

## Supplementary Materials

**Table S1.** GC/MS analysis of PAHs in ME particulate (MEP) extract.

Compound	Concentration (ng/mg MEP extract)
Naphthalene	1467.1 ± 20.9
Phenanthrene	195.7 ± 10.3
Anthracene	101.5 ± 2.2
Acenaphthylene	96.9 ± 6.9
Pyrene	88.6 ± 1.8
Fluorene	66.9 ± 7.6
Fluoranthene	48.9 ± 2.3
Benzo(a)pyrene	20.2 ± 1.0
Benz(a)anthracene	17.0 ± 1.1
Benzo(g,h,i)perylene	16.1 ± 0.9
Indeno(1,2,3-c,d)pyrene	10.6 ± 0.7
Chrysene	7.1 ± 0.7
Benzo(b)fluoranthene	6.1 ± 0.6
Benzo(k)fluoranthene	5.8 ± 0.8
Acenaphthene	n.d.*
Dibenz(a,h)anthracene	n.d.*

Note. The results were extracted from Ueng *et al.* (2005), *Toxicol. Sci.* 87: 483–496.

Each value represents the mean ± SD for three determinations.

\* n.d.: not detectable.

**Table S2.** Metabolite identification from the extracts of rat testis using  $^1\text{H}$  NMR spectroscopy

Hydrophilic Metabolite	Chemical Shift (ppm) and Multiplicity <sup>a</sup>
Acetate	1.92 (s)
Adenosine	4.27 (q), 4.44 (q), 6.10 (d)* <sup>b</sup> , 8.24 (s), 8.35 (s)
Alanine	1.48 (d)*, 3.78 (q)
Ascorbate	3.74 (m), 3.99 (t)*
Aspartate	2.65 (q), 2.81 (q)*
Betaine	3.28 (s)*, 3.89 (s)
Creatine	3.03 (s), 3.94 (s)*
Ethanolamine	3.10 (t)*, 3.81 (t)
Glucose	3.23 (t), 3.35 (t), 3.40 (m)*, 3.47 (t), 3.52 (t), 3.69 (t), 3.73 (q), 3.76 (t), 3.82 (m), 3.89 (q), 4.63 (d), 5.23 (d)
Glutamate	2.02 (m), 2.12 (m), 2.36 (m)*, 3.74 (t)
Glutathione	2.13 (q), 2.55 (m), 3.80 (t)*, 4.56 (t)
Glycine	3.53 (s)
Inositol	3.52 (q), 3.65 (t)*, 4.05 (t)
Lactate	1.33 (d)*, 4.10 (q)
Leucine	0.95 (t)*, 1.70 (m), 3.73 (m)
Phosphocholine	3.22 (s)*, 3.58 (m), 4.15 (m)
Phosphoethanolamine	3.21 (t), 3.97 (m)*
Trimethylamine	2.86 (s)
Tyrosine	6.90 (d)*, 7.20 (d)
Valine	0.98 (d), 1.04 (d)*
Hydrophobic Metabolite	Chemical Shift (ppm) and Multiplicity
Cholesterol	0.68* (s), 1.01 (s), 3.53 (m)
Lipid hydroperoxide/conjugated diene	4.30 (m), 7.53 (s), 7.71* (s)
Phosphatidylcholine	3.32* (s), 3.95 (m), 4.07 (bm), 4.30 (bm)
Triglyceride	4.14 (d), 4.29 (d), 5.26* (m)
Fatty acyl chain( -CH=CH- )	5.30–5.41* (m)
Fatty acyl chain( -CH2- )	1.20–1.37* (m)
Fatty acyl chain( terminal CH3 )	0.80–0.91* (m)
Fatty acyl chain( -CH2-CO- )	2.26–2.33* (m)

<sup>a</sup> s, singlet; d, doublet; t, triplet; q, quartlet; bm, broad multiplet; m, multiplet

