

LAMPIRAN

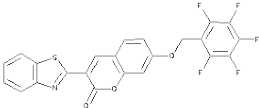
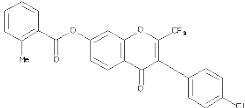
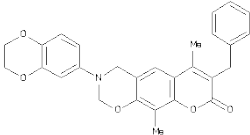
Lampiran 1 Daftar *Active Set Compound* ChEMBL

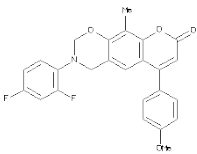
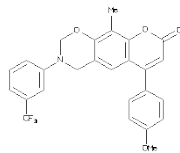
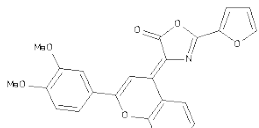
No	Molecule	Standard Value	Standard Unit	Activity Comment	Organism
1	CHEMBL3613 686	5,012	nM	Active	Homo Sapiens
2	CHEMBL2202 44	63,1	nM	Active	Homo Sapiens
3	CHEMBL2059 66	1,585	nM	Active	Homo Sapiens
4	CHEMBL5218 26	39,81	nM	Active	Homo Sapiens
5	CHEMBL5189 68	12,59	nM	Active	Homo Sapiens
6	CHEMBL2065 44	31,62	nM	Active	Homo Sapiens
7	CHEMBL1909 385	25,12	nM	Active	Homo Sapiens
8	CHEMBL4779 78	15,85	nM	Active	Homo Sapiens
9	CHEMBL2062 289	15,85	nM	Active	Homo Sapiens
10	CHEMBL5318 04	15,85	nM	Active	Homo Sapiens
11	CHEMBL2756 66	1,259	nM	Active	Homo Sapiens
12	CHEMBL1794 066	79,43	nM	Active	Homo Sapiens
13	CHEMBL1909 376	19,95	nM	Active	Homo Sapiens
14	CHEMBL1516 890	10	nM	Active	Homo Sapiens
15	CHEMBL1857	63,1	nM	Active	Homo Sapiens

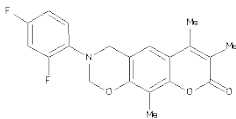
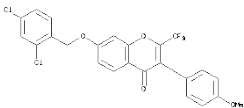
	10				
16	CHEMBL1882 40	15,85	nM	Active	Homo Sapiens
17	CHEMBL4757 61	5,012	nM	Active	Homo Sapiens
18	CHEMBL1909 357	25,12	nM	Active	Homo Sapiens
19	CHEMBL4347 29	25,12	nM	Active	Homo Sapiens
20	CHEMBL1794 073	19,95	nM	Active	Homo Sapiens
21	CHEMBL1768 57	79,43	nM	Active	Homo Sapiens
22	CHEMBL3465 51	12,59	nM	Active	Homo Sapiens
23	CHEMBL5133 0	12,59	nM	active	Homo Sapiens
24	CHEMBL1794 061	79,43	nM	Active	Homo Sapiens
25	CHEMBL3599 9	79,43	nM	Active	Homo Sapiens
26	CHEMBL1794 055	50,12	nM	Active	Homo Sapiens
27	CHEMBL5199 62	39,81	nM	Active	Homo Sapiens
28	CHEMBL3986 609	39,81	nM	Active	Homo Sapiens
29	CHEMBL2786 83	15,85	nM	Active	Homo Sapiens
30	CHEMBL2325 906	25,12	nM	Active	Homo Sapiens
31	CHEMBL1909 364	3,981	nM	Active	Homo Sapiens
32	CHEMBL4664 12	12,59	nM	Active	Homo Sapiens
33	CHEMBL4762 59	39,81	nM	Active	Homo Sapiens
34	CHEMBL3599 63	63,1	nM	Active	Homo Sapiens

