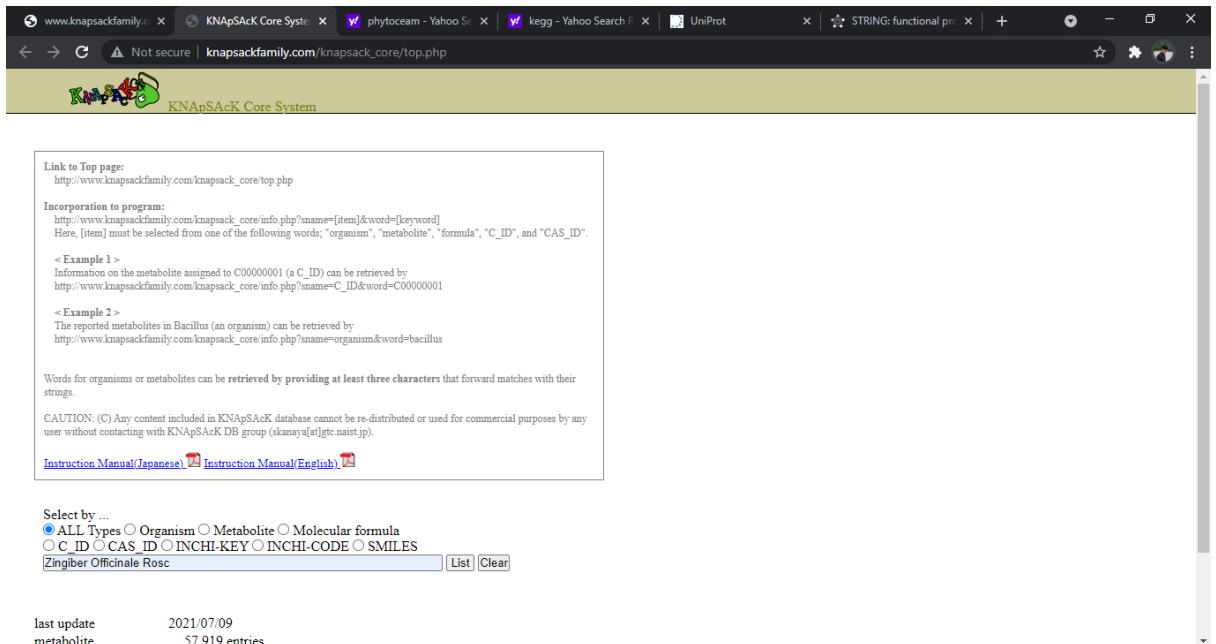


LAMPIRAN

1. Knapsack

Pertama buka webserver http://www.knapsackfamily.com/knapsack_core/top.php lalu akan muncul seperti gambar di bawah ini, pada kolom kosong di klik nama tanaman yang di gunakan



The screenshot shows a web browser window with the URL www.knapsackfamily.com/knapsack_core/top.php. The page title is "KNApSAcK Core System". The main content area contains a box with the following text:

Link to Top page:
http://www.knapsackfamily.com/knapsack_core/top.php



Incorporation to program:
http://www.knapsackfamily.com/knapsack_core/info.php?mname={item}&word={keyword}
Here, {item} must be selected from one of the following words; "organism", "metabolite", "formula", "C_ID", and "CAS_ID".

- Example 1 -
Information on the metabolite assigned to C00000001 (a C_ID) can be retrieved by
http://www.knapsackfamily.com/knapsack_core/info.php?mname=C_ID&word=C00000001

- Example 2 -
The reported metabolites in Bacillus (an organism) can be retrieved by
http://www.knapsackfamily.com/knapsack_core/info.php?mname=organism&word=bacillus

Words for organisms or metabolites can be retrieved by providing at least three characters that forward matches with their strings.

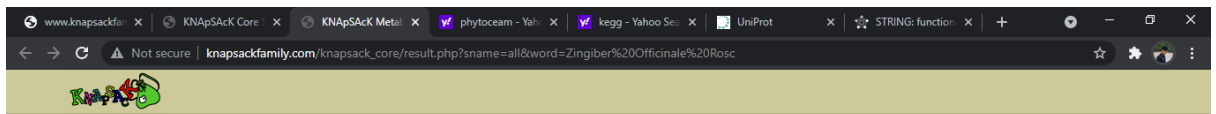
CAUTION: (C) Any content included in KNApSAcK database cannot be re-distributed or used for commercial purposes by any user without contacting with KNApSAcK DB group ([skanaya\[at\]gtc.naist.jp](mailto:skanaya[at]gtc.naist.jp)).

[Instruction Manual/Japanese](#)  [Instruction Manual/English](#) 

