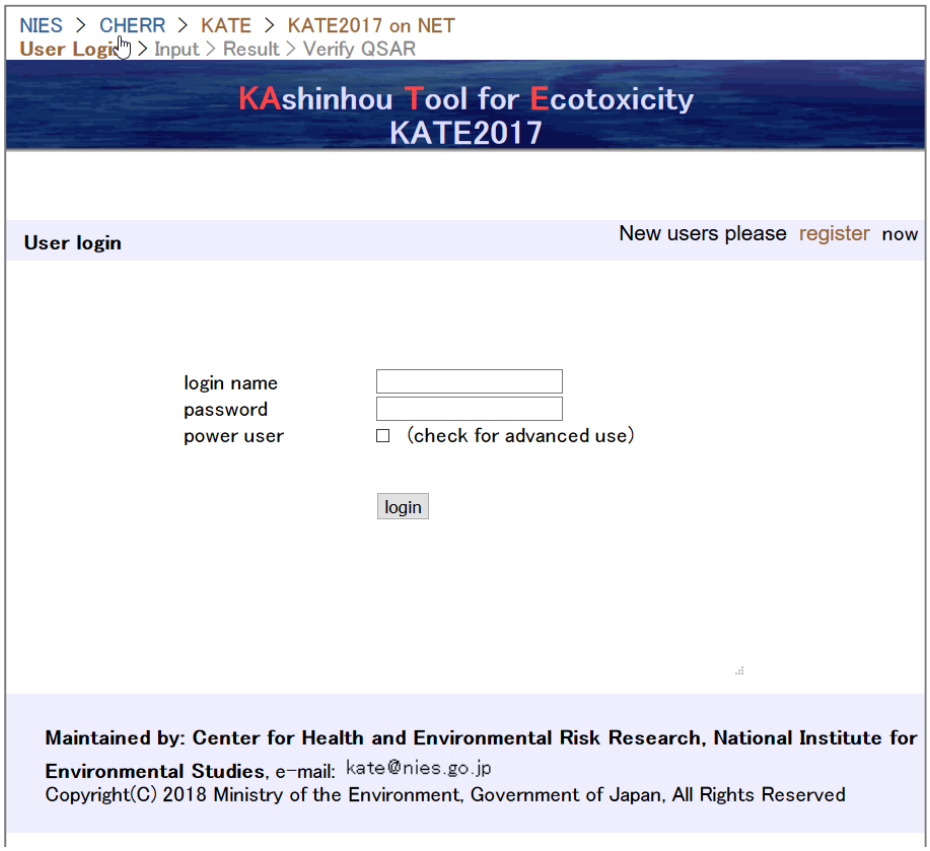
KATE2017 on NET beta version

http://kate.nies.go.jp

https://kate2.nies.go.jp/nies/

Operating manual 2018.03.29 (Modified on 2019.01.30)



- KATE2017 on NET was developed to predict the following ecotoxicity values:
  - 50% effective concentration (EC_{50}) and no-observed-effect concentration (NOEC) in the 72 h algal growth inhibition test
  - EC_{50} in the 48 h *Daphnia* acute immobilization test
  - NOEC in the 21 d *Daphnia magna* reproduction test
  - 50% lethal concentration (LC_{50}) in the 96 h fish acute toxicity test
  - NOEC in the fish early-life-stage toxicity test

Note that values predicted by KATE cannot be used to satisfy the requirement for ecotoxicity data that are necessary for notification regarding new chemical substances under the Japanese Act on the Evaluation of Chemical Substances and Regulation of Their Manufacture, etc. (Chemical Substances Control Law).

For inquiries about KATE, contact the Center for Health and Environmental Risk Research, National Institute for Environmental Studies at kate@nies.go.jp.

KATE2017 on NET beta version

KATE2017 on NET beta version is an updated version of KATE on NET, which is the internet version of KATE2011 (this version is available only in Japanese). The major differences between KATE2017 on NET beta version and KATE on NET are as follows:

■ Added features

• New reference data were added for *Daphnia* (acute) and fish (acute).

