao15	848.98--849.10	38.1	61	0.9	0.41
Tiao15	849.10--849.31	37.5	61.8	0.7	0.41
Tiao15	851.06--851.20	59.2	39.5	1.3	0.45
Tiao15	851.20--851.46	65.4	34.3	0.4	0.45
Tiao15	851.46--851.71	67.9	31.2	0.9	0.44
Tiao15	851.71--851.93	67.9	30.7	1.4	0.46
Ma205	768.85-768.88	46	44	10	0.38
Ma76	1800.4	60.1	34.4	5.5	0.62

Table S3. Results of the partial proximate analysis of the coals in the Xishanyao Formation of the Santanghu Basin (Data from Research Institute of Exploration and Development, Petro China Tuha Oilfield Company, the data with * in Well ID are the results of this study).

Well ID	Depth/m	Proximate analysis (%)			
		M_{ad} /%	A_d /%	V_{daf} /%	FC_{ad} /%
Tangqican1	722.29-722.49	6.42	3.61	31.76	61.55
Tangqican1	724.66-724.81	8.96	19.88	47.14	38.56
Tangqican1	726.49-726.59	13.48	4.1	38.04	51.41
Tangqican1	728.20-728.37	15.15	3.18	31.14	56.57
Tangqican1	728.52-728.69	15.32	5.17	37.97	49.81
Tangqican1	728.69-728.89	5.44	14.23	49.93	40.61
Tangqican1	729.13-729.22	14.42	5.04	38	50.39
Tangqican1	729.84-729.93	8.87	34.74	42.36	34.28
Tangqican1	729.93-730.03	10.59	7.34	33.66	54.96
Tangqican1	730.03-730.29	6.14	3.67	34.47	59.25
Tangqican1	730.71-730.78	9.2	36.97	48.33	29.57
Tangqican1	731.51-731.69	12.02	3.07	37.98	52.89
Tangqican1	735.71-735.95	5.14	28.69	53.3	31.59
Tangqican1	737.43-737.63	10.67	6.94	36.53	52.76
Tangqican1	738.13-738.30	7.79	13.64	41.07	46.93
Tangqican1	738.69-738.86	8.08	7.03	34.85	55.68
Tangqican1	739.26-739.43	6.02	20.44	44.68	41.37
Tangqican1	739.43-739.60	8.34	7.7	35.75	54.36
Tangqican1	740.62-740.79	8.3	10.34	34.55	53.81
Tangqican1	740.79-740.96	8.5	9.14	40.01	49.88
Tangqican1	740.96-741.16	9.78	5.22	39.25	51.95
Tangqican1	741.16-741.33	8.2	21.46	38.21	44.55
Tangqican1	741.73-741.93	5.95	3.64	35.92	58.08
Tangqican1	742.32-742.49	7.08	27.84	38.22	41.43
Tangqican1	742.49-742.66	7.08	26.88	38.92	41.5
Tangqican1	742.66-742.83	8.12	16.21	37.62	48.03
Tangqican1	742.83-743.00	8.64	6.35	34.55	56
Tangqican1	743.11-743.28	8.32	8.62	34.98	54.47
Tangqican1	743.45-743.62	7.72	13.01	38.16	49.64
Tangqican1	743.62-743.79	8.11	13.47	38.9	48.58
Tangqican1	745.66-745.84	6.44	4.26	35.81	57.5
Tangqican1	746.14-746.31	9.98	3.95	35.74	55.56
Tangqican1	746.31-746.48	9.22	9	37.48	51.65
Tangqican1	746.65-746.82	10.04	3.69	33.64	57.49
Tangqican1	746.82-746.90	7.42	6.63	37.95	53.64
Tangqican1	747.35-747.52	7.64	7.23	38.18	52.97
Tangqican1	748.18-748.35	7.54	12.91	34.91	52.41
Tangqican1	749.71-749.88	7.78	16.09	36.96	48.78
Tangqican1	749.88-750.00	8.32	6.48	36.25	54.66
Tangqican1	756.99-757.14	10.26	19.91	36.41	45.71
Tangqican1*	721.84-726.72	6.06	10.99	32.24	56.65
Tangqican1*	727.49-733.78	5.22	5.72	38.31	55.12
Tangqican1*	734.69-739.03	5.05	5.29	33.48	59.82
Tangqican1*	739.03-743.96	4.34	21.39	44.53	41.71
Tangqican1*	744.57-748.03	4.78	5.68	34.69	58.66
Tangqican1*	755.65-757.38	4.72	21.35	37.73	46.66
Tang1*	991.57-992.31	4.32	2.73	30.96	64.25

