Part. 1 Composition of the coal tar feedstock

Table s1 The definition of the 9 components

Item.		Detail composition
Non-polar components (with no polar group)	PAH-1	Aromatic hydrocarbons with 2 aromatic rings, *e.g. biphenyl, naphthalene, acenaphthene, acenaphthylene, fluorine*; partly hydrogenated aromatic hydrocarbons (ring number from 2 to 3) *and their ramification(total C number of the Alkyl substituents is less than 6)*
	PAH-2	3-ring aromatic hydrocarbons, *e.g. phenanthrene, anthracene and their ramification*
	PAH-3	4-ring aromatic hydrocarbons, *e.g. pyrene, benz[a]anthracene, chrysene, fluoranthene*
	PAH-4	5-ring aromatic hydrocarbons, *e.g. benzo[b]fluorathene, benzo[a]pyrene*
	H-1	Saturated hydrocarbons and alkene (C number from 18 to 32); cycloalkanes (one or two C6 rings, C number from 14 to 21, no aromatic and polar group)
	H-2	Aromatic hydrocarbons with long chain alkyl substituents (total C number of the Alkyl substituents is more than 8), *e.g. 7-butyl-1-hexylnaphthalene*
polar components	P-1	Heterocyclic components, *e.g. 9-fluorenone, carbazole, dibenzothiophene, 7,8-Benzoquinoline*
	P-2	Polar group containing components (expect phenols), *e.g. 1-Hexadecanol, 9-Fluorenol*
	P-3	Phenols

Table s2 Compounds in the coal tar feedstock (analyzed by GC-MS directly)

Item.	NO.	name	Peak area	CAS number	mass percentage %
PAH-1	1	Naphthalene	459.0284	91-20-3	0.0106
	2	Naphthalene,1,8-dimethyl-	961.3615	569-41-5	0.0222
	3	Naphthalene,1,2-dimethyl-	541.3071	573-98-8	0.0125
	4	Naphthalene,1,3-dimethyl-	489.3416	575-41-7	0.0113
	5	Naphthalene,1,7-dimethyl-	1377.085	575-37-1	0.0318
	6	Acenaphthene	8292.825	83-32-9	0.1915
	7	Naphthalene,1,2,3,4-tetrahydro-5,6,7,8-tetramethyl-	6084.292	19063-11-7	0.1405
	8	acenaphthylene	9817.146	208-96-8	0.2267
	9	Naphthalene, 1,2-dihydro-1,1,6-trimethyl-	1017.657	30364-38-6	0.0235
	10	Naphthalene,1,2,3,4-tetramethyl-	12917.75	3031-15-0	0.2983
	11	Naphthalene,1-methyl-7-(1-methylethyl)-	1130.249	490-65-3	0.0261
	12	2,6-Diisopropylnaphthalene	25116.65	24157-81-1	0.58
	13	1,4,5,8-Tetramethylnaphthalene	9353.787	2717-39-7	0.216
	14	Biphenyl	8847.124	92-52-4	0.2043
	15	1,1'-Biphenyl, 4-methyl-	4412.736	644-08-6	0.1019
	16	1,1’-Biphenyl,2-methyl-	4447.379	643-58-3	0.1027
	17	Diphenylethyne	4906.408	501-65-5	0.1133
	18	Fluorene	2780.153	86-73-7	0.0642
	19	9H-Fluorene,9,9-dimethyl-	978.6833	4569-45-3	0.0226
PAH-2	1	Phenanthrene	99280.06	85-01-8	2.2926
	2	Anthracene	76666.41	120-12-7	1.7704
	3	Naphthalene,1-phenyl-	60656.71	605-02-7	1.4007
	4	Phenanthrene,1-methyl-	52524.11	832-69-9	1.2129
	5	Phenanthrene,2-methyl-	71565.13	2531-84-2	1.6526
	6	Phenanthrene,3-methyl-	74994.85	832-71-3	1.7318
	7	Phenanthrene,4-methyl-	62051.12	832-64-4	1.4329

	8	Phenanthrene,9-methyl-	61678.7	883-20-5	1.4243
	9	Anthracene,1-methyl-	54494.47	610-48-0	1.2584
	10	Anthracene,2-methyl-	10839.13	613-12-7	0.2503
	11	Anthracene,2-ethyl-	4087.951	52251-71-5	0.0944
	12	Phenanthrene,3,6-dimethyl-	52268.62	1576-67-6	1.207
	13	Phenanthrene,2,7-dimethyl-	62042.46	1576-69-8	1.4327
	14	Phenanthrene,1,4-dimethyl-	25237.9	22349-59-3	0.5828
	15	Anthracene, 1,2-dimethyl-	54762.96	53666-94-7	1.2646
	16	Anthracene,1,4-dimethyl-	17477.72	781-92-0	0.4036
	17	Phenanthrene,2,3,5-trimethyl-	78099.79	3674-73-5	1.8035
	18	Phenanthrene,1-methyl-7-(1-methylethyl)-	99219.43	483-65-8	2.2912
	19	Naphthalene,2-phenyl-	60115.4	612-94-2	1.3882
	20	Phenanthrene,1-methyl-7-(1-methylethyl)-	178090	483-65-8	4.1125
	21	8-Isopropyl-1,3-dimethylphenanthrene	7301.151	-	0.1686
	22	9,10-Dimethylanthracene	28412.13	781-43-1	0.6561
	23	Naphthalene,2-(phenylmethyl)-	3667.897	613-59-2	0.0847
	24	8-Isopropyl-1,3-dimethylphenanthrene	52047.76	-	1.2019
	25	Phenanthrene,2,3,5-trimethyl-	68399.57	3674-73-5	1.5795
	26	9-Ethyl-10-methylanthracene	69140.08	19713-49-6	1.5966
	27	Phenanthrene,2,3,5-trimethyl-	66342.6	3674-73-5	1.532
	28	11H-Bzenzo[b]fluorene	74037.82	238-84-6	1.7097
	29	Phenanthrene,2,3,5-trimethyl-	67814.96	3674-73-5	1.566
	30	Phenanthrene,1-methyl-7-(1-methylethyl)-	114237.5	483-65-8	2.638
	31	8-Isopropyl-1,3-dimethylphenanthrene	23323.84	-	0.5386
	32	9-Ethyl-10-methylanthracene	14736.55	19713-49-6	0.3403
	33	Phenanthrene,2,3,5-trimethyl-	69707.37	3674-73-5	1.6097
	34	p-Terphenyl	5542.985	92-94-4	0.128
	35	Phenanthrene,1-methyl-7-(1-methylethyl)-	192843.9	483-65-8	4.4532
PAH-3	1	benz[a]anthracene	40485.44	56-55-3	0.9349
	2	Fluoranthene	44746.61	206-44-0	1.0333