• An ecotoxicity predicting function for the following alga and chronic endpoints was added:

Alga: 50% effective concentration (EC_{50}) and no-observed-effect concentration (NOEC) in the algal growth inhibition test (72 h)

Daphnia (chronic): NOEC in the *Daphnia magna* reproduction test (21 d)

Fish (chronic): NOEC in the fish early-life-stage toxicity test

• Toxicity data obtained by means of the limit test (e.g., a test used to identify compounds that show no effect at the highest concentration used in the test) were added. These data are presented in tables and graphs and are used to determine applicability domains based on chemical substructures.

■ Update of QSAR models

• The language used for chemical substructure searching was changed from Fragment Identification by Tree Structure (FITS) to SMiles ARbitrary Target Specification (SMARTS), and SMARTS substructure searching by means of the Chemistry Development Kit (CDK) was implemented.

• The definitions and classifications of chemical structures for the QSAR models were improved.

~~• For several of the QSARs, the new version uses not only log *P* values but other values such as log BCF as descriptors. In addition, multiple-regression equations, and activity–activity relationships (e.g., an equation to predict the chronic toxicity of a chemical to *Daphnia* by use of the acute toxicity of the chemical to *Daphnia*) have been introduced.~~ (Updated on January 30, 2019)

■ Improvement of displays and operations

~~• A Power User option checkbox was introduced on the login page.~~

~~a. When the box is checked (on), the software operates in an advanced mode (with more functionality) intended for expert users).~~

~~b. When the box is unchecked (off), the software operates in a simple mode intended for non-expert users.~~ (Updated on January 30, 2019)

• Several new pages were added.

1. New User Registration

Before using KATE for the first time, you must register a unique user name and password at https://kate2.nies.go.jp/nies/user_regist_input.php. The user name must have at least five characters.

If you forget your user name or password, you must reregister with a new user name and password. Note that user names that are unused for a long time are periodically removed.

2. Log In

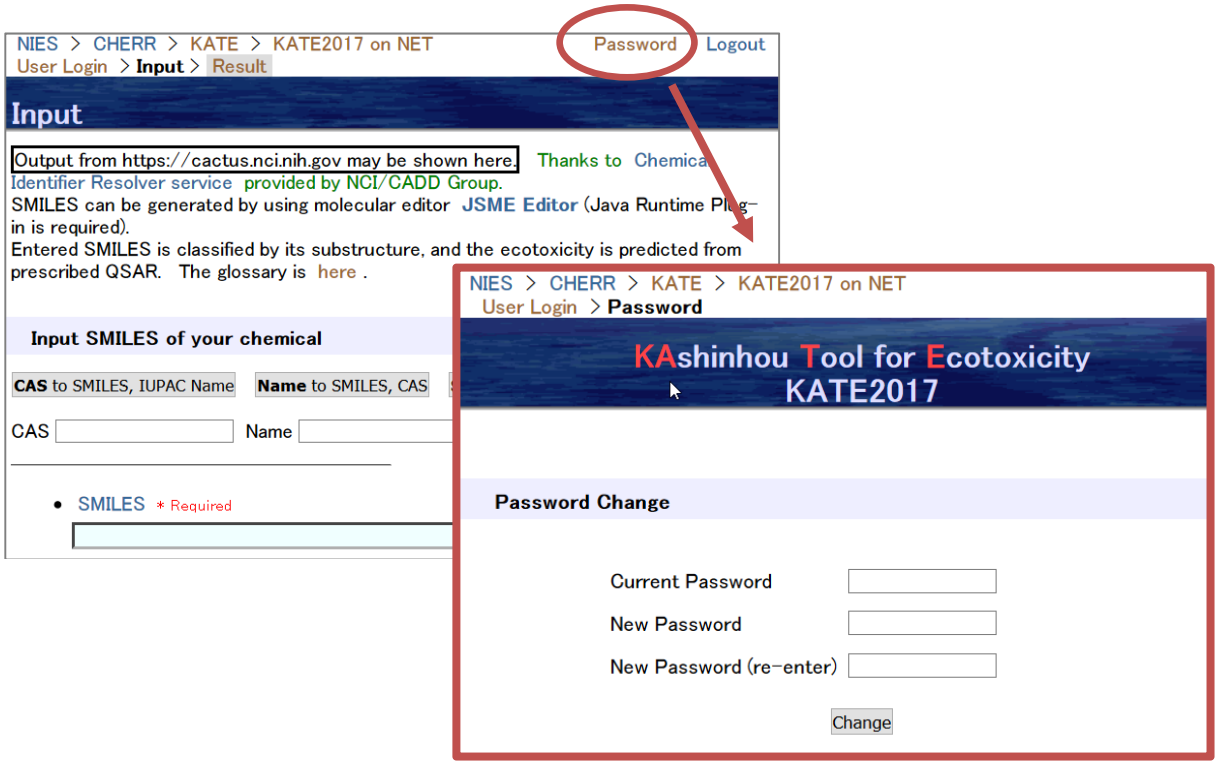
Log in at https://kate2.nies.go.jp/nies/index.php with the user name and password* registered in Step 1.

