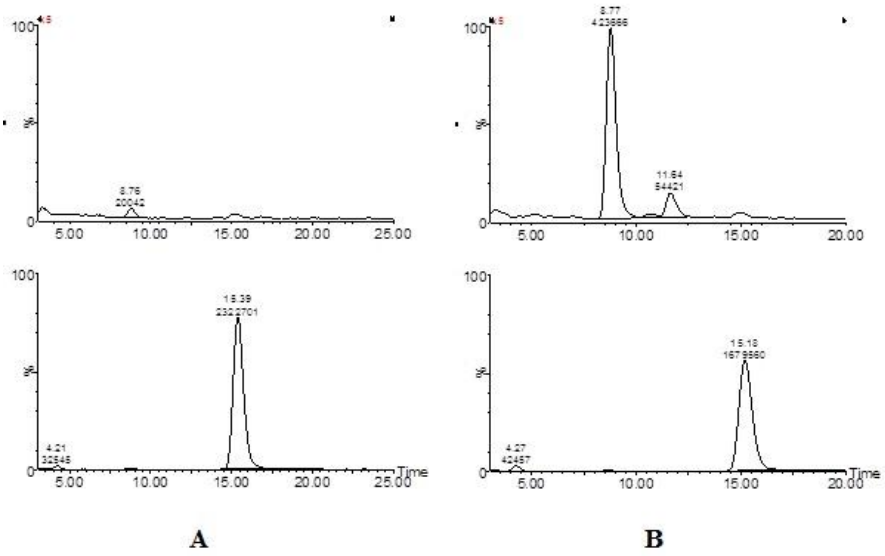
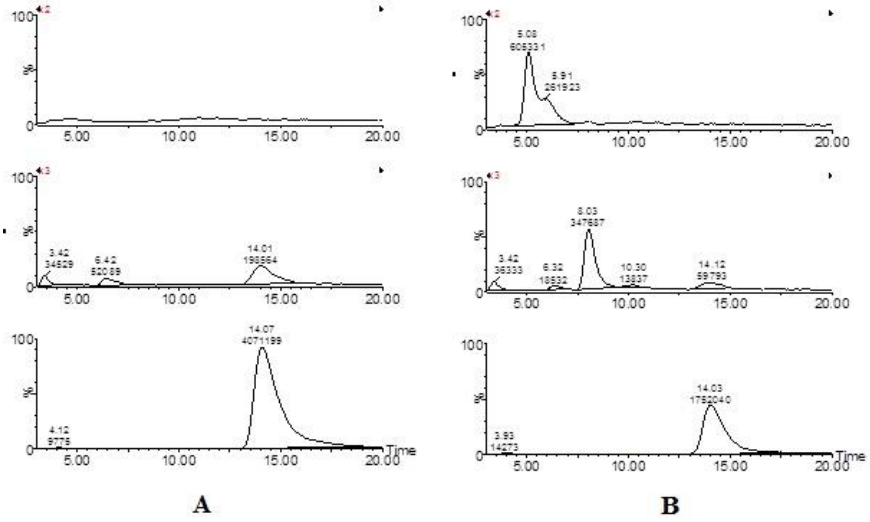
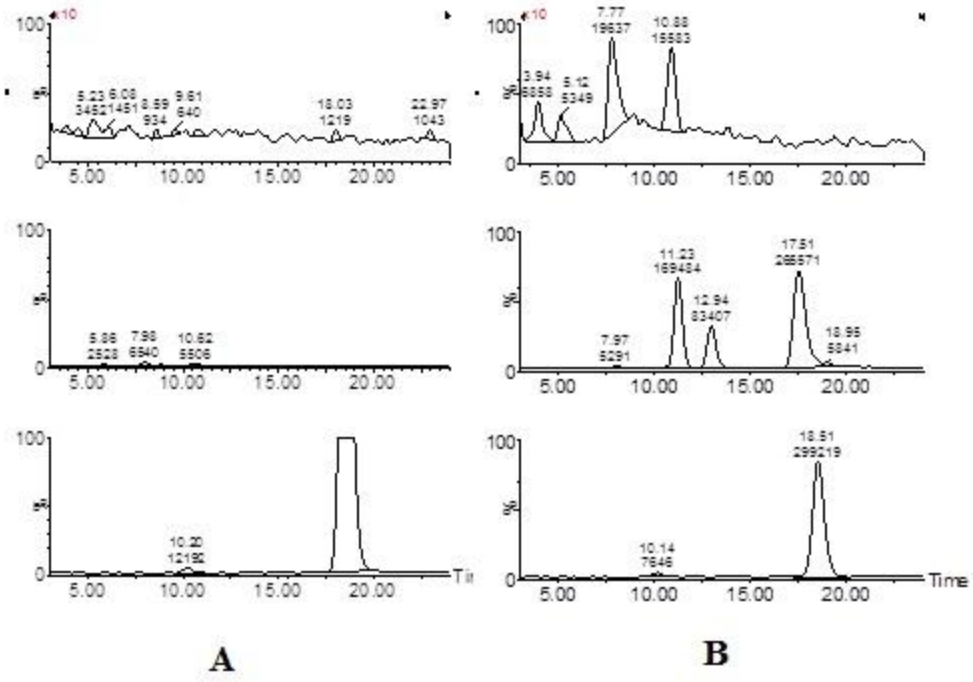


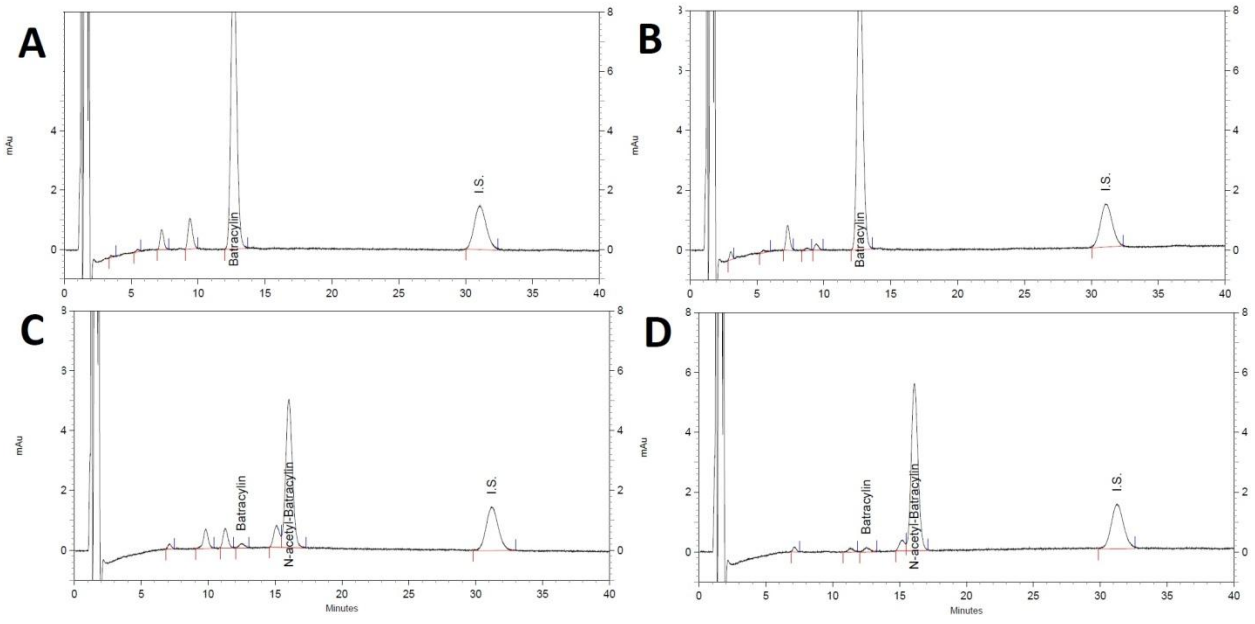
Supplementary Figure 1: Metabolites formed after 120-minute incubation of BAT (10 μM) with H. CYP1B1. Chromatogram intensity is set to 4.0e6. A) LC-MS chromatogram of control microsomes in the presence of NADPH. Top: MS scan m/z 266 (+16, 1-oxygen). Bottom: MS scan m/z 250 (parent); A) LC-MS chromatogram of CYP1B1 microsomes in the presence of NADPH. Top: MS scan m/z 266 (+16, 1-oxygen). Bottom: MS scan m/z 250 (parent).



