1. Download data

* curl -O <https://reactome.org/download/current/ChEBI2Reactome.txt>
* curl -O <https://reactome.org/download/current/NCBI2Reactome.txt>

Header for the files:

The columns within the mapping’s files follow a similar format:

1. Source database identifier, e.g. UniProt, ENSEMBL, NCBI Gene or ChEBI identifier
2. Reactome Pathway Stable identifier
3. URL
4. Event (Pathway or Reaction) Name
5. Evidence Code
6. Species
7. Appending header to the columns using command line

* (echo -e"ChEBI\_ID\tReactomePathway\_ID\tURL\tPathwayName\tEvidenceCode\tSpecies"; cat ChEBI2Reactome.txt;) > ChEBI2Reactome2.txt
* (echo -e “NCBI\_Gene\_ID\tReactomePathway\_ID\tURL\tPathwayName\tEvidenceCode\tSpecies"; cat NCBI2Reactome.txt;) > NCBI2Reactome2.txt

1. Appending prefix to the chebi\_id’s in order to match with the existing chebi\_id’s

* awk 'BEGIN{FS=OFS=","} {$1 = "CHEBI:"$1; print}' ChEBI2Reactome2.txt > ChEBI2Reactomefinal.txt

1. Loading on PostgreSQL

CREATE STATEMENTS:

* CREATE TABLE ncbi2reactome (ncbi\_gene\_id VARCHAR, reactome\_pathway\_id VARCHAR, pathway\_name VARCHAR, evidence\_code VARCHAR, species VARCHAR);
* CREATE TABLE chebi2reactome(chebi\_id VARCHAR, reactome\_pathway\_id VARCHAR, pathway\_name VARCHAR, evidence\_code VARCHAR, species VARCHAR);
* CREATE TABLE chebi2ndb (chebi\_id VARCHAR PRIMARY KEY, ndb\_id INTEGER, ndb\_name VARCHAR);

COPY STATEMENTS:

* COPY ncbi2reactome (ncbi\_gene\_id, reactome\_pathway\_id, pathway\_name, evidence\_code, species) FROM '/Users/aginni/Documents/Level-1/finaldatasets/NCBI2Reactometrim.txt' WITH (FORMAT CSV,HEADER,DELIMITER' ');
* COPY chebi2reactome (chebi\_id, reactome\_pathway\_id, pathway\_name, evidence\_code, species) FROM '/Users/aginni/Documents/Level-1/finaldatasets/ChEBI2Reactometrim.txt' WITH (FORMAT CSV,HEADER, DELIMITER' ');
* COPY chebi2ndb (chebi\_id, ndb\_id,ndb\_name) FROM '/Users/aginni/Documents/Level-1/finaldatasets/chebi2ndb.csv' WITH(FORMAT CSV, HEADER, DELIMITER',');

IGNORE:

* ALTER TABLE ncbi2reactome DROP CONSTRAINT ncbi2reactome\_pkey;
* ALTER TABLE chebi2ndb ADD CONSTRAINT chebi2ndb\_pkey PRIMARY KEY (chebi\_id,ndb\_id);
* ALTER TABLE ncbi2reactome ALTER COLUMN ncbi\_gene\_id TYPE VARCHAR;