~~■ Power User option checkbox~~

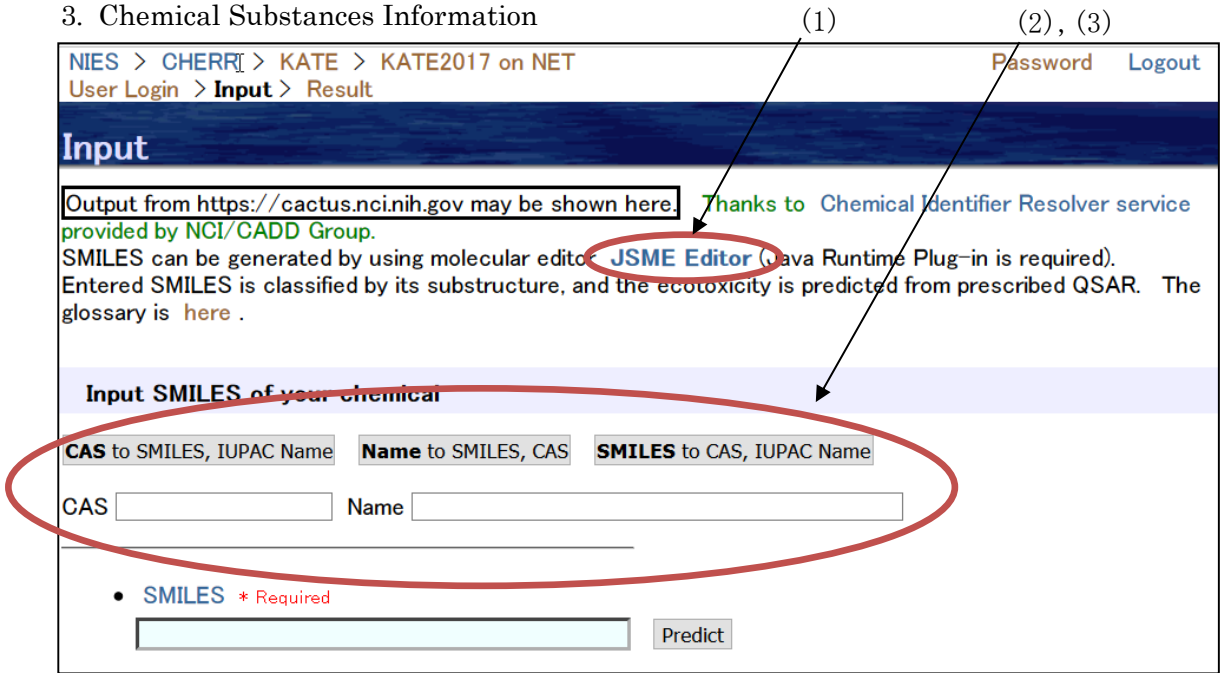
~~a. When the box is checked (on), the software operates in an advanced mode (with more functionality) intended for expert users.~~

