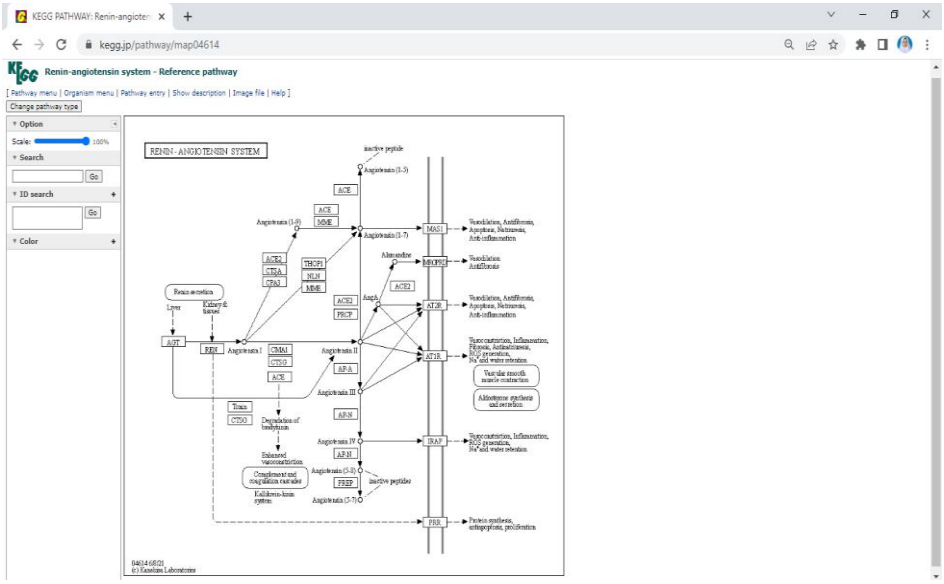
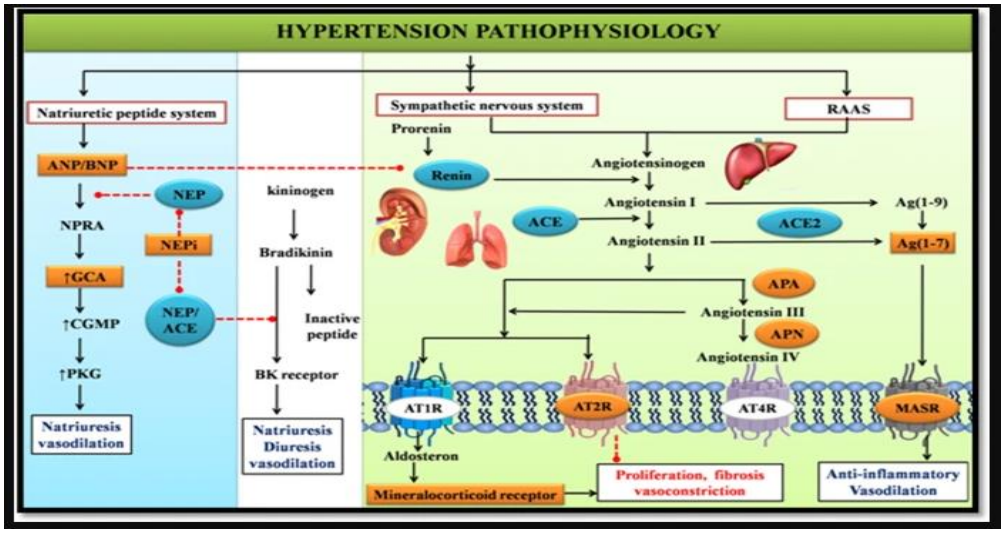
LAMPIRAN

