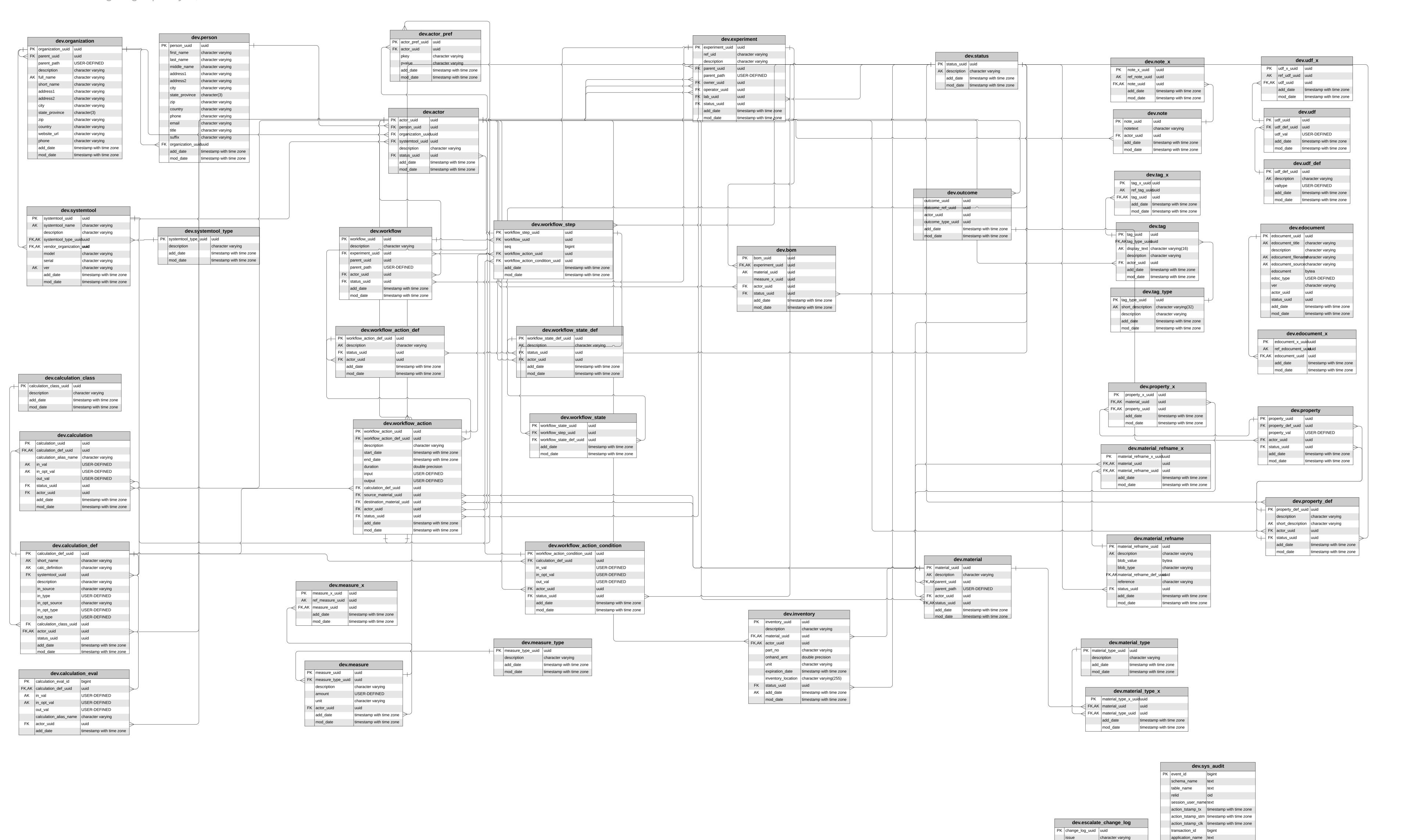
ESCALATE v3 Data Model

Haverford College - gc | July 6, 2020



dev.load perov desc _raw_inchikey character varying(255) character varying(255) _raw_smiles raw molweight double precision _raw_density double precision _raw_smiles_standard character varying(255 _raw_standard_molweight double precision character varying _prototype_ecpf4_256_6 _feat_atomcount_c _feat_atomcount_r _feat_avgpol double precision _feat_molpol double precision _feat_refractivity double precision _feat_aliphaticringcount _feat_aromaticringcount _feat_aliphaticatomcount _feat_aromaticatomcount _feat_bondcount feat carboaliphaticringcount _feat_carboaromaticringcount _feat_carboringcount _feat_chainatomcount feat chiralcentercount _feat_ringatomcount _feat_smallestringsize _feat_largestringsize _feat_heteroaliphaticringcount _feat_heteroaromaticringcount _feat_rotatablebondcount _feat_balabanindex double precision smallint _feat_cyclomaticnumber _feat_hyperwienerindex _feat_wienerindex smallint _feat_wienerpolarity _feat_minimalprojectionarea _feat_maximalprojectionarea double precision _feat_minimalprojectionradius double precision _feat_maximalprojectionradius double precision _feat_lengthperpendiculartotheminarea | double precision _feat_lengthperpendiculartothemaxarea |double precision _feat_vanderwaalsvolume double precision _feat_vanderwaalssurfacearea double precision _feat_asa double precision double precision _feat_asa+ _feat_asadouble precision _feat_asa_h double precision _feat_asa_p double precision _feat_polarsurfacearea double precision _feat_acceptorcount _feat_accsitecount _feat_donorcount _feat_donsitecount smallint _feat_fr_nh2 feat fr_nh1 smallint _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh _feat_fr_imine smallint _feat_fr_amidine _feat_fr_dihydropyridine _feat_fr_guanido _feat_fr_piperdine _feat_fr_piperzine _feat_fr_pyridine _feat_maximalprojectionsize double precision _feat_minimalprojectionsize double precision _feat_molsurfaceareavdwp double precision _feat_msareavdwp double precision _feat_molsurfaceareaasap double precision _feat_msareaasap double precision _feat_protpolarsurfacearea double precision _feat_protpsa double precision _feat_hacceptorcount _feat_hdonorcount _feat_charge_cnt _calc_chrg_per_vol double precision _calc_chrg_per_asadouble precision

dev.load_hc_inventory character varying(255) character varying(255) amount double precision character varying(255) update_date | timestamp with time zone create_date | timestamp with time zone updated_by | character varying(255) in_stock real remaining_sto**ck**al

dev.load_lbl_inventory reagent character varying(255) part_no character varying(255) amount double precision character varying(255) update_date | timestamp with time zone create_date | timestamp with time zone

dev.load_perov_desc_def short_name character varying(255) calc_definition | character varying(255) description character varying(255) systemtool_nameharacter varying(255) systemtool_ver | character varying(255) in_calc_source | character varying(255) in_type character varying(255) in_opt_calc_sour**cle**aracter varying(255) in_opt_type character varying(255) out_type character varying(255)

dev.load_perov_mol_image full_filenameharacter varying

filename character varying mol_name character varying _image bytea

object_type character varying

object_name character varying

character varying

character varying

character varying

timestamp with time zone

create_date timestamp with time zone

resolution

close_date

author

status

client_addr inet client_port integer

text

row_data USER-DEFINED

statement_only boolean

client_query

action

dev.escalate version

description character varying add_date | timestamp with time zone

AK short_name character varying

PK,AK ver_uuid uuid