

BAB V

KESIMPULAN DAN SARAN

A. Kesimpulan

Berdasarkan analisis hasil *docking* molekuler dari senyawa-senyawa *acetogenin* pada tanaman sirsak sebagai antikanker hati, dapat diambil kesimpulan bahwa:

1. Senyawa-senyawa *acetogenin* dari tanaman sirsak memiliki interaksi terhadap BCL-XL dan ERK1/2 sebagai antikanker hati yang ditunjukkan dengan besarnya energi ikatan dan kesesuaian model interaksi dengan ligan asli.
2. Senyawa *acetogenin* dengan model interaksi serupa ligan asli protein BCL-XL yaitu Corossolone melalui ikatan hidrogen konvensional dengan Asn:136; interaksi *pi-stacked* dengan Phe:105; serta ikatan alkil dan pi alkil dengan Ala:142, Ala:149, Arg:102, Arg:139, dan Leu:130. Sedangkan senyawa-senyawa *acetogenin* dengan model interaksi serupa ligan asli protein ERK1/2 yaitu Annocatacin B dan Muricin D, keduanya berinteraksi melalui ikatan alkil dengan Cys:164, Ile:54, Lys:52, Val:37.

B. Saran

1. Perlu dilakukan penelitian lebih lanjut mengenai analisis gugus fungsi yang terlibat dalam setiap interaksi guna mengetahui sisi aktif senyawa yang diteliti dan dapat digunakan sebagai acuan untuk modifikasi struktur menjadi senyawa yang lebih poten.
2. Perlu dilakukan analisis dengan metode lain guna membandingkan hasil *docking* terbaik terhadap senyawa-senyawa *acetogenin* tersebut.

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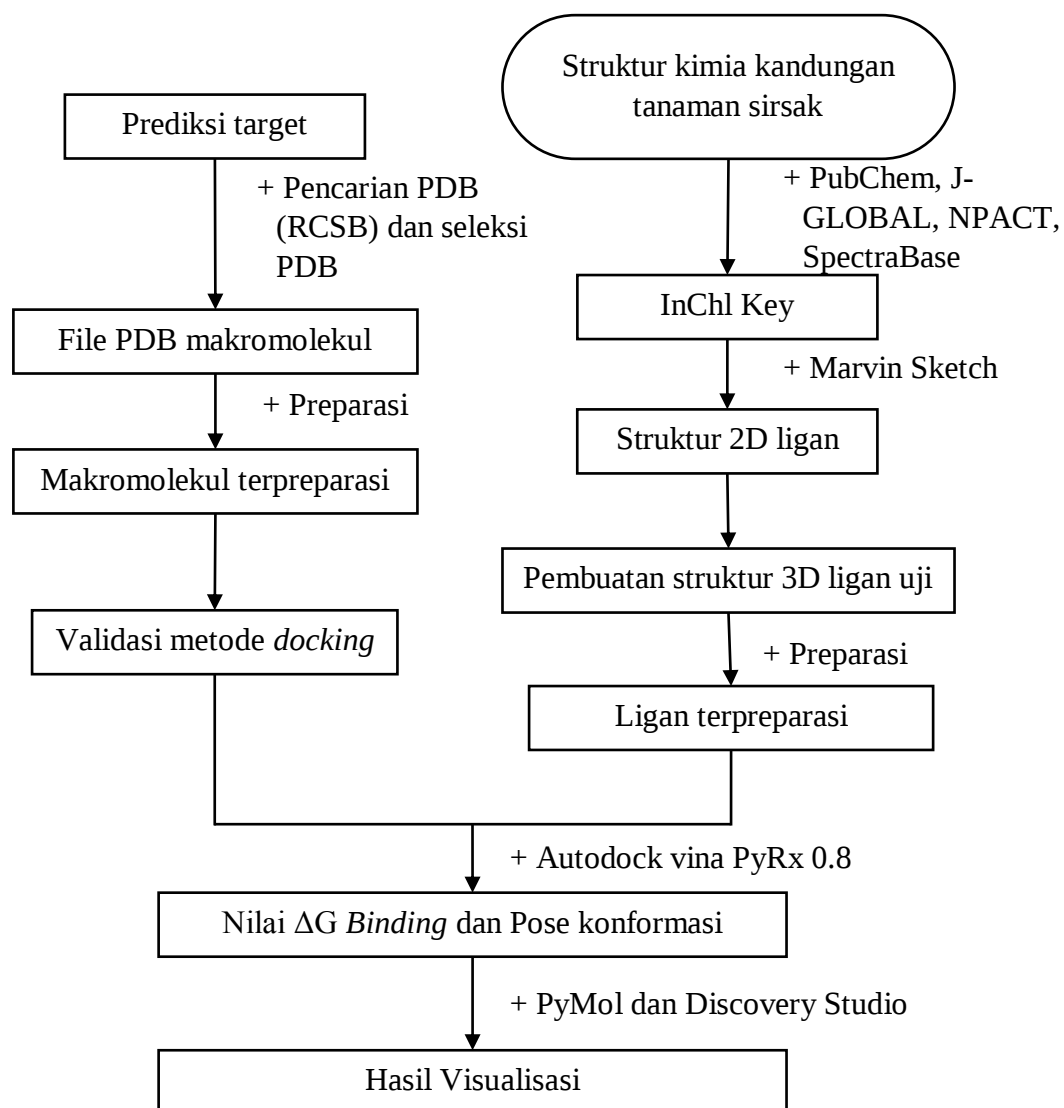
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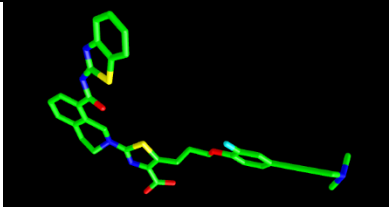
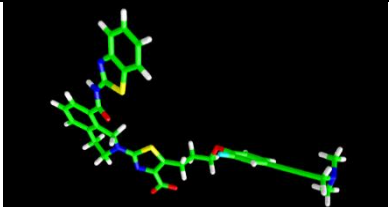
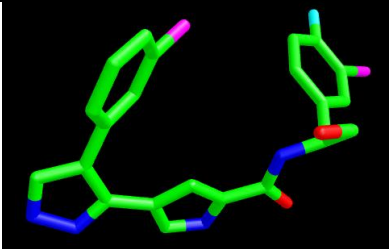
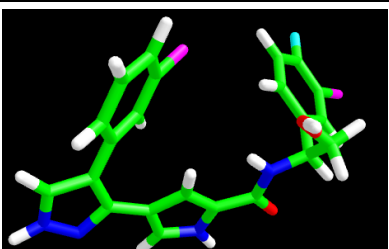
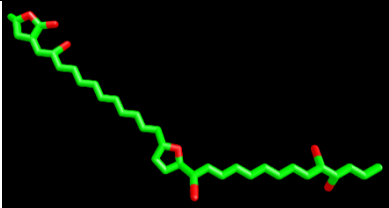
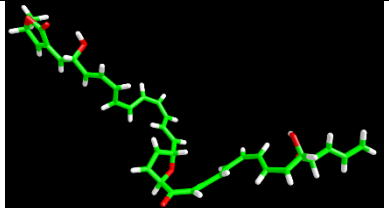
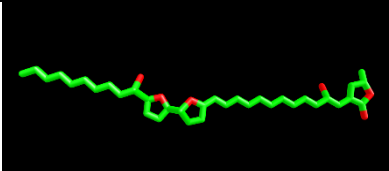
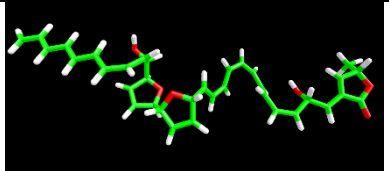
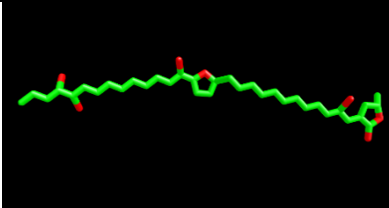
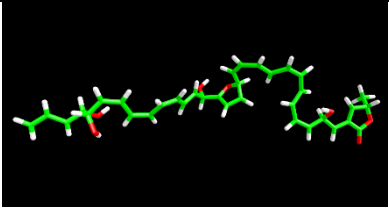
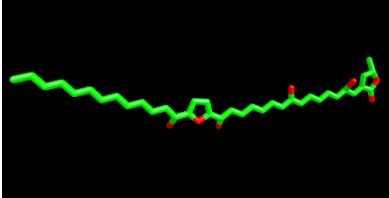
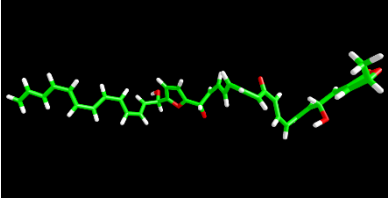
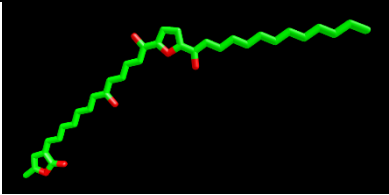
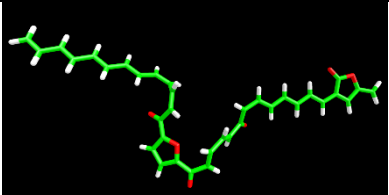
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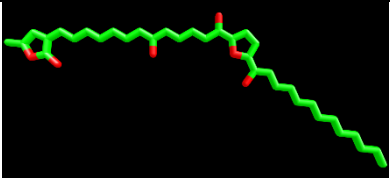
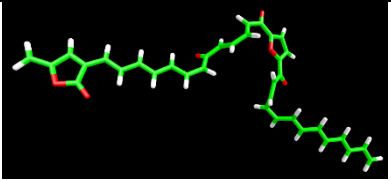
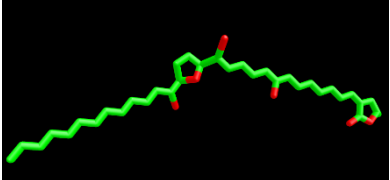
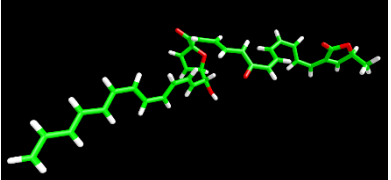
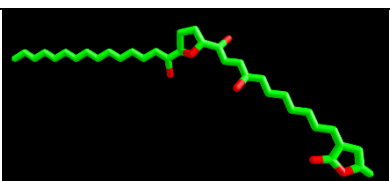
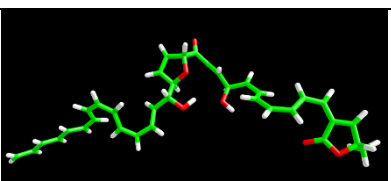
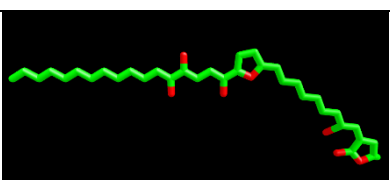
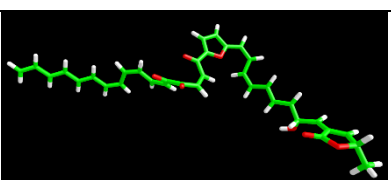
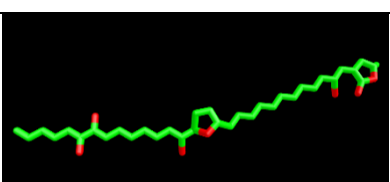
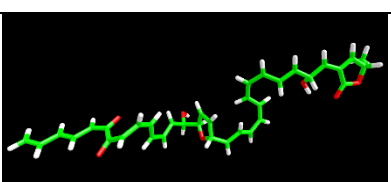
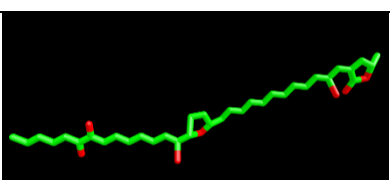
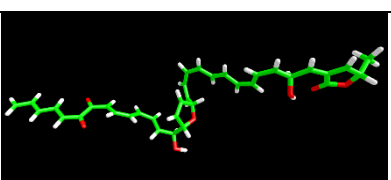
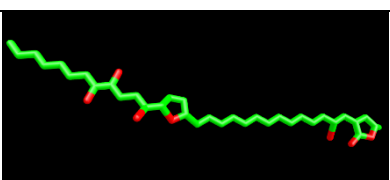
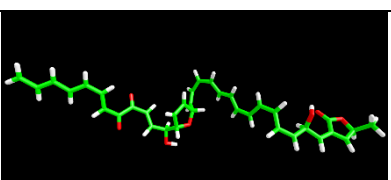
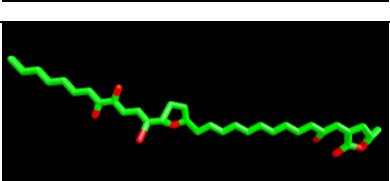
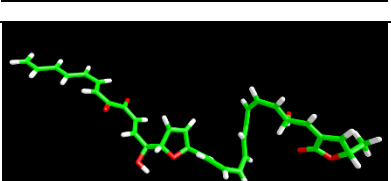
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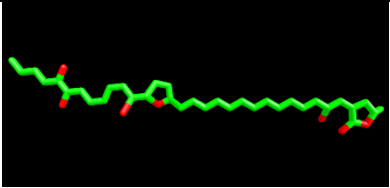
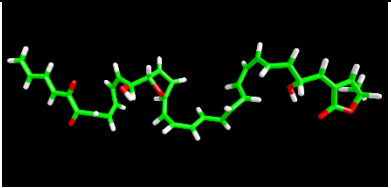
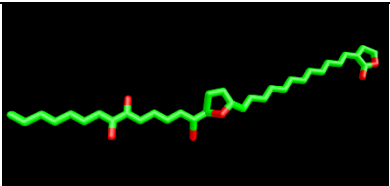
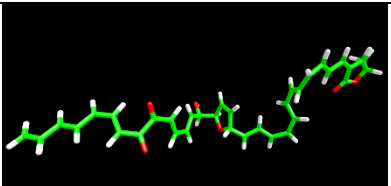
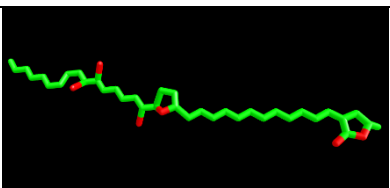
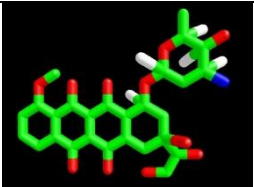
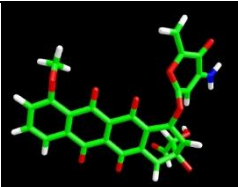
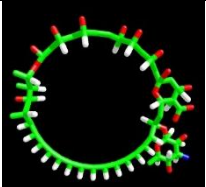
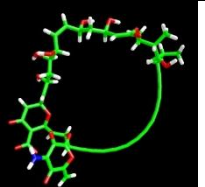
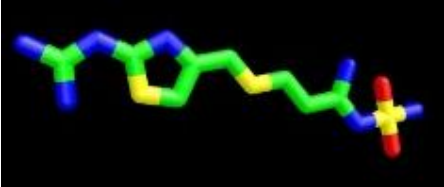
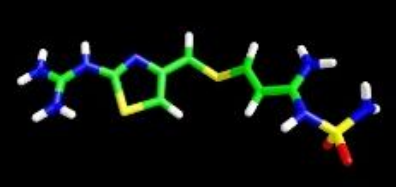
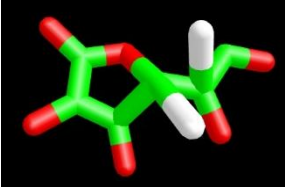
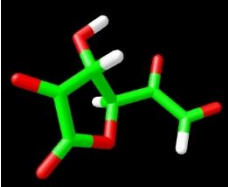
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Lampiran 1. Skema Jalannya Penelitian**Skema Jalannya Penelitian**