	3	Pyrene	21981.4	129-00-0	0.5076
	4	Pyrene,1-methyl-	43187.65	2381-21-7	0.9973
	5	Pyrene,1,3-dimethyl-	40364.19	64401-21-4	0.9321
	6	Pyrene,1,2-dimethyl-	41715.29	74869-48-0	0.9633
	7	Pyrene,1,6-dimethyl-	35436.13	27984-16-3	0.8183
	8	Triphenylene	69707.37	217-59-4	1.6097
	9	Chrysene	73271.33	218-01-9	1.692
	10	Chrysene,6-methyl-	952.7005	1705-85-7	0.022
PAH-4	1	Benzo[k]fluoranthene	57499.81	207-08-9	1.3278
	2	Perylene	37233.27	198-55-0	0.8598
	3	Benz[e]acephenanthrylene	29628.99	205-99-2	0.6842
	4	benzo[a]pyrene	71071.46	50-32-8	1.6412
H-1	1	nC17	11475.71		0.265
	2	nC18	7816.475		0.1805
	3	nC19	21552.68		0.4977
	4	nC20	4754.842		0.1098
	5	nC21	4495.014		0.1038
	6	nC22	5322.132		0.1229
	7	nC23	4482.023		0.1035
	8	nC24	6863.774		0.1585
	9	nC25	6699.217		0.1547
	10	nC26	9106.951		0.2103
	11	nC27	20894.46		0.4825
	12	nC28	38047.4		0.8786
	13	nC29	38532.41		0.8898
	14	nC30	37380.5		0.8632
	15	C32 isomer	28074.35		0.6483
	16	nC31	10665.92		0.2463
	17	nC32	2801.806		0.0647
	18	4-Tetradecene, (Z)-	1004.666	41446-65-5	0.0232

	19	Cyclohexane,2-butyl-1,1,3-trimethyl-	3226.191	54676-39-0	0.0745
	20	10-Heneicosene(c, t)	2983.685	95008-11-0	0.0689
	21	1-Docosene	5309.14	1599-67-3	0.1226
	22	1,7-Dimethyl-4-(1-methylethyl)cyclodecane	17620.63	645-10-3	0.4069
	23	1-Hexacosene	8634.931	18835-33-1	0.1994
	24	Phenanthrene, 9-dodecyltetradecahydro	5161.905	55334-01-5	0.1192
	25	1Hbenz[de]anthracene, hexadecahydro-6-octyl-	9453.388	7225-65-2	0.2183
	26	Squalene	14078.32	7683-64-9	0.3251
	27	Urs-12-ene	3546.644	464-97-1	0.0819
H-2	1	Benzene, decyl-	5659.907	104-72-3	0.1307
	2	Benzene, 1-heptyl-4-propyl	11913.09	-	0.2751
	3	(E)-1-(6,10-Dimethylundeca-5,9-dien-2-yl)-4-methylbenzene	10012.02	55968-43-9	0.2312
	4	Benzene, 1,3,5-tributyl-	22358.15	841-07-6	0.5163
	5	Naphthalene, 1,4-dimethyl-5-octyl-	37488.77	55000-53-8	0.8657
	6	Naphthalene,7-butyl-1-hexyl-	22830.17	55000-55-0	0.5272
	7	Naphthalene, 2,6-dimethyl-3-octyl-	24471.41	55000-54-9	0.5651
P-1	1	Dibenzofuran	13961.39	132-64-9	0.3224
	2	Pyridine,3-phenyl-	14528.68	1008-88-4	0.3355
	3	9H-Xanthene	14035.01	92-83-1	0.3241
	4	6H-Dibenzo[b,d]-pyran	3477.357	229-95-8	0.0803
	5	1,4,7-Trimethyl-2-azafluorene	27190.94	-	0.6279
	6	Naphtha[2,1-b]furan,1,2-dimethyl-	19162.27	-	0.4425
	7	Naphtha[2,1-b]furan,2,2-dimethyl-	26251.23	-	0.6062
	8	Benzo[b]naphtha[2,3-d]furan	11163.92	-	0.2578
	9	Benzo[kl]xanthenes	19387.46	-	0.4477
	10	9H-Xanthene	14043.67	92-83-1	0.3243
	11	3-(N,N-Dimethylamino)-9-methylcarbazole	16403.77	-	0.3788
	12	Naphtha[2,1-b]furan,1,2-dimethyl-	24436.77	-	0.5643
	13	Harmaline	4321.796	304-21-2	0.0998
	14	Benzeneethanol,.alpha.-[2-(dimethylamino)-1-methylethyl]-.alpha.-phenyl-,propanonate	19383.13	-	0.4476

	15	1-Isobenzofuranol,1,3-dihydro-3,3-dimethyl-1-phenyl-	14844.81	-	0.3428
	16	Benzo[d,E]isocoumarin,3,3-dimethyl-	5135.922	-	0.1186
	17	Naphtha[2,1-b:7,8-b']difuran,1,2,9,10-tetrahydro-2,9-dimethyl-	4165.9	-	0.0962
	18	1-Ethyl-3-formylindole	983.0137	-	0.0227
	19	1H,3H-Naphtho[1,8-cd]pyran,3a,4,5,6-tetrahydro-	783.8127	-	0.0181
	20	Lenacil	5183.557	2164-08-1	0.1197
	21	10-Acetyl-9,10-dihydroacridine	1468.025	-	0.0339
	22	2,5-Dimthylbenzoxazole	3356.104	5676-58-4	0.0775
	23	Quinoline	11047	91-22-5	0.2551
	24	Quinoline,2-methyl-	14468.06	91-63-4	0.3341
	25	Quinoline,8-methyl-	18274.53	611-32-5	0.422
	26	Pyridine,3-phenyl-	3269.495	1008-88-4	0.0755
	27	dl-5-Methyltryptophan	783.8127	-	0.0181
	28	Quinoline,2,3,4-trimethyl-	11488.7	2437-72-1	0.2653
	29	Isoquinoline,2-(2,2-dimethyl-1-oxopropyl)-1,2,3,4-tetrahydro-6,7-dimethoxy-	33071.7	-	0.7637
	30	Isoquinoline,3-methyl-	454.698	1125-80-0	0.0105
	31	Indoline,3-ethyl-2,3-dimethyl-	2736.849	-	0.0632
	32	7-(6-Methylpyridin-2-yl)hept-6-enal	22895.13	-	0.5287
	33	Quinoline,2,4,6-trimethyl-	528.3158	2243-89-2	0.0122
	34	Quinoline,2,3,4-trimethyl-	10280.5	2437-72-1	0.2374
	35	2,5-Dimethyl-4-phenylpyridine	480.6807	-	0.0111
	36	1,7-Phenanthroline	809.7955	230-46-6	0.0187
	37	Isoquinoline,1,2,3,4-tetrahydro-2,3-dimethyl-	4854.442	-	0.1121
	38	Quinoline, 2,3-dimethyl-	1662.896	1721-89-7	0.0384
	39	Quinoline,2,3,4-trimethyl-	5023.33	2243-89-2	0.116
	40	2-Methyl-3-phenylpyridine	26913.79	-	0.6215
	41	9H-Pyrido[3,4-b]indole,1-methyl-	5525.663	486-84-0	0.1276
	1	2-Buten-1-one,1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	4451.71	35044-68-9	0.1028
P-2	2	Methyl dehydroabietate	4113.934	1235-74-1	0.095
	3	[1,1'-Biphenyl]-4-methanol	6742.522	-	0.1557

