High Throughput Screening Assays Readme File for Supporting Data Files

Introduction

As part of the <u>West Virginia Chemical Spill research program</u>, NTP evaluated four chemicals related to the Elk River chemical spill in West Virginia in cell-based, high throughput screening (HTS) assays to identify potential toxicological/biological properties. A summary of the study findings was reported in a <u>December 2014</u> update.

Data Files Available for Download

A set of supporting data files for high throughput screening assays is available on this NTP data
Web page. The raw data and conclusions from the assays are available as Excel files. The key worksheet within the raw data file provides an explanation of variables. Links are provided in the conclusions file to protocols for each assay in PubChem. The concentration-response data of Elk River chemicals are analyzed using the developed pipeline. 1

Files can be downloaded individually or as a complete set for the study by using the *Download All* button. If you need assistance with the data files, please contact CEBS-Support@mail.nih.gov.

Access to Data Online

All data are available in the <u>Chemical Effects in Biological Systems (CEBS) database</u>. Access to the data is available by searching CEBS using the study numbers. Data from additional studies conducted on the chemicals are accessible by searching CEBS using the Chemical Abstracts Service Registry Number (CASRN) or chemical name (see Table 1).

Table 1. Elk River Spill Chemicals Tested for High Throughput Screening Assays

CASRN	Chemical Name
34885-03-5	4-Methylcyclohexanemethanol
770-35-4	Propylene glycol phenyl ether
105-08-8	1,4-Cyclohexanedimethanol
94-60-0	Dimethyl 1,4-cyclohexanedicarboxylate

Suggested Citation

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http://tools.niehs.nih.gov/cebs3/wvspill/index.cfm?action=main.dataReview&bin_id=751 [accessed *INSERT DATE*].

¹ Hsieh, J.-H.; Sedykh, A.; Huang, R.; Xia, M.; Tice, R. R. A Data Analysis Pipeline Accounting for Artifacts in Tox21 Quantitative High-Throughput Screening Assays. J Biomol Screen 2015, 1087057115581317.