

A Web-based Literature Identification Platform for the ECOTOXicology Knowledgebase, Powered by Deep Learning

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ECOTOX Knowledgebase

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Data last updated

**Sep 15,
2020**

See update totals

Recent chemicals with full searches completed and data extracted

Carbaryl

Clofibrate

Dibutyl phthalate

Dichloropropanes

Di-ethylhexyl phthalate

Gemfibrozil

Inorganic Chlorates

Mancozeb

Methomyl

Metrafenone

Octamethylcyclotetrasiloxane

Per- and Polyfluoroalkyl Substances (PFAS)

TBBPA (4,4'-(1-Methylethylidene)bis[2,6-...

Wy14643

Total in database

12,223

Chemicals

13,266

Species

50,932

References

1,018,565

Results

WELCOME TO ECOTOX VERSION 5!

Please click here to provide feedback so that we can continue to improve your experience.

About ECOTOX

The ECOTOXicology knowledgebase (ECOTOX) is a comprehensive, publicly available knowledgebase providing single chemical environmental toxicity data on aquatic life, terrestrial plants and wildlife.

[Learn More](#)

Getting Started

- Use [Search](#) if you know exact parameters or search terms (chemical, species, etc.)
- Use [Explore](#) to see what data may be available in ECOTOX (including data plots)
- [ECOTOX Quick User Guide](#) (2 pp, 141 K)
- [ECOTOX User Guide](#) (89 pp, 663 K)
- [ECOTOX Terms Appendix](#)

Other Links

- [Limitations](#)
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ECOTOX Pipeline

Develop
literature
search

Conduct
searches

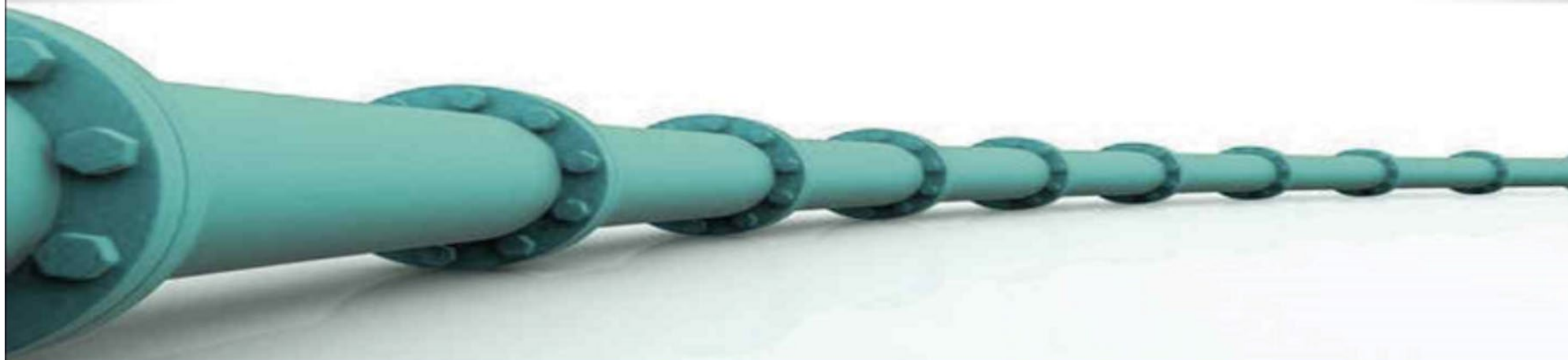
Identify
potentially
applicable
studies

Acquire
potentially
applicable
studies

Apply
ECOTOX
applicability
criteria

Code Data
into
ECOTOX

Systematic Review and Data Curation





SWIFT-Active Screener is a web-based, collaborative systematic review software application. Active Screener is designed to be easy-to-use, incorporating a simple, but powerful, graphical user interface with rich project management tools. What makes Active Screener special, however, is its behind-the-scenes application of state-of-the-art statistics designed to save screeners time and effort by automatically prioritizing articles as they are reviewed, using machine learning algorithms to push the most relevant articles to the top of the list.



IMPROVED RANKING
The computer suggests the next articles to screen based on previously reviewed articles.

USER FEEDBACK

User screening decisions are used to continuously refine the machine learning model.



Contents lists available at ScienceDirect

Environment International

journal homepage: www.elsevier.com/locate/envint



SWIFT-Active Screener: Accelerated document screening through active learning and integrated recall estimation

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Evidence mapping
Active learning
Machine learning
Document screening
Recall estimation

ABSTRACT

Background: In the screening phase of systematic review, researchers use detailed inclusion/exclusion criteria to decide whether each article in a set of candidate articles is relevant to the research question under consideration. A typical review may require screening thousands or tens of thousands of articles in and can utilize hundreds of person-hours of labor.

