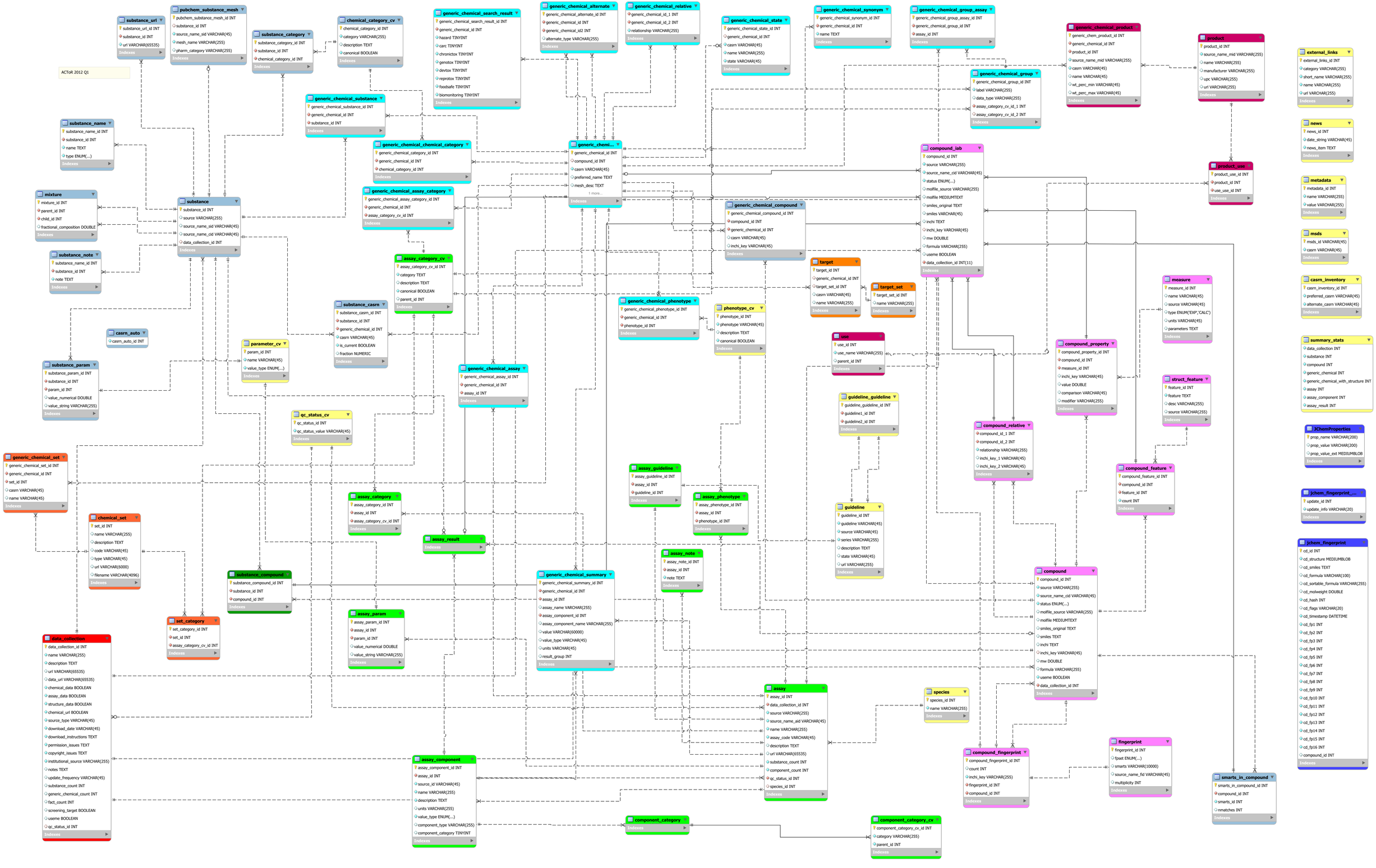
ACToR 2012 Q1
substance_url
substance_id INT
substance_id INT
url VARCHAR(65535)
Indexes
pubchem_substance_mesh
pubchem_substance_mesh_id INT
substance_id INT
source_name_sid VARCHAR(45)
mesh_name VARCHAR(255)
pharm_category VARCHAR(255)
Indexes
substance_category
substance_category_id INT
substance_id INT
chemical_category_id INT
Indexes
chemical_category_cv
chemical_category_id INT
category VARCHAR(255)
description TEXT
canonical BOOLEAN
Indexes
generic_chemical_search_result
generic_chemical_search_result_id INT
generic_chemical_id INT
hazard TINYINT
carc TINYINT
chronictox TINYINT
genotox TINYINT
devtox TINYINT
reprotox TINYINT
foodsafe TINYINT
biomonitoring TINYINT
Indexes
generic_chemical_alternate
generic_chemical_alternate_id INT
generic_chemical_id INT
generic_chemical_id2 INT
alternate_type VARCHAR(255)
Indexes
generic_chemical_relative
generic_chemical_id_1 INT
generic_chemical_id_2 INT
relationship VARCHAR(255)
Indexes
generic_chemical_state
generic_chemical_state_id INT
generic_chemical_id INT
casrn VARCHAR(45)
name VARCHAR(255)
state VARCHAR(45)
Indexes
generic_chemical_synonym
generic_chemical_synonym_id INT
generic_chemical_id INT
name TEXT
Indexes
generic_chemical_group_assay
generic_chemical_group_assay_id INT