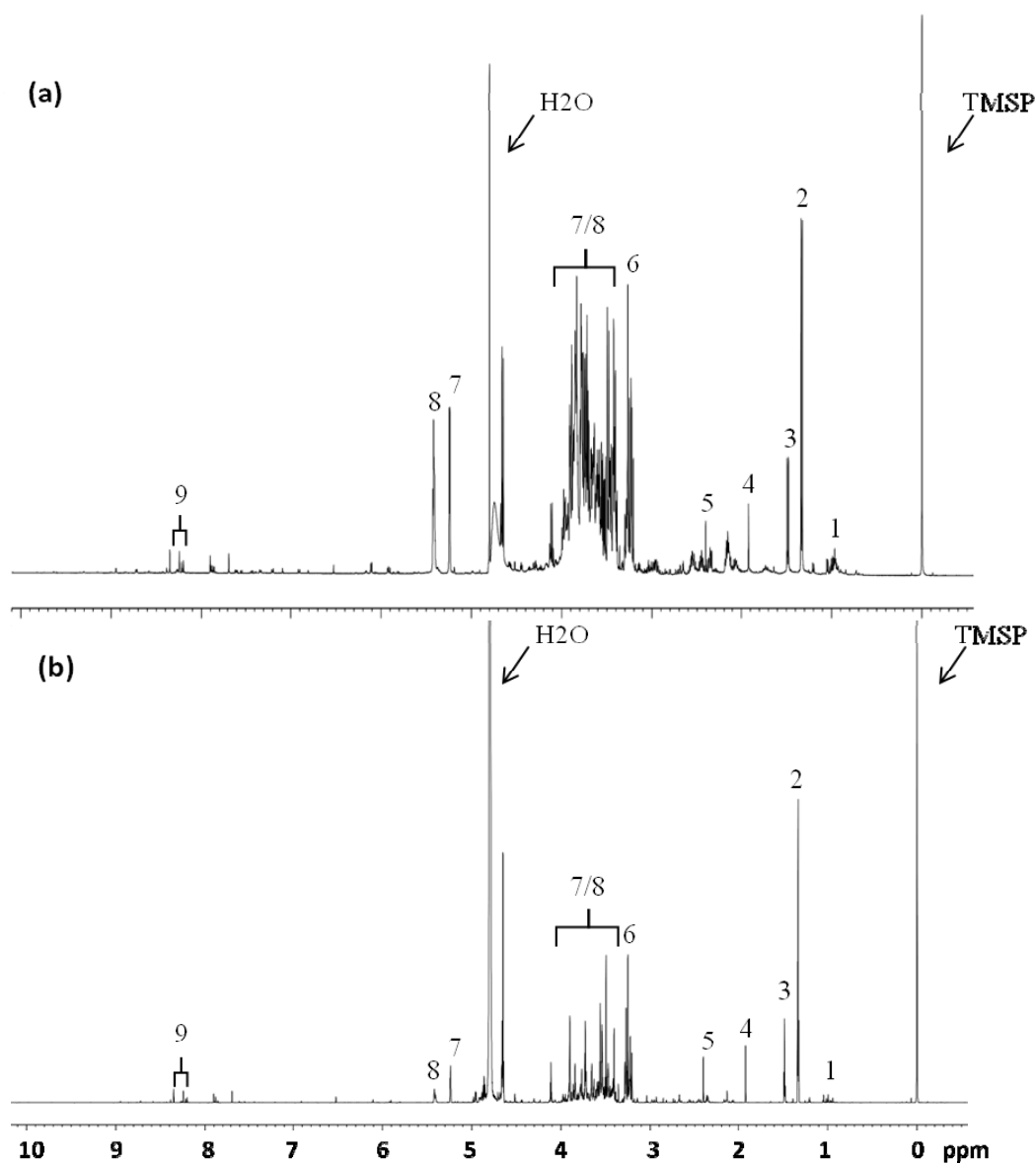
<sup>b</sup> \*, Peaks are selected to quantify and compare between treatments.

