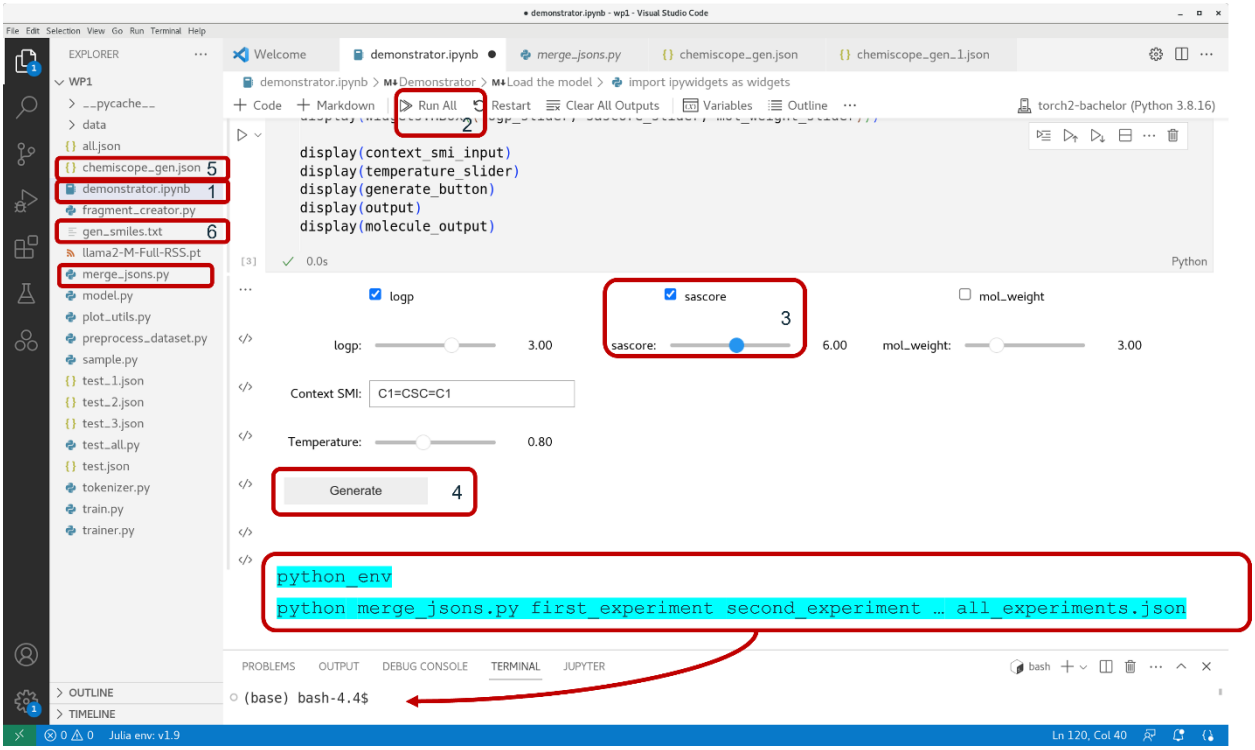
1.1 WP1 – AI & material search

The following instructions exemplifies a) how to generate some new molecules and b) how to submit them to a screening procedure. We assume a linux operating system.

1. Generate some compounds

Follow download and setup instructions given at https://github.com/Fraunhofer-SCAI/llamol. We suggest to use vscode to run the notebook.

- code .
    1. file explorer to the left → click on **demonstrator.ipynb** to open notebook
    2. if necessary, choose python environment **torch2-llamol**
    3. hit '**Run All**' button in top row, scroll down
    4. specify target properties
        a) tick box for desired property
        b) move slider and/or
        c) type in SMILES fragment
    5. hit **'Generate'** button at bottom of notebook. The output files *chemiscope_gen.json* and *gen_smiles.txt* will be generated . Scroll down to get a first overview.