Lampiran 2. Hasil Sebelum dan Sesudah Optimasi Ligan Uji

Ligan	Sebelum Optimasi	Sesudah Optimasi
Ligan BCL-XL		
Ligan ERK1/2		
Annocatacin A		
Annocatacin B		
Annocatalin		
Cis-annomontacin		
Corossolin		

Corossolone		
Cis-corossolone		
Longifolicin		
Muricatetrocin A		
Muricin A		
Muricin B		
Muricin C		
Muricin D		

Muricin F		
Muricin H		
Muricin I		
Doxorubicin		
Amfoterisin B		
Famotidin		
Vitamin C		

Lampiran 3. Hasil Uji Statistik

Uji *One-Sample Kolmogorov-Smirnov* ΔG_{bind} Hasil *Docking* Ligan terhadap Protein

BCL-XL

Ligan	$* \Delta G_{bind}$ (kkal/mol)			Signifikansi
	*R1	R2	R3	
Ligan asli	-11,2	-11,7	-11,6	0,929
Annocatacin A	-8,7	-8,9	-8,8	1,000
Annocatacin B	-8,0	-8,3	-8,4	0,960
Annocatalin	-8,8	-8,2	-7,9	0,991
Cis-annomontacin	-8,7	-8,5	-8,8	0,991
Cis-Corossolone	-7,6	-8,1	-8,2	0,904
Corossolin	-8,7	-9,0	-8,8	0,991
Corossolone	-9,0	-9,0	-8,7	0,766
Longifolicin	-8,4	-8,2	-8,4	0,766
Muricatetrocin A	-8,0	-8,7	-8,6	0,886
Muricin A	-8,1	-8,4	-8,4	0,766
Muricin B	-8,3	-8,4	-7,8	0,904
Muricin C	-8,3	-8,3	-7,7	0,766
Muricin D	-8,5	-8,5	-8,2	0,766
Muricin F	-8,9	-8,7	-9,2	0,999
Muricin H	-8,0	-8,4	-8,2	1,000
Muricin I	-8,5	-8,9	-8,3	0,991
Doxorubicin	-9,8	-9,8	-9,8	0,441
Amfoterisin B	-7,0	-7,0	-6,1	0,766
Famotidin	-6,5	-6,6	-6,5	0,766
Vitamin C	-5,9	-5,9	-5,9	-

*keterangan: ΔG_{bind} = *energy binding*; R = replikasi.

Uji *One-Sample Kolmogorov-Smirnov* Hasil *Docking* Ligan terhadap Protein
ERK1/2

Ligan	ΔG_{bind} (kkal/mol)			Signifikansi
	*R1	R2	R3	
Ligan asli	-10,5	-10,5	-10,6	0,766
Annocatacin A	-7,5	-7,9	-7,6	0,960
Annocatacin B	-8,1	-8,0	-8,0	0,766
Annocatalin	-8,0	-7,6	-7,8	1,000
Cis-annomontacin	-7,5	-7,9	-7,7	1,000
Cis-Corossolone	-7,5	-7,5	-7,9	0,766
Corossolin	-7,3	-7,4	-7,9	0,904
Corossolone	-7,8	-7,8	-7,5	0,766
Longifolicin	-7,8	-7,5	-7,4	0,960
Muricatetrocin A	-7,9	-7,7	-7,4	0,999
Muricin A	-8,0	-8,0	-8,0	-
Muricin B	-8,2	-8,0	-8,2	0,766
Muricin C	-7,9	-8,0	-8,1	1,000
Muricin D	-8,2	-8,1	-8,0	1,000
Muricin F	-7,7	-7,7	-7,3	0,766
Muricin H	-7,6	-7,4	-7,2	1,000
Muricin I	-7,7	-7,9	-7,4	0,999
Doxorubicin	-9,8	-9,9	-9,9	0,766
Amfoterisin B	-5,6	-5,3	-5,4	0,991
Famotidin	-6,2	-6,5	-6,3	0,991
Vitamin C	-5,5	-5,5	-5,5	-

*keterangan: ΔG_{bind} = *energy binding*; R = replikasi.

