

6 Supporting Information

Supplemental Material S1: Toxicity data for all chemicals is provided as a comma-separated value (csv) file in which rows correspond to chemicals. The first two columns include the DSSTox compound identifier (dsstox_cid) and the chemical name (name). Each of the remaining columns represent a target-organ toxicity in a particular repeat-dose testing study. Chemicals that are positive/negative/untested for a target-organ toxicity classification are denoted by 1/0/missing values, respectively.

Supplemental Material S2: ToxCast bioactivity data for all chemicals is provided as a comma-separated value (csv) file in which rows correspond to chemicals. The first two columns include the DSSTox compound identifier (dsstox_cid) and the chemical name (name). The remaining columns show ToxCast bioactivity assays. Chemicals that are positive/negative/untested in ToxCast are denoted by 1/0/missing value, respectively.

Supplemental Material S3: Chemical fingerprint data is provided as a comma-separated value (csv) file in which rows correspond to chemicals. The first two columns include the DSSTox compound identifier (dsstox_cid) and the chemical name (name). The remaining columns show chemical structure fingerprints. Chemicals that are positive/negative for a structure descriptor are denoted by 1/0, respectively.

Supplemental Material S4: Chemotype data is provided as a comma-separated value (csv) file in which rows correspond to chemicals. The first two columns include the DSSTox compound identifier (dsstox_cid) and the chemical name (name). The remaining columns show chemotypes. Chemicals that are positive/negative for a chemotype are denoted by 1/0, respectively.

Supplemental Material S5: Cross-validation performance results for the minimal data set across all machine learning algorithms, descriptor types, and target organ outcomes. This file provides the numeric data for the visualization shown in Figure 3 of the main manuscript.

This material is available free of charge via the internet at <http://pubs.acs.org>.