# Estimation of toxicity via T.E.S.T. (v5.1) and WebTEST

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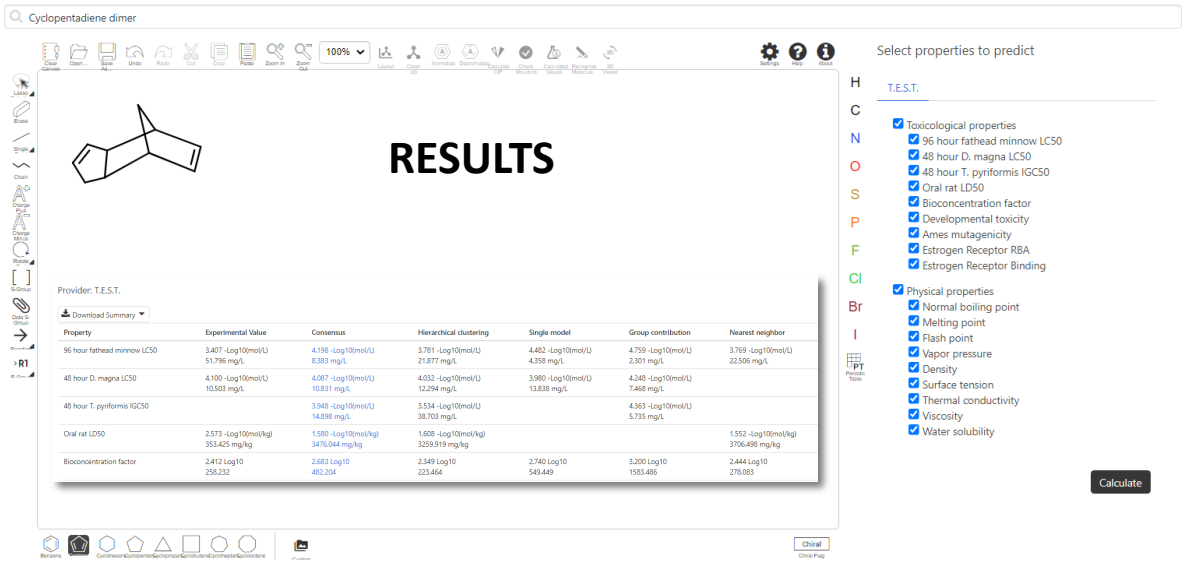
## OBJECTIVES

- Redesign of the interface
- Improved structure searching
- Improved calculation speed
- Incorporation of Chemical Transformation Simulator (CTS)
- Mac OS version of T.E.S.T.
- Web interface for running T.E.S.T. models (WebTEST)
- WebTEST models can be accessed via API calls

## APPROACH

- Downloadable T.E.S.T. Java application was redesigned to be more user friendly and run calculations faster
- T.E.S.T. was converted into a web-service based application (WebTEST)
- EPA's CTS web-service was incorporated into the single chemical mode of T.E.S.T. to estimate properties of breakdown products