generic_chemical_group_id INT
assay_id INT
Indexes
generic_chemical_product
generic_chem_product_id INT
generic_chemical_id INT
product_id INT
source_name_mid VARCHAR(255)
casrn VARCHAR(45)
name VARCHAR(45)
wt_perc_min VARCHAR(45)
wt_perc_max VARCHAR(45)
Indexes
product
product_id INT
source_name_mid VARCHAR(255)
name VARCHAR(255)
manufacturer VARCHAR(255)
upc VARCHAR(255)
url VARCHAR(255)
Indexes
external_links
external_links_id INT
category VARCHAR(255)
short_name VARCHAR(255)
name VARCHAR(255)
url VARCHAR(255)
Indexes
generic_chemical_group
generic_chemical_group_id INT
label VARCHAR(255)
data_type VARCHAR(255)
assay_category_cv_id_1 INT
assay_category_cv_id_2 INT
Indexes
generic_chemical_substance
generic_chemical_substance_id INT
generic_chemical_id INT
substance_id INT
Indexes
substance_name
substance_name_id INT
substance_id INT
name TEXT
type ENUM(...)
Indexes
generic_chemical_chemical_category
generic_chemical_category_id INT
generic_chemical_id INT
chemical_category_id INT
Indexes
generic_chemi...
generic_chemical_id INT
compound_id INT
casrn VARCHAR(45)
preferred_name TEXT
mesh_desc TEXT
1 more...
Indexes
news
news_id INT
date_string VARCHAR(45)
news_item TEXT
Indexes
compound_iab
compound_id INT
source VARCHAR(255)
source_name_cid VARCHAR(45)
status ENUM(...)
