

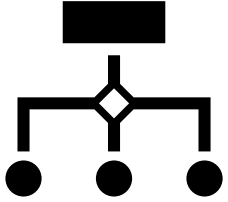
LSKB新機能のご紹介

AI 学習で作成した MoA データ と 意思決定支援 ツールの導入

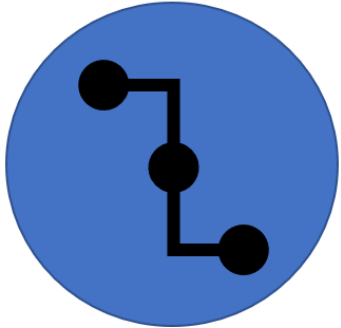
緑川 淳（株式会社ワールドフュージョン）

LSKB is scientific web

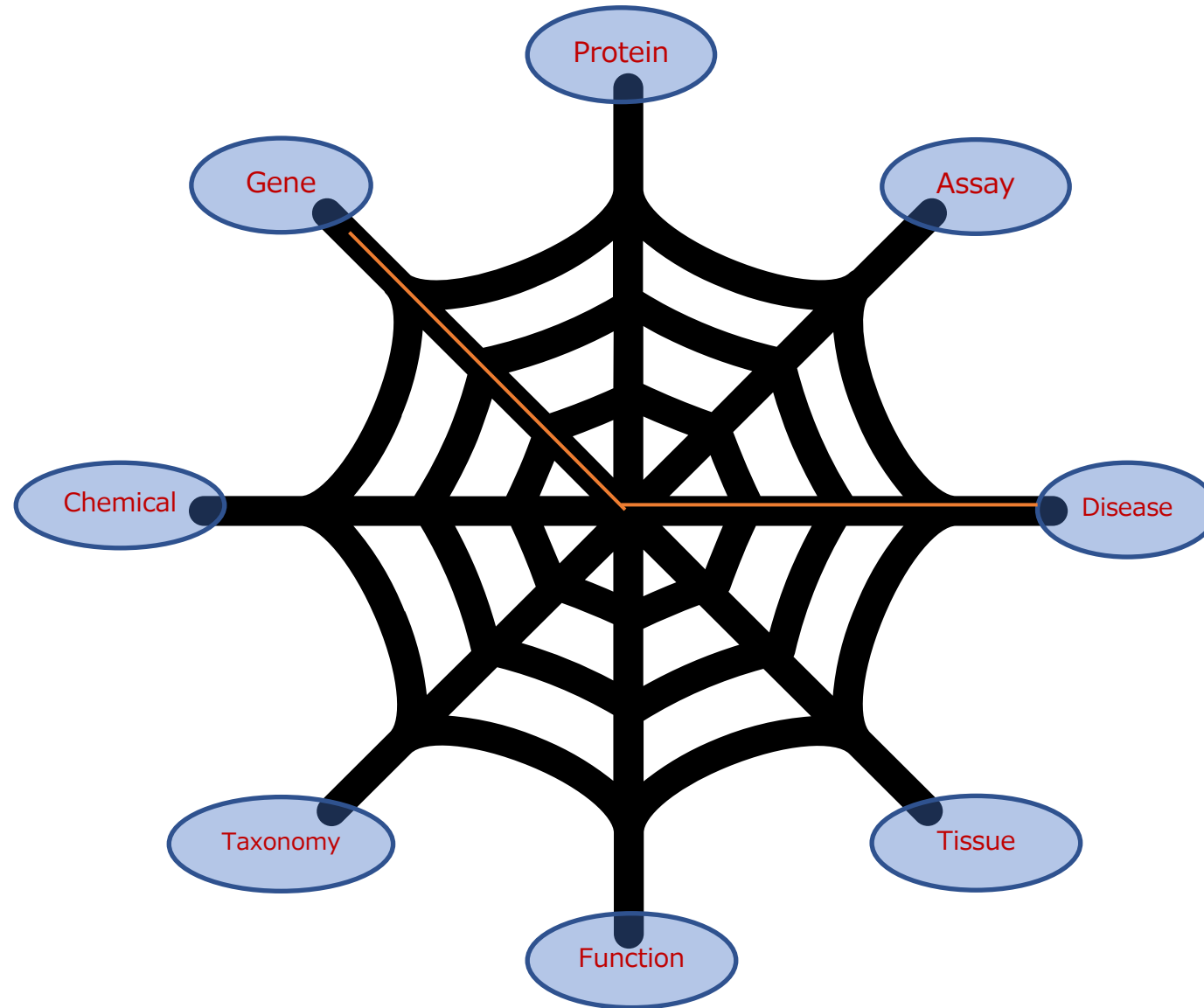
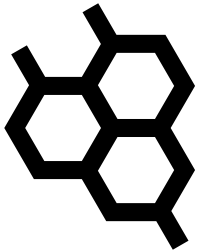
Ontology



