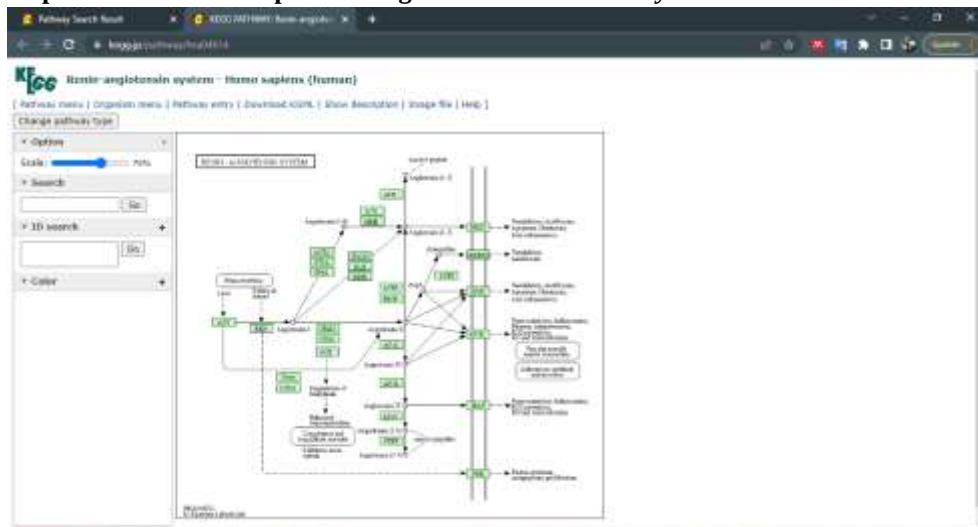


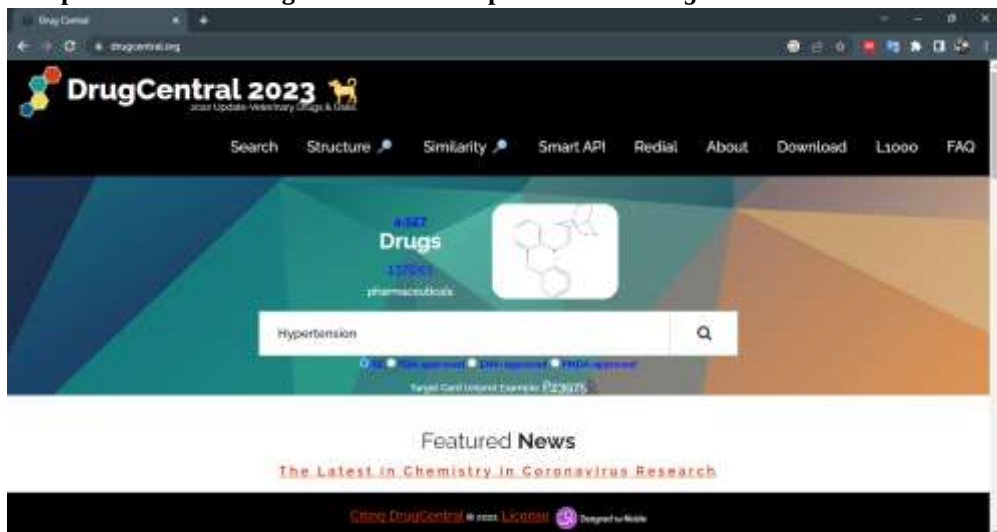
LAMPIRAN

Lampiran 1. Identifikasi protein target dari *KEGG Pathway*

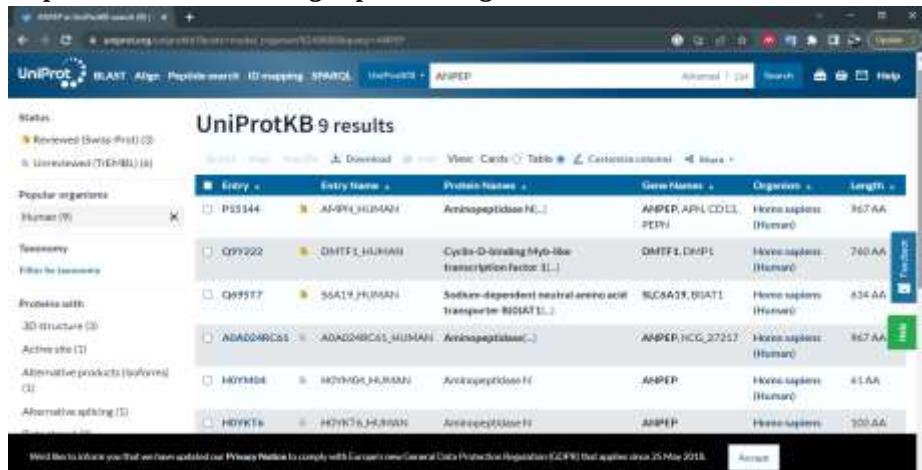


Jalur patofisiologi hipertensi melalui sistem RAS

Lampiran 2. Protein target obat sintesis hipertensi dari *DrugCentral*



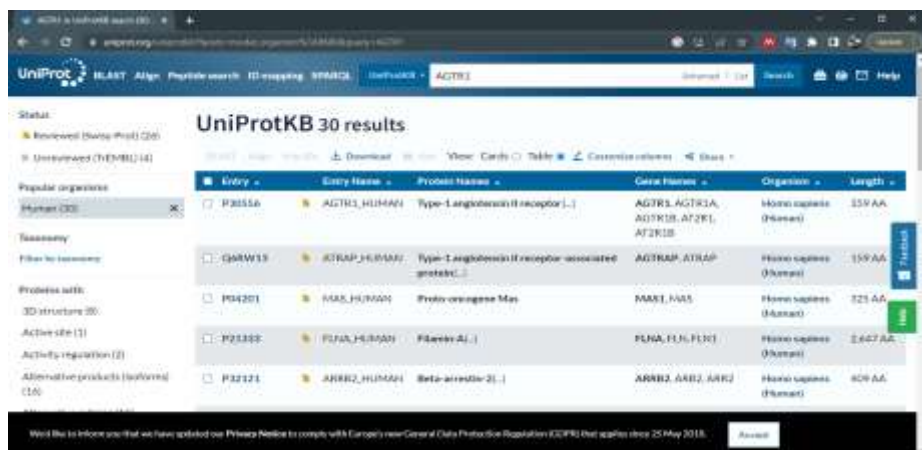
Lampiran 3. Validasi nama gen protein target dari UniProt



UniProtKB 9 results

Entry	Entry Name	Protein Name	Gene Name	Organism	Length
P51444	ANPEP_HUMAN	Aminopeptidase NC...	ANPEP, APPL, CD13, PCN1	Homo sapiens (Human)	967 AA
Q99222	DMTF1_HUMAN	Cyclic-D-binding Myo-like transcription factor 1L...	DMTF1, DMPL	Homo sapiens (Human)	740 AA
Q99777	S6AT1_HUMAN	Sodium-dependent neutral amino acid transporter B0DAT1L...	S6CAT1, S6AT1	Homo sapiens (Human)	634 AA
ADA204RC65	ADA204RC65_HUMAN	Aminopeptidase...	ANPEP, HCG_27317	Homo sapiens (Human)	967 AA
H0YH04	H0YH04_HUMAN	Aminopeptidase H...	ANPEP	Homo sapiens (Human)	61 AA
H0YH75	H0YH75_HUMAN	Aminopeptidase H...	ANPEP	Homo sapiens (Human)	305 AA