Methods: Here we introduce SWIFT-Active Screener, a web-based, collaborative systematic review software application, designed to reduce the overall screening burden required during this resource-intensive phase of the review process. To prioritize articles for review, SWIFT-Active Screener uses active learning, a type of machine learning that incorporates user feedback during screening. Meanwhile, a negative binomial model is employed to estimate the number of relevant articles remaining in the unscreened document list. Using a simulation involving 26 diverse systematic review datasets that were previously screened by reviewers, we evaluated both the document prioritization and recall estimation methods.

Results: On average, 95% of the relevant articles were identified after screening only 40% of the total reference list. In the 5 document sets with 5,000 or more references, 95% recall was achieved after screening only 34% of the available references, on average. Furthermore, the recall estimator we have proposed provides a useful, conservative estimate of the percentage of relevant documents identified during the screening process.

Conclusion: SWIFT-Active Screener can result in significant time savings compared to traditional screening and the savings are increased for larger project sizes. Moreover, the integration of explicit recall estimation during screening solves an important challenge faced by all machine learning systems for document screening: when to stop screening a prioritized reference list. The software is currently available in the form of a multi-user, collaborative, online web application.

1. Background

Systematic review is a formal, sequential process for identifying, assessing, and integrating the primary scientific literature with the aim of answering a specific, targeted question in pursuit of the current scientific consensus. This approach, already a cornerstone of evidence-based medicine, has recently gained significant popularity in several other disciplines including environmental health. It has been estimated

that more than 4,000 systematic reviews are conducted and published annually (Bastian et al., 2010), and while the precise time commitment can vary depending on the subject matter and protocol, reviews often require a year or more to complete (Ganann et al., 2010, Borah et al., 2016). Due to the large investment of resources necessary to develop and maintain a systematic review, there has been considerable recent interest in methods and techniques for using machine learning and automation to make this process more efficient (Tsafnat et al., 2014).



Screen Reference

 Add New Review

You have reached the predicted inclusion threshold and can stop screening.

Currently Screening: Level 1 - Title & Abstract



 Inclusion Color
 Exclusion Color

2021913: Functionality of sugars: physicochemical interactions in foods

Davis, E. A.; Am J Clin Nutr; 1995

Basic and selected functional properties of s and maple syrups, honey, and high-fructose Properties that relate to sweetness and prop component interaction as a basis for produc implications of such functionality are illustra energy foods and for the microwave heating of foods. Among the properties discussed are solubility, hygroscopicity, crystallinity, and viscosity. Interrelations among water mobility, water activity, and hydration of proteins, lipids, and carbohydrates are described in the context of food formulation. Application of polymer chemistry principles to explain functional properties of amorphous molecules is reviewed.

Active Screener can **reduce required screening by 50%** on most projects with more than 1,000 references

Main

Notes

Unique EcoTox Review Process: Unique Challenges/Opportunities

- The same type of review is **conducted repeatedly** (same questions, same process)
- Significant accumulation of **manually annotated datasets**
- Excluded items need to be documented with a **reason for exclusion**

