

LAMPIRAN

Lampiran 1. Pengumpulan data kandungan kimia dari Knapsack

Number of matched data: 26

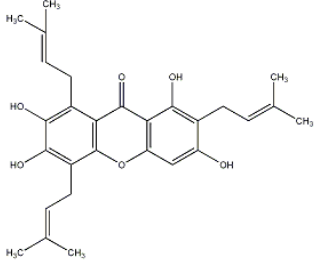
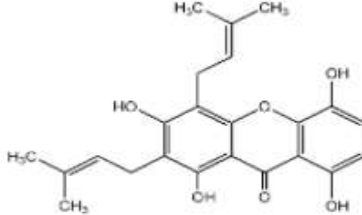
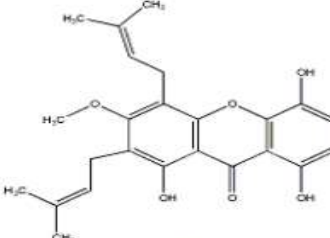
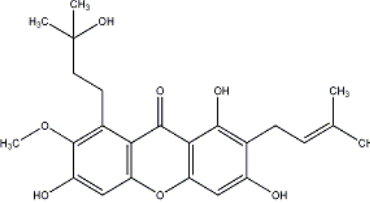
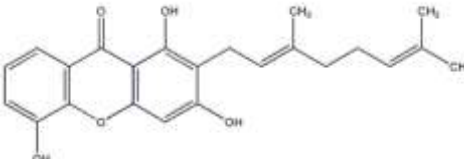
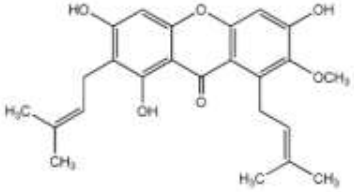
Pubmed ID	Pubmed Title	Molecular Formula	MW	Chemical Structure
C00000001	485-18-2	Daikotin	C15H12O7	504.05830274
C00000002	490-46-0	Epicatechin	C15H14O6	250.07903818
C00000003	5617-33-4	Amretosifone	C30H16O10	536.0686668
C00000004	7584-24-4	Cyanidin-3-O-glucoside	C27H26O11+	440.1083803
C00000005	41745-41-5	Procyanidin A2	C30H40O12	576.12677623
C00000006	2781-65-5	Orthoctic acid	C18H14O8	326.0661838
C00000007	31380-42-0	Gartarin	C24H24O6	396.1573883
C00000008	437-50-3	Gemtin	C14H10O5	258.05820343
C00000009	19275-44-6	1-isomangosin	C24H26O8	410.1720086
C00000010	6147-11-1	Mangosin	C24H26O8	410.1720086
C00000011	3542-72-1	1,1,6,7-tetrahydroxanthone	C13H10O6	250.05208799
C00000012	78821-30-9	Gemina	C18H16O6	302.08073603
C00000013	819-34-6	Madecasin	C15H10O6	262.04773809
C00000014	52517-52-0	Kanhydrotyrol	C18H16O6	302.08073603
C00000015	83-46-3	beta-Sitosterol	C28H48O	414.38616622
C00000016	27542-37-6	Talbotraflaxone	C30H40O10	540.10564886
C00000017	29082-85-1	Palugaside	C18H20O10	378.12336491
C00000018	38620-68-7, 18376-31-3	Cyanidin-3-sophoroside	C27H26O11	440.1083803
C00000019	34443-82-4	Cyanidin-3-O-galloylglucoside	C33H40O12+	572.21911875
C00000020	28636-67-3	Aslibin	C27H22O11	460.17821158
C00000021	12786-07-1	Procyanidin B3	C30H40O12	576.12677623
C00000022	92383-03-0	Procyanidin A1	C28H34O12	538.1083803
C00000023	384385-71-3	11-Hydroxy-1-benzoxepin	C14H18O7	286.1078379
C00000024	33960-41-9	beta-Hydroxytyrol	C18H16O6	302.08073603
C00000025	20921-57-7	beta-Mangosin	C24H26O6	396.1573883
C00000026	106807-05-4	Demethylcalabaxanthone	C24H22O5	378.14672361
C00000027	31271-01-5	garcinia-mangosin	C25H40O6	396.1572883
C00000028	463342-33-6	Garcinatanin	C21H20O6	360.12698837

