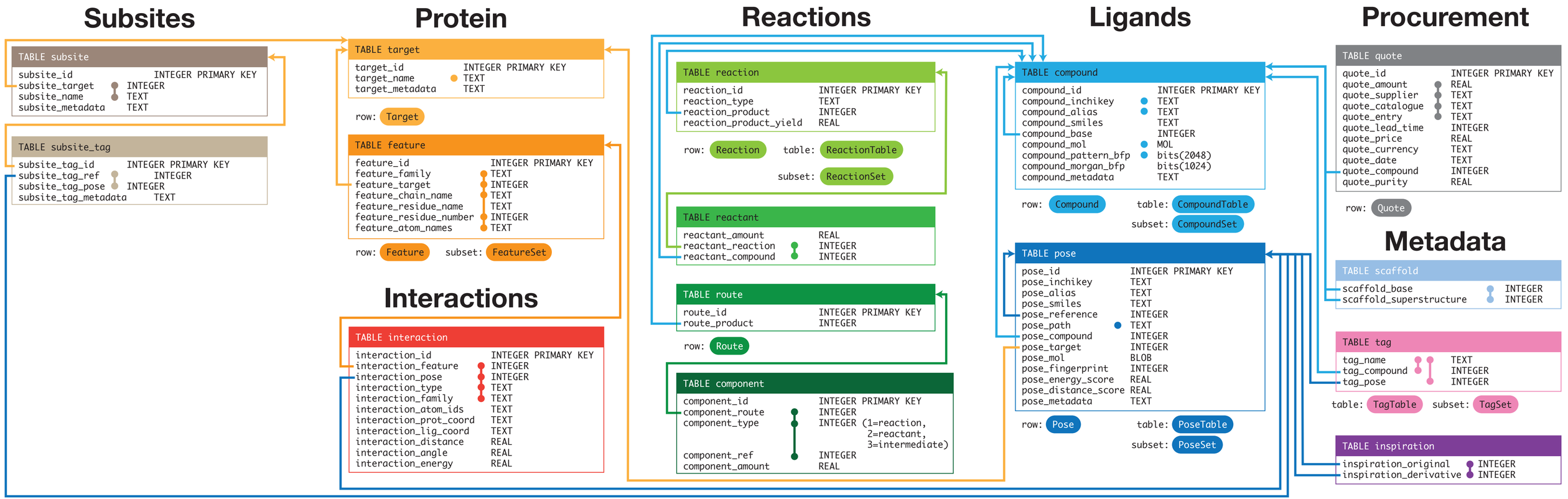

Subsites
TABLE subsite
subsite_id INTEGER PRIMARY KEY
subsite_target INTEGER
subsite_name TEXT
subsite_metadata TEXT
TABLE subsite_tag
subsite_tag_id INTEGER PRIMARY KEY
subsite_tag_ref INTEGER
subsite_tag_pose INTEGER
subsite_tag_metadata TEXT
Protein
TABLE target
target_id INTEGER PRIMARY KEY
target_name 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
Interactions
TABLE interaction
interaction_id INTEGER PRIMARY KEY
interaction_feature INTEGER
interaction_pose INTEGER
interaction_type TEXT
interaction_family TEXT
interaction_atom_ids TEXT
interaction_prot_coord TEXT
interaction_lig_coord TEXT
interaction_distance REAL
interaction_angle REAL
interaction_energy REAL
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
TABLE route
route_id INTEGER PRIMARY KEY
route_product INTEGER
row: Route
TABLE component
component_id INTEGER PRIMARY KEY
component_route INTEGER
component_type INTEGER (1=reaction, 2=reactant, 3=intermediate)
component_ref INTEGER
component_amount REAL
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 INTEGER
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 scaffold
scaffold_base INTEGER
scaffold_superstructure INTEGER
TABLE tag
tag_name TEXT
tag_compound INTEGER
tag_pose INTEGER
table: TagTable
subset: TagSet
TABLE inspiration
inspiration_original INTEGER
inspiration_derivative INTEGER

Single-Step Synthetis

SQL

reactant + reactant ⟶ reaction

Python

reactants product

Reaction : Compound + Compound ⟶ Compound

R1 C1 C2 C3

Python (Recipe)

reactions reactants product

Recipe : [Reaction],[Quote Ingredient + Quote Ingredient], Quote Ingredient

R1 x mg of C1 x mg of C2 x mg of C3

Two-Step Synthesis

SQL

reactant + reactant ⟶ reaction

reactant + reactant ⟶ reaction

Python

Reaction : Compound + Compound ⟶ Compound

R1 C1 C2 C3

Reaction : Compound + Compound ⟶ Compound

R2 C3 C4 C5

Python (Recipe)

reactions reactants product

Recipe : [Reaction R1 Reaction R1],[Quote Ingredient + Quote Ingredient], Quote Ingredient

