

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

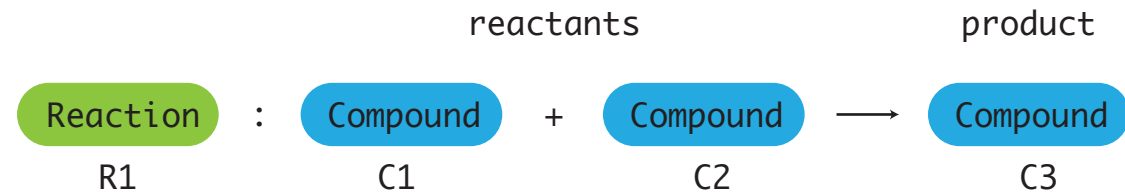
TABLE inspiration		
inspiration_original	INTEGER	
inspiration_derivative	INTEGER	

Single-Step Synthetis

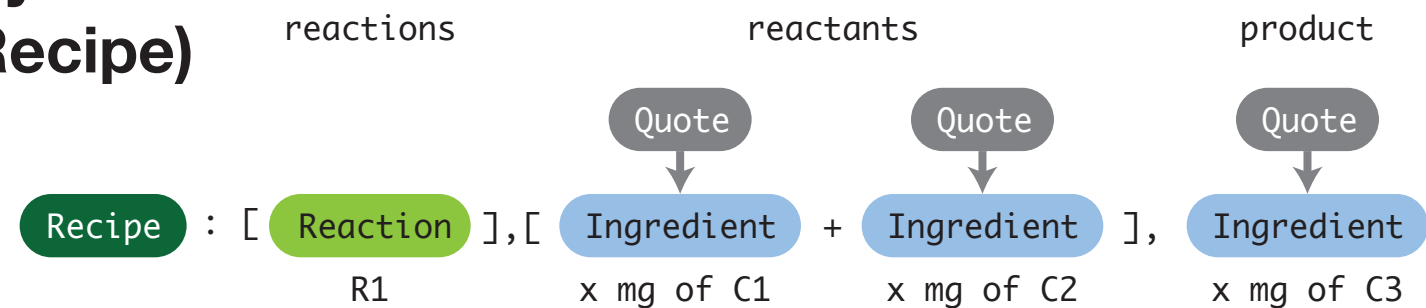
SQL



Python

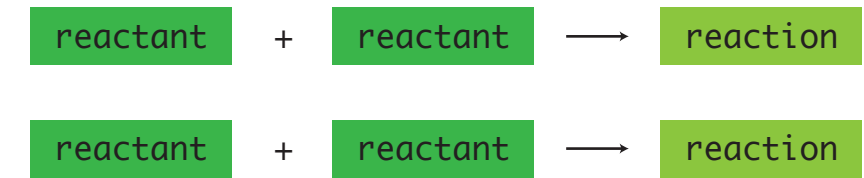


Python (Recipe)