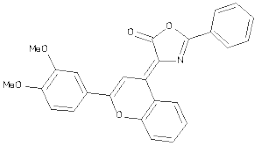
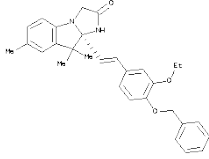
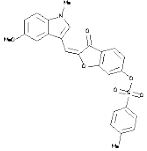
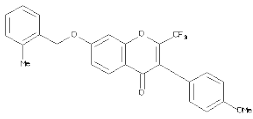
35	CHEMBL4689 63	50,12	nM	Active	Homo Sapiens
36	CHEMBL1031 15	25,12	nM	Active	Homo Sapiens
37	CHEMBL2698 83	12,59	nM	Active	Homo Sapiens
38	CHEMBL3618 94	15,85	nM	Active	Homo Sapiens
39	CHEMBL2721 65	39,81	nM	Active	Homo Sapiens
40	CHEMBL2705 44	31,62	nM	Active	Homo Sapiens

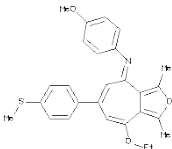
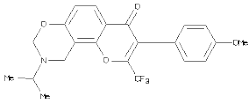
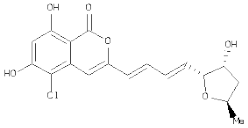
Lampiran 2. Identifikasi Kandidat Senyawa Hasil *Virtual Screening*

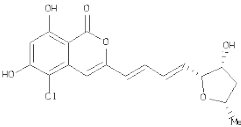
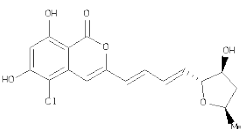
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1		ID	ZINC01797720
		ZINC	
		Sumber	IBScreen Natural Product
		Nama	<u>3-(1,3-benzothiazol-2-yl)-7-(2,3,4,5,6-pentafluorobenzyl)oxy-coumarin</u>
2		ID	ZINC01959510
		ZINC	
		Sumber	IBScreen Natural Product
		Nama	<u>2-methylbenzoic-acid-[3-(4-chlorophenyl)-4-keto-2-(trifluoromethyl)chromen-7-yl]-ester</u>
3		ID	ZINC02116890
		ZINC	
		Sumber	IBScreen Natural Product
		Nama	<u>7-benzyl-3-(2,3-dihydro-1,4-benzodioxin-6-yl)-</u>

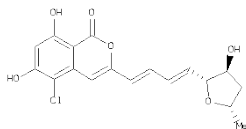
		<u>6,10-dimethyl-2,4-</u> <u>dihydropyrano[3,2-</u> <u>g][1,3]benzoxazin-</u>	
4		ID ZINC	ZINC02118366
		Sumber	IBScreen Natural Product
		Nama	<u>3-(2,4-difluorophenyl)-</u> <u>6-(4-methoxyphenyl)-</u> <u>10-methyl-2,4-</u> <u>dihydropyrano[3,2-</u> <u>g][1,3]benzoxazin-8-</u> <u>one</u>
5		ID ZINC	ZINC02124746
		Sumber	IBScreen Natural Product
		Nama	<u>6-(4-methoxyphenyl)-</u> <u>10-methyl-3-[3-</u> <u>(trifluoromethyl)phenyl</u> <u>]-2,4-</u> <u>dihydropyrano[3,2-</u> <u>g][1,3]benzoxazin-</u>
6		ID ZINC	ZINC02128015
		Sumber	IBScreen Natural

		Product
		Nama <u>4-[2-(3,4-dimethoxyphenyl)chromen-4-ylidene]-2-(2-furyl)oxazol-5-one</u>
7		ID ZINC02158547 ZINC
		Sumber IBScreen Natural Product
		Nama <u>3-(2,4-difluorophenyl)-6,7,10-trimethyl-2,4-dihydropyrano[3,2-g][1,3]benzoxazin-8-one</u>
8		ID ZINC02414186 ZINC
		Sumber IBScreen Natural Product
		Nama <u>7-(2,4-dichlorobenzyl)oxy-3-(4-methoxyphenyl)-2-(trifluoromethyl)chromone</u>
9		ID ZINC08789359 ZINC
		Sumber IBScreen Natural Product

