

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

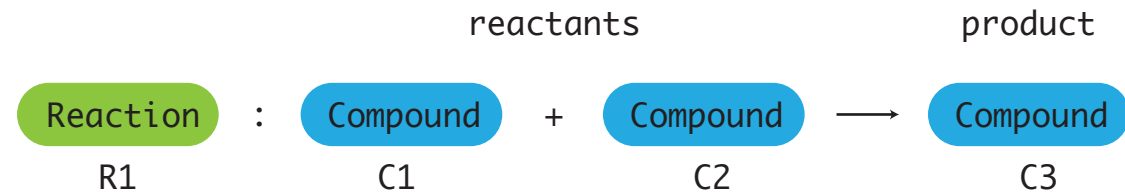
TABLE inspiration		
inspiration_original	INTEGER	
inspiration_derivative	INTEGER	

Single-Step Synthetis

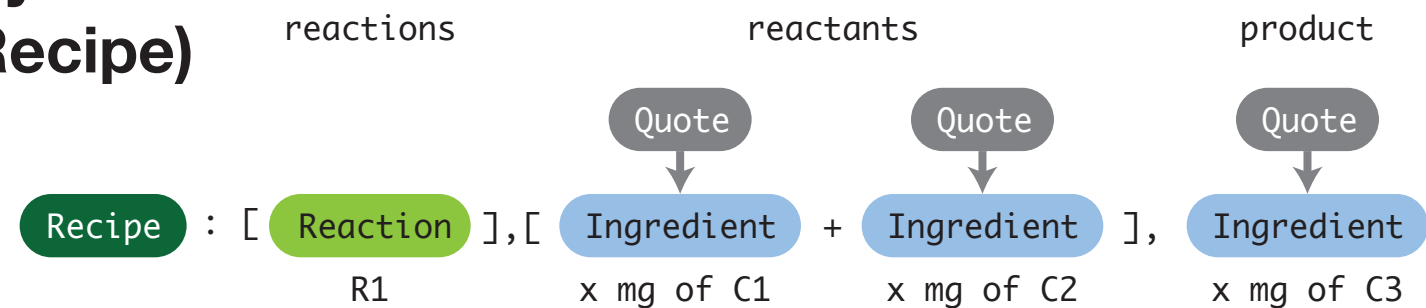
SQL



Python

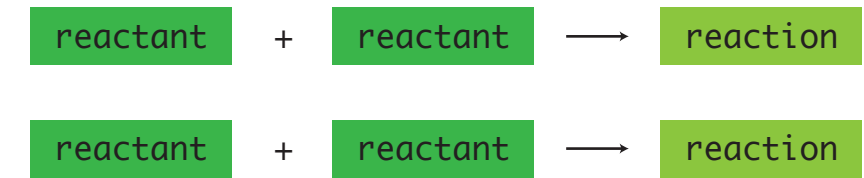


Python (Recipe)

