LAMPIRAN

1. Knapsack

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

😚 www.knapsackfamily.c 🗙 💿 KNApSAcK Core Syste: 🗙 😾 phytoceam - Yahoo Se 🗙 😾 kegg - Yahoo Search R 🗙 📑 Un	iProt X 🟚 STRING: functional pro X + 💿 🚽 🗗 X
← → C ▲ Not secure knapsackfamily.com/knapsack_core/top.php	🖈 🖈 🏀 🗄
KNApSAcK Core System	
Link to Top page: http://www.knapsackfamily.com/knapsack_core/top.php	
Incorporation to program: http://www.lampackfmmly.com/mapsack_core/info.php?imanne=[item]&vood=[keyword] Here, [item] must be safected from one of the following words; "organism", "metabolite", "formula", "C_ID", and "CAS_ID".	
< Example 1 > Information on the metaboline amigned to C00000001 (a C_ID) can be retrieved by http://www.tangaackfamily.com/kangaack_core info.php/name=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?sname=organism&word=bacillus</example>	
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 (akanaya[arlgtc.naintjp).	
Instruction Manual/Japanese) 22 Instruction Manual(English)	
Select by	
● ALL Types ○ Organism ○ Metabolite ○ Molecular formula ○ C_ID ○ CAS_ID ○ INCHI-KEY ○ INCHI-CODE ○ SMILES	
Zingiber Officinale Rosc	
last update 2021/07/09	
metabolite 57,919 entries	•

Setelah itu klik list dan akan muncul seperti gambar di bawah

www.knapsackfar	× S KNApSAcK Co	re 🗄 🗙 🕥 KNApSAcK Metal: 🗙 😾 phyto	ceam - Yah 🗙 📔 💅 kegg - Yahoo S	šea × ∣ <u>Ω</u> UniProt	× 🌸 STRING: function × +	•			, ,
→ C 🔻	Not secure knapsac	kfamily.com/knapsack_core/result.php?snar	ne=all&word=Zingiber%20Officir	nale%20Rosc			☆	*	۲
RAND									
nnut type = all	nout word = Zingiber O	fficinale Posc							
input type – all , i	nput word – Zingiber O	ilicinale Rosc							
Number of match	ed data :25								
		Metabolite	Molecular formula	Mw	Organism or InChlKey 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	3387-41-5	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.				
C00036574	532929-69-4	4-Gingesulfonic acid	C15H22O6S	330.11370917	Zingiber officinale ROSCOE				
C00036619	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 gunkan 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



Dan setelah itu akan muncul seperti gambar di bawah ini

sackfan 🗙 🛛 🕄	KNApSAcK Core 🗄 🗙 📔 🌍 KNApSAcK Metal: 🗙 📔 💅	kegg - Yahoo Sea 🗙 🛛 🛄 UniProt	× 🔤 🍲 STRI	NG: function: 🗙 🛛 🎬 Dr.	Duke's Phytoc × +	o		Ø	×
n phytoche	m.nal.usda.gov/phytochem/plants/show/2129?et=l					\$) *	۲	
	Show all ro	ws. Click on column headings	to sort table by th	at column					-
# Activity	Chemical	Part All	Low PPM	High PPM Std	IDev [*] 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			*				ł
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	*				
¥ 67									*