Select by ...
 ALL Types Organism Metabolite Molecular formula
 C_ID CAS_ID INCHI-KEY INCHI-CODE SMILES

last update 2021/07/09
metabolite 57,919 entries

Setelah itu klik list dan akan muncul seperti gambar di bawah



Input type = all , Input word = Zingiber Officinale Rosc

Number of matched data :25

C ID	CAS ID	Metabolite	Molecular formula	Mw	Organism or InChIKey etc.
C00000135	464-48-2	(-)-Camphor	C10H16O	152.12011513	Zingiber officinale ROSC.
C00000805	80-56-8	(+)-alpha-Pinene	C10H16	136.12520051	Zingiber officinale ROSC.
C00000816	127-91-3	beta-Pinene	C10H16	136.12520051	Zingiber officinale ROSC.
C00000861	586-62-9	alpha-Terpinolene	C10H16	136.12520051	Zingiber officinale ROSC.
C00003029	79-92-5	Camphene	C10H16	136.12520051	Zingiber officinale ROSC.
C00003035	141-27-5	trans-Citral	C10H16O	152.12011513	Zingiber officinale ROSC.
C00003111	469-61-4	alpha-Cedrene	C15H24	204.18780077	Zingiber officinale ROSC.
C00003130	502-61-4	alpha-Farnesene	C15H24	204.18780077	Zingiber officinale ROSC.
C00011720	23986-74-5	Germacrene D	C15H24	204.18780077	Zingiber officinale ROSC.
C00021859	22469-52-9	(+)-Cyclosativene	C15H24	204.18780077	Zingiber officinale ROSC.
C00030758	112-12-9	2-Undecanone	C11H22O	170.16706532	Zingiber officinale ROSC.
C00031258	3367-41-5	Sabinene	C10H16	136.12520051	Zingiber officinale ROSC.
C00031475	23513-08-8	(S)-8-Gingerol	C19H30O4	322.21440945	Zingiber officinale ROSC.
C00034994	36752-54-2	10-Shogaol	C21H32O3	332.23514489	Zingiber officinale ROSC.
C00034999	7785-70-8	1R,5R-(+)-alpha-Pinene	C10H16	136.12520051	Zingiber officinale ROSC.
C00035032	53172-04-6	[7]-Paradol	C18H28O3	292.20384476	Zingiber officinale ROSC.
C00035035	36700-45-5	[8]-Shogaol	C19H28O3	304.20384476	Zingiber officinale ROSC.
C00035036	53172-05-7	[9]-Paradol	C20H32O3	320.23514489	Zingiber officinale ROSC.
C00035042	598-07-2	alpha-Linalool	C10H18O	154.1357652	Zingiber officinale ROSC.
C00035574	532929-69-4	4-Gingesulfonic acid	C15H22O6S	330.11370917	Zingiber officinale ROSCOE
C00035519	145937-21-9	6-Gingesulfonic acid	C17H26O6S	358.14500929	Zingiber officinale ROSCOE
C00037817	532929-70-7	Shogasulfonic acid A	C21H26O8S	438.13483854	Zingiber officinale ROSCOE
C00037818	532929-71-8	Shogasulfonic acid B	C20H24O8S	424.11918847	Zingiber officinale ROSCOE
C00037819	532929-72-9	Shogasulfonic acid C	C19H22O8S	410.10353841	Zingiber officinale ROSCOE
C00037820	532929-73-0	Shogasulfonic acid D	C21H26O10S	470.12466778	Zingiber officinale ROSCOE

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Dan kita bisa melihat senyawa pada tanaman tersebut

2. Phytochem

Di gunakan untuk melihat senyawa yang ada di dalam tanaman tersebut, untuk melakukannya masuk ke webserver

<https://phytochem.nal.usda.gov/phytochem/search/list>. lalu klik pada enter dan masukan nama tanaman yang digunakan, dan kolom di sebelah masukan plant untuk tanaman

USDA Dr. Duke's Phytochemical and Ethnobotanical Databases
U.S. DEPARTMENT OF AGRICULTURE

Search Help About Contact Us Disclaimer

Dr. Duke's Phytochemical and Ethnobotanical databases facilitate in-depth plant, chemical, bioactivity, and ethnobotany searches using scientific or common names. Search results can be downloaded in PDF or spreadsheet form. Of interest to pharmaceutical, nutritional, and biomedical research, as well alternative therapies and herbal products.

Search for in

Hint: To browse or limit your search, select an entity type from the dropdown list next to the search box. [Help](#)

2,376 entities found (showing 1 - 20) - Click on an entity to view details

1 2 3 4 5 6 7 8 9 10 .. 119 Next

Key: **A** = Biological Activity **C** = Chemical **E** = Ethnobotany Plant **P** = Plant **S** = Syndrome **U** = Ethnobotany Use