C00000029	76986-28-4	Garcoside B	C23H22O6	394.14163844
C00000030	76986-27-8	Garcoside C	C23H22O7	414.16183118
C00000031	107390-06-9	Garcoside D	C24H28O7	428.18203321
C00000032	112649-21-5	Garcoside E	C26H32O6	454.21906075
C00000033	463342-33-4	Mangostanol	C24H26O7	426.10782019
C00000034	184857-72-2	Mangostanol	C24H26O7	426.10782019
C00000035	88485-76-2	Mangostanol C	C24H26O6	442.16257871
C00000036	886450-77-7	Mangostanol D	C23H24O6	396.1573883
C00000037	896450-76-6	Mangostanol E	C24H26O6	444.17841787
C00000038	106197-40-6	Mangostanol	C23H24O6	380.16237388
C00000039	437715-44-8	Mangostanol A	C28H28O6	460.18868883
C00000040	59785-61-0	Triacetoxanthone	C23H20O5	376.13107375
C00000041	40738-44-1	Tovophyllin A	C28H30O6	462.20423899
C00000042	40738-45-2	Tovophyllin B	C28H28O6	460.18868883
C00000043	1010089-70-0	1,2-Dihydro-1,8,10-trihydroxy-2-(2-hydroxypropyl)-9-(3-methylbut-2-enyl)flav(5,7)-ol-one	C29H40O7	412.13220312
C00000044	1010089-79-0	6-Deoxy-7-demethylmangostanol	C23H24O6	396.1572883
C00000045	147782-04-5	Gutiferone C	C18H16O6	302.08073603
C00000046	15071-46-8	3-Hydroxytyrol	C18H16O6	302.08073603
C00000047	463342-41-6	O-Hydroxyprocyanidin	C23H22O7	440.18203321
C00000048	112649-48-4	BR-Xanthone A	C23H24O6	396.1572883
C00000049	864815-33-5	Dulcioxanthone D	C28H28O6	460.18868883
C00000050	15424-75-9	Fuscoxanthone C	C26H28O6	438.20423899
C00000051	147887-34-1	Gutiferone A	C18H16O6	302.08073603
C00000052	211568-69-3	1,3,7-Triacetoxanthone	C14H10O6	274.04773809
C00000053	102814-07-6	Dulcioxanthone D	C18H16O6	302.08073603
C00000054	437715-43-8	Mangostanol	C24H26O7	426.10782019
C00000055	462856-77-5	(16E)-1,6-Dihydroxy-8-(3-hydroxy-3-methylbut-1-enyl)-3,7-dimethoxy-2-(3-methylbut-2-enyl)xanthone	C28H38O7	440.18203321
C00000056	462856-78-6	(16E)-1-Hydroxy-8-(3-hydroxy-3-methylbut-1-enyl)-3,6,7-trimethoxy-2-(3-methylbut-2-enyl)xanthone	C28H38O7	444.19810331
C00000057	463342-36-1	1,8-Dihydroxy-2-(2-hydroxy-3-methylbut-3-enyl)-3,7-dimethoxy-6-(3-methylbut-2-enyl)xanthone	C29H40O7	440.18203321

