

Reactions

TABLE reaction	
reaction_id	INTEGER PRIMARY KEY
reaction_type	TEXT
reaction_product	INTEGER
reaction_product_yield	REAL

row: Reaction table: ReactionTable

subset: ReactionSet

TABLE reactant	
reactant_amount	REAL
reactant_reaction	INTEGER
reactant_compound	INTEGER

Protein

TABLE target	
target_id	INTEGER PRIMARY KEY
target_name	TEXT
target_metadata	TEXT

row: Target

TABLE feature	
feature_id	INTEGER PRIMARY KEY
feature_family	TEXT
feature_target	INTEGER
feature_chain_name	TEXT
feature_residue_name	TEXT
feature_residue_number	INTEGER
feature_atom_names	TEXT

row: Feature subset: FeatureSet

Ligands

TABLE compound	
compound_id	INTEGER PRIMARY KEY
compound_inchikey	TEXT
compound_alias	TEXT
compound_smiles	TEXT
compound_base	INTEGER
compound_mol	MOL
compound_pattern_bfp	bits(2048)
compound_morgan_bfp	bits(1024)
compound_metadata	TEXT

row: Compound table: CompoundTable

subset: CompoundSet

TABLE pose	
pose_id	INTEGER PRIMARY KEY
pose_inchikey	TEXT
pose_alias	TEXT
pose_smiles	TEXT
pose_reference	INTEGER
pose_path	TEXT
pose_compound	INTEGER
pose_target	INTEGER
pose_mol	BLOB
pose_fingerprint	BLOB
pose_energy_score	REAL
pose_distance_score	REAL
pose_metadata	TEXT

row: Pose table: PoseTable

subset: PoseSet

Procurement

TABLE quote	
quote_id	INTEGER PRIMARY KEY
quote_amount	REAL
quote_supplier	TEXT
quote_catalogue	TEXT
quote_entry	TEXT
quote_lead_time	INTEGER
quote_price	REAL
quote_currency	TEXT
quote_date	TEXT
quote_compound	INTEGER
quote_purity	REAL

row: Quote

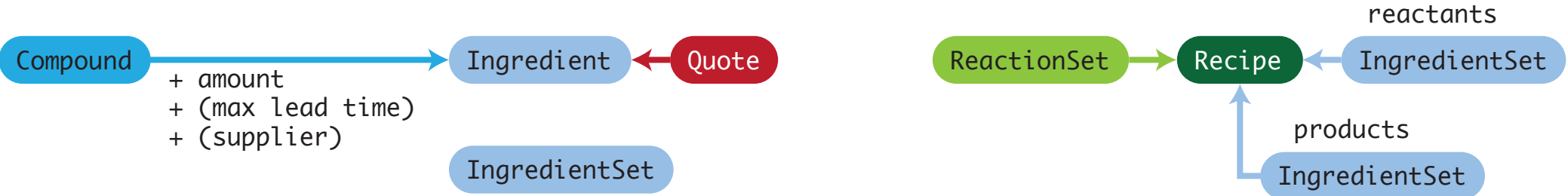
Metadata

TABLE tag	
tag_name	TEXT
tag_compound	INTEGER
tag_pose	INTEGER

table: TagTable subset: TagSet

TABLE inspiration	
inspiration_original	INTEGER
inspiration_derivative	INTEGER

Derived Classes



Single-Step Synthetis

SQL reactant + reactant \longrightarrow reaction

Python Reaction : Compound + Compound \longrightarrow Compound
R1 C1 C2 C3

Python (Recipe) reactions reactants product

Recipe : [Reaction], [Ingredient + Ingredient], Ingredient
R1 x mg of C1 x mg of C2 x mg of C3

Quote Quote Quote

↓ ↓ ↓

Two-Step Synthesis

SQL reactant + reactant \longrightarrow reaction

reactant + reactant \longrightarrow reaction

Python Reaction : Compound + Compound \longrightarrow Compound
R1 C1 C2 C3

Reaction : Compound + Compound \longrightarrow Compound
R2 C3 C4 C5

Python (Recipe) reactions reactants product

Recipe : [Reaction], [Ingredient + Ingredient], Ingredient
R1 x mg of C1 x mg of C2 x mg of C5

Quote Quote

↓ ↓

+ Ingredient

 x mg of C3