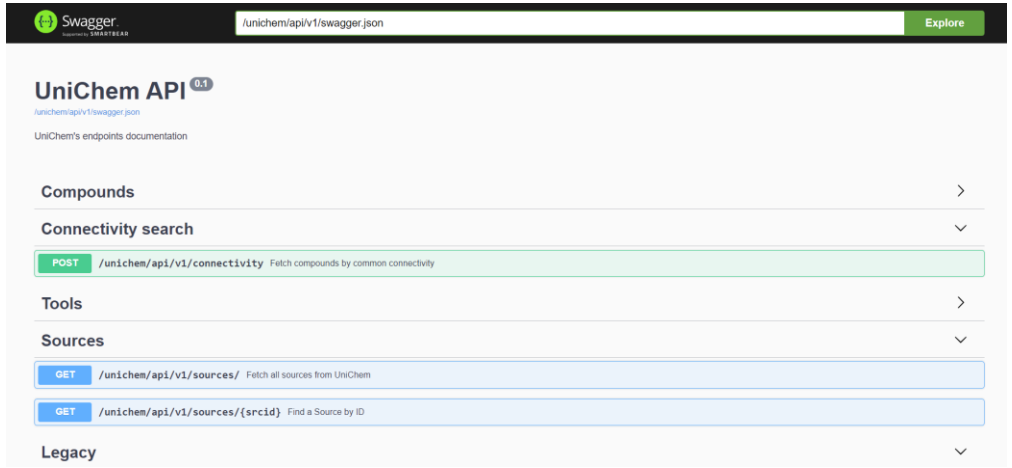
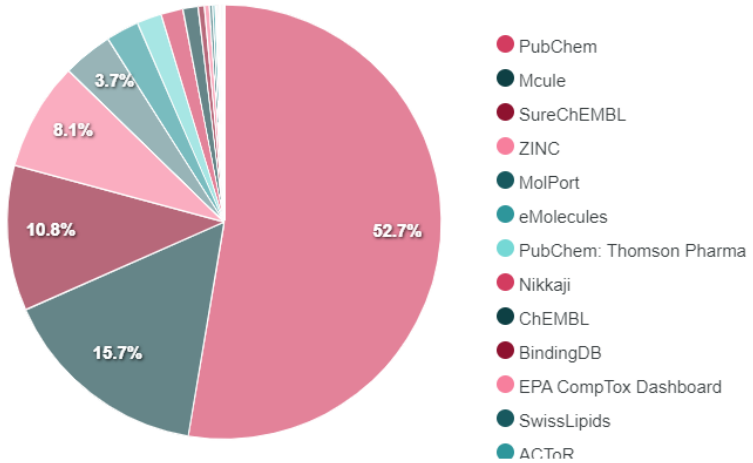
# Drug repositioning web application using compound API

BY SARAWOOT SOMIN

# Compound API online

https://www.ebi.ac.uk/unichem/api/docs#/




This is non-redundant database of pointers between chemical structures and EMBL-EBI chemistry resources. Its purpose is to optimise the efficiency with which structure-based hyperlinks may be built and maintained between chemistry-based resources, and is particularly suitable for creating such links 'on the fly' (by use of REST web services).

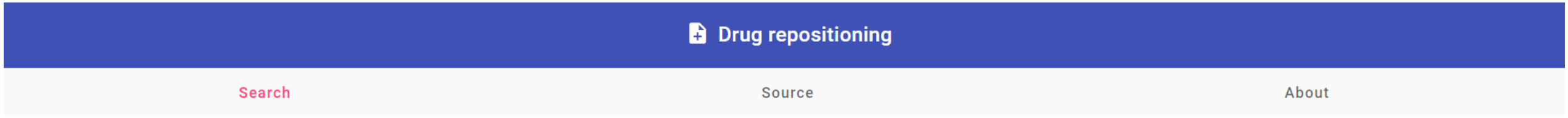
# The web application

There are three tabs, including “Search”, “Source” and “About”

- “Search” tab is to fetch multiple source data sets for a given compound with common connectivity to a given id (UCI) on the database source.

- “Source” tab is to show all source of the compounds.