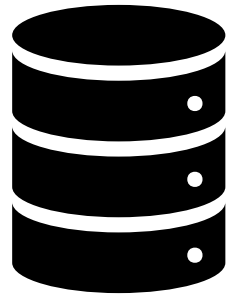
Interaction



Structure

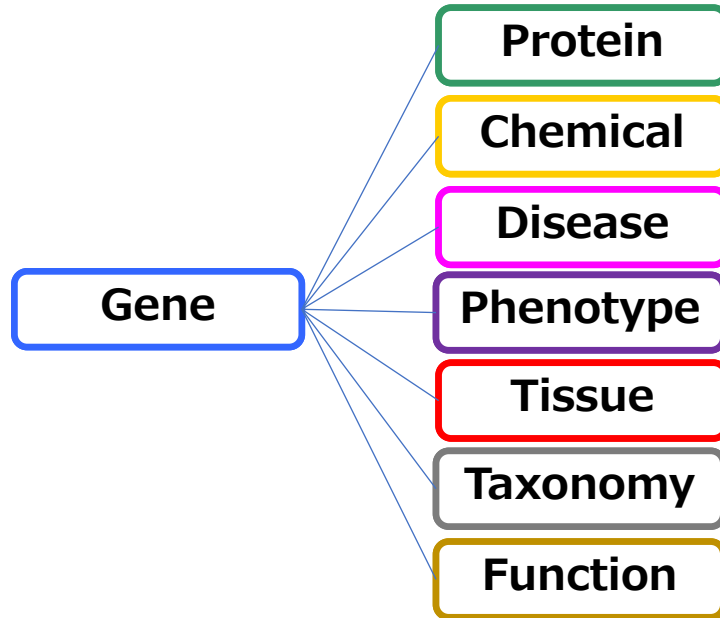
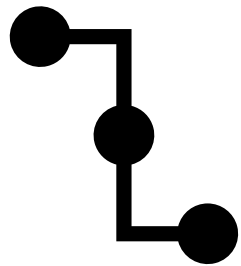


Contents

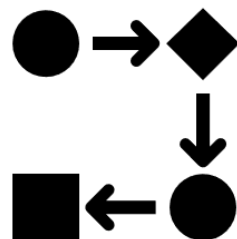


LSKB Interaction

Interaction



GO-MoA database



1) Text-Mining

- 20 years of PubMed literature (3 levels)
- Clinical Trial
- Assay Description

2) Assay Data

- Target Gene/Protein - Chemical
- Activities Endpoint
- Mode : Inhibition agonism/antagonism
- Expression: up/down regulation
- GWAS

