DjangoAPI

Install

Install the enviroment

In the root folder execute "python manage.py runserver"

Run

```
% python manage.py runserver
```

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.

In order to be able to aggregate the data by parent compound, some pre-processing has to be done to data as they exist in the database. Each substance is standardised according to the following protocol:

- Use the process_smiles.std method from this repository to standardize, discard mixtures, discard compound with metal ions, and remove all salts.
- Neutralize all charges.

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.

Output example

On clicking the 'Extract' button, two output files are generated, one with quantitative and the other with qualitative data. Both have a caption summarising the filtering criteria applied. After this caption, they both have a table with the data aggergated by parent compound. The table contains several fixed columns, namely 6 at the begining:

- inchi_key: Parent compound's InChIKey.

- study_count: Number of relevant studies (according to the current filtering scheme) in which the compound appears.
- dose_min: Minimum dose at which the compound has been tested among the relevant studies.
- dose_max: Maximum dose at which the compound has been tested among the relevant studies.
- min_observation_dose: Minimum dose for which a relevant finding (according to the current filtering scheme) has been reported for the compound.
- is_active: Boolean indicating whether the substance has been found to have any toxicity according to the current finding-related filtering criteria. And two at the end:
- subst_id: All substance IDs corresponding to the parent compound.
- std_smiles: Smiles string corresponding to the standardised parent compound.

Between these two groups, 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 the number of studies that report the finding in the qualitative file, and the minimum dose at which the finding is reported in the quantitative file.

This is an example of the qualitative output:

Study-level filters:									
	Species: Rat								
	Dose range: 1 to 100 mg/kg								
Finding-level filters:									
	Parameter: Histopathological|Liver								
	Observation: Histopathological|Degeneration								
	Sex: Male								
	Treatment-related only								
inchi_key	study_count	dose_min	dose_max	min_observation_dose	Liver_Degeneration, vacuolar	Liver_Degeneration, cystic	Liver_Degeneration, hydropic	subst_id	std_smiles
BPRHUIZ(	2	2	100	2	2			AZ_GGA_229587807	CC(C)c1nc(
OVCDSSH	1	30	100	100			1	GGA-SAD-0053, GGA-SAD-0038	CCN(CC)Cc
XGALLCV:	1	1	10	1		1		AZ_GGA_200002321	COc1cc2nc

This is an example of the quantitative output:

Study-level filters:									
	Species: Rat								
	Dose range: 1 to 100 mg/kg								
Finding-level filters:									
	Parameter: Histopathological|Liver								
	Observation: Histopathological|Degeneration								
	Sex: Male								
	Treatment-related only								
inchi_key	study_count	dose_min	dose_max	min_observation_dose	Liver_Degeneration, vacuolar	Liver_Degeneration, cystic	Liver_Degeneration, hydropic	subst_id	std_smiles
BPRHUIZ(	2	2	100	2	2			AZ_GGA_229	CC(C)c1nc(
OVCDSSH	1	30	100	100			100	GGA-SAD-00	CCN(CC)Cc
XGALLCV:	1	1	10	1		1		AZ_GGA_200	COc1cc2nc