

Supplementary Material

Effect of Solvent Treatment on the Composition and Structure of Santanghu Long Flame Coal and Its Rapid Pyrolysis Products

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Table S1

Alkanes detected in SLFC and SLFC-L

Species	Peak	Compound	CAS	RC (area %)	
				SLFC	SLFC-L
Normal alkanes (NAs)	15	Decane	124-18-5	2.06	1.90
	23	Undecane	1120-21-4	0.85	0.85
	34	Dodecane	112-40-3	1.25	1.09
	40	Tridecane	629-50-5	0.93	0.88
	45	Tetradecane	629-59-4	0.79	0.74
	53	Hexadecane	544-76-3	-	0.99
	54	Pentadecane	629-62-9	0.99	-
	62	Nonadecane	629-92-5	-	0.60
	63	Hexadecane	544-76-3	0.65	-
	69	Heptadecane	629-78-7	1.03	0.81
	75	Pentadecane	629-62-9	-	0.67
	76	Octadecane	593-45-3	0.77	-
	79	Eicosane	112-95-8	-	0.78
	80	Nonadecane	629-92-5	0.81	-
	84	Heneicosane	629-94-7	0.89	-
	104	Tetratetracontane	7098-22-8	6.76	5.64
Branched alkanes (BAs)	49	2,6,10-Trimethyldodecane	3891-98-3	-	0.56
	50	2,6,10-Trimethyltridecane	3891-99-4	0.53	-
	65	2,6,10-Trimethyldodecane	3891-98-3	0.32	-
	83	3-Ethyl-5-(2-ethylbutyl)octadecane	55282-12-7	-	0.81
	87	Dodecane,5,8-diethyl-	24251-86-3	0.97	-
Cyclic alkanes	93	Heptadecane,2,3-dimethyl-	61868-03-9	2.00	-
	33	Nonylcyclopropane	74663-85-7	0.79	-
	39	1-Heptyl-2-methylcyclopropane	74663-91-5	0.89	-
	106	Cyclohexane,1,1'-dodecylidenebis[4-methyl-	55334-09-3	3.02	-
	108	Cyclohexane,1,3,5-trimethyl-2-octadecyl-	55282-34-3	8.46	6.91

Table S2

Olefines detected in SLFC and SLFC-L

Peak	Compound	CAS	RC (area %)	
			SLFC	SLFC-L
10	2-Methylbicyclo[4.3.0]non-1(6)-ene	60223-07-6	0.26	-
14	1-Decene	872-05-9	0.57	-
17	p-Mentha-1,5,8-triene	21195-59-5	0.40	-
18	(3E,5E)-2,6-Dimethyl-1,3,5,7-octatetrene	460-01-5	-	0.88
22	3-Dodecene,(Z)-	7239-23-8	1.42	-
32	1-Dodecene	112-41-4	-	0.67
38	1-Tridecene	2437-56-1	-	0.85
42	Bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene	2443-46-1	0.77	-
44	1-Tetradecene	1120-36-1	0.67	0.78
52	Cetene	629-73-2	0.57	0.60
60	1-Nonadecene	18435-45-5	-	0.42
67	1-Heptadecene	6765-39-5	-	0.42
68	5-Octadecene,(E)-	7206-21-5	0.36	-
70	5-Methyl-1-undecene	74630-38-9	-	2.26
71	Tridecane,7-methylene-	19780-80-4	2.35	-
73	Heneicosene	27400-79-9	-	0.53
74	1-Heptadecene	6765-39-5	0.45	-
77	1-Docosene	1599-67-3	-	0.63
78	1-Nonadecene	18435-45-5	0.55	-
88	17-Pentatriacontene	6971-40-0	-	0.70
92	1-Hexacosene	18835-33-1	-	1.09
99	17-Pentatriacontene	6971-40-0	2.13	-
103	Squalene	111-02-4	3.22	3.07

Table S3

Arenes detected in SLFC and SLFC-L

Species	Peak	Compound	CAS	RC (area %)	
				SLFC	SLFC-L
Monocyclic aromatics (MAs)	1	1,3,5-Cycloheptatriene	108-88-3	1.96	-
	6	p-Xylene	106-42-3	1.21	-
	7	1,2-xylene	95-47-6	-	1.55
	8	Ethylbenzene	100-41-4	1.74	-
	11	1-ethyl-2-methyl-Benzene	611-14-3	0.67	-
	13	Mesitylene	108-67-8	-	0.60
	16	Benzene,(1-methylethyl)-	98-82-8	0.77	-
	20	1,2,4,5-Tetramethylbenzene	95-93-2	0.36	-
	26	Benzene,2,4-diethyl-1-methyl-	1758-85-6	-	0.28
	28	Benzene, 1-ethyl-2,4-dimethyl-	874-41-9	0.81	-
Polycyclic aromatic hydrocarbon (PAHs)	51	Benzene, octyl-	2189-60-8	-	0.63
	56	1,1,4,5,6-Pentamethyl-2,3-dihydro-1H-indene	16204-67-4	0.40	-
	30	1H-Indene, 3-methyl-	767-60-2	0.75	1.23
	41	7H-Benzocycloheptene	264-09-5	-	0.81
	43	1-Methylnaphthalene	90-12-0	0.71	0.88
	46	Naphthalene,1-(2-propen-1-yl)-	2489-86-3	-	0.42
	47	1,4-Dimethylnaphthalene	571-58-4	0.34	-
	48	1,7-Dimethylnaphthalene	575-37-1	-	0.42
	64	1,4,5-Trimethylnaphthalene	2131-41-1	0.83	1.13
	66	Naphthalene,1,6-dimethyl-4-(1-methylethyl)-	483-78-3	0.28	-
	90	Retene	483-65-8	1.25	-