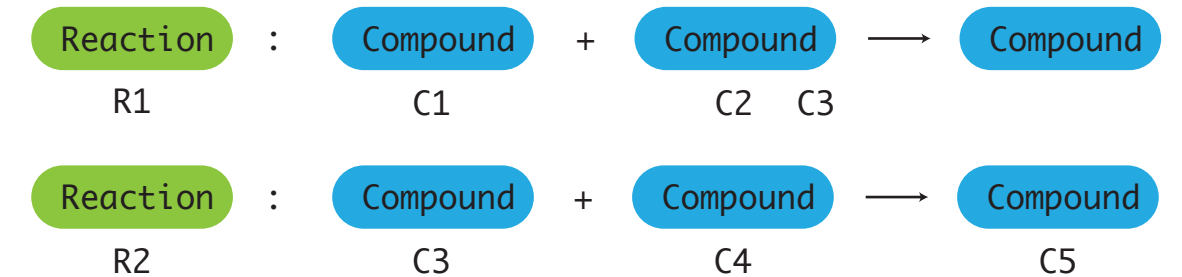


Two-Step Synthesis

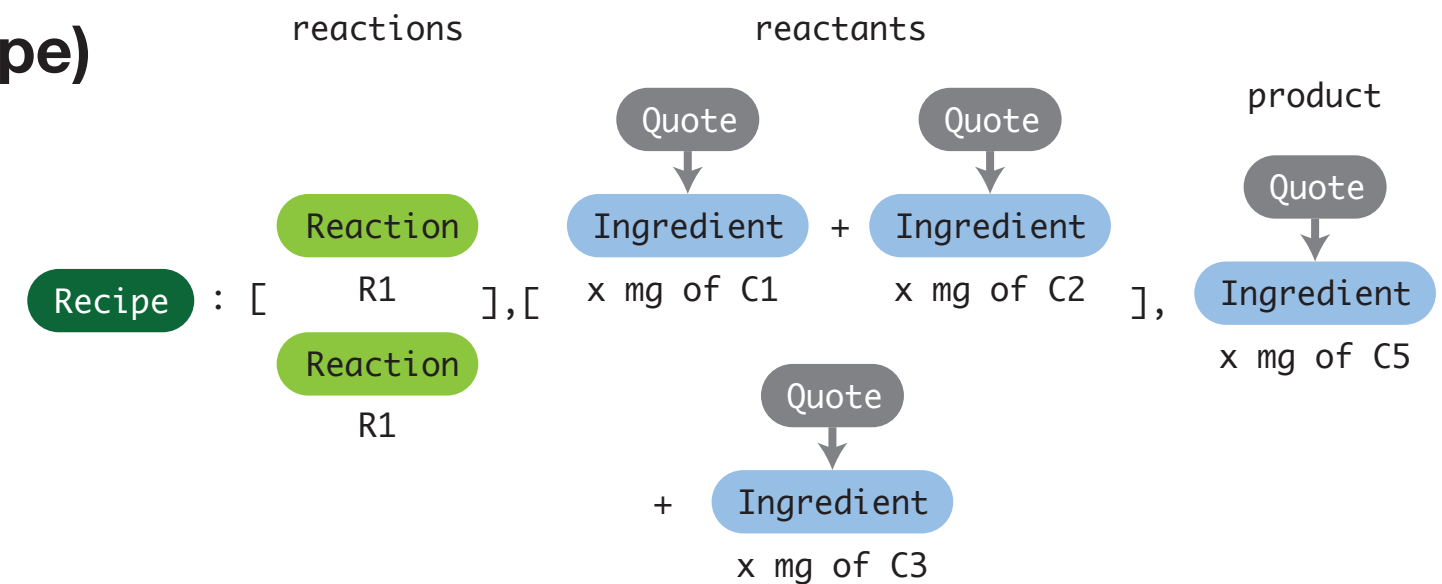
SQL



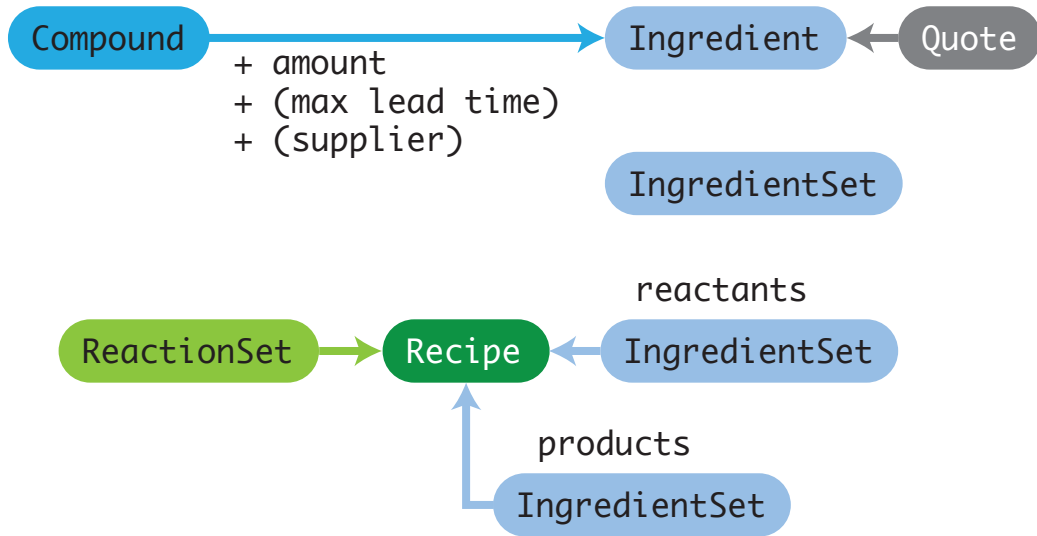
Python



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

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

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

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

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

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

Metadata

TagModel		
id		BigAuto(PK)
name	●	Char[60]

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