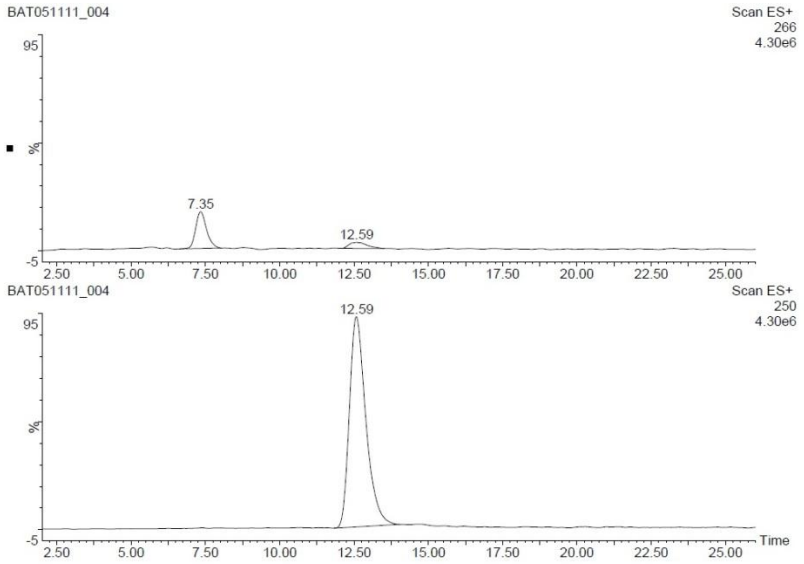
Supplementary Figure 2: Metabolites formed after 120-minute incubation of BAT (10 μM) with liver microsomes from 3MC treated rats. Chromatogram intensity is set to 3.0e6. A) LC-MS chromatogram of RLM in the absence of NADPH. Top: MS scan m/z 282 (+32, 2-oxygen). Middle MS scan m/z 266 (+16 oxygen). Bottom: MS scan m/z 250 (parent); B) LC-MS chromatogram of RLM in the presence of NADPH. Top: MS scan m/z 282 (+32, 2-oxygen). Middle MS scan m/z 266 (+16 oxygen). Bottom: MS scan m/z 250 (parent).



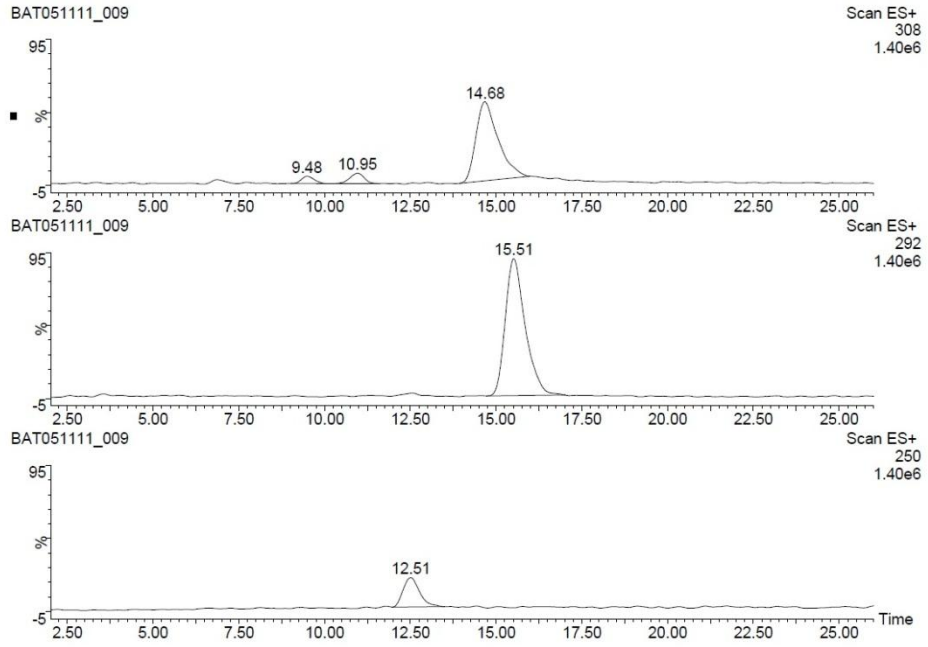