Tang1	993.40-993.42	7.59	2.86	27.23	65.33
Tang1	998.10-998.45	2.89	2.35	32.68	62.09
Tang1*	1000.46-1001.79	4.42	3.34	30.04	64.63
Tang1	1005.8	5.43	1.78	26.66	66.14
Tang1	1007.9	4.84	3.01	37.15	55.01
Tang1	1013.95-1014.30	3.01	2.4	28.37	66.23
Tang1*	1017.74-1019.46	3.82	2.71	32.16	63.47
Tang1	1026.78-1027.13	1.79	5.25	37.59	55.38
Tang3	1186.30-1186.32	6.94	2.58	45.11	49.76
Tiao15	843.72--844.01	8.19	4.39	32.26	
Tiao15	843.98-844.00	5.52	4.89	32.95	60.25
Tiao15	844.73--845.00	8.77	4.33	28.65	
Tiao15	845.68-845.70	5.8	4.32	35.25	58.36
Tiao15	846.80--847.10	8.88	4.6	31.35	
Tiao15	847.10--847.40	8.52	4.82	29.7	
Tiao15	847.40--847.70	8.2	6.68	27.56	
Tiao15	847.70--848.00	8.79	5.88	29.3	
Tiao15	848.00--848.26	7.74	9.58	27.72	
Tiao15	848.41--848.69	7.76	9.82	26.93	
Tiao15	848.69--848.86	7.99	5.98	29.9	
Tiao15	848.98--849.10	8.47	5.42	32.92	
Tiao15	849.10--849.31	8.4	4	29.67	
Tiao15	851.06--851.20	8.89	3.24	35.99	
Tiao15	851.20--851.46	8.79	3.08	38.55	
Tiao15	851.46--851.71	8.69	2.94	38.15	
Tiao15	851.71--851.93	8.89	5.93	40.77	
Ma76	1800.4	3.71	29.47	4.17	62.66
Ma76*	1805.74-1806.54	2.28	31.01	39.29	40.93
Ma205	768.77-768.79	7.73	3.1	46.19	48.12

Table S4. Coalbed Methane Isotope Data (Tiaohu and Malang sags data from [46]; Surat Basin data from [66]; Bowen Basin data from [65]; Erlian Basin data from [67]).

Basin/Sag	Well ID	Depth	Sample ID	δC^{13}-(CH_4) ‰	$C_1/(C_2+C_3)$	δD-(CH_4) ‰	Data Source
Tiaohu sag	Bei 2	1879.32	B2-1	-55.5	117.65	-215.6	[46]
			B2-2	-54.5	117.65	-215.2	
			B2-3	-54.1	117.65	-215.1	
Malang sag	Ma 491	1489.00	M491-1	-63.6	139.32	-267.2	[46]
			M491-2	-64.1	139.32	-267.5	
	Tang 1-5	1080.00	T1-5-1	-54.7	2515.75	-248.2	
			T1-5-2	-54.8	2515.75	-248.4	
			T1-5-3	-55.2	2515.75	-248	
	Tang 1	993.00	T1-1	-54.8	203.65	-239.3	
			T1-2	-54.9	203.65	-239.1	
			T1-3	-55.3	203.65	-238.9	
Surat Basin			Walloon Subgroup Juandah Coal Measures	-53.3	9970	-233	[66]
				-53.6	9700	-229	
				-53.4	9960	-231	
				-53.9	190	-227	
				-54.1	9950	-234	
				-55	9940	-236	
				-54.5	706	-235	
				-54	206	-232	

