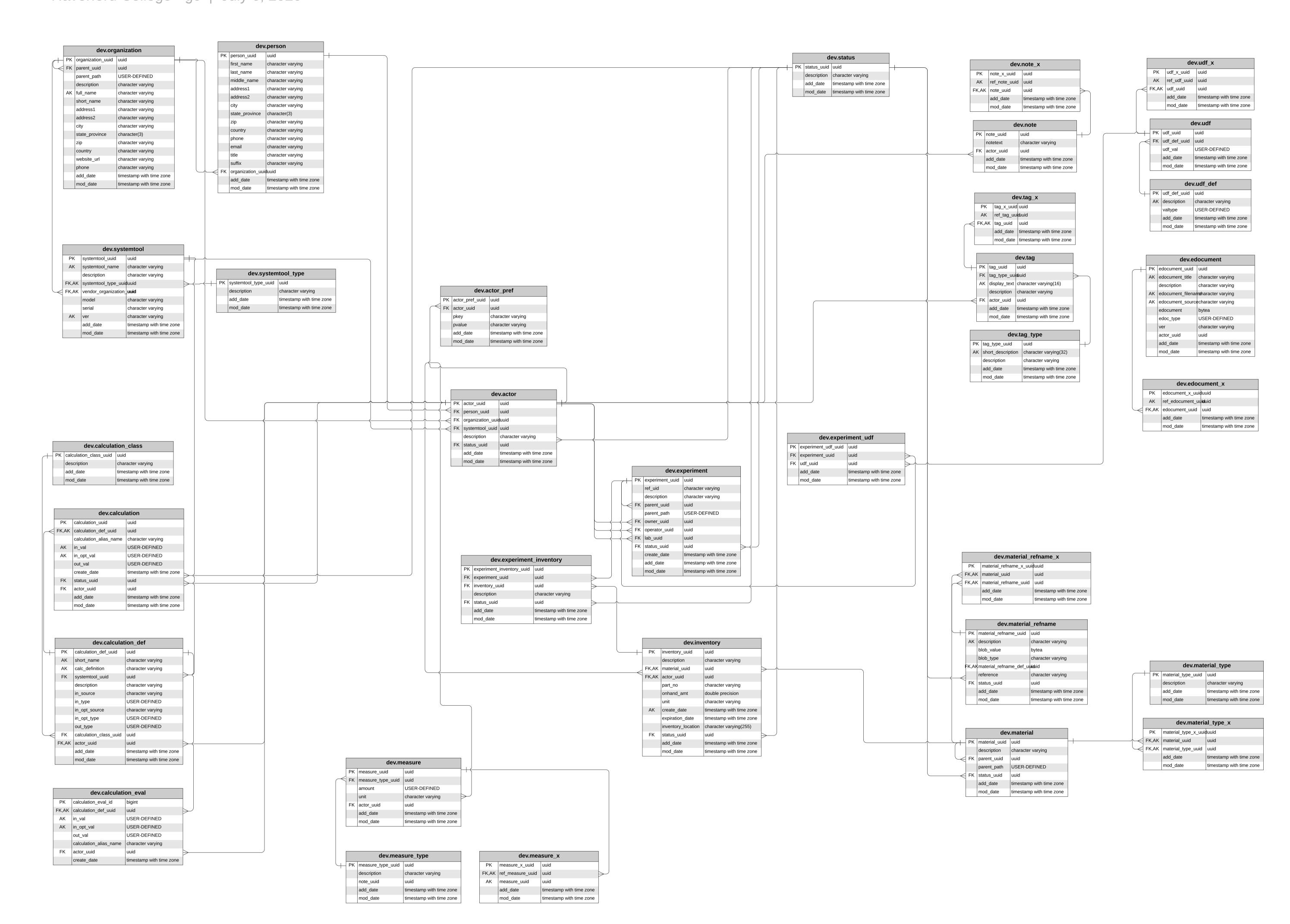
ESCALATE v3 Data Model

Haverford College - gc | July 6, 2020



reagent character varying(255)
part_no character varying(255)
amount double precision
units character varying(255)
update_date create_date updated_by in_stock real
remaining_stocksal

