Subsites

TABLE subsite INTEGER PRIMARY KEY subsite_id INTEGER subsite_target ■ TEXT subsite_name TEXT subsite_metadata

TABLE subsite_tag INTEGER PRIMARY KEY subsite_taq_id

INTEGER subsite_tag_ref TEXT subsite_tag_metadata

Protein

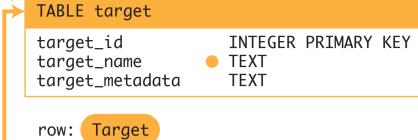


TABLE feature

INTEGER PRIMARY KEY feature_id TEXT feature family INTEGER feature_target feature_chain_name TEXT TEXT feature_residue_name INTEGER feature residue number → TEXT feature atom names

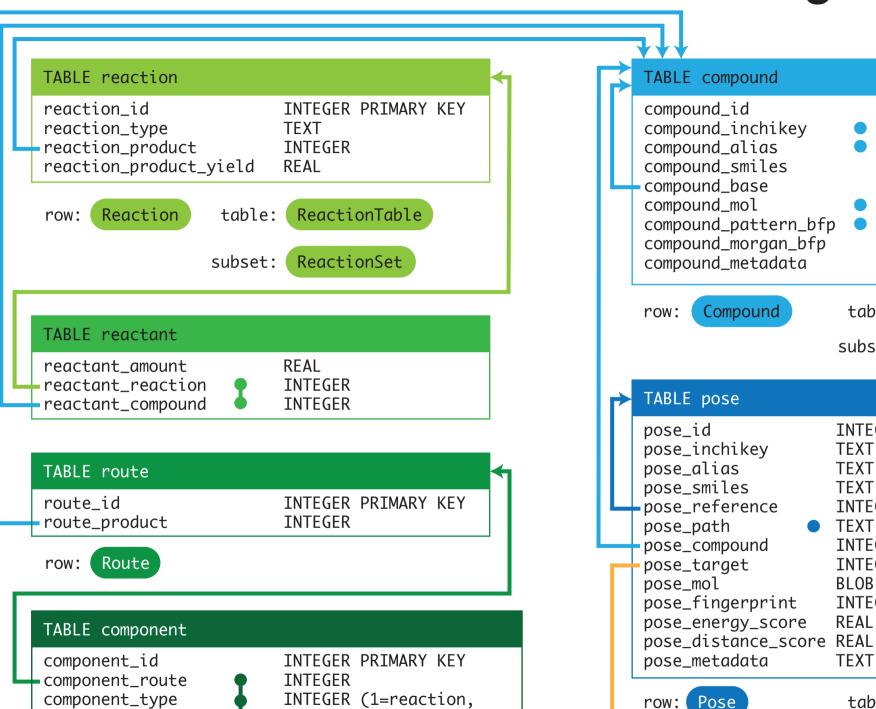
row: Feature

subset: FeatureSet

Interactions

TABLE interaction INTEGER PRIMARY KEY interaction id interaction feature INTEGER interaction_pose **♦** TEXT interaction_type **♦** TEXT interaction_family TEXT interaction_atom_ids TEXT interaction_prot_coord interaction_lig_coord TEXT interaction_distance REAL REAL interaction_anale REAL interaction_energy

Reactions



INTEGER

REAL

component_ref

component_amount

2=reactant,

3=intermediate)

Ligands

TEXT

TEXT

TEXT

MOL

TEXT

INTEGER

bits(2048)

bits(1024)

table: CompoundTable

subset: CompoundSet

INTEGER PRIMARY KEY

table: PoseTable

subset: PoseSet

TEXT

TEXT

TEXT

TEXT

INTEGER

INTEGER

INTEGER

INTEGER

BLOB

TEXT

INTEGER PRIMARY KFY

Procurement

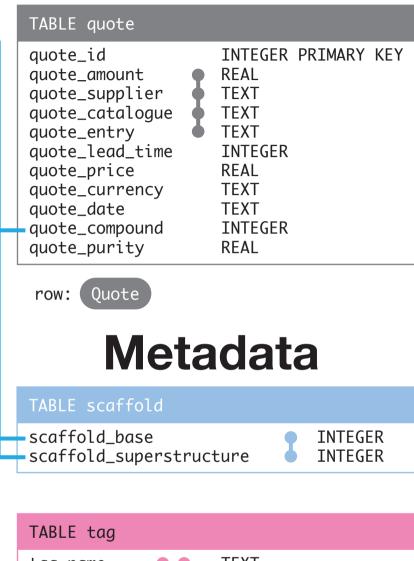




table: TagTable subset: TagSet

TABLE inspiration

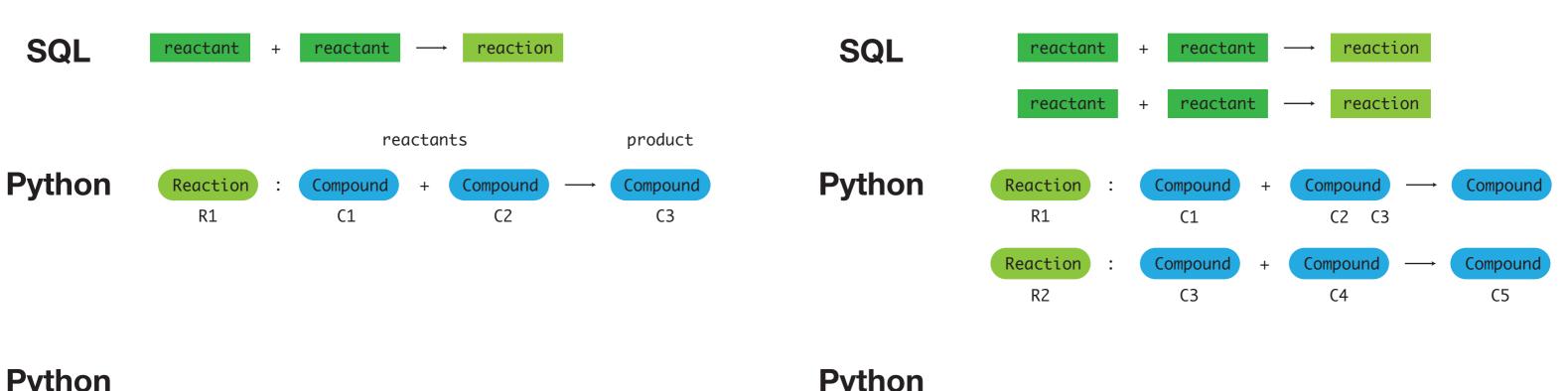
inspiration_original INTEGER inspiration_derivative 🌢 INTEGER

Single-Step Synthetis

Two-Step Synthesis

Ingredient

x mg of C3





Derived Classes