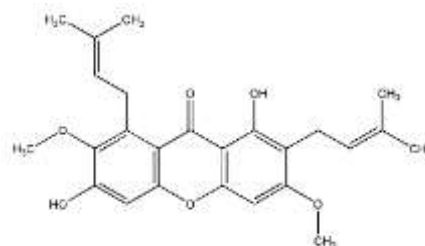
Accession	Gene	Gene ID	Gene Name	Gene Type	Gene Length	Gene Location
C0003433	46342-34-9		1-Hydroxy-5-(2-hydroxy-3-methylbut-3-enyl)-3,6,7-trimethoxy-2-(3-methylbut-2-enyl)xanthone	C28H30O7	454	19910331
C0003455	5663-17-7		2,4,5-Trihydroxy-1-methoxyanthrone	C14H10O6	274	04773805
C0003493	119713-07-0		5 <i>S</i> -Xanthone B	C14H10O6	274	04773805
C0003543	46342-35-0		1,8-Dihydroxy-8-(2-hydroxy-3-methylbut-3-enyl)-5,7-dimethoxy-2-(3-methylbut-2-enyl)xanthone	C28H30O7	445	19360325
C0003833	86295-18-2		8-Hydroxycathoxanthone G	C24H20O6	410	17203656
C0003881	130774-35-5		Cathoxanthone G	C24H20O6	394	17502394
C0003927	864974-49-2		3-Methylxanthone A	C23H24O6	396	1572885
C0003943	50816-23-4		Troxycanthone A	C23H22O6	378	14672381
C0003953	30-47-1		Xanthone	C13H8O2	198	0324285
C0004035	360255-68-0		Garcinangosone D	C19H20O5	382	11033324
C0004052	360255-65-7		Garcinangosone A	C28H30O6	465	19558665
C0004059	360255-66-8		Garcinangosone B	C24H24O6	408	1572885
C0004063	360255-67-9		Garcinangosone C	C23H24O7	412	15220312
C0004071	437711-45-0		Mangostenone B	C28H30O6	462	20423669
C0004079	164672-85-9		Criboxanthone	C48H60O13	834	32514168
C0004084	869296-01-1		Mangoxanthone	C23H24O6	396	1572885
C0004094	35349-85-9		5-Hydroxycathoxanthone	C24H24O6	408	1572885
C0004102	1268161-44-8		Garcinangosaxanthone A	C21H18O6	366	11033307
C0004109	1268161-45-0		Garcinangosaxanthone B	C23H24O7	412	15220312
C0004129	1268161-46-1		Garcinangosaxanthone C	C19H22O5	330	14672381
C0004133	1261983-35-6		Garcinangosaxanthone D	C23H22O6	394	14163844
C0004137	1301563-57-7		Garcinangosaxanthone E	C24H26O7	426	16785319
C0004139	1632448-64-6		Garcinangosaxanthone F	C28H32O7	480	21480338
C0004143	1632448-65-7		Garcinangosaxanthone G	C28H34O7	482	23045944
C0004151	1242436-70-5		Mangostenone F	C24H24O6	408	1572885
C0004152	1242436-71-6		Mangostenone G	C23H22O6	394	14163844
C0004158	862955-26-9		Mangostegone	C24H24O7	424	15220312
C0004161	1262527-36-5		1'-2'-Dihydroxyphyllin A	C28H32O6	464	21988875
C0004171	104537-94-3		6-Deoxy-gamma-mangosin	C23H24O5	380	16237388
C0004173	30209-77-3		O-Deethyltorboxanthone	C18H14O6	326	07903816
C0004180	39011-96-6		Calabaxanthone	C24H24O6	392	16237388
C0004203	28063-85-6		1-Isomangosin hydrate	C24H28O7	428	18380025
C0004208	118498-86-3		Alloxanthone E	C24H24O7	424	15220312