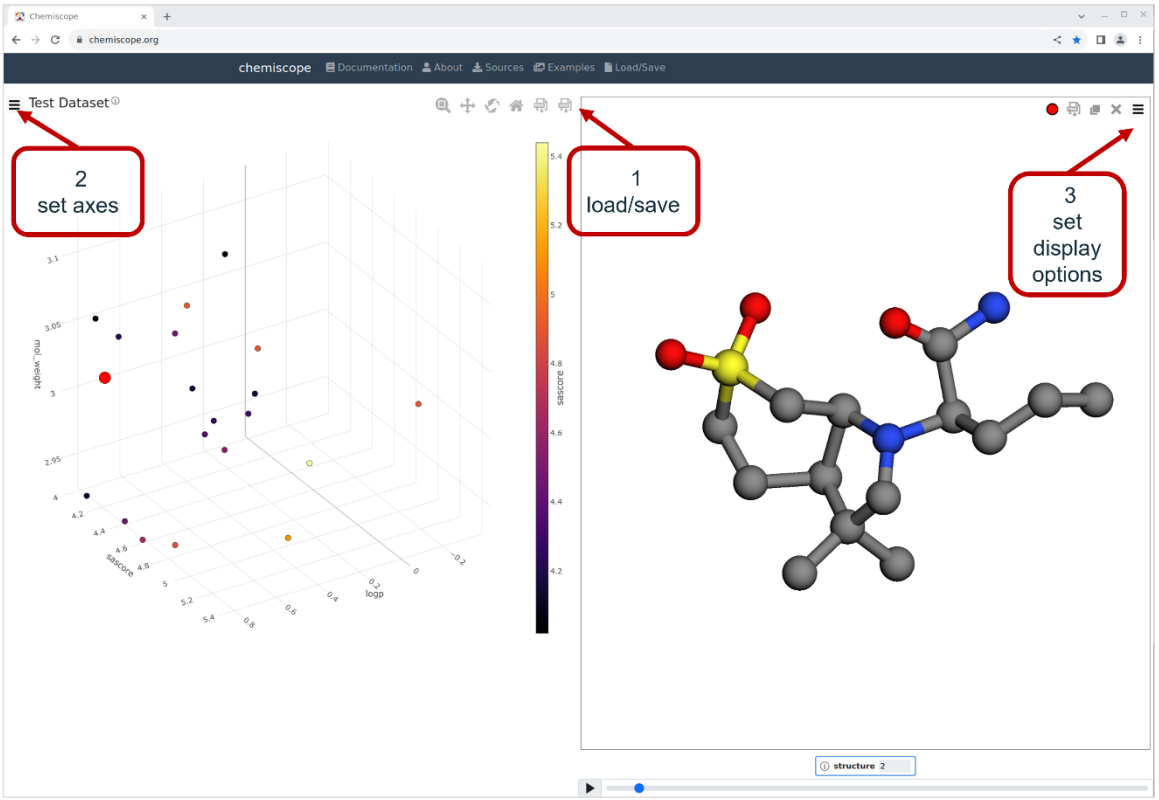


- in case you run several experiments, you have to rename the output files (else they will be overwritten), e.g. mv chemiscope_gen.json first_experiment.json
- to compile the results
    - enter python_env in the bottom terminal window
    - python merge_jsons.py first_experiment second_experiment … all_experiments.json