molfile_source VARCHAR(255)
molfile MEDIUMTEXT
smiles_original TEXT
smiles VARCHAR(45)
inchi TEXT
inchi_key VARCHAR(45)
mw DOUBLE
formula VARCHAR(255)
useme BOOLEAN
data_collection_id INT(11)
Indexes
product_use
product_use_id INT
product_id INT
use_use_id INT
Indexes
metadata
metadata_id INT
name VARCHAR(255)
value VARCHAR(255)
Indexes
mixture
mixture_id INT
parent_id INT
child_id INT
fractional_composition DOUBLE
Indexes
substance
substance_id INT
source VARCHAR(255)
source_name_sid VARCHAR(45)
source_name_cid VARCHAR(45)
data_collection_id INT
Indexes
generic_chemical_assay_category
generic_chemical_assay_category_id INT
generic_chemical_id INT
assay_category_cv_id INT
Indexes
generic_chemical_compound
generic_chemical_compound_id INT
compound_id INT
generic_chemical_id INT
casrn VARCHAR(45)
inchi_key VARCHAR(45)
Indexes
msds
msds_id VARCHAR(45)
casrn VARCHAR(45)
Indexes
substance_note
substance_name_id INT
substance_id INT
note TEXT
Indexes
assay_category_cv
assay_category_cv_id INT
category TEXT
description TEXT
canonical BOOLEAN
parent_id INT
Indexes
target
target_id INT
generic_chemical_id INT
target_set_id INT
casrn VARCHAR(45)
name VARCHAR(255)
Indexes
target_set
target_set_id INT
name VARCHAR(255)
Indexes
measure
measure_id INT
name VARCHAR(45)
source VARCHAR(45)
type ENUM('EXP','CALC')
units VARCHAR(45)
parameters TEXT
Indexes
casrn_inventory
casrn_inventory_id INT
preferred_casrn VARCHAR(45)
alternate_casrn VARCHAR(45)
Indexes
substance_casrn
substance_casrn_id INT
substance_id INT
generic_chemical_id INT
casrn VARCHAR(45)
is_current BOOLEAN
fraction NUMERIC
Indexes
generic_chemical_phenotype
generic_chemical_phenotype_id INT
generic_chemical_id INT
phenotype_id INT
Indexes
phenotype_cv
phenotype_id INT
phenotype VARCHAR(45)
description TEXT
canonical BOOLEAN
Indexes
casrn_auto
casrn_auto_id INT
parameter_cv
param_id INT
name VARCHAR(45)
value_type ENUM(...)
Indexes
use
use_id INT
use_name VARCHAR(255)
parent_id INT
Indexes
compound_property
compound_property_id INT
compound_id INT
measure_id INT
inchi_key VARCHAR(45)
value DOUBLE
comparison VARCHAR(45)
modifier VARCHAR(255)
Indexes
summary_stats
data_collection INT
substance INT
compound INT
generic_chemical INT
generic_chemical_with_structure INT
assay INT
assay_component INT
assay_result INT
substance_param
substance_param_id INT
substance_id INT
param_id INT
value_numerical DOUBLE
value_string VARCHAR(255)
Indexes
generic_chemical_assay
generic_chemical_assay_id INT
generic_chemical_id INT
assay_id INT
Indexes
struct_feature
feature_id INT
feature TEXT
desc VARCHAR(255)
source VARCHAR(255)
Indexes
guideline_guideline
guideline_guideline_id INT
guideline1_id INT
guideline2_id INT
Indexes
qc_status_cv
qc_status_id INT
qc_status_value VARCHAR(45)
Indexes
compound_relative
compound_id_1 INT
compound_id_2 INT
relationship VARCHAR(255)
inchi_key_1 VARCHAR(45)
inchi_key_2 VARCHAR(45)
Indexes
JChemProperties
prop_name VARCHAR(200)
prop_value VARCHAR(200)
prop_value_ext MEDIUMBLOB
Indexes
generic_chemical_set
generic_chemical_set_id INT
generic_chemical_id INT
set_id INT
casrn VARCHAR(45)
name VARCHAR(45)
Indexes
assay_guideline
assay_guideline_id INT
assay_id INT
guideline_id INT
Indexes
assay_phenotype
assay_phenotype_id INT
assay_id INT
phenotype_id INT
Indexes
compound_feature
compound_feature_id INT
compound_id INT
feature_id INT
count INT
Indexes
assay_category
assay_category_id INT
assay_id INT
assay_category_cv_id INT
Indexes
guideline
guideline_id INT
guideline VARCHAR(45)
source VARCHAR(45)
series VARCHAR(255)
description TEXT
state VARCHAR(45)
url VARCHAR(255)
Indexes
jchem_fingerprint_...