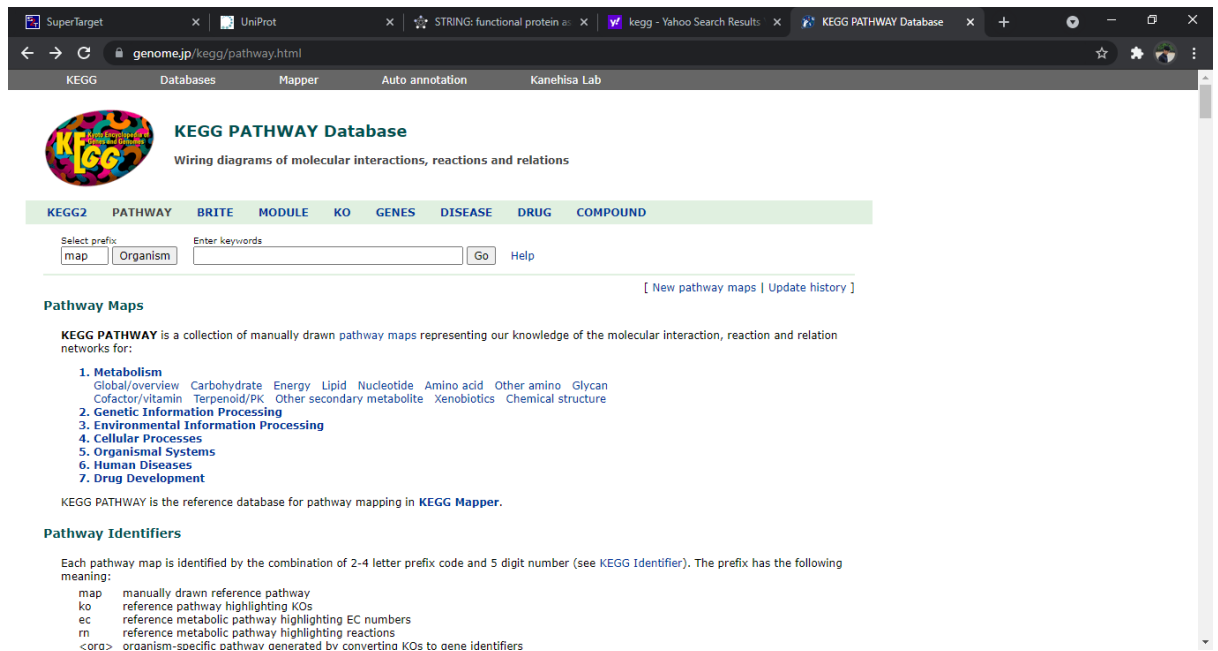
Dan setelah itu akan muncul seperti gambar di bawah ini

Show all rows. Click on column headings to sort table by that column

# Activity	Chemical	Part	All	Low PPM	High PPM	StdDev	Reference
0	(+)-6-GINGEROL	Root		--	--		*
0	(+)-ALPHA-CURCUMENE	Essential Oil		--	--		*
0	(+)-ANGELICOIDENOL	Rhizome		--	14.0		*
0	(+)-BETA-PHELLANDRENE	Essential Oil		--	--		*
0	(+)-BORNEOL	Rhizome Essent. Oil		--	--		*
0	1,5-EPOXY-3-EPIHYDROXY-1-(3,4-DIHYDROXY-5-METHOXY-PHENYL)-7-(4-HYDROXY-3-METHOXY-PHENYL)-HEPTANE	Rhizome		--	--		*
0	1,5-EPOXY-3-HYDROXY-1-(3,4-DIHYDROXY-5-METHOXY-PHENYL)-7-(4-HYDROXY-3-METHOXY-PHENYL)-HEPTANE	Rhizome		--	--		*
0	1,5-EPOXY-3-HYDROXY-1-(4-HYDROXY-3,5-DIMETHOXY-PHENYL)-7-(4-HYDROXY-3-METHOXY-PHENYL)-HEPTANE	Rhizome		--	--		*
67	1,8-CINEOLE	Rhizome Essent. Oil		26000.0	100000.0		*

3. Kegg

Dilakukan untuk menentukan pathway yg digunakan, untuk melakukan dengan webserver setelah itu <https://www.genome.jp/kegg/pathway.html> lalu akan muncul seperti gambar di bawah ini



The screenshot shows the KEGG PATHWAY Database homepage. At the top, there is a navigation bar with tabs for KEGG, Databases, Mapper, Auto annotation, and Kanehisa Lab. Below this is the KEGG logo and the text 'KEGG PATHWAY Database' and 'Wiring diagrams of molecular interactions, reactions and relations'. A search bar is present with a 'Select prefix' dropdown set to 'map' and an 'Organism' dropdown. Below the search bar, there is a list of 'Pathway Maps' categories: 1. Metabolism (with sub-categories like Global/overview, Carbohydrate, Energy, Lipid, Nucleotide, Amino acid, Other amino, Glycan, Cofactor/vitamin, Terpenoid/PK, Other secondary metabolite, Xenobiotics, Chemical structure), 2. Genetic Information Processing, 3. Environmental Information Processing, 4. Cellular Processes, 5. Organismal Systems, 6. Human Diseases, and 7. Drug Development. A 'Pathway Identifiers' section explains the 2-4 letter prefix code and 5 digit number used for identification.

Pada enter keywords masukan nama penyakit yang kita akan gunakan dan klik tombol go

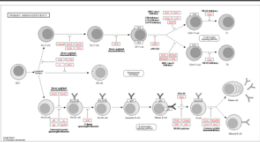
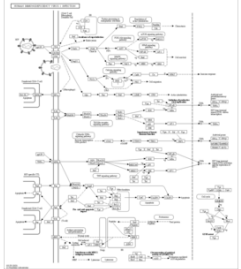
SuperTarget x UniProt x STRING: functional protein a... x kegg - Yahoo Search Results x Pathway Search Result x

kegg.jp/kegg-bin/search_pathway_text?map=map&keyword=immuno&mode=1&viewImage=true

