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Supplemental Material

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

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Text S1. Graphical User Interface (GUI) installation

The GUI installer requires Java 8 (https://www.oracle.com/java/technologies/javase/javase-jdk8-downloads.html) under Windows or Mac OS operating system. Our first version of GUI package can be downloaded in the Supplementary Information named "HExpMetDB.rar". The most updated GUI package is also available as an open access Java library at:

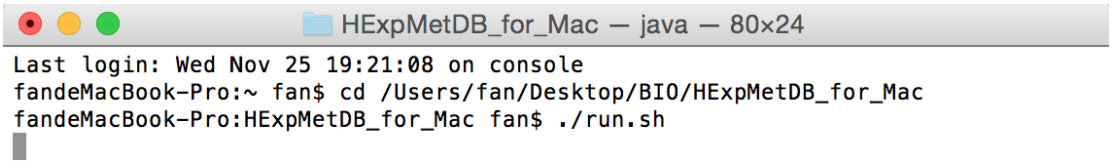
https://github.com/FangLabNTU/HExpMetDB

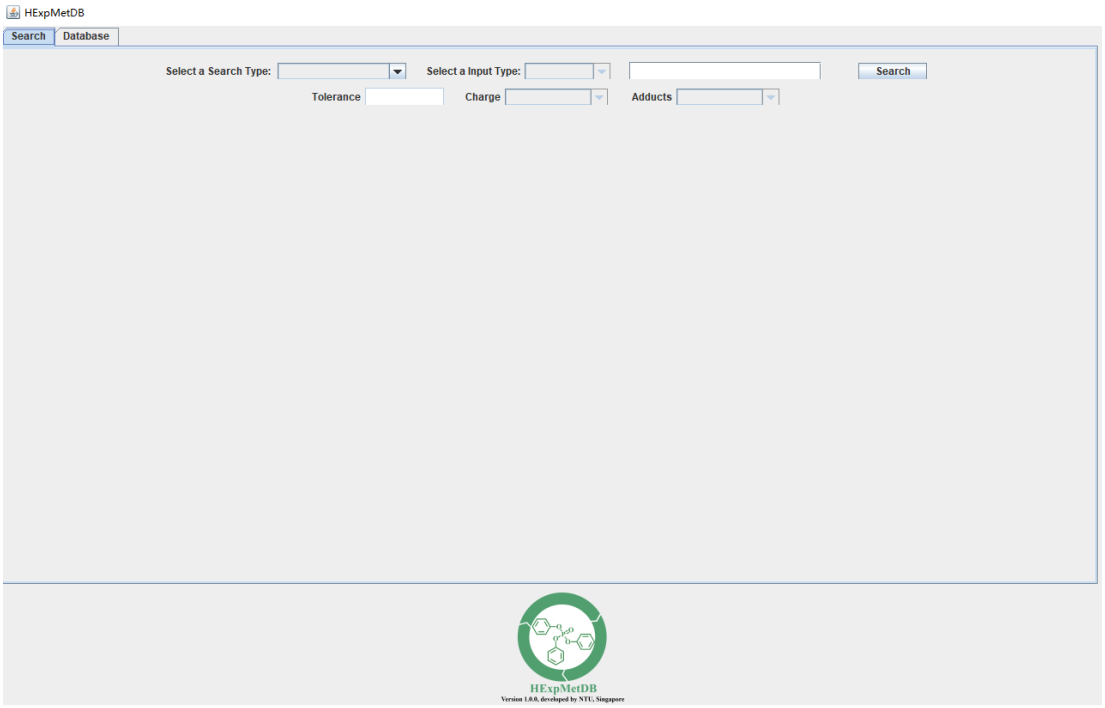
Step 1: Download package "HExpMetDB.zip for Win" or "HExpMetDB.zip for Mac" and unzip the file.

Step 2: For Windows system: Open the file → Double lick the "run.bat" file, then the GUI will be automatically opened (maybe wait for a few seconds);

For **Mac OS** system: The snapshot of the file list can be found below. Open "Terminal.app" → Enter "cd+space+file path of "run.sh" in HExpMetDB package + carriage return" (e.g., cd+space+/Users/fan/Desktop/BIO/HExpMetDB_for_Mac+carriage return) → Enter "./run.sh", then the GUI will be opened (shown as following figure).