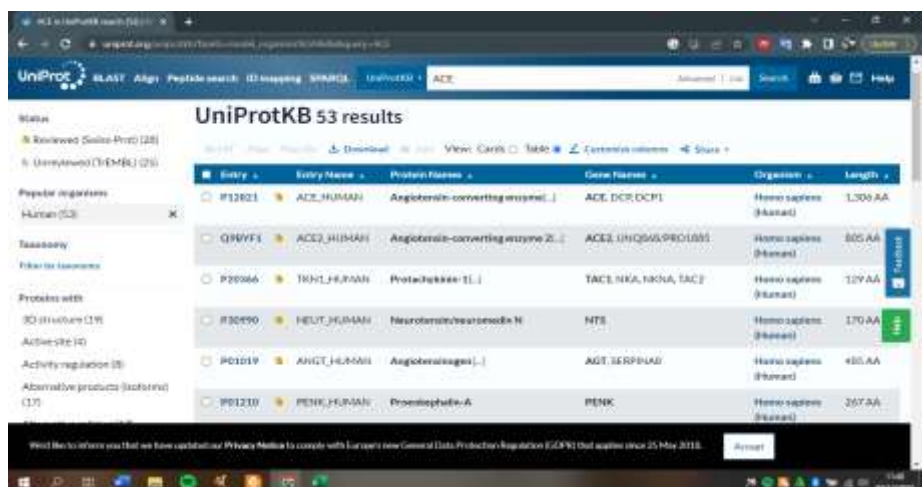
Alanyl aminopeptidase



UniProtKB 30 results

Entry	Entry Name	Protein Name	Gene Name	Organism	Length
P35556	AGTR1_HUMAN	Type-1 angiotensin II receptor...	AGTR1, AGTR1A, AGTR1B, AT2R1	Homo sapiens (Human)	359 AA
Q9ARW5	ATRAP_HUMAN	Type-1 angiotensin II receptor-associated protein...	ATRAP, ATRAP	Homo sapiens (Human)	159 AA
P04201	MAS_HUMAN	Protein oncogene Mas	MAS1, MAS	Homo sapiens (Human)	321 AA
P25355	PLN1_HUMAN	Filamin A1...	PLN1, FLN, FLN1	Homo sapiens (Human)	2,647 AA
P32121	ARRB2_HUMAN	Beta-arrestin-2...	ARRB2, ARB2, ARB2	Homo sapiens (Human)	609 AA

Angiotensin II receptor type 1

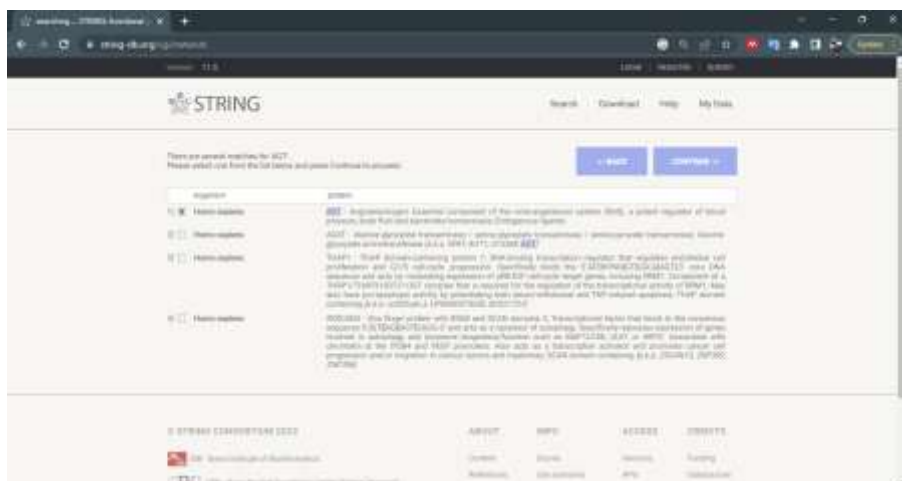
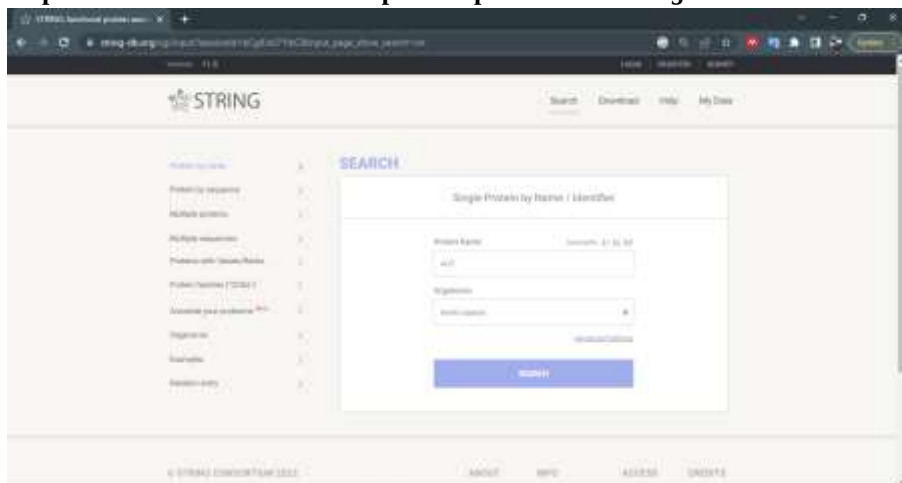


