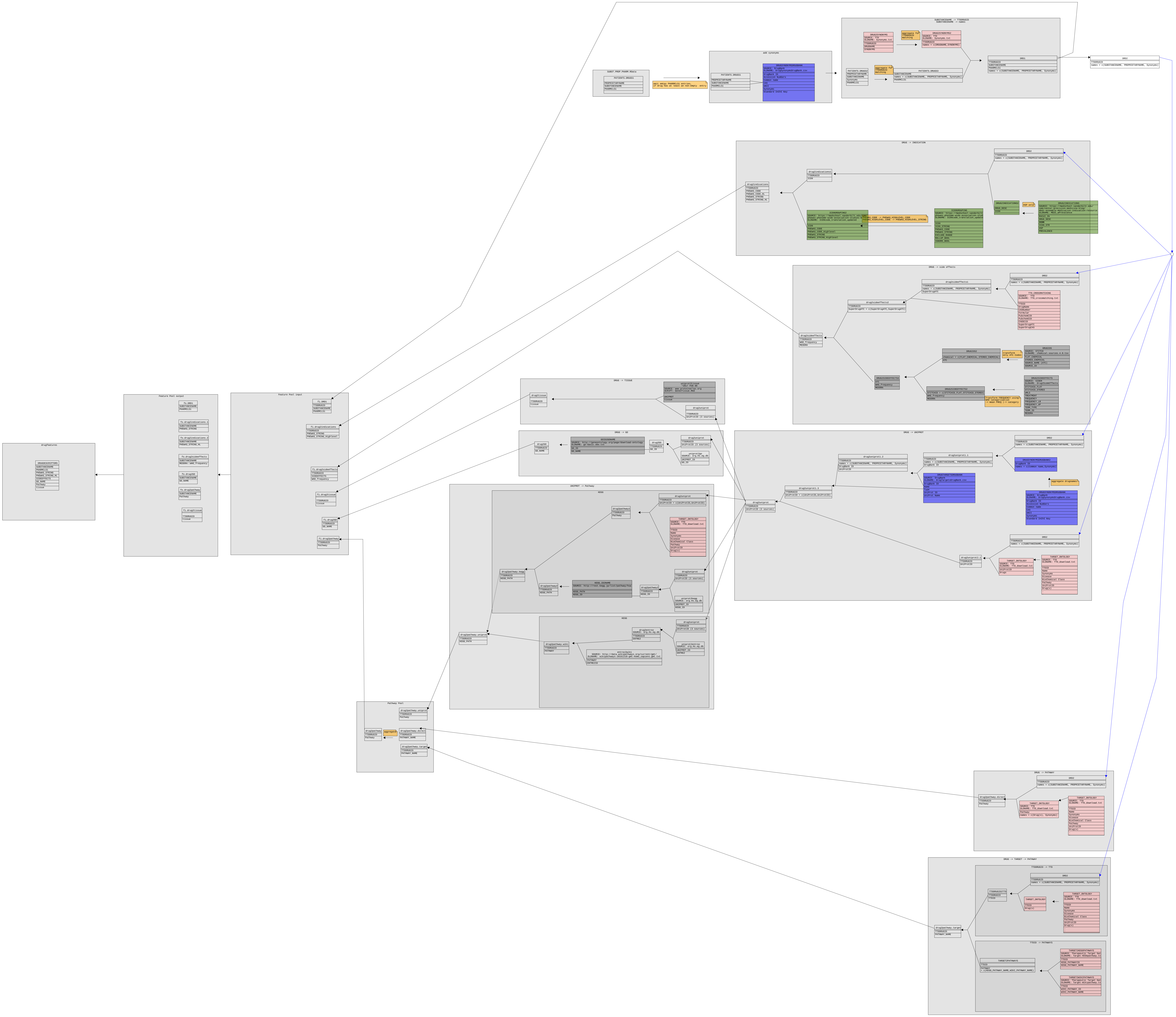
SUBST.PROP.PHARM.RData
PATIENTS.DRUGS1
PROPRIETARYNAME
SUBSTANCENAME
PHARMCLS1
omit emtpy PHARMCLS1 entries,
if drug has at least an non-empty entry
add synonyms
PATIENTS.DRUGS1
PROPRIETARYNAME
SUBSTANCENAME
PHARMCLS1
DRUGSYNONYMSDRUGBANK
SOURCE: DrugBank
OLDNAME: DrugSynonymsDrugBank.csv
DrugBank ID
Accession Numbers
Common name
CAS
UNII
Synonyms
Standard InChI Key
SUBSTANCENAME -> TTDDRUGID
SUBSTANCENAME -> names
DRUG2SYNONYMS
SOURCE: TTD
OLDNAME: Synonyms.txt
TTDDRUGID
DRUGNAME
SYNONYMS
aggregate for TTDDRUGID matching
DRUG2SYNONYMS2
SOURCE: TTD
OLDNAME: Synonyms.txt
TTDDRUGID
names = c(DRUGNAME,SYNONYMS)
PATIENTS.DRUGS2
PROPRIETARYNAME
SUBSTANCENAME
Synonyms
PHARMCLS1
aggregate for TTDDRUGID matching
PATIENTS.DRUGS3
SUBSTANCENAME
names = c(SUBSTANCENAME, PROPRIETARYNAME, Synonyms)
PHARMCLS1
DRD1
TTDDRUGID
SUBSTANCENAME
PHARMCLS1
names = c(SUBSTANCENAME, PROPRIETARYNAME, Synonyms)
DRD2
TTDDRUGID
names = c(SUBSTANCENAME, PROPRIETARYNAME, Synonyms)
DRUG -> INDICATION
DRD2
TTDDRUGID
names = c(SUBSTANCENAME, PROPRIETARYNAME, Synonyms)
drug2indications1
TTDDRUGID
ICD9
drug2indications
TTDDRUGID
PHEWAS_CODE
PHEWAS_CODE_HL
PHEWAS_STRING
PHEWAS_STRING_HL
DRUG2INDICATIONS2
DRUG_DESC
ICD9
HSP only
DRUG2INDICATIONS
SOURCE: https://medschool.vanderbilt.edu/cpm/center-precision-medicine-blog/medi-ensemble-medication-indication-resource
OLDNAME: MEDI_wPrevalence
RXCUI_IN
DRUG_DESC
ICD9
ICD9_STR
HSP
PREVALENCE
ICD9GROUPING2
SOURCE: https://medschool.vanderbilt.edu/cpm/phewas-phenome-wide-association-studies-0
OLDNAME: ICD9code_translation_updated
ICD9
PHEWAS_CODE
PHEWAS_CODE_Highlevel
PHEWAS_STRING
PHEWAS_STRING_Highlevel
PHEWAS_CODE -> PHEWAS_HIGHLEVEL_CODE
PHEWAS_HIGHLEVEL_CODE -> PHEWAS_HIGHLEVEL_STRING
ICD9GROUPING
SOURCE: https://medschool.vanderbilt
