

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

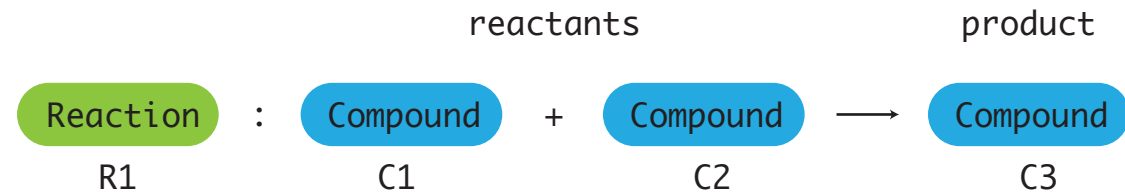
TABLE inspiration		
inspiration_original	INTEGER	
inspiration_derivative	INTEGER	

Single-Step Synthesis

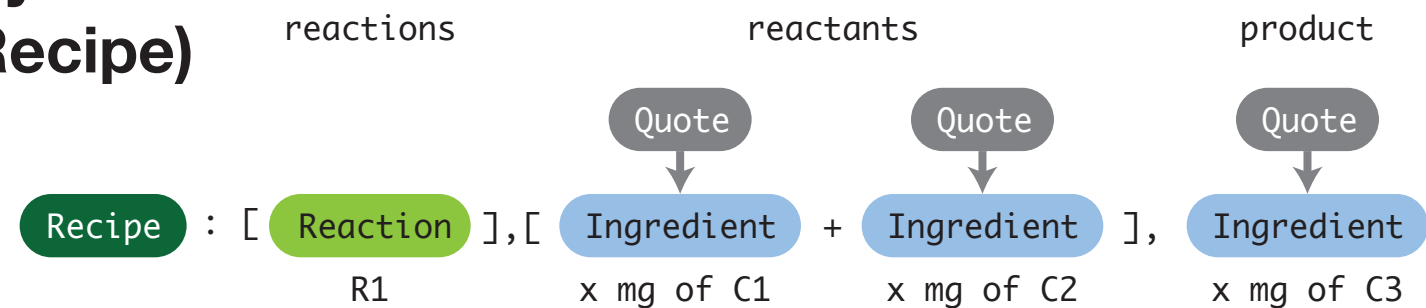
SQL



Python

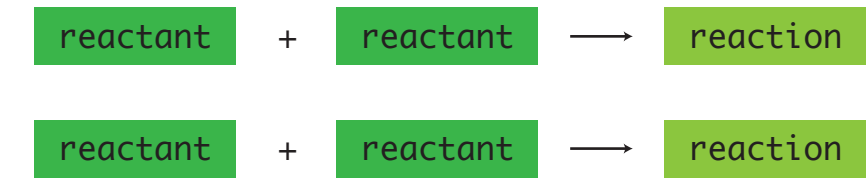


Python (Recipe)