3) Curated Annotation

- Disease Target
- Gene Ontology
- Pathway

4) AI Curated Annotation

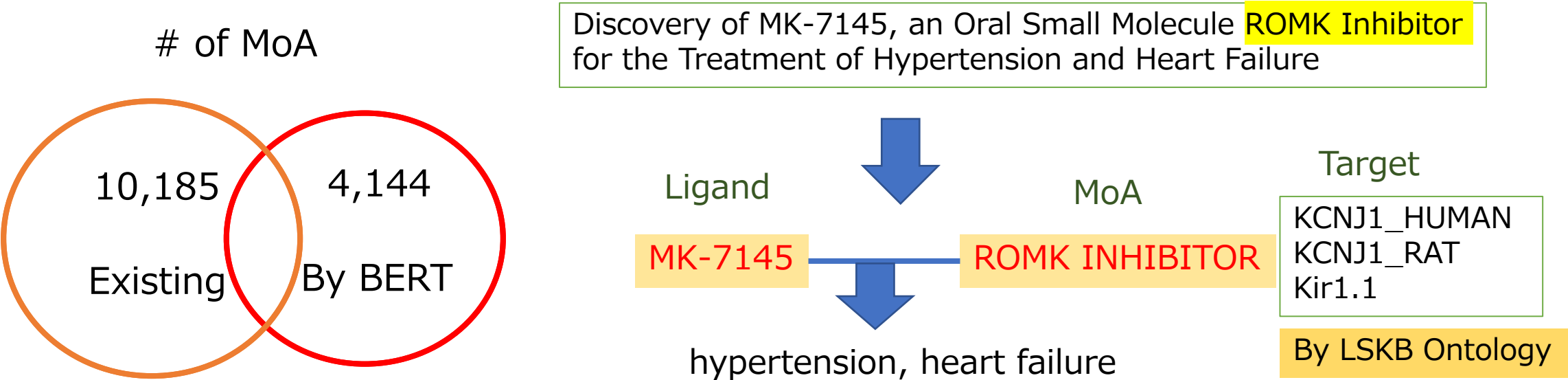
- Mechanism of Action
- Gene RIF

5) Misc

- Protein Pocket Similarity
- GO-MoA database

AI Curated Annotation

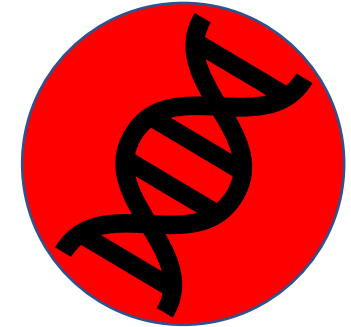
- 新規MoAの抽出



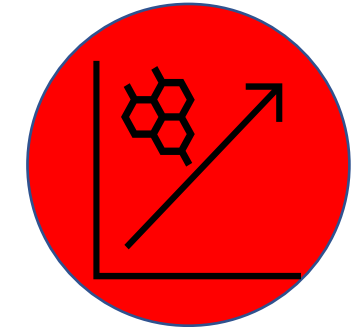
ラベル	Recall(再現率)	Precision(精度)	F1 Score
MoA	98.30%	95.30%	96.80%