Table S4

Oxygen-containing organic compounds detected in SLFC and SLFC-L

Species	Peak	Compound	CAS	RC (area %)	
				SLFC	SLFC-L
Alcohols	4	Bicyclo[2.2.1]hept-2-en-7-ol	53783-87-2	0.26	-
	5	D-erythro-L-galacto-Octopyranose, α-(8CI)	5329-49-7	0.55	-
	9	Z,Z-2,5-Pentadecadien-1-ol	139185-79-8	0.49	-
	21	1-Undecanol	112-42-5	-	0.99
	24	3-Cyclohexen-1-ol,5-methylene-6-(1-methylethenyl)-	54274-41-8	0.34	-
	31	2-Hydroxytetralin	530-91-6	-	0.35
	36	(1-Benzyl-cyclopropyl)-methanol	108546-79-8	-	0.42
	37	1-Naphthalenol,1,2,3,4-tetrahydro-3-methyl-	3344-45-4	0.45	0.81
	55	2,9-Heptadecadiene-4,6-diyn-8-ol, (Z,E)-	50816-77-8	-	0.39
	61	Hexadecanol; 1-Cetanol	36653-82-4	0.38	-
	72	3,7,11-Trimethyl-1-dodecanol	6750-34-1	0.43	0.39
	91	Lycopene,1,2-dihydro-1-hydroxy	105-92-0	-	0.46
	107	1-Hentetracontanol	40710-42-7	-	2.61
	109	Octacosanol	557-61-9	-	26.60
	110	1-Hexacosanol	506-52-5	22.81	-
Carboxylic acids (CAs)	27	Methyl 4,6-tetradecadiynoate	NA	0.24	-
	57	2-Oxiraneoctanoic acid,3-octyl-, (2R,3S)-rel-	24560-98-3	-	0.28
	58	2,5-Octadecadiynoic acid,methyl ester	57156-91-9	-	0.39
	59	Naproxen	22204-53-1	0.42	-
	81	Ethyliso-allocholate	47676-48-2	0.47	-
	82	Kaur-16-ene-3,7,15,18-tetrol,7,18-diacetate, (3a,4b,7b,15a)- (9CI)	70902-37-3	-	0.46
	85	Ethyliso-allocholate	47676-48-2	-	1.27
	86	Lauric acid (1aR)-1α,2,5,5a,6,9,10,10α-octahydro-5aβ-hydroxy-4-hydroxymethyl-1,1,7,9α-tetramet	77508-68-0	-	0.85
	95	Oleic acid,eicosyl este	22393-88-0	-	1.48
	96	7,8-Epoxy lanostan-11-ol,3-acetoxy-Lauric acid (1aR)-1α,2,5,5a,6,9,10,10α-octahydro-5aβ-hydroxy-4-hydroxymethyl-1,1,7,9α-tetramet	NA	-	0.92
	97	9,19-Cyclolanostan-3-ol,24,24-epoxymethano-, acetate	77508-68-0	1.03	-
	98	5H-Cyclopropa(3,4)benz(1,2-e)azulen-5-one,1,1a-1b-4,4a,7a-7b,8,9,9a-decahydro-7b-9-9a-trihydroxy-3-hydroxymethyl-1,1,6,8-tetramethyl-4a-methoxy-,9,9a-	NA	-	1.94
	100		54870-24-5	-	2.47

		didecanoate			
	101	Oleic acid,eicosyl ester	22393-88-0	1.17	-
	105	Oleic acid,3-(octadecyloxy)propyl ester	17367-41-8	1.72	-
Ethers	29	Naphthalene,1,2,3,4-tetrahydro-1-methoxy-	1008-18-0	-	0.78
	89	5a-Cholestan-3-one, cyclic-1,2-ethanediylaetal	25328-53-4	0.81	-
	94	Tetradecane,1-(tetradecyloxy)-	5412-98-6	-	1.09
	102	1,1'-[Ethylenebis(oxy)]bis[(Z)-9-octadecene]	17367-13-4	6.48	-
Aldehydes	25	3-O-Benzyl-d-glucose	10230-17-8	0.59	-
	35	5,8-Decadien-2-one,5,9-dimethyl-,(E)-	130876 -99-2	0.43	-

Table S5

Other heteroatom-containing organic compounds detected in SLFC and SLFC-L

Peak	Compound	CAS	RC (area %)	
			SLFC	SLFC-L
2	1,1,2-trichloroethane	79-00-5	-	3.42
3	Tetrachloroethylene	127-18-4	-	5.92
12	P-methylampeamine	1964/11/9	0.40	-
19	Hexachloroethane	67-72-1	-	1.66