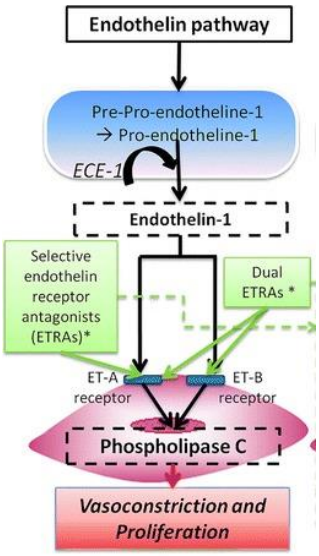
Lampiran 1. Identifikasi protein target



Sistem renin angiotensin-aldosteron

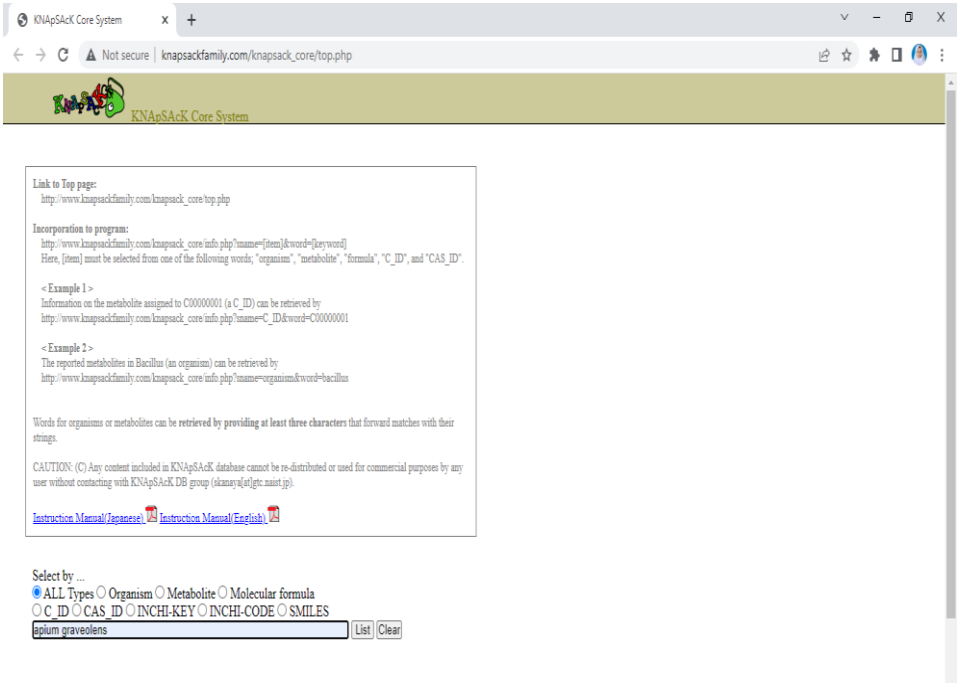


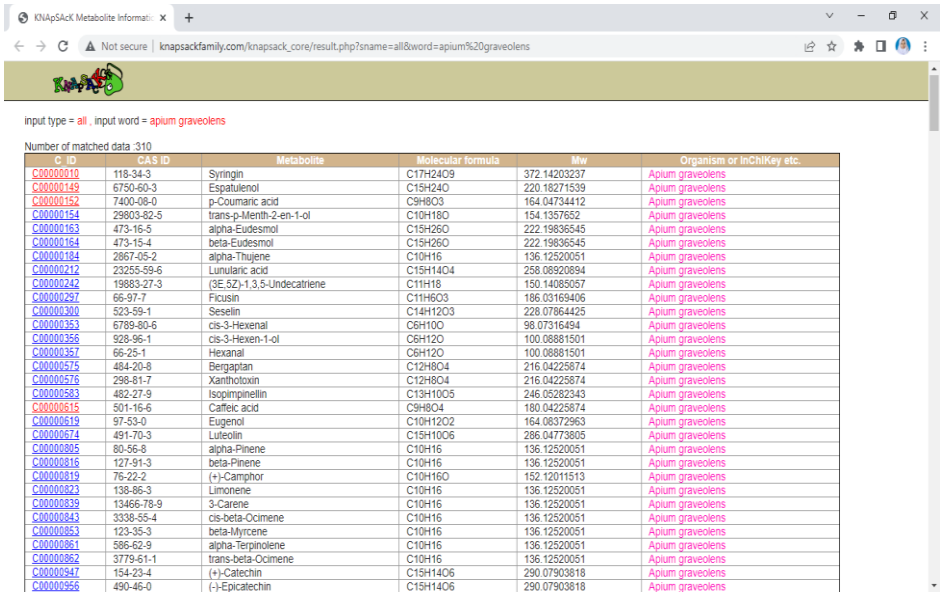
Patofisiologi hipertensi



Endothelin pathway in hypertension

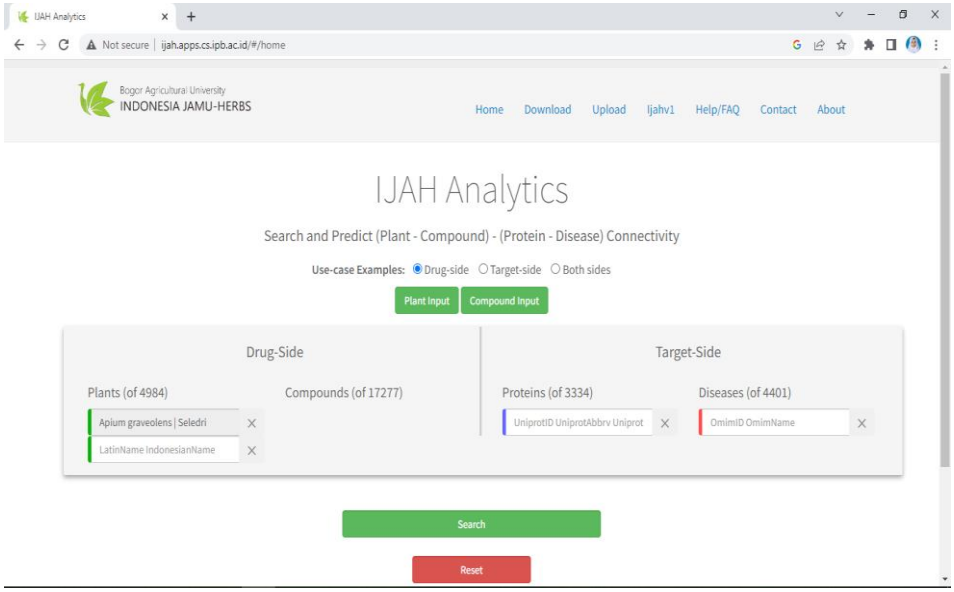
Lampiran 2. Kandungan senyawa kimia dari KNApSAcK