copyright	2020/6/21 3:00
cyp450_AB	2020/11/23 15:50
ecbased_AB	2020/11/23 15:46
HExpMetDB.class	2020/11/25 15:44
HExpMetDB.java	2020/11/25 15:44
hgut_AB	2020/11/23 15:42
Index$1.class	2020/11/25 15:44
Index$2.class	2020/11/25 15:44
Index$3.class	2020/11/25 15:44
Index.class	2020/11/25 15:44
phaseII_AB	2020/11/23 15:48
run	2020/11/25 15:46
run.sh	2020/11/25 15:50
total_matter	2020/11/25 11:00





Text S2. HExpMetDB Functionality

We have developed a Java GUI client program running on JVM 1.8 under Windows and Mac OS operating system. Upon startup, it preloads the detailed information of all substances into a table. Users can pose queries by specifying a few keywords and retrieve their desired information in milliseconds. The HExpMetDB GUI contains compound search tab and database tab: When users open the database tab, users can browse our database and choose the parameters they want to display on the interface (Figure S2). Under the search tab, users can search chemicals as demonstrated in Figure S3. Specifically, the GUI allows users to do the following functions: (1) a single chemical search using a Chemical Abstracts Service Registry Number (CASRN), molecular formula, mass-charge-ratio (m/z) or adduct (Figure S3A); (2) searching predicted metabolites of a single chemical using the metabolite search module (Figure S3B); (3) searching predicted metabolites using the m/z, adducts or molecular formula (Figure S3C). Information including human exposure, animal toxicity LD_{50}, ToxPi Score, their HQ (Hazard Quotient, LD_{50} based) and Risk Index (ToxPi based) values as well as their ranking and confidence intervals were all given in "HExpMetDB" GUI. This platform would assist in a broad array of human exposure research and to facilitate chemical risk prioritization and metabolite identification.