3. Kegg

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

	🔒 Su	perTarget	t	× 🛄 ι	UniProt		× 🌸	STRING: funct	tional protein a	as 🗙 📔 📝 kegg - Yahoo Search Results 🔪	× 👔 KEGG PA	THWAY Database	× H	F	0	-	٥	×
÷	>	G	🔒 geno	m e.jp /kegg/pat	thway.html											☆ :	* 🏀	
		KEGG	(Databases	Mapper		Auto ann	notation	Kaneh	iisa Lab								<u>^</u>
		KC		KEGG P/ Wiring diag	ATHWAY	Datab ular inte	ase eractions,	, reactions a	nd relation	ıs								l
	K	GG2	PATHWA	Y BRITE	MODULE	ко	GENES	DISEASE	DRUG	COMPOUND								
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										[New pathway maps (pdate history]							
	Pa	thway	/ Maps															
		KEGG F	PATHWAY i ks for:	s a collection o	f manually draw	n pathwa	ay maps re	epresenting o	ur knowledg	e of the molecular interaction, reaction	and relation							
		1. M G 2. G 3. E 4. C 5. O 6. H 7. D	letabolism ilobal/overvi ofactor/vita cenetic Info nvironmen cellular Pro organismal luman Dise orug Develo	iew Carbohydr min Terpenoid ormation Proc tal Informatio cesses Systems ases opment	rate Energy L i/PK Other sec cessing on Processing	ipid Nuo ondary m	cleotide /	Amino acid C Xenobiotics	Other amino Chemical s	Glycan tructure								
		KEGG P	ATHWAY is	the reference d	atabase for path	hway maj	pping in K	EGG Mapper										
	Pa	thway	/ Identifie	ers														
		Each pa meanin	athway map g:	is identified by	the combinatio	n of 2-4	letter prefi	ix code and 5	digit numbe	er (see KEGG Identifier). The prefix has	the following							
		map ko	manual referen	ly drawn refere ce pathway higi	nce pathway hlighting KOs													
		ec rn	referen	ce metabolic pa ce metabolic pa	athway highlight athway highlight	ing EC nu ing react	umbers ions											
		<000	o> ordanis	m-specific path	way generated	bv conve	rtina KOs I	to aene identi	ifiers									Ŧ

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

tombol go

🚼 SuperTarg	get 🗙 🛛 📑 UniProt 🗙 🛛 🤹 STRIM	IG: functional protein as $$ × $$	💅 kegg - Yahoo Search Results 🐂 🗙	🔀 Pathway Search Result 🛛 🗙	+ • - •	×
\leftrightarrow \Rightarrow C	kegg.jp /kegg-bin/search_pathway_text?map=map&keyword	l=immuno&mode=1&vie	wlmage=true		🖈 🔹 😽	:
Path Number of e Page : 1	nway Text Search entries in a page 20 V Hide thumbnail Go of 2 Items : 1 - 20 of 32 Top Previous New	t				•
Entry	Thumbnail Image	Name	Description	Object	Legend	
map05340		Primary immunodeficiency	Primary immunodeficiencies (PIs) are a heterogeneous group of disorders, which affect cellular and h	l 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 immunodeficency virus 1 infection map04064: NF-kappa	PIP S6K1/2 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

🚼 SuperTarget	× 🔝 UniProt	🗴 🏽 🏚 STRING: functional protein as 🗴 🖌 🌠 kegg - Yahoo Search Results 🗙 🛛 🦉 Pathway Search Result 💿 🗙 🗍 🕇	• - • ×
\leftrightarrow \Rightarrow G	bioinformatics.charite.de/supertarge	t/index.php?site=pathway	🔤 🖈 🌲 😽 E
	44	SuperTarget 🌰 🌰	Î
	Home Dru	gs Targets Pathways Ontologies Cyp450s Adv.search Help/FAQ	
		Organism Please choose organism Pathway: Please choose the organism first Display selected pathway	
	Diogeo ongbio, java to bo obio t	ues the natural viewleation and at	
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	This wor	The second of th	•

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



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/

🛄 UniProt		🔅 STRING: functional protein ass	soci 🗙 📔 💆 kegg - Yahoo Search Res	sults Yaha 🗙 📔 🔀 Pathway Search Result	× +	• - • ×
\leftrightarrow \rightarrow C \square uniprot.org						🖈 🌲 🏀 E
UniProt	X	UniProtKB -			4. 1.1887	Advanced - Q Search
BLAST Align Retrieve/ID n	mapp	ng Peptide search SPARQL		A PL-		Help Contact
The mission of UniProt is to pr	ovide	the scientific community with	a comprehensive, high-quality	and freely accessible resource of prot	ein sequence and functional inf	ormation.
UniProtKB UniProt Knowledgebase		UniRef	UniParc	Proteomes	New U CoV-2 receptr genera	niProt portal for the latest SARS- coronavirus protein entries and ors, updated independent of the Il UniProt release cycle.
Swiss-Prot (565,254) Manually annotated and reviewed.		Sequence clusters	Sequence archive	Proteome sets	View Recep	SARS-CoV-2 Proteins and otors
Records with information extracted from literature and curator-evaluated					News Forthcoming changes There are currently no cha	nges planned
TrEMBL (219,174,961)			Supporting data		UniProt release 2021_03 The importance of being di predictions for intrinsically	isordered MobiDB-lite disordered regions
Automatically annotated and not reviewed.		Literature citations	Taxonomy	Subcellular locations	UniProtKB via AWS Open D	Data and Amazo
Records that await full manual annotation.		Cross-ref. databases জু ম দ ক্ট্র	Diseases XXX	Keywords	With a little help from my f subcellular location visualiz codes for combinatorial evi	friend SwissBioPics zation Change of evidence idence •
https://www.uniprot.org/keywords					Rews archive	