Two Main Goals

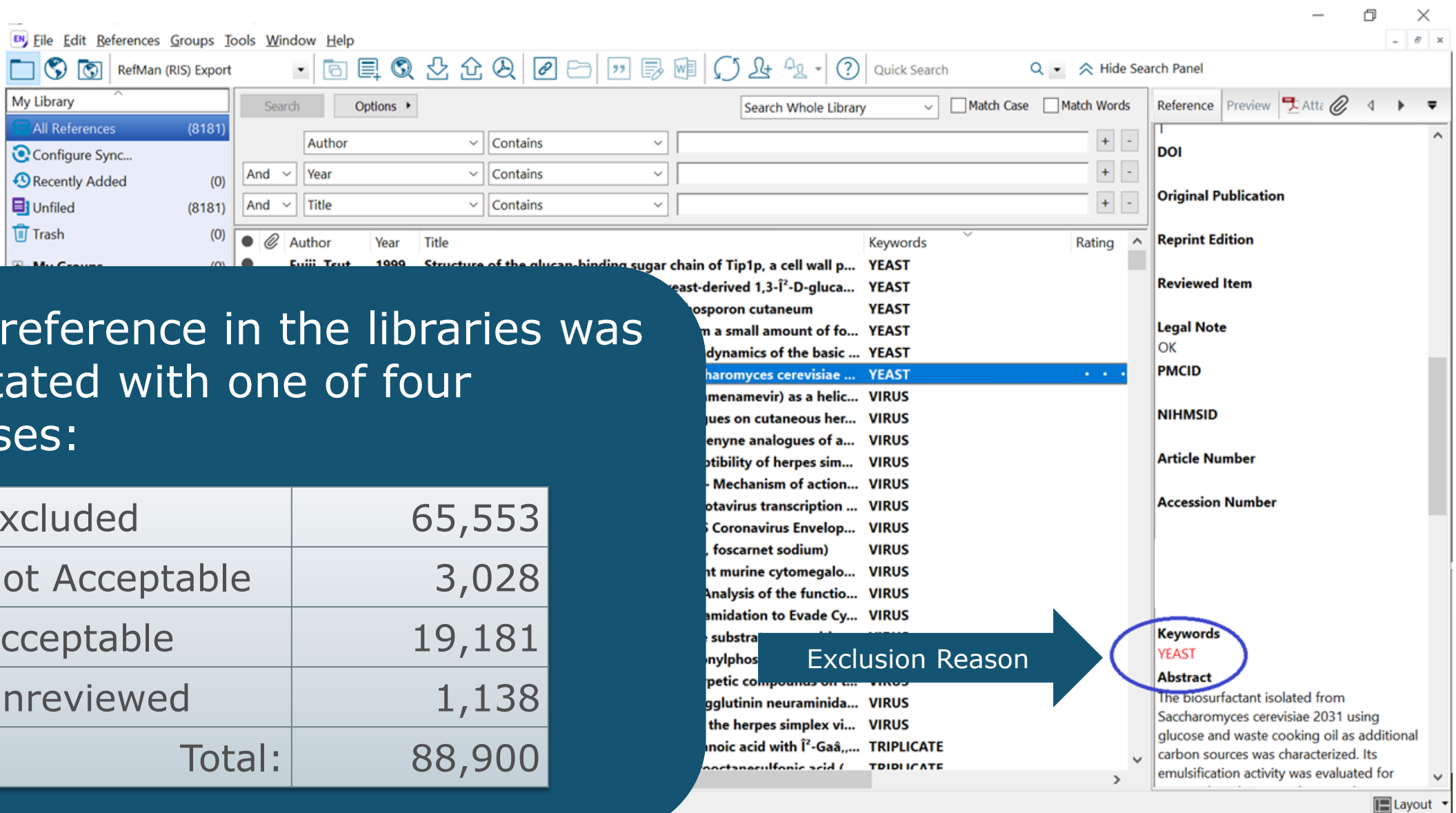
Use available data to:

1. Predict **which articles to exclude** (improved prioritization)
2. Predict **why each article should be excluded** (exclusion reason detection)

Existing Datasets

Each reference in the libraries was annotated with one of four statuses:

Excluded	65,553
Not Acceptable	3,028
Acceptable	19,181
Unreviewed	1,138
Total:	88,900



Existing Datasets

- Excluded articles also were associated with a reason for exclusion.
- The top 20 reasons make up over 95% of the data. The remaining terms were combined as an "Other" category.

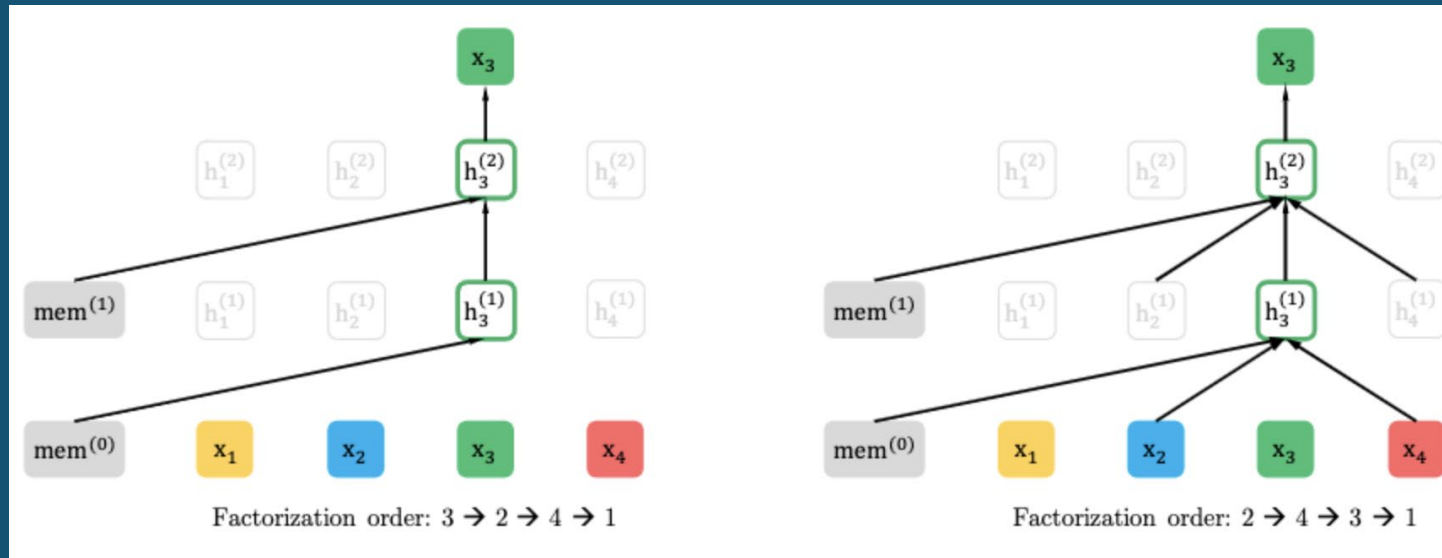
Exclusion Reason	Refs	Percentage
HUMAN HEALTH	19609	30.41%
CHEM METHODS	16745	25.97%
NO TOXICANT	8074	12.52%
FATE	5184	8.04%
BACTERIA	2961	4.59%
REVIEW	2251	3.49%
SURVEY	1696	2.63%
MIXTURE	1101	1.71%
NON-ENGLISH	1003	1.56%
ABSTRACT	939	1.46%
IN VITRO	805	1.25%
OTHER	701	1.09%
.....
BIOLOGICAL TOXICANT	105	0.16%
	64,480	