## RESULTS



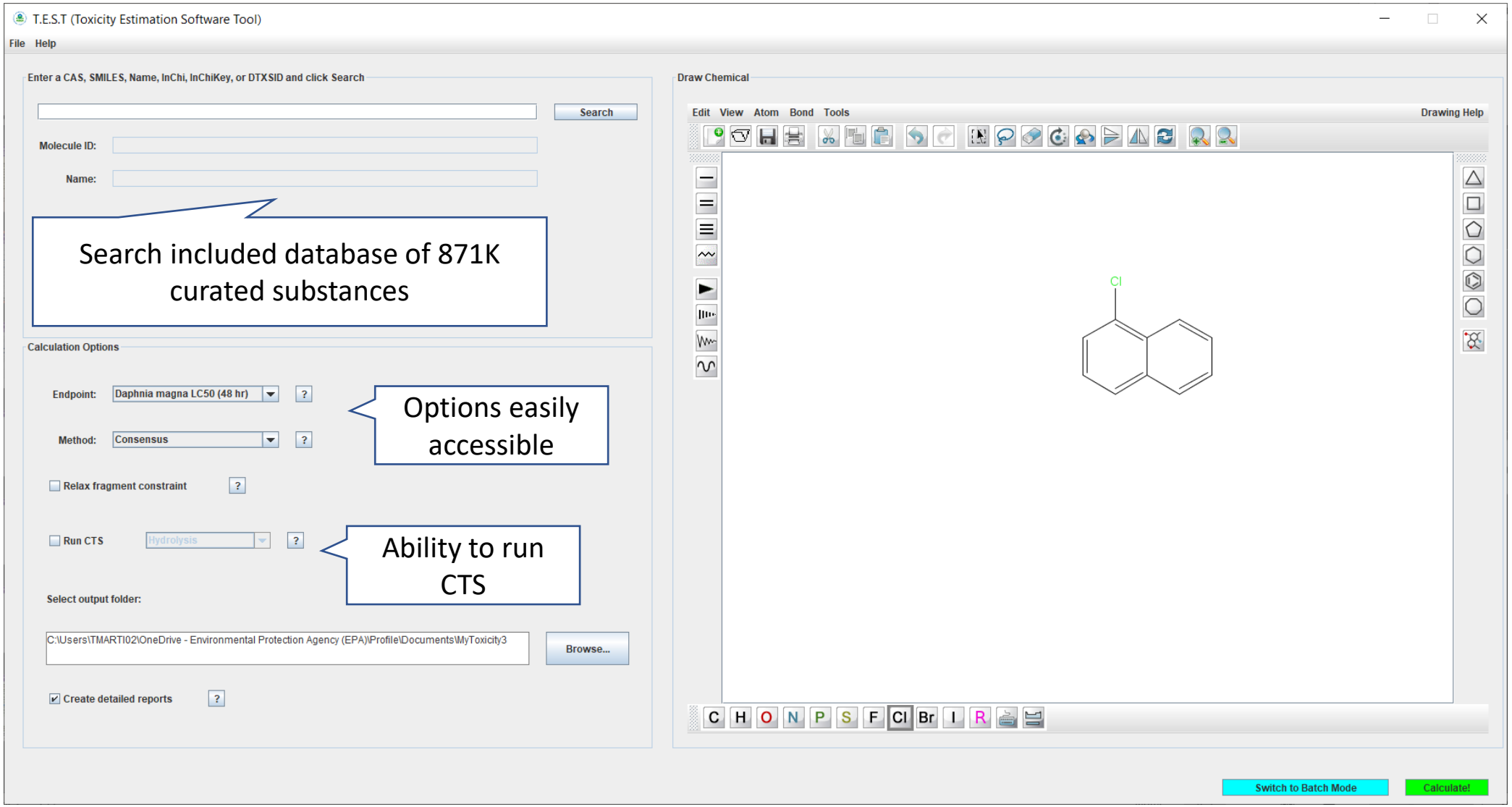

## IMPACT

- T.E.S.T. has been made more accessible by redesigning the application and providing a web-based version.
- T.E.S.T. can now estimate the toxicity of environmental breakdown products via CTS

**For more information:** martin.todd@epa.gov;
https://www.epa.gov/chemical-research/toxicity-estimation-software-tool-test;
https://comptox.epa.gov/dashboard/predictions/index