UniProtKB 53 results

Entry	Entry Name	Protein Name	Gene Name	Organism	Length
P12821	ACE_HUMAN	Angiotensin-converting enzyme...	ACE, DCR, DCP1	Homo sapiens (Human)	1,206 AA
Q9BYF1	ACE2_HUMAN	Angiotensin-converting enzyme 2L...	ACE2, UNQ564/PRO1051	Homo sapiens (Human)	805 AA
P25966	TRO1_HUMAN	Protachikin-1L...	TAC1, NKA, NKNA, TAC2	Homo sapiens (Human)	129 AA
P30490	NEUT_HUMAN	Neurotensin/neurokinin B	NTS	Homo sapiens (Human)	170 AA
P01019	ANGT_HUMAN	Angiotensinogen...	AGT, SERPINH1	Homo sapiens (Human)	485 AA
P01210	PENK_HUMAN	Prometkephelin-A	PENK	Homo sapiens (Human)	267 AA

Angiotensin-converting enzyme

Lampiran 4. Identifikasi interaksi protein-protein dari *String*



Lampiran 5. Data kandungan senyawa kimia tanaman dari KNpSack

input type = **ss** input word = **Monarda citrifolia**

number of matched data: 107

id	cas	name	chem	mw	chem name in wikipedia
200001374	5544-30-9	Methyl phosphoride a	C18-08H4O8	436.3422515	Monarda citrifolia L
200001375	01446-20-9	1-Propanol	C3H8O	74.1268644	Monarda citrifolia L
200001376	11961-75-5	Phenyl	C6H5	94.11636595	Monarda citrifolia L
200001379	92-61-5	Scopolamine	C19H27NO	312.0425874	Monarda citrifolia L
200001382	2465-22-8	Isorham	C18H21O	253.0473442	Monarda citrifolia L
200001384	493-39-4	Coniferylaldehyde	C12H14O2	178.0629479	Monarda citrifolia L
200001385	72-44-0	Alcohol	C14H18O	210.0427876	Monarda citrifolia L
200001389	6095-71-8	1-Hydroxy-2-methoxyanthracene	C18H15O2	254.0576881	Monarda citrifolia L
200001390	602-64-2	Anthracene	C14H10	202.0517137	Monarda citrifolia L
200001393	474-08-8	Linalyl	C15H18O	210.0526343	Monarda citrifolia L
200001394	474-28-8	Monoterpene	C15H18O	210.0526343	Monarda citrifolia L
200001395	117-92-2	Alcohol	C15H18O	210.0526343	Monarda citrifolia L
200001396	84-54-8	2-Methylanthracene	C18H14	232.0607555	Monarda citrifolia L
200001397	14200-40-1	Agonist	C18H22O11	414.1762119	Monarda citrifolia L
200001398	475-99-1	Alcohol	C19H20O	268.328021	Monarda citrifolia L
200001399	3945-80-8	Monoterpene	C18H22O11	390.3821188	Monarda citrifolia L
200001400	2150-61-2	Agonist	C17H24O11	434.1759191	Monarda citrifolia L
200001401	186-86-1	Agonist	C18H22O	268.328021	Monarda citrifolia L
200001402	71-75-1	Uronic acid	C18H22O	268.328021	Monarda citrifolia L
200001403	82-46-5	1-Oxa-1,2-dioxane	C18H22O	268.328021	Monarda citrifolia L
200001404	18465-297-7	Agonist	C17H24O11	330.0759258	Monarda citrifolia L
200001405	60072-15-6	Agonist 1,2-dimethyl ether 4-galactose	C22H40O11	460.7304833	Monarda citrifolia L
200001406	528-18-3	Karaphyll	C18H18O	266.0477882	Monarda citrifolia L
200001407	17555-94-9	Monoterpene	C17H22O11	364.3847529	Monarda citrifolia L
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200001409	183-18-4	Alcohol	C18H22O11	440.3209148	Monarda citrifolia L
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Lampiran 6. Data kandungan senyawa kimia tanaman dari IJAH Analytics

