# Improving the Efficiency of Literature Identification for the ECOTOXicology Knowledgebase Using Deep Learning

Sciome

*Enabling Science via Analytical Informatics*

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## Introduction

The ECOTOXicology Knowledgebase (ECOTOX) is a comprehensive, publicly available resource providing single chemical environmental toxicity data on aquatic life, terrestrial plants and wildlife. The database is updated quarterly, and to identify relevant references and extract pertinent data, the ECOTOX data curation pipeline employs a methodical process similar to the initial stages of systematic review. This labor-intensive workflow requires curators to regularly evaluate tens of thousands of candidate references, the majority of which are then rejected as not relevant. After the careful review of hundreds of thousands of potentially relevant articles, the ECOTOX database currently (as of March 2022) contains data for 12,485 chemicals and 13,709 species manually extracted from 53,020 references. The availability of this extensive dataset of historical screening decisions provided us with the opportunity to develop high performance, state-of-the-art neural network classifiers to partially automate title and abstract screening and to categorize (e.g., human health, fate, chemical methods) rejected references.

https://cfpub.epa.gov/ecotox/

*Note: The views expressed in this poster are those of the authors and do not necessarily reflect the views or policies of the U.S. EPA.*

## Material and Methods

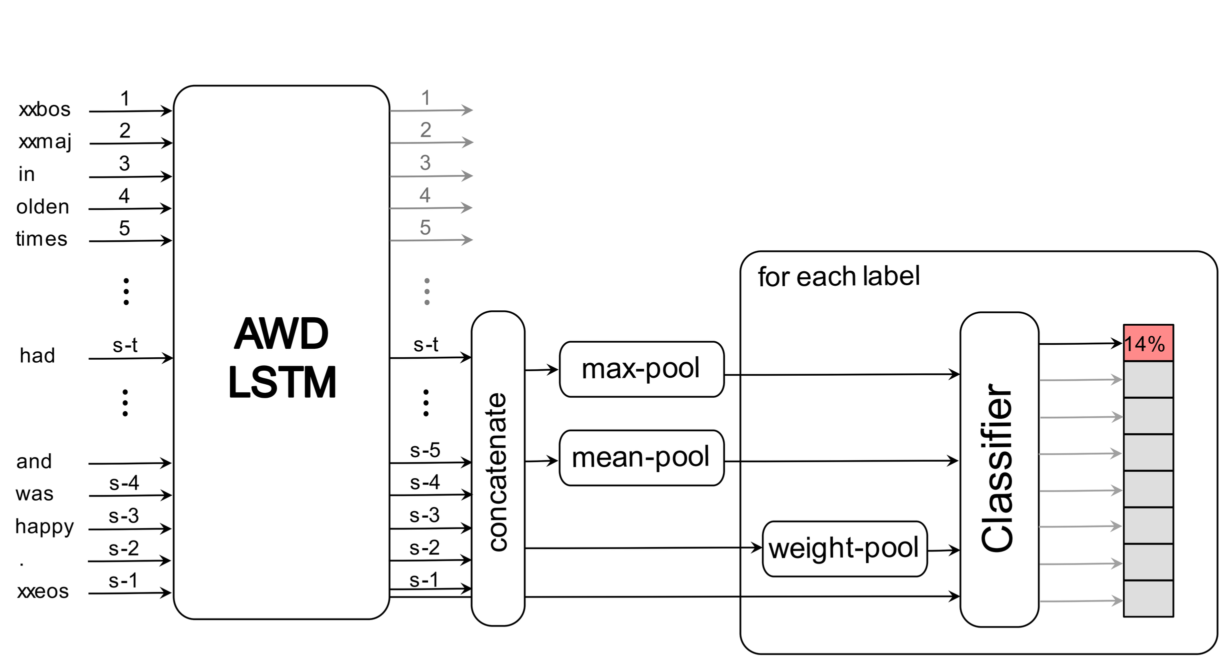
We experimented on a subset of 88,900 articles spanning nearly 100 chemicals from the ECOTOX database. Out of these, 65,553 were excluded after manual screening, and annotated with a reason for exclusion.

