

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

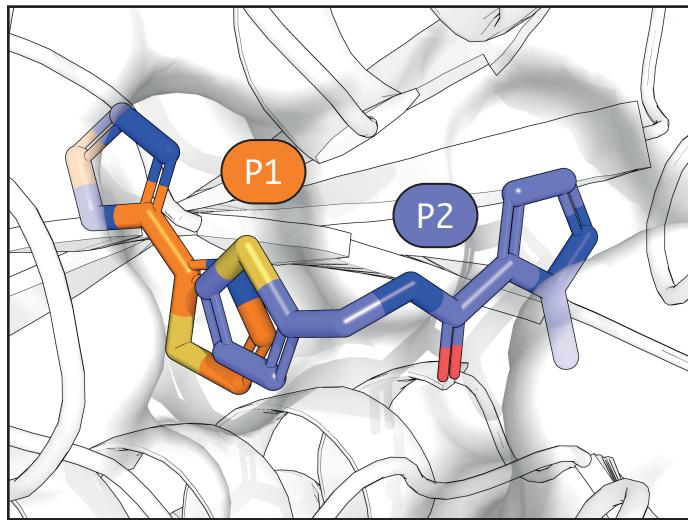
TABLE	scaffold
	scaffold_base INTEGER
	scaffold_superstructure INTEGER

TABLE	tag
	tag_name TEXT
	tag_compound INTEGER
	tag_pose INTEGER

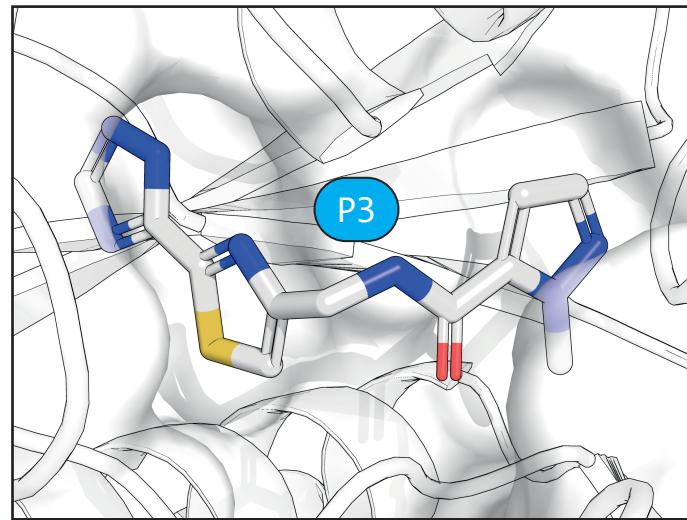
table: TagTable subset: TagSet

TABLE	inspiration
	inspiration_original INTEGER
	inspiration_derivative INTEGER

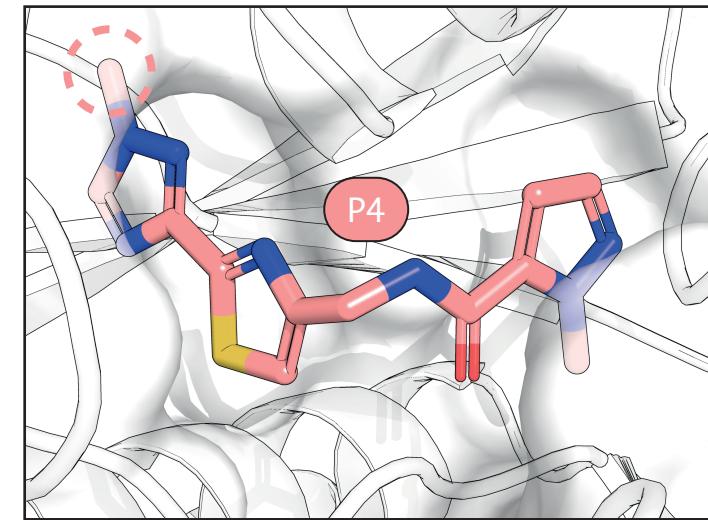
a) Fragment Inspirations



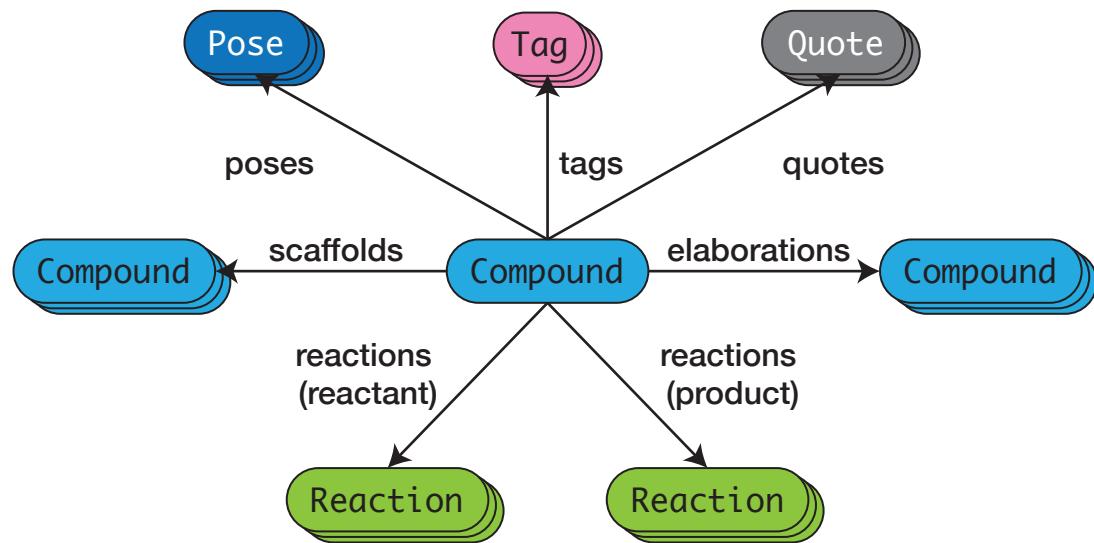
b) Fragment Merge (Scaffold)



c) Fragment Merge (Elaborated)



d) Compound Relations



e) Pose Relations