IJAH Analytics
Search and Predict (Plant - Compound) - (Protein - Disease) Connectivity

Use-case Examples: ☒ Drug-side ☐ Target-side ☐ Both sides

Drug-Side

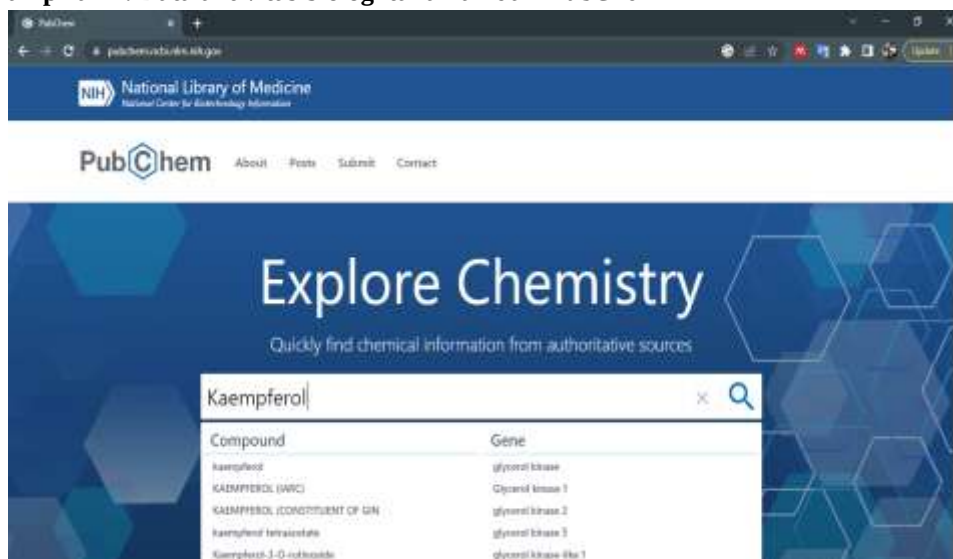
Target-Side

Plants (of 4064) Compounds (of 17277) Proteins (of 3334) Diseases (of 4421)

Kembang Kiri (Rengasulita) X UniprotKB: uniprotKB:K18191 X Disorder Knowledge X



Lampiran 7. Data aktivitas biologi tanaman dari PubChem



NIH National Library of Medicine
National Center for Biotechnology Information

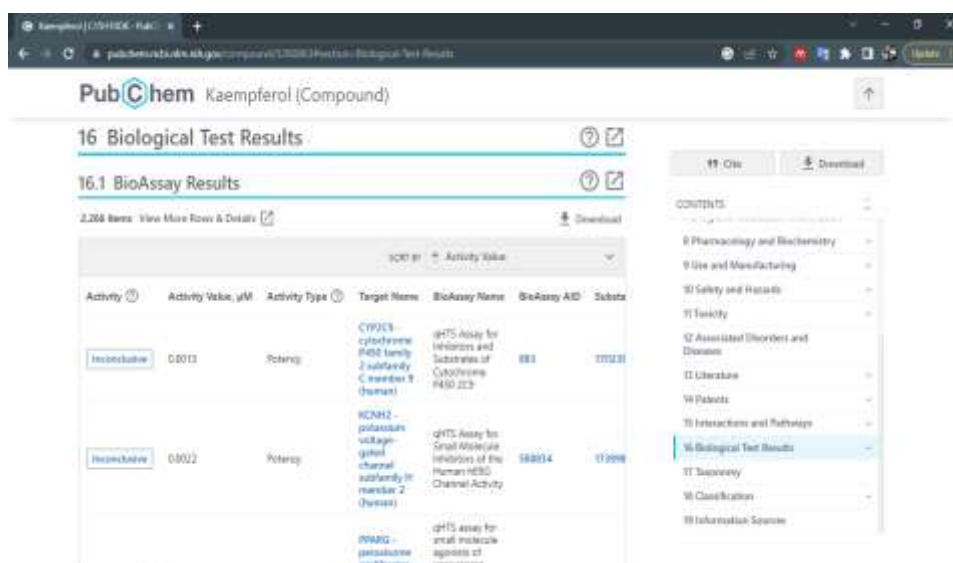
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Quickly find chemical information from authoritative sources