Pathway Text Search

Number of entries in a page

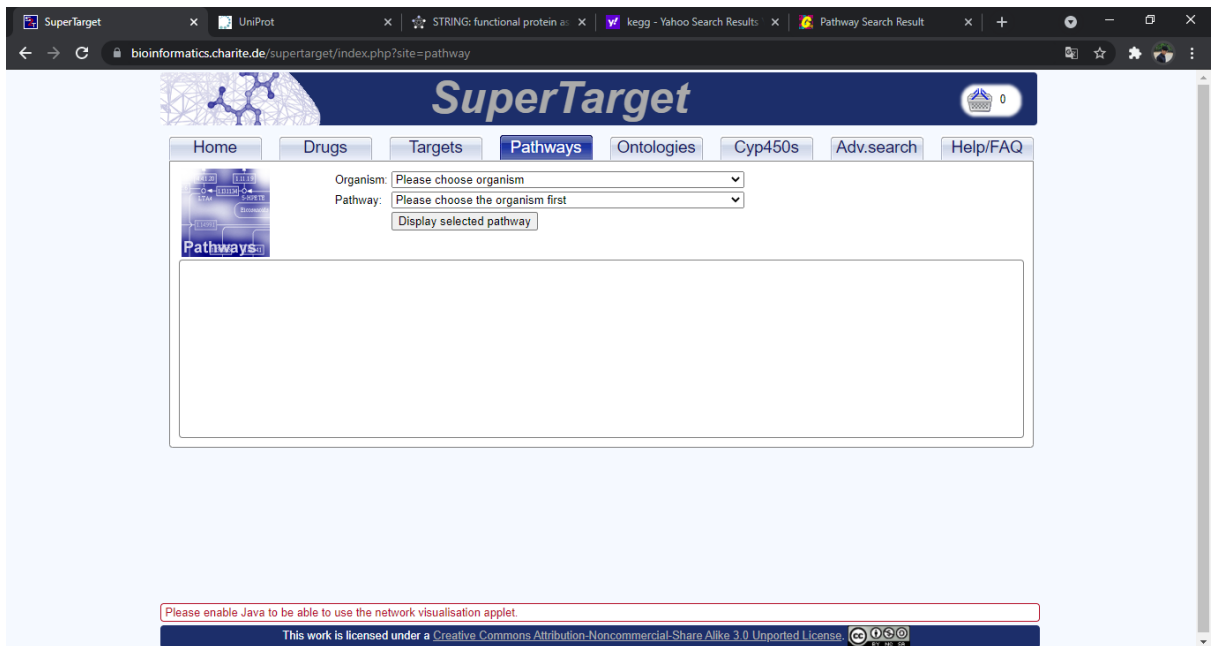
Page: of 2 Items: 1 - 20 of 32

Entry	Thumbnail Image	Name	Description	Object	Legend
map05340		Primary immunodeficiency	Primary immunodeficiencies (PIs) are a heterogeneous group of disorders, which affect cellular and h...	...I receptor signaling pathway map05340: Primary immunodeficiency	...age B cell receptor signaling pathway PRIMARY IMMUNODEFICIENCY B cell TAP1 CD4+ T cell CD8+ T cell ...
map05170		Human immunodeficiency virus 1 infection	Human immunodeficiency virus type 1 (HIV-1), the causative agent of AIDS (acquired immunodeficiency...	... K02580 (NFKB1), K04735 (RELA) map05170: Human immunodeficiency virus 1 infection map04064: NF-kappa...	PIP 56K1/2 mTOR AKT PI3K HUMAN IMMUNODEFICIENCY VIRUS 1 INFECTION NF kB NFkB signaling pathway...

Hasil akan menunjukan pathway yang akan kita gunakan

4. SuperTarget

Dilakukan dengan membuka SuperTarget untuk mengetahui target yang kita gunakan



Dimasukkan pada organism yaitu homo sapiens dan pada pathway di masukan yang kita cari di kegg

05340 8/9/19
(c) Kanehisa Laboratories

Target	Drug	Interaction
Adenosine deaminase	1gx1	show
Adenosine deaminase	1um1	show
Adenosine deaminase	ACT1MHQ05	show
Adenosine deaminase	AIDS210536	show
Adenosine deaminase	AIDS210539	show
Adenosine deaminase	Antistenocardin	show
Adenosine deaminase	Arabinosyladenine	show
Adenosine deaminase	CHEBI:141697	show
Adenosine deaminase	CHEBI:256468	show

Dan akan mendapatkan hasil di mana di sebelah kiri ada nama protein target yang akan kita pakai

5. Uniport

Dilakukan untuk mengetahui nama protein target secara global dan di gunakan di webserver <https://www.uniprot.org/>

The mission of UniProt is to provide the scientific community with a comprehensive, high-quality and freely accessible resource of protein sequence and functional information.

UniProtKB
UniProt Knowledgebase
Swiss-Prot (565,254)
Manually annotated and reviewed.
Records with information extracted from literature and curator-evaluated computational analysis.
TrEMBL (219,174,961)
Automatically annotated and not reviewed.
Records that await full manual annotation.

UniRef
Sequence clusters

UniParc
Sequence archive

Proteomes
Proteome sets

Supporting data
Literature citations
Taxonomy
Subcellular locations
Cross-ref. databases
Diseases
Keywords

News
Forthcoming changes
There are currently no changes planned.
UniProt release 2021_03
The importance of being disordered | MobiDB-lite predictions for intrinsically disordered regions | UniProtKB via AWS Open Data and Amazo...
UniProt release 2021_02
With a little help from my friend | SwissBioPics subcellular location visualization | Change of evidence codes for combinatorial evidence
News archive

Pada bagian kolom kosong di isi nama protein yang akan kita gunakan

UniProtKB 2021_03 results

UniProtKB consists of two sections:
Reviewed (Swiss-Prot) - Manually annotated
 Records with information extracted from literature and curator-evaluated computational analysis.
Unreviewed (TrEMBL) - Computationally analyzed
 Records that await full manual annotation.