4	1,1'-Biphenyl, 2-methoxy-	24813.52	86-26-0	0.573
5	1,1-Dimethyl-2-(diphenylmethylene)hydrazone	9782.502	-	0.2259
6	9H-Fluoren-9-ol	39177.64	1689-64-1	0.9047
7	5H-Dibenzo[a,d]cyclohepten-5-ol,10,11-dihydro	1970.358	1210-34-0	0.0455
8	10H-Dibenzo[b,E]thiopyran-10-one,2-ethyl-	3308.469	-	0.0764
9	9H-Fluorene-2,7-diamine	45521.76	-	1.0512
10	Benzylamine,4-(1-methylethyl)-N,.alpha.-diphenyl-	22081	-	0.5099
11	2-Hydroxymethyl-10-methylanthracene	5815.804	-	0.1343
12	1-Acetyl-4,6,8-trimethylazulene	14675.92	-	0.3389
13	2-Methyl-3,4-diphenyl-2-cyclopenten-1-one	3351.774	-	0.0774
14	6-hydroxy-7-methyl-9-oxopodocarpane	4945.382	-	0.1142
15	9,10-Anthracenedione	25597.33	84-65-1	0.5911
16	Pregnenolone-7,9(11)-dien	974.3528	-	0.0225
17	Cyclopentene-1-carboxylic acid,4-[2-(diphenylmethyl)-2-propen-1-yl]-,methyl ester	4378.092	-	0.1011
18	1-(10-Methylanthracene-9-yl)ethanone	2334.116	-	0.0539
19	9,10-Anthracenedione,2-(1,1-dimethylethyl)-	3425.392	84-47-9	0.0791
20	Bicyclo[3.1.0]hex-3-en-2-one,6,6-diphenyl-	11198.56	-	0.2586
21	2-Ethyl-3-methylene-indan-1-one	7833.797	-	0.1809
22	2-Acetoxy-3-methoxybiphenylene	12164.25	-	0.2809
23	Naphthalene,6-methoxy-2-(1-buten-3-yl)-	1489.677	-	0.0344
24	1-(10-Methylanthracen-9-yl)ethanone	2472.691	-	0.0571
25	11H-Cyclopenta[a]phenanthren-17-ol,12,13,16,17-tetrahydro-3-methoxy-13-methyl	3425.392	-	0.0791
26	Estra-1,3,5,7,9-pentaen-17-one,3-(acetyloxy)-	11198.56	-	0.2586
27	9,10-Anthracenedione,1,8-dimethoxy-	7833.797	-	0.1809
28	1-Phenanthrenecarboxaldehyde, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1α,4aβ,10aα)]-	12164.25	13601-88-2	0.2809
29	1,2,3,4-Tetrahydro-1,4-ethanoanthracene,9,10-dimethoxy-	1489.677	-	0.0344
30	7-Methylindan-1-one	31768.23	-	0.7336
31	9,10-Anthracenedione,1,8-dimethoxy-	3425.392	-	0.0791
32	1-Phenylcyclopenthlamine	11198.56	-	0.2586
33	Quinoline,2,4-dimethyl-	7833.797	1198-37-4	0.1809

	34	Dimethylphthalate	12164.25	131-11-3	0.2809
	35	1-Naphthalenamine,N,N-dimethyl-	20322.83	86-56-6	0.4693
	1	2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, (4bS-trans)-	4360.77	511-15-9	0.1007
	2	2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, (4bS-trans)-	4789.485	511-15-9	0.1106
	3	1-Naphthalenol	4802.477	90-15-3	0.1109
	4	1-Naphthalenol,2-methyl-	14303.5	-	0.3303
	5	1-Naphthalenol,4-methyl-	13437.41	-	0.3103
	6	1-Naphthalenol,2-methyl-	16473.06	-	0.3804
	7	1-Naphthol,6,7-dimethyl-	16053	-	0.3707
	8	1-Naphthol,2,4-dimethyl-	25142.63	-	0.5806
P-3	9	1-Naphthol,1,6-dimethyl-	30317.53	-	0.7001
	10	p-butyl phenol	19088.65	1638-22-8	0.4408
	11	7-Hydroxycadalene	19526.03	2102-75-2	0.4509
	12	Octyl phenol	9102.621	-	0.2102
	13	o-butyl phenol	4767.833	3180-09-4	0.1101
	14	1-anthrol	6517.338	-	0.1505
	15	1-Hydroxypyrene	14758.2	5315-79-7	0.3408
	16	5-Amino-1-naphthol	3914.733	83-55-6	0.1604
	17	Phenol,2,5-bis(1,1-dimethylethyl)-	3078.955	5875-45-6	0.1418

Part. 2 Complementary information for Analysis process

1. HPLC

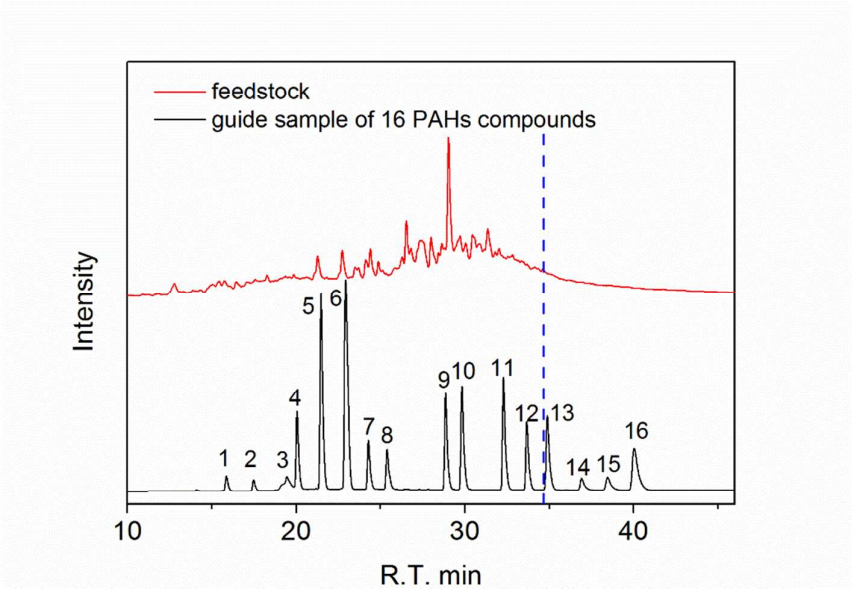

Fig. s1. The HPLC graph for coal tar feed stock (distillate >300°C) and the 16 PAHs guide sample(λ= 270nm)

The HPLC graph for the coal tar feedstock (>300°C) and the 16 PAHs guide sample are shown in **Fig. s1**. The chromatographic column of the HPLC system was Eclipse PAH (Agilent) and mobile phase was acetonitrile/H_2O. The details of analysis conditions and compounds in the guild sample are listed in supporting information (**Table s3, s4**).

Since HPLC system uses an UV-detector, compounds with little UV absorption, e.g. saturated hydrocarbons, would not give responding signal on the graph. While for most of the PAHs components, significant responses (may not be the maximum value, but with relatively strong intensity) can be found under λ= 270nm. The peak of PAHs compound with larger molecular weights appears latter during the analysis process, and no peaks of compounds in coal tar feedstock can be detected when the retention time is more than 34.45min. It indicates that there is few aromatic compound with more than 5 aromatic rings existing in the coal tar feedstock.

Table s3 Chromatographic conditions for HPLC spectrum of 16 PAHs standard sample

Column	Eclipse PAH (Agilent) 4.6×250mm 5μm
Sample concentration	0.2g coal tar sample dissolved in 5ml THF; 0.0004g/ml for each PAHs compounds in the guild sample (use methanol as solvent)
Mobile phase	acetonitrile/H_2O
Flow rate	1ml/min
Column temperature	40°C
Gradient elution	from 15min to 60min, the volume percent of acetonitrile in mobile phase changes from 40% to 100%

Table s4 Compounds in the 16 PAHs standard sample

NO.*	R. time (min)	Name	λ_{max} (nm)	Boiling points (^oC)
1	15.695	naphthalene	219	217
2	17.304	acenaphthene	225	279
3	19.299	acenaphthylene	228	280
4	19.866	fluorene	210	298
5	21.302	phenanthrene	251	336
6	22.781	anthracene	251	340
7	24.136	fluoranthene	232	384
8	25.244	pyrene	238	393
9	28.775	benz[a]anthracene	287	437
10	29.779	chrysene	267	448
11	32.251	benzo[b]fluorathene	258	481
12	33.674	benzo[k]fluorathene	240	480
13	34.918	benzo[a]pyrene	295	495
14	37.046	dibenz[a,h]anthracene	296	524
15	38.650	benzo[g,h,i]perylene	210	550
16	40.325	Indeno[1,2,3-cd]pyrene	251	Not found

*corresponding to the numbers in **Fig s1**.