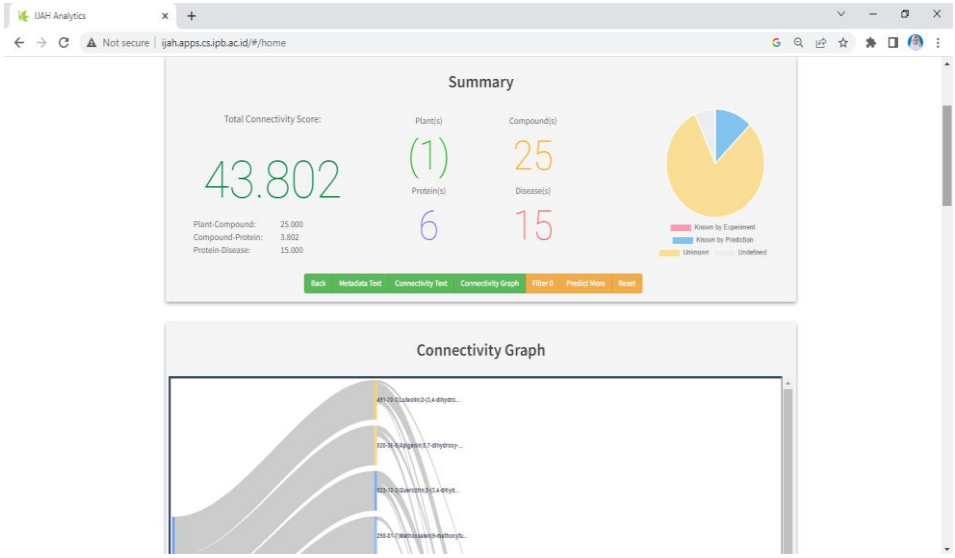




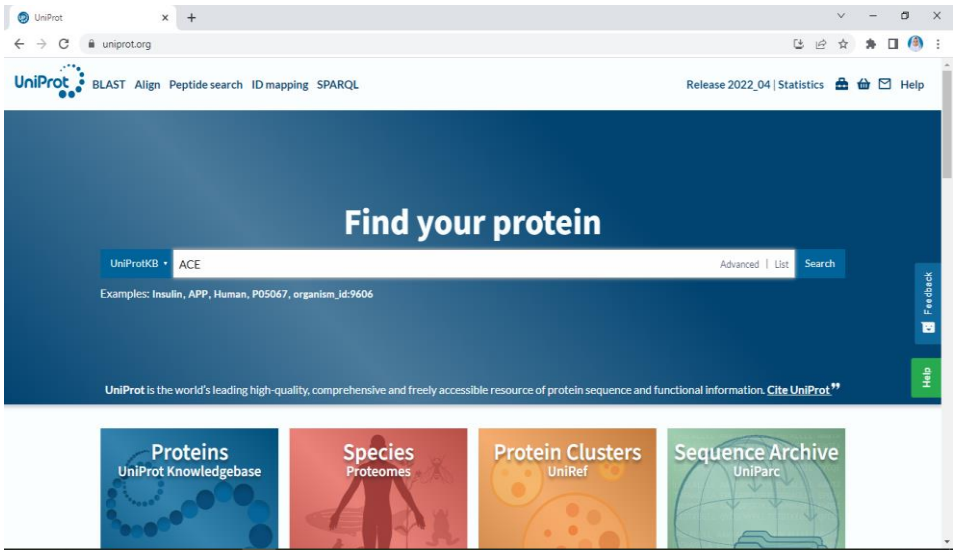
c# ↓	cr_LS ID	Metabolite	Molecular formula	Mw	Organism or InChIKey etc.
C00000010	118-34-3	Syringin	C17H24O9	372.14203237	Apium graveolens
C00000149	6750-60-3	Espatulenol	C15H24O	220.18271539	Apium graveolens
C00000152	7400-08-0	p-Coumaric acid	C9H8O3	164.04734412	Apium graveolens
C00000154	29803-82-5	trans-p-Menth-2-en-1-ol	C10H18O	154.1357652	Apium graveolens
C00000163	473-16-5	alpha-Eudesmol	C15H26O	222.19836545	Apium graveolens
C00000164	473-15-4	beta-Eudesmol	C15H26O	222.19836545	Apium graveolens
C00000184	2867-05-2	alpha-Thujene	C10H16	136.12520051	Apium graveolens
C00000212	23255-59-6	Lunularic acid	C15H14O4	258.08920894	Apium graveolens
C00000242	19883-27-3	(3E,5Z)-1,3,5-Undecatriene	C11H18	150.14085057	Apium graveolens
C00000297	66-97-7	Ficusin	C11H6O3	186.03169406	Apium graveolens
C00000300	523-59-1	Seselin	C14H12O3	228.07864425	Apium graveolens
C00000353	6789-80-6	cis-3-Hexenal	C6H10O	98.07316494	Apium graveolens
C00000356	928-96-1	cis-3-Hexen-1-ol	C6H12O	100.08881501	Apium graveolens
C00000357	66-25-1	Hexanal	C6H12O	100.08881501	Apium graveolens
C00000575	484-20-8	Bergaptan	C12H8O4	216.04225874	Apium graveolens
C00000576	298-81-7	Xanthotoxin	C12H8O4	216.04225874	Apium graveolens
C00000583	482-27-9	Isopimpinellin	C13H10O5	246.05282343	Apium graveolens
C00000615	501-16-6	Caffeic acid	C9H8O4	180.04225874	Apium graveolens
C00000619	97-53-0	Eugenol	C10H12O2	164.08372963	Apium graveolens
C00000674	491-70-3	Luteolin	C15H10O6	286.04773805	Apium graveolens
C00000805	80-56-8	alpha-Pinene	C10H16	136.12520051	Apium graveolens
C00000816	127-91-3	beta-Pinene	C10H16	136.12520051	Apium graveolens
C00000819	76-22-2	(+)-Camphor	C10H16O	152.12011513	Apium graveolens
C00000823	138-86-3	Limonene	C10H16	136.12520051	Apium graveolens
C00000839	13466-78-9	3-Carene	C10H16	136.12520051	Apium graveolens
C00000843	3338-55-4	cis-beta-Ocimene	C10H16	136.12520051	Apium graveolens
C00000853	123-35-3	beta-Myrcene	C10H16	136.12520051	Apium graveolens
C00000861	586-62-9	alpha-Terpinolene	C10H16	136.12520051	Apium graveolens
C00000862	3779-61-1	trans-beta-Ocimene	C10H16	136.12520051	Apium graveolens
C00000947	154-23-4	(+)-Catechin	C15H14O6	290.07903818	Apium graveolens
C00000956	490-46-0	(-)-Epicatechin	C15H14O6	290.07903818	Apium graveolens

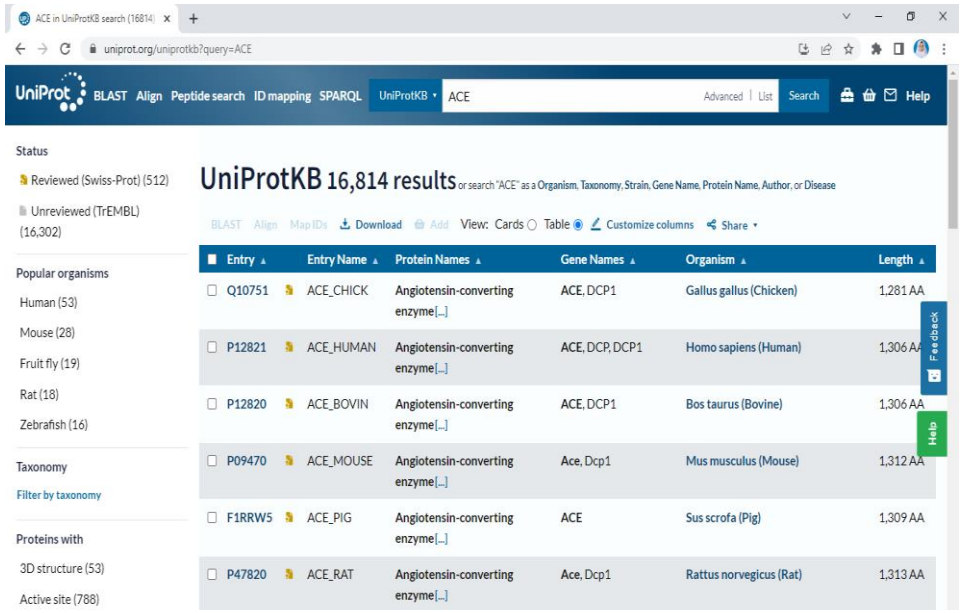
Lampiran 3. Pencarian kandungan kimia dari IJAH *analytics*