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_mol_image

full_filename character varying mol_name character varying bytea

_feat_refractivity _feat_aliphaticringcount	double precision
feat aliphaticringcount	double precision
	smallint
_feat_aromaticringcount	smallint
_feat_aliphaticatomcount	smallint
_feat_aromaticatomcount	smallint
feat bondcount	smallint
 feat_carboaliphaticringcount	smallint
	smallint
	smallint
_feat_chainatomcount	smallint
feat chiralcentercount	smallint
	smallint
_feat_ringatomcount	
_feat_smallestringsize	smallint
_feat_largestringsize	smallint
_feat_heteroaliphaticringcount	smallint
_feat_heteroaromaticringcount	smallint
_feat_rotatablebondcount	smallint
_feat_balabanindex	double precision
_feat_cyclomaticnumber	smallint
_feat_hyperwienerindex	smallint
_feat_wienerindex	smallint
_feat_wienerpolarity	smallint
_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	double precision
_feat_vanderwaalssurfacearea	double precision
_feat_asa	double precision
_feat_asa+	double precision
_feat_asa-	double precision
feat asa h	double precision
feat asa p	double precision
	double precision
feat acceptorcount	smallint
feat accsitecount	smallint
 _feat_donorcount	smallint
	smallint
i leat donsitecount	
_feat_donsitecount	smallint
	smallint smallint
feat_fr_nh2 _feat_fr_nh1	smallint
feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0	smallint smallint
_feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn	smallint smallint smallint
feat_fr_nh2feat_fr_nh1feat_fr_nh0feat_fr_quatnfeat_fr_arn	smallint smallint smallint smallint
feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh	smallint smallint smallint smallint smallint
feat_fr_nh2feat_fr_nh1feat_fr_nh0feat_fr_quatnfeat_fr_arnfeat_fr_ar_nhfeat_fr_imine	smallint smallint smallint smallint smallint smallint
feat_fr_nh2feat_fr_nh1feat_fr_nh0feat_fr_quatnfeat_fr_arnfeat_fr_ar_nhfeat_fr_iminefeat_fr_amidine	smallint smallint smallint smallint smallint smallint smallint
feat_fr_nh2feat_fr_nh1feat_fr_nh0feat_fr_quatnfeat_fr_arnfeat_fr_ar_nhfeat_fr_iminefeat_fr_amidinefeat_fr_dihydropyridine	smallint smallint smallint smallint smallint smallint smallint smallint
feat_fr_nh2feat_fr_nh1feat_fr_nh0feat_fr_quatnfeat_fr_arnfeat_fr_ar_nhfeat_fr_iminefeat_fr_amidinefeat_fr_dihydropyridinefeat_fr_guanido	smallint
feat_fr_nh2feat_fr_nh1feat_fr_nh0feat_fr_quatnfeat_fr_arnfeat_fr_ar_nhfeat_fr_iminefeat_fr_dihydropyridinefeat_fr_guanidofeat_fr_piperdine	smallint
_feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh _feat_fr_imine _feat_fr_amidine _feat_fr_dihydropyridine _feat_fr_guanido _feat_fr_piperdine _feat_fr_piperzine	smallint
_feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh _feat_fr_imine _feat_fr_dihydropyridine _feat_fr_guanido _feat_fr_piperdine _feat_fr_piperzine _feat_fr_pyridine	smallint
feat_fr_nh2feat_fr_nh1feat_fr_nh0feat_fr_quatnfeat_fr_arnfeat_fr_ar_nhfeat_fr_iminefeat_fr_amidinefeat_fr_dihydropyridinefeat_fr_guanidofeat_fr_piperdinefeat_fr_piperzinefeat_fr_pyridinefeat_maximalprojectionsize	smallint double precision
_feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh _feat_fr_amidine _feat_fr_dihydropyridine _feat_fr_guanido _feat_fr_piperdine _feat_fr_piperzine _feat_fr_pyridine _feat_maximalprojectionsize _feat_minimalprojectionsize	smallint double precision double precision
feat_fr_nh2feat_fr_nh1feat_fr_nh0feat_fr_quatnfeat_fr_arnfeat_fr_ar_nhfeat_fr_iminefeat_fr_dihydropyridinefeat_fr_guanidofeat_fr_piperdinefeat_fr_piperzinefeat_fr_pyridinefeat_maximalprojectionsizefeat_molsurfaceareavdwp	smallint double precision double precision double precision
_feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh _feat_fr_imine _feat_fr_amidine _feat_fr_dihydropyridine _feat_fr_guanido _feat_fr_piperdine _feat_fr_piperzine _feat_fr_pyridine _feat_maximalprojectionsize _feat_molsurfaceareavdwp _feat_msareavdwp	smallint double precision double precision double precision double precision
_feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh _feat_fr_amidine _feat_fr_dihydropyridine _feat_fr_guanido _feat_fr_piperdine _feat_fr_piperzine _feat_fr_pyridine _feat_maximalprojectionsize _feat_molsurfaceareavdwp _feat_molsurfaceareaasap	smallint double precision double precision double precision double precision double precision double precision
_feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh _feat_fr_imine _feat_fr_amidine _feat_fr_dihydropyridine _feat_fr_guanido _feat_fr_piperdine _feat_fr_piperzine _feat_fr_pyridine _feat_maximalprojectionsize _feat_molsurfaceareavdwp _feat_msareavdwp	smallint double precision double precision double precision double precision
_feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh _feat_fr_amidine _feat_fr_dihydropyridine _feat_fr_guanido _feat_fr_piperdine _feat_fr_piperzine _feat_fr_pyridine _feat_maximalprojectionsize _feat_molsurfaceareavdwp _feat_molsurfaceareaasap	smallint double precision double precision double precision double precision double precision double precision
_feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh _feat_fr_imine _feat_fr_amidine _feat_fr_dihydropyridine _feat_fr_guanido _feat_fr_piperdine _feat_fr_piperzine _feat_fr_pyridine _feat_maximalprojectionsize _feat_molsurfaceareavdwp _feat_molsurfaceareasap _feat_msareaasap	smallint double precision
_feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh _feat_fr_amidine _feat_fr_dihydropyridine _feat_fr_guanido _feat_fr_piperdine _feat_fr_piperzine _feat_fr_pyridine _feat_maximalprojectionsize _feat_molsurfaceareavdwp _feat_molsurfaceareaasap _feat_protpolarsurfacearea	smallint double precision
_feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh _feat_fr_amidine _feat_fr_dihydropyridine _feat_fr_guanido _feat_fr_piperdine _feat_fr_piperzine _feat_maximalprojectionsize _feat_maximalprojectionsize _feat_molsurfaceareavdwp _feat_molsurfaceareaasap _feat_molsurfaceareaasap _feat_protpolarsurfacearea _feat_protpsa	smallint double precision
_feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh _feat_fr_imine _feat_fr_amidine _feat_fr_dihydropyridine _feat_fr_guanido _feat_fr_piperdine _feat_fr_piperzine _feat_maximalprojectionsize _feat_molsurfaceareavdwp _feat_molsurfaceareaasap _feat_msareaasap _feat_protpolarsurfacearea _feat_hacceptorcount	smallint double precision smallint
_feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh _feat_fr_amidine _feat_fr_dihydropyridine _feat_fr_guanido _feat_fr_piperdine _feat_fr_piperzine _feat_maximalprojectionsize _feat_maximalprojectionsize _feat_molsurfaceareavdwp _feat_msareavdwp _feat_msareavdwp _feat_msareasap _feat_protpolarsurfacearea _feat_protpsa _feat_hacceptorcount _feat_hdonorcount	smallint double precision smallint smallint
_feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh _feat_fr_imine _feat_fr_amidine _feat_fr_dihydropyridine _feat_fr_guanido _feat_fr_piperdine _feat_fr_piperzine _feat_maximalprojectionsize _feat_maximalprojectionsize _feat_molsurfaceareavdwp _feat_msareavdwp _feat_msareavdwp _feat_msareasap _feat_protpolarsurfacearea _feat_protpsa _feat_hacceptorcount _feat_hdonorcount _feat_charge_cnt	smallint double precision smallint smallint smallint