Supplementary Figure 3: Metabolites formed after 120-minute incubation of NAB (10 μM) with liver microsomes from 3MC treated rats. Chromatogram intensity is set to 5.0e5. A) LC-MS chromatogram of RLM in the absence of NADPH. Top: MS scan m/z 324 (+32, 2-oxygen). Middle MS scan m/z 308 (+16 oxygen). Bottom: MS scan m/z 292 (parent); B) LC-MS chromatogram of RLM in the presence of NADPH. Top: MS scan m/z 324 (+32, 2-oxygen). Middle MS scan m/z 308 (+16 oxygen). Bottom: MS scan m/z 292 (parent).



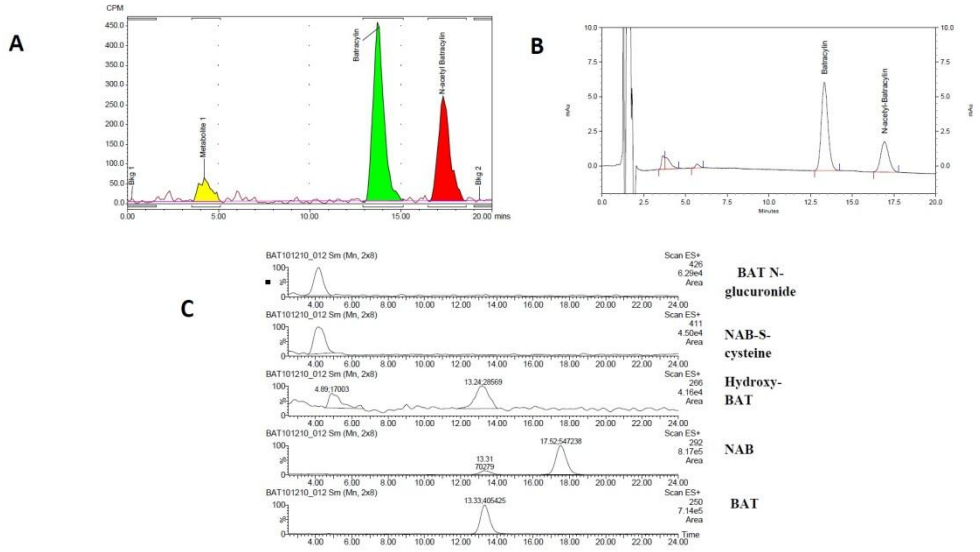
Supplementary Figure 4: UV chromatograms showing metabolites formed after 120-minute incubation with 10 μM BAT (A-B) or NAB (C-D) in the presence of NADPH-fortified rat cDNA expressing microsomes: CYP1A1 (A and C), CYP1A2 (B and D).