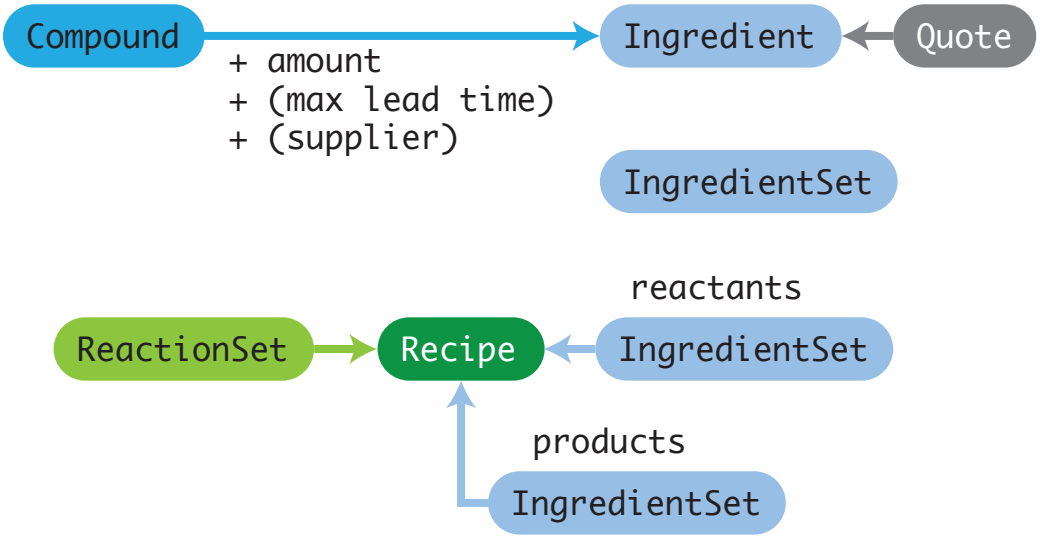
x mg of C1 x mg of C2 x mg of C5

Quote

\+ Ingredient

x mg of C3

Derived Classes



Subsites

SubsiteModel

id	BigAuto(PK)
target	**ForeignKey(Target)**
name	Char[30]
metadata	JSON
poses	**M2M(Pose, SubsiteMember)**

SubsiteMember

id	BigAuto(PK)
subsite	**ForeignKey(Subsite)**
pose	**ForeignKey(Pose)**
atom_ids	JSON
metadata	JSON

Protein

TargetModel

id	BigAuto(PK)
name	Char[60]
metadata	JSON

FeatureModel

id	BigAuto(PK)
family	Char[30]
target	**ForeignKey(Target)**
chain_name	Char[5]
residue_name	Char[10]
residue_number	PositiveSmallInteger
atom_names	JSON

Interactions

InteractionModel

id	BigAuto(PK)
feature	**ForeignKey(Feature)**
pose	**ForeignKey(Pose)**
type	Char[30]
family	Char[30]
atom_ids	JSON
prot_coord	JSON
lig_coord	JSON
distance	REAL
angle	REAL
energy	REAL

Reactions

ReactionModel

id	BigAuto(PK)
type	Char[60]
product	**ForeignKey(Compound)**
product_yield	Float

ReactantModel

id	BigAuto(PK)
amount	Float
reaction	**ForeignKey(Reaction)**
compound	**ForeignKey(Compound)**
solvent	**ForeignKey(Solvent)**

SolventModel

id	BigAuto(PK)
name	Char[30]
metadata	JSON

TABLE route

route_id	INTEGER PRIMARY KEY
route_product	INTEGER

TABLE component

component_id	INTEGER PRIMARY KEY
component_route	INTEGER
component_type	INTEGER (1=reaction, 2=reactant, 3=intermediate)
component_ref	INTEGER
component_amount	REAL

Ligands

CompoundModel

id	BigAuto(PK)
inchikey	Char[27]
alias	Char[60]
smiles	Char[90]
mol	Generated(Mol)
pattern_bfp	Generated(Binary)
metadata	JSON
scaffolds	**M2M(self, “elaborations”)**
tags	**M2M(Tag, “compounds”)**

PoseModel

id	BigAuto(PK)
inchikey	Char[27]
alias	Char[60]
smiles	Char[90]
reference	**ForeignKey(Pose)**
path	FilePath[200]
compound	**ForeignKey(Compound)**
target	**ForeignKey(Target)**
mol	Mol
fingerprinted	Boolean
energy_score	Float
distance_score	Float
metadata	JSON
inspirations	**M2M(self, “derivatives”)**
tags	**M2M(Tag, “poses”)**

Procurement

QuoteModel

id	BigAuto(PK)
amount	Float
supplier	Char[60]
catalogue	Char[90]
entry	Char[60]
lead_time	Float
price	Decimal(8.2)
currency	Char[3]
date	Date
compound	**ForeignKey(Compound)**
purity	Float

Metadata

TagModel

id	BigAuto(PK)
name	Char[60]