

# 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

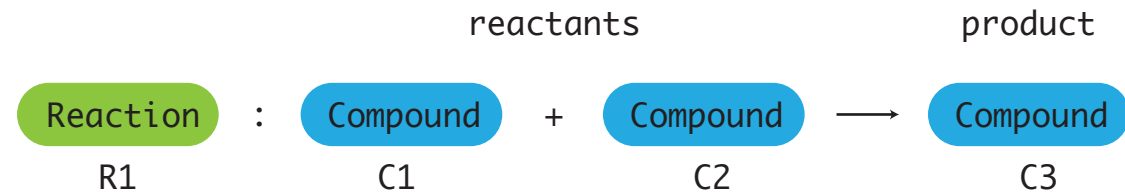
TABLE inspiration		
inspiration_original	INTEGER	
inspiration_derivative	INTEGER	

# Single-Step Synthetis

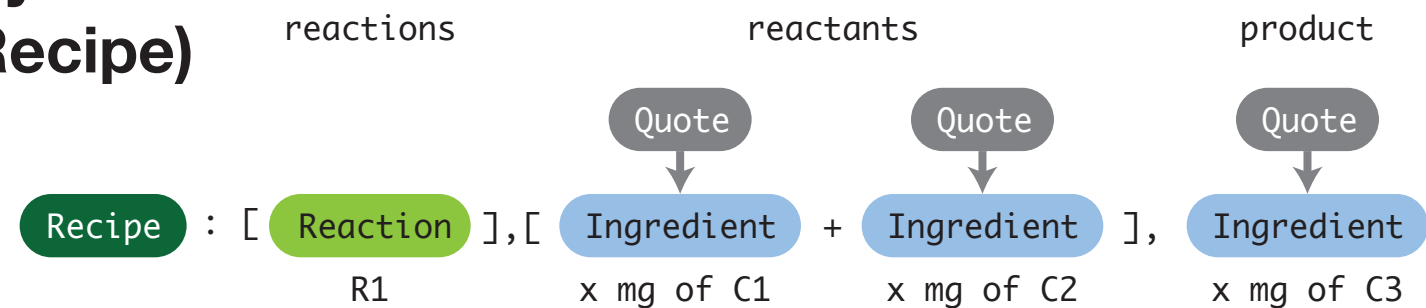
# SQL



# Python

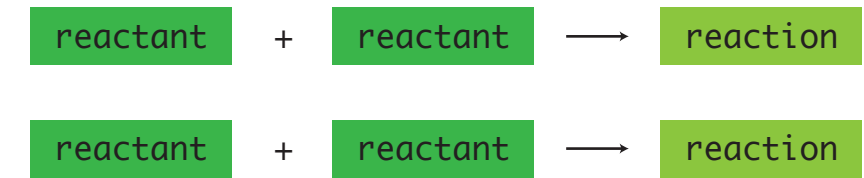


# Python (Recipe)

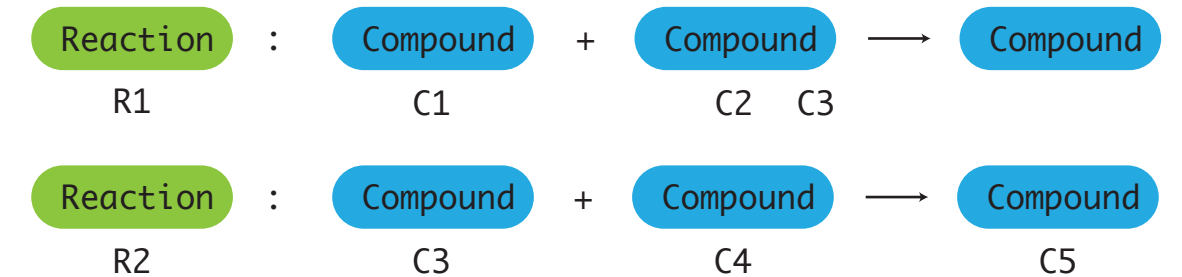


# Two-Step Synthesis

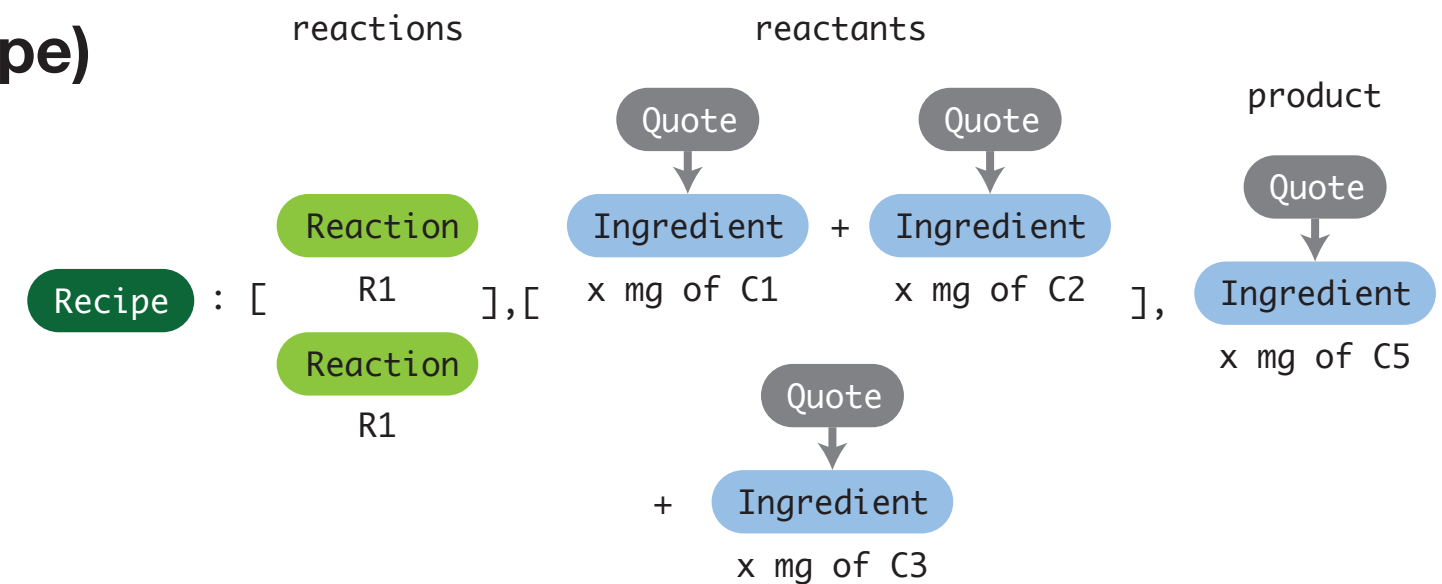
# SQL



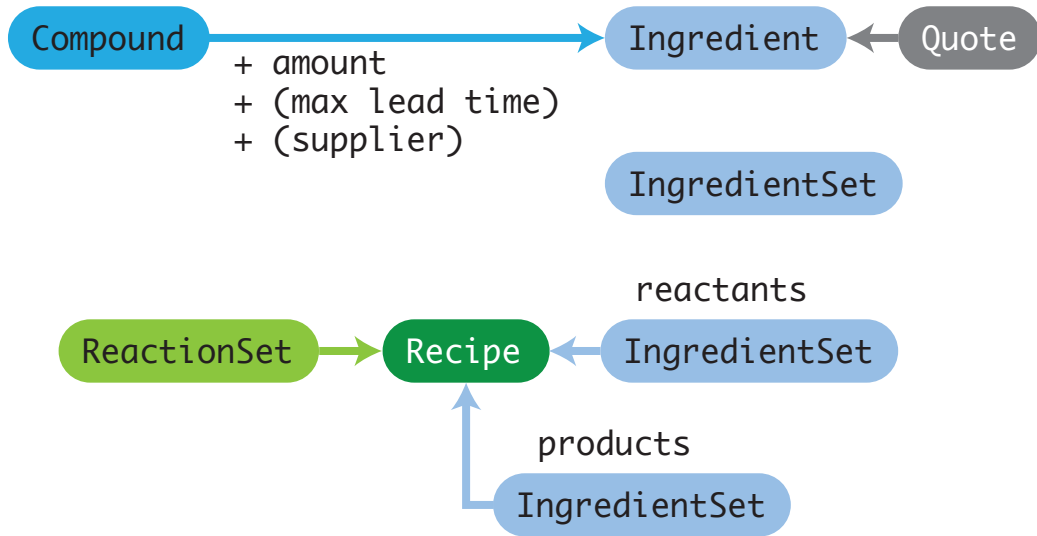
# Python





# Python (Recipe)





# Derived Classes




# Subsites

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







  

SubsiteMember	
id	BigAuto(PK)
subsite	 <b>ForeignKey(Subsite)</b>
pose	 <b>ForeignKey(Pose)</b>
atom_ids	JSON
metadata	JSON





# Protein

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

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

# Interactions

InteractionModel	
id	BigAuto(PK)
feature	 <b>ForeignKey(Feature)</b>
pose	 <b>ForeignKey(Pose)</b>
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	<b>ForeignKey(Compound)</b>
product_yield	Float






ReactantModel	
amount	Float
reaction	 <b>ForeignKey("Reaction")</b>
compound	 <b>ForeignKey("Compound")</b>

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	<b>M2M(self, "elaborations")</b>
tags	<b>M2M(Tag, "compounds")</b>

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

# 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	<b>ForeignKey(Compound)</b>
purity	Float

# Metadata

TagModel	
id	BigAuto(PK)
name	 Char[60]