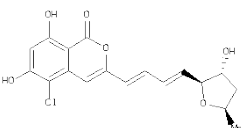
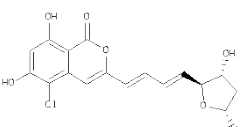
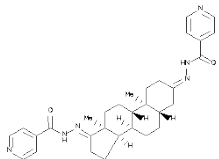
	Nama <u>4-[2-(3,4-dimethoxyphenyl)chromen-4-ylidene]-2-phenyl-oxazol-5-one</u>
10 	ID ZINC08918631 ZINC Sumber IBScreen Natural Product Nama <u>2-(4-benzyloxy-3-ethoxy-phenyl)vinyl-trimethyl-BLAHone</u>
11 	ID ZINC09423665 ZINC Sumber IBScreen Natural Product Nama <u>2-[(5-methoxy-1-methyl-indol-3-yl)methylene]-6-(p-tolylsulfonyloxy)benzofuran-3-one</u>
12 	ID ZINC11865231 ZINC Sumber IBScreen Natural Product Nama <u>3-(4-methoxyphenyl)-7-(o-tolylmethoxy)-2-(trifluoromethyl)chromone</u>

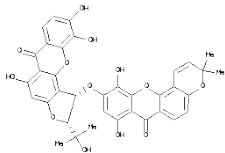
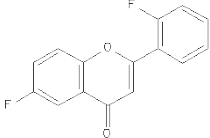
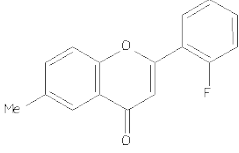
		<u>en-4-one</u>	
13		ID	ZINC12659531
		ZINC	
		Sumber	IBScreen Natural Product
		Nama	<u>8-ethoxy-N-(4-methoxyphenyl)-1,3-dimethyl-6-(4-methylsulfanylphenyl)cyclohepta[c]furan-4-imine</u>
14		ID	ZINC13733891
		ZINC	
		Sumber	IBScreen Natural Product
		Nama	<u>9-isopropyl-3-(4-methoxyphenyl)-2-(trifluoromethyl)-8,10-dihydropyrano[2,3-f][1,3]benzoxazin-4-one</u>
15		ID	ZINC31168678
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		Sumber	IBScreen Natural Product
		Nama	<u>5-chloro-6,8-dihydroxy-3-[(1E,3E)-</u>

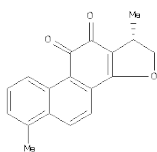
		<u>4-[(2R,3R,5R)-3-hydroxy-5-methyl-tetrahydrofuran-2-yl]buta-1,3-die</u>	
16		ID	ZINC31168682
		ZINC	
		Sumber	IBScreen Natural Product
		Nama	<u>5-chloro-6,8-dihydroxy-3-[(1E,3E)-4-[(2R,3R,5S)-3-hydroxy-5-methyl-tetrahydrofuran-2-yl]buta-1,3-die</u>
17		ID	ZINC31168686
		ZINC	
		Sumber	IBScreen Natural Product
		Nama	<u>5-chloro-6,8-dihydroxy-3-[(1E,3E)-4-[(2R,3S,5R)-3-hydroxy-5-methyl-tetrahydrofuran-2-yl]buta-1,3-die</u>
18		ID	ZINC31168690
		ZINC	
		Sumber	IBScreen Natural