LSKB is scientific web

Bioinformatics



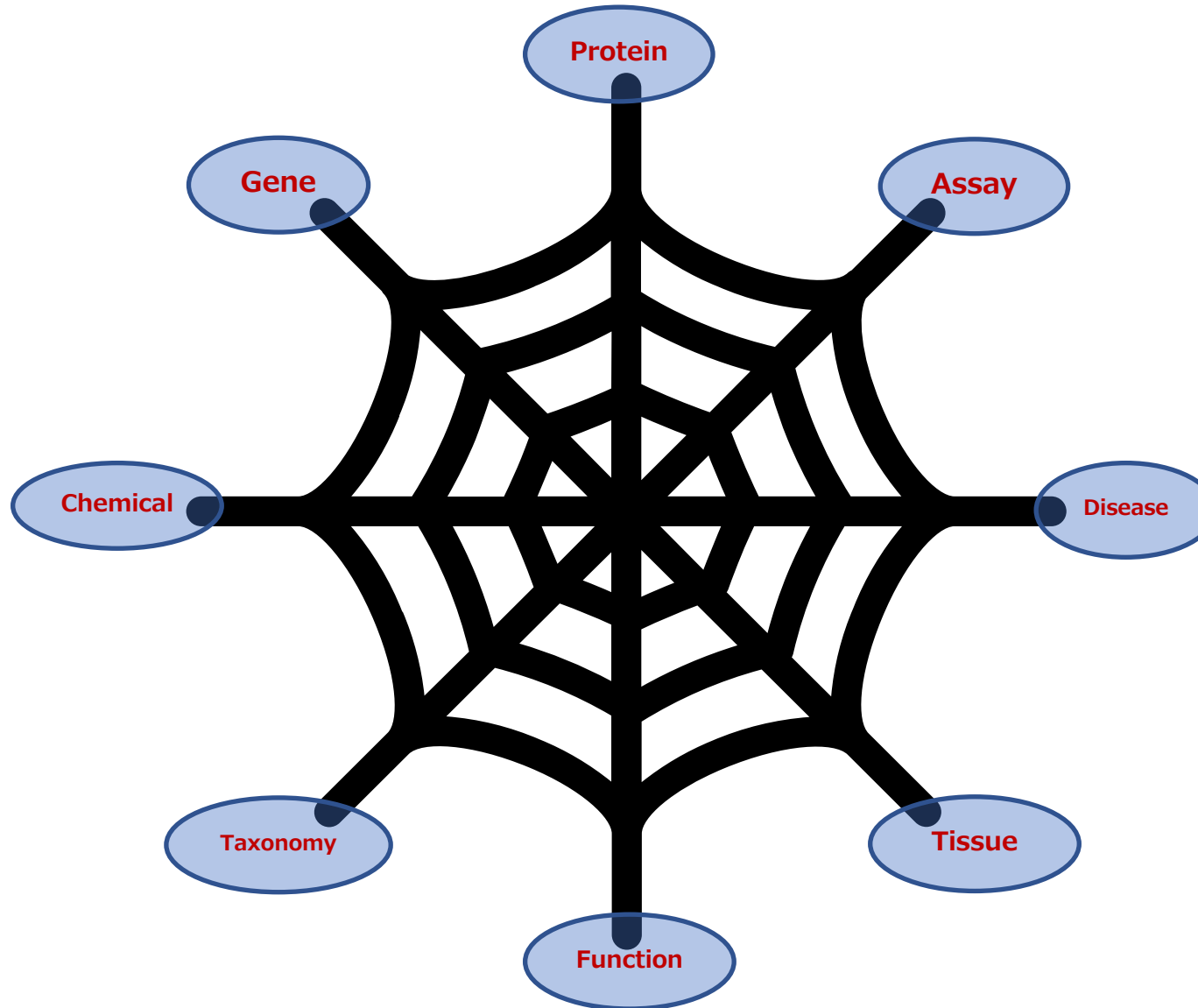
Cheminformatics



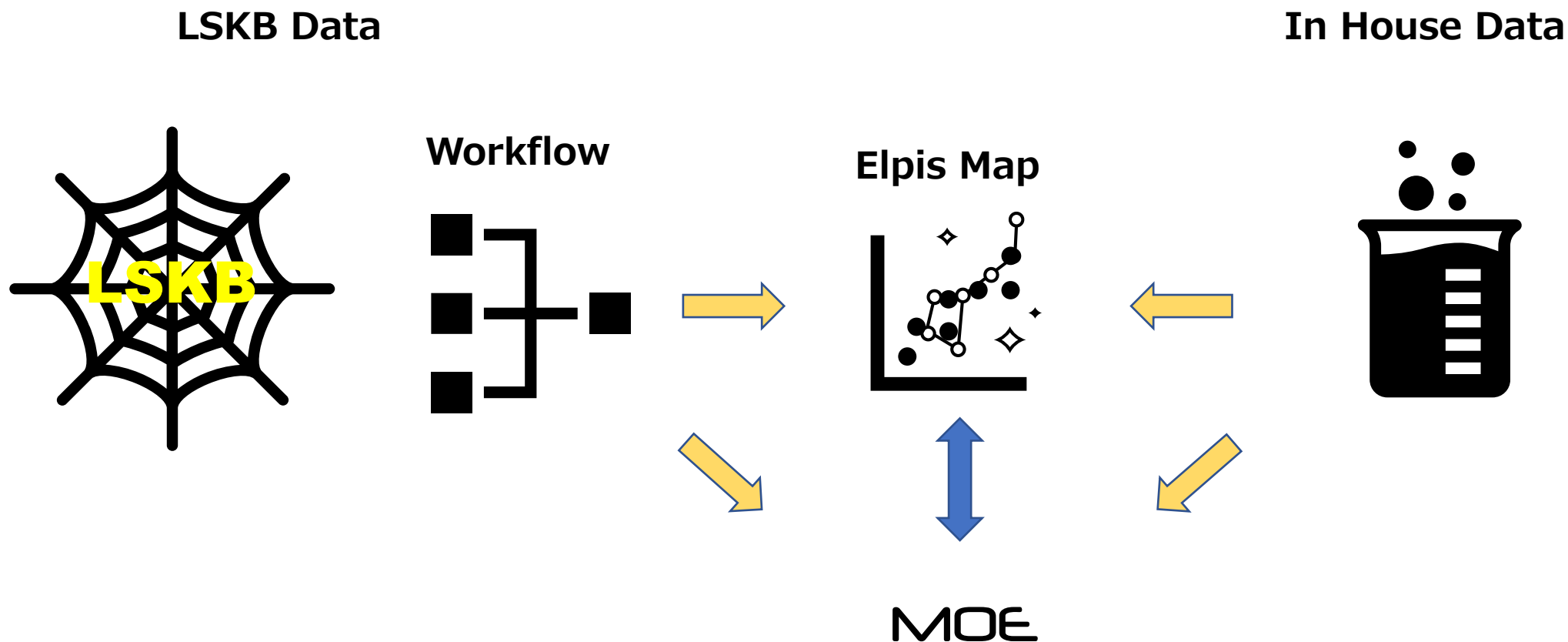
Exploration



Analysis



Elpis Map : Decision Support Tool



Current Workflow

Begin workflow process

Seek compounds by structure search using single compound by sketch

Seek compounds by Exact match w/o chirality from dataset: Small Molecules Collection

Edit...

(optional) Click to open the dialog, to choose/drop items store into result table...

Result Tables

COMPOUND

Input keywords as gene/protein identifier.

Acceptable Gene/Protein identifier types are,

- Entrez GeneID
- Gene Symbol
- UniProt Entry Name/Accession
- Ensembl GeneID/ProteinID/TranscriptID
- RefSeq Accession

Multiple identifiers/keywords delimited by newline, tab, colon, semicolon and/or comma, allowed.
Input keyword type(s) are automatically detected for each.

PK3CA_HUMAN
PK3CB_HUMAN
PK3CG_HUMAN

Ortholog conversion

(optional) Click to open the dialog, to choose/drop items store into result table...