Accession	Gene	Gene ID	Gene Name	Gene Type	Gene Length	Gene Location
C0004209	326032-86-0		Isomangosone U	C18H14O6	326	11013224
C0004222	356285-65-7		Garcinangosone A	C28H30O6	460	19558663
C0004226	356285-66-8		Garcinangosone B	C24H24O6	408	1572885
C0004229	356285-67-9		Garcinangosone C	C23H24O7	412	15220312
C0004234	457711-45-0		Mangostenone B	C28H30O6	462	20423669
C0004236	164672-81-9		Criboxanthone	C48H60O13	834	32514168
C0004239	864096-01-1		Mangoxanthone	C23H24O6	396	1572885
C0004245	35349-85-9		5-Hydroxycathoxanthone	C24H24O6	408	1572885
C0004247	1268161-44-9		Garcinangosaxanthone A	C21H18O6	366	11033307
C0004258	1268161-45-0		Garcinangosaxanthone B	C23H24O7	412	15220312
C0004265	1268161-46-1		Garcinangosaxanthone C	C19H22O5	330	14672381
C0004270	1261983-35-6		Garcinangosaxanthone D	C23H22O6	394	14163844
C0004271	1261983-57-7		Garcinangosaxanthone E	C24H26O7	426	16785319
C0004272	1632448-64-6		Garcinangosaxanthone F	C28H32O7	480	21480338
C0004273	1632448-65-7		Garcinangosaxanthone G	C28H34O7	482	23045944
C0004285	1242436-70-5		Mangostenone F	C24H24O6	408	1572885
C0004287	1242436-71-6		Mangostenone G	C23H22O6	394	14163844
C0004289	862955-26-9		Mangostegone	C24H24O7	424	15220312
C0004291	1262527-36-5		1'-2'-Dihydroxyphyllin A	C28H32O6	464	21988875
C0004293	104537-94-3		6-Deoxy-gamma-mangosin	C23H24O5	380	16237388
C0004295	30209-77-3		O-Deethyltorboxanthone	C18H14O6	326	07903816
C0004298	39011-96-6		Calabaxanthone	C24H24O6	392	16237388
C0004303	28063-85-6		1-Isomangosin hydrate	C24H28O7	428	18380025
C0004308	118498-86-3		Alloxanthone E	C24H24O7	424	15220312
C0004309	153432-49-1		Mangostenone	C14H12O6	276	06338812
C0004361	326204-89-0		Mangosin	C19H18O6	326	11542369
C0004461	1188186-51-1		1,7-Dihydroxy-3-methoxy-4-prenylxanthone	C19H18O6	326	11542369
C0005295	1182036-52-4		11-Hydroxy-5-O-methyl-1-isomangosin	C25H28O7	440	18380025
C0005298	118227-98-4		1,8-Dihydroxy-3-methoxy-2-prenylxanthone	C19H18O6	326	11542369
C0005787	118187-11-6		1,8,8-Trihydroxy-3-methyl-2-prenylxanthone	C19H18O6	342	11033301

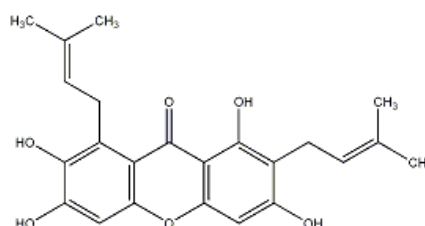
Lampiran 2. Pengumpulan data aktivitas biologis dari PubChem

Metabolit	Struktur
Garcinone E	 <p>The structure of Garcinone E is a xanthone derivative. It features a central xanthone core with a carbonyl group at position 9. It has hydroxyl groups at positions 1, 2, 4, 5, and 7. There are three prenyl side chains attached at positions 3, 6, and 8, each consisting of a propene chain with a methyl group at the terminal end.</p>
Gartanin	 <p>The structure of Gartanin is a xanthone derivative. It has a carbonyl group at position 9 and hydroxyl groups at positions 1, 2, 4, 5, and 7. It features a prenyl side chain at position 3 and a 3-methylbut-2-enyl side chain at position 6.</p>
8-Hydroxycudraxanthone G	 <p>The structure of 8-Hydroxycudraxanthone G is a xanthone derivative. It has a carbonyl group at position 9 and hydroxyl groups at positions 1, 2, 4, 5, 7, and 8. It features a prenyl side chain at position 3 and a 3-methylbut-2-enyl side chain at position 6. There is also a methoxy group at position 10.</p>
Garcinone D	 <p>The structure of Garcinone D is a xanthone derivative. It has a carbonyl group at position 9 and hydroxyl groups at positions 1, 2, 4, 5, and 7. It features a prenyl side chain at position 3, a 3-methylbut-2-enyl side chain at position 6, and a 2-hydroxypropan-2-yl side chain at position 8. There is also a methoxy group at position 10.</p>
Mangostinon	 <p>The structure of Mangostinon is a xanthone derivative. It has a carbonyl group at position 9 and hydroxyl groups at positions 1, 2, 4, and 5. It features a long prenyl side chain at position 3, which is a 3-methylbut-2-enyl chain with a methyl group at the terminal end.</p>
alpha-Mangostin	 <p>The structure of alpha-Mangostin is a xanthone derivative. It has a carbonyl group at position 9 and hydroxyl groups at positions 1, 2, 4, 5, and 7. It features a prenyl side chain at position 3, a 3-methylbut-2-enyl side chain at position 6, and a methoxy group at position 10.</p>

