CDD json connections - Overview

Protocols

class:string
id:int
created_at:date
modified_at:date
name:string
description:string
category:string
data_set:dict ({:name->"TB", :id->12})
readout_definitions: json array
calculations: json array
run: json array

Readout Definitions

class:string
id:int
name:string
data_type:{"Number", "Date", "Text"}
calculation: int (id)
precision_type: f'decimal place",
"significant figure, or ommitted}
precision_number: int

n — 1

1 — n

n — n

Runs

class:string
id:int
conditions:string
person:string
run_ date:date

Calculations

class:string
id:int
mean_type
scope
inputs:dict (input names =>
readout_ definition id)
outputs: diet (output names=>
readout_ definition_id)

Protocol Data

batch:int (batch_id)
molecule:int (molecule_id)
run:int (run_id)
well:dict
readouts:dict
(readout_d efinition_ id=>value)

Note: value can be numbers, strings,
value dictionary (see Value)

Value

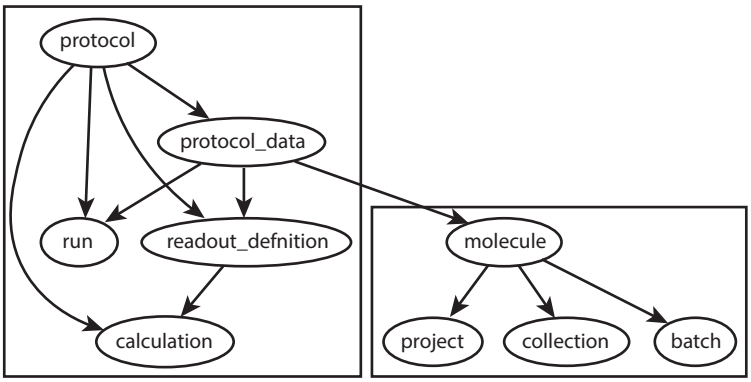
value::int/string
modifier:string
note:string
outlier_type:{1,2,0, or ommitted}

Molecules

class:string
id:int
created_at:date
modified_ at:date
name:string
synonyms:json array (string)
cdd_registry_number:string
smiles:string
cxsmiles:id (cxsmiles identifier)
inchi_key:string
udfs:dict (user defined fields) collections:array
(array of collections the molecule belongs to)
projects:array
batches:array
formula:string
composition
isotope_ composition
topological_polar _surface_ area
log_p
dot_disconneted_formula
num _rotatable_ bonds
numb_h_bond_donors
numb_h_bond_acceptors
exact_mass
num_rule_of_S_violations
molecular_weight
heavy_atom_count

Batches

class:string
id:int
name:string
molecules:json
projects:array (json of projects)
created_at:date
modified_at:date
batch_fields:dict
formula_weight:float



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