2. Simulated distillation

The simulated distillation of the raw coal tar (low temperature coal tar) was conducted by ASTM D7169-11, and the results are shown in **Fig. s2**. It shows that about 95% of the raw coal tar are with boiling points less than 491^oC.

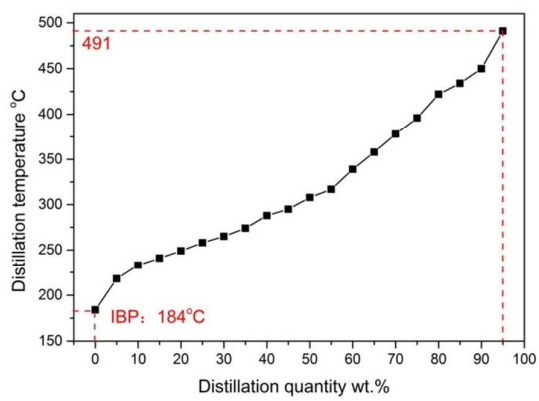

Fig. s2 simulated distillation of the low temperature coal tar

3. The total content of phenols

The total content of phenols in the coal tar distillate with boiling points less than 300^oC and the raw coal tar (all distillation fraction) were analyzed by the method presented in YB/T 5080-93, and the results can be found in **Table s5**. The main principle of the method is an acid-base reaction between phenolic compounds and sodium hydroxide solution. In practice, oil sample was diluted by toluene, removed water by adding anhydrous sodium sulfate, and then put into an instrument named "dual-ball measuring pipe" with sodium hydroxide solution(10% $NaOH/H_2O$). After 1 hour's standing, the volume increase of the aqueous phase (A) was recorded, and the mass percentage of phenols in oil sample is calculated by the following equation:

$$X = \frac{1.035 \times A}{G} \times 100\%$$

Where G means the mass of raw sample, constant 1.035 was the approximate average density of phenols in the coal tar sample. What's more, the phenolic compounds in coal tar distillate less than 300^oC and the low temperature coal tar (all distillation fraction) were also enriched by alkali extraction and analyzed by GCMS, and the results are also listed in **Table s5**.

Since the coal tar distillate >300°C is ca. 50 w.t. % in the low temperature coal tar, it can be found that almost all phenolic compounds were distilled from the low temperature coal tar before the temperature reached 300°C. From **Table s5**, a consistency can be found between the two methods. However, because the GC-MS analysis would suffer quantitative troublesome due to the varying response signals on different materials, the consistency might be with few uncertainties.

Table s5. the determination of phenolic compounds

Analysis using GB/T 24207-2009		Mass percentage %	
		The low temperature coal tar (all distillation fraction)	coal tar distillate less than 300°C
	Total phenols content	26.04	51.98
GCMS analysis		mass percentage %	
		The low temperature coal tar (all distillation fraction)	coal tar distillate less than 300°C
	phenol	0.50	1.02
	Methylphenol	15.96	32.00
	Phenol, ethyl- and methyl-	7.96	16.12
	Phenol, alkylene-	0.08	0.13
	Naphthalenol	1.14	0.60
	total phenols content)	25.64	49.87

4. GC-MS

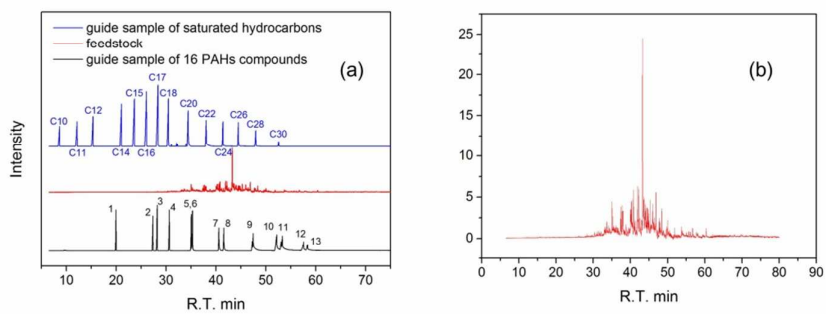

Fig. s3 GC-MS analysis of the feedstock
(a) comparison between total ion chromatogram of feedstock, guide sample of PAHs compounds (numbers for PAHs are corresponding to **Table. s2**) and saturated hydrocarbons
(b) the total ion chromatogram of feedstock

Fig. s3 presents the performance of GC-MS analysis for the feedstock, guide sample of PAHs compounds and saturated hydrocarbons. The concentration of sample were as following: 0.5g coal tar sample dissolved in 5ml THF; 0.0004g/ml for each PAHs or saturated hydrocarbons compounds in the guild sample (use methanol as solvent). Compounds in the guide sample of saturated hydrocarbons (from C10-C30) can be fully detected by the GCMS, while for the guide sample of 16 PAHs compounds, only 13 compounds can be found, and the last compound appeared in the graph is benzo[a]pyrene (T_b=495°C). It reveals that the GCMS process adopted in this study can hardly detected aromatic compounds with more than 5 rings (or compounds with T_b larger than a certain value which is between 495 °C and 524 °C). However, **Fig. 3b** shows that only slight peaks can be found when the retention time is larger than 57 min and those peaks were identified as non-aromatic hydrocarbons or some compounds with both polar group and a long chain structure by the mass spectral library. It indicates that the GCMS process adopted in this study can identify most of compounds existing in the coal tar feedstock. This result is conformed with the conclusion made in the analysis process of HPLC and simulated distillation.

5. SGCC-GC-MS

To evaluate the influence of "heavy compounds" in the composition analysis and enhance the selectivity in analysis process, we conducted a silica gel column chromatography process(SGCC). Compounds in coal tar which can't be detected by the GC-MS are supposed to be with high boiling point and/or strong polarity, and they also tend to stay in the retentate on the silica gel column. Thus, the amount of irreversible adsorption can be a proper index to estimate the influence of "heavy compounds" in composition analysis by the GCMS method.

The SGCC experiment was carried out on a column(1.5cm×70cm) filled by silica-gel with partical size from 37 to 344 um. Organic compounds sequentially flowing out through the SGCC were monitored by a UV-absorbance detector at 254 nm. The SGCC process divide the coal tar feedstock into 17 fractions by the solvents elution process and the UV-absorbance detector, and the results are listed in **Table s6 and s7.**

The SGCC-GC-MS analysis identified around 240 kinds of compounds in the coal tar feedstock, which is much more than that identified by the GC-MS (around 140 kinds). However, the content of the 9 kinds of major components were similar between the two method, as shown in Fig. s4.