Lampiran 4. Data Hasil *Docking* Molekuler dengan Autodock Vina

1. Replikasi 1 Hasil *Docking* terhadap Protein BCL-XL

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Ligan asli	-11 ,2	0	0
2	Ligan asli	-9 ,6	11 ,053	4 ,569
3	Ligan asli	-9 ,5	11 ,881	4 ,24
4	Ligan asli	-9 ,5	13 ,089	4 ,779
5	Ligan asli	-9 ,5	12 ,673	4 ,366
6	Ligan asli	-9 ,4	11 ,452	4 ,864
7	Ligan asli	-9 ,3	11 ,268	3 ,931
8	Ligan asli	-9 ,3	11 ,652	4 ,641
9	Ligan asli	-9 ,3	11 ,48	4 ,8

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatacin A	-8 ,7	0	0
2	Annocatacin A	-8	5 ,669	3 ,123
3	Annocatacin A	-8	2 ,911	1 ,747
4	Annocatacin A	-7 ,9	5 ,431	3 ,562
5	Annocatacin A	-7 ,9	12 ,644	2 ,023
6	Annocatacin A	-7 ,9	1 ,933	1 ,42
7	Annocatacin A	-7 ,7	7 ,024	3 ,582
8	Annocatacin A	-7 ,7	14 ,277	3 ,597
9	Annocatacin A	-7 ,5	7 ,626	4 ,666

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatacin B	-8	0	0
2	Annocatacin B	-7 ,9	6 ,093	3 ,635
3	Annocatacin B	-7 ,7	6 ,803	3 ,455
4	Annocatacin B	-7 ,7	9 ,412	2 ,766
5	Annocatacin B	-7 ,7	3 ,08	1 ,843
6	Annocatacin B	-7 ,6	9 ,034	2 ,597
7	Annocatacin B	-7 ,4	6 ,527	3 ,751
8	Annocatacin B	-7 ,4	2 ,634	1 ,863
9	Annocatacin B	-7 ,3	9 ,373	2 ,444

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatalin	-8 ,8	0	0
2	Annocatalin	-8 ,4	3 ,123	1 ,822
3	Annocatalin	-7 ,9	2 ,465	1 ,613
4	Annocatalin	-7 ,9	13 ,315	3 ,556
5	Annocatalin	-7 ,8	6 ,29	3 ,43
6	Annocatalin	-7 ,7	5 ,756	3 ,992
7	Annocatalin	-7 ,7	11 ,013	3 ,627
8	Annocatalin	-7 ,7	5 ,604	4 ,156
9	Annocatalin	-7 ,7	9 ,708	3 ,885

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annomontacin cis	-8 ,7	0	0
2	Annomontacin cis	-8 ,5	2 ,196	1 ,416
3	Annomontacin cis	-8 ,4	13 ,172	2 ,961
4	Annomontacin cis	-8 ,1	4 ,22	2 ,604
5	Annomontacin cis	-7 ,9	12 ,573	2 ,877
6	Annomontacin cis	-7 ,9	12 ,71	3 ,846
7	Annomontacin cis	-7 ,8	2 ,29	1 ,504
8	Annomontacin cis	-7 ,7	13 ,347	2 ,918
9	Annomontacin cis	-7 ,7	5 ,44	3 ,252

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Cis-Corossolone	-7 ,6	0	0
2	Cis-Corossolone	-7 ,5	9 ,884	2 ,647
3	Cis-Corossolone	-7 ,4	6 ,756	2 ,719
4	Cis-Corossolone	-7 ,4	10 ,052	2 ,983
5	Cis-Corossolone	-7 ,3	10 ,27	2 ,597
6	Cis-Corossolone	-7 ,3	9 ,468	3 ,833
7	Cis-Corossolone	-7 ,2	9 ,419	2 ,933
8	Cis-Corossolone	-7 ,2	9 ,632	2 ,369
9	Cis-Corossolone	-7 ,1	10 ,371	2 ,666

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Corossolin	-8 ,7	0	0
2	Corossolin	-8 ,7	12 ,903	2 ,919
3	Corossolin	-8 ,4	12 ,531	3 ,71
4	Corossolin	-8 ,4	4 ,334	2 ,297
5	Corossolin	-8 ,3	4 ,524	2 ,593
6	Corossolin	-8 ,2	2 ,004	1 ,578
7	Corossolin	-8	7 ,61	4 ,97
8	Corossolin	-7 ,8	12 ,727	5 ,611
9	Corossolin	-7 ,8	5 ,782	4 ,099

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Corossolone	-9	0	0
2	Corossolone	-8 ,5	2 ,148	1 ,553
3	Corossolone	-8 ,5	2 ,383	1 ,785
4	Corossolone	-8 ,4	5 ,846	3 ,864
5	Corossolone	-8 ,3	11 ,645	3 ,413
6	Corossolone	-8 ,3	2 ,258	1 ,54
7	Corossolone	-8 ,2	11 ,537	4 ,511
8	Corossolone	-8 ,1	11 ,572	3 ,904
9	Corossolone	-7 ,8	8 ,283	3 ,975

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Longifolicin	-8 ,4	0	0
2	Longifolicin	-8 ,2	11 ,486	4 ,326
3	Longifolicin	-8 ,1	3 ,335	1 ,803
4	Longifolicin	-7 ,9	11 ,33	5 ,453
5	Longifolicin	-7 ,8	11 ,268	4 ,762
6	Longifolicin	-7 ,7	8 ,522	4 ,59
7	Longifolicin	-7 ,7	3 ,357	1 ,606
8	Longifolicin	-7 ,7	9 ,565	5 ,138
9	Longifolicin	-7 ,7	3 ,526	1 ,916

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricatetrocin A	-8	0	0
2	Muricatetrocin A	-7 ,9	4 ,946	3 ,082
3	Muricatetrocin A	-7 ,8	3 ,47	2 ,047
4	Muricatetrocin A	-7 ,8	10 ,58	3 ,238
5	Muricatetrocin A	-7 ,8	6 ,877	3 ,799
6	Muricatetrocin A	-7 ,7	4 ,999	3 ,087
7	Muricatetrocin A	-7 ,6	6 ,135	3 ,623
8	Muricatetrocin A	-7 ,5	5 ,494	3 ,279
9	Muricatetrocin A	-7 ,5	6 ,043	3 ,458

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin A	-8 ,1	0	0
2	Muricin A	-7 ,9	3 ,311	2 ,161
3	Muricin A	-7 ,5	10 ,79	1 ,721
4	Muricin A	-7 ,3	2 ,07	1 ,365
5	Muricin A	-7 ,2	6 ,38	3 ,647
6	Muricin A	-7 ,2	5 ,367	2 ,052
7	Muricin A	-7 ,1	6 ,962	3 ,614
8	Muricin A	-7 ,1	10 ,991	1 ,754
9	Muricin A	-7	11 ,459	3 ,14

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin B	-8 ,3	0	0
2	Muricin B	-8 ,3	7 ,81	5 ,079
3	Muricin B	-8 ,2	2 ,405	1 ,474
4	Muricin B	-8	5 ,309	3 ,315
5	Muricin B	-8	8 ,682	5 ,76
6	Muricin B	-7 ,9	10 ,296	5 ,496
7	Muricin B	-7 ,9	6 ,326	3 ,636
8	Muricin B	-7 ,8	8 ,174	5 ,1
9	Muricin B	-7 ,8	8 ,134	4 ,078

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin C	-8 ,3	0	0
2	Muricin C	-8 ,3	3 ,294	2 ,127
3	Muricin C	-8 ,2	11 ,754	2 ,468
4	Muricin C	-7 ,7	12 ,486	5 ,287
5	Muricin C	-7 ,6	5 ,935	3 ,473
6	Muricin C	-7 ,6	5 ,384	3 ,148
7	Muricin C	-7 ,5	3 ,835	2 ,3
8	Muricin C	-7 ,4	6 ,033	3 ,279
9	Muricin C	-7 ,4	10 ,032	2 ,968

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin D	-8 ,5	0	0
2	Muricin D	-8	12 ,116	3 ,829
3	Muricin D	-8	11 ,469	2 ,795
4	Muricin D	-7 ,9	2 ,408	1 ,613
5	Muricin D	-7 ,9	10 ,945	2 ,657
6	Muricin D	-7 ,7	6 ,759	3 ,59
7	Muricin D	-7 ,5	10 ,341	3 ,076
8	Muricin D	-7 ,4	10 ,371	2 ,548
9	Muricin D	-7 ,3	12 ,84	3 ,911

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin F	-8 ,9	0	0
2	Muricin F	-8 ,4	13 ,476	2 ,179
3	Muricin F	-8 ,3	6 ,275	4 ,744
4	Muricin F	-8 ,2	7 ,262	4 ,352
5	Muricin F	-8 ,2	8 ,237	4 ,788
6	Muricin F	-8 ,1	8 ,217	5 ,32
7	Muricin F	-8 ,1	7 ,826	4 ,62
8	Muricin F	-8 ,1	6 ,896	3 ,847
9	Muricin F	-8 ,1	5 ,272	3 ,121