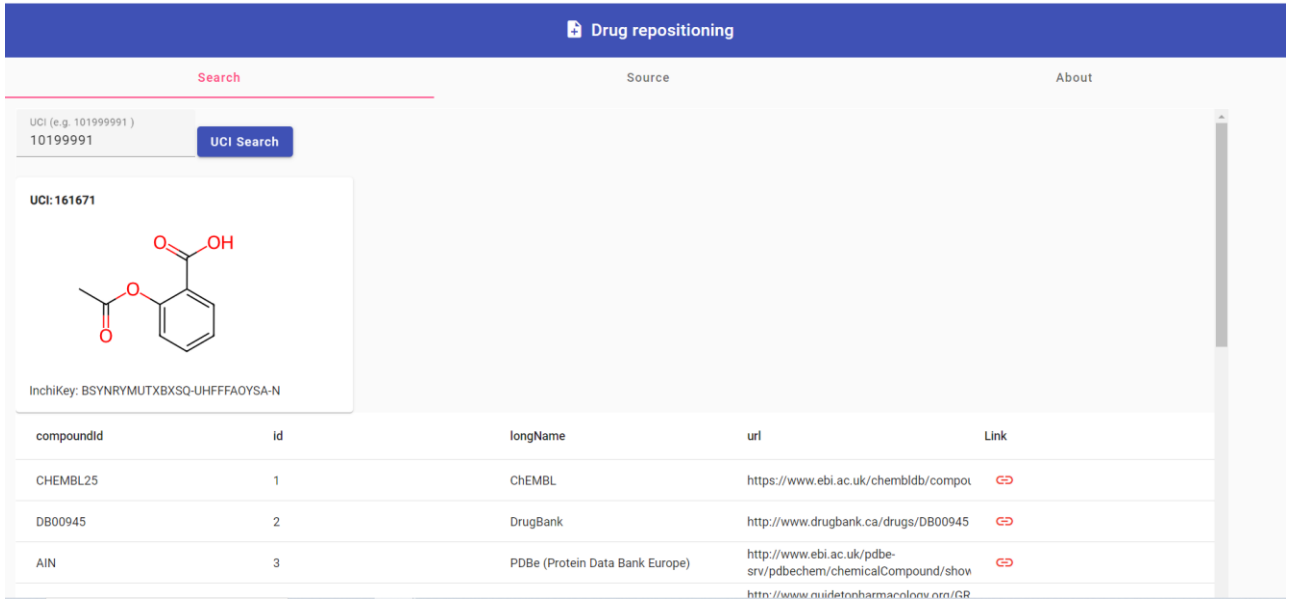
- “About” tab is to show the author information and the overview of the proposal.



# Search feature

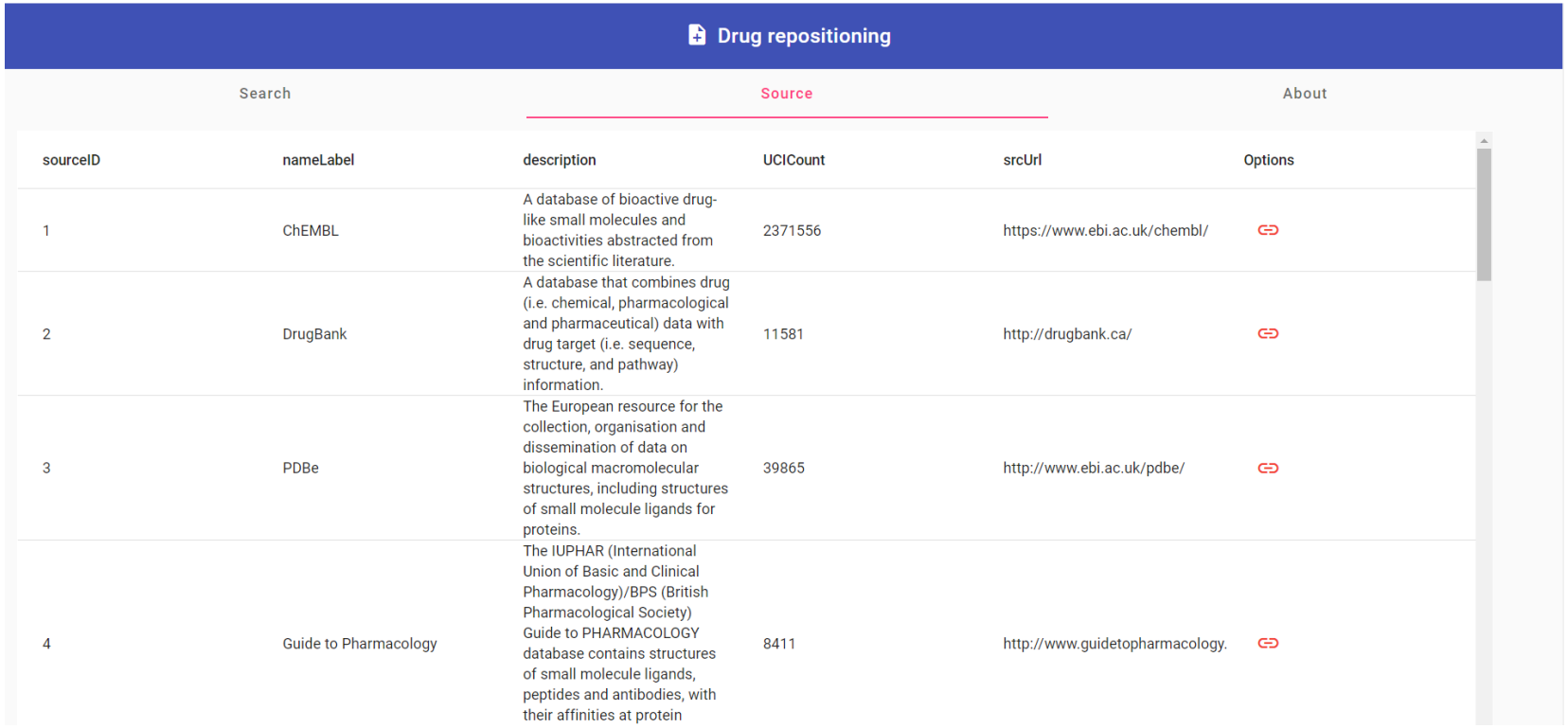
- The web application recommend retrieves the compounds from different sources by UCI search.