Kaempferol

Compound	Gene
kaempferol	glycerol kinase
KADAMFEROL (WCI)	Glycerol kinase 1
KADAMFEROL (CONSTITUENT OF GIN)	glycerol kinase 2
kaempferol tetraacetate	glycerol kinase 3
Kaempferol-3-O-rutinoside	glycerol kinase like 1



PubChem Kaempferol (Compound)

16 Biological Test Results

16.1 BioAssay Results

2,268 Items View More Rows & Details Download

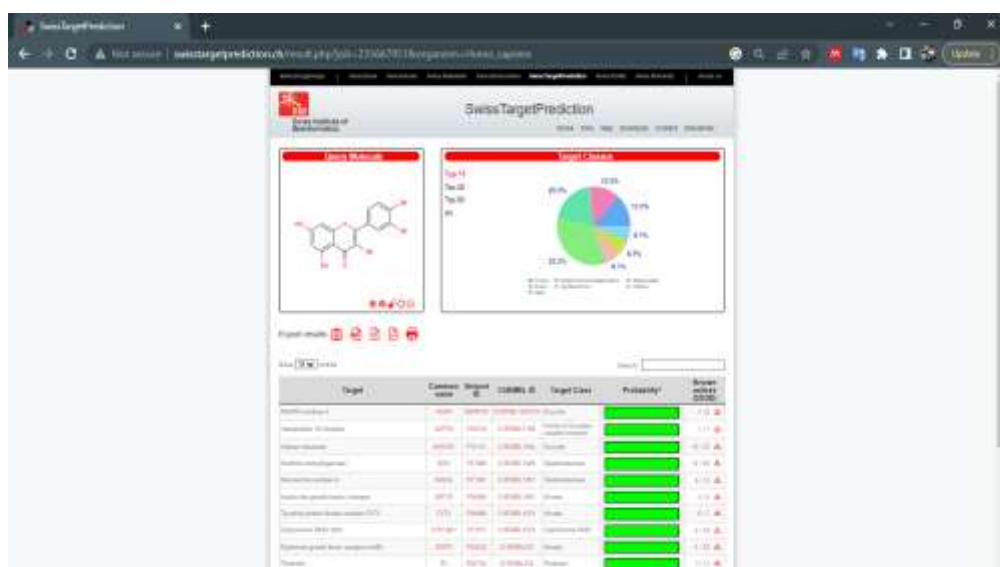
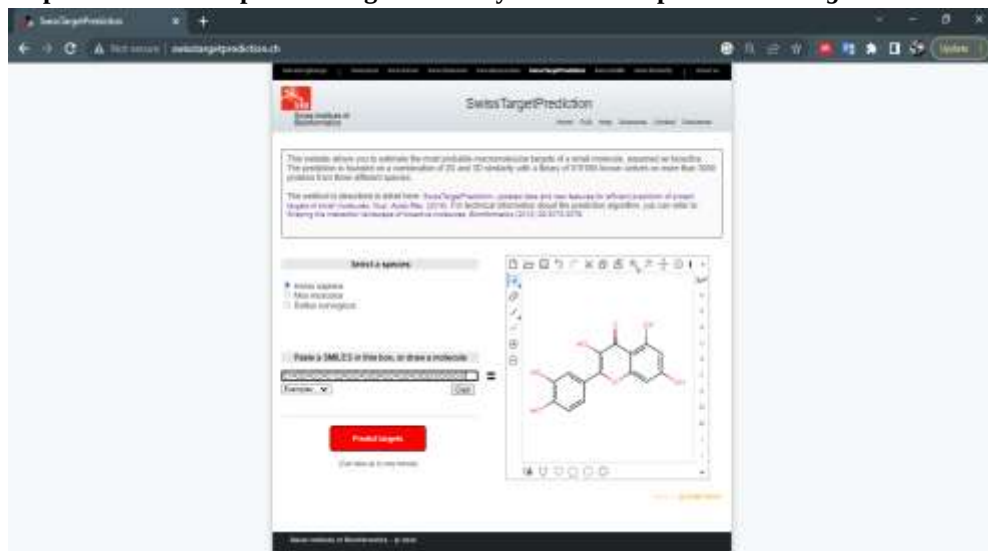
Activity	Activity Value, μ M	Activity Type	Target Name	BioAssay Name	BioAssay AID	Substrate
Inconclusive	0.0013	Potency	CYP2C8 - cytochrome P450 family 2 subfamily C member 8 (human)	gHTS Assay for Inhibitors and Substrates of Cytochrome P450 2C8	883	1112331
Inconclusive	0.0022	Potency	KCNH2 - potassium voltage-gated channel subfamily H member 2 (human)	gHTS Assay for Small Molecule Inhibitors of the Human hERG Channel Activity	588014	112098
Inconclusive		Potency	PP2A8G - proteinase activator	gHTS assay for small molecule agonists of proteinase		