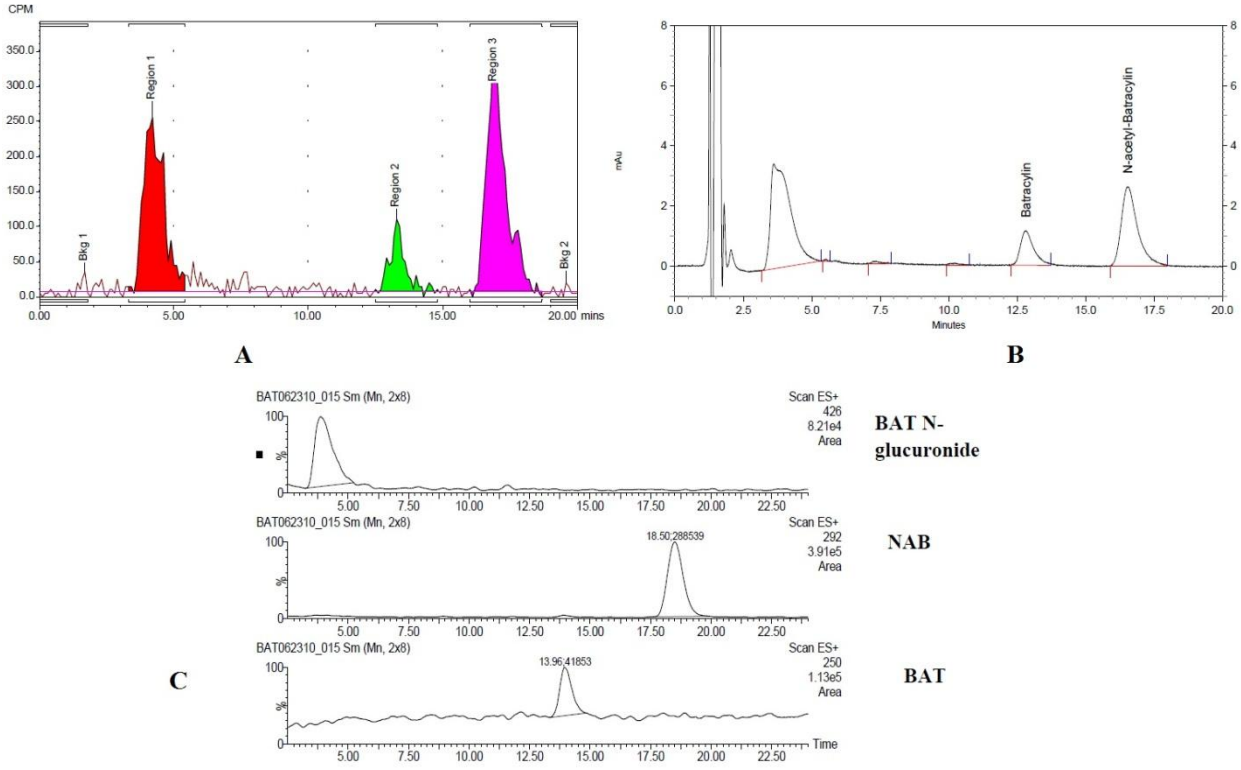
Supplementary Figure 5: LC/MS chromatograms of DLM incubations containing BAT (10 μM). Metabolites formed after 120-minute incubations with DLM in the presence of NADPH (concentrated sample).