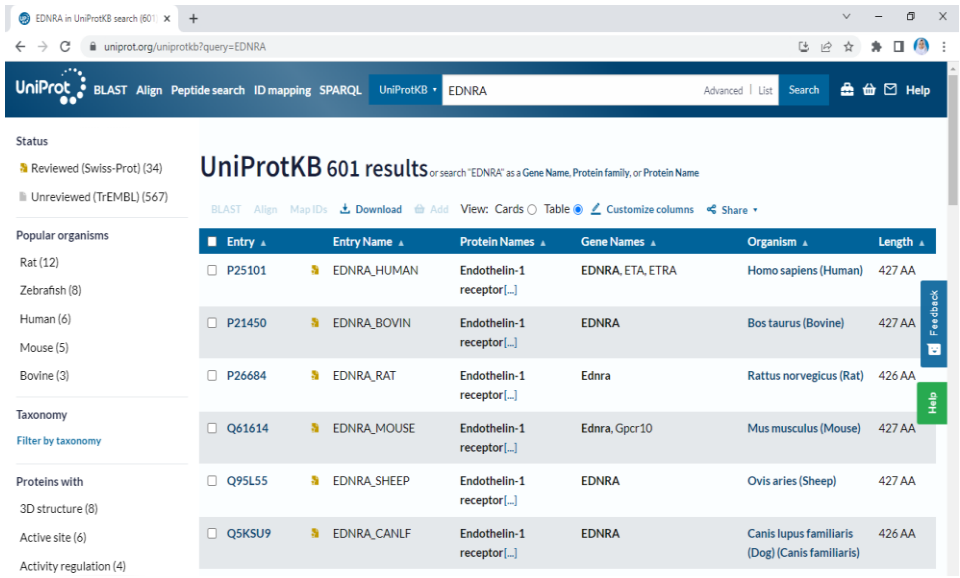


Lampiran 4. Validasi nama gen



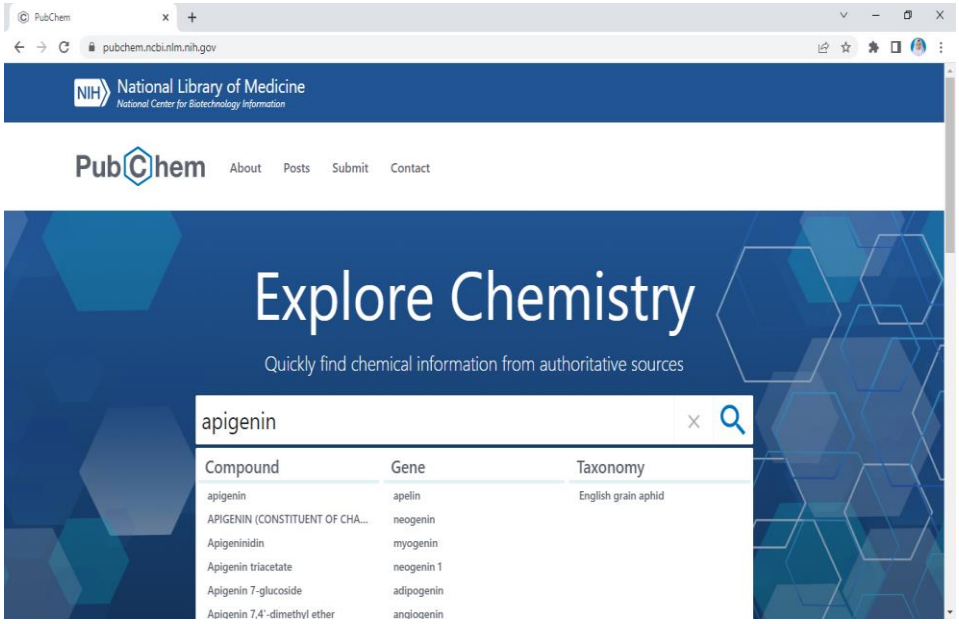


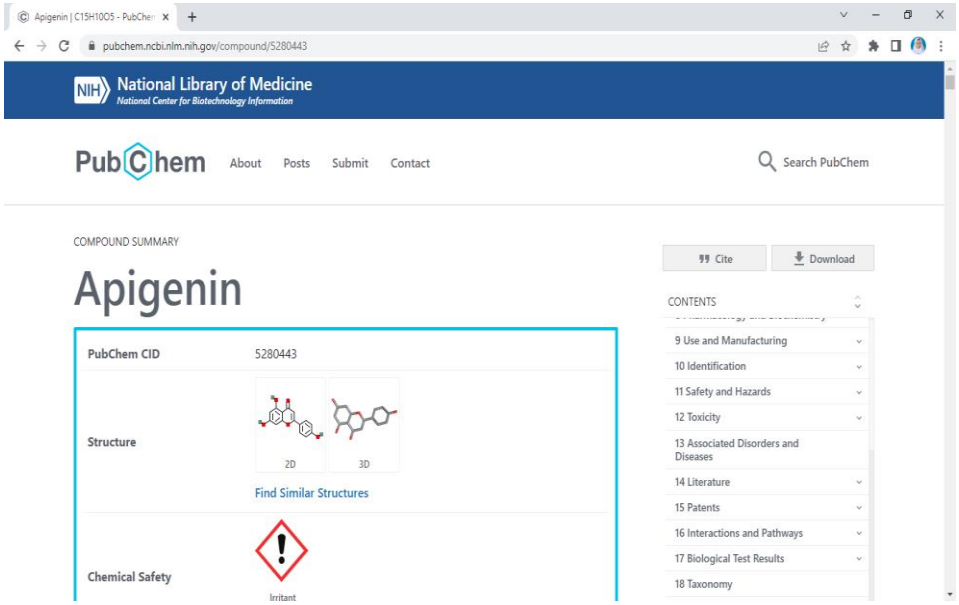
Angiotensin-converting enzyme

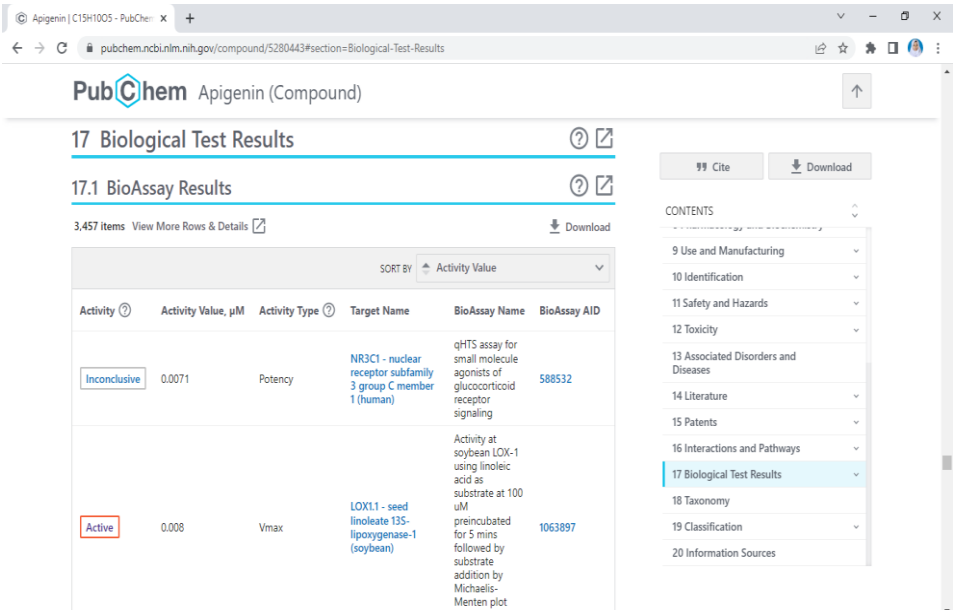


Endothelin Receptor Type A

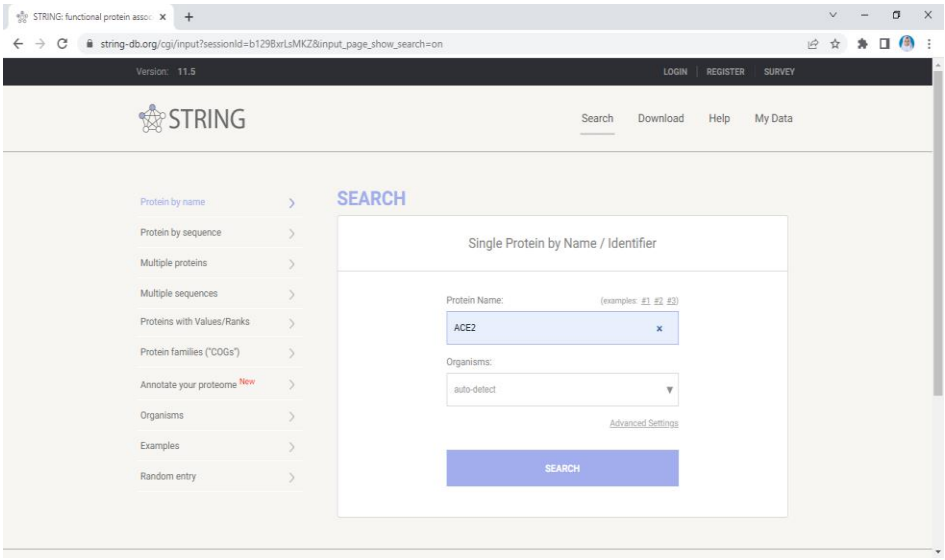
Lampiran 5. Percarian aktivitas biologi kandungan senyawa