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin H	-8	0	0
2	Muricin H	-7 ,9	12 ,062	4 ,008
3	Muricin H	-7 ,7	12 ,827	3 ,947
4	Muricin H	-7 ,7	11 ,769	3 ,056
5	Muricin H	-7 ,6	10 ,952	2 ,747
6	Muricin H	-7 ,5	10 ,545	2 ,403
7	Muricin H	-7 ,4	10 ,884	2 ,77
8	Muricin H	-7 ,4	10 ,05	2 ,828
9	Muricin H	-7 ,3	7 ,762	3 ,016

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin I	-8 ,5	0	0
2	Muricin I	-8 ,1	11 ,193	6 ,847
3	Muricin I	-7 ,9	7 ,427	4 ,721
4	Muricin I	-7 ,9	8 ,586	5 ,06
5	Muricin I	-7 ,8	8 ,206	4 ,848
6	Muricin I	-7 ,8	12 ,147	6 ,585
7	Muricin I	-7 ,8	9 ,192	6 ,828
8	Muricin I	-7 ,8	9 ,525	6 ,087
9	Muricin I	-7 ,7	10 ,633	6 ,755

2. Replikasi 2 Hasil Docking terhadap Protein BCL-XL

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Ligan asli	-11 ,7	0	0
2	Ligan asli	-9 ,9	12 ,854	4 ,499
3	Ligan asli	-9 ,7	11 ,934	4 ,155
4	Ligan asli	-9 ,7	13 ,043	4 ,754
5	Ligan asli	-9 ,6	11 ,464	4 ,337
6	Ligan asli	-9 ,5	11 ,916	4 ,34
7	Ligan asli	-9 ,5	11 ,518	4 ,117
8	Ligan asli	-9 ,5	13 ,016	4 ,782
9	Ligan asli	-9 ,1	12 ,024	4 ,532

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatacin A	-8 ,9	0	0
2	Annocatacin A	-8 ,7	13 ,376	1 ,648
3	Annocatacin A	-8 ,5	12 ,536	2 ,249
4	Annocatacin A	-8 ,3	14 ,565	2 ,703
5	Annocatacin A	-8	12 ,062	4 ,031
6	Annocatacin A	-7 ,7	4 ,41	2 ,829
7	Annocatacin A	-7 ,7	14 ,612	2 ,938
8	Annocatacin A	-7 ,7	13 ,215	5 ,197
9	Annocatacin A	-7 ,6	14 ,544	3 ,089

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatacin B	-8 ,3	0	0
2	Annocatacin B	-8 ,1	2 ,694	1 ,56
3	Annocatacin B	-8 ,1	12 ,164	3 ,363
4	Annocatacin B	-7 ,9	2 ,83	1 ,492
5	Annocatacin B	-7 ,9	2 ,34	1 ,373
6	Annocatacin B	-7 ,7	2 ,642	1 ,723
7	Annocatacin B	-7 ,7	6 ,011	3 ,372
8	Annocatacin B	-7 ,5	3 ,373	1 ,605
9	Annocatacin B	-7 ,3	3 ,001	1 ,435

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatalin	-8 ,2	0	0
2	Annocatalin	-8 ,1	1 ,922	1 ,327
3	Annocatalin	-8	13 ,881	2 ,878
4	Annocatalin	-7 ,9	14 ,522	1 ,641
5	Annocatalin	-7 ,9	5 ,647	3 ,535
6	Annocatalin	-7 ,7	11 ,021	5 ,126
7	Annocatalin	-7 ,4	9 ,657	3 ,638
8	Annocatalin	-7 ,3	8 ,023	3 ,052
9	Annocatalin	-7 ,3	14 ,858	2 ,026

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annomontacin cis	-8 ,5	0	0
2	Annomontacin cis	-8 ,2	2 ,847	1 ,884
3	Annomontacin cis	-8 ,1	12 ,587	4 ,462
4	Annomontacin cis	-8	11 ,542	3 ,145
5	Annomontacin cis	-7 ,9	12 ,058	3
6	Annomontacin cis	-7 ,9	11 ,741	3 ,184
7	Annomontacin cis	-7 ,7	11 ,206	3 ,247
8	Annomontacin cis	-7 ,5	10 ,548	2 ,79
9	Annomontacin cis	-7 ,5	8 ,319	3 ,448

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Cis-Corossolone	-8 ,1	0	0
2	Cis-Corossolone	-7 ,7	12 ,213	4 ,276
3	Cis-Corossolone	-7 ,6	6 ,861	3 ,545
4	Cis-Corossolone	-7 ,5	4 ,889	3 ,144
5	Cis-Corossolone	-7 ,3	10 ,495	3 ,151
6	Cis-Corossolone	-7 ,2	12 ,532	4 ,342
7	Cis-Corossolone	-7 ,2	9 ,925	2 ,684
8	Cis-Corossolone	-7 ,2	10 ,273	2 ,368
9	Cis-Corossolone	-7 ,1	4 ,568	3 ,118

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Corossolin	-9	0	0
2	Corossolin	-8 ,8	2 ,121	1 ,603
3	Corossolin	-8 ,5	11 ,258	4 ,086
4	Corossolin	-8 ,5	12 ,87	2 ,732
5	Corossolin	-8 ,1	5 ,567	3 ,538
6	Corossolin	-8	6 ,874	3 ,614
7	Corossolin	-7 ,9	4 ,9	2 ,461
8	Corossolin	-7 ,8	5 ,693	4 ,079
9	Corossolin	-7 ,8	7 ,043	3 ,888

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Corossolone	-9	0	0
2	Corossolone	-8 ,6	12 ,691	2 ,878
3	Corossolone	-8 ,6	1 ,824	1 ,157
4	Corossolone	-8 ,4	2 ,104	1 ,35
5	Corossolone	-8 ,4	5 ,872	3 ,975
6	Corossolone	-8 ,3	11 ,75	4 ,249
7	Corossolone	-8 ,3	11 ,472	4 ,328
8	Corossolone	-8 ,2	7 ,694	3 ,961
9	Corossolone	-8 ,1	6 ,327	4 ,558

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Longifolicin	-8 ,2	0	0
2	Longifolicin	-7 ,9	3 ,807	2 ,287
3	Longifolicin	-7 ,8	13 ,527	3 ,459
4	Longifolicin	-7 ,7	2 ,921	1 ,782
5	Longifolicin	-7 ,6	10 ,942	3 ,905
6	Longifolicin	-7 ,6	11 ,643	3 ,176
7	Longifolicin	-7 ,5	12 ,044	4 ,262
8	Longifolicin	-7 ,5	10 ,348	4 ,621
9	Longifolicin	-7 ,4	10 ,458	4 ,283

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricatetrocin A	-8 ,7	0	0
2	Muricatetrocin A	-8 ,3	11 ,972	4 ,418
3	Muricatetrocin A	-8 ,3	2 ,146	1 ,456
4	Muricatetrocin A	-8 ,3	14 ,136	3 ,16
5	Muricatetrocin A	-8 ,2	13 ,053	2 ,959
6	Muricatetrocin A	-8 ,2	13 ,474	2 ,587
7	Muricatetrocin A	-8 ,2	6 ,973	5 ,007
8	Muricatetrocin A	-8 ,1	13 ,228	4 ,249
9	Muricatetrocin A	-8	14 ,267	3 ,562

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin A	-8 ,4	0	0
2	Muricin A	-8 ,2	14 ,167	4 ,753
3	Muricin A	-8 ,1	2 ,474	1 ,678
4	Muricin A	-8	13 ,704	4 ,639
5	Muricin A	-7 ,9	13 ,919	4 ,877
6	Muricin A	-7 ,9	8 ,874	5 ,05
7	Muricin A	-7 ,9	13 ,667	6 ,213
8	Muricin A	-7 ,8	14 ,32	1 ,672
9	Muricin A	-7 ,8	8 ,001	4 ,855

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin B	-8 ,4	0	0
2	Muricin B	-8	6 ,59	3 ,959
3	Muricin B	-7 ,9	6 ,845	3 ,772
4	Muricin B	-7 ,9	4 ,081	2 ,591
5	Muricin B	-7 ,8	5 ,283	4 ,048
6	Muricin B	-7 ,7	7 ,728	4 ,747
7	Muricin B	-7 ,5	11 ,537	4 ,886
8	Muricin B	-7 ,4	6 ,593	4 ,103
9	Muricin B	-7 ,4	8 ,704	3 ,758

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin C	-8 ,3	0	0
2	Muricin C	-8	11 ,895	4 ,096
3	Muricin C	-7 ,7	5 ,873	3 ,467
4	Muricin C	-7 ,5	7 ,074	3 ,38
5	Muricin C	-7 ,5	4 ,224	1 ,933
6	Muricin C	-7 ,4	7 ,149	3 ,611
7	Muricin C	-7 ,3	5 ,944	3 ,49
8	Muricin C	-7 ,3	4 ,535	2 ,846
9	Muricin C	-7 ,3	6 ,743	3 ,609

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin D	-8 ,5	0	0
2	Muricin D	-8 ,3	11 ,973	3 ,905
3	Muricin D	-8	2 ,038	1 ,286
4	Muricin D	-8	4 ,166	2 ,702
5	Muricin D	-7 ,9	10 ,631	2 ,418
6	Muricin D	-7 ,7	3 ,285	2 ,249
7	Muricin D	-7 ,7	10 ,194	2 ,564
8	Muricin D	-7 ,6	3 ,993	2 ,157
9	Muricin D	-7 ,6	11 ,254	2 ,575