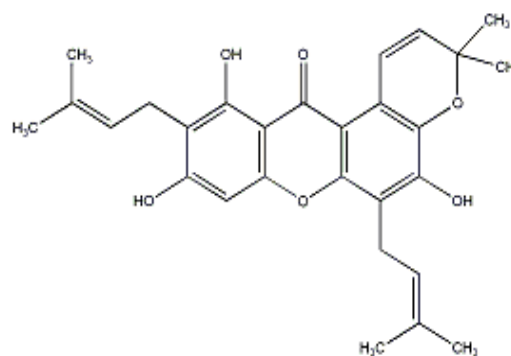
beta-Mangostin



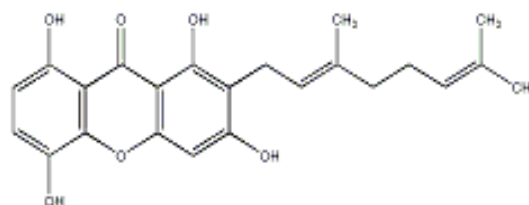
gamma-Mangostin



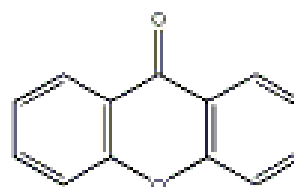
Tovophyllin A



Smeathxanthone A



Xanthone



Lampiran 3. Identifikasi prediksi target protein dari SwissTargetprediksi

DATA SWISSTARGET PREDICTION KESELURUHAN - Microsoft Excel

No	CAS ID	Metabolite	Smile	Target
1	882505-18-2	8-Hydroxycuraxantone G	<chem>CC1=CCC1=C(C2=C(C1=O)OC3=C(C2=O)C=C3)OC4=CC(=O)O4</chem>	0
2	0101016147	alpha-mangostin	<chem>CC1=CCC1=C(C2=C(C1=O)OC3=C(C2=O)C=C(C3=O)OC4=CC(=O)O4</chem>	0
3	20931-37-7	Beta-mangostin	<chem>CC1=CCC1=C(C2=C(C1=O)OC3=C(C2=O)C=C(C3=O)OC4=CC(=O)O4</chem>	0
4	31271-07-5	Gamma-mangostin	<chem>CC1=CCC1=C(C2=C(C1=O)OC3=C(C2=O)C=C(C3=O)OC4=CC(=O)O4</chem>	0
5	107390-08-9	Garcinone D	<chem>CC1=CCC1=C(C2=C(C1=O)OC3=C(C2=O)C=C(C3=O)OC4=CC(=O)O4</chem>	RELA
6	112649-21-5	Garcinone E	<chem>CC1=CCC1=C(C2=C(C1=O)OC3=C(C2=O)C=C(C3=O)OC4=CC(=O)O4</chem>	0
7	33390-42-0	Garitanin	<chem>CC1=CCC1=C(C2=C(C1=O)OC3=C(C2=O)C=C(C3=O)OC4=CC(=O)O4</chem>	0
8	166197-40-6	Mangostinon	<chem>CC1=CCC1=C(C2=C(C1=O)OC3=C(C2=O)C=C(C3=O)OC4=CC(=O)O4</chem>	0
9	864974-49-2	Smacthaxanthone A	<chem>CC1=CCC1=C(C2=C(C1=O)OC3=C(C2=O)C=C(C3=O)OC4=CC(=O)O4</chem>	0
10	40738-44-1	Tovophyllin A	<chem>CC1=CCC1=C(C2=C(C1=O)OC3=C(C2=O)C=C(C3=O)OC4=CC(=O)O4</chem>	0
11	90-47-1	Xanthone	<chem>C1=CC=C2C=C1C=O)C3=CC=CC=C3O2</chem>	0