# Estimation of toxicity via T.E.S.T. (v5.1) and WebTEST

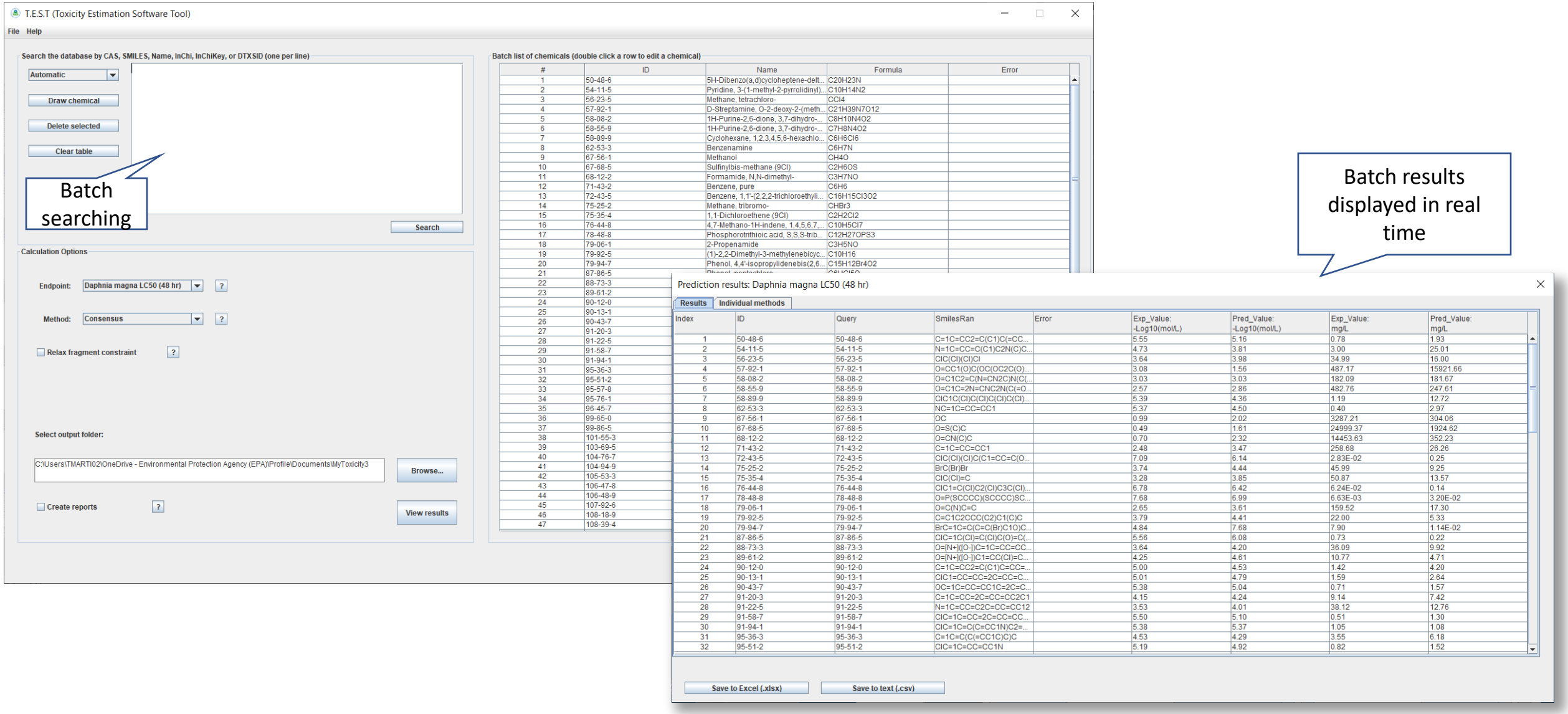
## T.E.S.T 5.1. Single Chemical Mode




https://www.epa.gov/chemical-research/toxicity-estimation-software-tool-test

# Estimation of toxicity via T.E.S.T. (v5.1) and WebTEST

## T.E.S.T 5.1. Batch Mode



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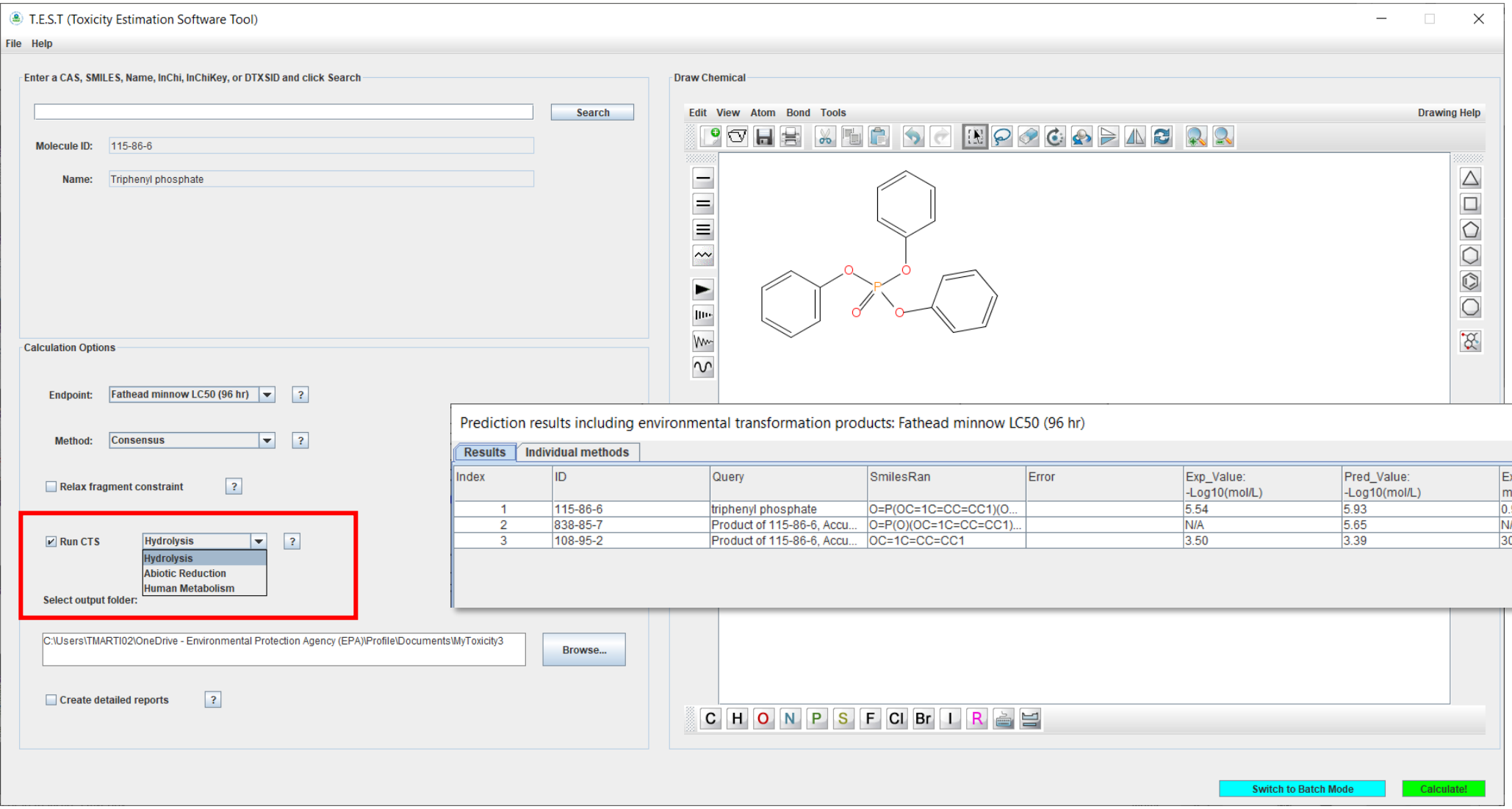
## CTS Integration: estimate properties of breakdown products




Prediction results including environmental transformation products: Fathead minnow LC50 (96 hr)

Results | Individual methods

| Index | ID | Query | SmilesRan | Error | Exp_Value: -Log10(mol/L) | Pred_Value: -Log10(mol/L) | Exp_Value: mg/L | Pred_Value: mg/L |
|---|---|---|---|---|---|---|---|---|
| 1 | 115-86-6 | triphenyl phosphate | O=P(OC=1C=CC=CC1)(O... | | 5.54 | 5.93 | 0.93 | 0.39 |
| 2 | 838-85-7 | Product of 115-86-6, Accu... | O=P(O)(OC=1C=CC=CC1)... | | N/A | 5.65 | N/A | 0.56 |
| 3 | 108-95-2 | Product of 115-86-6, Accu... | OC=1C=CC=CC1 | | 3.50 | 3.39 | 30.11 | 38.69 |