Result Tables

GENE/PROTEIN

Retrieve activities associated with compounds for proteins in

Items available

Load Datafile

Load text file containing Gene/Protein identifiers

Load SD File, with properties

Seek Gene/Protein

Seek Gene/Protein by category associated

Seek Gene/Protein by EC number

Seek Gene/Protein by PDB IDs

Seek Gene/Protein by arbitrary keyword(s)

Seek Assay Targets by TaxID

Seek Compounds

Seek Compounds by LSKB ChemID

Seek Compounds by Patent ID

Seek Compounds by Compounds currently held

Seek Compounds by MoA/function associated

Retrieve protein-ligand Pairs, by Action Type

Compound list handling (Dummy)

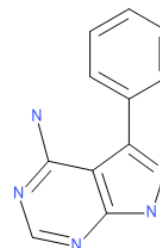
Retriever, using Keys/IDs in workflow

Retrieve PDB entries associated with protein(s)

Get Disease summary by compound identifier

Get Disease/Chemical/Function association by compound identifier

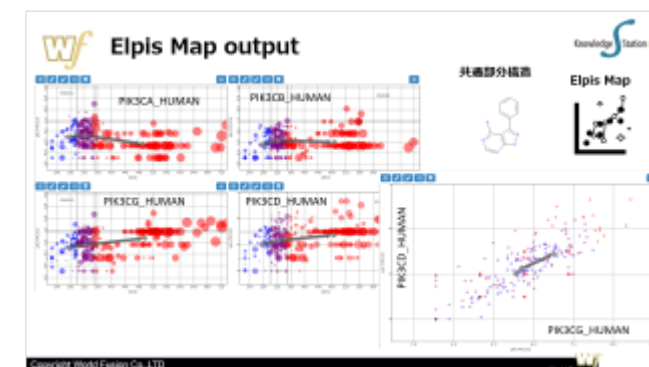
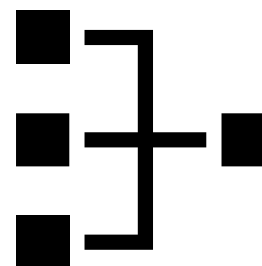
部分構造を指定