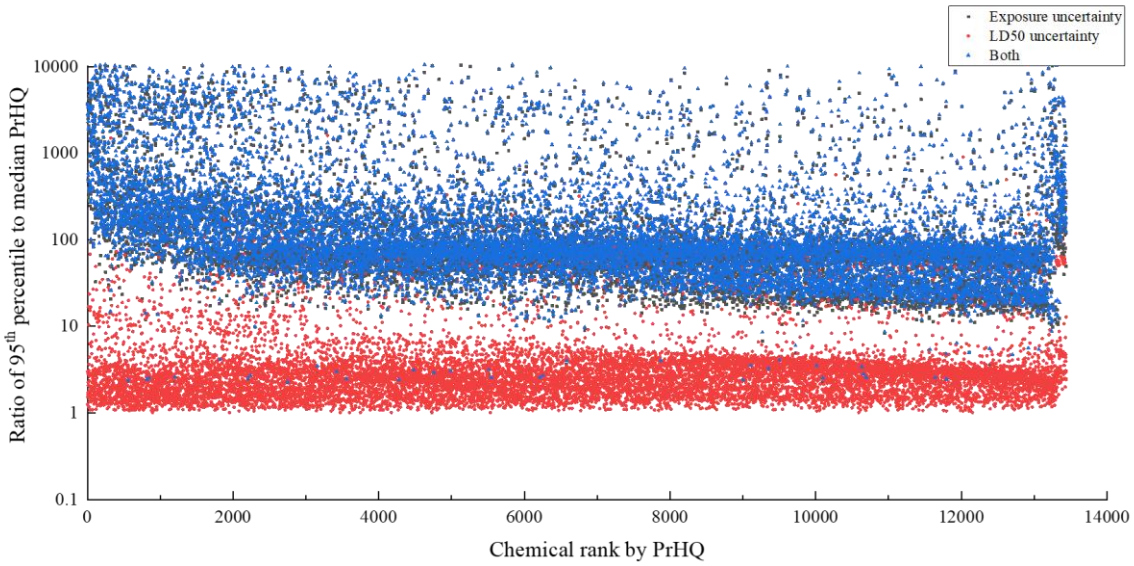
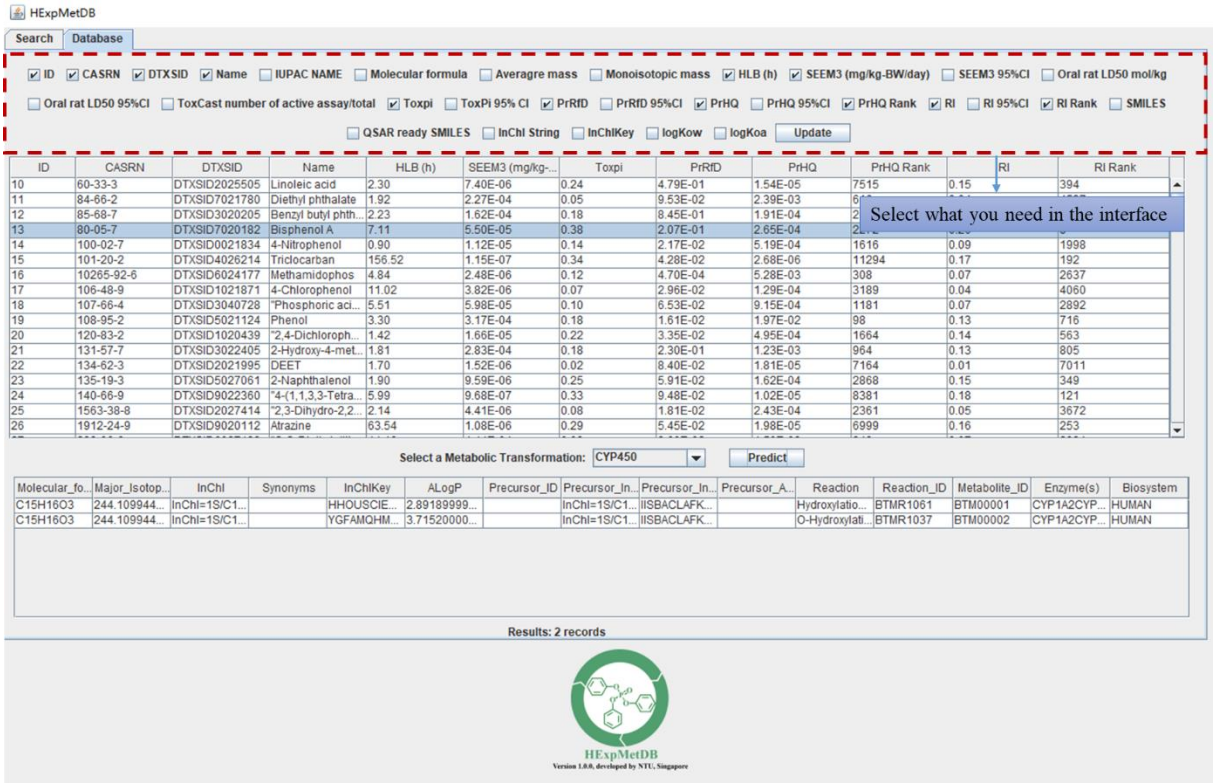
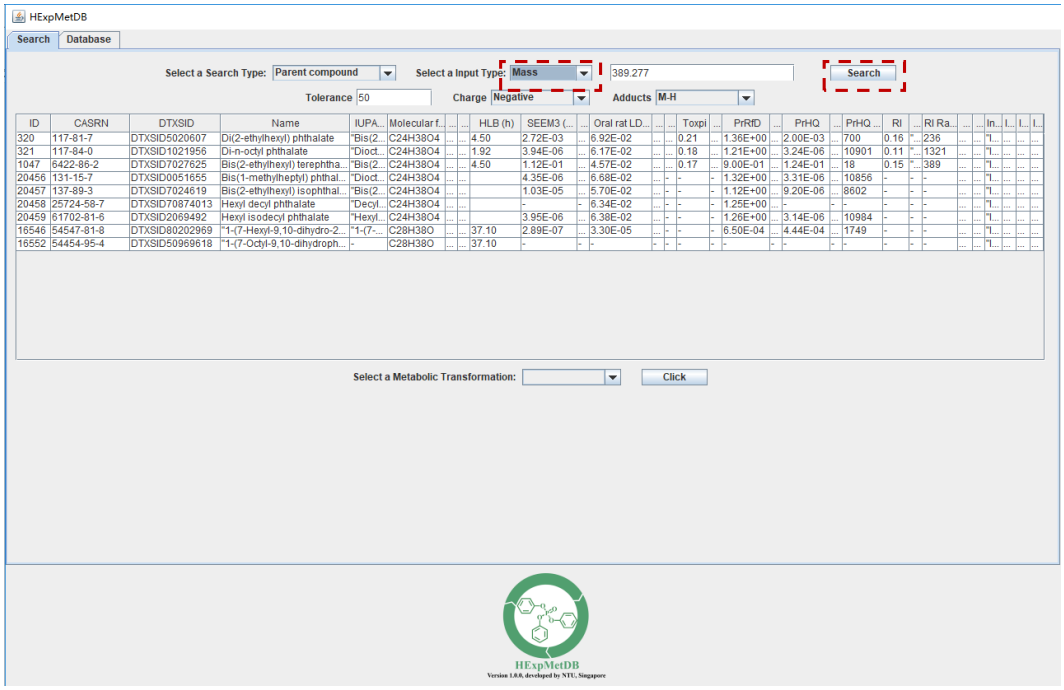


Figure S1. Relative contributions of exposure and LD_{50} prediction uncertainty to differences between the 95th percentile and median PrHQ. Monte Carlo analysis of both exposure and LD_{50} prediction uncertainty gives distributions that can be characterized by the ratio of the PrHQ for the 95th percentile to the median.