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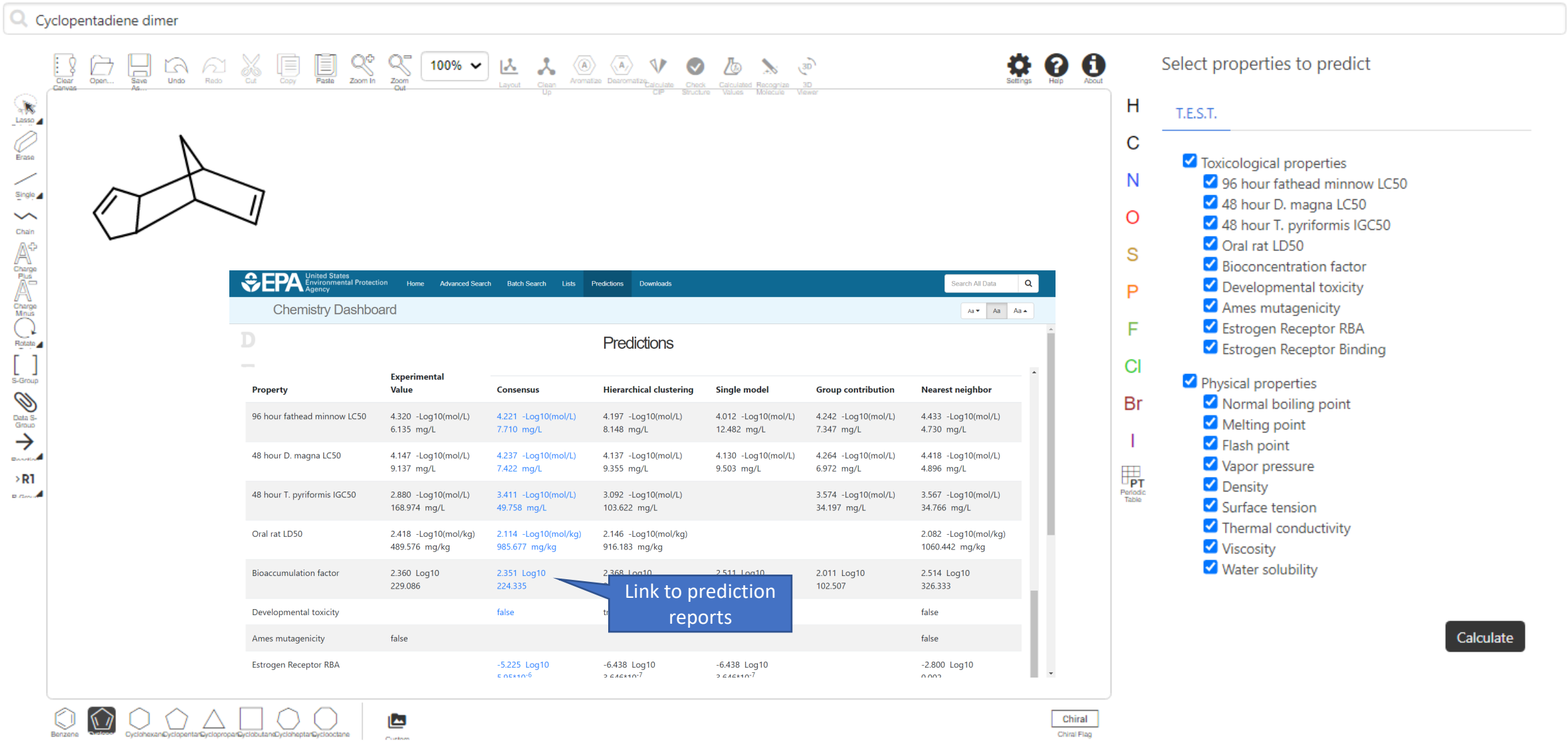
## WebTEST Interface

