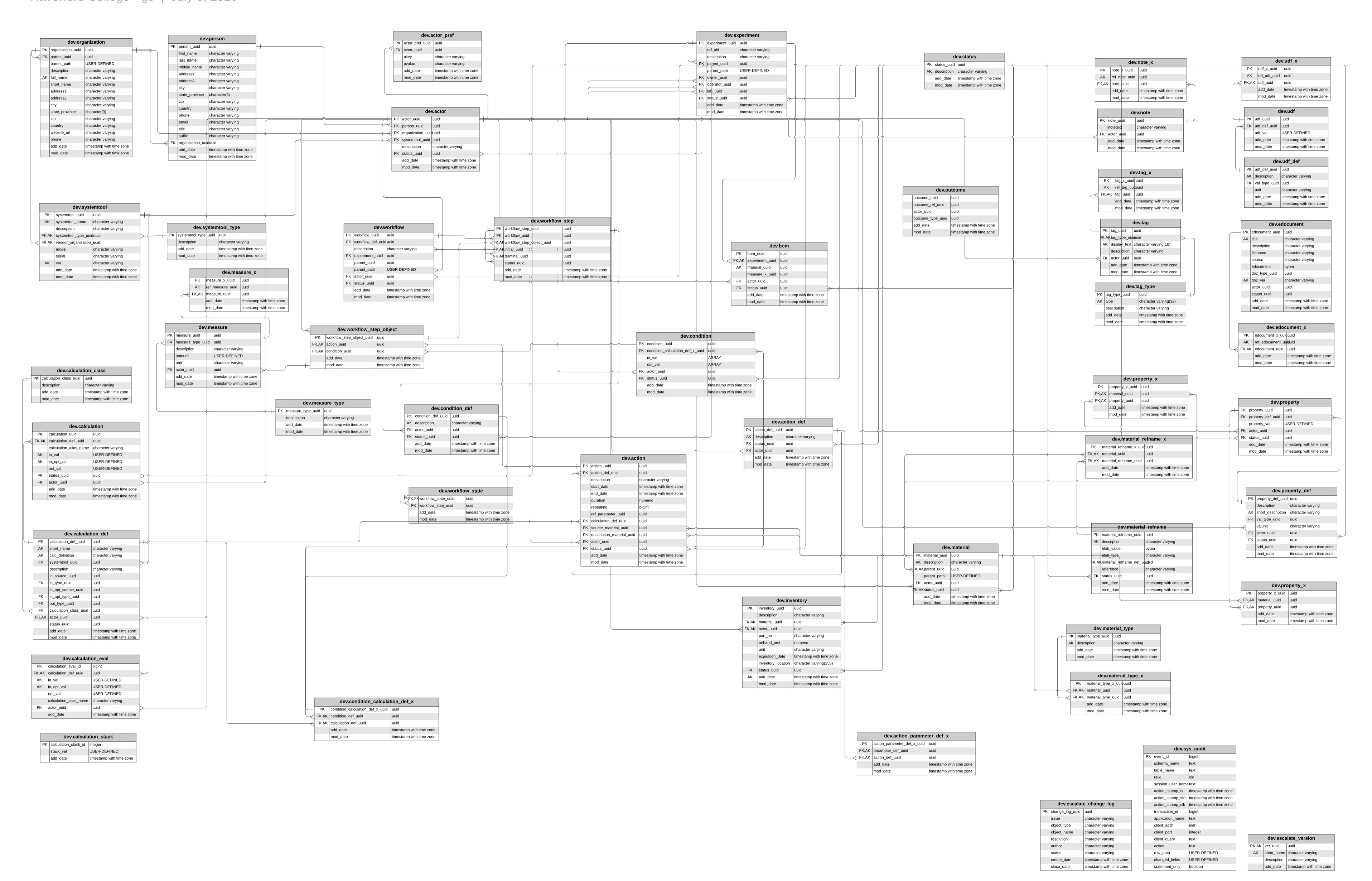
ESCALATE v3 Data Model

Haverford College - gc | July 6, 2020



dev.load perov desc _raw_inchikey character varying(255) _raw_smiles character varying (255 raw molweight double precision _raw_density double precision _raw_smiles_standard character varying(255) _raw_standard_molweight double precision _prototype_ecpf4_256_6 character varying _feat_atomcount_c _feat_atomcount_n double precision _feat_avgpol _feat_molpol double precision _feat_refractivity double precision _feat_aliphaticringcount smallint _feat_aromaticringcount smallint _feat_aliphaticatomcount _feat_aromaticatomcount _feat_bondcount feat carboaliphaticringcount _feat_carboaromaticringcount _feat_carboringcount _feat_chainatomcount smallint _feat_chiralcentercount _feat_ringatomcount _feat_smallestringsize _feat_largestringsize _feat_heteroaliphaticringcount _feat_heteroaromaticringcount _feat_rotatablebondcount _feat_balabanindex double precision _feat_cyclomaticnumber _feat_hyperwienerindex smallint smallint _feat_wienerindex _feat_wienerpolarity _feat_minimalprojectionarea double precision _feat_maximalprojectionarea double precision _feat_minimalprojectionradius double precision _feat_maximalprojectionradius double precision _feat_lengthperpendiculartotheminarea | double precision _feat_lengthperpendiculartothemaxarea |double precision _feat_vanderwaalsvolume _feat_vanderwaalssurfacearea double precision _feat_asa double precision _feat_asa+ double precision _feat_asadouble precision _feat_asa_h double precision _feat_asa_p double precision _feat_polarsurfacearea double precision _feat_acceptorcount _feat_accsitecount smallint _feat_donorcount smallint _feat_donsitecount smallint _feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_ar_nh smallint _feat_fr_imine smallint _feat_fr_amidine _feat_fr_dihydropyridine _feat_fr_guanido smallint _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 smallint _feat_hdonorcount smallint _feat_charge_cnt double precision _calc_chrg_per_vol double precision _calc_chrg_per_asa-

reagent character varying(255)
part_no character varying(255)
amount double precision
units character varying(255)
update_date timestamp with time zone
create_date timestamp with time zone
updated_by character varying(255)
in_stock real
remaining_stockal

reagent character varying(255)
part_no character varying(255)
amount double precision
units 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 description systemtool_nametharacter varying(255)
systemtool_ver in_calc_source in_type character varying(255)
in_opt_calc_sourcearacter varying(255)
in_opt_type character varying(255)
out_type character varying(255)
character varying(255)
character varying(255)
character varying(255)
character varying(255)

full_filename character varying mol_name character varying jimage bytea