RDTextractor

!! Requires python3.6!!

Installation

```
pip install -r requirements.txt
python setup.py install
```

Once it's installed, you can run the extractor by typing:

% extract -h

Introduction

This tool is designed to extract data from the *in vivo* repeat-dose toxicity (RDT) studies' database generated within the context of the eTOX project. These data are expanded using an histopathological observation and an anatomical entity ontologies. The histopathological ontology is obtained from Novartis and can be used under the Apache License 2.0. The anatomical entities ontology is extracted from the following paper:

Hayamizu TF, Mangan M, Corradi JP, Kadin JA, Ringwald M. Genome Biol. 2005; 6(3): R29

The script can work with version 2016.1 or with later versions. For the former, you need to request access to the data files from us and place these files in the data folder. For the latter, you need to have the Oracle database provided by Lhasa installed and run the script from the Oracle server. Additionally, you'll need to set up the ORACLE_HOME and LD_LIBRARY_PATH environment variables. This project is an extension of the work published in the following paper:

 López-Massaguer O, Pinto-Gil K, Sanz F, Amberg A, Anger LT, Stolte M, Ravagli C, Marc P, Pastor M. Toxicol Sci. 2018 Mar; 162(1): 287–300.

Manual

Exract studies' findings based on the given filtering and the organs' and morphological changes' ontologies-based expansions of these findings.

- Required arguments:
 - -a / --organ ORGAN Anatomical entity that the finding refers to (case insensitive). You can filter for more than one organ by passing a blank space-separated list.
- Optional arguments:
 - Version-related arguments:
 - -v / --version {local, oracle}Vitic database version (default: oracle).
 - -n / --hostIf working with the Oracle database, provide the Oracle DB's host.
 - -d / --sid SID If working with the Oracle database, provide the Oracle SID's.

 -b / --dbname DBname If working with Vitic's Oracle database, provide the DB's name if necessary for querying.

- -u / --user USER If working with the Oracle database, provide the Oracle database user name.
- -p / --passw PASSW If working with the Oracle database, provide the Oracle database password.
- -c / --port PASSW If working with the Oracle database, the Oracle database port (default: 1521).
- Study design-related arguments:
 - -i / --min_exposure MIN_EXPOSUREMinimum exposure period (days).
 - -e / --max_exposure MAX_EXPOSURE Maximum exposure period (days).
 - -r / --route {Cutaneous, Diertary, Oral, Oral gavage, Intragastric, Nasogastric, Oropharyngeal, Endotracheal, Intra-articular, Intradermal, Intraesophageal, Intraileal, Intramuscular, Subcutaneous, Intraocular, Intraperitoneal, Intrathecal, Intrauterine, Intravenous, Intravenous bolus, Intravenous drip, Parenteral, Nasal, Respiratory (inhalation), Percutaneous, Rectal, Vaginal, Subarachnoid} Administration route (case insensitive).
 You can filter for more than one administration route by passing a blank space-separated list.
 - -s / --species {Mouse, Rat, Hamster, Guinea pig, Rabbit, Dog, Pig, Marmoset, Monkey,
 Baboon} Species (case insensitive). You can filter for more than one species by passing a blank space-separated list.
- Finding-related arguments:
 - -m / --observation OBSERVATION Morphological change type that the finding refers to (case insensitive). You can filter for more than one morphological change by passing a blank space-separated list.
 - -t / --treatment_related Keep only treatment-related findings.
 - -x / --sex {F,M,Both} Finding's sex sex.
- Output-related arguments:
 - -o / --output_basename OUTPUT_BASENAME Output file base name. Two output files will be generated: basename_quant.tsv and basename_qual.tsv, with quantitative and qualitative results respectively. (default: output).

Use examples

- 1. Extract all studies with liver-related findings
 - vitic 2016.1:

```
extract -v local -a liver
```

latest vitic:

```
extract -v oracle -d ORACLE_SID -u ORACLE_USER -p ORACLE_PASSWORD -a liver
```

2. Extract all studies with liver- and kidney-related findings

Note that you can filter for more than one organ by passing a blank space-separated list.

• vitic 2016.1:

```
extract -v local -a liver kidney
```

latest vitic:

```
extract -v oracle -d ORACLE_SID -u ORACLE_USER -p ORACLE_PASSWORD -a liver kidney
```

3. Extract only studies of interest

Filter the studies of interest based on exposure time (days), administration route, and species. Note that for route and species you can filter for more than one value by passing a blank space-separated list.

• Using long arguments:

```
extract -v local --organ liver --min_exposure 1 --max_exposure 10 --route ORAL -- species MOUSE RAT
```

• Using short arguments:

```
extract -v local -a liver -i 1 -e 10 -r ORAL -s MOUSE RAT
```

4. Extract treatment-related findings only

```
extract -v local -a liver -i 1 -e 10 -r ORAL -s MOUSE RAT -t
```

5. Output example

After extracting data using this tool, two output files are generated, one with quantitative and the other with qualitative data. Both have five common columns, namely:

- subst id: Substance ID.
- study_count: Number of relevant studies (according to the current filtering scheme) in which the substance appears.
- dose_max: Maximum dose at which the substance has been tested among the relevant studies.
- dose_min: Minimum dose at which the substance has been tested among the relevant studies.
- is_active: Boolean indicating whether the substance has been found to have any toxicity according to the current finding-related filtering criteria.

After these, there is a column for each relevant finding. In these columns a value is provided if the finding is reported for the given substance, and it is empty otherwise. The value will be 1 in the qualitative file and the minimum dose at which the finding is reported in the quantitative file.



This is an example of the quantitative output:



You can also run a script that displays the available options by typing:

Manual

[%] getRDToptions -h

show all the available options for any of the selected fields.

- Optional arguments:
 - Version-related arguments:
 - -v / --version {local, oracle}Vitic database version (default: oracle).
 - -n / --host If working with the Oracle database, provide the Oracle DB's host.
 - -d / --sid SID If working with the Oracle database, provide the Oracle SID's.
 - -b / --dbname DBname If working with Vitic's Oracle database, provide the DB's name if necessary for querying.
 - -u / --user USER If working with the Oracle database, provide the Oracle database user name.
 - -p / --passw PASSW If working with the Oracle database, provide the Oracle database password.
 - -c / --port PASSW If working with the Oracle database, the Oracle database port (default: 1521).
 - Study design-related arguments:
 - -e / --exposure Get exposure range for the whole DB.
 - -r / --route Get all route options for the whole DB.
 - -s / --species Get all species options for the whole DB.
 - o Finding-related arguments:
 - -a / --organGet all anatomical entity options for the whole DB.
 - -m / --observation Get all morphological change options for the whole DB.
 - Output-related arguments:
 - -o / --output_name OUTPUT_NAMEOutput file name (default: standard output).