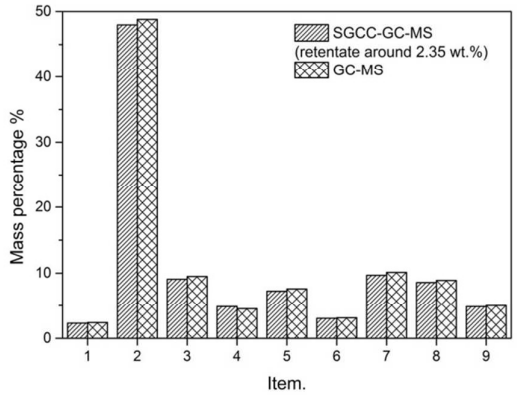

Fig. s4. Comparison between GC-MS method and SGCC-GC-MS method on the analysis of the coal tar feedstock

1. PAH-1; 2. PAH-2; 3. PAH-3; 4. PAH-4; 5. H-1; 6. H-2; 7. P-1; 8. P-2; 9. P-3

The extraction products were also analysised by the SGCC process, and the results show that the mass percentage of retentates for all extraction products was less than 1%. It reveals that compounds in retentate of SGCC process also tend to stay at the extraction residual. It is also indicated that the high boiling compounds has little influence on the analysis of extraction products.

Since SGCC-GC-MS obtained similar results with that of the GC-MS method mentioned above, the study still use the GC-MS directly to analyze composition of extraction products. However, for the analysis of residual for certain SFE process, the influence of "heavy compounds" can't be ignored.

5. conclusion

In consequence, there are little aromatic hydrocarbons with more than 5 aromatic rings in the coal tar feedstock, and about 97% of the low temperature coal tar are with boiling points less than 501°C. During the distillation process, most of phenols in the coal tar feedstock are stayed in the distillate less than 300°C. The GCMS process adopted in this study can identify most of compounds existing in the coal tar feedstock and be suitable for the analysis of extraction product . While for the analysis of residual for certain SFE process, the influence of "heavy compounds" can't be ignored.

Table s6 the composition of coal tar feedstock (obtained by SGCC-GC-MS)

Solvent	Elution fraction	Mass percentage %									
		PAH-1	PAH-2	PAH-3	PAH-4	H-1	H-2	P-1	P-2	P-3	Sum %
n-pentane	F-1	-	-	-	-	5.7985	-	-	-	-	5.7985
	F-2	-	-	-	-	1.5901	0.3954	0.0019	0.1157	-	2.1031
n-pentane: n-hexane (1:1)	F-3	1.7091	-	-	-	-	2.636	-	0.09	-	4.4351
	F-4	0.4974	-	-	-	-	-	1.6112	0.9898	0.0048	3.1032
	F-5	0.0624	20.2028	0.8415	-	-	-	1.674	-	-	22.7807
	F-6	0.0011	4.8725	0.9301	-	-	-	0.6702	0.9	-	7.3739
	F-7	0.0371	15.2615	-	-	-	-	0.5379	0.0724	-	15.9089
n-hexane	F-8	0.001	6.6229	6.8099	4.8558	-	-	0.0013	1.6068	0.0064	19.9041
	F-9	-	-	-	-	-	-	0.8486	1.5507	-	2.3993
n-hexane: CH_2Cl_2 (1:1)	F-10	-	-	-	-	-	-	0.2069	0.6068	-	0.8137
	F-11	-	-	-	-	-	-	0.0291	0.4162	0.0969	0.5422
	F-12	-	-	-	-	-	-	0.1712	0.2987	0.1065	0.5764
	F-13	-	-	-	-	-	-	-	-	4.3184	4.3184
ethyl acetate	F-14	-	-	-	-	-	-	1.3933	0.7698	0.144	2.3071
acetonitrile	F-15	-	-	-	-	-	-	1.5685	0.7149	0.087	2.3704
methanol	F-16	-	-	-	-	-	-	0.9693	0.4484	0.0684	1.4861
sum		2.3081	46.9597	8.5815	4.8558	7.3886	3.0314	9.6834	8.5802	4.8324	96.2211
retentate		3.7789									

Table s7 the compounds in coal tar feedstock (analyzed by SGCC-GC-MS)

Item	NO.	name	CAS number	mass percentage %
	1	Naphthalene	91-20-3	0.0096
	2	Naphthalene,1-methyl-	90-12-0	0.002
	3	Naphthalene,1-ethyl-	1127-76-0	0.0039
	4	Naphthalene,1,8-dimethyl-	569-41-5	0.0193
	5	Naphthalene,1,2-dimethyl-	573-98-8	0.0118
	6	Naphthalene,1,3-dimethyl-	575-41-7	0.0107
	7	Naphthalene,1,7-dimethyl-	575-37-1	0.0301
	8	Naphthalene,1,5-dimethyl-	571-61-9	0.0022
	9	Naphthalene,1,2,3,4-tetrahydro-1,1,6-trimethyl-	475-03-6	0.0008
	10	Acenaphthene	83-32-9	0.1814
	11	Naphthalene,1,2,3,4-tetrahydro-5,6,7,8-tetramethyl-	19063-11-7	0.1331
	12	acenaphthylene	208-96-8	0.2147
	13	Naphthalene, 1,2-dihydro-1,1,6-trimethyl-	30364-38-6	0.0223
PAH-1	14	Naphthalene,1,2,3,4-tetramethyl-	3031-15-0	0.2825
	15	Naphthalene,1-methyl-7-(1-methylethyl)-	490-65-3	0.0247
	16	Cadina-1(10),6,8-triene	1460-96-4	0.0007
	17	2,6-Diisopropylnaphthalene	24157-81-1	0.5493
	18	1,1'-Biphenyl, 4-methyl-	644-08-6	0.0009
	19	Cadina-1(10),6,8-triene	1460-96-4	0.001
	20	1,4,5,8-Tetramethylnaphthalene	2717-39-7	0.2046
	21	Naphthalene,1,6-dimethyl-4-(1-methylethyl)-	483-78-3	0.0002
	22	Benzene,1,2-dimethyl-4-(phenyl methyl)-	13540-56-2	0.0003
	23	Naphthalene,1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-	483-77-2	0.0007
	24	1-Methyl-10,18-bisnorabieta-8,11,13-triene	-	0.0011
	25	2,4-Diphenyl-4-methyl-1-pentene	-	0.0001
	26	4,4’-Diacethldiphenylmethane	-	0.0011
	27	Biphenyl	92-52-4	0.1935

	28	1,1'-Biphenyl, 4-methyl-	644-08-6	0.0965
	29	1,1’-Biphenyl,2-methyl-	643-58-3	0.0973
	30	2,2'-Dimethylbiphenyl	605-39-0	0.0005
	31	Benzene,1,1’-methylenbis[4-methyl-	4957-14-6	0.0007
	32	Diphenylethyne	501-65-5	0.1073
	33	Benzene,1-methyl-3-[(4-methylphenyl)methyl]-	21895-16-9	0.0003
	34	Propyne,1,3-diphenyl-	-	0.0007
	35	Benzene,1,1’-(1,3-butadiyne-1,4-diyl)bis-	886-66-8	0.0006
	36	Fluorene	86-73-7	0.0608
	37	9H-Fluorene,2-methyl-	1430-97-3	0.0002
	38	9H-Fluorene,3-methyl-	2523-39-9	0.0005
	39	9H-Fluorene,1-methyl-	1730-37-6	0.0009
	40	9H-Fluorene, 2-methyl-	1430-97-3	0.0009
	41	9H-Fluorene,1-methyl-	1730-37-6	0.0002
	42	9H-Fluorene,2,3-dimethyl-	4612-63-9	0.0021
	43	Anthracene,9,10-dihydro-2-methyl	-	0.0008
	44	9H-Fluorene,2,3-dimethyl-	4612-63-9	0.0098
	45	9H-Fluorene,9,9-dimethyl-	4569-45-3	0.0214
	46	Anthracene,9,10-dihydro-9,10-dimethyl-	-	0.003
	47	9-Methyl-S-octahydroanthracene	-	0.0007
	48	Anthracene,9,10-dihydro-9,10-dimethyl-	-	0.0003
	1	Phenanthrene	85-01-8	1.9704
	2	Anthracene	120-12-7	1.5216
	3	Naphthalene,1-phenyl-	605-02-7	1.2038
	4	Phenanthrene,1-methyl-	832-69-9	1.0424
PAH-2	5	Phenanthrene,2-methyl-	2531-84-2	1.4203
	6	Phenanthrene,3-methyl-	832-71-3	1.4884
	7	Phenanthrene,4-methyl-	832-64-4	1.2315
	8	Phenanthrene,9-methyl-	883-20-5	1.2241
	9	Anthracene,1-methyl-	610-48-0	1.0815