Deep Learning

1. ULMFit Classifier (Howard and Ruder, 2018)

2. BERT (Devlin, et al, 2019)

3. XLNet (Yang, et al, 2019)



“Attention” in neural networks

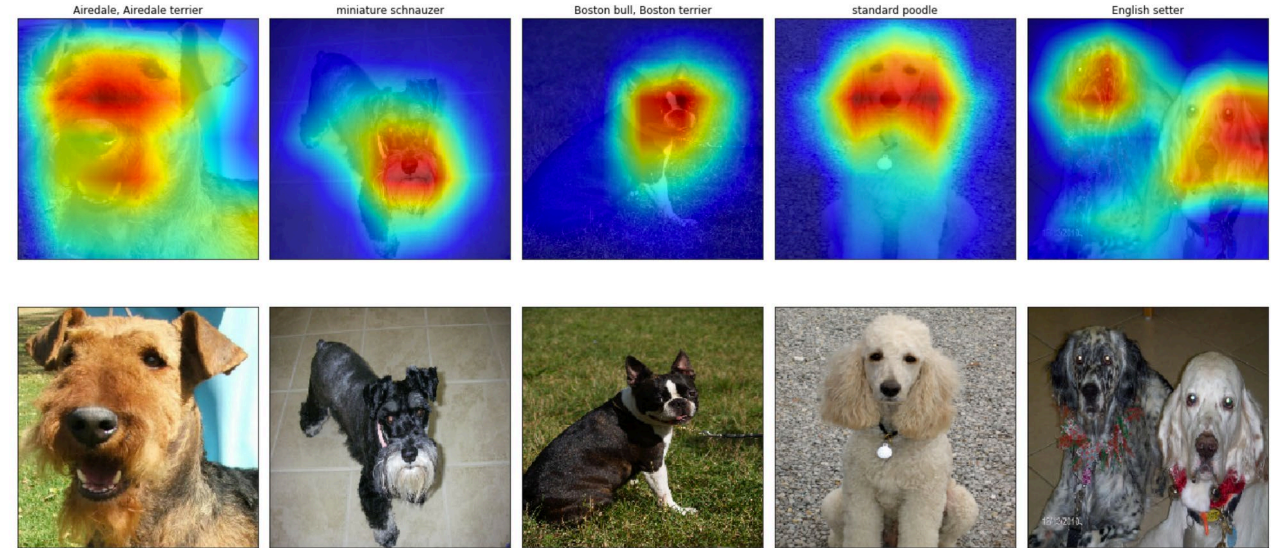
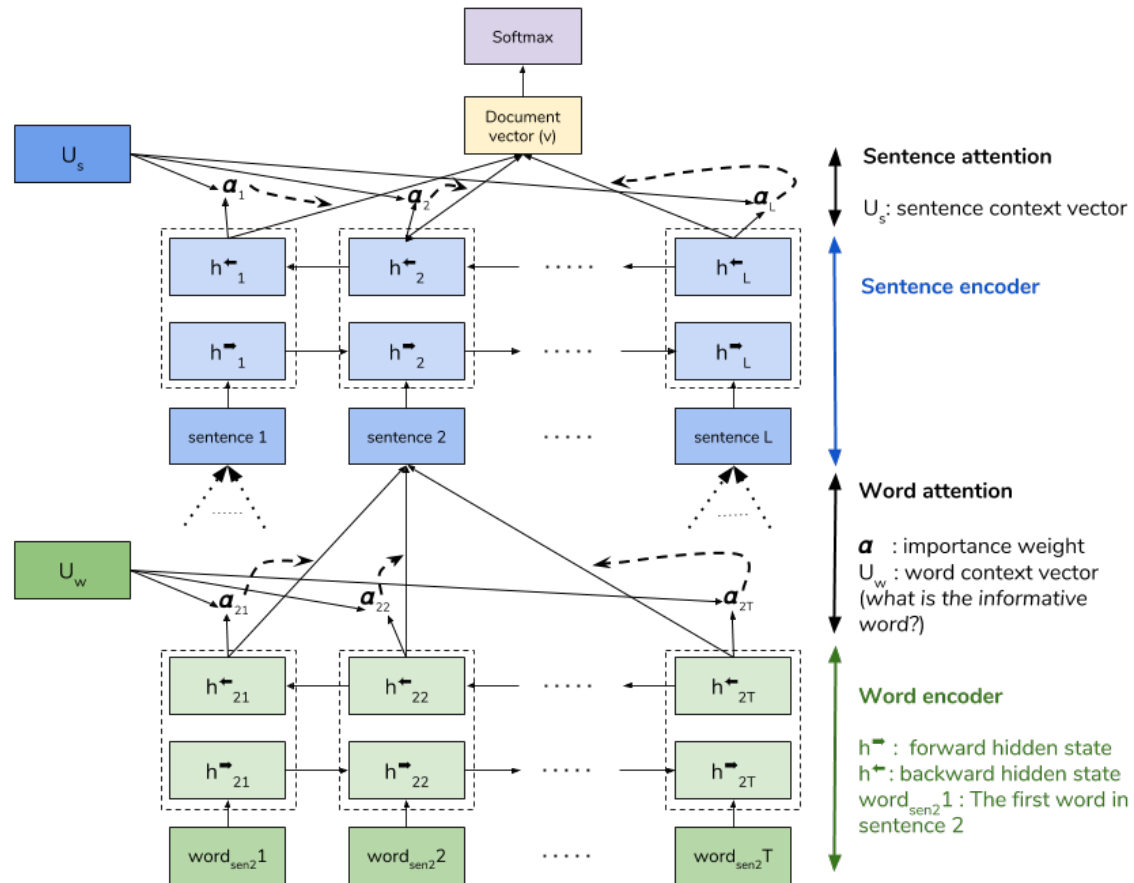


