

## Supplemental Information

**Table S1 MCAs detected in the products from coal oxidation**

peak	MCAs	SLL	SFB	JCA
<b>1</b>	butanoic acid	×	×	
<b>2</b>	chloroacetic acid	×	×	×
<b>3</b>	2-chloropropanoic acid		×	
<b>4</b>	pentanoic acid	×	×	
<b>5</b>	dichloroacetic acid	×	×	×
<b>6</b>	2,2-dichloropropanoic acid	×	×	×
<b>7</b>	2-chlorobutanoic acid	×	×	
<b>9</b>	trichloroacetic acid	×	×	×
<b>10</b>	hexanoic acid	×	×	
<b>11</b>	2,2-dichlorobutanoic acid	×	×	
<b>13</b>	heptanoic acid	×	×	
<b>15</b>	2,3,3-trichloroacrylic acid	×	×	
<b>16</b>	2,2-dichloro-3-methylbutanoic acid		×	
<b>17</b>	2,2-dichloropentanoic acid	×	×	
<b>20</b>	3,5-dimethylheptanoic acid	×	×	
<b>22</b>	2,2,3-trichlorobutanoic acid	×	×	
<b>25</b>	2-chloroheptanoic acid		×	
<b>26</b>	2,2,3,3-tetrachloropropanoic acid	×	×	
<b>28</b>	nonanoic acid		×	
<b>29</b>	2,2,3-trichloro-3-methylbutanoic acid		×	
<b>32</b>	4-methylnonanoic acid	×	×	
<b>33</b>	decanoic acid	×	×	
<b>34</b>	2,2,3-trichloropentanoic acid		×	
<b>35</b>	2,2-dichlorooctanoic acid	×	×	
<b>41</b>	9-methyldecanoic acid	×		
<b>43</b>	dodecanoic acid	×	×	
<b>49</b>	tetradecanoic acid	×		
<b>59</b>	palmitic acid	×	×	

**Table S2 DCAs detected in the products from coal oxidation**

peak	DCAs	SLL	SFB	JCA
<b>14</b>	succinic acid	×		
<b>18</b>	2-methylsuccinic acid	×	×	
<b>19</b>	2-chloro-2-methylmalonic acid	×	×	
<b>23</b>	2-chlorosuccinic acid	×	×	
<b>24</b>	glutaric acid	×	×	
<b>27</b>	2,3-dichlorosuccinic acid	×	×	
<b>36</b>	heptanedioic acid	×	×	
<b>40</b>	2-chloro-3-(dichloromethyl)fumaric acid	×	×	
<b>45</b>	nonanedioic acid		×	
<b>47</b>	decanedioic acid		×	
<b>51</b>	undecanedioic acid	×	×	