**Table S3.** Metabolite identification from the extracts of rat liver using  $^1\text{H}$  NMR spectroscopy.

Hydrophilic Metabolite	Chemical Shift (ppm) and Multiplicity <sup>a</sup>
Acetylcarnitine	3.18 (s)
Arginine	1.64 (m)* <sup>b</sup> , 1.71 (m), 1.88 (m), 1.91 (m)
Ascorbate	4.51 (d)
Creatine	3.04 (s)*, 3.94 (s)
Fumarate	6.52 (s)
Glucose	3.23 (t), 3.35 (t), 3.40 (m), 3.47 (t), 3.52 (t), 3.69 (t), 3.73 (q)*, 3.76 (t), 3.82 (m), 3.89 (q), 4.63 (d), 5.23 (d)
Glutamine	2.14 (m)*, 2.45 (m)
Inosine	4.27 (q), 4.31 (q), 6.10 (d), 8.24 (s)*, 8.34 (s)
Isoleucine	0.99 (t)*, 1.01 (d)
Isopropanol	1.20 (d)
Kynurenine	6.79 (d), 6.89 (d), 7.43 (t)*, 7.85 (d)
Maltose	3.42 (t), 3.58 (m), 3.64 (t), 3.69 (m), 3.76 (m), 3.85 (m), 3.92 (m), 3.98 (t), 5.22 (d), 5.40 (t)*
Succinate	2.40 (s)
Theophylline	3.40 (s), 3.56 (s), 7.68 (s)*
Trimethylamine	2.86 (s)
Trimethylamine N-oxide	3.23 (s)
Uridine	4.22 (t), 4.34 (t), 5.90 (q), 7.85 (d)*
Xanthine	7.88 (s)
Hydrophobic Metabolite	Chemical Shift (ppm) and Multiplicity
Cholesterol	0.68 (s), 1.01* (s), 3.53 (m)
Cholesteryl ester	0.68 (s), 1.03* (s), 4.60 (m)
Phosphatidylcholine	3.32* (s), 3.95 (m), 4.07 (bm), 4.30 (bm)
Triglyceride	4.14 (d), 4.29 (d), 5.26* (m)
Fatty acyl chain( -CH=CH- )	5.30–5.41* (m)
Fatty acyl chain( -CH <sub>2</sub> - )	1.20–1.37* (m)
Fatty acyl chain( terminal CH <sub>3</sub> )	0.80–0.91* (m)
Fatty acyl chain( -CH <sub>2</sub> -CO- )	2.26–2.33* (m)