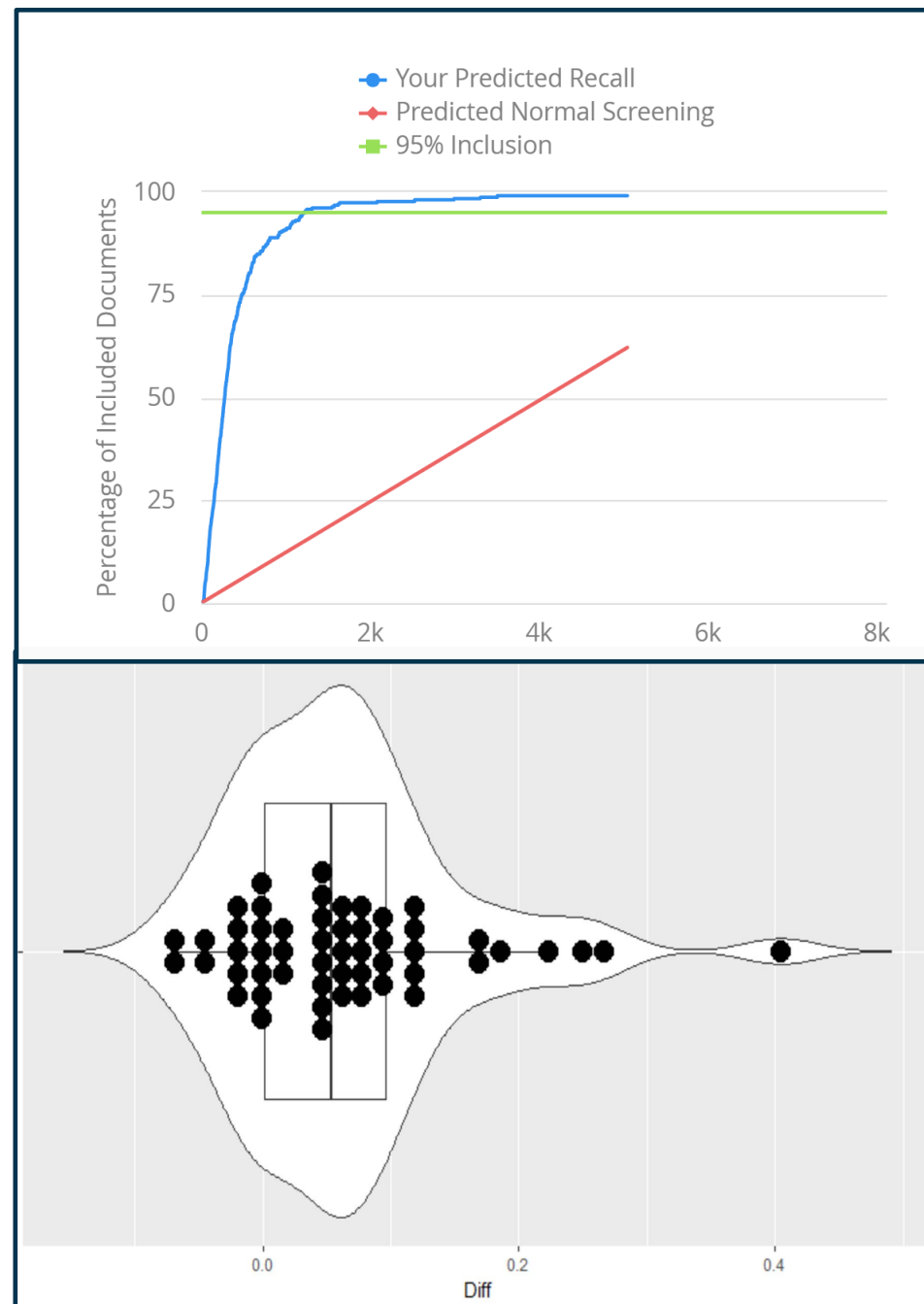
Table 10: Final Exclusion Reason Classification Model