https://comptox.epa.gov/dashboard/predictions/index



# Estimation of toxicity via T.E.S.T. (v5.1) and WebTEST

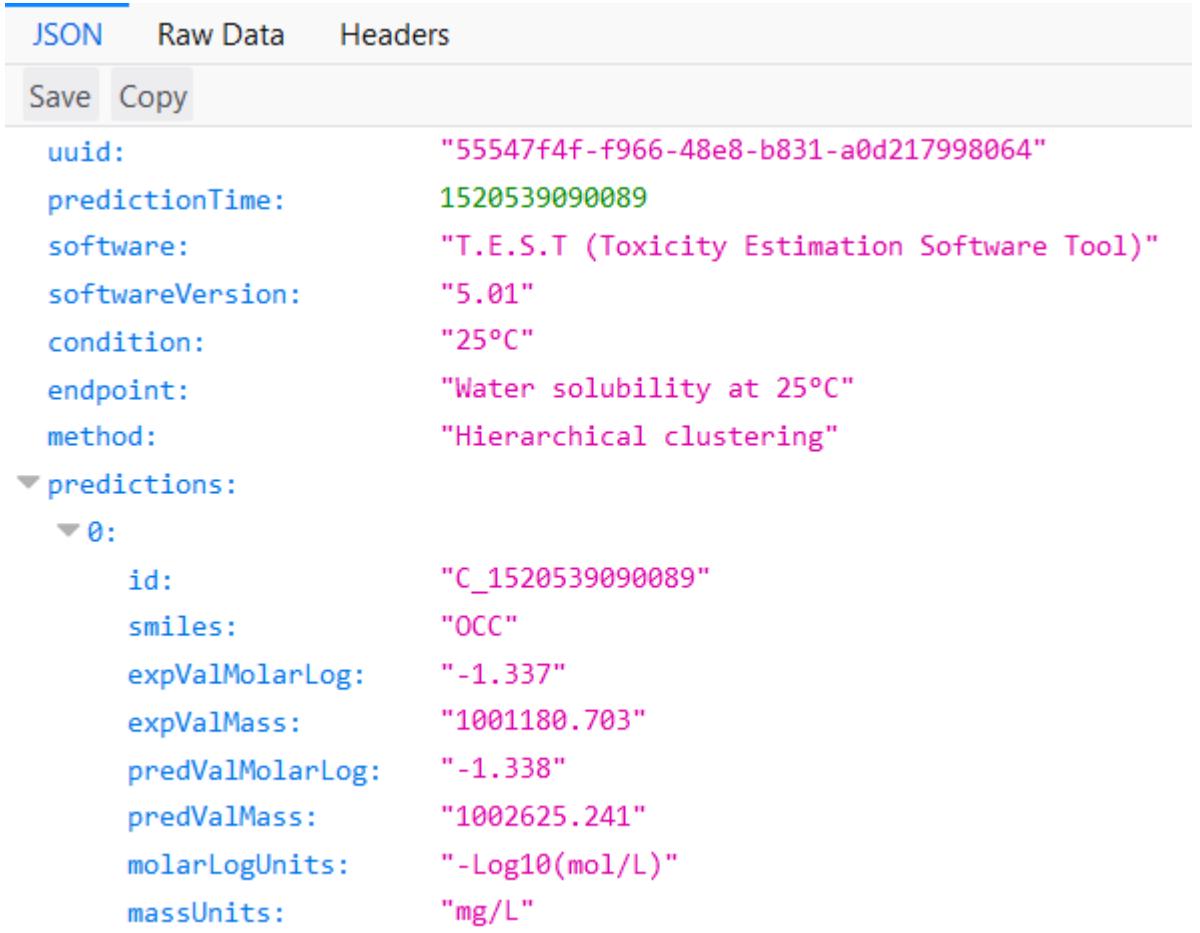
## WebTEST "GET" API Call

URL/endpointAbbreviation?smiles=desiredSmiles&method=methodAbbreviation

where URL = https://comptox.epa.gov/dashboard/web-test/

| Method | Abbreviation |
|---|---|
| Hierarchical clustering | hc |
| Single model | sm |
| Nearest neighbor | nn |
| Group contribution | gc |
| Consensus | consensus (default) |

| Endpoint | Abbreviation |
|---|---|
| Fathead minnow LC50 (96 hr) | LC50 |
| Daphnia magna LC50 (48 hr) | LC50DM |
| T. pyriformis IGC50 (48 hr) | IGC50 |
| Oral rat LD50 | LD50 |
| Bioaccumulation factor | BCF |
| Developmental Toxicity | DevTox |
| Mutagenicity | Mutagenicity |
| Normal boiling point | BP |
| … | … |



# Estimation of toxicity via T.E.S.T. (v5.1) and WebTEST

## Summary

- T.E.S.T. can now search EPA's DSSTOX database
- Calculations are performed faster
- Properties of environmental breakdown products can now be estimated using CTS
- Calculations can now be run on the web using WebTEST using a graphical interface and API calls

## Future work

- Map all data sets to DSSTOX identifiers
- Add additional data and endpoints/properties
- Add models to predict properties of PFAS
- Replace legacy QSAR methods with python web-service based methods (e.g. SVM, RF, DNN)
- Make single chemical output display in the software rather than web browser
- Batch mode of WebTEST

## References

U.S. EPA (2020). "User's Guide for T.E.S.T. (version 5.1) (Toxicity Estimation Software Tool): A Program to Estimate Toxicity from Molecular Structure."