**Supplementary Table 1.** Correlations among TCE metabolites in serum and liver in TCE-treated mice in a sub-acute study (600 mg/kg/d for 5 days).

| | | TCA in serum | DCA in serum | DCVG in serum | DCVC in serum | TCA in liver | DCA in liver | TCOH in liver | DCVG in liver |
|---|---|---|---|---|---|---|---|---|---|
| DCVG in liver | $\rho$ | -0.49 | 0.54 | 0.77 | 0.67 | -0.10 | 0.09 | 0.40 | 1 |
| | $q$ | - | - | - | **0.017** | - | - | - | |
| | n | 21 | 17 | 6 | 19 | 26 | 26 | 25 | 26 |
| TCOH in liver | $\rho$ | -0.28 | 0.13 | -0.1 | 0.26 | -0.28 | -0.12 | 1 | |
| | $q$ | - | - | - | - | - | - | | |
| | n | 20 | 16 | 5 | 18 | 25 | 25 | 25 | |
| DCA in liver | $\rho$ | 0.78 | 0.19 | 0.37 | 0.00 | 0.74 | 1 | | |
| | $q$ | **0.001** | - | - | - | **0.001** | | | |
| | n | 21 | 17 | 6 | 19 | 26 | 26 | | |
| TCA in liver | $\rho$ | 0.62 | -0.24 | -0.2 | -0.09 | 1 | | | |
| | $q$ | **0.020** | - | - | - | | | | |
| | n | 21 | 17 | 6 | 19 | 26 | | | |
| DCVC in serum | $\rho$ | -0.48 | 0.03 | 0.54 | 1 | | | | |
| | $q$ | - | - | - | | | | | |
| | n | 19 | 15 | 7 | 20 | | | | |
| DCVG in serum | $\rho$ | -0.29 | -0.31 | 1 | | | | | |
| | $q$ | - | - | | | | | | |
| | n | 7 | 6 | 7 | | | | | |
| DCA in serum | $\rho$ | -0.11 | 1 | | | | | | |
| | $q$ | - | | | | | | | |
| | n | 18 | 18 | | | | | | |
| TCA in serum | $\rho$ | 1 | | | | | | | |
| | $q$ | | | | | | | | |
| | n | 22 | | | | | | | |

Table displays Spearman rank correlation ($\rho$), false discovery rate-corrected significance value ($q$), and the number of data points with matching values in the same animal (n). Empty cell indicates that no correlation value was computed. Dash (-) indicates that the correlation was not significant ($q>0.1$).

**Supplementary Table 2.** Correlations among TCE metabolites and toxicity phenotypes in the liver of TCE-treated mice in a sub-acute study (600 mg/kg/d for 5 days). Data from vehicle-treated samples were not included in the analyses.

| | | TCA | DCA | TCOH | DCVG | Liver/Body weight ratio | *Acox1* | *Cyp4a10* | Hepato-cellular proliferation |
|---|---|---|---|---|---|---|---|---|---|
| Hepatocellular proliferation | $\rho$ | 0.22 | 0.30 | -0.43 | -0.39 | 0.16 | 0.23 | 0.27 | 1 |
| | $q$ | - | - | - | - | - | - | - | |
| | n | 23 | 23 | 22 | 23 | 24 | 20 | 20 | 24 |
| *Cyp4a10* | $\rho$ | 0.63 | 0.79 | -0.13 | 0.00 | 0.35 | 0.68 | 1 | |
| | $q$ | **0.022** | **<0.001** | - | - | - | **0.006** | | |
| | n | 19 | 19 | 18 | 19 | 20 | 20 | 20 | |
| *Acox1* | $\rho$ | 0.60 | 0.89 | -0.15 | 0.11 | 0.09 | 1 | | |
| | $q$ | **0.031** | **<0.001** | - | - | - | | | |
| | n | 19 | 19 | 18 | 19 | 20 | 20 | | |
| Liver/Body weight ratio | $\rho$ | -0.03 | 0.15 | -0.42 | -0.38 | 1 | | | |
| | $q$ | - | - | - | - | | | | |
| | n | 26 | 26 | 25 | 26 | 27 | | | |
| DCVG | $\rho$ | -0.10 | 0.09 | 0.40 | 1 | | | | |
| | $q$ | - | - | - | | | | | |
| | n | 26 | 26 | 25 | 26 | | | | |
| TCOH | $\rho$ | -0.28 | -0.12 | 1 | | | | | |
| | $q$ | - | - | | | | | | |
| | n | 25 | 25 | 25 | | | | | |
| DCA | $\rho$ | 0.74 | 1 | | | | | | |
| | $q$ | **<0.001** | | | | | | | |
| | n | 26 | 26 | | | | | | |
| TCA | $\rho$ | 1 | | | | | | | |
| | $q$ | | | | | | | | |
| | n | 26 | | | | | | | |

Table displays Spearman rank correlation ($\rho$), false discovery rate-corrected significance value ($q$), and the number of data points with matching values in the same animal (n). Empty cell indicates that no correlation value was computed. Dash (-) indicates that the correlation was not significant ($q>0.1$).