	ULMFit 2019			ULMFit 2020			BioBERT			Final Hybrid Model		
	P	R	F	P	R	F	P	R	F	diff		
HUMAN HEALTH	71.66%	60.90%	65.84%	65.06%	72.80%	68.72%	68.09%	54.29%	60.41%	-6.60%	+11.90%	+2.88%
CHEM METHODS	75.36%	75.16%	75.26%	76.50%	76.64%	76.57%	81.21%	71.91%	76.28%	+1.14%	+1.48%	+1.31%
FATE	69.01%	63.80%	66.31%	61.61%	70.99%	65.97%	71.05%	60.67%	65.45%	-7.40%	+7.19%	-0.34%
BACTERIA	66.49%	37.72%	48.13%	41.19%	67.53%	51.17%	41.51%	81.54%	55.02%	-24.98%	+43.82%	+6.89%
REVIEW	58.38%	66.55%	62.20%	56.94%	60.18%	58.52%	69.10%	72.36%	70.69%	+10.72%	+5.81%	+8.49%
SURVEY	45.85%	62.70%	52.97%	61.75%	52.96%	57.02%	63.74%	64.73%	64.23%	+17.89%	+2.03%	+11.26%
MIXTURE	64.50%	45.23%	53.17%	61.18%	55.03%	57.94%	50.45%	65.29%	56.92%	-3.32%	+9.80%	+4.77%
NON-ENGLISH	75.11%	60.36%	66.94%	63.77%	76.47%	69.55%	87.73%	85.02%	86.35%	+12.62%	+24.66%	+19.41%
ABSTRACT	53.73%	53.73%	53.73%	47.25%	64.18%	54.43%	74.14%	63.70%	68.53%	+20.41%	+9.97%	+14.80%
IN VITRO	38.72%	61.31%	47.47%	71.14%	39.85%	51.08%	63.13%	51.12%	56.49%	+24.41%	-10.19%	+9.02%
OTHER	3.70%	25.93%	6.48%	39.39%	6.84%	11.66%	32.35%	17.01%	22.30%	+28.65%	-8.92%	+15.82%
REFS CHECKED	66.19%	53.18%	58.97%	54.03%	48.55%	51.15%	63.41%	67.10%	65.20%	-2.78%	+13.92%	+6.23%
NO CONC	22.77%	42.59%	29.68%	51.28%	39.60%	44.69%	63.49%	38.46%	47.90%	+40.72%	-4.13%	+18.22%
MODELING	72.73%	34.78%	47.06%	57.50%	69.70%	63.01%	42.11%	72.73%	53.33%	-15.23%	+34.92%	+15.95%
NO SOURCE	48.11%	68.46%	56.51%	75.19%	52.43%	61.78%	76.51%	61.62%	68.26%	+28.40%	-6.84%	+11.75%
METHODS	60.00%	66.67%	63.16%	78.57%	55.00%	64.71%	58.33%	52.50%	55.26%	+18.57%	-11.67%	+1.55%
NO EFFECT	7.84%	40.00%	13.11%	33.33%	5.88%	10.00%	36.00%	8.82%	14.17%	+28.16%	-31.18%	+1.06%
FOOD	28.57%	32.00%	30.19%	63.64%	25.00%	35.90%	36.67%	39.29%	37.93%	+8.10%	+7.29%	+7.74%
YEAST	84.31%	87.76%	86.00%	87.50%	82.35%	84.85%	88.46%	90.20%	89.32%	+4.15%	+2.44%	+3.32%
PUBL AS	10.81%	33.33%	16.33%	28.13%	48.65%	35.64%	66.67%	70.27%	68.42%	+55.86%	+36.94%	+52.09%
NO DURATION	8.33%	66.67%	14.81%	50.00%	29.17%	36.84%	85.71%	50.00%	63.16%	+77.38%	-16.67%	+48.35%
Macro average	49.15%	54.23%	48.30%	58.33%	52.37%	52.91%	62.85%	58.98%	59.32%	+13.70%	+4.75%	+11.02%
Weighted average	60.45%	60.89%	59.23%	60.45%	60.89%	59.23%	63.23%	62.04%	61.30%	+2.78%	+1.15%	+2.07%

Results: Acceptable / Not Acceptable

Evaluated whether machine learning can be used to classify documents as Acceptable vs Not Acceptable / Excluded and found that:

- Using Active Screener can save users 50% of screening effort for many datasets.
- Augmenting standard model with pretrained model via transfer learning provides additional benefits (mean **improvement of 9.5% WSS** over the standard Active Screener prioritization model, but several datasets had significantly larger gains).