Filter by: Reviewed (24) Swiss-Prot, Unreviewed (551) TrEMBL

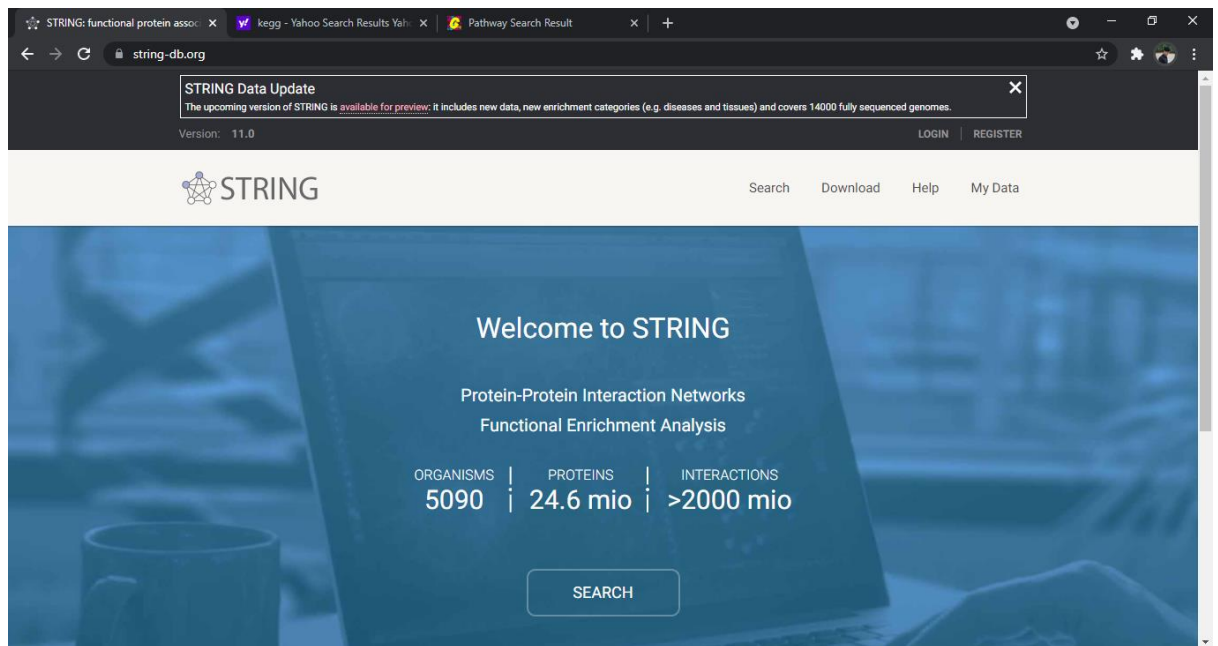
Popular organisms: Human (10), Bovine (6), Mouse (6)

Entry	Entry name	Protein names	Gene names	Organism	Length
P29965	CD40L_HUMAN	CD40 ligand	CD40LG CD40L, TNFSF5, TRAP	Homo sapiens (Human)	261
Q9Z2V2	CD40L_RAT	CD40 ligand	Cd40lg Cd40l, Tnfsf5	Rattus norvegicus (Rat)	260
P27548	CD40L_MOUSE	CD40 ligand	Cd40lg Cd40l, Tnfsf5	Mus musculus (Mouse)	260
O97626	CD40L_CANLF	CD40 ligand	CD40LG CD40L, TNFSF5	Canis lupus familiaris (Dog) (Canis familiaris)	260
O97605	CD40L_FELICA	CD40 ligand	CD40LG CD40L, TNFSF5	Felis catus (Cat) (Felis silvestris catus)	260

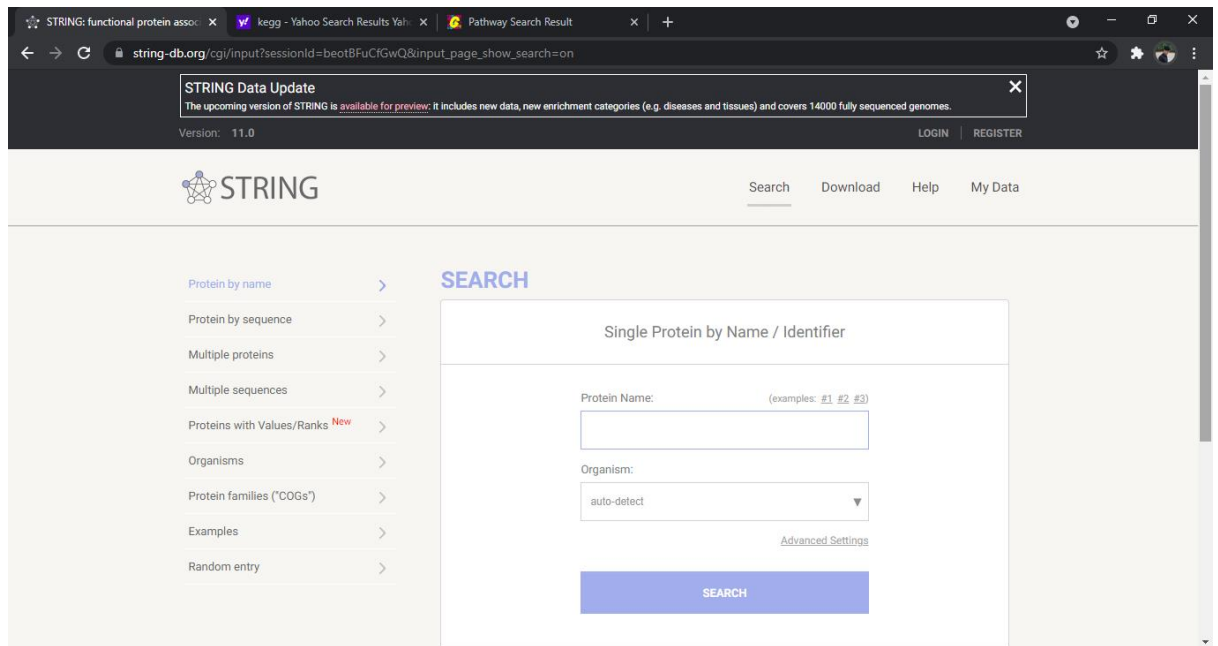
Akan mendapatkan hasil seperti ini yang kita ambil pada bagian organism homo sapiens dan di copy entry untuk dimasukkan ke dalam string