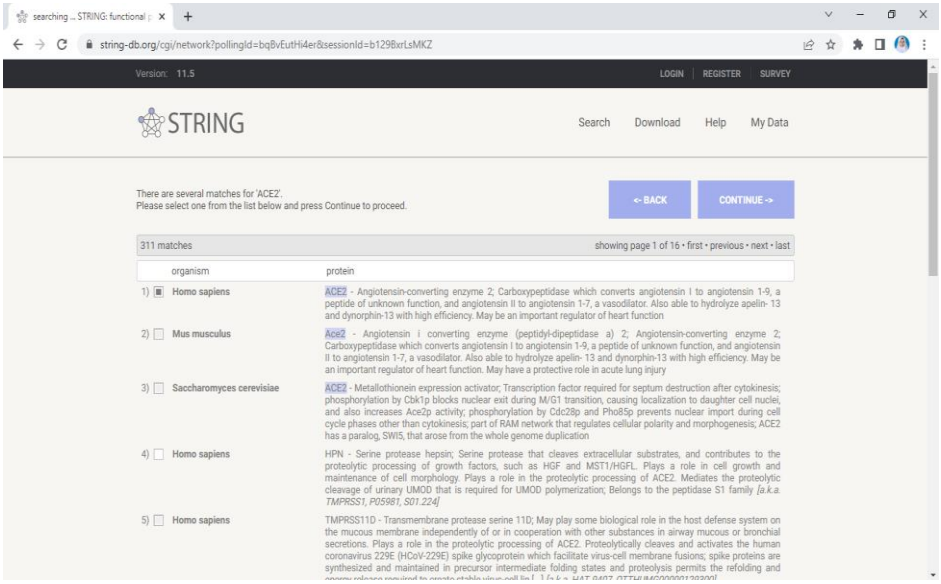


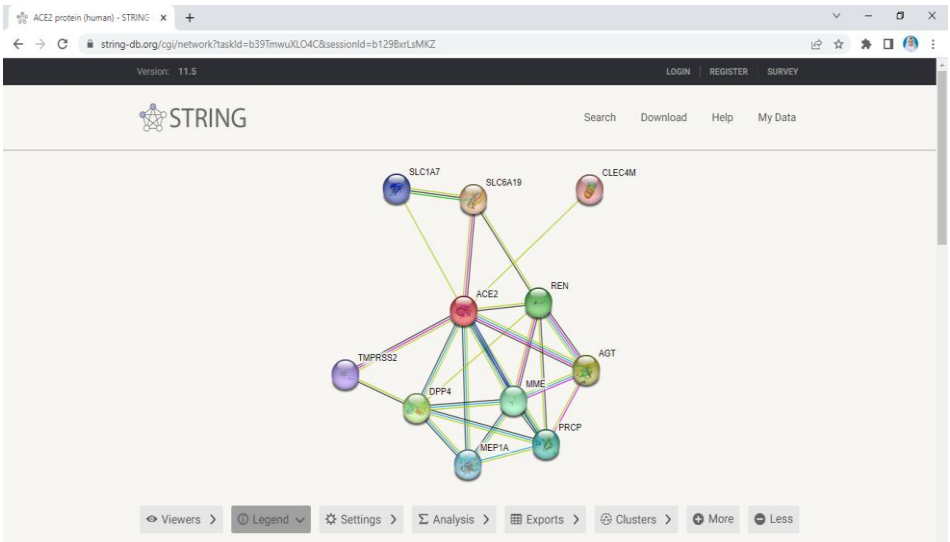




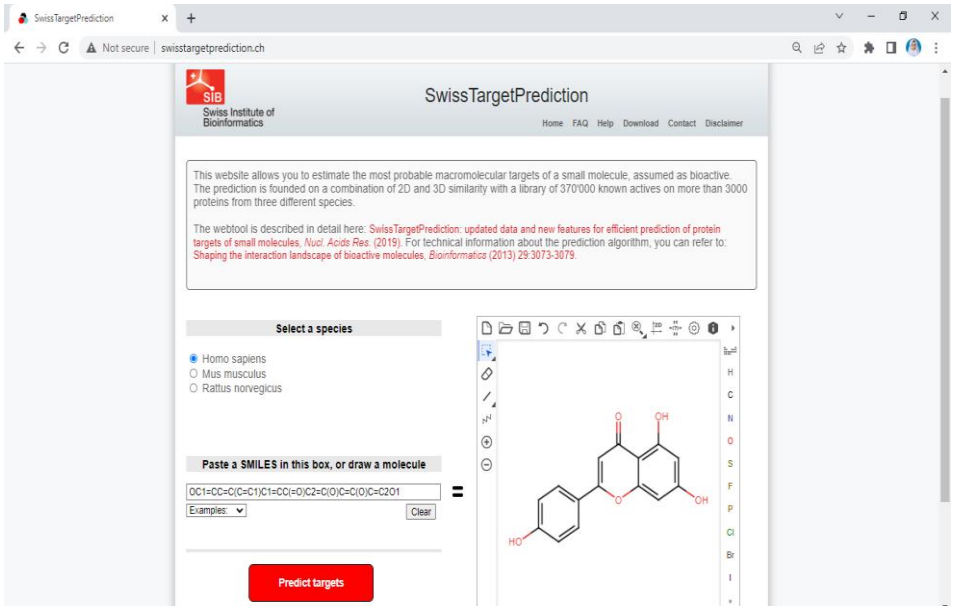
Lampiran 6. Interaksi protein-protein

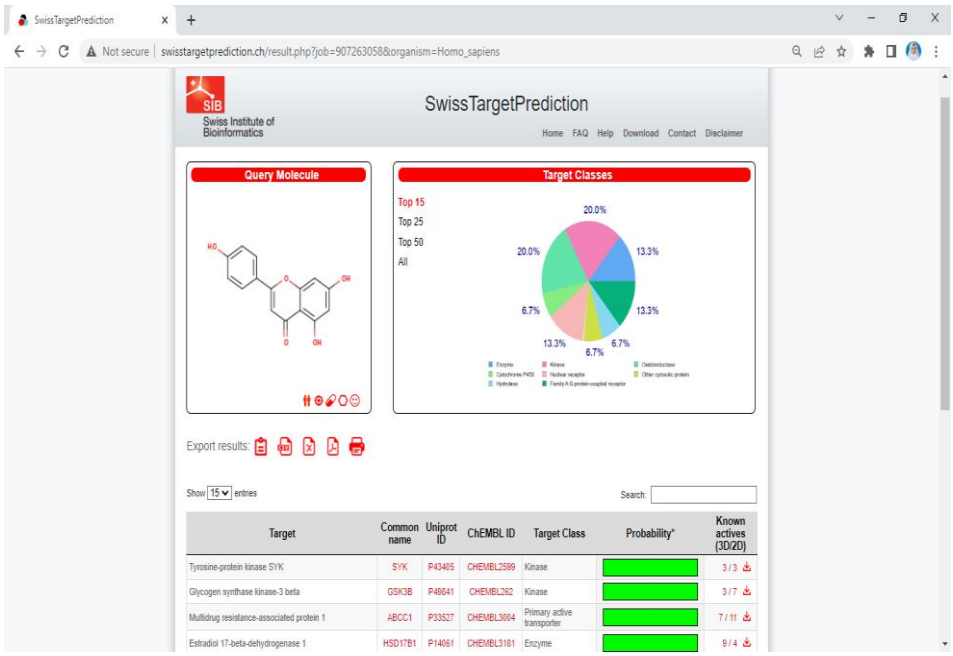



searching ... STRING: functional
string-db.org/cgi/network?pollingId=bq8vEutHi4er&sessionId=b129BxrLsMKZ
Version: 11.5
LOGIN | REGISTER | SURVEY
STRING
Search Download Help My Data
There are several matches for 'ACE2'.
Please select one from the list below and press Continue to proceed.
<- BACK
CONTINUE ->
311 matches
showing page 1 of 16 • first • previous • next • last
organism
protein
1) Homo sapiens
ACE2 - Angiotensin-converting enzyme 2; Carboxypeptidase which converts angiotensin I to angiotensin 1-9, a peptide of unknown function, and angiotensin II to angiotensin 1-7, a vasodilator. Also able to hydrolyze apelin- 13 and dynorphin-13 with high efficiency. May be an important regulator of heart function
2) Mus musculus
Ace2 - Angiotensin i converting enzyme (peptidyl-dipeptidase a) 2; Angiotensin-converting enzyme 2; Carboxypeptidase which converts angiotensin I to angiotensin 1-9, a peptide of unknown function, and angiotensin II to angiotensin 1-7, a vasodilator. Also able to hydrolyze apelin- 13 and dynorphin-13 with high efficiency. May be an important regulator of heart function. May have a protective role in acute lung injury
3) Saccharomyces cerevisiae
