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Supplemental Material

Risk-Based Chemical Ranking and Generating a Prioritized Human Exposome Database

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Figure S1. Relative contributions of exposure and LD₅₀ prediction uncertainty to differences between the 95th percentile and median PrHQ. Monte Carlo analysis of both exposure and LD₅₀ prediction uncertainty gives distributions that can be characterized by the ratio of the PrHQ for the 95th percentile to the median.

Figure S2. Database parameter selection display function.

Figure S3. Searching functions of HExpMetDB GUI. Using DHEP (117-81-7) as an example: (A) searching a chemical and its parameters by mass-charge-ratio (m/z); (B) searching predicted metabolites of a single chemical using the metabolite search module; and (C) searching predicted metabolites by the m/z.

Additional File- Excel Document