	10	Anthracene,2-methyl-	613-12-7	0.2151
	11	Anthracene,2-ethyl-	52251-71-5	0.0811
	12	Phenanthrene,3,6-dimethyl-	1576-67-6	1.0374
	13	Phenanthrene,2,7-dimethyl-	1576-69-8	1.2313
	14	Phenanthrene,1,4-dimethyl-	22349-59-3	0.5009
	15	Anthracene, 1,2-dimethyl-	53666-94-7	1.0869
	16	Anthracene,1,4-dimethyl-	781-92-0	0.3469
	17	Phenanthrene,2,3,5-trimethyl-	3674-73-5	1.55
	18	Phenanthrene,1-methyl-7-(1-methylethyl)-	483-65-8	1.9692
	19	Naphthalene,2-phenyl-	612-94-2	1.1931
	20	Phenanthrene,1-methyl-7-(1-methylethyl)-	483-65-8	3.5345
	21	8-Isopropyl-1,3-dimethylphenanthrene	-	0.1449
	22	9,10-Dimethylanthracene	781-43-1	0.5639
	23	Naphthalene,2-(phenylmethyl)-	613-59-2	0.0728
	24	8-Isopropyl-1,3-dimethylphenanthrene	-	1.033
	25	Phenanthrene,2,3,5-trimethyl-	3674-73-5	1.3575
	26	9-Ethyl-10-methylanthracene	19713-49-6	1.3722
	27	Phenanthrene,2,3,5-trimethyl-	3674-73-5	1.3167
	28	11H-Bzenzo[b]fluorene	238-84-6	1.4694
	29	Phenanthrene,2,3,5-trimethyl-	3674-73-5	1.3459
	30	Phenanthrene,1-methyl-7-(1-methylethyl)-	483-65-8	6.2672
	31	8-Isopropyl-1,3-dimethylphenanthrene	-	0.4629
	32	9-Ethyl-10-methylanthracene	19713-49-6	0.2925
	33	Phenanthrene,2,3,5-trimethyl-	3674-73-5	1.3835
	34	p-Terphenyl	92-94-4	0.11
	35	Phenanthrene,1-methyl-7-(1-methylethyl)-	483-65-8	4.8369
PAH-3	1	benz[a]anthracene	56-55-3	0.8415
	2	Fluoranthene	206-44-0	0.9301
	3	Pyrene	129-00-0	0.4569
	4	Pyrene,1-methyl-	2381-21-7	0.8977

	5	11H-Benzo[b]fluorene	30777-19-6	0.0075
	6	Pyrene,1,3-dimethyl-	64401-21-4	0.839
	7	Pyrene,1,2-dimethyl-	74869-48-0	0.8671
	8	Pyrene,1,6-dimethyl-	27984-16-3	0.7366
	9	Triphenylene	217-59-4	1.4489
	10	Chrysene	218-01-9	1.523
	11	Chrysene,6-methyl-	1705-85-7	0.0261
	12	Chrysene,5-methyl-	3697-24-3	0.0068
	13	Chrysene,4-methyl-	3351-30-2	0.0003
PAH-4	1	Benzo[k]fluoranthene	207-08-9	1.4279
	2	Perylene	198-55-0	0.9246
	3	Benz[e]acephenanthrylene	205-99-2	0.7358
	4	Benzo[k]fluoranthene	203-33-8	0.0026
	5	benzo[a]pyrene	50-32-8	1.7649
H-1	1	nC17		0.257
	2	nC18		0.175
	3	nC19		0.4826
	4	nC20		0.1065
	5	nC21		0.1006
	6	nC22		0.1192
	7	nC23		0.1004
	8	nC24		0.1537
	9	nC25		0.15
	10	nC26		0.2039
	11	nC27		0.4678
	12	nC28		0.8519
	13	nC29		0.8628
	14	nC30		0.837
	15	C32 isomer		0.6286
	16	nC31		0.2388

	17	nC32		0.0627
	18	4-Tetradecene, (Z)-	41446-65-5	0.0225
	19	Cyclohexane,2-butyl-1,1,3-trimethyl-	54676-39-0	0.0722
	20	10-Heneicosene(c, t)	95008-11-0	0.0668
	21	1-Docosene	1599-67-3	0.1189
	22	1,7-Dimethyl-4-(1-methylethyl)cyclodecane	645-10-3	0.3945
	23	1-Hexacosene	18835-33-1	0.1933
	24	Phenanthrene, 9-dodecyltetradecahydro	55334-01-5	0.1156
	25	1Hbenz[de]anthracene, hexadecahydro-6-octyl-	7225-65-2	0.2117
	26	Squalene	7683-64-9	0.3152
	27	Urs-12-ene	464-97-1	0.0794
H-2	1	Benzene, decyl-	104-72-3	0.127345
	2	Benzene, 1-heptyl-4-propyl	-	0.268011
	3	(E)-1-(6,10-Dimethylundeca-5,9-dien-2-yl)-4-methylbenzene	55968-43-9	0.225294
	4	Benzene, 1,3,5-tributyl-	841-07-6	0.503065
	5	Naphthalene, 1,4-dimethyl-5-octyl-	55000-53-8	0.843418
	6	Naphthalene,7-butyl-1-hexyl-	55000-55-0	0.51363
	7	Naphthalene, 2,6-dimethyl-3-octyl-	55000-54-9	0.550605
P-1	1	Pyrimido[1,2-a]azepine, 2,3,4,6,7,8,9,10-octahydro-	6674-22-2	0.0022
	2	Dibenzofuran	132-64-9	0.3073
	3	Pyridine,3-phenyl-	1008-88-4	0.3198
	4	9H-Xanthene	92-83-1	0.309
	5	6H-Dibenzo[b,d]-pyran	229-95-8	0.0765
	6	1,4,7-Trimethyl-2-azafluorene	-	0.5986
	7	Naphtha[2,1-b]furan,1,2-dimethyl-	-	0.4218
	8	Naphtha[2,1-b]furan,2,2-dimethyl-	-	0.5779
	9	Xanthenes,9,9-dimethyl-	-	0.0017
	10	Benzo[b]naphtha[2,3-d]furan	-	0.2458
	11	Benzo[kl]xanthenes	-	0.4268
	12	9H-Xanthene	92-83-1	0.3091