19 Cit Download

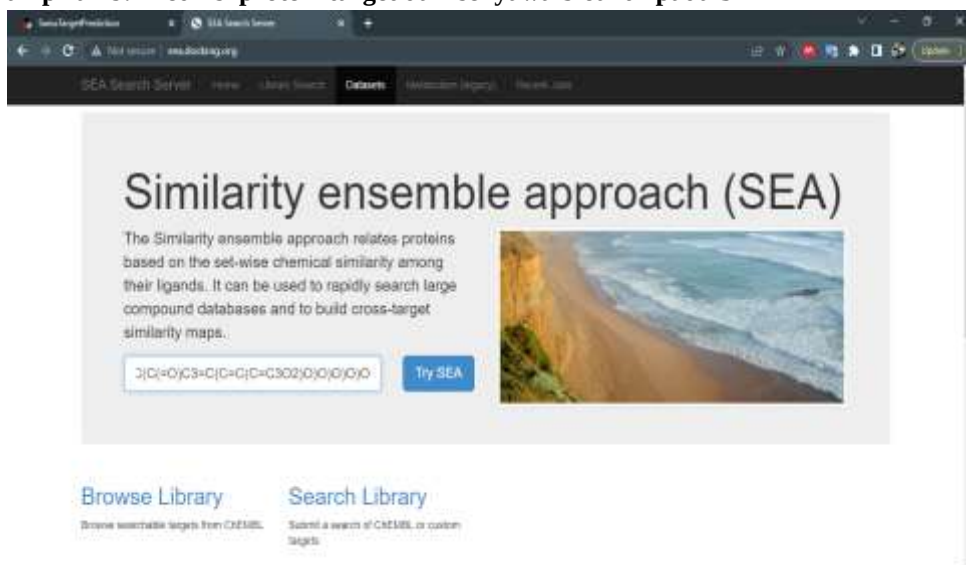
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- 9 Use and Manufacturing
- 10 Safety and Hazards
- 11 Toxicity
- 12 Associated Disorders and Diseases
- 13 Literature
- 14 Patents
- 15 Interactions and Pathways
- 16 Biological Test Results
- 17 Toxicology
- 18 Classification
- 19 Information Sources

Lampiran 8. Prediksi protein target dari senyawa bioaktif pada *Swiss Target Prediction*



Lampiran 9. Prediksi protein target dari senyawa bioaktif pada SEA



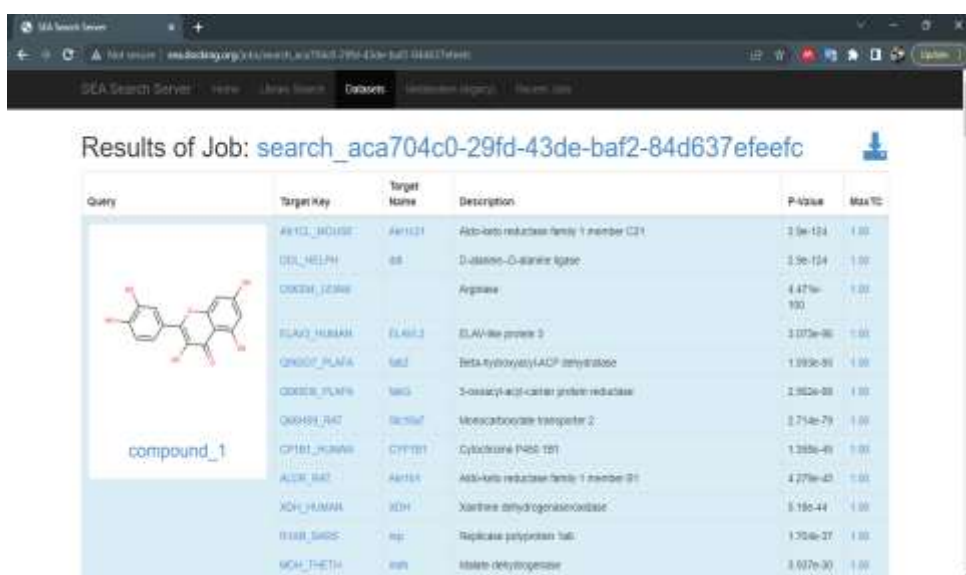
Similarity ensemble approach (SEA)