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin F	-8 ,7	0	0
2	Muricin F	-8 ,5	4 ,854	2 ,918
3	Muricin F	-8 ,4	8 ,08	4 ,627
4	Muricin F	-8 ,3	2 ,087	1 ,363
5	Muricin F	-8 ,3	14 ,036	3 ,317
6	Muricin F	-8 ,3	3 ,893	1 ,95
7	Muricin F	-8 ,2	5 ,791	3 ,491
8	Muricin F	-8 ,2	7 ,893	4 ,682
9	Muricin F	-8	9 ,87	5 ,347

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin H	-8 ,4	0	0
2	Muricin H	-8	6 ,97	4 ,32
3	Muricin H	-8	12 ,012	3 ,876
4	Muricin H	-7 ,9	9 ,238	5 ,799
5	Muricin H	-7 ,8	11 ,856	4 ,206
6	Muricin H	-7 ,7	11 ,896	3 ,86
7	Muricin H	-7 ,6	8 ,71	5 ,873
8	Muricin H	-7 ,5	7 ,288	4 ,307
9	Muricin H	-7 ,5	12 ,066	5 ,643

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin I	-8 ,9	0	0
2	Muricin I	-8 ,8	10 ,679	6 ,086
3	Muricin I	-8 ,3	10 ,099	5 ,465
4	Muricin I	-8 ,2	2 ,216	1 ,658
5	Muricin I	-8	10 ,108	4 ,212
6	Muricin I	-8	3 ,818	2 ,287
7	Muricin I	-8	2 ,215	1 ,569
8	Muricin I	-8	10 ,067	5 ,694
9	Muricin I	-7 ,9	9 ,944	6 ,012

3. Replikasi 3 Hasil *Docking* terhadap Protein BCL-XL

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Ligan asli	-11 ,6	0	0
2	Ligan asli	-10	12 ,833	4 ,18
3	Ligan asli	-9 ,9	11 ,185	4 ,513
4	Ligan asli	-9 ,8	13 ,135	4 ,717
5	Ligan asli	-9 ,8	11 ,89	4 ,173
6	Ligan asli	-9 ,7	11 ,581	4 ,99
7	Ligan asli	-9 ,5	11 ,398	4 ,167
8	Ligan asli	-9 ,5	5 ,423	3 ,455
9	Ligan asli	-9	13 ,136	4 ,812

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatacin A	-8 ,8	0	0
2	Annocatacin A	-8 ,1	5 ,549	3 ,172
3	Annocatacin A	-7 ,7	14 ,087	4 ,713
4	Annocatacin A	-7 ,7	7 ,685	4 ,457
5	Annocatacin A	-7 ,7	13 ,493	4 ,71
6	Annocatacin A	-7 ,6	9 ,111	5 ,376
7	Annocatacin A	-7 ,5	9 ,955	5 ,286
8	Annocatacin A	-7 ,5	5 ,763	3 ,46
9	Annocatacin A	-7 ,4	10 ,606	4 ,821

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatacin B	-8 ,4	0	0
2	Annocatacin B	-8 ,2	5 ,957	3 ,522
3	Annocatacin B	-8 ,2	6 ,24	3 ,001
4	Annocatacin B	-8 ,1	6 ,632	3 ,379
5	Annocatacin B	-8 ,1	6 ,367	3 ,296
6	Annocatacin B	-7 ,9	3 ,96	2 ,51
7	Annocatacin B	-7 ,9	3 ,984	1 ,84
8	Annocatacin B	-7 ,8	6 ,838	4 ,013
9	Annocatacin B	-7 ,8	3 ,895	1 ,997

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatalin	-7 ,9	0	0
2	Annocatalin	-7 ,9	13 ,996	3 ,288
3	Annocatalin	-7 ,8	2 ,524	1 ,72
4	Annocatalin	-7 ,8	5 ,479	3 ,191
5	Annocatalin	-7 ,6	5 ,497	3 ,389
6	Annocatalin	-7 ,4	6 ,996	3 ,445
7	Annocatalin	-7 ,4	9 ,75	4 ,124
8	Annocatalin	-7 ,3	8 ,283	3 ,692
9	Annocatalin	-7 ,3	5 ,671	3 ,906

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annomontacin cis	-8 ,8	0	0
2	Annomontacin cis	-8 ,6	3 ,876	1 ,936
3	Annomontacin cis	-8 ,3	12 ,671	3 ,3
4	Annomontacin cis	-8	11 ,871	3 ,842
5	Annomontacin cis	-7 ,9	13 ,176	3 ,351
6	Annomontacin cis	-7 ,7	13 ,162	3 ,79
7	Annomontacin cis	-7 ,7	12 ,538	2 ,681
8	Annomontacin cis	-7 ,6	12 ,516	2 ,978
9	Annomontacin cis	-7 ,5	9 ,185	3 ,982

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Cis-Corossolone	-8 ,2	0	0
2	Cis-Corossolone	-7 ,8	9 ,344	2 ,696
3	Cis-Corossolone	-7 ,8	9 ,367	3 ,132
4	Cis-Corossolone	-7 ,6	11 ,11	3 ,896
5	Cis-Corossolone	-7 ,5	10 ,3	2 ,606
6	Cis-Corossolone	-7 ,4	9 ,91	2 ,272
7	Cis-Corossolone	-7 ,4	7 ,343	3 ,665
8	Cis-Corossolone	-7 ,4	10 ,481	2 ,913
9	Cis-Corossolone	-7 ,4	11 ,511	3 ,367

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Corossolin	-8 ,8	0	0
2	Corossolin	-8 ,4	11 ,815	3 ,807
3	Corossolin	-8 ,3	6 ,978	3 ,787
4	Corossolin	-8 ,2	5 ,986	4 ,228
5	Corossolin	-8 ,1	2 ,982	1 ,931
6	Corossolin	-8	12 ,409	3 ,039
7	Corossolin	-8	5 ,455	3 ,533
8	Corossolin	-8	5 ,319	3 ,132
9	Corossolin	-7 ,9	5 ,819	4 ,287

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Corossolone	-8 ,7	0	0
2	Corossolone	-8 ,7	13 ,228	3 ,434
3	Corossolone	-8 ,5	7 ,377	4 ,514
4	Corossolone	-8 ,4	8 ,682	5 ,09
5	Corossolone	-8 ,2	7 ,152	4 ,552
6	Corossolone	-8 ,2	9 ,137	5 ,688
7	Corossolone	-8 ,1	5 ,73	3 ,24
8	Corossolone	-8 ,1	3 ,172	1 ,928
9	Corossolone	-8	12 ,612	3 ,882

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Longifolicin	-8 ,4	0	0
2	Longifolicin	-8 ,4	12 ,132	3 ,18
3	Longifolicin	-7 ,9	11 ,619	3 ,977
4	Longifolicin	-7 ,8	10 ,601	4 ,005
5	Longifolicin	-7 ,8	9 ,839	4 ,198
6	Longifolicin	-7 ,8	11 ,146	4 ,623
7	Longifolicin	-7 ,8	12 ,623	3 ,108
8	Longifolicin	-7 ,8	5 ,432	3 ,876
9	Longifolicin	-7 ,8	7 ,162	4 ,741

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricatetrocin A	-8 ,6	0	0
2	Muricatetrocin A	-8 ,4	12 ,673	4 ,574
3	Muricatetrocin A	-8 ,1	12 ,279	3 ,37
4	Muricatetrocin A	-8 ,1	4 ,661	2 ,953
5	Muricatetrocin A	-8	11 ,757	4 ,322
6	Muricatetrocin A	-7 ,9	12 ,572	4 ,312
7	Muricatetrocin A	-7 ,9	12 ,93	3 ,518
8	Muricatetrocin A	-7 ,8	13 ,208	3 ,467
9	Muricatetrocin A	-7 ,8	2 ,243	1 ,509

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin A	-8 ,4	0	0
2	Muricin A	-8 ,4	13 ,768	4 ,484
3	Muricin A	-8 ,1	5 ,693	3 ,372
4	Muricin A	-7 ,9	13 ,364	4 ,783
5	Muricin A	-7 ,9	7 ,294	5 ,241
6	Muricin A	-7 ,9	8 ,105	4 ,594
7	Muricin A	-7 ,9	14 ,186	3 ,582
8	Muricin A	-7 ,9	7 ,401	5 ,115
9	Muricin A	-7 ,8	13 ,492	5 ,011

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin B	-7 ,8	0	0
2	Muricin B	-7 ,8	2 ,471	1 ,84
3	Muricin B	-7 ,7	12 ,404	4 ,825
4	Muricin B	-7 ,6	10 ,606	2 ,929
5	Muricin B	-7 ,6	11 ,17	3 ,432
6	Muricin B	-7 ,5	11 ,768	4 ,341
7	Muricin B	-7 ,5	11 ,577	3 ,738
8	Muricin B	-7 ,4	12 ,081	2 ,565
9	Muricin B	-7 ,3	10 ,409	3 ,933

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin C	-7 ,7	0	0
2	Muricin C	-7 ,6	10 ,595	2 ,509
3	Muricin C	-7 ,5	11 ,931	4 ,909
4	Muricin C	-7 ,4	7 ,178	3 ,829
5	Muricin C	-7 ,3	4 ,777	2 ,921
6	Muricin C	-7 ,3	12 ,357	5 ,862
7	Muricin C	-7 ,2	7 ,741	3 ,793
8	Muricin C	-7 ,2	5 ,796	3 ,424
9	Muricin C	-7 ,2	11 ,49	3 ,262