phewas-phenome-wide-association-stud
OLDNAME: ICD9code_translation_update
ICD9
ICD9_STRING
PHEWAS_CODE
PHEWAS_STRING
EXCLUDE_RANGE
ROLLUP_BOOL
IGNORE_BOOL
DRUG -> side effects
DRD2
TTDDRUGID
names = c(SUBSTANCENAME, PROPRIETARYNAME, Synonyms)
drug2sideeffects1
TTDDRUGID
names = c(SUBSTANCENAME, PROPRIETARYNAME, Synonyms)
SuperDrugATC
TTD_CROSSMATCHING
SOURCE: TTD
OLDNAME: TTD_crossmatching.txt
TTDID
DrugName
CASNumber
Formular
PubchemCID
PubchemSID
ChEBIID
SuperDrugATC
SuperDrugCAS
drug2sideeffects2
TTDDRUGID
SuperDrugATC = c(SuperDrugATC,SuperDrugATC)
drug2sideeffects
TTDDRUGID
WHO_frequency
MEDDRA
DRUGIDS2
chemical = c(FLAT_CHEMICAL,STEREO_CHEMICAL)
ATC
transform only ATC Codes
DRUGIDS
SOURCE: STITCH
OLDNAME: chemical.sources.4.0.tsv
FLAT_CHEMICAL
STEREO_CHEMICAL
SOURCE_NAME (ATC)
SOURCE_ID
DRUG2SIDEEFFECTS3
ATC
WHO_frequency
MEDDRA
DRUG2SIDEEFFECTS2
STITCHID = c(STITCHID_FLAT,STITCHID_STEREO)
WHO_frequency
MEDDRA
Transform FREQUENCY using WHO categorisation
-> mean FREQ |-> category
DRUG2SIDEEFFECTS
SOURCE: SIDER
OLDNAME: Drug2SideEffects
STITCHID_FLAT
STITCHID_STEREO
UMLS
TREATMENT
FREQUENCY
FREQUENCY_LB
FREQUENCY_UP
TERM_TYPE
TERM_ID
MEDDRA
DRUG -> TISSUE
drug2tissue
TTDDRUGID
tissue
uniprot2tissue
*2017 FEB 08
SOURCE: www.proteinatlas.org
SCRIPT: Gene2Tissue.Rmd
UNIPROT
tissue
drug2uniprot
TTDDRUGID
UniProtID (3 sources)
DRUG -> GO
drug2GO
TTDDRUGID
GO_NAME
GOID2GONAME
SOURCE: http://geneontology.org/page/download-ontology
OLDNAME: go-basic.obo.txt
GO_ID
GO_NAME
drug2GO
TTDDRUGID
GO_ID
drug2uniprot
TTDDRUGID
UniProtID (3 sources)
uniprot2go
SOURCE: org.Hs.eg.db
UNIPROT_ID
GO_ID
DRUG -> UNIPROT
DRD2
TTDDRUGID
names = c(SUBSTANCENAME, PROPRIETARYNAME, Synonyms)
drug2uniprot1.1
TTDDRUGID
names = c(SUBSTANCENAME, PROPRIETARYNAME, Synonyms)
DrugBank ID
DRUGSYNONYMSDRUGBANK2