- The system also display the chemical structure following the UCI search.



# Source feature

The web application shows all sources of the compounds.




| sourceID | nameLabel | description | UCICount | srcUrl | Options |
|---|---|---|---|---|---|
| 1 | ChEMBL | A database of bioactive drug-like small molecules and bioactivities abstracted from the scientific literature. | 2371556 | https://www.ebi.ac.uk/chembl/ | |
| 2 | DrugBank | A database that combines drug (i.e. chemical, pharmacological and pharmaceutical) data with drug target (i.e. sequence, structure, and pathway) information. | 11581 | http://drugbank.ca/ | |
| 3 | PDBe | The European resource for the collection, organisation and dissemination of data on biological macromolecular structures, including structures of small molecule ligands for proteins. | 39865 | http://www.ebi.ac.uk/pdbe/ | |
| 4 | Guide to Pharmacology | The IUPHAR (International Union of Basic and Clinical Pharmacology)/BPS (British Pharmacological Society) Guide to PHARMACOLOGY database contains structures of small molecule ligands, peptides and antibodies, with their affinities at protein | 8411 | http://www.guidetopharmacology. | |

# About feature

## Author information, and the research of interest

Drug repositioning

Search | Source | About

### Author

Objective: Doing research can provide me with opportunities for using and improving my programming and analytical skill. I have a true passion for developing methods and applications to solve difficult problems in computer science and biological fields. Proficient in programming, I can be flexible to develop solutions to various problems in different environments. After spending several years on postgraduate degrees, including working as a system analyst and a programmer, I am excellent at identifying and analysing problems and developing a solution to address those problems.

- PhD degree: Computational Modelling and Systems Biology, Faculty of Agriculture and Life Sciences, Lincoln University, New Zealand (2020-Current).
- PhD degree (outstanding): Computer Science, King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand (2012-2018).
- Master degree : Computer Science, King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand (2008-2011).
- Bachelor degree : Computer Science, King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand (2001-2004).

Figure 1. Drug repositioning approaches for drug discovery and validation.

### Proposal

Drug repositioning, also known as drug repurposing, seeks to identify FDA-approved drugs for the treatment of various diseases (Hodos et al., 2016). This strategy, alternatively referred to as drug repositioning, rediscovery, or reprofiling, aims to uncover new therapeutic applications for preapproved drugs or existing medications. The fundamental concept behind repurposing is to identify novel beneficial effects for a specific ailment in a previously clinically utilized drug or one that faced setbacks in later stages of development (Chong and Sullivan, 2007). Drug repositioning is involved in two main procedures, as figure 1.