6. String

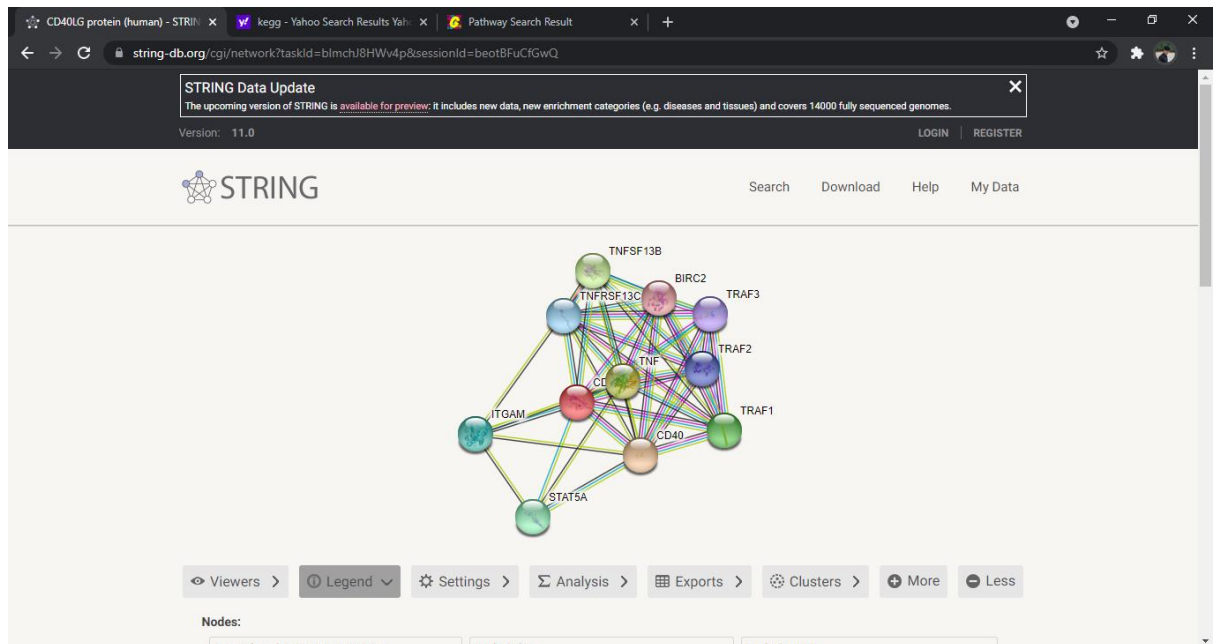
String dilakukan untuk melihat antara ikatan protein dengan protein yang digunakan dan dilakukan dengan *web server* <https://string-db.org/>



Klik pada search



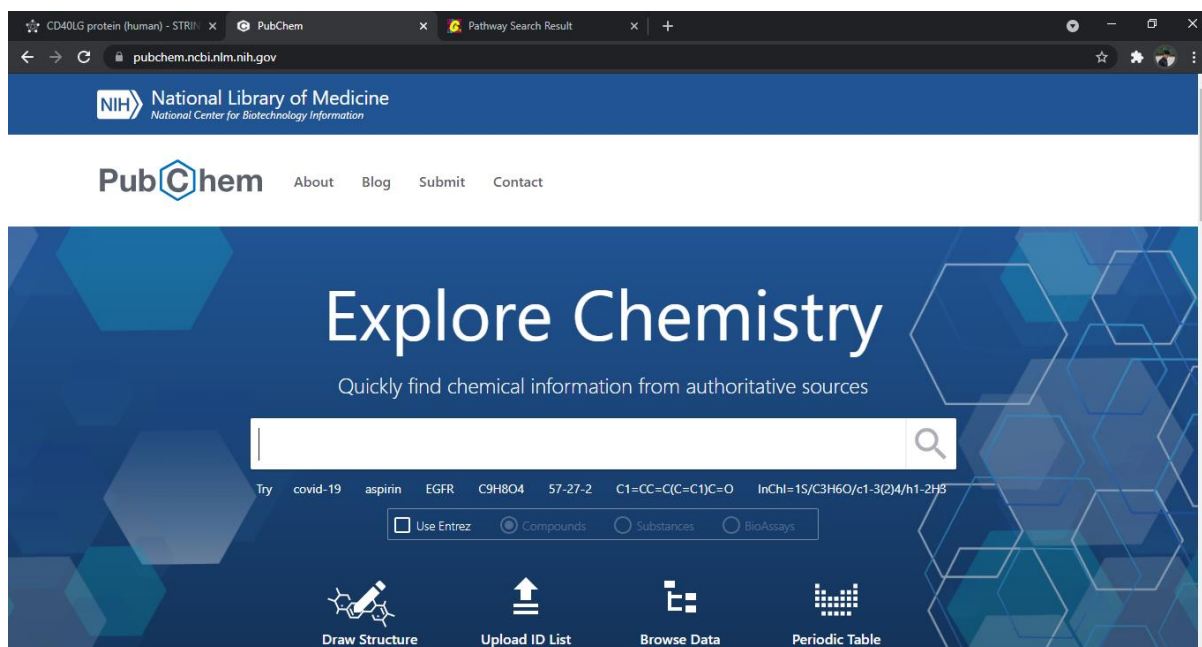
Dan di masukan nama protein target yang di gunakan atau nomor entry yang ada di uniport dan organism pilih homo sapiens