dev.load perov desc

character varying(255

double precision

double precision

double precision

double precision

double precision

smallint

character varying

character varying(255)

character varying(255)

_raw_inchikey

_raw_molweight

_raw_smiles_standard

_raw_standard_molweight

_prototype_ecpf4_256_6

_feat_atomcount_c

_feat_atomcount_n

_feat_avgpol

_feat_molpol

_raw_density

_raw_smiles

dev.sys_audit							
PK	event_id	bigint		dev.escalate_change_log			
	schema_name	text		PK	cha	ange_log_uuic	uuid
	table_name	text			iss	ue	character varying
	relid	oid			object_type		character varying
	session_user_name	text			object_name		character varying
	action_tstamp_tx	timestamp with time zone			resolution		character varying
	action_tstamp_stm	timestamp with time zone			author		character varying
	action_tstamp_clk	timestamp with time zone			status		character varying
	transaction_id	bigint			create_date		timestamp with time zor
	application_name	text			close_date		timestamp with time zor
	client_addr	inet	'				
	client_port	integer					
	client_query	text		dev.escalate_version			
	action	text		PK,	AK	ver_uuid	uuid
	row_data	USER-DEFINED		Ał	<	short_name	character varying
	changed_fields	USER-DEFINED				description	character varying
	statement_only	boolean				add_date	timestamp with time zone
			-				