**Supplementary Table 3.** Correlations among TCE metabolites in serum and liver in TCE-treated mice in a sub-chronic study (100 or 400 mg/kg/d for 1, 2 or 4 wks).
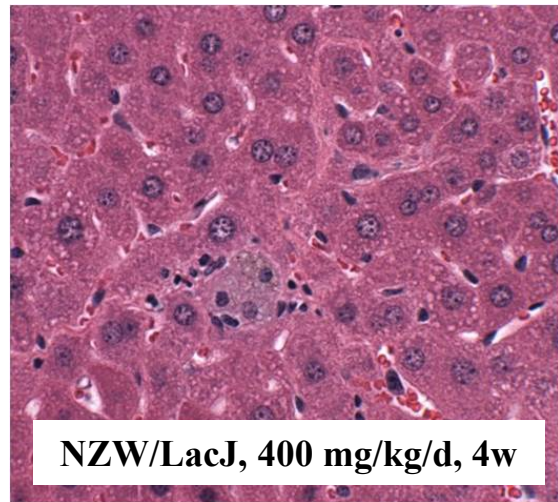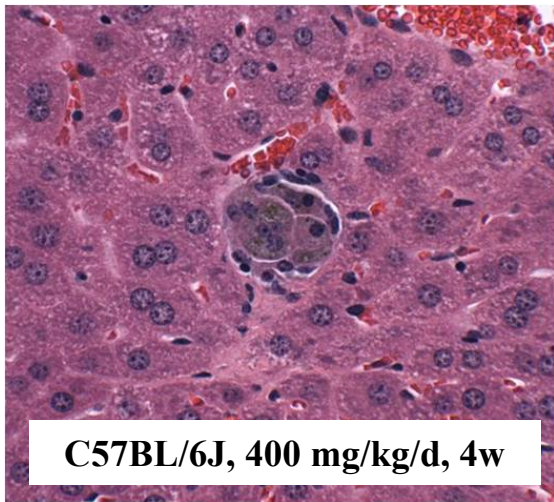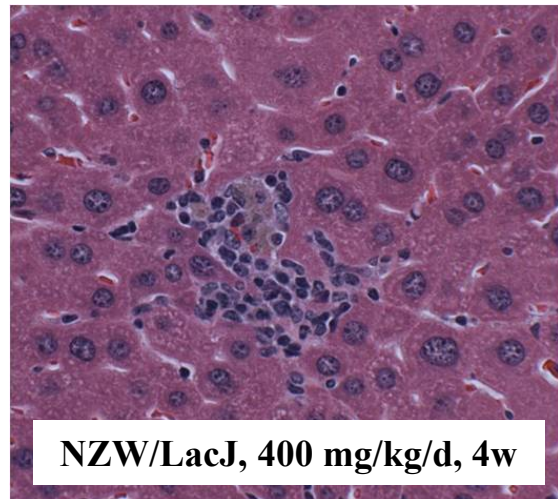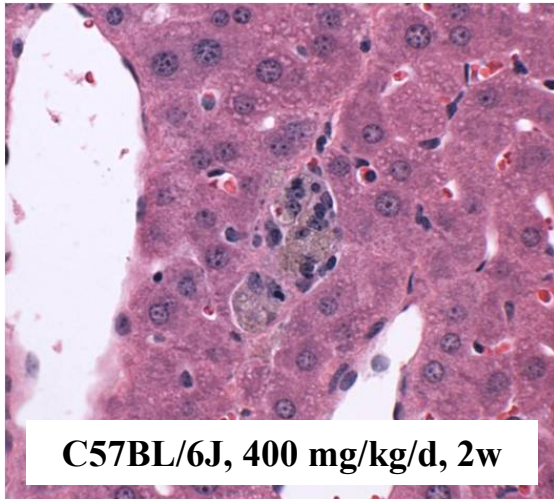
| | | TCA in serum | DCA in serum | TCA in liver | DCA in liver | TCOH in liver | DCVG in liver |
|---|---|---|---|---|---|---|---|
| DCVG in liver | $\rho$ | 0.04 | -0.09 | 0.20 | -0.13 | 0.41 | 1 |
| | $q$ | - | - | - | - | - | |
| | n | 15 | 15 | 16 | 16 | 16 | 16 |
| TCOH in liver | $\rho$ | 0.65 | 0.72 | 0.60 | 0.65 | 1 | |
| | $q$ | **<0.001** | **<0.001** | **<0.001** | **<0.001** | | |
| | n | 36 | 36 | 37 | 37 | 37 | |
| DCA in liver | $\rho$ | 0.83 | 0.97 | 0.90 | 1 | | |
| | $q$ | **<0.001** | **<0.001** | **<0.001** | | | |
| | n | 40 | 42 | 43 | 43 | | |
| TCA in liver | $\rho$ | 0.90 | 0.91 | 1 | | | |
| | $q$ | **<0.001** | **<0.001** | | | | |
| | n | 40 | 42 | 43 | | | |
| DCA in serum | $\rho$ | 0.87 | 1 | | | | |
| | $q$ | **<0.001** | | | | | |
| | n | 39 | 42 | | | | |
| TCA in serum | $\rho$ | 1 | | | | | |
| | $q$ | | | | | | |
| | n | 40 | | | | | |