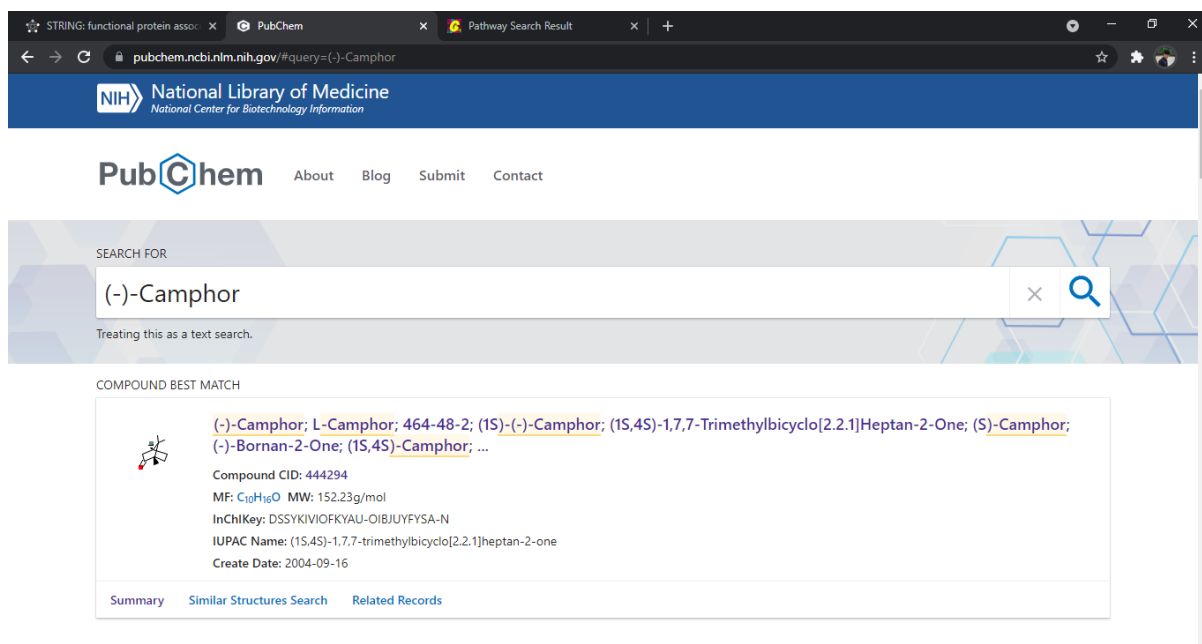
Akan muncul hasil seperti ini dan diamati protein yang berikatan

7. Pubchem

Digunakan untuk mengeliminasi senyawa yang mempunyai target dan di lakukan dengan webserver <https://pubchem.ncbi.nlm.nih.gov/>



Pada kolom tersebut diisi dengan senyawa yang kita dapat tadi menggunakan knapsack



Dan setelah dimasukkan namanya akan muncul seperti ini dan di klik salah satu

PubChem (-)-Camphor (Compound)

15 Biological Test Results

15.1 BioAssay Results

624 items View More Rows & Details

SORT BY Activity Value

Activity	Activity Value, μM	Activity Type	Target Name	BioAssay Name	BioAssay AID	Substances
Inactive	19.3312	Potency	AR - androgen receptor (human)	qHTS assay to identify small molecule antagonists of the androgen receptor (AR) signaling pathway using the MDA cell line in the presence of 0.5 nM R1881	1259243	251919
Active	19.4938	Potency	JUN - Jun proto-oncogene, AP-1 transcription factor subunit (human)	qHTS assay to identify small molecule agonists of the AP-1 signaling pathway	1159526	251919