~~b. When the box is unchecked (off), the software operates in a simple mode intended for non-expert users.~~ (Updated on January 30, 2019)

*The password can be changed.



3. Chemical Substances Information

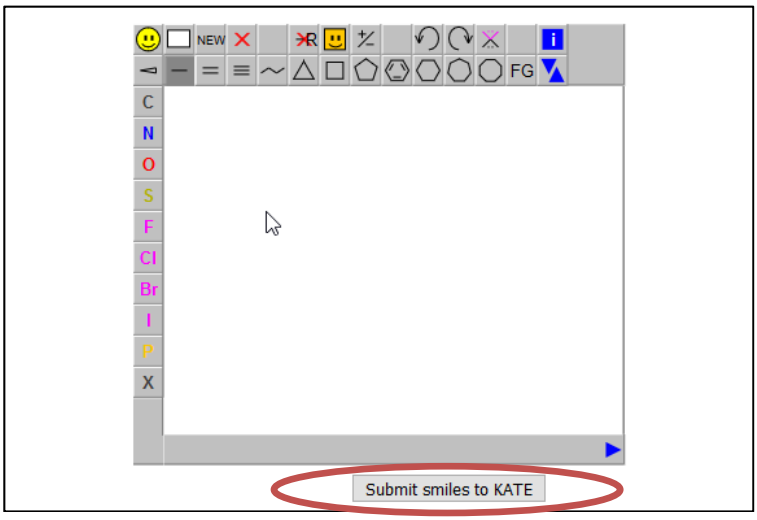


Input the chemical substances information using SMILES. SMILES strings can be generated by using (1) JSME Molecule Editor, (2) the CAS to SMILES, IUPAC Name function, or (3) the Name to SMILES, CAS function. Details are provided below.

Any supplementary information (e.g., log *P*) are displayed on the result page. Such supplementary information is not mandatory.

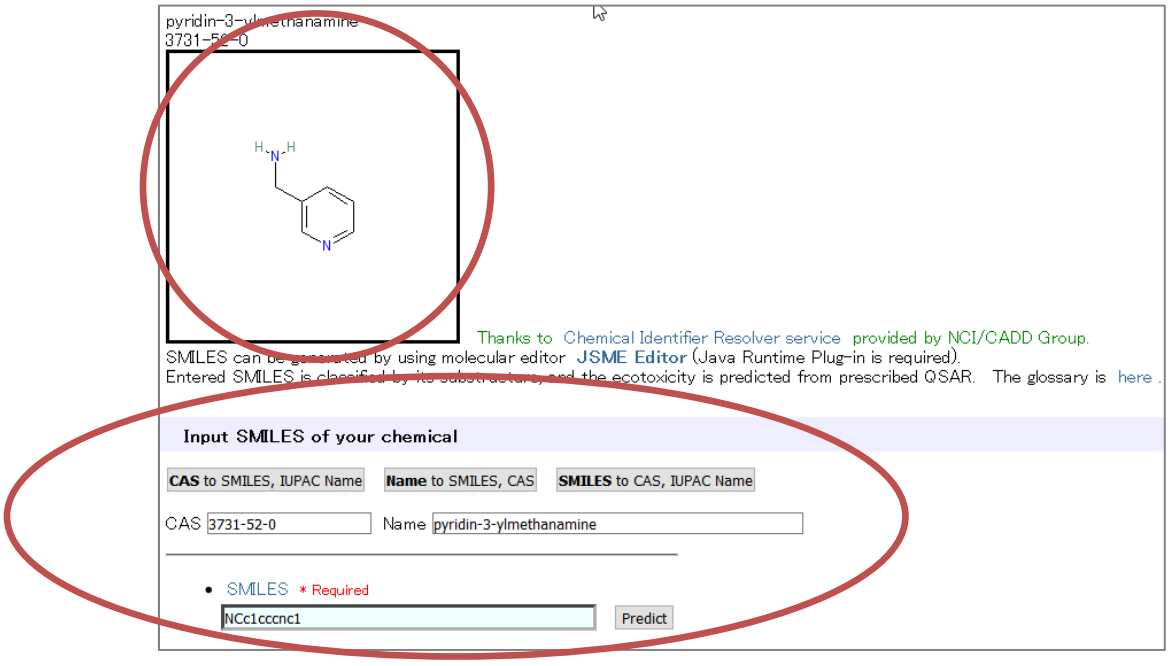
3.1. JSME Molecule Editor. Note that the molecule editor requires the Java Runtime Plug-in.