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin D	-8 ,2	0	0
2	Muricin D	-8	12 ,222	4 ,733
3	Muricin D	-8	11 ,854	3 ,95
4	Muricin D	-7 ,9	11 ,129	2 ,457
5	Muricin D	-7 ,8	10 ,563	2 ,906
6	Muricin D	-7 ,8	6 ,726	3 ,29
7	Muricin D	-7 ,8	7 ,071	3 ,449
8	Muricin D	-7 ,7	1 ,543	1 ,077
9	Muricin D	-7 ,7	10 ,119	2 ,652

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin F	-9 ,2	0	0
2	Muricin F	-8 ,5	3 ,494	1 ,947
3	Muricin F	-8 ,4	6 ,616	4 ,75
4	Muricin F	-8 ,3	5 ,546	3 ,031
5	Muricin F	-8 ,3	5 ,923	3 ,177
6	Muricin F	-8 ,1	7 ,584	4 ,243
7	Muricin F	-8 ,1	9 ,254	4 ,841
8	Muricin F	-8 ,1	11 ,794	3 ,393
9	Muricin F	-8	6 ,246	4 ,518

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin H	-8 ,2	0	0
2	Muricin H	-8 ,1	12 ,253	5 ,264
3	Muricin H	-7 ,9	8 ,08	5 ,124
4	Muricin H	-7 ,9	2 ,618	1 ,596
5	Muricin H	-7 ,8	8 ,221	5 ,317
6	Muricin H	-7 ,7	8 ,862	5 ,182
7	Muricin H	-7 ,7	11 ,358	6 ,87
8	Muricin H	-7 ,6	14 ,181	6 ,038
9	Muricin H	-7 ,5	10 ,416	6 ,947

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin I	-8 ,3	0	0
2	Muricin I	-8 ,3	4 ,999	2 ,609
3	Muricin I	-8 ,1	5 ,692	3 ,469
4	Muricin I	-8 ,1	13 ,915	4 ,436
5	Muricin I	-7 ,8	6 ,632	3 ,829
6	Muricin I	-7 ,7	11 ,066	4 ,877
7	Muricin I	-7 ,7	13 ,278	3 ,013
8	Muricin I	-7 ,6	13 ,63	4 ,565
9	Muricin I	-7 ,6	12 ,807	6 ,132

4. Replikasi 1 Hasil *Docking* terhadap Protein ERK1/2

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Ligan asli	-10 ,5	0	0
2	Ligan asli	-9 ,8	4 ,091	2 ,947
3	Ligan asli	-9 ,7	9 ,106	4 ,086
4	Ligan asli	-9 ,6	5 ,085	3 ,577
5	Ligan asli	-9 ,6	9 ,312	3 ,532
6	Ligan asli	-9 ,4	4 ,709	3 ,319
7	Ligan asli	-9 ,4	4 ,749	3 ,499
8	Ligan asli	-8 ,9	3 ,414	2 ,706
9	Ligan asli	-8 ,9	9 ,309	3 ,848

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatacin A	-7 ,5	0	0
2	Annocatacin A	-7 ,5	10 ,522	2 ,694
3	Annocatacin A	-7 ,4	4 ,271	1 ,448
4	Annocatacin A	-7 ,3	1 ,995	1 ,466
5	Annocatacin A	-7 ,2	10 ,644	1 ,86
6	Annocatacin A	-7 ,1	10 ,702	2 ,011
7	Annocatacin A	-7	4 ,852	2 ,682
8	Annocatacin A	-6 ,9	9 ,867	2 ,848
9	Annocatacin A	-6 ,8	10 ,595	2 ,609

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatacin B	-8 ,1	0	0
2	Annocatacin B	-7 ,5	10 ,832	2 ,765
3	Annocatacin B	-7 ,3	4 ,938	2 ,829
4	Annocatacin B	-7 ,2	3 ,602	1 ,924
5	Annocatacin B	-7 ,2	4 ,683	3 ,043
6	Annocatacin B	-7	8 ,983	3 ,222
7	Annocatacin B	-7	4 ,741	2 ,954
8	Annocatacin B	-6 ,8	10 ,027	3 ,005
9	Annocatacin B	-6 ,6	10 ,123	5 ,447

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatalin	-8	0	0
2	Annocatalin	-7 ,7	3 ,526	2 ,306
3	Annocatalin	-7 ,6	2 ,431	1 ,478
4	Annocatalin	-7 ,5	10 ,363	2 ,526
5	Annocatalin	-7 ,2	4 ,845	2 ,901
6	Annocatalin	-7 ,1	4 ,627	3 ,024
7	Annocatalin	-7 ,1	4 ,991	2 ,149
8	Annocatalin	-7	10 ,545	3 ,085
9	Annocatalin	-6 ,9	4 ,475	1 ,977

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annomontacin cis	-7 ,5	0	0
2	Annomontacin cis	-7 ,4	9 ,1	2 ,832
3	Annomontacin cis	-7 ,2	5 ,028	2 ,434
4	Annomontacin cis	-7 ,1	8 ,18	4 ,464
5	Annomontacin cis	-7 ,1	9 ,971	2 ,569
6	Annomontacin cis	-7	10 ,078	2 ,21
7	Annomontacin cis	-6 ,9	11 ,374	4 ,891
8	Annomontacin cis	-6 ,9	8 ,027	4 ,143
9	Annomontacin cis	-6 ,9	9 ,01	4 ,326

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Cis-Corossolone	-7 ,5	0	0
2	Cis-Corossolone	-7 ,5	3 ,801	1 ,737
3	Cis-Corossolone	-7 ,4	9 ,574	2 ,814
4	Cis-Corossolone	-7 ,4	4 ,265	2 ,45
5	Cis-Corossolone	-7 ,4	9 ,36	2 ,985
6	Cis-Corossolone	-7 ,2	3 ,79	1 ,765
7	Cis-Corossolone	-7 ,1	9 ,815	2 ,576
8	Cis-Corossolone	-7 ,1	6 ,479	3 ,164
9	Cis-Corossolone	-6 ,9	3 ,13	1 ,3

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Corossolin	-7 ,3	0	0
2	Corossolin	-7 ,2	10 ,705	3 ,072
3	Corossolin	-7	5 ,858	2 ,824
4	Corossolin	-6 ,9	10 ,481	3 ,366
5	Corossolin	-6 ,9	10 ,874	3 ,901
6	Corossolin	-6 ,8	8 ,902	5 ,709
7	Corossolin	-6 ,8	10 ,672	3 ,413
8	Corossolin	-6 ,7	11 ,204	6 ,756
9	Corossolin	-6 ,7	5 ,928	3 ,207

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Corossolone	-7 ,8	0	0
2	Corossolone	-7 ,4	3 ,751	1 ,695
3	Corossolone	-6 ,9	11 ,276	5 ,973
4	Corossolone	-6 ,8	5 ,647	3 ,075
5	Corossolone	-6 ,7	10 ,013	6 ,382
6	Corossolone	-6 ,6	5 ,324	2 ,605
7	Corossolone	-6 ,5	6 ,084	3 ,165
8	Corossolone	-6 ,5	6 ,189	2 ,852
9	Corossolone	-6 ,5	8 ,927	5 ,395

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Longifolicin	-7 ,8	0	0
2	Longifolicin	-7 ,6	2 ,359	1 ,564
3	Longifolicin	-7 ,5	10 ,515	2 ,376
4	Longifolicin	-7 ,3	4 ,821	1 ,509
5	Longifolicin	-7 ,1	9 ,679	3 ,369
6	Longifolicin	-7	4 ,44	2 ,344
7	Longifolicin	-7	10 ,403	3 ,059
8	Longifolicin	-6 ,9	8 ,755	2 ,22
9	Longifolicin	-6 ,9	5 ,22	2 ,184

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricatetrocin A	-7 ,9	0	0
2	Muricatetrocin A	-7 ,7	3 ,449	1 ,24
3	Muricatetrocin A	-7 ,4	3 ,795	2 ,045
4	Muricatetrocin A	-7 ,2	2 ,017	1 ,335
5	Muricatetrocin A	-7 ,2	7 ,375	2 ,858
6	Muricatetrocin A	-7 ,1	10 ,993	2 ,249
7	Muricatetrocin A	-7 ,1	7 ,289	3 ,247
8	Muricatetrocin A	-7	3 ,031	1 ,97
9	Muricatetrocin A	-6 ,9	10 ,257	2 ,652

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin A	-8	0	0
2	Muricin A	-7 ,8	3 ,239	2 ,094
3	Muricin A	-7 ,7	3 ,434	1 ,651
4	Muricin A	-7 ,3	4 ,162	2 ,263
5	Muricin A	-7 ,2	9 ,343	5 ,457
6	Muricin A	-7 ,1	7 ,35	1 ,949
7	Muricin A	-7	4 ,482	2 ,553
8	Muricin A	-7	9 ,558	5 ,431
9	Muricin A	-7	4 ,846	2 ,487

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin B	-8 ,2	0	0
2	Muricin B	-7 ,7	2 ,756	2 ,12
3	Muricin B	-7 ,3	10 ,56	1 ,774
4	Muricin B	-7 ,1	10 ,952	1 ,56
5	Muricin B	-6 ,9	10 ,332	1 ,846
6	Muricin B	-6 ,2	10 ,141	4 ,217
7	Muricin B	-6 ,1	10 ,201	5 ,439
8	Muricin B	-6 ,1	8 ,245	5 ,172
9	Muricin B	-6 ,1	10 ,786	2 ,266