1 **Figure S2.** Database parameter selection display function.

A



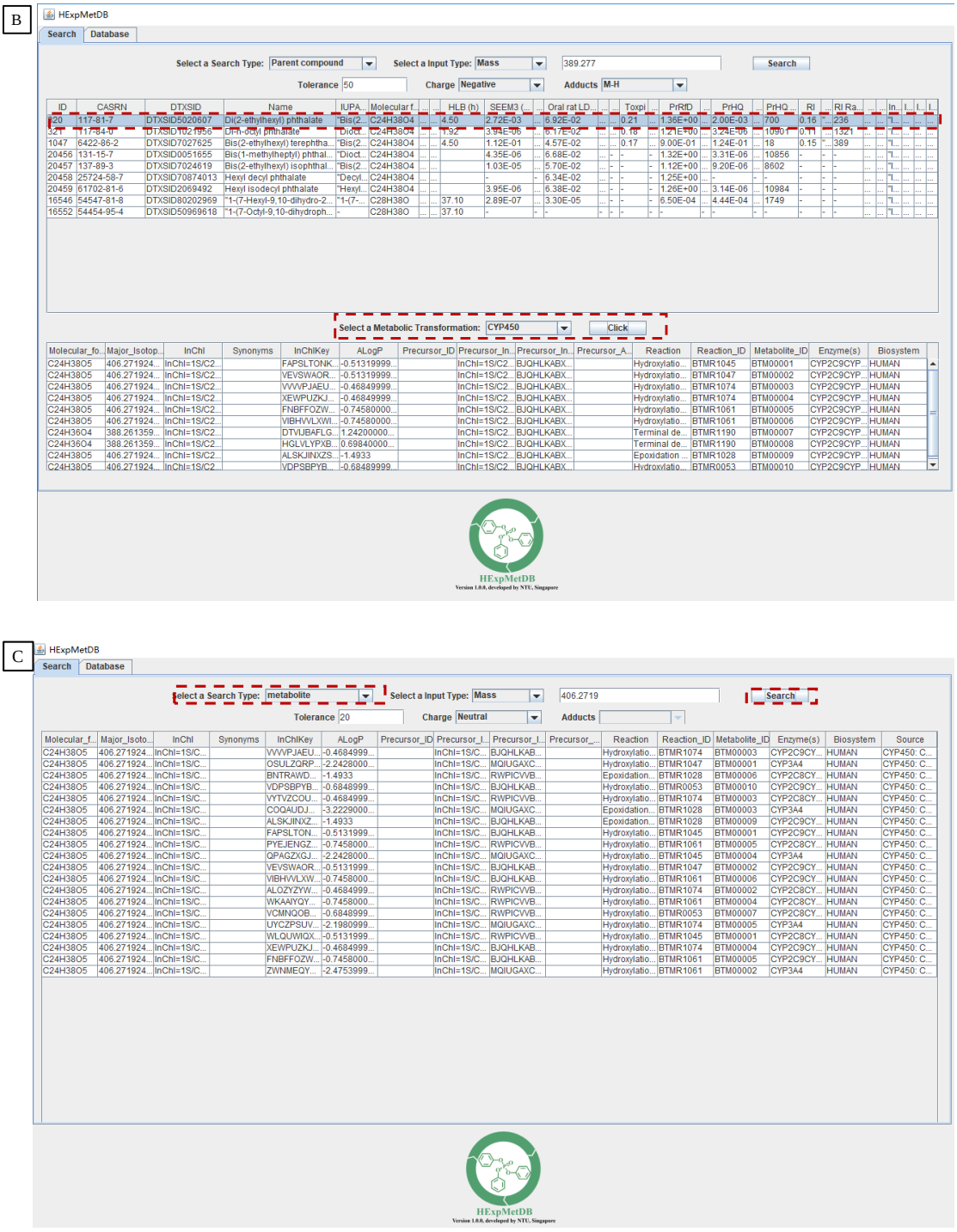


Figure S3. Searching functions of HExpMetDB GUI. Using DHEP (117-81-7) as an example: (A) searching a chemical and its parameters by mass-charge-ratio (m/z); (B) searching predicted metabolites of a single chemical using the metabolite search module; and (C) searching predicted metabolites by the m/z.