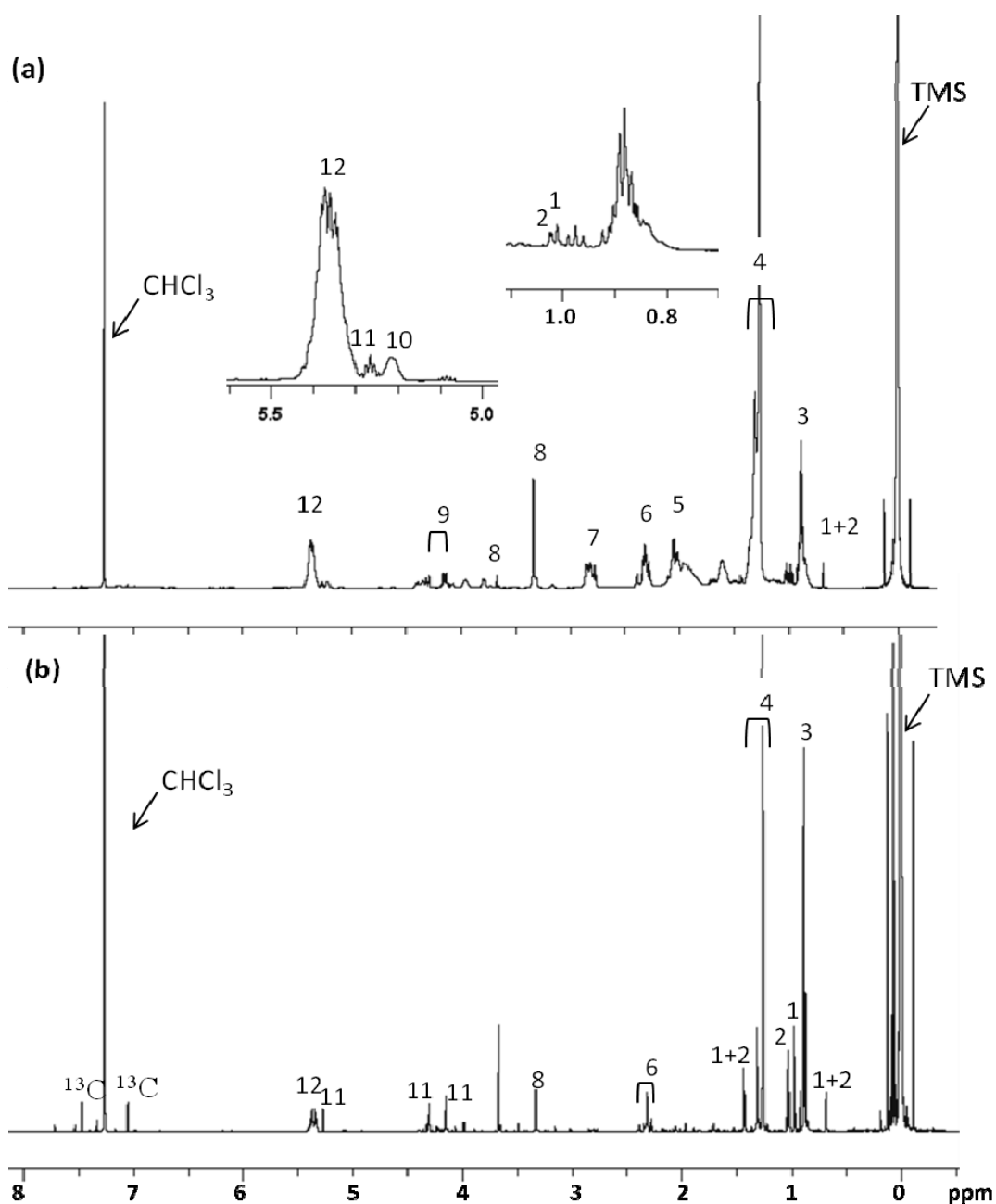
<sup>a</sup> s, singlet; d, doublet; t, triplet; q, quartlet; bm, broad multiplet; m, multiplet

<sup>b</sup> \*, Peaks are selected to quantify and compare between treatments.



**Figure S1.** Representative  $^1\text{H}$  NMR (a) and  $p$ -JRES NMR (b) spectra from the hydrophilic metabolites of the rat liver.

1. Isoleucine; 2. Lactate; 3. Alanine; 4. Succinate; 5. Acetate; 6. Trimethylamine N-oxide; 7. Glucose; 8. Maltose; 9. Inosine.



**Figure S2.** Representative  $^1\text{H}$  NMR (a) and  $p$ -JRES NMR (b) spectra from the hydrophobic metabolites of the rat liver.

1. Cholesterol; 2. Cholesteryl ester; 3. Fatty acyl chain terminal  $\text{CH}_3$ ; 4. Fatty acyl chain  $(\text{CH}_2)_n$ ; 5. Fatty acyl chain  $-\text{CH}_2\text{CH}=\text{}$ ; 6. Fatty acyl chain  $-\text{CH}_2\text{-CO}$ ; 7. Fatty acyl chain  $=\text{CHCH}_2\text{CH}=\text{}$ ; 8. Phosphatidylcholine; 9. Glycerol backbone C-1  $\text{H}_2$ /C-3  $\text{H}_2$ ; 10. Phospholipid glycerol backbone C-2  $\text{H}_2$ ; 11. Triglyceride glycerol backbone C-2  $\text{H}_2$ ; 12. Fatty acyl chain  $-\text{HC}=\text{CH}-$ . The peaks labeled  $^{13}\text{C}$  are the Carbon-13 satellite of  $\text{CHCl}_3$ .