DrugBank ID
names = c(Common name,Synonyms)
aggregate drugnames
DRUGSYNONYMSDRUGBANK
SOURCE: DrugBank
OLDNAME: DrugSynonymsDrugBank.csv
DrugBank ID
Accession Numbers
Common name
CAS
UNII
Synonyms
Standard InChI Key
drug2uniprot1.2
TTDDRUGID
names = c(SUBSTANCENAME, PROPRIETARYNAME, Synonyms)
DrugBank ID
UniProtID
DRUGTARGETSDRUGBANK
SOURCE: DrugBank
OLDNAME: DrugTargetsDrugBank.csv
DrugBank ID
Name
Type
UniProt ID
UniProt Name
drug2uniprot1.3
TTDDRUGID
UniProtID = c(UniProtID,UniProtID)
drug2uniprot
TTDDRUGID
UniProtID (3 sources)
DRD2
TTDDRUGID
names = c(SUBSTANCENAME, PROPRIETARYNAME, Synonyms)
drug2uniprot2.1
TTDDRUGID
UniProtID
TARGET_ONTOLOGY
SOURCE: TTD
OLDNAME: TTD_download.txt
UniProtID
Drugs
TARGET_ONTOLOGY
SOURCE: TTD
OLDNAME: TTD_download.txt
TTDID
Name
Synonyms
Disease
BioChemical Class
Pathway
UniProtID
Drug(s)
UNIPROT -> Pathway
KEGG
drug2uniprot
TTDDRUGID
UniProtID = c(UniProtID,UniProtID)
drug2pathway1
TTDDRUGID
Pathway
TARGET_ONTOLOGY
SOURCE: TTD
OLDNAME: TTD_download.txt
TTDID
Name
Synonyms
Disease
BioChemical Class
Pathway
UniProtID
Drug(s)
drug2pathway.kegg
TTDDRUGID
KEGG_PATH
drug2pathway2
TTDDRUGID
KEGG_PATH
KEGG_ID2NAME
SOURCE: http://rest.kegg.jp/list/pathway/hsa
KEGG_PATH
KEGG_ID
drug2pathway2
TTDDRUGID
KEGG_ID
drug2uniprot
TTDDRUGID
UniProtID (3 sources)
uniprot2kegg
SOURCE: org.Hs.eg.db
UNIPROT_ID
KEGG_ID
KEGG
drug2uniprot
TTDDRUGID
UniProtID (3 sources)
drug2entrez
SOURCE: org.Hs.eg.db
TTDDRUGID
ENTREZ
uniprot2entrez
SOURCE: org.Hs.eg.db
UNIPROT_ID
ENTREZ
drug2pathway.wiki
TTDDRUGID
PATHWAY
entrez2wiki
SOURCE: http://data.wikipathways.org/current/gmt/
OLDNAME: wikipathways-20161210-gmt-Homo_sapiens.gmt.txt
PATHWAY
ENTREZID
drug2pathway.uniprot
TTDDRUGID
KEGG_PATH
Pathway Pool
drug2pathway.uniprot
TTDDRUGID
Pathway
drug2pathway
TTDDRUGID
Pathway
aggregate
