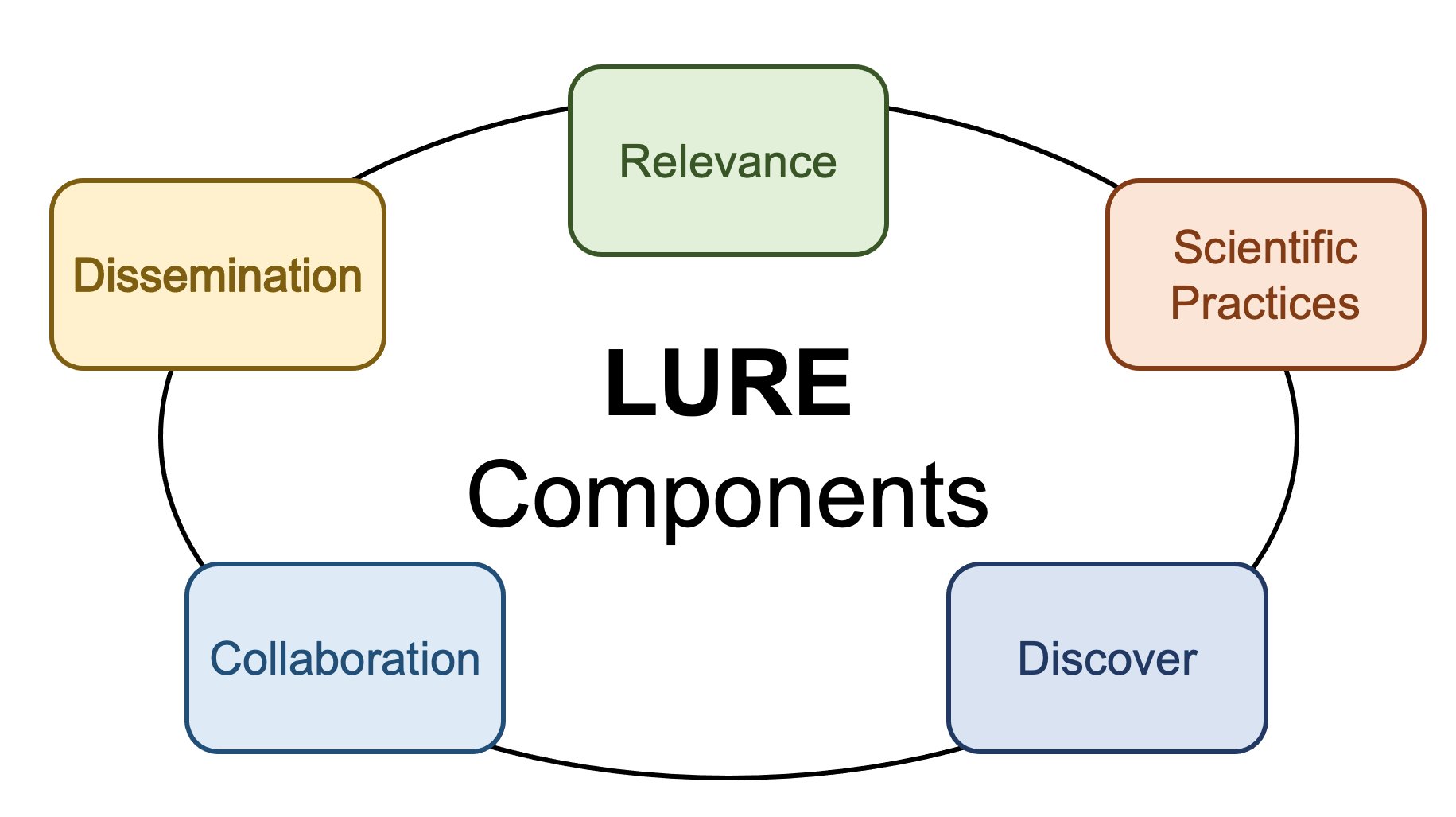
Title: Pharmacokinetics Lab (PK LURE)



**Objectives**

The purpose of this lab is to:

1. Students will be able to conduct searches on publicly available databases and interpret results (Pubchem and SwissADME).
2. Students will be able to compare and contrast chemical ADME properties in small groups to determine which chemical is more likely to have a biological effect in the consumer.
3. Students will formulate hypotheses to determine outcomes of chemical interactions within the body.
4. Students will conduct literature searches to support their formulated hypothesis.