**Table S3 BCAs detected in the products from coal oxidation**

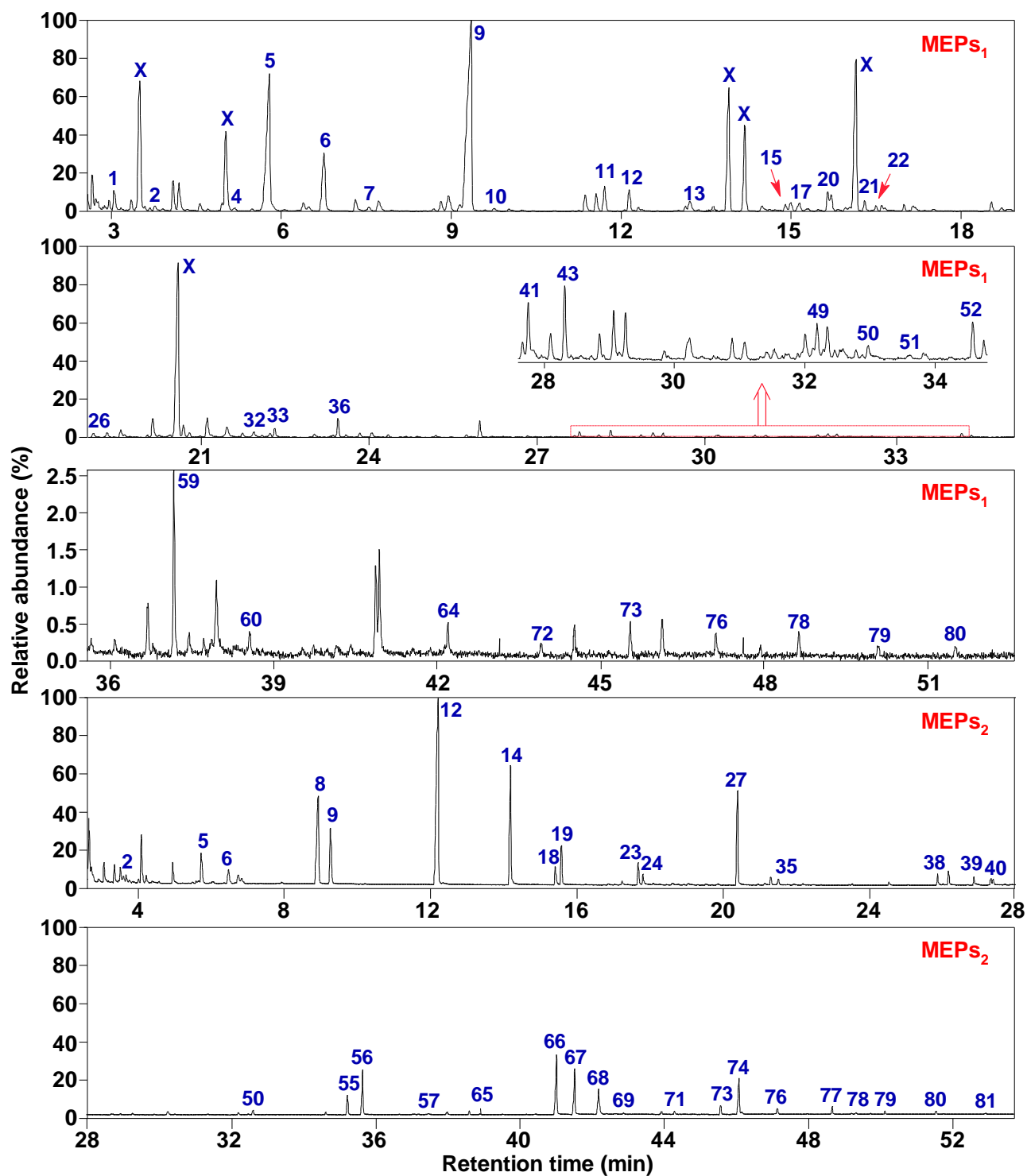
peak	BCAs	SLL	SFB	JCA
21	benzoic acid	×	×	
30	3-chlorobenzoic acid		×	
31	4-chlorobenzoic acid		×	
37	2-chloro-4-methylbenzoic acid		×	
39	phthalic acid	×	×	×
42	isophthalic acid		×	
44	2,5-dichloro-4-methylbenzoic acid		×	
46	3-chlorophthalic acid		×	×
48	4-chlorophthalic acid		×	
50	4-chloro-5-methylphthalic acid	×	×	
52	4-chloro-5-ethylphthalic acid	×	×	
53	4-chloro-5-isopropylphthalic acid		×	
54	2,3,4-trichloro-5,6-dimethylbenzoic acid		×	
55	benzene-1,2,3-tricarboxylic acid	×	×	×
56	benzene-1,2,4-tricarboxylic acid	×	×	×
57	3,5-dichloro-4-methylphthalic acid		×	
58	benzene-1,3,5-tricarboxylic acid		×	
62	4-chlorobenzene-1,2,3-tricarboxylic acid	×	×	×
63	5-methylbenzene-1,2,4-tricarboxylic acid		×	
64	6-chlorobenzene-1,2,4-tricarboxylic acid	×	×	×
65	6-chloro-5-methylbenzene-1,2,4-tricarboxylic acid	×	×	
66	benzene-1,2,3,4-tetracarboxylic acid	×	×	×
67	benzene-1,2,3,5-tetracarboxylic acid	×	×	×
68	benzene-1,2,4,5-tetracarboxylic acid	×	×	×
69	5-chlorobenzene-1,2,3,4-tetracarboxylic acid	×	×	×
70	3-chlorobenzene-1,2,4,5-tetracarboxylic acid		×	×
71	5-chloro-6-methylbenzene-1,2,3,4-tetracarboxylic acid	×	×	
74	benzene-1,2,3,4,5-pentacarboxylic acid	×	×	×
75	6-chlorobenzene-1,2,3,4,5-pentacarboxylic acid		×	×
77	benzene-1,2,3,4,5,6-hexacarboxylic acid	×	×	×