Draw a chemical structure and click the Submit smiles to KATE button.



3.2. CAS to SMILES, IUPAC Name

Enter a CAS registry number formatted as XXXXX-XX-X (e.g., 27271-55-2) and then click the *CAS to SMILES, IUPAC Name* button to display the chemical structure, IUPAC name, and SMILES string.



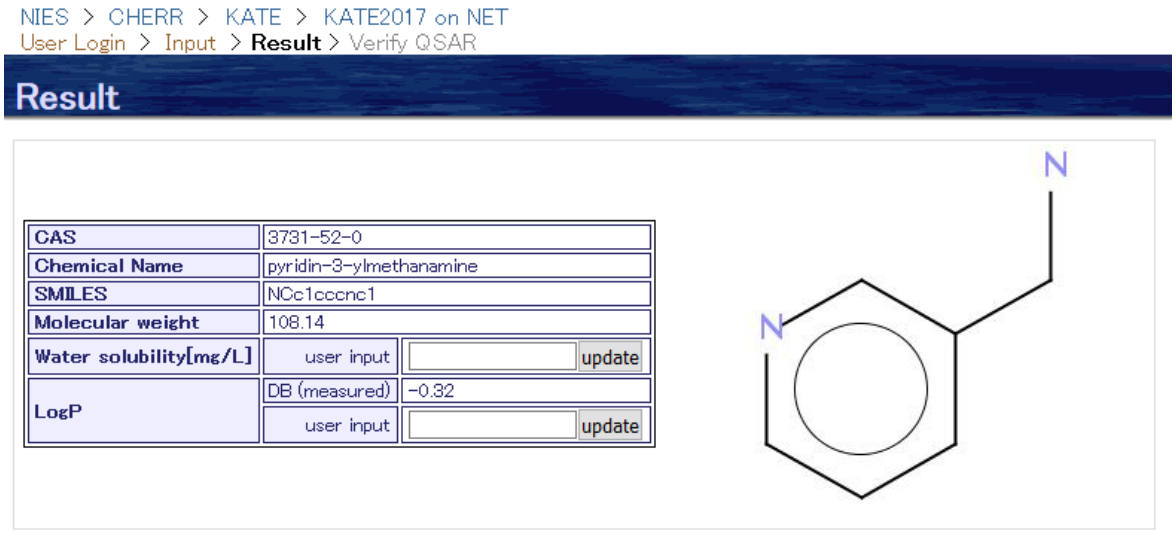
3.3. Name to SMILES, CAS

Enter a name in the Name box and then click the Name to SMILES, CAS button to obtain the chemical structure, CAS registry number, and SMILES string.