**Lab Procedures**

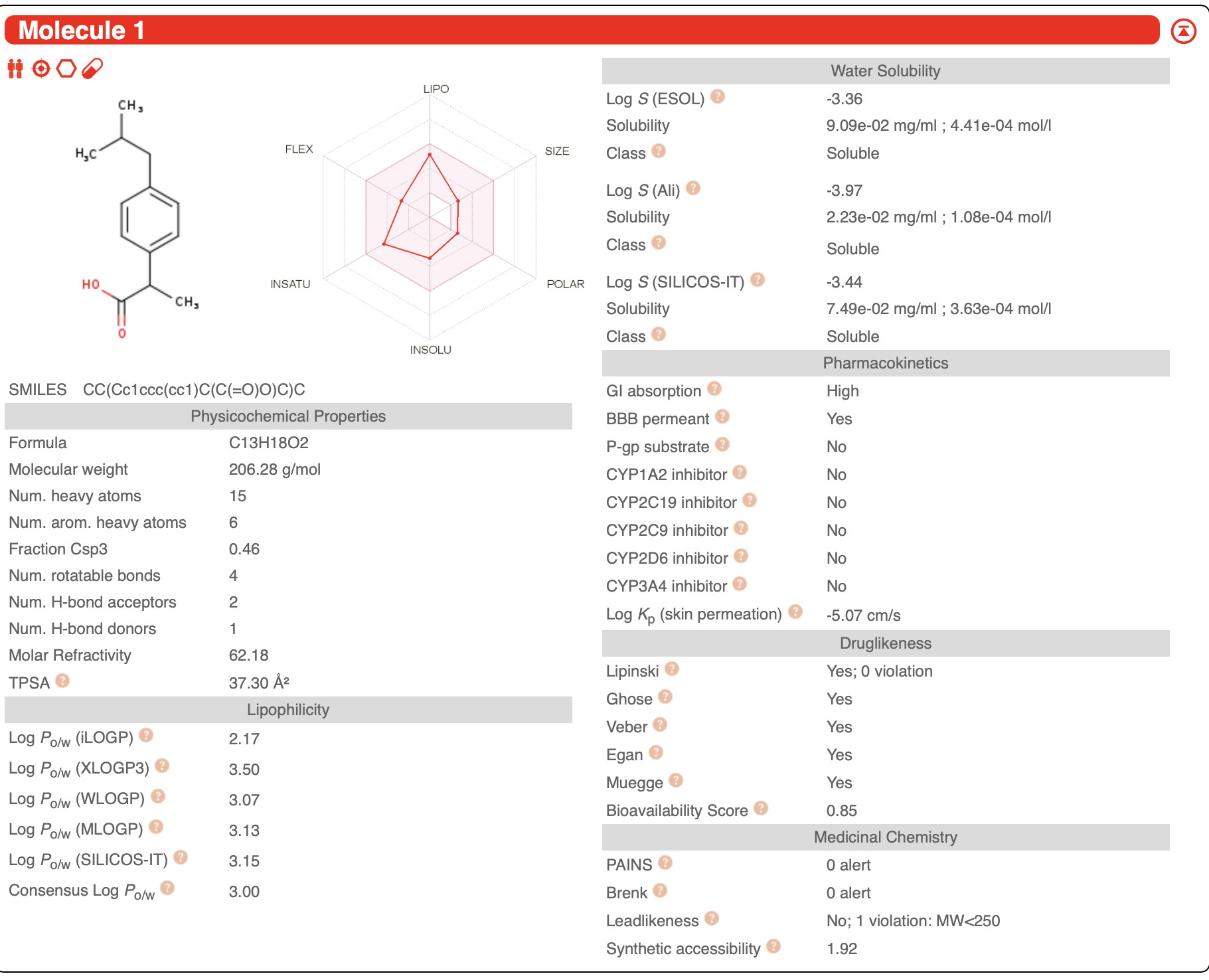
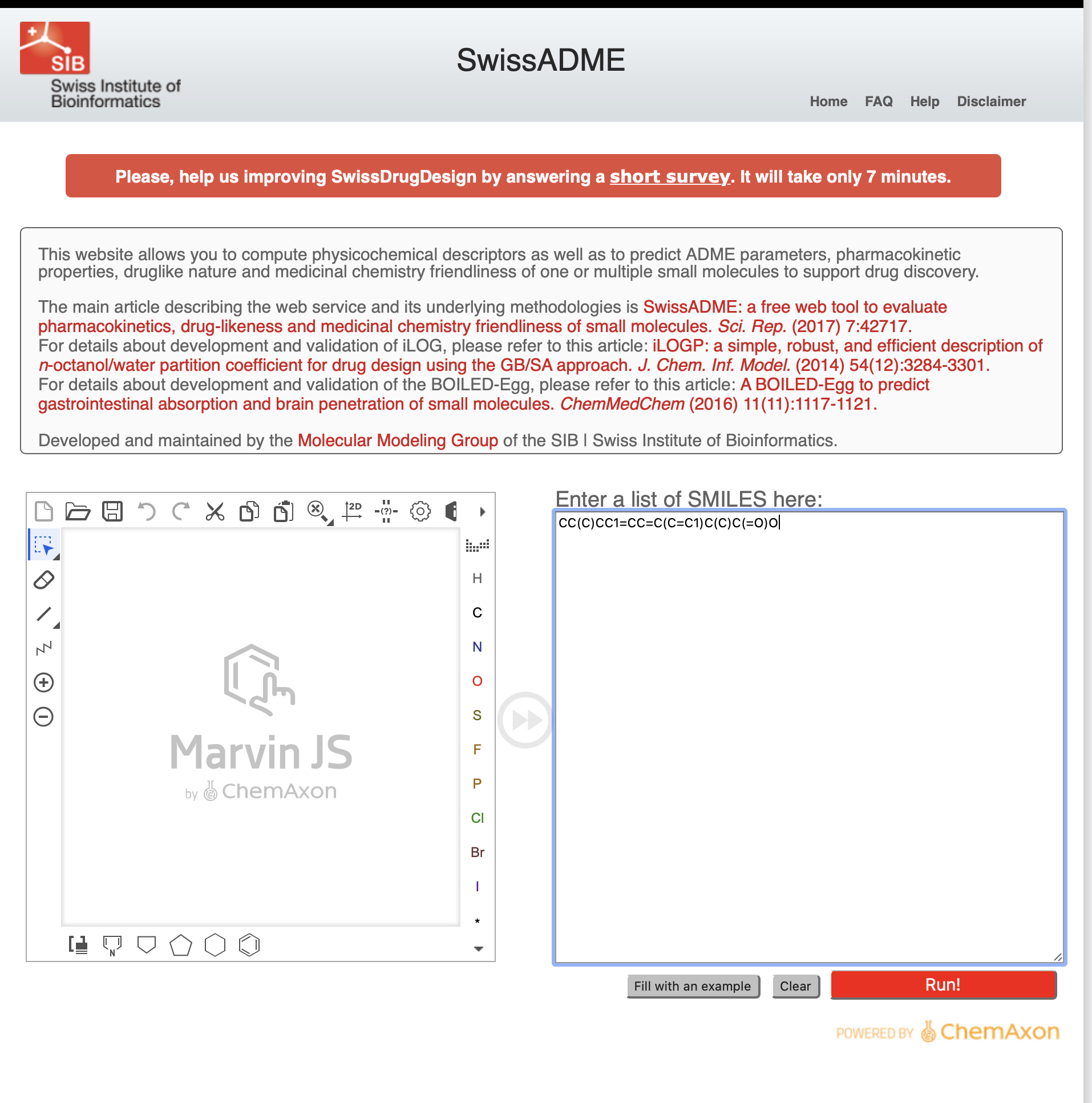
Step 1: Each student will select a chemical from “List of chemicals signup” worksheet in:

[List of Chemicals sign up sheet](https://docs.google.com/spreadsheets/d/1OhBm9e7Gi8-lflFc1w-0YsMmopOB8CL8F0o-VU2hK9Y/edit#gid=0) and be sure that chemical also exists on worksheet #3 “ADME\_ChemList” and sign up for that chemical

Step 2: Go to PubChem: <https://pubchem.ncbi.nlm.nih.gov/> and get chemical information and enter it in “Swiss ADME info selected chemical hypothesis” (yellow highlighted column) -worksheet in: [Swiss ADME info selected chemical hypthesis](https://docs.google.com/spreadsheets/d/1OhBm9e7Gi8-lflFc1w-0YsMmopOB8CL8F0o-VU2hK9Y/edit#gid=45808038) worksheet 2

Step 3: Go to Swiss ADME site: <http://www.swissadme.ch/> and

1. Navigate to “Enter a list of SMILES here:” and in the text box enter your CanonicalSMILES (2.1.4 from pubchem)
2. Click Run
3. Compare your ADME to ADME information found here: [ADME\_ChemList](https://docs.google.com/spreadsheets/d/1OhBm9e7Gi8-lflFc1w-0YsMmopOB8CL8F0o-VU2hK9Y/edit#gid=45808038) worksheet #3 ADME\_ChemList



Step 4: As a group share and compare ADME properties and decide “which of your group’s chemicals is most likely to have a biological effect in the consumer” enter that info in “Swiss ADME info selected chemical hypothesis” (yellow highlighted column) -worksheet in:

[Swiss ADME info selected chemical hypthesis](https://docs.google.com/spreadsheets/d/1OhBm9e7Gi8-lflFc1w-0YsMmopOB8CL8F0o-VU2hK9Y/edit#gid=45808038) Worksheet 2

Step 5: Identify which ADME parameter(s) is/are used to predict that your selected chemical would have a biological effect on the consumer?

Step 6: Come up with a hypothesis (make sure directional) about how an animal (wild, domestic, or human) would interact with selected chemical and what the outcome would be.

Step 7: Identify literature to support hypothesis and enter Author. year. Title. journal. DOI of that manuscript.

Step 8: Draft a short (no more than 2 sentences) summary of how the reference you found supports or refutes your hypothesis.

Step 9: Select a representative from your group to share ADME features of your chemical of interest and describe rationale for your hypothesis with the rest of class.

Homework - Step 10: Navigate to the [Turi Paper](https://drive.google.com/file/d/1qzEdETIss9x1rTxU9VRoczknx5wvXc7n/view?usp=sharing) and take a look at the tables of chemicals separated into chemical classes. Navigate to [ADME\_ChemList](https://docs.google.com/spreadsheets/d/1OhBm9e7Gi8-lflFc1w-0YsMmopOB8CL8F0o-VU2hK9Y/edit#gid=45808038) worksheet #3 ADME\_ChemList and sign up for 5 chemicals per person and specify on the worksheet what species of sagebrush each of your 5 chemicals came from.

Helpful Links

SwissADME Paper: <https://pubmed.ncbi.nlm.nih.gov/28256516/>