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

cd40ligand in UniProtKB	× 🔅 STRING: fun	ctional protein associ $ imes $	<mark> 111</mark> kegg	g - Yahoo Search Results Y	'ah 🗙 📔 🔀 Pathway Search Res	sult × +	• - •	ı ×
\leftrightarrow \rightarrow C \square uniprot.org/		0ligand&sort=score					\$	٠
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UniProtKB 2	021_03	results					Help Col	ket 👻
Reviewed (Swiss-Pn Records with information ep analysis. Unreviewed (TrEMBI Records that await full man	tracted from literation L) - Computationa L) annotation.	notated ure and curator~evalua Ily analyzed	ted com	putational	The UniProt Knowledgebas information on proteins, wi the core data mandatory for name or description, taxon information as possible is a reg Help	e (UniProtKB) is the central hub for the collection th accurate, consistent and rich annotation. In ad or each UniProtKB entry (mainly, the amino acid s omic data and citation information), as much ann dded. IniProtKB help video Other tutorials and vide	of functional dition to capturin equence, protein otation os 土 Download	g ds
Filter by ⁱ	SBLAST ≡ Alig	n 🛨 Download 🟦 Ad	d to bask	et 🖉 Columns	>	1 to 25 of 3	575 🕨 Show 2	<u>'</u> 5 ¥
Reviewed (24)	Entry 🖨	Entry name 🖨		Protein names 🖨	Gene names 🖨	Organism 🖨	Length 🖨	Z
Unreviewed (551)	P29965	CD40L_HUMAN	<u>.</u>	CD40 ligand	CD40LG CD40L, TNFSF5, TRAP	Homo sapiens (Human)	261	
Popular organisms	Q9Z2V2	CD40L_RAT		CD40 ligand	Cd40lg Cd40l, Tnfsf5	Rattus norvegicus (Rat)	260	
Human (10)	P27548	CD40L_MOUSE		CD40 ligand	Cd40lg Cd40l, Tnfsf5	Mus musculus (Mouse)	260	
Bovine (6)	097626	CD40L_CANLF		CD40 ligand	CD40LG CD40L, TNFSF5	Canis lupus familiaris (Dog) (Canis familiaris)	260	
Mouse (6)	□ 007605	CD40L FELCA		CD40 ligand	CD40LC CD40L TNESES	Falie catue (Cat) (Falie eilveetrie catue)	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

STRING Data Update The upcoming version of STRING is available	able for previo	t includes new data, new enrichment categories (e.g. diseases and t	tissues) and covers 14000 fully sequen	ced genomes.	×		
Version: 11.0				LOGIN	REGISTER		
STRING			Search Download	Help	My Data		
Protein by name	>	SEARCH					
Protein by sequence	>	Single Protein by	Name / Identifier				
Multiple proteins	>						
Multiple sequences	>	Protein Name:	(examples: #1 #2 #3)				
Proteins with Values/Ranks New	>						
Organisms	>	Organism:					
Protein families ("COGs")	>	auto-detect	v				
Examples	>		Advanced Settings				
Random entry	>						

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

C is string-db.org/cgi/network?taskld=blmch/8HWv4p8xsessionId=beot8FuCfGwQ STRING Data Update Image: Comparison of STRING is available for preview: It includes new data, new enrichment categories (e.g. diseases and tissue) and covers 14000 fully sequenced genomes.) :
STRING Data Update X The upcoming version of STRING is <u>available for proview</u> : it includes new data, new enrichment categories (e.g. diseases and tissues) and covers 14000 fully sequenced genomes.	^
Version: 11.0 LOGIN REGISTER	
STRING Search Download Help My Data	
THEREFISE THAF3 TRAF3 TRAF1	
♦ Viewers > ① Legend ∨ ☆ Settings > ∑ Analysis > ⊞ Exports > ④ Clusters > ④ More ● Less ↓	
Nodes:	