ACE2 - Metallothionein expression activator; Transcription factor required for septum destruction after cytokinesis; phosphorylation by Cbk1p blocks nuclear exit during M/G1 transition, causing localization to daughter cell nuclei, and also increases Ace2p activity; phosphorylation by Cdc28p and Pho85p prevents nuclear import during cell cycle phases other than cytokinesis; part of RAM network that regulates cellular polarity and morphogenesis; ACE2 has a paralog, SWI5, that arose from the whole genome duplication
4) Homo sapiens
HPN - Serine protease hepsin; Serine protease that cleaves extracellular substrates, and contributes to the proteolytic processing of growth factors, such as HGF and MST1/HGFL. Plays a role in cell growth and maintenance of cell morphology. Plays a role in the proteolytic processing of ACE2. Mediates the proteolytic cleavage of urinary UMOD that is required for UMOD polymerization; Belongs to the peptidase S1 family [a.k.a. TMPRSS1, P05981, S01.224]
5) Homo sapiens
TMPRSS11D - Transmembrane protease serine 11D; May play some biological role in the host defense system on the mucous membrane independently of or in cooperation with other substances in airway mucous or bronchial secretions. Plays a role in the proteolytic processing of ACE2. Proteolytically cleaves and activates the human coronavirus 229E (HCoV-229E) spike glycoprotein which facilitate virus-cell membrane fusions; spike proteins are synthesized and maintained in precursor intermediate folding states and proteolysis permits the refolding and