The Similarity ensemble approach relates proteins based on the set-wise chemical similarity among their ligands. It can be used to rapidly search large compound databases and to build cross-target similarity maps.

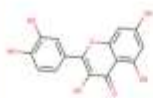
O=C(O)C3=C(C(=C(C=C3O2)O)O)O)O [Try SEA](#)

[Browse Library](#)
Browse searchable targets from ChEMBL

[Search Library](#)
Submit a search of ChEMBL or custom targets



Results of Job: [search_aca704c0-29fd-43de-baf2-84d637efeefc](#)

Query	Target Key	Target Name	Description	P-Value	Max TC
 compound_1	AKR1C1_MOUSE	Akr1c1	Aldo-keto reductase family 1 member C21	2.9e-124	1.00
	DEL_HELPH	DEL	D-aldose-O-amine ligase	2.9e-124	1.00
	ARGIN_HUMAN	Arginase	Arginase	4.47e-100	1.00
	ELAVL3_HUMAN	ELAVL3	ELAV-like protein 3	3.073e-96	1.00
	QNGDPT_PLAFA	fat3	Beta-xyloxyacyl-CoA dehydrogenase	1.993e-91	1.00
	QOQDSE_PLAFA	fat5	5-oxoacyl-CoA carboxyl-protein reductase	2.902e-88	1.00
	QK6H9L_P407	SLC35A7	Monocarboxylate transporter 2	2.754e-79	1.00
	CYP1B1_HUMAN	CYP1B1	Cyclooxane P450 1B1	1.385e-49	0.99
	AKR1A_MOUSE	Akr1a	Aldo-keto reductase family 1 member B1	4.277e-45	1.00
	XDH_HUMAN	XDH	Xanthine dehydrogenase	5.18e-44	1.00
	R10R_SARS	rep	Replicase polypeptide tail	1.504e-27	1.00
	MCH_THETA	mch	Maltate dehydrogenase	8.037e-30	1.00

Lampiran 10. Prediksi protein target dari senyawa bioaktif pada *SuperPred*

Here you can run a [target prediction](#) for your input compound.

There are different ways to start the classification:

- Search a compound by its name via PubChem
- Create a structure by SMILES string
- Draw your structure
- Load a molecule by clicking on inchikey (optional)

Pubchem Name :

Quercetin

Enter a compound name to search via PubChem

SMILES:

eg. CC1=CC(=C(C=C1)OC(=C)C=C1C(=O)O

Enter a SMILES string to search by defined structure

Additionally predicted targets

Search:

Target Name	UniProt ID	PDB Visualization	TTD ID	Probability	Model accuracy
Tyrosyl-DNA phosphodiesterase 1	D4H4B8.1075138	Q3MUW6	6P4D	Not Available	76.49%
DNA (apurinic or apyrimidinic site) lyase	D4H4B8.2610	P27093	6B7W	T13348	88.21%
Monamine oxidase A	D4H4B8.1501	P21337	2Z5Y	Not Available	87.49%
DNA topoisomerase II alpha	D4H4B8.1806	P11388	6ZV3	T17048	78.29%
Arachidonate 12-Lipoxygenase	D4H4B8.3607	P18064	3C9L	Not Available	85.49%
Transferrin	D4H4B8.3194	P02768	6SLG	T08462	88.21%
Thyroid hormone receptor alpha	D4H4B8.1860	P10327	3LZ	T70091	78.29%

Lampiran 11. Visualisasi *network pharmacology* menggunakan *software Cytoscape*