Akan muncul hasil seperti ini dan diamati protein yang berikatan

7. Pubchem

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



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

🔅 STRING: functional protein asso × 📀 PubChem	X 🦉 Pathway Search Result X +	• - • ×
← → C ■ pubchem.ncbi.nlm.nih.gov/#query=(-)-Camphor		🖈 🖨 😽 E
NIH National Library of Medicine National Center for Biotechnology Information		
	Submit Contact	
SEARCH FOR		
(-)-Camphor		×Q
Treating this as a text search.		
COMPOUND BEST MATCH		
(-)-Camphor; L-Camphor; (-)-Bornan-2-One; (15,45)- Compound CID: 444294 MF: C10H160 MW: 152.23g/mol InChIKey: DSSYKIVIOFK/AU-OIBJU' IUPAC Name: (15.45)-1.7.7-trimethy Create Date: 2004-09-16	464-48-2; (1S <mark>)-(-)-Camphor</mark> ; (1S,4S)-1,7,7-Trimethylbicyclo[2.2.1]Heptan-2-One; (Camphor; (FYSA-N /bicyclo[2.2.1]heptan-2-one	S <mark>)-Camphor</mark> ;
Summary Similar Structures Search Related R	ecords	

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

☆ STRING: fu ← → C	Inctional protein assoc	× G (-)-Camphor	C10H16O - PubCh ×	Pathway Sear Biological-Test-R	ch Result X	+					0 	- c	7 🙊	×		
	PubCh	em (-)-Cam	nphor (Comp	ound)							\uparrow			^		
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	Activity (?) Activity Value, µM Activity Type (?		_	SORT BY	Activity Value		~		6 Chemical Vendors	. I 6						
			Activity Type	Target Name	Rio Assau Namo	Rio Assau AID	Substa		8 Pharmacology and B	iochemistry	~					
	Activity	Activity value, pivi	curry value, pin Activity Type 🕞		BIOASSay Name	bioAssay Hame bioAssay Alb St			9 Use and Manufactur	ing	~					
					qHTS assay to identify small				10 Safety and Hazards		~					
					molecule antagonists of							11 Toxicity		~		
	Incetting	10 2212	Determine	AR - androgen	the androgen receptor (AR)	1250242	251010		12 Literature		~					
	Inactive	19.3312	Potency	receptor signaling 1259243 251919 (human) pathway using 13 Pa	signaling 1259245 251919 pathway using		251919		1259243 251919		13 Patents		~			1
					the MDA cell line in the presence of 0.5				14 Biomolecular Interactions and v Pathways		~					
					nM R1881				15 Biological Test Resu	lts	~					
				JUN - Jun proto-	gHTS assay to				16 Classification		~					
		40,4020		oncogene, AP-1	identify small molecule	4450500	254040		17 Information Source	5						
https://pubchem.r	Active ncbi.nlm.nih.gov/comp	19.4938 ound/444294#section=Bio	Potency logical-Test-Results	transcription factor subunit (human)	agonists of the AP-1 signaling pathway	1159526	251919							•		

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

% Se	sion: New Se	ssion Select Lavout	Anns	s Tools Help								-	٥	×
THE	Open Ctrl+O Open Recent				2 4	* • •		Enter search term				- 🔺	• •	
	Save Ctrl+S Save As Ctrl+Shift+S Close New Network		Ex		□ ☆ _ Q \$	Recent Sessions	Welcome to Cytoscape							×
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T Anno	Print Quit	Ctrl+P Ctrl+Q		Network from File Network from File Syst Network from File Table from File Table from RLL Table from RLL Styles from File	Alt+T		ndexbio.org	Ivacaftor C	author Styl	yes Demo	TCGA Colorectal Cancer	Yeast Gene Inte	teractions	~
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Setelah Itu klik import dan klik network from file lalu pilih file dan open