		-52.2	172	-236
		-51.4	241	-235
		-52.2	308	-230
		-52.9	621	-233
		-52.7	198	-231
		-51.2	224	-231
		-52.4	496	-226
		-52.4	576	-226
		-50.8	1655	-223
		-52.1	496	-222
		-51.8	1653	-222
		-52.3	1976	-221
		-53.1	210	-225
		-54.7	1932	-224
		-55.2	4981	-221
		-54	9968	-212
		-56	9970	-202
		-55.2	9969	-224
		-55.3	9962	-223
		-51.9	4978	-221
		-51.5	3320	-225
		-51.3	1992	-225
Surat Basin	Desorption 2 Juandah Coal Measures	-50.9	3317	-227
		-51.7	3318	-223
		-49.2	3315	-221
		-49.4	2486	-219
		-49.9	3313	-226
		-47.7	3315	-224
		-47.8	1986	-220
		-47.5	9944	-213
		-48.5	3300	-224
		-48.1	9924	-222
		-58.5	311	-202
		-54.3	354	-203
		-53.6	1880	-209
		-53.4	496	-213
		-52.7	1984	-208
		-53.9	1984	-208
		-54	3303	-210
		-53.2	3313	-212
Surat Basin	Taroom Coal Measures	-52.2	2455	-216
		-52.1	4960	-213
		-51.7	3303	-214
		-51.7	3303	-216
		-50.9	3307	-213
		-50.3	2478	-213
		-49.3	1978	-212
		-47.4	1982	-216
		-46.8	1984	-214
		-49.2	2475	-216
		-47.3	1986	-215
Surat Basin	Taroom Coal Measures	-50.1	149	-215
		-51.1	116	-214

				-50.2	105	-215	
				-53.9	659	-214	
				-54.4	1585	-212	
		272.8		-56.6		-212.1	
	Upper seam north of fault	187.3		-56.7		-212	
		332.3		-56.6		-212.2	
		176.6		-56.3		-207.5	
	Upper seam south of fault	118.7		-62.2		-209.6	
Bowen Basin		208.1		-48		-205.4	[65]
		332.9		-56.7		-212.7	
	Lower seam north of fault	237.5		-58		-215.8	
		411.4		-54.3		-211	
		227.5		-58.9		-211	
	Lower seam south of fault	107.5		-61.7		-214.7	
		280.8		-56.6		-207	
				-62.5	1532	-275	
Erlian Basin				-60.3	3035	-270.2	[67]
				-60.1	2854	-270.8	

Table S5. Hydrogeological types and mineralization of coal seam water of Santanghu Basin (Structural units' data from [70], Well data from Research Institute of Exploration and Development, Petro China Tuha Oilfield Company). The date with * in Well ID are the results of this study.

Structural units/Well ID	Mineralization（mg/L）	Water chemical type	Hydrogeological type	Data Source
Kumusu sag	1800-3400	Na-Cl-SO_4	confined weak runoff	[70]
Hanshuiquan sag	1400-3100	Na-Cl-SO_4	confined weak runoff	[70]
Tiaohu sag	2400-5000	Na-Cl-SO_4	open local stagnation	[70]
Malang sag	1000-5000	Na-HCO_3-SO_4	open local stagnation	[70]
Naomaohu sag	1000-3000	Na-Cl-SO_4	confined weak runoff	[70]
Ma 18*	3882	HCO_3-Na		
Ma 206*	5625-5657	Na_2SO_4		
Ma 214*	3827	$NaHCO_3$		
Ma 208*	3880	$NaHCO_3$		
Ma 209*	3155	$NaHCO_3$		
Ma 203*	1160	Na_2SO_4		
Ma 205*	4778	$NaHCO_3$		
Ma 202*	2241	Na_2SO_4		
Ma 201*	2382	$NaHCO_3$		
Xi 9-13*	2398	$NaHCO_3$		
Xi 9-11*	2865	$NaHCO_3$		