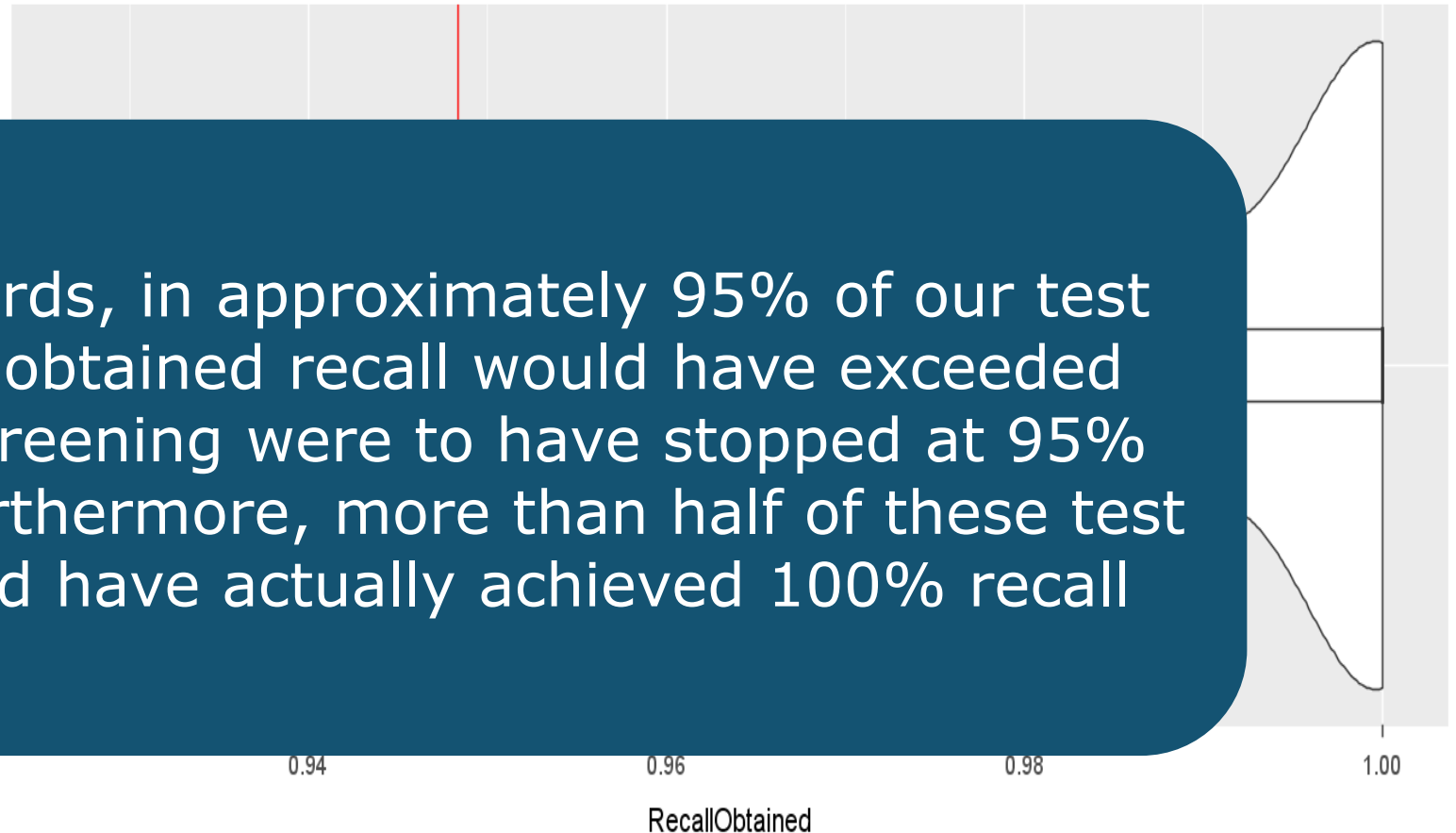


Recall Estimation

For Active Screener
estimate of 95%
recall, the
of actual
like this..