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin C	-7 ,9	0	0
2	Muricin C	-7 ,6	1 ,924	1 ,216
3	Muricin C	-7 ,6	10 ,207	2 ,486
4	Muricin C	-7 ,5	2 ,725	1 ,463
5	Muricin C	-7 ,3	2 ,42	1 ,486
6	Muricin C	-7 ,2	3 ,954	2 ,298
7	Muricin C	-6 ,9	7 ,246	3 ,856
8	Muricin C	-6 ,9	5 ,082	2 ,627
9	Muricin C	-6 ,8	6 ,576	2 ,197

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin D	-8 ,2	0	0
2	Muricin D	-7 ,9	5 ,106	2 ,423
3	Muricin D	-7 ,8	3 ,583	1 ,821
4	Muricin D	-7 ,7	10 ,705	2 ,154
5	Muricin D	-7 ,5	5 ,749	2 ,691
6	Muricin D	-7 ,5	5 ,188	2 ,61
7	Muricin D	-7 ,3	7 ,51	2 ,697
8	Muricin D	-7 ,3	9 ,835	5 ,012
9	Muricin D	-7 ,1	10 ,683	2 ,899

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin F	-7 ,7	0	0
2	Muricin F	-7 ,5	9 ,948	3 ,192
3	Muricin F	-7 ,4	5 ,797	2 ,928
4	Muricin F	-7 ,4	2	1 ,224
5	Muricin F	-7 ,3	2 ,198	1 ,475
6	Muricin F	-7 ,3	2 ,798	1 ,622
7	Muricin F	-7 ,3	6 ,888	3 ,605
8	Muricin F	-7 ,2	5 ,88	2 ,999
9	Muricin F	-7 ,2	9 ,756	3 ,164

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin H	-7 ,6	0	0
2	Muricin H	-7 ,3	10 ,517	2 ,474
3	Muricin H	-6 ,9	7 ,527	2 ,61
4	Muricin H	-6 ,9	10 ,43	2 ,887
5	Muricin H	-6 ,8	8 ,742	4 ,984
6	Muricin H	-6 ,7	4 ,544	2 ,553
7	Muricin H	-6 ,5	10 ,418	3 ,274
8	Muricin H	-6 ,4	8 ,615	4 ,932
9	Muricin H	-6 ,3	10 ,871	6 ,971

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin I	-7 ,7	0	0
2	Muricin I	-7 ,3	10 ,35	2 ,42
3	Muricin I	-7 ,2	5 ,792	2 ,768
4	Muricin I	-7	3 ,927	2 ,356
5	Muricin I	-6 ,9	9 ,453	3 ,541
6	Muricin I	-6 ,9	2 ,067	1 ,373
7	Muricin I	-6 ,8	9 ,825	2 ,65
8	Muricin I	-6 ,8	8 ,513	4 ,539
9	Muricin I	-6 ,7	12 ,453	4 ,148

5. Replikasi 2 Hasil *Docking* terhadap Protein ERK1/2

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Ligan asli	-10 ,5	0	0
2	Ligan asli	-9 ,8	4 ,069	2 ,949
3	Ligan asli	-9 ,7	9 ,093	4 ,086
4	Ligan asli	-9 ,7	5 ,083	3 ,561
5	Ligan asli	-9 ,6	9 ,261	3 ,537
6	Ligan asli	-9 ,4	4 ,656	3 ,465
7	Ligan asli	-9 ,2	4 ,95	3 ,618
8	Ligan asli	-9 ,1	4 ,781	3 ,352
9	Ligan asli	-8 ,8	6 ,101	4 ,318

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatacin A	-7 ,9	0	0
2	Annocatacin A	-7 ,8	10 ,739	1 ,287
3	Annocatacin A	-7 ,4	10 ,667	1 ,553
4	Annocatacin A	-7 ,2	10 ,572	2 ,425
5	Annocatacin A	-6 ,8	4 ,517	2 ,171
6	Annocatacin A	-6 ,8	5 ,212	2 ,95
7	Annocatacin A	-6 ,7	4 ,416	2 ,74
8	Annocatacin A	-6 ,6	5 ,131	2 ,947
9	Annocatacin A	-6 ,5	10 ,36	2 ,895

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatacin B	-8	0	0
2	Annocatacin B	-8	10 ,655	2 ,332
3	Annocatacin B	-7 ,8	10 ,102	2 ,336
4	Annocatacin B	-7 ,4	10 ,122	3 ,058
5	Annocatacin B	-7 ,3	10 ,978	2 ,701
6	Annocatacin B	-7 ,2	4 ,829	2 ,676
7	Annocatacin B	-7 ,1	10 ,306	2 ,908
8	Annocatacin B	-6 ,9	8 ,802	3 ,35
9	Annocatacin B	-6 ,9	10 ,528	3 ,456

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatalin	-7 ,6	0	0
2	Annocatalin	-7 ,3	2 ,46	1 ,757
3	Annocatalin	-7 ,2	4 ,348	2 ,334
4	Annocatalin	-7 ,2	2 ,647	1 ,704
5	Annocatalin	-7 ,1	8 ,531	3 ,174
6	Annocatalin	-7	4 ,276	1 ,457
7	Annocatalin	-6 ,8	9 ,647	2 ,926
8	Annocatalin	-6 ,8	6 ,428	1 ,84
9	Annocatalin	-6 ,6	3 ,45	1 ,713

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annomontacin cis	-7 ,9	0	0
2	Annomontacin cis	-7 ,2	9 ,677	2 ,781
3	Annomontacin cis	-6 ,9	7 ,722	4 ,64
4	Annomontacin cis	-6 ,9	10 ,779	5 ,225
5	Annomontacin cis	-6 ,9	10 ,073	3 ,315
6	Annomontacin cis	-6 ,9	10 ,753	5 ,411
7	Annomontacin cis	-6 ,7	7 ,202	4 ,606
8	Annomontacin cis	-6 ,6	11 ,266	6 ,262
9	Annomontacin cis	-6 ,6	11 ,202	4 ,618

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Cis-Corossolone	-7 ,5	0	0
2	Cis-Corossolone	-7	3 ,358	1 ,045
3	Cis-Corossolone	-6 ,8	7 ,97	3 ,267
4	Cis-Corossolone	-6 ,8	7 ,945	4 ,331
5	Cis-Corossolone	-6 ,7	10 ,226	4 ,173
6	Cis-Corossolone	-6 ,6	4 ,025	2 ,012
7	Cis-Corossolone	-6 ,5	4 ,781	2 ,367
8	Cis-Corossolone	-6 ,5	2 ,132	1 ,419
9	Cis-Corossolone	-6 ,4	10 ,018	2 ,135

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Corossolin	-7 ,4	0	0
2	Corossolin	-7 ,4	10 ,232	2 ,455
3	Corossolin	-7 ,3	10 ,024	1 ,917
4	Corossolin	-7 ,3	10 ,435	1 ,814
5	Corossolin	-7 ,2	3 ,411	1 ,59
6	Corossolin	-7 ,1	3 ,146	1 ,628
7	Corossolin	-7	9 ,934	3 ,121
8	Corossolin	-7	10 ,242	2 ,655
9	Corossolin	-6 ,9	3 ,898	1 ,836

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Corossolone	-7 ,8	0	0
2	Corossolone	-7 ,4	3 ,22	1 ,875
3	Corossolone	-7 ,1	6 ,558	2 ,483
4	Corossolone	-6 ,9	9 ,411	5 ,68
5	Corossolone	-6 ,7	10 ,662	3 ,688
6	Corossolone	-6 ,7	10 ,024	6 ,79
7	Corossolone	-6 ,6	10 ,247	3 ,38
8	Corossolone	-6 ,5	6 ,097	3 ,947
9	Corossolone	-6 ,5	10 ,272	6 ,621

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Longifolicin	-7 ,5	0	0
2	Longifolicin	-7 ,4	5 ,401	1 ,787
3	Longifolicin	-7 ,4	2 ,728	1 ,672
4	Longifolicin	-7 ,4	2 ,112	1 ,36
5	Longifolicin	-7 ,1	3 ,741	1 ,861
6	Longifolicin	-7	4 ,74	2 ,797
7	Longifolicin	-6 ,9	9 ,652	3 ,47
8	Longifolicin	-6 ,8	10 ,078	3 ,308
9	Longifolicin	-6 ,8	8 ,118	2 ,703

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricatetrocin A	-7 ,7	0	0
2	Muricatetrocin A	-7 ,2	3 ,835	1 ,741
3	Muricatetrocin A	-7 ,2	4 ,373	2 ,056
4	Muricatetrocin A	-7 ,2	9 ,132	4 ,622
5	Muricatetrocin A	-7 ,1	4 ,093	1 ,858
6	Muricatetrocin A	-7	9 ,911	3 ,965
7	Muricatetrocin A	-7	11 ,11	7 ,238
8	Muricatetrocin A	-6 ,9	9 ,973	5 ,539
9	Muricatetrocin A	-6 ,8	6 ,751	4 ,249

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin A	-8	0	0
2	Muricin A	-7 ,8	10 ,668	1 ,596
3	Muricin A	-7 ,7	10 ,575	2 ,099
4	Muricin A	-7 ,2	10 ,927	2 ,738
5	Muricin A	-7 ,2	4 ,027	1 ,913
6	Muricin A	-7	4 ,646	2 ,392
7	Muricin A	-6 ,9	10 ,332	3 ,125
8	Muricin A	-6 ,9	9 ,342	5 ,835
9	Muricin A	-6 ,9	9 ,335	6 ,168

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin B	-8	0	0
2	Muricin B	-7 ,7	1 ,681	1 ,239
3	Muricin B	-7 ,6	2 ,844	1 ,815
4	Muricin B	-6 ,9	3 ,893	2 ,154
5	Muricin B	-6 ,7	4 ,971	2 ,982
6	Muricin B	-6 ,7	3 ,345	2 ,364
7	Muricin B	-6 ,7	4 ,261	3 ,094
8	Muricin B	-6 ,6	5 ,275	3 ,021
9	Muricin B	-6 ,5	6 ,388	4 ,528