13	3-(N,N-Dimethylamino)-9-methylcarbazole	-	0.3611
14	Naphtha[2,1-b]furan,1,2-dimethyl-	-	0.5379
15	Benzo[h]quinoline,2,4-dimethyl-	605-67-4	0.0013
16	Harmaline	304-21-2	0.0951
17	Benzeneethanol,.alpha.-[2-(dimethylamino)-1-methylethyl]-.alpha.-phenyl-,propanonate	-	0.4267
18	1-Isobenzofuranol,1,3-dihydro-3,3-dimethyl-1-phenyl-	-	0.3268
19	Benzo[d,E]isocoumarin,3,3-dimethyl-	-	0.1131
20	Xanthenes,9,9-dimethyl-	-	0.0021
21	Naphtha[2,1-b:7,8-b']difuran,1,2,9,10-tetrahydro-2,9-dimethyl-	-	0.0917
22	1-Ethyl-3-formylindole	-	0.0216
23	5H-Dibenz[b, f]azepine,10,11-dihydro-5-nitroso-	-	0.0075
24	1H,3H-Naphtho[1,8-cd]pyran,3a,4,5,6-tetrahydro-	-	0.0173
25	Lenacil	2164-08-1	0.1141
26	carbazol-9-ylmethanol	-	0.0075
27	10-Acetyl-9,10-dihydroacridine	-	0.0323
28	2,5-Dimthylbenzoxazole	5676-58-4	0.0739
29	Quinoline	91-22-5	0.2432
30	Quinoline,2-methyl-	91-63-4	0.3185
31	Quinoline,8-methyl-	611-32-5	0.4023
32	Quinoline,2,7-dimethyl-	93-37-8	0.0065
33	Pyridine,3-phenyl-	1008-88-4	0.072
34	dl-5-Methyltryptophan	-	0.0173
35	Quinoline,2,3,4-trimethyl-	2437-72-1	0.2529
36	2,4-Diamino-5-benzyl-6-methylthieno[2,3-d]pyrimidine	-	0.0067
37	Isoquinoline,2-(2,2-dimethyl-1-oxopropyl)-1,2,3,4-tetrahydro-6,7-dimethoxy-	-	0.728
38	Isoquinoline,3-methyl-	1125-80-0	0.01
39	Indoline,3-ethyl-2,3-dimethyl-	-	0.0602
40	7-(6-Methylpyridin-2-yl)hept-6-enal	-	0.504
41	Quinoline,2,4,6-trimethyl-	2243-89-2	0.0116
42	Quinoline,2,3,4-trimethyl-	2437-72-1	0.2263

	43	2,5-Dimethyl-4-phenylpyridine	-	0.0106
	44	1,7-Phenanthroline	230-46-6	0.0178
	45	Isoquinoline,1,2,3,4-tetrahydro-2,3-dimethyl-	-	0.1069
	46	Quinoline, 2,3-dimethyl-	1721-89-7	0.0366
	47	Quinoline,2,3,4-trimethyl-	2243-89-2	0.1106
	48	2-Methyl-3-phenylpyridine	-	0.5925
	49	2,5-Dimethyl-4-phenylpyridine	-	0.0011
	50	9H-Pyrido[3,4-b]indole,1-methyl-	486-84-0	0.1216
P-2	1	2-Dodencen-1-yl(-) succinic anhydride	-	0.0008
	2	Cyclododecanemethanol	-	0.0015
	3	Boldenone	846-48-0	0.0074
	4	2-Buten-1-one,1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	35044-68-9	0.0974
	5	3-Buten-2-one,4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	14901-07-6	0.0086
	6	Methyl dehydroabietate	1235-74-1	0.09
	7	1,1’-Biphenyl,3-ethoxy-	-	0.0007
	8	[1,1’-Biphenyl]-4-methanol	-	0.1475
	9	[1,1’-Biphenyl]-4-carboxaldhyde	-	0.0849
	10	1,1'-Biphenyl, 2-methoxy-	86-26-0	0.5427
	11	1,1-Dimethyl-2-(diphenylmethylene)hydrazone	-	0.214
	12	9H-Fluoren-9-ol	1689-64-1	0.8569
	13	5H-Dibenzo[a,d]cyclohepten-5-ol,10,11-dihydro	1210-34-0	0.0431
	14	10H-Dibenzo[b,E]thiopyran-10-one,2-ethyl-	-	0.0724
	15	9H-Fluorene-2,7-diamine	-	0.9957
	16	Benzylamine,4-(1-methylethyl)-N,.alpha.-diphenyl-	-	0.483
	17	Nortriptyline	72-69-5	0.0009
	18	2-Hydroxymethyl-10-methylanthracene	-	0.1272
	19	1-Acetyl-4,6,8-trimethylazulene	-	0.321
	20	2-Methyl-3,4-diphenyl-2-cyclopenten-1-one	-	0.0733
	21	6-hydroxy-7-methyl-9-oxopodocarpane	-	0.1082
	22	9,10-Anthracenedione	84-65-1	0.5599

	23	Pregnenolone-7,9(11)-dien	-	0.0213
	24	Cyclopentene-1-carboxylic acid,4-[2-(diphenylmethyl)-2-propen-1-yl]-,methyl ester	-	0.0958
	25	Pregna-5,8,16-triene-3.beta.-ol-20-one acetate	-	0.0003
	26	1-(10-Methylanthracene-9-yl)ethanone	-	0.0511
	27	9,10-Anthracenedione,2-(1,1-dimethylethyl)-	84-47-9	0.0749
	28	Bicyclo[3.1.0]hex-3-en-2-one,6,6-diphenyl-	-	0.2449
	29	2-Ethyl-3-methylene-indan-1-one	-	0.1713
	30	2-Acetoxy-3-methoxybiphenylene	-	0.2661
	31	Naphthalene,6-methoxy-2-(1-buten-3-yl)-	-	0.0326
	32	1-(10-Methylanthracen-9-yl)ethanone	-	0.0541
	33	Estra-1,3,5(10),9(11)-tetraen-17-one, 3-methoxy-	-	0.0069
	34	3-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-2-(1-methylethyl)-, acetate, (4bs-trans)-	15340-79-1	0.0009
	35	11H-Cyclopenta[a]phenanthren-17-ol,12,13,16,17-tetrahydro-3-methoxy-13-methyl	-	0.0749
	36	Estra-1,3,5,7,9-pentaen-17-one,3-(acetyloxy)-	-	0.2449
	37	9,10-Anthracenedione,1,8-dimethoxy-	-	0.1713
	38	1-Phenanthrenecarboxaldehyde, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1α,4aβ,10aα)]-	13601-88-2	0.2661
	39	1,2,3,4-Tetrahydro-1,4-ethanoanthracene,9,10-dimethoxy-	-	0.0326
	40	7-Methylindan-1-one	-	0.6949
	41	9,10-Anthracenedione,1,8-dimethoxy-	-	0.0749
	42	1-Phenylcyclopenthlamine	-	0.2449
	43	Quinoline,2,4-dimethyl-	1198-37-4	0.1713
	44	Dimethylphthalate	131-11-3	0.2661
	45	1H-Inden-1-one, 2,3-dihydro-2,6-dimethyl-	-	0.0326
	46	o-Hydroxyacetophenonylidene-4,5-dimethyl-O-phenylenediamine	-	0.0031
	47	Benzene,1-(1,1-dimethylethyl)-3,5-dimethyl-2,4,6-trinitro-	81-15-2	0.0008
	48	1-Naphthalenamine,N,N-dimethyl-	86-56-6	0.4445
P-3:	1	Phenol,2-(1-phenylethyl)-	4237-44-9	0.001
	2	Phenol,4-(2-phenylethenyl)-,(E)-	-	0.0038
	3	Phenol,p-1-indanyl-	-	0.0064
	4	2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, (4bS-trans)-	511-15-9	0.0969

