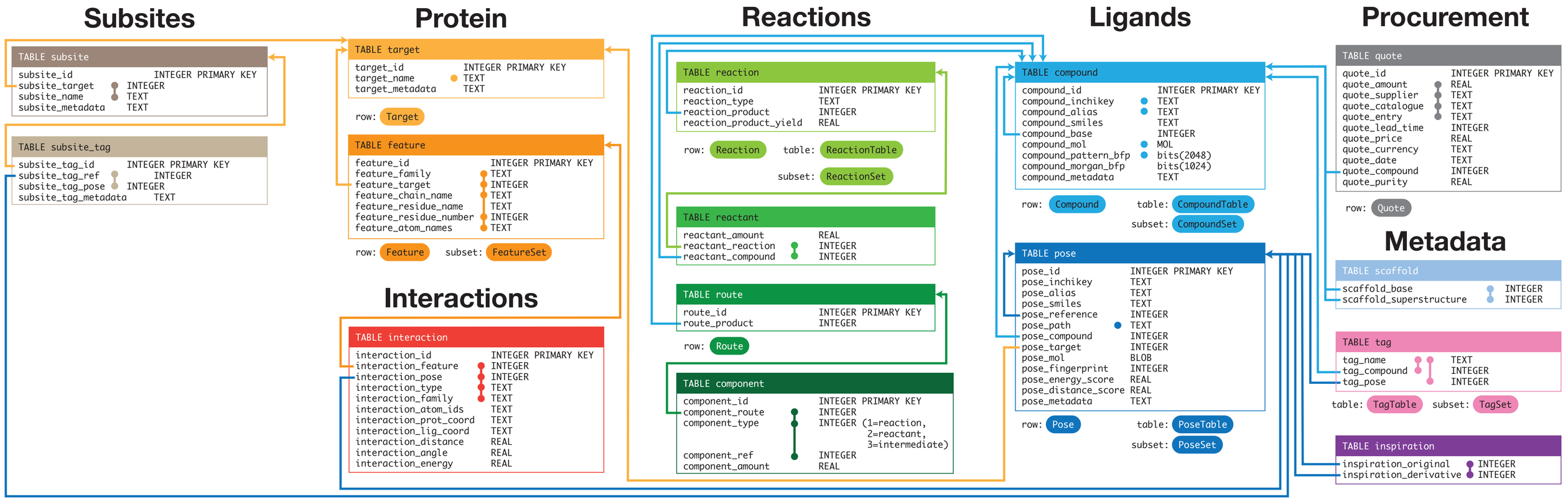

Subsites
TABLE subsite
subsite_id INTEGER PRIMARY KEY
subsite_target INTEGER
subsite_name TEXT
subsite_metadata TEXT
TABLE subsite_tag
subsite_tag_id INTEGER PRIMARY KEY
subsite_tag_ref INTEGER
subsite_tag_pose INTEGER
subsite_tag_metadata TEXT
Protein
TABLE target
target_id INTEGER PRIMARY KEY
target_name 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

reactant + reactant ⟶ reaction

Python

reactants product

Reaction : Compound + Compound ⟶ Compound

R1 C1 C2 C3

Python (Recipe)

reactions reactants product

Recipe : [Reaction],[Quote Ingredient + Quote Ingredient], Quote Ingredient

R1 x mg of C1 x mg of C2 x mg of C3

Two-Step Synthesis

SQL

reactant + reactant ⟶ reaction

reactant + reactant ⟶ reaction

Python

Reaction : Compound + Compound ⟶ Compound

R1 C1 C2 C3

Reaction : Compound + Compound ⟶ Compound

R2 C3 C4 C5

Python (Recipe)

reactions reactants product

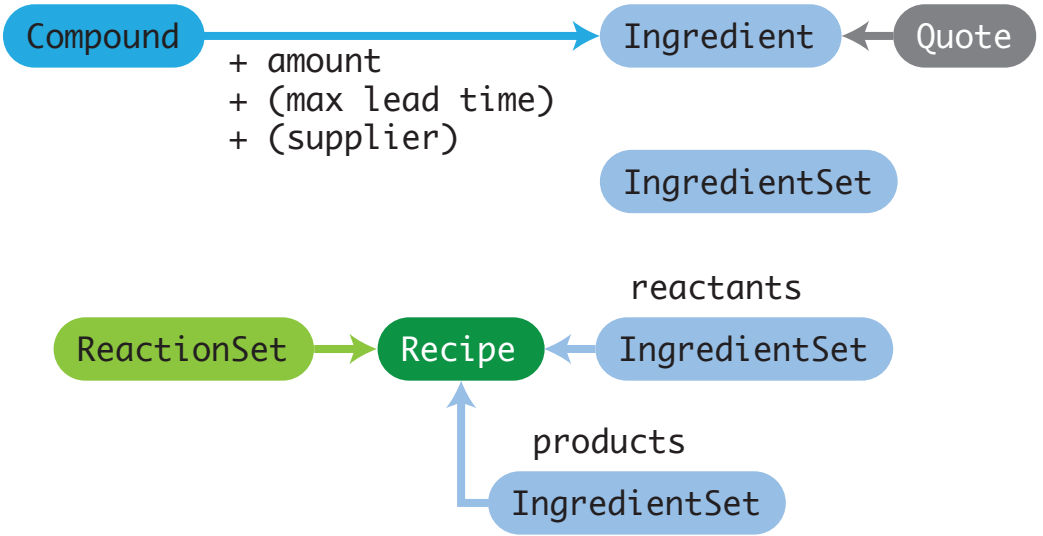
Recipe : [Reaction R1 Reaction R1],[Quote Ingredient + Quote Ingredient], Quote Ingredient