**Table S4 HCs detected in the products from coal oxidation**

peak	HCs	SLL	SFB	JCA
<b>60</b>	icosane	×	×	
<b>61</b>	henicosane		×	
<b>72</b>	tricosane	×	×	×
<b>73</b>	tetracosane	×	×	×
<b>76</b>	pentacosane	×	×	×
<b>78</b>	hexacosane	×	×	×
<b>79</b>	heptacosane	×	×	×
<b>80</b>	octacosane	×	×	×
<b>81</b>	nonacosane	×	×	×
<b>82</b>	triacontane		×	
<b>83</b>	hentriacontane		×	
<b>84</b>	dotriacontane		×	

**Table S5 OSs detected in the products from coal oxidation**

peak	OSs	SLL	SFB	JCA
<b>8</b>	ethyl 2,2-dichloroacetate	×	×	×
<b>12</b>	ethyl 2,2,2-trichloroacetate	×	×	×
<b>38</b>	propane-1,2,3-tricarboxylic acid	×	×	



**Figure S1** Total ion chromatograms of  $P_{SLL}$  (X stands for unknown species)

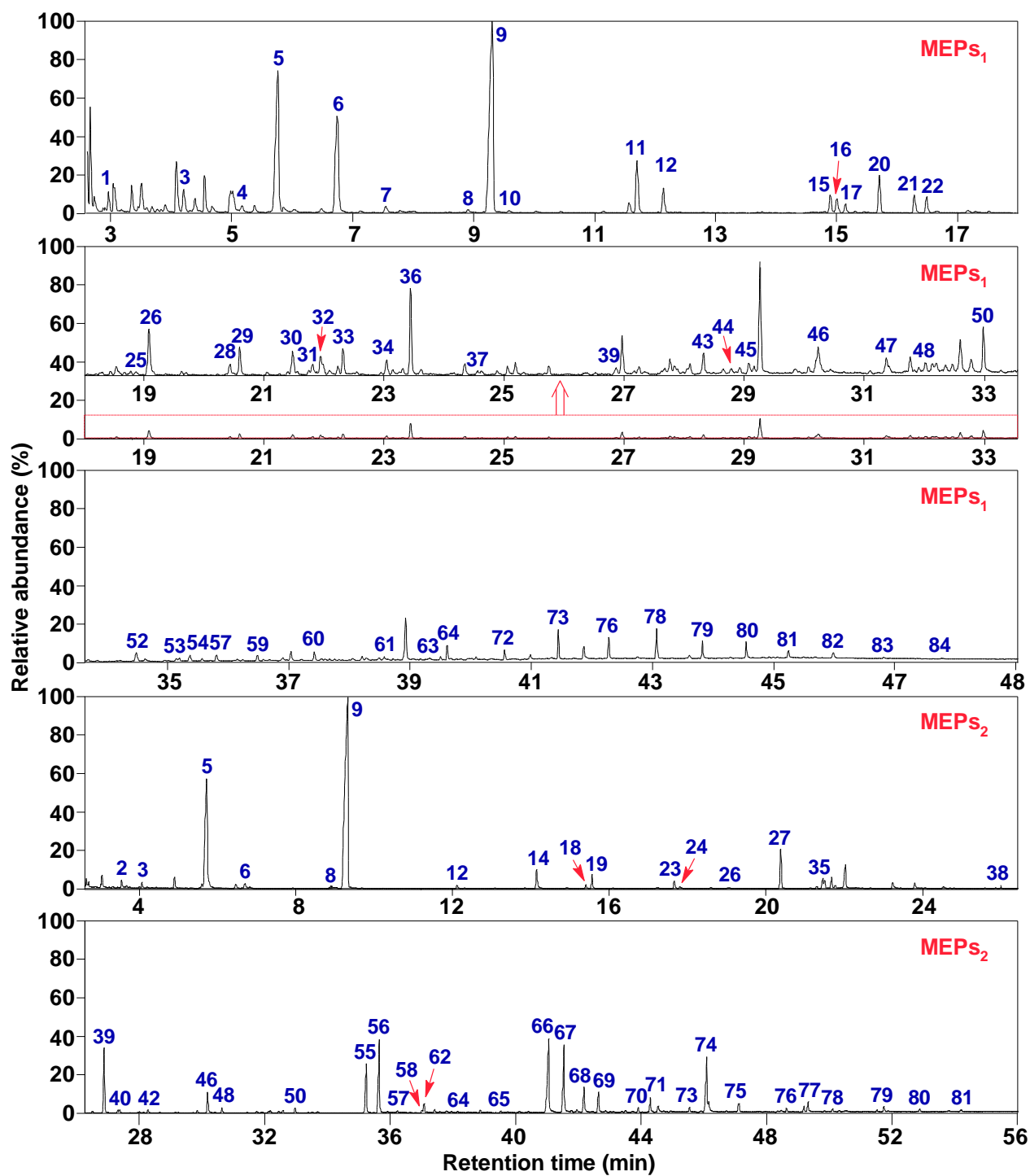
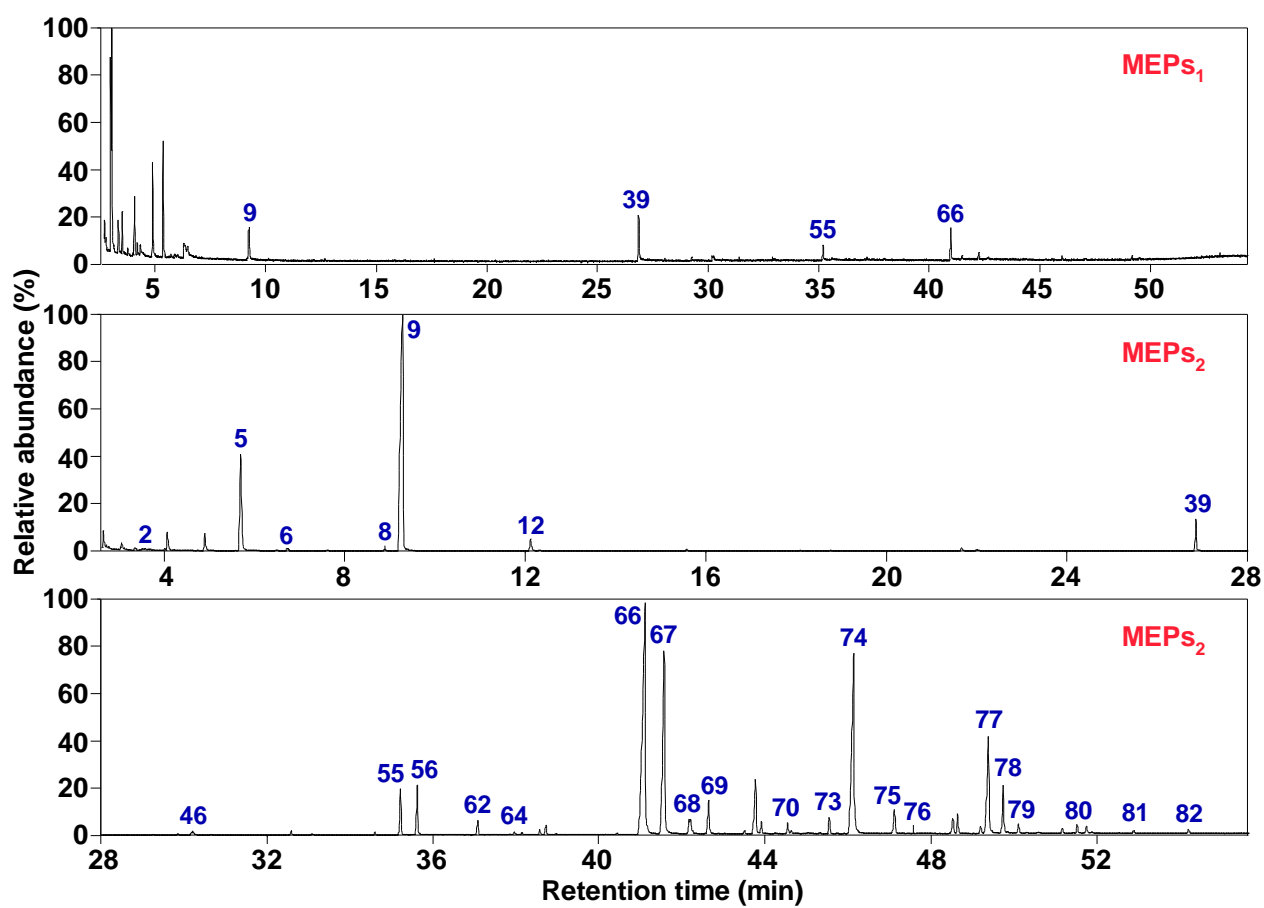


Figure S2 Total ion chromatograms of  $P_{SFB}$



**Figure S3** Total ion chromatograms of P<sub>JCA</sub>