References were cleaned prior to processing:

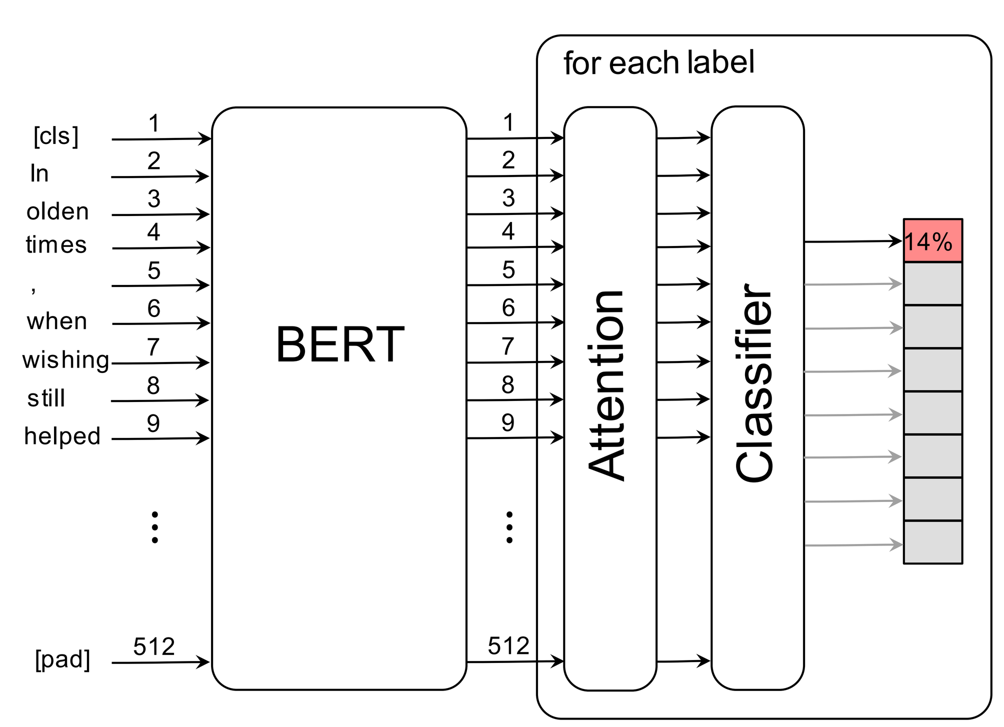
- Encoding problems were corrected and html entities were normalized
- Boilerplate text such as 'Abstract:', 'All rights reserved', et c. were stripped using regexes
- Abstracts were parsed to strip keywords from the abstract body
- Abstracts were parsed to strip copyright statements from the abstract body
- Keywords, journal, and publisher information were each given their own dedicated field

We trained modified versions of ULM-FiT and BERT-large to identify the 22 most frequent exclusion criteria in ECOTOX, as well the other criteria in one label (OTHER).

The final model used in ECOTOX is a hybrid meta-model which delegates decision to either UML-FiT (Howard 2018, arXiv:1801.06146) or BERT (Devlin 2019, doi 10.18653/v1/N19-1423) depending on which performs best on each label. References without abstracts are processed by a dedicated titles-only classifier.




UML-FiT adapted to highlight information salient to each label We modify the classification layer of UML-FiT by adding the weight-pooled hidden state vector, using weights derived from word-level attention (Yang 2016, doi: 10.18653/v1/n16-1174). The attention weights are trained separately for each label.




**BERT adapted to highlight information salient to each label** We modify the classification layer of BERT by replacing the pre-classification layer with a scaled dot-product attention head (Vaswani 2017, arXiv:1706.03762). The attention heads are trained separately for each label.