DATA SWISSTARGET PREDICTION KESELURUHAN - Microsoft Excel

Protein kinase C beta

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Knesses
Cytochrome P450 9A1	CYP19A1	P11511	CHEMBL1876	Cytochrome P450	0.66940123	7 / 6
Nuclear factor NF-kappa-B p50 subunit	RELA	Q04066	CHEMBL1519	Transcription factor	0.66940123	7 / 2
Isocitrate dehydrogenase (NADP) cytoplasmic	IDH3	Q75674	CHEMBL3907625	Enzyme	0.18235581	2 / 2
Arachidonate 15-lipoxygenase	ALOX15	P98050	CHEMBL2993	Enzyme	0.18235581	4 / 1
Arachidonate 12-lipoxygenase	ALOX12	P98054	CHEMBL3687	Enzyme	0.18235581	6 / 1
Fatty acid synthase	FASN	P49327	CHEMBL4159	Transferase	0.18235581	5 / 3
Cyclooxygenase-1	PTGS1	P23219	CHEMBL3221	Oxidoreductase	0.12892674	1 / 2
Cyclooxygenase-2	PTGS2	P33054	CHEMBL293	Oxidoreductase	0.12892674	1 / 3
Nuclear factor NF-kappa-B p105 subunit	NFkB1	P28636	CHEMBL3251	Other cytosolic protein	0.11880367	0 / 2
Axin1/beta-catenin	CTNMB1	P32222	CHEMBL5960	Unclassified protein	0.11880367	1 / 0
Tyrosine-protein kinase SRC	SRC	P12931	CHEMBL267	Kinase	0.11880367	5 / 0
Protein kinase C iota	PRKCI	P41743	CHEMBL2598	Kinase	0.11880367	1 / 0
TNF-alpha	TNF	P01379	CHEMBL3825	Secreted protein	0.11880367	2 / 0
Protein kinase C delta	PRKCD	Q05653	CHEMBL2990	Kinase	0.11880367	59 / 0
Protein kinase C beta	PRKCB	P05771	CHEMBL3040	Kinase	0.11880367	69 / 0
Protein kinase C epsilon	PRKCE	Q02156	CHEMBL3582	Kinase	0.11880367	61 / 0
Tropomyosin, cardiac muscle	TNNC1 TNNT2 TNNT3	P83316 P45179 P29429	CHEMBL2095263	Unclassified protein	0.11880367	2 / 0
Maternal embryonic leucine zipper kinase	MEK1	Q14688	CHEMBL4578	Kinase	0.11880367	301 / 6
Heat shock protein HSP 90-beta	HSP90AB1	P08238	CHEMBL4303	Other cytosolic protein	0.11880367	17 / 0
Pyruvate dehydrogenase kinase isoform 1	PKDL	Q15118	CHEMBL4766	Kinase	0.11880367	52 / 0
Glucagon receptor	GCGR	P42871	CHEMBL1985	Family G G protein-coupled receptor	0.11880367	62 / 0
Heat shock protein HSP 90-alpha	HSP90AA1	P07900	CHEMBL1880	Other cytosolic protein	0.11880367	62 / 0
Protein kinase C alpha	PRKCA	P17052	CHEMBL299	Kinase	0.11880367	60 / 0