5	2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, (4bS-trans)-	511-15-9	0.1065
6	1-Naphthalenol	90-15-3	0.1067
7	1-Naphthalenol,2-methyl-	-	0.3179
8	1-Naphthalenol,4-methyl-	-	0.2987
9	1-Naphthalenol,2-methyl-	-	0.3661
10	1-Naphthol,6,7-dimethyl-	-	0.3568
11	1-Naphthol,2,4-dimethyl-	-	0.5588
12	1-Naphthol,1,6-dimethyl-	-	0.6739
13	p-butyl phenol	1638-22-8	0.4243
14	7-Hydroxycadalene	2102-75-2	0.434
15	Octyl phenol	-	0.2023
16	o-butyl phenol	3180-09-4	0.106
17	1-anthrol	-	0.1449
18	1-Hydroxypyrene	5315-79-7	0.328
19	1,2-Benzenediol,4-methyl-	452-86-8	0.0086
20	1,4-Benzenediol,2,5-dimethyl-	615-90-7	0.1354
21	5-Amino-1-naphthol	83-55-6	0.087
22	Phenol,2,5-bis(1,1-dimethylethyl)-	5875-45-6	0.0684

Part 3 The detail of extraction conditions and results

Table s8. Mass percentage of major components in extraction product

Items	T (K)	P (MPa)	Mass percentage in extraction product (w_1 %)								
			PAHs-1	PAHs-2	PAHs-3	PAHs-4	H-1	H-2	P-1	P-2	P-3
1	490	5.5	4.60	70.77	2.62	1.00	7.62	4.35	5.57	3.57	0.00
2	500	8.0	3.11	63.30	11.50	1.10	7.04	3.41	5.17	5.38	0.00
3	510	4.0	8.37	69.10	0.58	1.00	9.22	3.98	4.07	3.67	0.00
4	520	6.5	4.15	66.42	7.24	0.00	5.50	4.01	6.50	6.2	0.00
5	530	9.0	3.41	57.82	13.57	1.15	7.87	3.69	5.28	7.28	0.00
6	540	5.0	6.81	62.13	2.10	0.00	6.20	3.21	6.85	8.56	4.15
7	550	7.5	4.02	57.67	9.69	0.00	5.46	3.88	9.00	9.23	1.08
8	560	3.5	12.12	51.57	0.00	0.00	12.86	1.79	9.33	11.18	1.2
9	570	6.0	5.64	48.13	3.77	3.5	5.64	2.77	13.48	13.82	3.3
10	580	8.5	4.25	42.69	5.38	1.94	6.12	3.54	16.29	13.8	6.00
11	590	4.5	9.01	32.81	0.00	0.00	9.51	1.44	23.60	22.26	1.44
12	600	7.0	5.10	37.26	2.19	1.12	5.85	2.38	24.01	21.25	0.83
13	490	3.5	9.31	68.33	0.00	0.00	11.43	4.44	3.65	2.85	0.00
14	490	9.0	2.80	58.09	11.33	5.26	9.22	3.77	5.23	4.26	0.00
15	600	3.5	13.86	30.74	0.00	0.00	11.43	1.31	19.15	21.38	2.12
16	600	9.0	4.66	31.33	3.05	3.11	5.11	3.88	20.67	18.03	10.15

Table s9. Extraction yield of major components in extraction product

Items	T (K)	P (MPa)	Extraction yield (y_1 %)								
			PAHs-1	PAHs-2	PAHs-3	PAHs-4	H-1	H-2	P-1	P-2	P-3
1	490	5.5	92.21	69.76	13.25	10.67	48.11	67.29	26.48	19.30	0.00
2	500	8.0	95.69	95.90	89.42	18.04	68.32	81.08	37.78	44.70	0.00
3	510	4.0	93.36	37.90	1.63	5.94	32.39	34.26	10.77	11.04	0.00
4	520	6.5	94.61	74.46	41.66	0.00	39.50	70.56	35.15	38.12	0.00
5	530	9.0	98.06	81.64	98.34	17.57	71.18	81.77	35.96	56.38	0.00
6	540	5.0	96.40	43.24	7.50	0.00	27.64	35.06	22.99	32.67	28.20
7	550	7.5	95.55	67.48	58.19	0.00	40.92	71.25	50.79	59.23	12.34
8	560	3.5	94.36	19.75	0.00	0.12	31.54	10.76	17.23	23.48	4.49
9	570	6.0	92.11	38.67	15.55	30.44	29.03	34.93	52.24	60.90	25.89
10	580	8.5	94.50	46.72	30.22	22.98	42.90	60.81	85.99	82.83	64.10
11	590	4.5	89.67	16.05	0.00	0.00	29.80	11.06	55.69	59.73	6.88
12	600	7.0	88.59	31.82	9.60	10.35	32.00	31.90	98.89	99.52	6.92
13	490	3.5	92.51	33.39	0.00	0.00	35.78	34.05	8.60	7.64	0.00
14	490	9.0	95.29	97.15	97.25	95.20	98.77	98.95	42.19	39.07	0.00
15	600	3.5	88.54	9.65	0.00	0.00	23.00	6.46	29.01	36.83	6.50
16	600	9.0	94.79	31.31	15.64	33.64	32.71	60.86	99.63	98.82	99.02

Table. S10 Mass equilibrium accounting for each experiment

Items	T (K)	P (MPa)	Mass of feedstock (g)	Mass of extraction product (g)	Yield of each experiment (%)	Mass loss (%)
1	490	5.5	100.13	48.11	48.05	1.21
2	500	8.0	100.71	73.95	73.43	2.04
3	510	4.0	100.22	26.77	26.71	2.09
4	520	6.5	100.03	54.72	54.7	1.09
5	530	9.0	99.87	68.92	69.01	1.77
6	540	5.0	99.91	33.97	34	0.82
7	550	7.5	99.89	57.11	57.17	1.12
8	560	3.5	100.11	18.69	18.67	0.48
9	570	6.0	100	39.22	39.22	1.62
10	580	8.5	100.32	53.42	53.25	3.31
11	590	4.5	99.99	23.88	23.88	1.01
12	600	7.0	99.9	41.68	41.72	2.78
13	490	3.5	100.24	23.85	23.79	2.50
14	490	9.0	100.17	81.63	81.49	1.19
15	600	3.5	100.13	15.33	15.31	1.63
16	600	9.0	100.31	48.78	48.63	2.77

Part 4. TIC graphs of extraction products and residual in the sequential extraction process

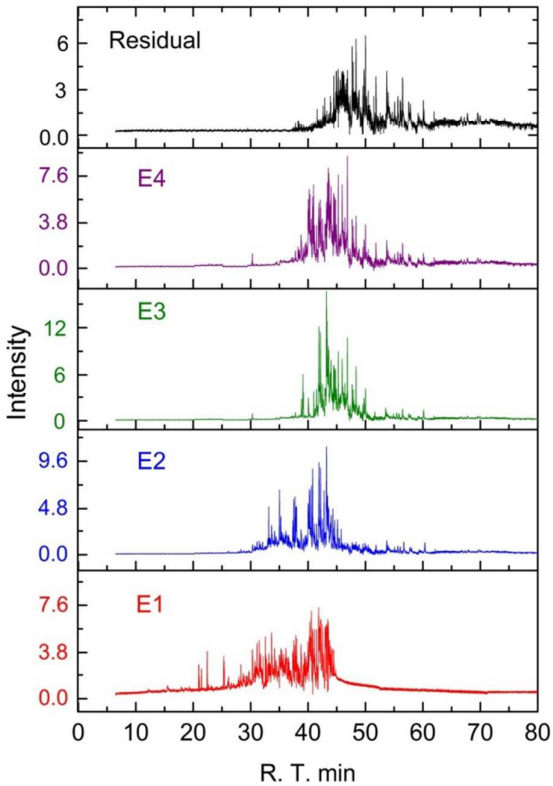

Fig. s5 TIC graph of extraction products and the residual in the sequential extraction process (the residual was pretreated by SGCC)