

# Pockets

TABLE pocket	
pocket_id	INTEGER PRIMARY KEY
pocket_target	INTEGER
pocket_name	TEXT
pocket_metadata	TEXT

TABLE pocket_tag	
pocket_tag_ref	INTEGER
pocket_tag_pose	INTEGER
pocket_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

# 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 tag	
tag_name	TEXT
tag_compound	INTEGER
tag_pose	INTEGER

table: TagTable subset: TagSet

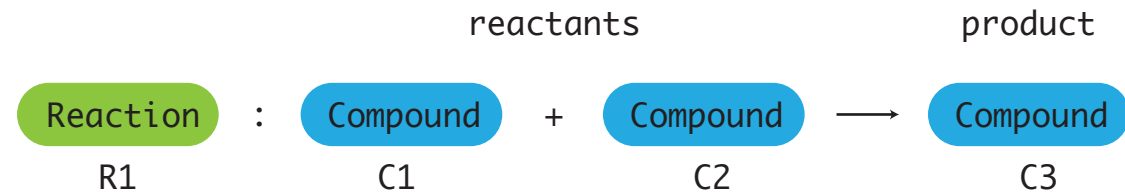
TABLE inspiration	
inspiration_original	INTEGER
inspiration_derivative	INTEGER

# Single-Step Synthesis

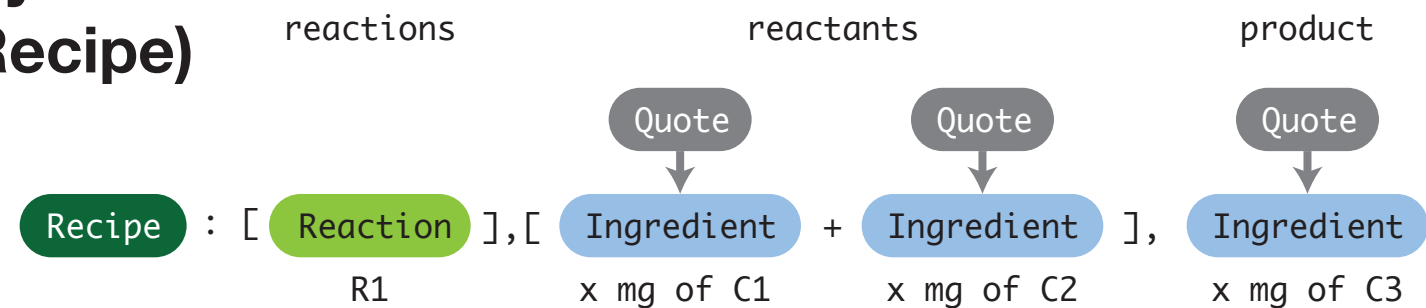
# SQL



# Python

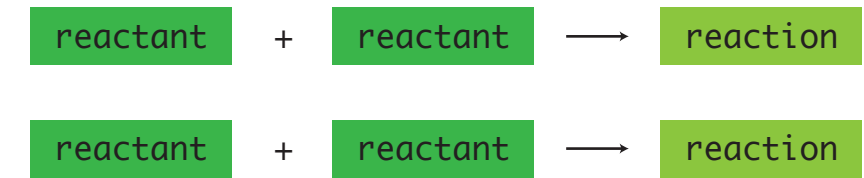


# Python (Recipe)

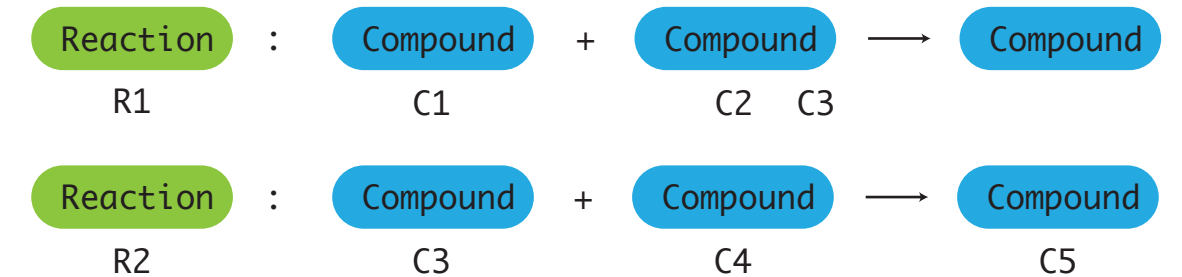


# Two-Step Synthesis

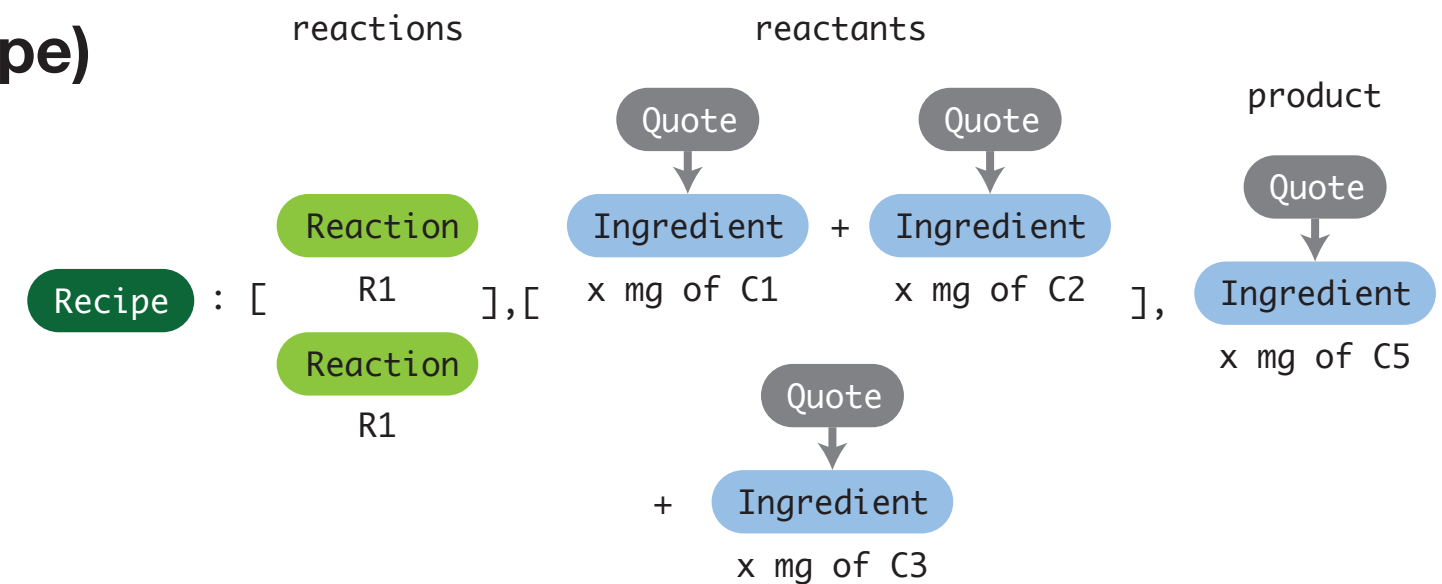
# SQL



# Python



# Python (Recipe)



# Derived Classes