		Product	
		Nama	<u>5-chloro-6,8-</u> <u>dihydroxy-3-[(1E,3E)-</u> <u>4-[(2R,3S,5S)-3-</u> <u>hydroxy-5-methyl-</u> <u>tetrahydrofuran-2-</u> <u>yl]buta-1,3-die</u>
19		ID	ZINC35464494
		ZINC	
		Sumber	IBScreen Natural Product
		Nama	<u>5-chloro-6,8-</u> <u>dihydroxy-3-[(1E,3E)-</u> <u>4-[(2S,3S,5R)-3-</u> <u>hydroxy-5-methyl-</u> <u>tetrahydrofuran-2-</u> <u>yl]buta-1,3-die</u>
20		ID	ZINC35464497
		ZINC	
		Sumber	IBScreen Natural Product
		Nama	<u>5-chloro-6,8-</u> <u>dihydroxy-3-[(1E,3E)-</u> <u>4-[(2S,3S,5S)-3-</u> <u>hydroxy-5-methyl-</u> <u>tetrahydrofuran-2-</u> <u>yl]buta-1,3-die</u>

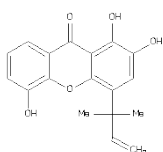
21		ID	ZINC35464499
		ZINC	
		Sumber	IBScreen Natural Product
		Nama	<u>5-chloro-6,8-dihydroxy-3-[(1E,3E)-4-[(2S,3R,5R)-3-hydroxy-5-methyl-tetrahydrofuran-2-yl]buta-1,3-die</u>
22		ID	ZINC35464502
		ZINC	
		Sumber	IBScreen Natural Product
		Nama	<u>5-chloro-6,8-dihydroxy-3-[(1E,3E)-4-[(2S,3R,5S)-3-hydroxy-5-methyl-tetrahydrofuran-2-yl]buta-1,3-die</u>
23		ID	ZINC59409300
		ZINC	
		Sumber	IBScreen Natural Product
		Nama	<u>N-[(E)-[(5S,8R,9S,10S,13S,14R,17E)-10,13-</u>

		<u>dimethyl-17-(pyridine-4-carbonylhydrazono)-2,4,5,6,7,8,9,11</u>
24		ID ZINC85488756 ZINC Sumber IBScreen Natural Product Nama <u>8,11-dihydroxy-3,3-dimethyl-10-[[1S,2R)-5,9,10-trihydroxy-2-(1-hydroxy-1-methyl-ethyl)-6-oxo-1,2-di</u>
25		ID ZINC00522078 ZINC Sumber IBScreen Natural Product Nama <u>6-fluoro-2-(2-fluorophenyl)chromone</u>
26		ID ZINC00522115 ZINC Sumber IBScreen Natural Product Nama <u>2-(2-fluorophenyl)-6-methyl-chromone</u>
27		ID ZINC08681480 ZINC Sumber TCM Database



Nama	<u>Dihydrotanshinone i</u>
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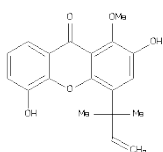
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ZINC	
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Sumber	TCM Database
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Nama	<u>4-(1,1-dimethylprop-2-enyl)-1,2,5-trihydroxy-xanthen-9-one</u>
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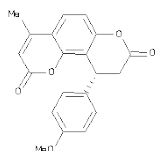
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Sumber	TCM Database
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Nama	<u>4-(1,1-dimethylprop-2-enyl)-2,5-dihydroxy-1-methoxy-xanthen-9-one</u>
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30



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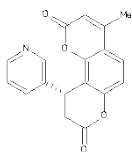
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Sumber	IBScreen Natural Product
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Nama	<u>(10R)-10-(4-methoxyphenyl)-4-methyl-9,10-dihydropyrano[2,3-f]chromene-2,8-dione</u>
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31

ID	ZINC96221612
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ZINC

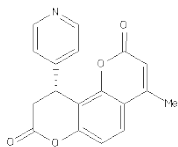
Sumber IBScreen Natural
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Nama (10R)-4-methyl-10-(3-pyridyl)-9,10-dihydropyrano[2,3-f]chromene-2,8-dione

32

ID ZINC96221980

ZINC



Sumber IBScreen Natural
Product

Nama (10R)-4-methyl-10-(4-pyridyl)-9,10-dihydropyrano[2,3-f]chromene-2,8-dione