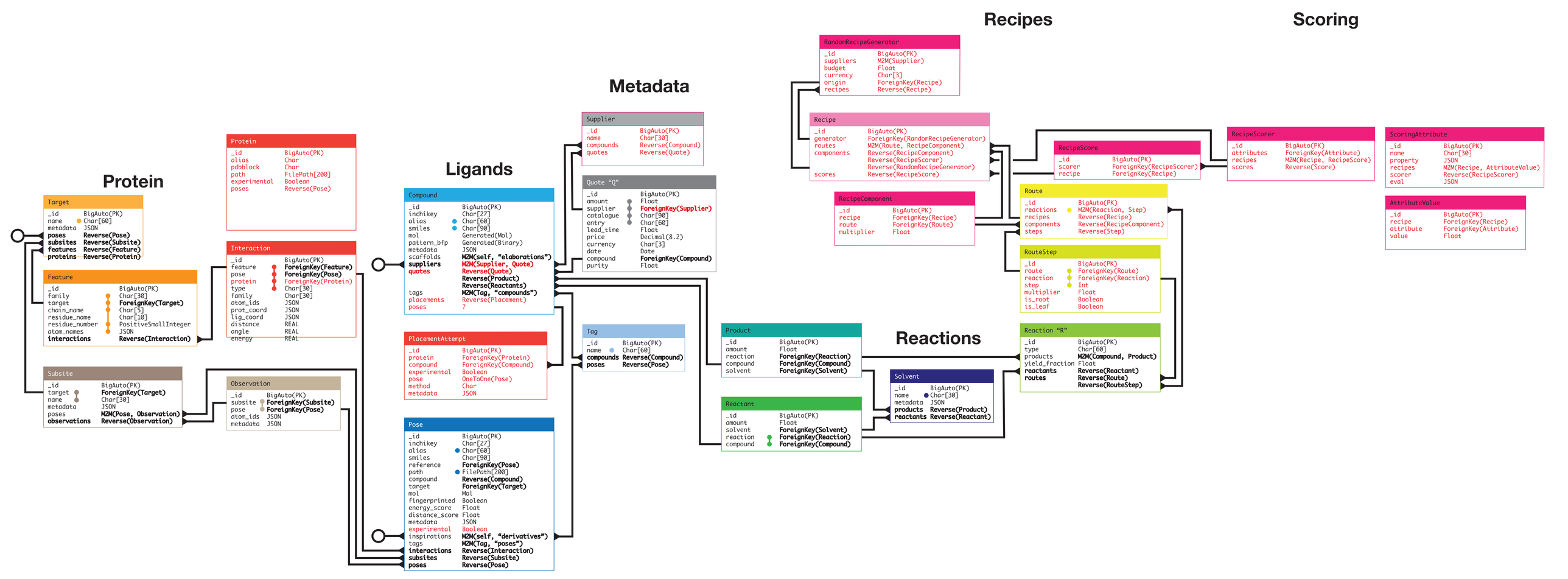
x mg of C1 x mg of C2 x mg of C5

+ Quote Ingredient

x mg of C3

Derived Classes




Protein
Target
_id BigAuto(PK)
name Char[60]
metadata JSON
poses Reverse(Pose)
subsites Reverse(Subsite)
features Reverse(Feature)
proteins Reverse(Protein)
Feature
_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)
Subsite
_id BigAuto(PK)
target ForeignKey(Target)
name Char[30]
metadata JSON
poses M2M(Pose, Observation)
observations Reverse(Observation)
Protein
_id BigAuto(PK)
alias Char
pdbblock Char
path FilePath[200]
experimental Boolean
poses Reverse(Pose)
Interaction
_id BigAuto(PK)
feature ForeignKey(Feature)
pose ForeignKey(Pose)
protein ForeignKey(Protein)
type Char[30]
family Char[30]
atom_ids JSON
prot_coord JSON
lig_coord JSON
distance REAL
angle REAL
energy REAL
Observation
_id BigAuto(PK)
subsite ForeignKey(Subsite)
pose ForeignKey(Pose)
atom_ids JSON
metadata JSON
Ligands
Compound
_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)
Reverse(Product)
Reverse(Reactants)
tags M2M(Tag, "compounds")
placements Reverse(Placement)
poses ?
PlacementAttempt
_id BigAuto(PK)
protein ForeignKey(Protein)
compound ForeignKey(Compound)
experimental Boolean
pose OneToOne(Pose)
method Char
metadata JSON
Pose
_id BigAuto(PK)
inchikey Char[27]
alias Char[60]
smiles Char[90]
reference ForeignKey(Pose)
path FilePath[200]
compound Reverse(Compound)
target ForeignKey(Target)
mol Mol
fingerprinted Boolean
energy_score Float
distance_score Float
metadata JSON
experimental Boolean
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
Tag
_id BigAuto(PK)
name Char[60]
compounds Reverse(Compound)
poses Reverse(Pose)
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)
Reactions
Solvent
_id BigAuto(PK)
name Char[30]
metadata JSON
products Reverse(Product)
reactants Reverse(Reactant)
Reaction "R"
_id BigAuto(PK)
type Char[60]
products M2M(Compound, Product)
yield_fraction Float
reactants Reverse(Reactant)
routes Reverse(Route)
Reverse(RouteStep)
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(RecipeScorer)
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
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