## Results

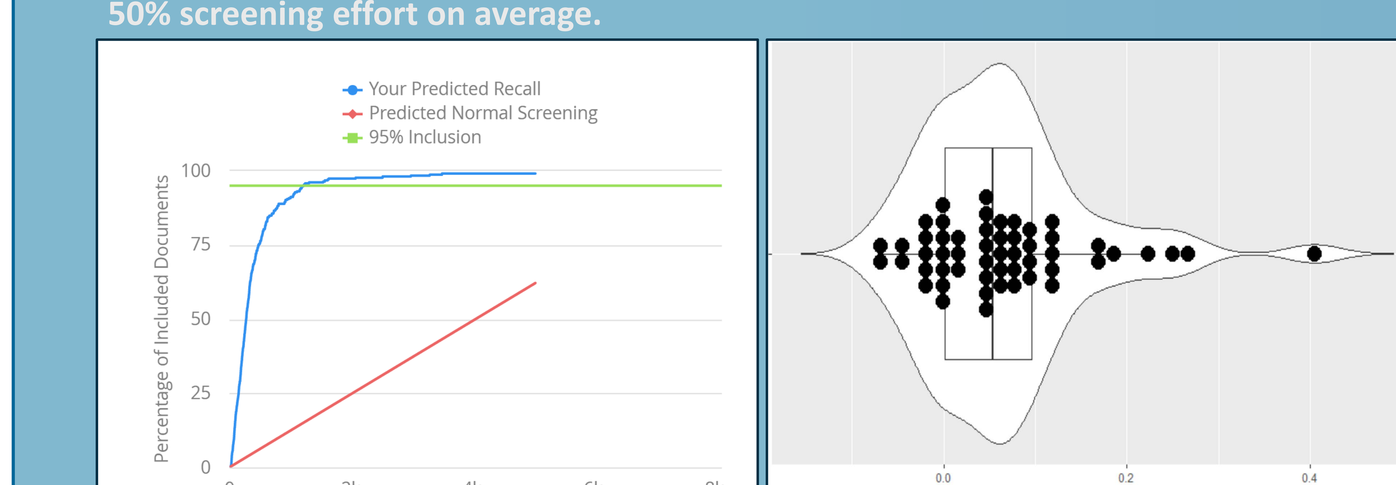
*Table 1*: **Final performance, cross validated over 5 folds. P denotes precision, R denotes recall (sensitivity), F denotes the $F_1$ measure.**

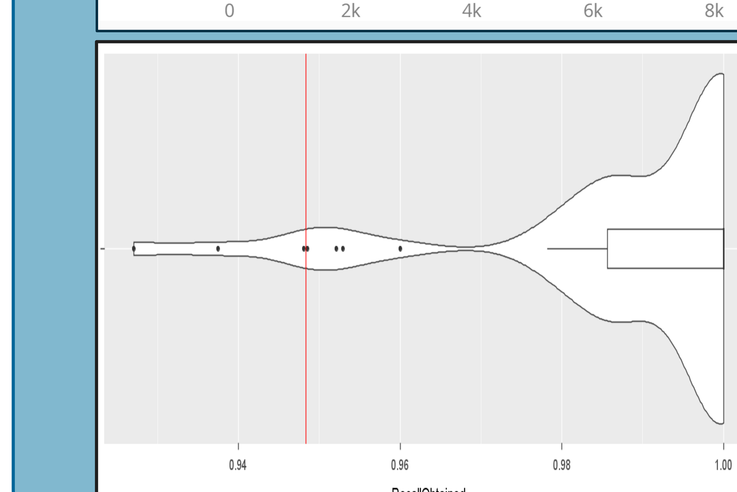
| | P | R | F |
|---|---|---|---|
| HUMAN HEALTH | 67.09% | 60.06% | 55.30% |
| CHEM METHODS | 77.61% | 73.16% | 74.51% |
| FATE | 55.01% | 70.04% | 58.29% |
| BACTERIA | 65.30% | 66.41% | 64.71% |
| REVIEW | 71.78% | 66.98% | 69.07% |
| SURVEY | 61.71% | 65.99% | 63.50% |
| MIXTURE | 51.22% | 60.43% | 55.09% |
| NON-ENGLISH | 80.70% | 78.13% | 77.64% |
| ABSTRACT | 62.19% | 63.72% | 57.51% |
| IN VITRO | 48.59% | 39.94% | 39.37% |
| OTHER | 19.48% | 24.20% | 18.57% |
| REFS CHECKED | 67.20% | 66.19% | 66.01% |
| NO CONC | 42.64% | 34.91% | 36.89% |
| MODELING | 51.68% | 41.55% | 44.24% |
| NO SOURCE | 71.76% | 52.61% | 58.07% |
| METHODS | 80.91% | 39.63% | 52.18% |
| NO EFFECT | 20.25% | 23.26% | 17.03% |
| FOOD | 32.83% | 45.70% | 37.56% |
| YEAST | 66.24% | 84.24% | 73.12% |
| PUBL AS | 79.01% | 58.07% | 66.11% |
| NO DURATION | 80.48% | 48.23% | 58.35% |
| BIOLOGICAL TOXICANT | 53.29% | 28.55% | 30.34% |
| NO TOXICANT | 67.09% | 60.06% | 55.30% |
| Macro average | 56.81% | 54.66% | 51.92% |
| Weighted average | 73.70% | 64.04% | 62.31% |