ターゲットタンパク質を指定

PIK3CA_HUMAN
PIK3CB_HUMAN
PIK3CG_HUMAN
PIK3CD_HUMAN

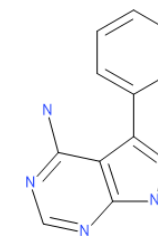
Workflow



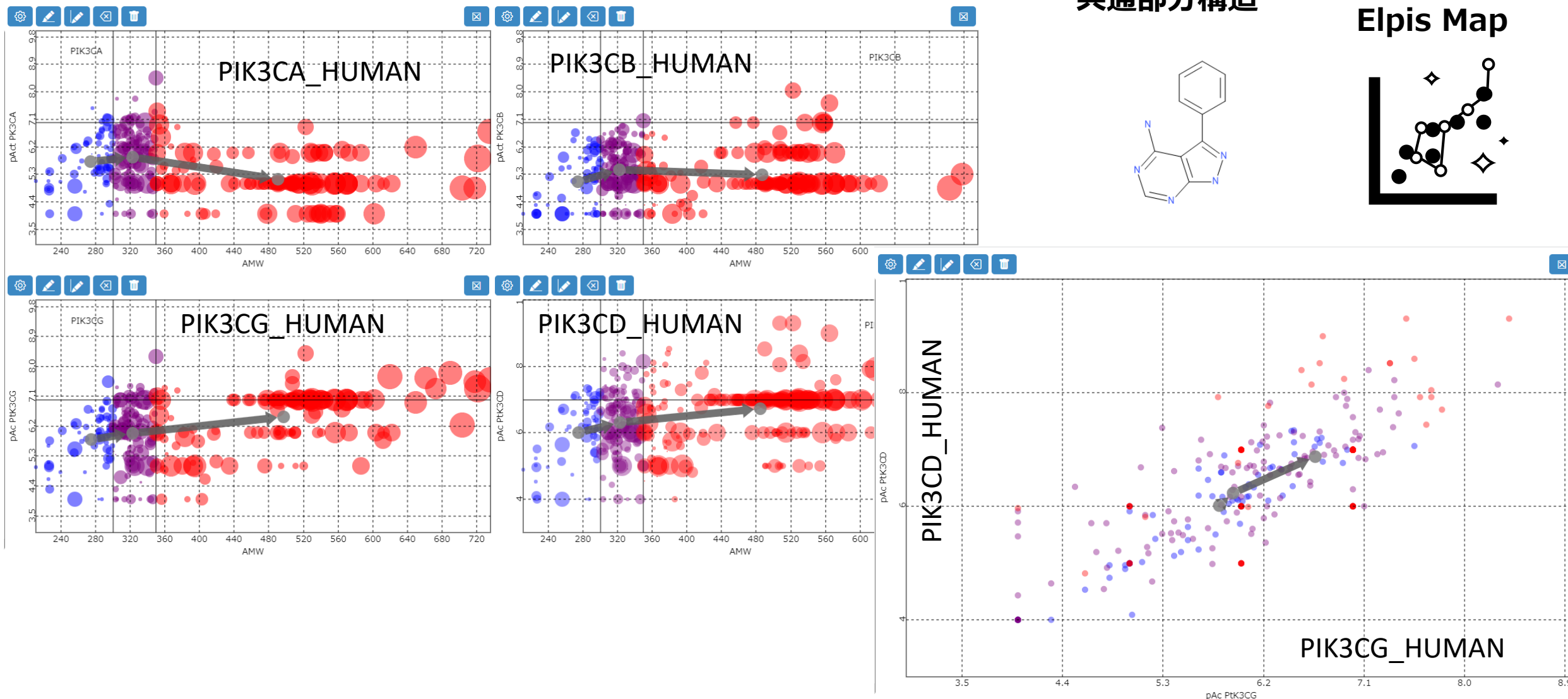
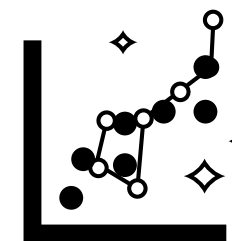


Elpis Map output

共通部分構造



Elpis Map





LSKB Ver.7

1. GUI を刷新
 - Top Menu の再構成
 - 新しいテーブルの導入
2. Deep Learning により 抽出した MoA の追加
 - ターゲット/Ligand/疾患との関連性の拡大
3. GO-MoAの Update
 - 新規 MoAの追加と 不要なアノテーションの整理
 - 疾患から 新しい ターゲット、ターゲット遺伝子から新たな適応症、化合物から 新たな適応症の探索
4. Workflowの Update
 - 目的とするデータ収集を可能に
 - 処理の自動化
 - LSKBのデータベースを最大限に活用できる探索ツール
5. Elpis Mapの搭載
 - LSKB 搭載データと 自社データの比較が容易
 - 意思決定を強力にサポート

etc

ご清聴ありがとうございました。

アンケートにご協力をお願いいたします。

<https://www.lskb.jp/cbi2021>

ご質問は

support@lskb.jp

までお願いいたします。