Table displays Spearman rank correlation ($\rho$), false discovery rate-corrected significance value ($q$), and the number of data points with matching values in the same animal (n). Empty cell indicates that no correlation value was computed. Dash (-) indicates that the correlation was not significant ($q>0.1$).

**Supplementary Table 4.** Correlations among TCE metabolites and toxicity phenotypes in the liver of TCE-treated mice in a sub-chronic study (100 or 400 mg/kg/d for 1, 2 or 4 wks). Data from vehicle-treated samples were not included in the analyses.

| | | TCA | DCA | TCOH | DCVG | Liver/Body weight ratio | *Acox1* | *Cyp4a10* | Hepato-cellular proliferation |
|---|---|---|---|---|---|---|---|---|---|
| Hepatocellular proliferation | $\rho$ | 0.13 | 0.09 | -0.09 | -0.24 | -0.25 | -0.26 | -0.43 | 1 |
| | $q$ | - | - | - | - | - | - | **0.0515** | |
| | n | 35 | 35 | 32 | 14 | 34 | 28 | 28 | 35 |
| *Cyp4a10* | $\rho$ | 0.65 | 0.58 | 0.36 | 0.50 | 0.68 | 0.39 | 1 | |
| | $q$ | **<0.001** | **0.001** | **0.089** | - | **<0.001** | **0.045** | | |
| | n | 35 | 35 | 31 | 12 | 34 | 35 | 35 | |
| *Acox1* | $\rho$ | 0.44 | 0.45 | 0.48 | 0.11 | 0.34 | 1 | | |
| | $q$ | **0.022** | **0.020** | **0.020** | - | **0.092** | | | |
| | n | 35 | 35 | 31 | 12 | 34 | 35 | | |
| Liver/Body weight ratio | $\rho$ | 0.47 | 0.43 | 0.34 | 0.16 | 1 | | | |
| | $q$ | **0.007** | **0.017** | **0.083** | - | | | | |
| | n | 41 | 41 | 36 | 16 | 41 | | | |
| DCVG | $\rho$ | 0.20 | -0.13 | 0.41 | 1 | | | | |
| | $q$ | - | - | - | | | | | |
| | n | 16 | 16 | 16 | 16 | | | | |
| TCOH | $\rho$ | 0.60 | 0.65 | 1 | | | | | |
| | $q$ | **<0.001** | **<0.001** | | | | | | |
| | n | 37 | 37 | 37 | | | | | |
| DCA | $\rho$ | 0.90 | 1 | | | | | | |
| | $q$ | **<0.001** | | | | | | | |
| | n | 43 | 43 | | | | | | |
| TCA | $\rho$ | 1 | | | | | | | |
| | $q$ | | | | | | | | |
| | n | 43 | | | | | | | |

Table displays Spearman rank correlation ($\rho$), false discovery rate-corrected significance value ($q$), and the number of data points with matching values in the same animal (n). Empty cell indicates that no correlation value was computed. Dash (-) indicates that the correlation was not significant ($q>0.1$).

**Supplementary Figure 1.** Hemosiderin depositions observed in liver from TCE-treated group. Deposition of yellowish-brown pigments was a result of phagocytized red blood cells in macrophages in liver.