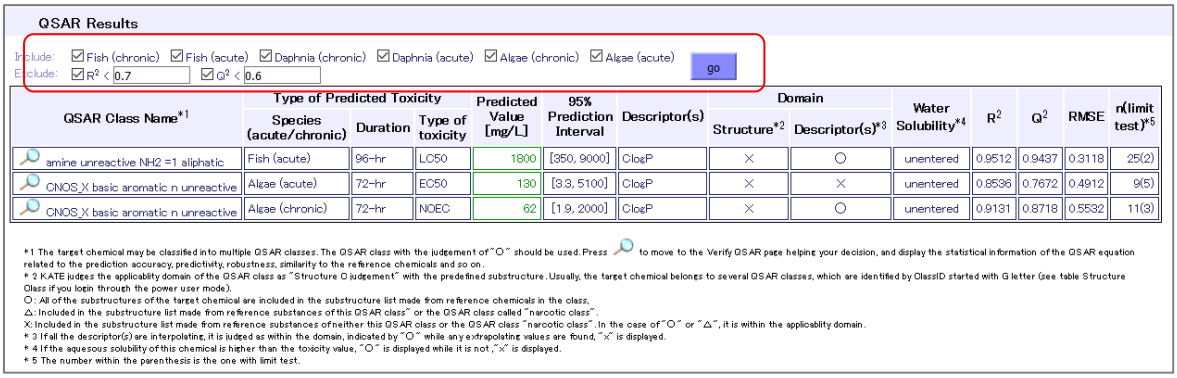
4. Result Page

The top of the result page shows the SMILES string and supplemental information that were inputted, along with the molecular weight calculated from the inputted information.

If you do not input a measured log *P* value of the chemical for which you want to predict the toxicity, KATE will use a ClogP value calculated by means of an algorithm developed by BioByte Co. and included in the ClogP program offered by Daylight Chemical Information Systems. Owing to restrictions in the licensing contract, calculated ClogP values cannot be displayed.



The middle of the result page displays the chemical substance classes, and the Algae (Alga), *Daphnia*, and Fish toxicity values predicted by KATE.

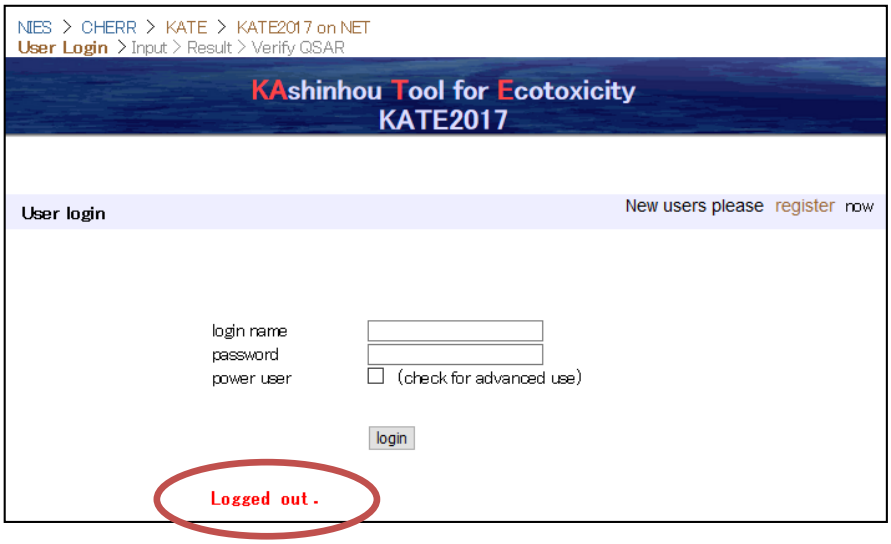


5. Viewing details and Comparison with Reference Substances

On the result page on page 7, click on the magnifying glass icon next to the class category to see the regression line and structural formulas of the reference substances for that class.

6. Log Out

Log out after you finish using KATE. If you terminate your session without logging out, your last set of prediction results will remain on the server. If you forget to log out, you can delete the last set of prediction results by logging in again with the same user name and then logging out.



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