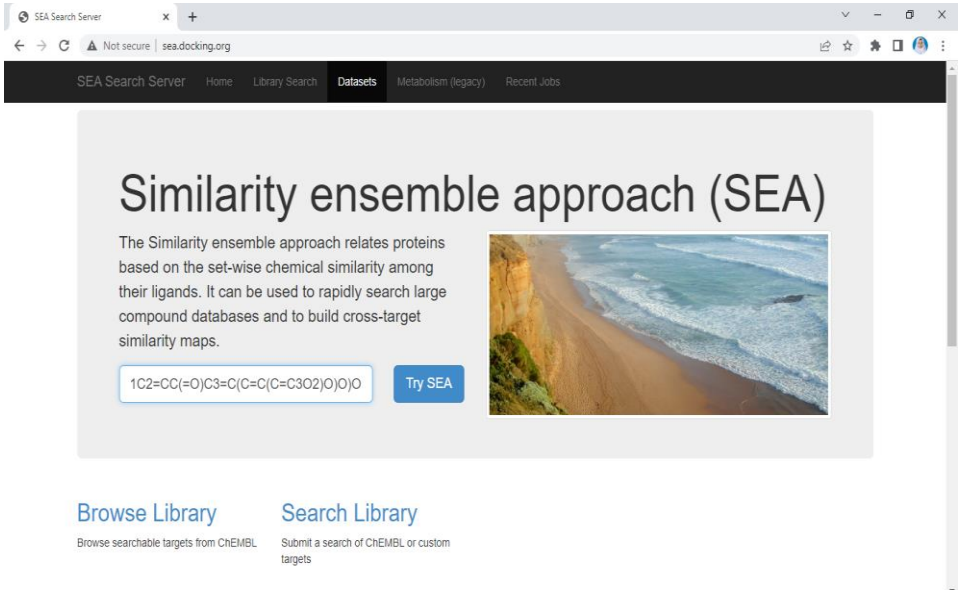

ACE2 protein (human) - STRING
string-db.org/cgi/network?taskId=b39TmwuXLO4C&sessionId=b129BxrLsMKZ
Version: 11.5
LOGIN | REGISTER | SURVEY
STRING
Search Download Help My Data
SLC1A7
SLC6A19
CLEC4M
ACE2
REN
TMPRSS2
AGT
MME
DPP4
PRCP
MEP1A
Viewers
Legend
Settings
Analysis
Exports
Clusters
More
Less

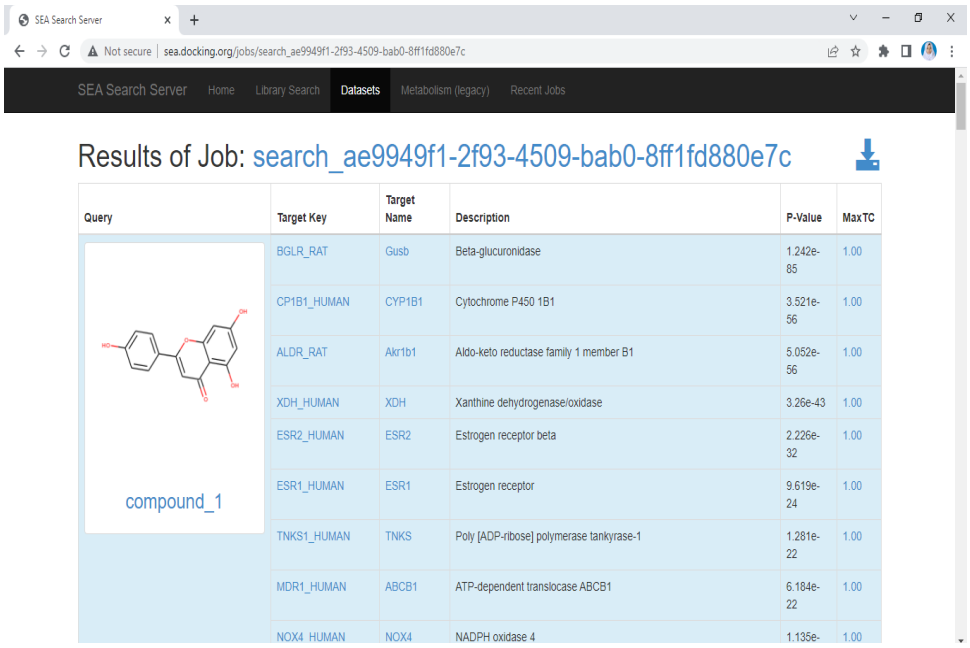
Lampiran 7. Data protein target dari *Swiss Target Prediction*





