

# Charge for EPI Suite Review

## General charge to the Science Advisory Board

The Agency is primarily interested in the SAB's review of the supporting science, functionality, and appropriate use of EPI Suite. While SAB should feel free to comment broadly, specific responses to the following technical questions would be welcomed.

1. Supporting Science
  - A. Comprehensiveness
    - i. Are there additional properties which should be included in upgrades to EPI Suite for its various specified uses (PMN, P2, ???)? (An example might be Characteristic Travel Distance.) Can any be dropped?
    - ii. Are there additional sets of existing measured data which should be included in upgrades to EPI Suite? Are there specific measurements with the potential to improve EPI Suite estimates so much that an effort should be made to collect them?
    - iii. Are there other capabilities that should be included in upgrades to EPI Suite? The Agency is especially interested in the SAB's views on uncertainty analysis and if/how information on how good the estimates are can be conveyed to users.
  - B. Method accuracy and validation
    - i. Is the accuracy of the modules in the EPI Suite sufficient for its various specified uses?
    - ii. Have the modules been adequately validated, and have they been published in the peer-reviewed technical literature or elsewhere?
    - iii. Are some modules more accurate/better validated than others, and if so, which need more work?
    - iv. To the extent that modules work together to generate estimates, do they do so correctly?
  - C. Estimation Methods and Alternates

- i. Are the estimation methods in EPI Suite up-to-date and generally accepted by the scientific community for its various specified uses?
- ii. Are there other estimation methods which should be considered in upgrading EPI Suite?

2. Functionality (Program documentation; user interface; convenience features)

- A. How convenient is the software and does it have all the necessary features?
- B. Are there places where EPI Suite user's guide (and other program documentation) does not clearly explain EPI's design and use? How can these be improved?
- C. Are there aspects of the user interface (i.e., the initial, structure/data entry screen; and the results screens) that need to be corrected, redesigned, or otherwise improved? Do the results screens display all the desired information?
- D. Currently one enters a chemical structure in EPI Suite using SMILES and CAS; are there other ways to describe the structure (e.g., ability to input a structure by drawing it), that should be added?
- E. The EPI Suite has many convenience features, such as the ability to accept batchwise entry of chemical structures, and automatic display of measured values for some (but not all) properties. Are there other features that could enhance convenience and overall utility for users?
- F. Are property estimates expressed in correct/appropriate units?
- G. Is adequate information on accuracy/validation conveyed to the user by the program documentation and/or the program itself?

3. Appropriate Use

- A. Currently Identified Uses: review of PMNs, P2 decisions, predicting physical/chemical properties and environmental fate and transport properties for HPV Challenge chemicals, to begin the assessment of exposure, and other routine OPPT uses. It is important to understand that EPI Suite is intended to be used in the absence of

measured data and not take their place.

- i. Is the science incorporated into EPI Suite adequate for each of these current uses?
- ii. If not, what improvements are needed to make EPI Suite adequate and what alternate approach could be used in the interim?

B. Potential Additional Uses