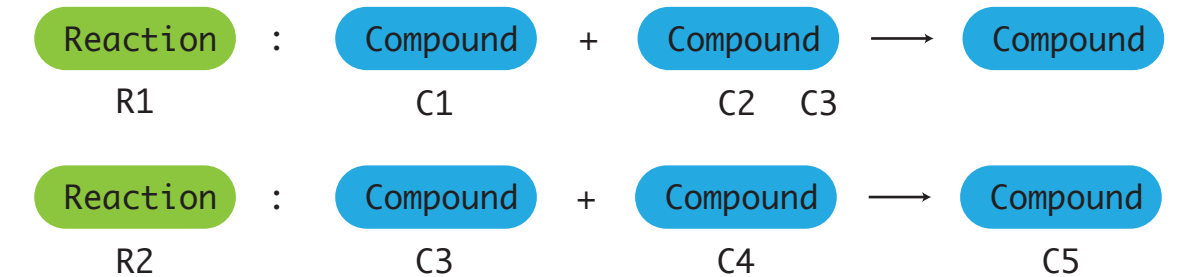


Two-Step Synthesis

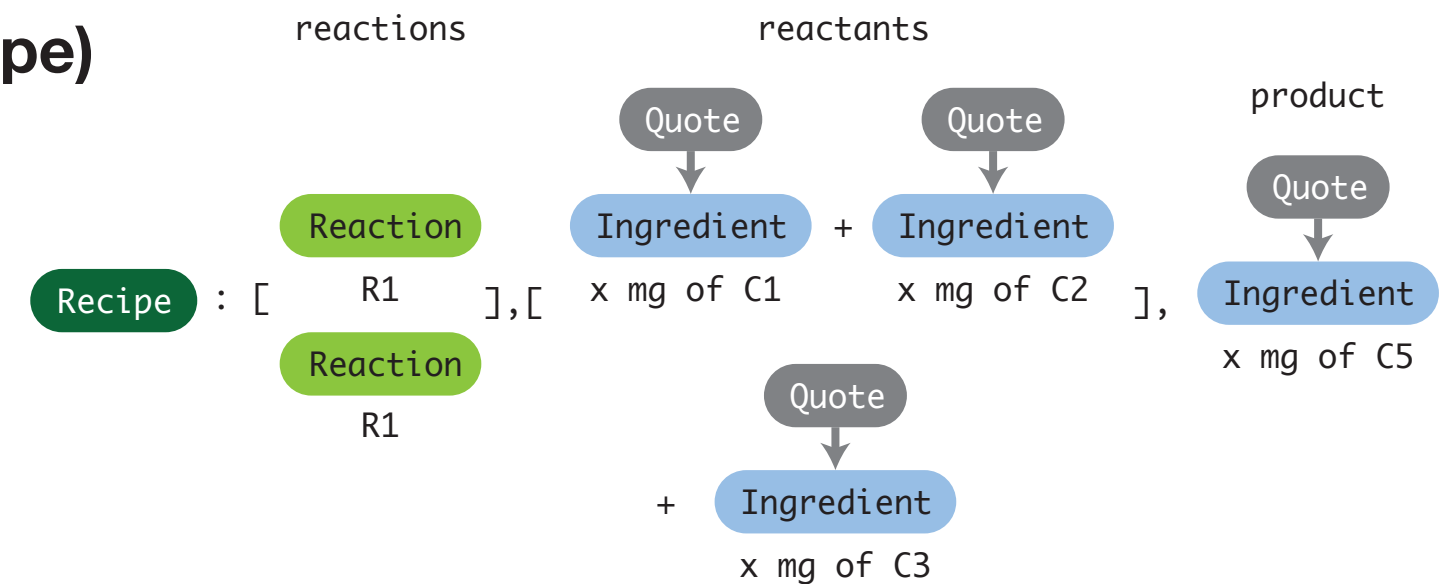
SQL



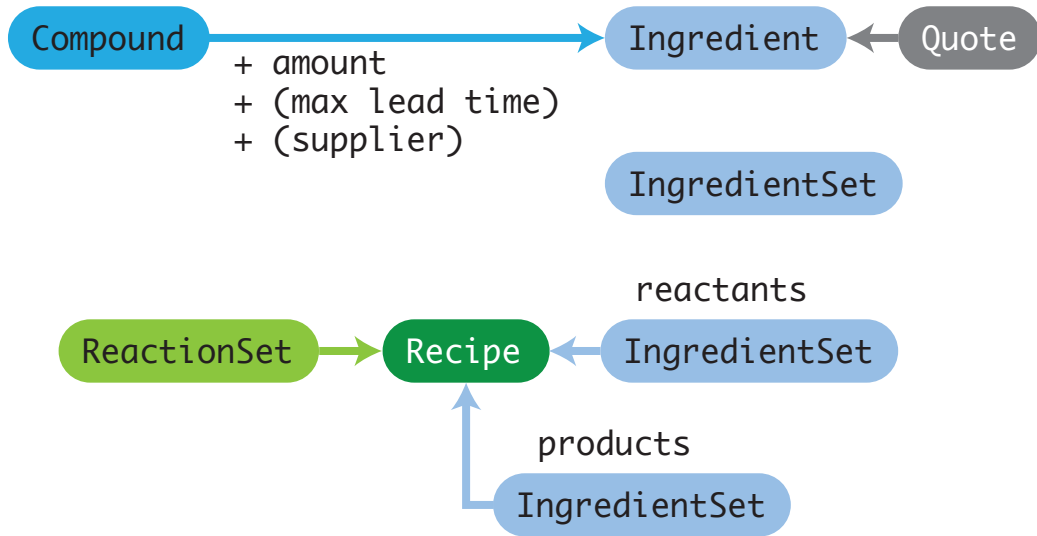
Python



Python (Recipe)



Derived Classes



Protein

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

Model: Target QuerySet: TargetSet

Table: TargetTable

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

Model: Feature

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

Model: Subsite

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

Model: SubsiteMember

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

Model: Interaction

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")

Model: Compound QuerySet: CompoundSet

Table: CompoundTable

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")

Model: Pose QuerySet: PoseSet

Table: PoseTable

Reactions

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

Model: Reaction

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

Model: Reactant

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

Model: Solvent

Metadata

TagModel	
id	BigAuto(PK)
name	Char[60]

Model: Tag

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

Model: Quote