update_id INT
update_info VARCHAR(20)
Indexes
chemical_set
set_id INT
name VARCHAR(255)
description TEXT
code VARCHAR(45)
type VARCHAR(45)
url VARCHAR(6000)
filename VARCHAR(4096)
Indexes
assay_result
Indexes
substance_compound
substance_compound_id INT
substance_id INT
compound_id INT
Indexes
generic_chemical_summary
generic_chemical_summary_id INT
generic_chemical_id INT
assay_id INT
assay_name VARCHAR(255)
assay_component_id INT
assay_component_name VARCHAR(255)
value VARCHAR(60000)
value_type VARCHAR(45)
units VARCHAR(45)
result_group INT
Indexes
assay_note
assay_note_id INT
assay_id INT
note TEXT
Indexes
compound
compound_id INT
source VARCHAR(255)
source_name_cid VARCHAR(45)
status ENUM(...)
molfile_source VARCHAR(255)
molfile MEDIUMTEXT
smiles_original TEXT
smiles TEXT
inchi TEXT
inchi_key VARCHAR(45)
mw DOUBLE
formula VARCHAR(255)
useme BOOLEAN
data_collection_id INT
Indexes
jchem_fingerprint
cd_id INT
cd_structure MEDIUMBLOB
cd_smiles TEXT
cd_formula VARCHAR(100)
cd_sortable_formula VARCHAR(255)
cd_molweight DOUBLE
cd_hash INT
cd_flags VARCHAR(20)
cd_timestamp DATETIME
cd_fp1 INT
cd_fp2 INT
cd_fp3 INT
cd_fp4 INT
cd_fp5 INT
cd_fp6 INT
cd_fp7 INT
cd_fp8 INT
cd_fp9 INT
cd_fp10 INT
cd_fp11 INT
cd_fp12 INT
cd_fp13 INT
cd_fp14 INT
cd_fp15 INT
cd_fp16 INT
compound_id INT
Indexes
set_category
set_category_id INT
set_id INT
assay_category_cv_id INT
Indexes
assay_param
assay_param_id INT
assay_id INT
param_id INT
value_numerical DOUBLE
value_string VARCHAR(255)
Indexes
data_collection
data_collection_id INT
name VARCHAR(255)
description TEXT
url VARCHAR(65535)
data_url VARCHAR(65535)
chemical_data BOOLEAN
assay_data BOOLEAN
structure_data BOOLEAN
chemical_url BOOLEAN
source_type VARCHAR(45)
download_date VARCHAR(45)
download_instructions TEXT
permission_issues TEXT
copyright_issues TEXT
institutional_source VARCHAR(255)
notes TEXT
update_frequency VARCHAR(45)
substance_count INT
generic_chemical_count INT
fact_count INT
screening_target BOOLEAN
useme BOOLEAN
qc_status_id INT
Indexes
assay
assay_id INT
data_collection_id INT
source VARCHAR(255)
source_name_aid VARCHAR(45)
name VARCHAR(255)
assay_code VARCHAR(45)
description TEXT
url VARCHAR(65535)
substance_count INT
component_count INT
qc_status_id INT
species_id INT
Indexes
species
species_id INT
name VARCHAR(255)
Indexes
compound_fingerprint
compound_fingerprint_id INT
count INT
inchi_key VARCHAR(255)
fingerprint_id INT
compound_id INT
Indexes
fingerprint
fingerprint_id INT
fpset ENUM(...)
smarts VARCHAR(10000)
source_name_fid VARCHAR(45)
multiplicity INT
Indexes
smarts_in_compound
smarts_in_compound_id INT
compound_id INT
smarts_id INT
nmatches INT
Indexes
assay_component
assay_component_id INT
assay_id INT
source_id VARCHAR(45)
name VARCHAR(255)
description TEXT
units VARCHAR(255)
value_type ENUM(...)
component_type VARCHAR(255)
component_category TINYINT
Indexes
component_category
Indexes
component_category_cv
component_category_cv_id INT
category VARCHAR(255)
parent_id INT
Indexes