1. Check searching by CAS, name, and smiles
2. Check URLS for experimental values in link at top of reports, see ToxPredictor.Application.Calculations. PredictToxicityWebPageCreator.getSourceTag
3. Make sure it can create images properly if not present in the chemicals dashboard – see CreateImageFromTrainingPredictionSDFs
4. Make user’s guide is correct in the version that’s in installanywhere
5. Run all endpoints for benzene- make reports look OK
6. Run all methods for benzene for fathead minnow toxicity
7. Test relax fragment constraint
8. Test run CTS
9. Test create detailed reports
10. Test batch searching by CAS, smiles, name, DTXSID (automatic)
11. Test importing by file: SDF, list of cas numbers, list of smiles string, batch import by training/test set
12. Test batch run saving to excel, text, html
13. See if batch run of TEST prediction set matches the text file
14. Test run from command line: TEST\_2020\_03\_18\_EPA\_Github\TEST deployment\test run from command line\ToxPredictor.Application.Calculations.RunFromCommandLine\0 run cas list csv 2024\_03\_21.bat