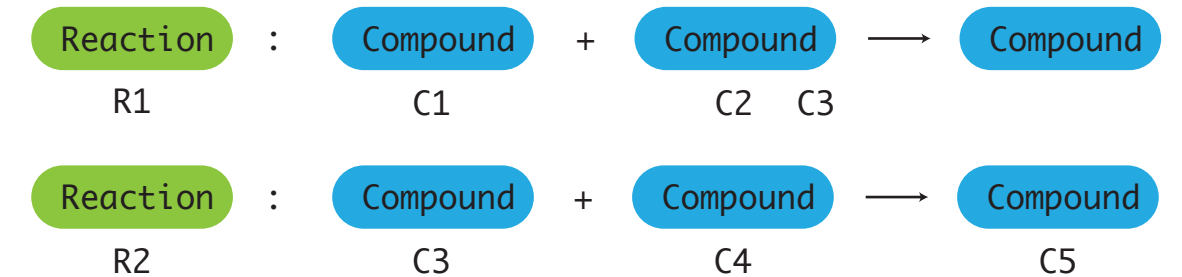


Two-Step Synthesis

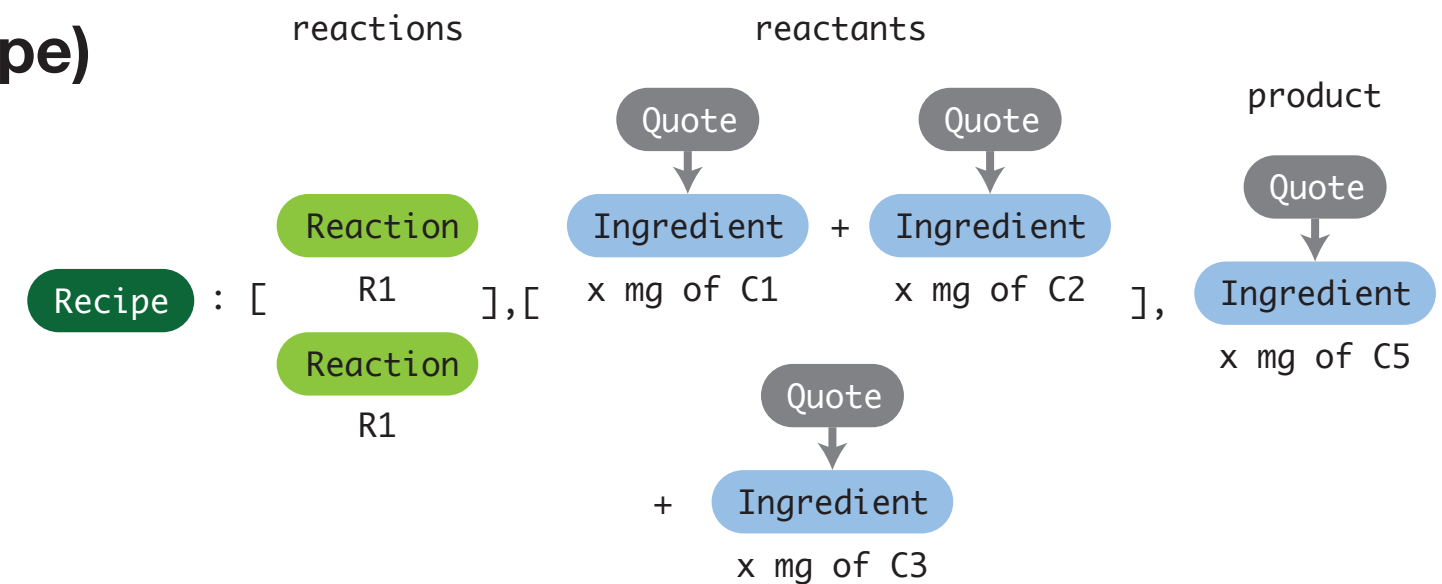
SQL



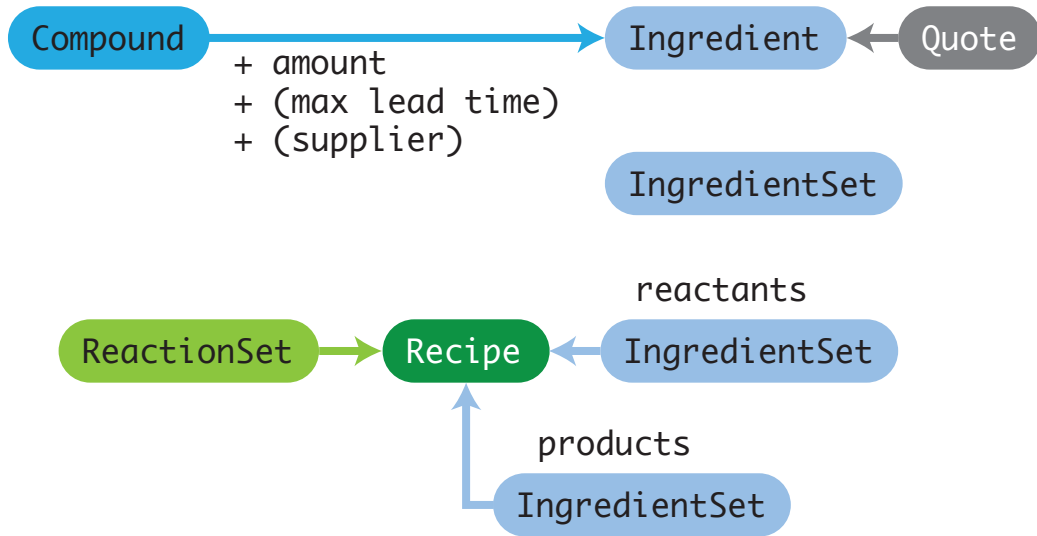
Python



Python (Recipe)



