Metabolism and Distribution of Benzo[*a*]pyrene-7,8-dione (B[*a*]P-7,8-dione) in Human Lung Cells by Liquid Chromatography Tandem Mass Spectrometry: Detection of an Adenine B[*a*]P-7,8dione Adduct.

Meng Huang, [†] Xiaojing Liu, [‡] Sankha S. Basu, [‡] Li Zhang, [†] Mary E. Kushman, [†] Ronald G. Harvey, [§] Ian A. Blair, [‡] and Trevor M. Penning ^{*,†}

[†] Center of Excellence in Environmental Toxicology and [‡] Center for Cancer Pharmacology,

Department of Pharmacology, Perelman School of Medicine, University of Pennsylvania, Philadelphia, Pennsylvania 19104, United States

[§] The Ben May Department for Cancer Research, University of Chicago, Chicago, Illinois 60637, United States

Supporting Information Available

Distribution of $1,3-[^{3}H_{2}]-B[a]P-7,8$ -dione radioactivity in three human lung cell lines (Figure S-1).

HPLC radio-chromatograms and UV chromatograms (348 nm) of extracts from organic phase of media in H358 cells (Figure S-2) and HBEC-KT cells (Figure S-3).

Figure S-1. Distribution of 2 μ M 1,3-[³H₂]-B[*a*]P-7,8-dione in A549 (A), H358 (B) and HBEC-KT (C) cells. (\blacklozenge : aqueous phase of media; \blacksquare : organic phase of media; \blacktriangle : cell lysate pellets; *: aqueous phase of cell lysate supernatants; \bullet : organic phase of cell lysate supernatants.) A549, H358 and HBEC-KT cells (5×10^6) were incubated with 1,3-[³H₂]-B[*a*]P-7,8-dione (2 μ M, 1

 \times 10⁵ cpm/nmol, 0.2 % DMSO) in HBSS buffer containing 1 mM sodium pyruvate. The culture media and the cells were collected separately over time and were extracted with ethyl acetate before counting. The mean ± SD for triplicate determinations are shown.

Figure S-2. HPLC radio-chromatogram (A) and UV chromatogram (348 nm) (B) of extracts from organic phase of media in H358 cells at 24h. H358 cells (5×10^{6}) were treated with [1,3-³H]-B[*a*]P-7,8-dione (2 μ M, 1 × 10⁵ cpm/nmol, 0.2 % DMSO) in the same manner as described in the legend of Figure 1. The culture media were collected at 24 h, and subsequently acidified with 0.1% formic acid before extraction with ethyl acetate. The extracts were analyzed on a HPLC-UV-RAM.

Figure S-3. HPLC radio-chromatogram (A) and UV chromatogram (348 nm) (B) of extracts from organic phase of media in HBEC-KT cells at 24h. HBEC-KT cells (5×10^6) were treated with $[1,3-^{3}H]$ -B[*a*]P-7,8-dione (2 μ M, 1 \times 10⁵ cpm/nmol, 0.2 % DMSO) in the same manner as described in the legend of Figure 1. The culture media were collected at 24 h, and subsequently acidified with 0.1% formic acid before extraction with ethyl acetate. The extracts were analyzed on a HPLC-UV-RAM.





Figure S-2.



Figure S-3.