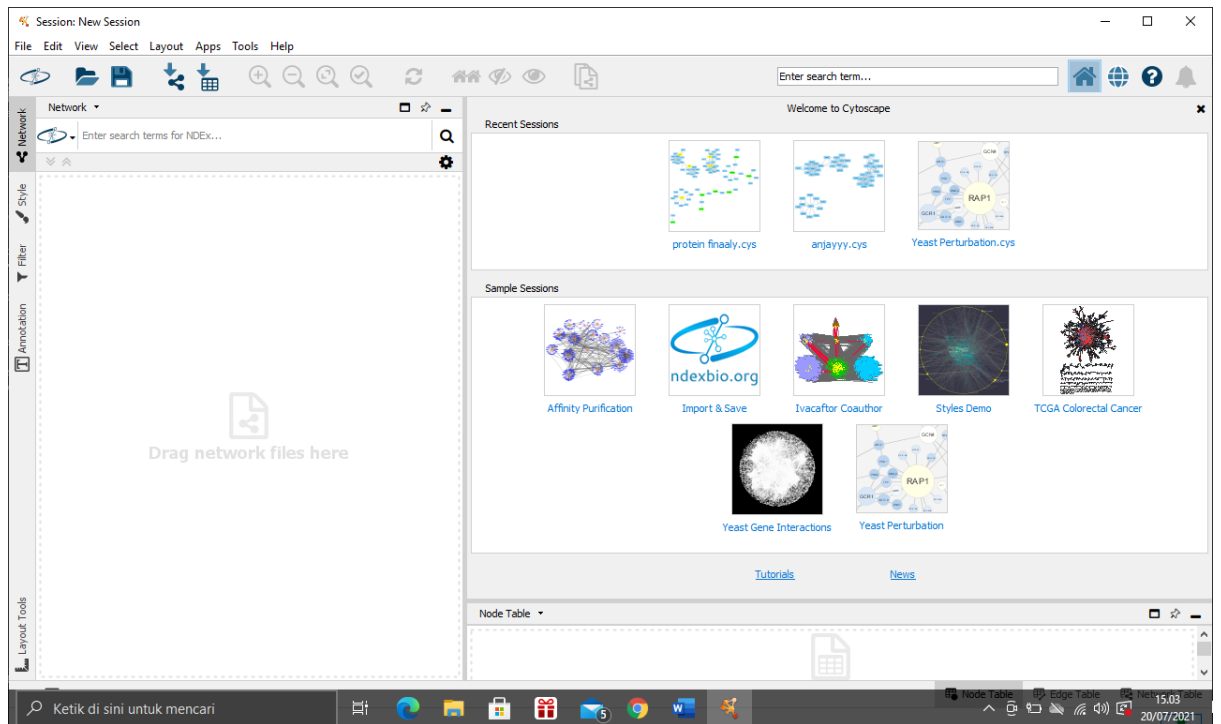
CONTENTS

- 6 Chemical Vendors
- 7 Drug and Medication Information
- 8 Pharmacology and Biochemistry
- 9 Use and Manufacturing
- 10 Safety and Hazards
- 11 Toxicity
- 12 Literature
- 13 Patents
- 14 Biomolecular Interactions and Pathways
- 15 Biological Test Results
- 16 Classification
- 17 Information Sources

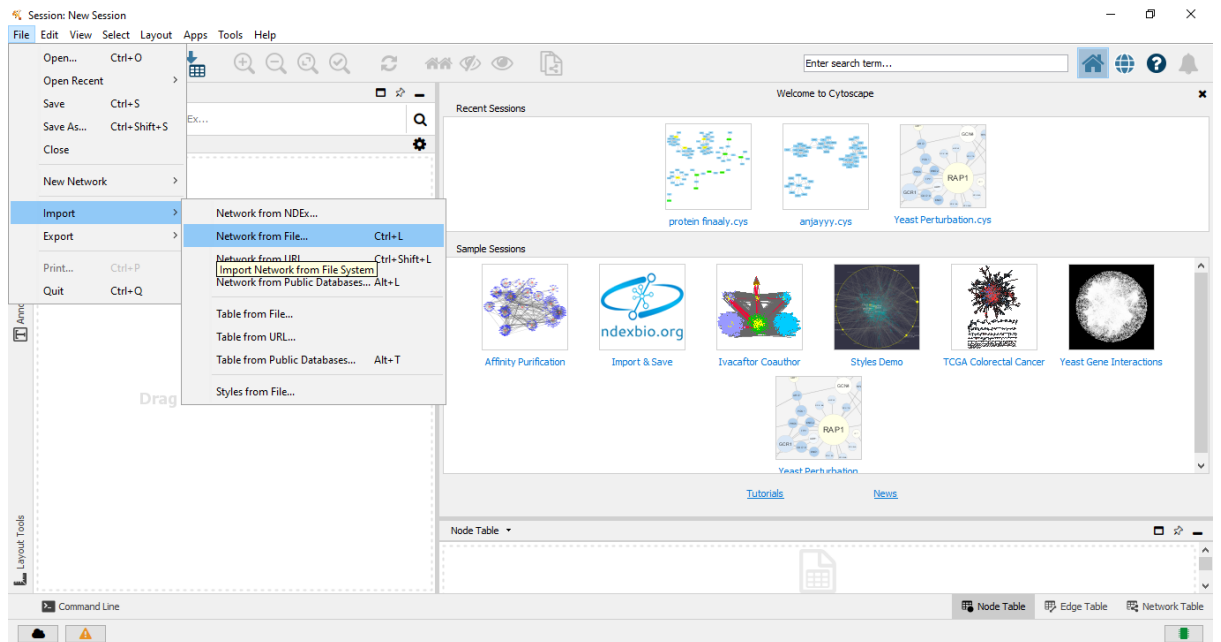
Kemudian di klink biological test result dan di download dalam format excel akan terlihat apakah ada target dalam senyawa tersebut

8. Cytoscape

Dilakukan dengan aplikasi digunakan sebagai untuk membentuk network pharmacology



Lalu pilih file



Setelah itu klik import dan klik network from file lalu pilih file dan open