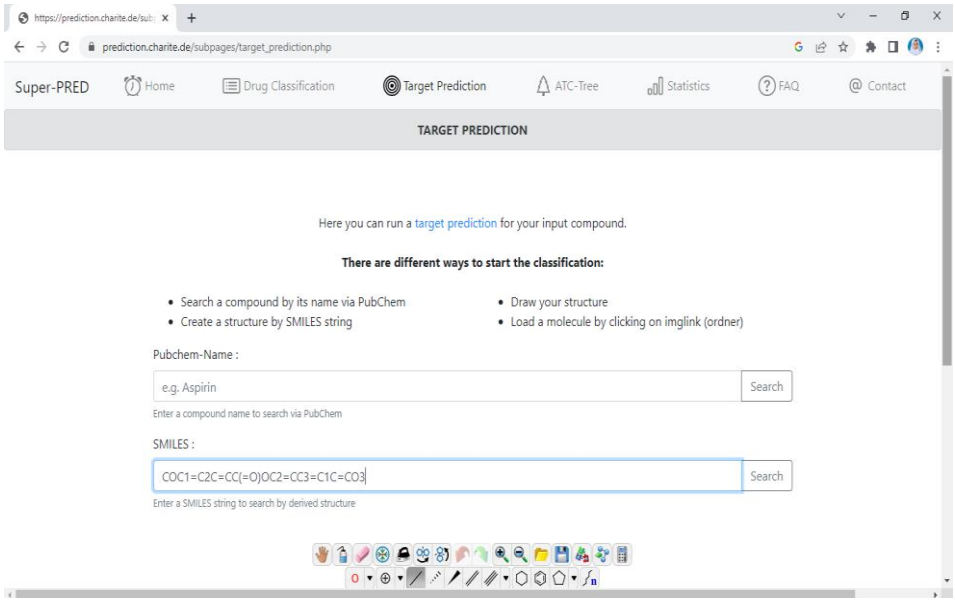
Lampiran 8. Data protein target dari SEA

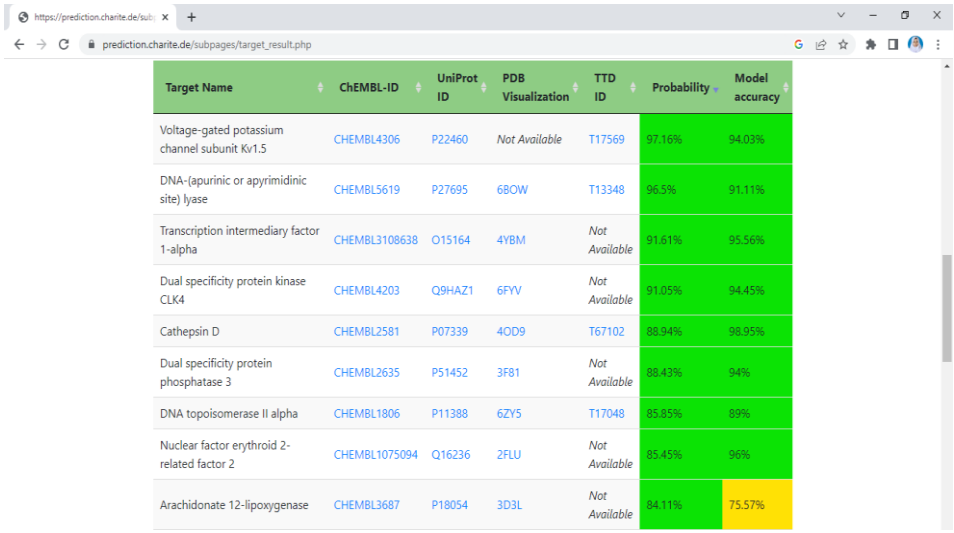




Query	Target Key	Target Name	Description	P-Value	MaxTC
compound_1	BGLR_RAT	Gusb	Beta-glucuronidase	1.242e-85	1.00
	CP1B1_HUMAN	CYP1B1	Cytochrome P450 1B1	3.521e-56	1.00
	ALDR_RAT	Akr1b1	Aldo-keto reductase family 1 member B1	5.052e-56	1.00
	XDH_HUMAN	XDH	Xanthine dehydrogenase/oxidase	3.26e-43	1.00
	ESR2_HUMAN	ESR2	Estrogen receptor beta	2.226e-32	1.00
	ESR1_HUMAN	ESR1	Estrogen receptor	9.619e-24	1.00
	TNKS1_HUMAN	TNKS	Poly [ADP-ribose] polymerase tankyrase-1	1.281e-22	1.00
	MDR1_HUMAN	ABCB1	ATP-dependent translocase ABCB1	6.184e-22	1.00
	NOX4_HUMAN	NOX4	NADPH oxidase 4	1.135e-	1.00

Lampiran 9. Data protein target dari SuperPred





Target Name	ChEMBL-ID	UniProt ID	PDB Visualization	TTD ID	Probability	Model accuracy
Voltage-gated potassium channel subunit Kv1.5	CHEMBL4306	P22460	*Not Available*	T17569	97.16%	94.03%
DNA-(apurinic or apyrimidinic site) lyase	CHEMBL5619	P27695	6BOW	T13348	96.5%	91.11%
Transcription intermediary factor 1-alpha	CHEMBL3108638	O15164	4YBM	*Not Available*	91.61%	95.56%
Dual specificity protein kinase CLK4	CHEMBL4203	Q9HAZ1	6FYV	*Not Available*	91.05%	94.45%
Cathepsin D	CHEMBL2581	P07339	4OD9	T67102	88.94%	98.95%
Dual specificity protein phosphatase 3	CHEMBL2635	P51452	3F81	*Not Available*	88.43%	94%
DNA topoisomerase II alpha	CHEMBL1806	P11388	6ZY5	T17048	85.85%	89%
Nuclear factor erythroid 2-related factor 2	CHEMBL1075094	Q16236	2FLU	*Not Available*	85.45%	96%
Arachidonate 12-lipoxygenase	CHEMBL3687	P18054	3D3L	*Not Available*	84.11%	75.57%

Lampiran 10. Senyawa hasil prediksi dari Swiss Tatget Prediction, SEA, SuperPred

Senyawa	***Swiss target prediction*** Nama protein target	**Nilai Probability**	**SEA** Nama protein target	**Max Tc**	**SuperPred** Nama protein target	**Nilai Probability**
Apigenin	TNKS	1	TNKS	1		
	TNKS2	1	TNKS2	1		
			MPO	1		
			DPP4	1		
Luteolin	MMP9	1	MMP9	1		
	TNKS	1	TNKS	1		
	TNKS2	1	TNKS2	1		
			DPP4	1		
Caffeic acid	MMP1	0,72	MMP1	1		
	MMP9	0,72	MMP9	1		
			DPP4	1		
3-n Butylphthalide					ANPEP	82,83%
Bergapten					ANPEP	73,63%

Lampiran 11. Visualisasi network pharmacology menggunakan *Cytoscape*