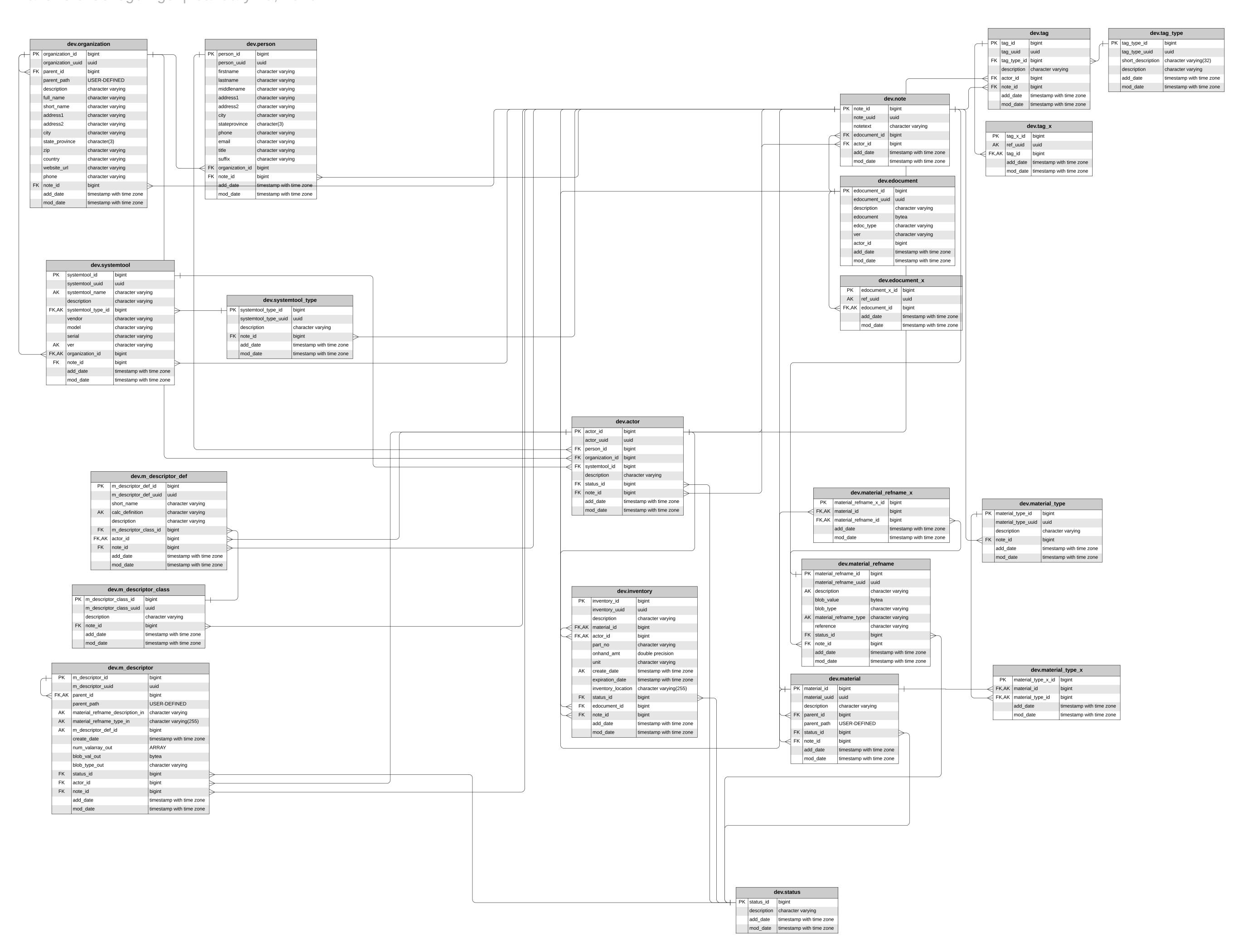
ESCALATE v3 Data Model

Haverford College - gc | January 29, 2020



dev.load_hc_inventory character varying(255) character varying(255) double precision character varying(255) update_date | timestamp with time zone create_date timestamp with time zone

dev.load_lbl_inventory reagent character varying(255) character varying(255) 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)

dev.load_perov_mol_image filename character varying fileno integer _image bytea

dev.load_chem_inventory	
ChemicalName	character varying(255
ChemicalAbbreviation	character varying(255
MolecularWeight	character varying(255
Density	character varying(255
InChl	character varying(255
InChlKey	character varying(255
ChemicalCategory	character varying(255
CanonicalSMILES	character varying(255
MolecularFormula	character varying(255
PubChemID	character varying(255
CatalogDescr	character varying(255
Synonyms	character varying(255
CatalogNo	character varying(255
Sigma-Aldrich URL	character varying(255
PrimaryInformationSource	character varying(255
StandardizedSMILES	character varying(255

dev.load_perov_desc _raw_inchikey character varying(255) _raw_smiles character varying(255) _raw_molweight double precision _raw_smiles_standard character varying(255) _raw_standard_molweight double precision _prototype_ecpf4_256_6 character varying(256) _feat_atomcount_c double precision _feat_atomcount_n double precision _feat_avgpol double precision _feat_molpol double precision _feat_refractivity double precision _feat_aliphaticringcount double precision _feat_aromaticringcount double precision _feat_aliphaticatomcount double precision _feat_aromaticatomcount double precision _feat_bondcount double precision _feat_carboaliphaticringcount double precision double precision $_$ feat $_$ carboaromaticringcount _feat_carboringcount double precision _feat_chainatomcount double precision _feat_chiralcentercount double precision _feat_ringatomcount double precision double precision _feat_smallestringsize _feat_largestringsize double precision double precision _feat_heteroaliphaticringcount _feat_heteroaromaticringcount double precision _feat_rotatablebondcount double precision _feat_balabanindex double precision double precision _feat_cyclomaticnumber _feat_hyperwienerindex double precision _feat_wienerindex double precision _feat_wienerpolarity double precision _feat_minimalprojectionarea double precision double precision _feat_maximalprojectionarea _feat_minimalprojectionradius double precision _feat_maximalprojectionradius double precision _feat_lengthperpendiculartotheminarea | double precision _feat_lengthperpendiculartothemaxarea | double precision _feat_vanderwaalsvolume double precision 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 double precision _feat_accsitecount double precision _feat_donorcount double precision _feat_fr_nh2 double precision _feat_fr_nh1 double precision _feat_fr_nh0 double precision _feat_fr_quatn double precision _feat_fr_arn double precision _feat_fr_ar_nh double precision _feat_fr_imine double precision _feat_fr_amidine double precision _feat_fr_dihydropyridine double precision _feat_fr_guanido double precision _feat_fr_piperdine double precision _feat_fr_piperzine double precision _feat_fr_pyridine double precision _feat_maximalprojectionsize double precision _feat_minimalprojectionsize double precision _feat_molsurfaceareavdwp double precision _feat_msareavdwp double precision _feat_molsurfaceareaasap double precision double precision _feat_msareaasap _feat_protpolarsurfacearea double precision _feat_protpsa double precision _feat_hacceptorcount double precision

_feat_hdonorcount

double precision