drug2pathway.direct
TTDDRUGID
PATHWAY_NAME
drug2pathway.target
TTDDRUGID
PATHWAY_NAME
DRUG -> PATHWAY
DRD2
TTDDRUGID
names = c(SUBSTANCENAME, PROPRIETARYNAME, Synonyms)
drug2pathway.direct
TTDDRUGID
Pathway
TARGET_ONTOLOGY
SOURCE: TTD
OLDNAME: TTD_download.txt
Pathway
names = c(Drug(s), Synonyms)
TARGET_ONTOLOGY
SOURCE: TTD
OLDNAME: TTD_download.txt
TTDID
Name
Synonyms
Disease
BioChemical Class
Pathway
UniProtID
Drug(s)
DRUG -> TARGET -> PATHWAY
TTDDRUGID -> TTD
DRD2
TTDDRUGID
names = c(SUBSTANCENAME, PROPRIETARYNAME, Synonyms)
TTDDRUGID2TTD
TTDDRUGID
TTDID
TARGET_ONTOLOGY
TTDID
Drug(s)
TARGET_ONTOLOGY
SOURCE: TTD
OLDNAME: TTD_download.txt
TTDID
Name
Synonyms
Disease
BioChemical Class
Pathway
UniProtID
Drug(s)
drug2pathway.target
TTDDRUGID
PATHWAY_NAME
TTDID -> PATHWAYS
TARGET2PATHWAYS
TTDID
PATHWAY
= c(KEGG_PATHWAY_NAME,WIKI_PATHWAY_NAME)
TARGET2KEGGPATHWAYS
SOURCE: Therapeutic Target Dat
OLDNAME: Target-KEGGpathway.tx
TTDID
KEGG_PATHWAYID
KEGG_PATHWAY_NAME
TARGET2WIKIPATHWAYS
SOURCE: Therapeutic Target Dat
OLDNAME: Target-Wikipathway.tx
TTDID
WIKI_PATHWAY_ID
WIKI_PATHWAY_NAME
Feature Pool input
fi.DRD1
TTDDRUGID
SUBSTANCENAME
PHARMCLS1
fi.drug2indications
TTDDRUGID
PHEWAS_STRING
PHEWAS_STRING_Highlevel
fi.drug2sideeffects
TTDDRUGID
SIDEEFFECTS
WHO_frequency
fi.drug2tissue
TTDDRUGID
tissue
fi.drug2GO
TTDDRUGID
GO_NAME
fi.drug2pathway
TTDDRUGID
Pathway
Feature Pool output
fo.DRD1
SUBSTANCENAME
PHARMCLS1
fo.drug2indications.1
SUBSTANCENAME
PHEWAS_STRING
fo.drug2indications.2
SUBSTANCENAME
PHEWAS_STRING_HL
fo.drug2sideeffects
SUBSTANCENAME
MEDDRA::WHO_frequency
fo.drug2GO
SUBSTANCENAME
GO_NAME
fo.drug2pathway
SUBSTANCENAME
Pathway
fi.drug2tissue
TTDDRUGID
tissue
drugfeatures
DRUGDESCRIPTORS
SUBSTANCENAME
PHARMCLS1
PHEWAS_STRING
PHEWAS_STRING_HL
SIDEEFFECTS
GO_NAME
Pathway
tissue