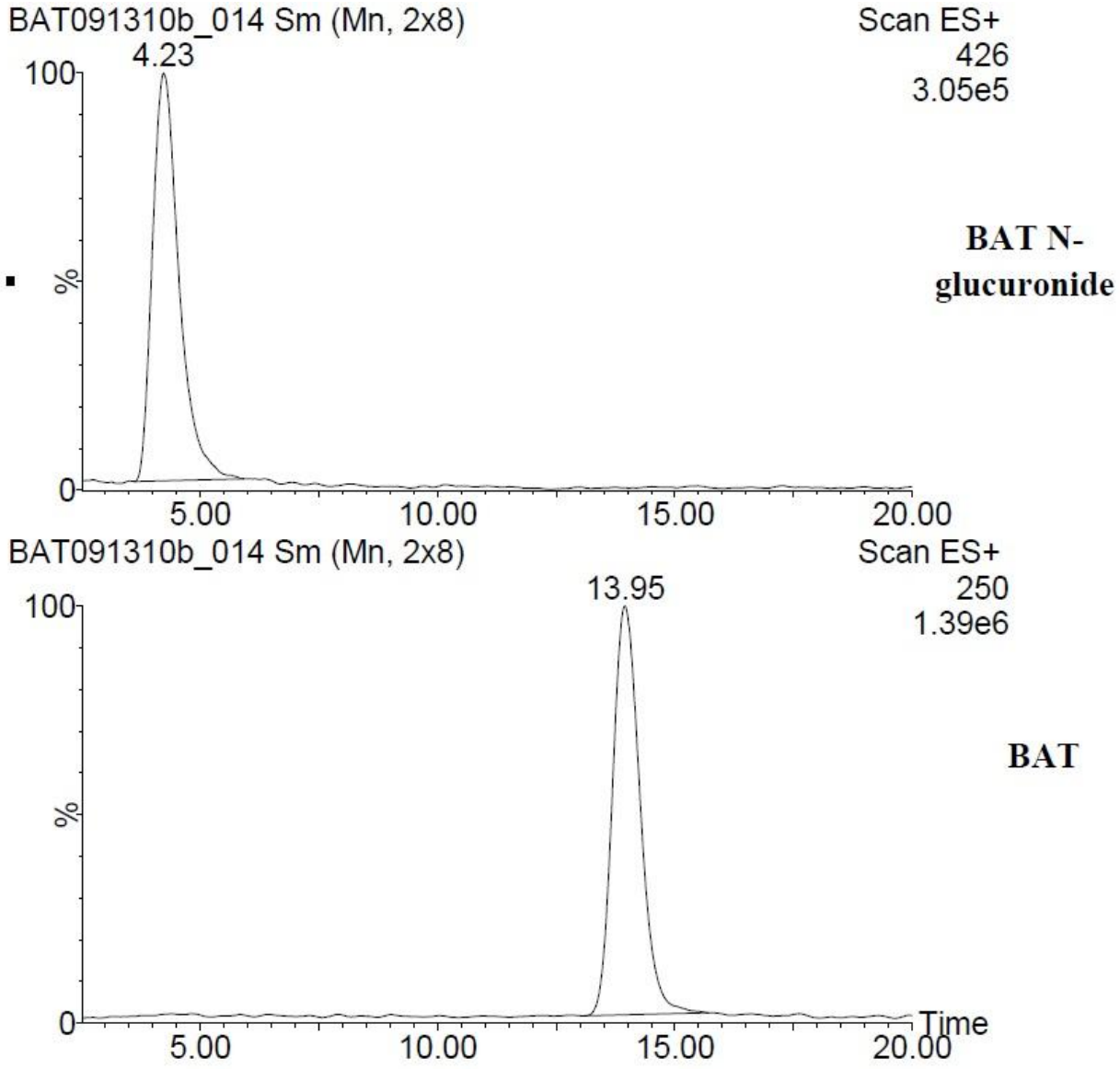
Supplementary Figure 6: LC/MS Chromatograms of metabolites formed in 120-minute incubations with DLM. NAB (10 μM) incubations with NADPH (concentrated sample).



Supplementary Figure 7: Radiochromatogram (A), UV chromatogram (B) and ion chromatograms (C) of the hepatocyte culture supernatant following 6-hours incubation of human hepatocytes with 10 µM 14C-BAT (A, B) or in parallel cold incubations (C).



Supplementary Figure 8: Radiochromatogram (A), UV chromatogram (B) and ion chromatograms (C) of the hepatocyte culture supernatant following 6-hr incubation of SD rat hepatocytes with 10 µM 14C-BAT (A, B) or in parallel cold incubations (C). Supplementary Figure 8: Radiochromatogram (A), UV chromatogram (B) and ion chromatograms (C) of the hepatocyte culture supernatant following 6-hr incubation of SD rat hepatocytes with 10 µM 14C-BAT (A, B) or in parallel cold incubations (C).



Supplementary Figure 9: Dog hepatocytes incubated with 25 μM BAT sent from NCI.