2. Inspect results

continue with file *chemiscope_gen.json*

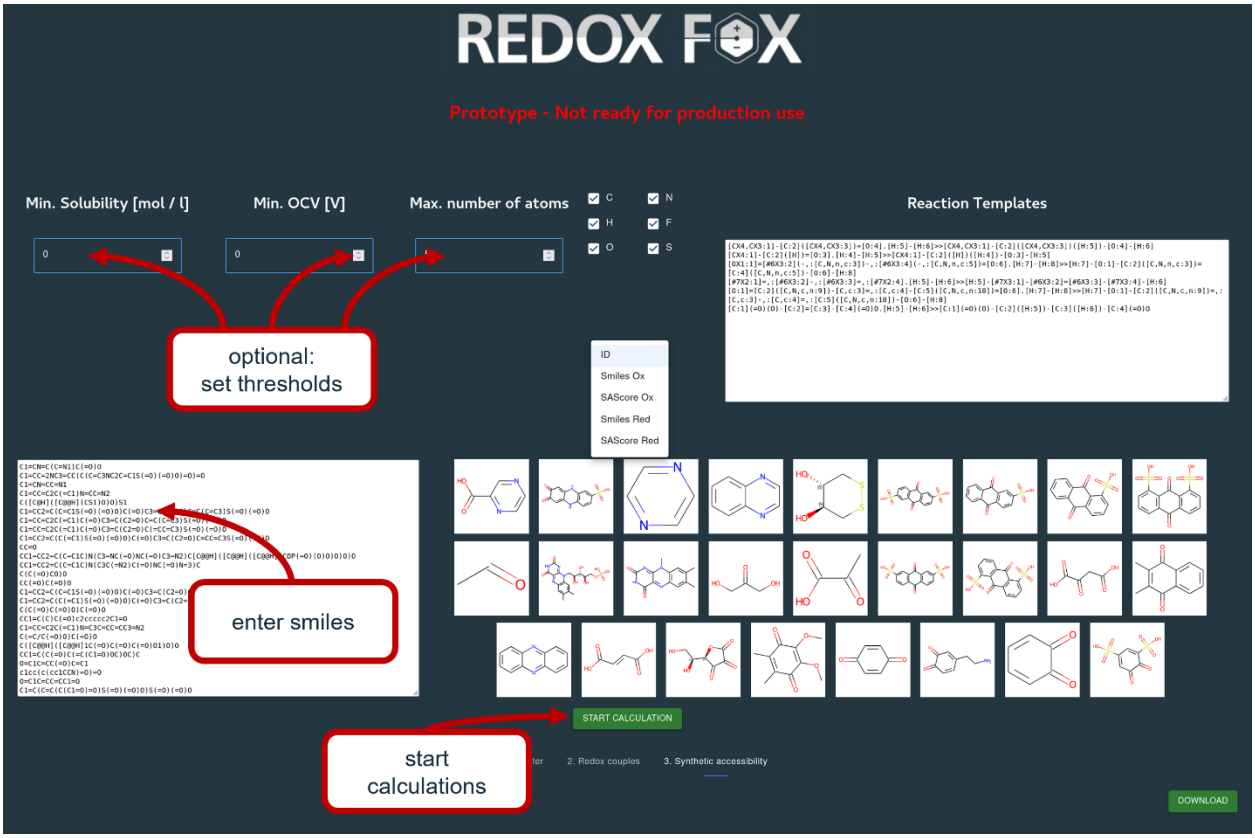
- open https://chemiscope.org in browser
  - press **'load/save'** button in middle of top row
  - upload *chemiscope_gen.json*
  - optional: press menu icon in top left corner to adapt 'Map settings'



3. Carry out screening experiment

continue with file *gen_smiles.txt*

- mark and copy content of file, i.e. list of smiles
- open www.redoxfox.scai.fraunhofer.de
  - replace default smiles in the white field on the left
    - mark & delete SMILES
    - paste list of copied SMILES
  - optional: adjust threshold criteria (fields above)
  - hit green **'START CALCULATION'** button
  - if posolyt/negolyte pairs survive. i.e. step 7 is reached:



4. Draw your own candidate or fragment SMILES

open cheminfo.org/flavor/malaria/Utilities/SMILES_generator___checker/index.html

- Draw molecule → SMILES appears in box below
- Copy & paste into
  - Redoxfox → run screening –OR--
  - Demonstrator: field **'Context Smi'** → use your molecule as seed structure for derivatives

When you are done: