

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

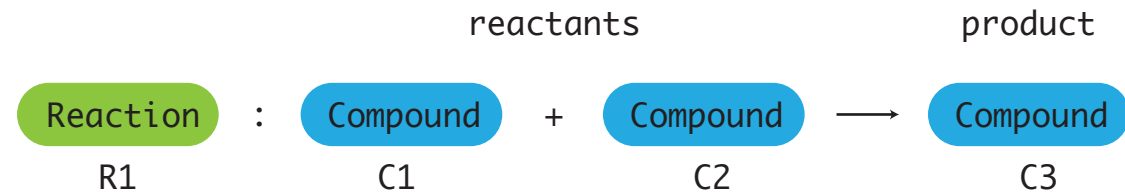
TABLE inspiration		
inspiration_original	INTEGER	
inspiration_derivative	INTEGER	

Single-Step Synthesis

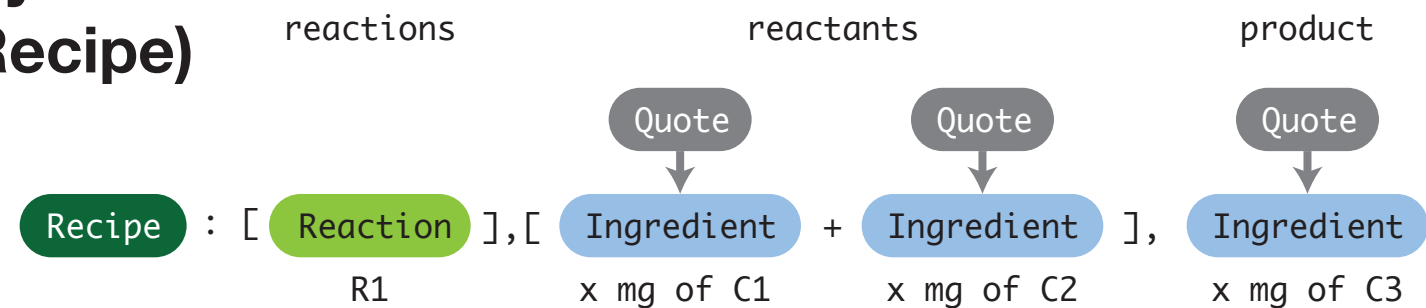
SQL



Python

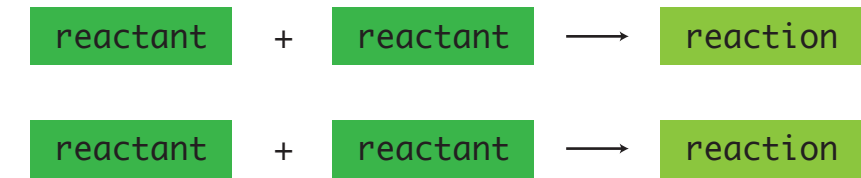


Python (Recipe)

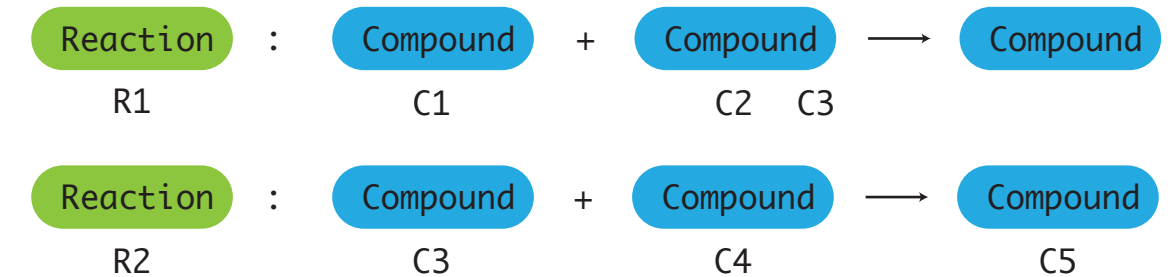


Two-Step Synthesis

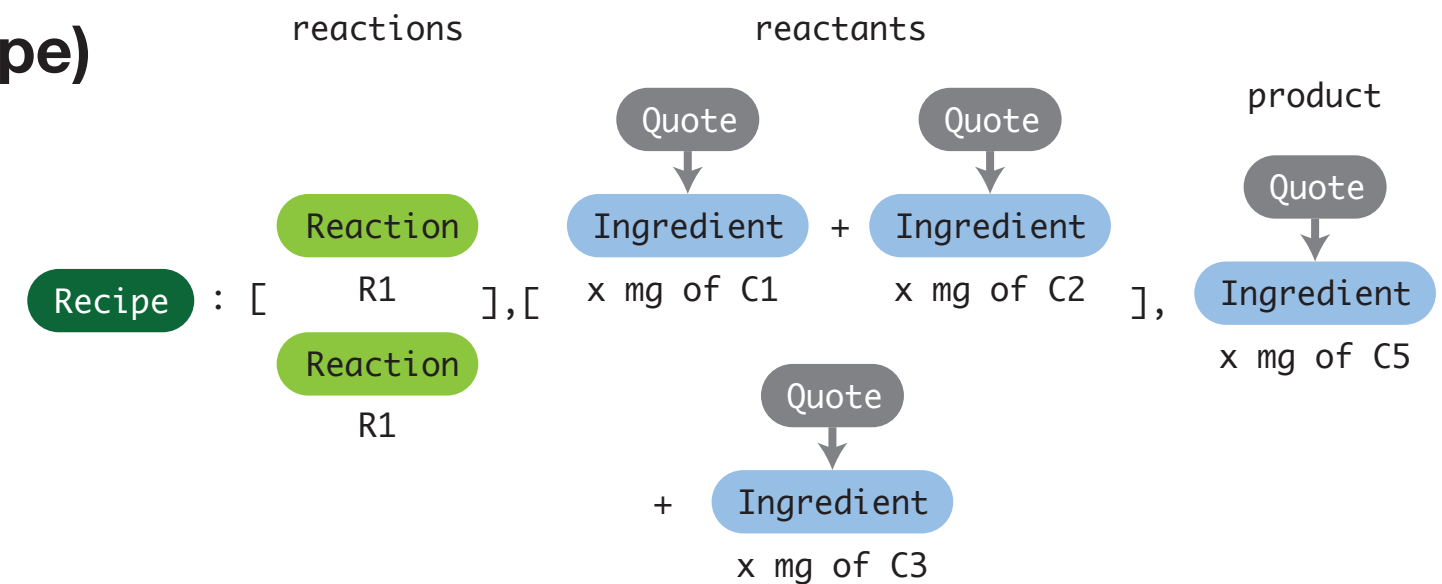
SQL



Python



Python (Recipe)



Derived Classes