Derived Classes



Protein

TargetModel	
_id	BigAuto(PK)
name	Char[60]
metadata	JSON
poses	Reverse(Pose)
subsites	Reverse(Subsite)
features	Reverse(Feature)

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	Reverse(Interaction)

SubsiteModel	
_id	BigAuto(PK)
target	ForeignKey(Target)
name	Char[30]
metadata	JSON
poses	M2M(Pose, Observation)
observations	Reverse(Observation)

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

ObservationModel	
_id	BigAuto(PK)
subsite	ForeignKey(Subsite)
pose	ForeignKey(Pose)
atom_ids	JSON
metadata	JSON

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")
suppliers	M2M(Supplier, Quote)
quotes	Reverse(Quote)
tags	Reverse(Product)
	Reverse(Reactants)
	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")
interactions	Reverse(Interaction)
subsites	Reverse(Subsite)
poses	Reverse(Pose)

Metadata

Supplier	
_id	BigAuto(PK)
name	Char[30]
compounds	Reverse(Compound)
quotes	Reverse(Quote)

Quote "Q"	
_id	BigAuto(PK)
amount	Float
supplier	ForeignKey(Supplier)
catalogue	Char[90]
entry	Char[60]
lead_time	Float
price	Decimal(8.2)
currency	Char[3]
date	Date
compound	ForeignKey(Compound)
purity	Float

TagModel	
_id	BigAuto(PK)
name	Char[60]
compounds	Reverse(Compound)
poses	Reverse(Pose)

Recipes

RandomRecipeGenerator	
_id	BigAuto(PK)
suppliers	M2M(Supplier)
budget	Float
currency	Char[3]
origin	ForeignKey(Recipe)
recipes	Reverse(Recipe)

Recipe	
_id	BigAuto(PK)
generator	ForeignKey(RandomRecipeGenerator)
routes	M2M(Route, RecipeComponent)
components	Reverse(RecipeComponent)
	Reverse(RandomRecipeGenerator)
scores	Reverse(RecipeScore)

RecipeComponent	
_id	BigAuto(PK)
recipe	ForeignKey(Recipe)
route	ForeignKey(Route)
multiplier	Float

Route	
_id	BigAuto(PK)
reactions	M2M(Reaction, Step)
recipes	Reverse(Recipe)
components	Reverse(RecipeComponent)
steps	Reverse(Step)

RouteStep	
_id	BigAuto(PK)
route	ForeignKey(Route)
reaction	ForeignKey(Reaction)
step	Int
multiplier	Float
is_root	Boolean
is_leaf	Boolean

Reaction "R"	
_id	BigAuto(PK)
type	Char[60]
products	M2M(Compound, Product)
yield_fraction	Float
reactants	Reverse(Reactant)
routes	Reverse(Route)
	Reverse(RouteStep)

Reactions

Product	
_id	BigAuto(PK)
amount	Float
reaction	ForeignKey(Reaction)
compound	ForeignKey(Compound)
solvent	ForeignKey(Solvent)

Reactant	
_id	BigAuto(PK)
amount	Float
solvent	ForeignKey(Solvent)
reaction	ForeignKey(Reaction)
compound	ForeignKey(Compound)

SolventModel	
_id	BigAuto(PK)
name	Char[30]
metadata	JSON
products	Reverse(Product)
reactants	Reverse(Reactant)

Scoring

RecipeScore	
_id	BigAuto(PK)
scorer	ForeignKey(RecipeScorer)
recipe	ForeignKey(Recipe)

RecipeScorer	
_id	BigAuto(PK)
attributes	ForeignKey(Attribute)
recipes	M2M(Recipe, RecipeScore)
scores	Reverse(Score)

ScoringAttribute	
_id	BigAuto(PK)
name	Char[30]
property	JSON
recipes	M2M(Recipe, AttributeValue)
scorer	Reverse(RecipeScorer)
eval	JSON

AttributeValue	
_id	BigAuto(PK)
recipe	ForeignKey(Recipe)
attribute	ForeignKey(Attribute)
value	Float