(Measure
distinct c

In other words, in approximately 95% of our test cases, the obtained recall would have exceeded 94.8% if screening were to have stopped at 95% estimate; furthermore, more than half of these test cases would have actually achieved 100% recall





Screen Reference

+ Add New Review

Currently Screening: Level 1 - Title & Abstract



Inclusion Color

Exclusion Color

3044610: Monte-Carlo-derived insights into dose-kerma-collision kerma inter-relationships for 50 keV-25 MeV photon beams in water, aluminum and copper

Kumar, S., Deshpande, D. D., Nahum, A. E.; Physics in Medicine and Biology; Pg501-519; 2015

Abstract: The relationships between D, K and K-col are of fundamental importance in radiation dosimetry. These relationships are critically influenced by secondary electron transport, which makes Monte- Carlo (MC) simulation indispensable; we have used MC codes DOSRZnrc and FLURZnrc. Computations of the ratios D/K and D/K-col in three materials (water,

Include/Exclude Question

Include this reference? *

- ☐ Yes, retain the reference for full-text review
- ☒ No, exclude the reference from full-text review

Exclusion Reasons

If the reference is excluded, why?

- ☒ CHEM METHODS
- ☐ HUMAN HEALTH
- ☐ FATE
- ☐ REVIEW
- ☐ BACTERIA
- ☐ NON-ENGLISH

****Active Screener for EcoTox****

Save and Next

Display Instructions



Screen Reference

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Currently Screening: Level 1 - Title & Abstract



Inclusion Color

Exclusion Color

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****Active Screener for EcoTox******1. Improved prioritization with Deep Learning / Transfer Learning**

Save and Next

Display Instructions



Screen Reference

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****Active Screener for EcoTox****

1. Improved prioritization with Deep Learning / Transfer Learning

2. Customized EcoTox Forms

Exclusion Reasons

If the reference is excluded, why?

- ☒ CHEM METHODS
- ☐ HUMAN HEALTH
- ☐ FATE
- ☐ REVIEW
- ☐ BACTERIA
- ☐ NON-ENGLISH

Save and Next

Display Instructions



Screen Reference

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Inclusion Color

Exclusion Color

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Exclusion Reasons

If the reference is excluded, why?

- ☒ CHEM METHODS
- ☐ HUMAN HEALTH
- ☐ FATE
- ☐ REVIEW
- ☐ BACTERIA
- ☐ NON-ENGLISH

Save and Next

Display Instructions

****Active Screener for EcoTox****

1. Improved prioritization with Deep Learning / Transfer Learning
2. Customized EcoTox Forms
3. Automatic Detection of Exclusion Reason



Screen Reference

+ Add New Review

Currently Screening: Level 1 - Title & Abstract



Inclusion Color

Exclusion Color

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- ☐ HUMAN HEALTH
- ☐ FATE
- ☐ REVIEW
- ☐ BACTERIA
- ☐ NON-ENGLISH

Save and Next

Display Instructions

****Active Screener for EcoTox****

1. Improved prioritization with Deep Learning / Transfer Learning
2. Customized EcoTox Forms
3. Automatic Detection of Exclusion Reason
4. Exclusion Reason Keyword Highlighting

Summary

- Standard Active Screener application saves users 50% screening time
- EcoTox Active Screener uses Deep Learning to:
 - Save an additional 9.5+% screening time
 - Accurately predict exclusion reasons
 - Explain its predictions using attention-highlighting

Next Steps

“**Phase III**” of the project...

- **Manuscript** about results so far
- **Field testing** and **iterative refinements**
- Automatic highlighting of phrases in the **relevant articles**
- Ways to **incorporate new data** and ongoing model improvements
- Natural language processing to **automate extraction**

Bioinformatics

- ✓ Next-Generation Sequence data analysis
- ✓ Microarray data analysis
- ✓ Structural & Functional genomics
- ✓ SNP/Genotype analysis & GWAS
- ✓ Biostatistics and Mathematical Modeling

Cheminformatics

- ✓ Quantitative Structure-Activity Relationship (QSAR) modeling
- ✓ Computational Toxicity Predictions
- ✓ Active site and Protein-Protein Docking
- ✓ Pharmacophore Modeling

Text-Mining and Literature Review

- ✓ Document Tagging and Visualization
- ✓ Full-Text Conversion and Search
- ✓ Document Clustering, Ranking & Classification
- ✓ Literature Prioritization and Screening
- ✓ Data extraction
- ✓ rapid Evidence Mapping (rEM) and systematic reviews
- ✓ Web mining and information retrieval

Data Science and Analytics

- ✓ Integration and visualization of large volumes of heterogeneous data
- ✓ Development and implementation of Deep Learning methodologies for predictive science
- ✓ Automated Image analysis using artificial intelligence
- ✓ Natural Language Processing (NLP) methods using Deep Learning

Software Development

- ✓ Requirements gathering
- ✓ Software architecture design
- ✓ User interface design
- ✓ Implementation, deployment
- ✓ User support

More info about Sciome and
Active Screener at our
website:

www.sciome.com

ANY
QUESTIONS?