*Table 2*: **Fuzzy Kappa scores for human- and model-screened Exclusion Reasons on 4427 new abstracts. Model performance is already on par with some human screeners. Work is ongoing to further improve performance for future datasets.**

| | Screener 1 | Screener 2 | Screener 3 | Screener 4 | Screener 5 | MODEL |
|---|---|---|---|---|---|---|
| Screener 1 | 1 | 0.674 | 0.565 | 0.601 | 0.963 | 0.425 |
| Screener 2 | | 1 | 0.559 | 0.644 | 0.769 | 0.470 |
| Screener 3 | | | 1 | 0.651 | 0.792 | 0.511 |
| Screener 4 | | | | 1 | 0.638 | 0.552 |
| Screener 5 | | | | | 1 | 0.502 |

*Figure 2*: **Using the extensive database of manually screened data also improved efficiency of binary inclusion/exclusion prediction. (A) Baseline model saves users 50% screening effort on average.**



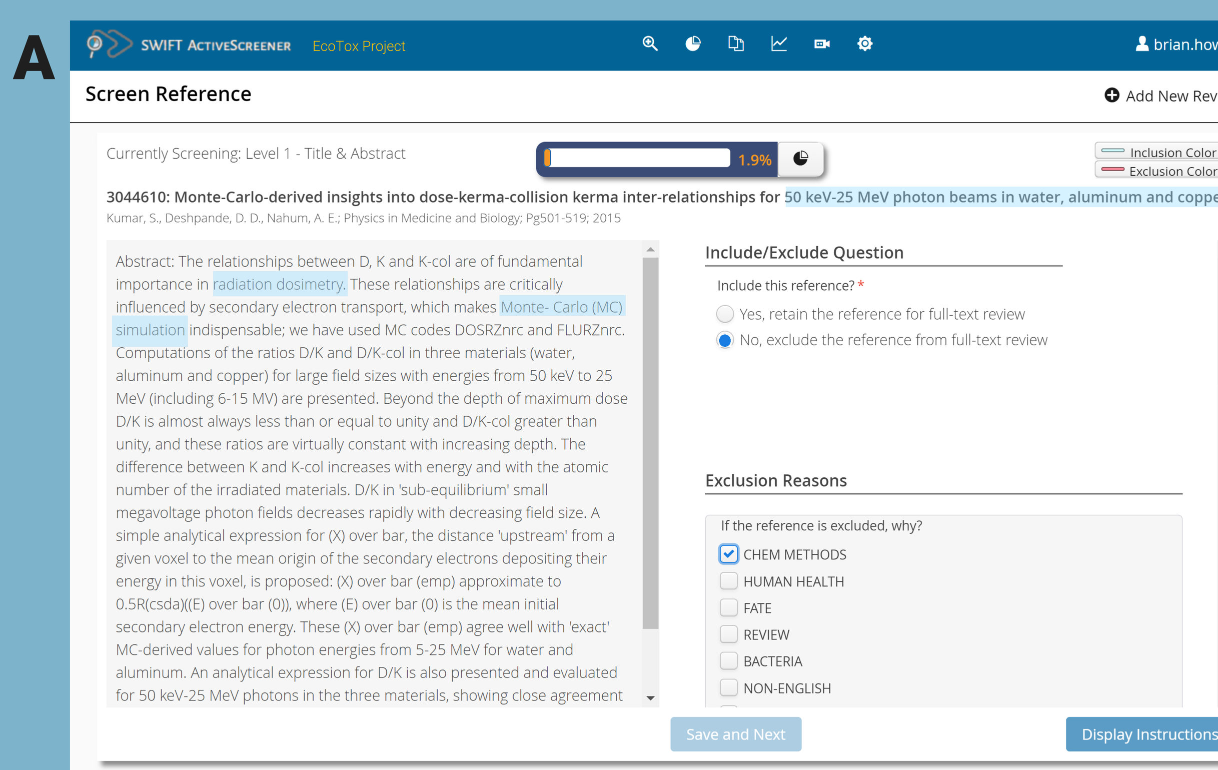




**(B) Augmenting standard model with pretrained model via transfer learning provides additional benefits (mean improvement of 9.5% WSS over the baseline prioritization model, but several datasets had significantly larger gains)**

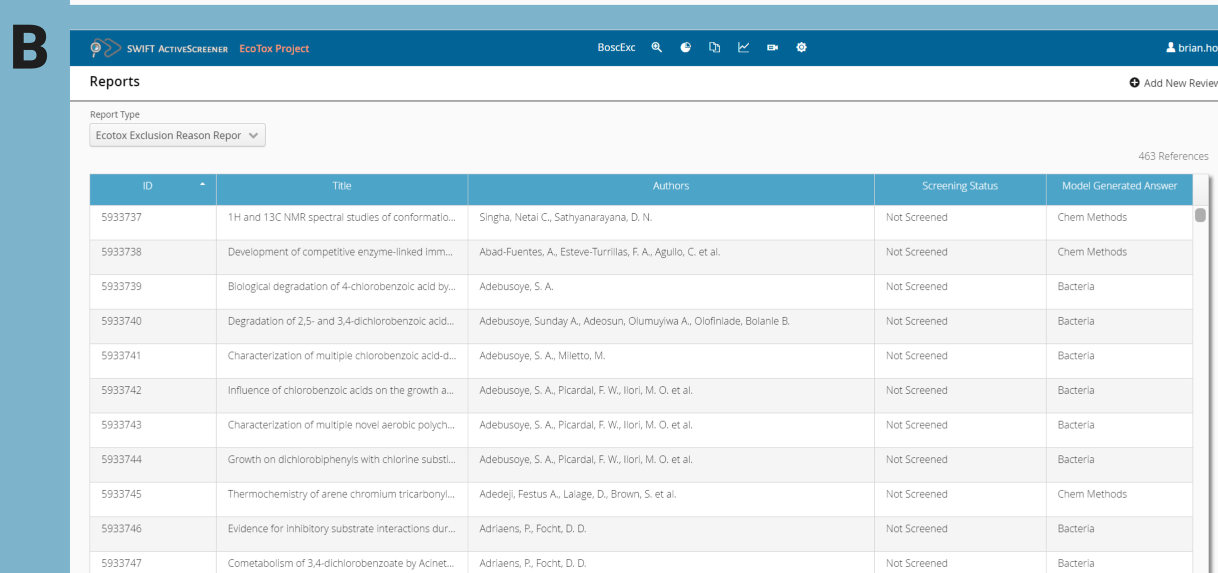
**(C) 95% Recall estimate was accurate lower bound in majority of 75 test cases.**

## SWIFT-Active Screener for EcoTox

A



B



The screens above show several of the enhancements made to SWIFT Active Screener (Howard 2020, doi:10.1016/j.envint.2020.105623) to support literature curation for EcoTox. In A) we can see an abstract presented to the user for screening. Articles are prioritized for review using a deep learning neural network. For excluded articles, an exclusion reason is suggested by the computer and supporting words and phrases are highlighted. The system also includes several custom reports B) created in support of the EcoTox literature review process.

## Conclusions

- EcoTox Active Screener uses Deep Learning to:
  - Save an additional 9.5+% screening time (above baseline 50%)
  - Accurately predict exclusion reasons (60-80% F1 score for common reasons)
  - Explain its predictions using attention-highlighting
- The system is being piloted at EPA, and several refinements are planned.

**For further information**
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