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin C	-8	0	0
2	Muricin C	-7 ,7	3 ,15	1 ,641
3	Muricin C	-7 ,4	2 ,648	1 ,969
4	Muricin C	-7 ,3	5 ,001	2 ,552
5	Muricin C	-7 ,2	2 ,294	1 ,623
6	Muricin C	-7 ,1	6 ,437	2 ,105
7	Muricin C	-7	2 ,255	1 ,453
8	Muricin C	-6 ,9	9 ,541	3 ,055
9	Muricin C	-6 ,9	2 ,768	1 ,556

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin D	-8 ,1	0	0
2	Muricin D	-7 ,8	3 ,712	1 ,803
3	Muricin D	-7 ,8	3 ,102	1 ,514
4	Muricin D	-7 ,7	3 ,698	1 ,701
5	Muricin D	-7 ,7	5 ,107	2 ,342
6	Muricin D	-7 ,5	6 ,041	2 ,933
7	Muricin D	-7 ,5	5 ,242	2 ,452
8	Muricin D	-7 ,2	9 ,59	4 ,697
9	Muricin D	-7 ,2	9 ,613	4 ,887

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin F	-7 ,7	0	0
2	Muricin F	-7 ,7	2 ,495	1 ,341
3	Muricin F	-7 ,5	10 ,12	2 ,45
4	Muricin F	-7 ,3	3 ,065	1 ,85
5	Muricin F	-7 ,2	9 ,06	2 ,69
6	Muricin F	-7 ,1	4 ,302	2 ,207
7	Muricin F	-7	10 ,237	1 ,931
8	Muricin F	-7	3 ,401	2 ,161
9	Muricin F	-7	9 ,481	2 ,787

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin H	-7 ,4	0	0
2	Muricin H	-7 ,3	10 ,762	2 ,353
3	Muricin H	-7 ,1	10 ,139	2 ,364
4	Muricin H	-7	8 ,266	3 ,44
5	Muricin H	-7	2 ,898	1 ,647
6	Muricin H	-7	4 ,732	2 ,974
7	Muricin H	-6 ,8	7 ,843	4 ,32
8	Muricin H	-6 ,7	5 ,063	2 ,194
9	Muricin H	-6 ,6	4 ,428	2 ,957

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin I	-7 ,9	0	0
2	Muricin I	-7	9 ,644	2 ,68
3	Muricin I	-6 ,9	9 ,513	4 ,936
4	Muricin I	-6 ,8	9 ,741	3 ,201
5	Muricin I	-6 ,8	8 ,377	4 ,555
6	Muricin I	-6 ,7	9 ,65	4 ,523
7	Muricin I	-6 ,7	4 ,347	2 ,618
8	Muricin I	-6 ,7	9 ,485	5 ,285
9	Muricin I	-6 ,7	9 ,67	5 ,087

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Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Ligan asli	-10 ,6	0	0
2	Ligan asli	-9 ,9	3 ,896	2 ,651
3	Ligan asli	-9 ,8	9 ,187	4 ,254
4	Ligan asli	-9 ,7	4 ,944	3 ,337
5	Ligan asli	-9 ,7	9 ,449	3 ,327
6	Ligan asli	-9 ,6	4 ,549	3 ,32
7	Ligan asli	-9 ,6	4 ,445	2 ,994
8	Ligan asli	-9 ,5	9 ,661	3 ,629
9	Ligan asli	-9 ,2	2 ,984	1 ,934

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatacin A	-7 ,6	0	0
2	Annocatacin A	-7 ,4	9 ,962	2 ,115
3	Annocatacin A	-7 ,4	3 ,074	1 ,672
4	Annocatacin A	-7 ,4	1 ,978	1 ,339
5	Annocatacin A	-7 ,1	10 ,231	2 ,016
6	Annocatacin A	-7	3 ,907	1 ,842
7	Annocatacin A	-6 ,8	10 ,311	1 ,986
8	Annocatacin A	-6 ,8	4 ,334	2 ,465
9	Annocatacin A	-6 ,7	10 ,651	1 ,636

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatacin B	-8	0	0
2	Annocatacin B	-7 ,3	4 ,134	2 ,492
3	Annocatacin B	-7 ,3	5 ,947	2 ,733
4	Annocatacin B	-7 ,2	5 ,939	2 ,728
5	Annocatacin B	-7	10 ,455	2 ,727
6	Annocatacin B	-6 ,7	7 ,123	3 ,823
7	Annocatacin B	-6 ,7	6 ,351	2 ,814
8	Annocatacin B	-6 ,5	5 ,69	2 ,622
9	Annocatacin B	-6 ,5	10 ,349	2 ,217

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annocatalin	-7 ,8	0	0
2	Annocatalin	-7 ,4	4 ,883	2 ,157
3	Annocatalin	-7 ,3	4 ,416	2 ,213
4	Annocatalin	-7 ,2	4 ,271	2 ,139
5	Annocatalin	-6 ,9	5 ,152	3 ,088
6	Annocatalin	-6 ,8	10 ,549	5 ,079
7	Annocatalin	-6 ,8	10 ,09	1 ,927
8	Annocatalin	-6 ,6	10 ,103	3 ,171
9	Annocatalin	-6 ,6	10 ,163	3 ,54

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Annomontacin cis	-7 ,7	0	0
2	Annomontacin cis	-7 ,6	8 ,588	2 ,415
3	Annomontacin cis	-7 ,5	3 ,976	2 ,035
4	Annomontacin cis	-7 ,3	2 ,704	1 ,376
5	Annomontacin cis	-7 ,2	9 ,12	2 ,741
6	Annomontacin cis	-7 ,1	8 ,282	3 ,557
7	Annomontacin cis	-7 ,1	9 ,443	2 ,93
8	Annomontacin cis	-7	8 ,681	3 ,941
9	Annomontacin cis	-6 ,8	10 ,362	5 ,68

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Cis-Corossolone	-7 ,9	0	0
2	Cis-Corossolone	-6 ,5	3 ,227	1 ,165
3	Cis-Corossolone	-6 ,4	9 ,99	5 ,805
4	Cis-Corossolone	-6 ,3	5 ,166	2 ,482
5	Cis-Corossolone	-6 ,3	10 ,735	3 ,48
6	Cis-Corossolone	-6 ,3	10 ,37	3 ,941
7	Cis-Corossolone	-6 ,2	10 ,711	7 ,024
8	Cis-Corossolone	-6 ,1	10 ,491	5 ,986
9	Cis-Corossolone	-6	10 ,561	8 ,279

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Corossolin	-7 ,9	0	0
2	Corossolin	-7 ,5	3 ,304	1 ,226
3	Corossolin	-7 ,2	3 ,459	1 ,616
4	Corossolin	-7	10 ,627	2 ,535
5	Corossolin	-6 ,8	4 ,757	2 ,458
6	Corossolin	-6 ,8	4 ,37	2 ,51
7	Corossolin	-6 ,8	6 ,367	3 ,119
8	Corossolin	-6 ,6	10 ,05	5 ,422
9	Corossolin	-6 ,6	6 ,756	3 ,219

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Corossolone	-7 ,5	0	0
2	Corossolone	-7 ,5	9 ,587	2 ,898
3	Corossolone	-7 ,3	2 ,073	1 ,404
4	Corossolone	-6 ,9	8 ,847	3 ,455
5	Corossolone	-6 ,8	7 ,486	1 ,902
6	Corossolone	-6 ,7	3 ,258	1 ,674
7	Corossolone	-6 ,7	9 ,584	4 ,466
8	Corossolone	-6 ,5	7 ,856	3 ,554
9	Corossolone	-6 ,5	10 ,843	5 ,609

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Longifolicin	-7 ,4	0	0
2	Longifolicin	-7 ,2	4 ,592	2 ,523
3	Longifolicin	-7 ,1	9 ,156	5 ,706
4	Longifolicin	-6 ,9	6 ,798	3 ,371
5	Longifolicin	-6 ,7	7 ,993	5 ,047
6	Longifolicin	-6 ,7	9 ,01	5 ,542
7	Longifolicin	-6 ,7	9 ,611	7 ,557
8	Longifolicin	-6 ,6	8 ,913	5 ,502
9	Longifolicin	-6 ,6	7 ,081	3 ,832

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricatetrocin A	-7 ,4	0	0
2	Muricatetrocin A	-7 ,4	3 ,146	1 ,633
3	Muricatetrocin A	-7 ,2	10 ,113	2 ,947
4	Muricatetrocin A	-7 ,1	5 ,08	2 ,123
5	Muricatetrocin A	-6 ,7	8 ,547	4 ,779
6	Muricatetrocin A	-6 ,7	5 ,432	2 ,225
7	Muricatetrocin A	-6 ,5	4 ,534	2 ,103
8	Muricatetrocin A	-6 ,5	8 ,375	2 ,753
9	Muricatetrocin A	-6 ,5	8 ,769	3 ,992

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin A	-8	0	0
2	Muricin A	-7 ,8	3 ,424	1 ,95
3	Muricin A	-7 ,6	10 ,512	1 ,531
4	Muricin A	-6 ,8	4 ,704	2 ,14
5	Muricin A	-6 ,8	2 ,248	1 ,355
6	Muricin A	-6 ,8	10 ,333	2 ,282
7	Muricin A	-6 ,6	9 ,165	5 ,074
8	Muricin A	-6 ,6	4 ,01	2 ,187
9	Muricin A	-6 ,5	4 ,535	2 ,863

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin B	-8 ,2	0	0
2	Muricin B	-7 ,9	3 ,167	1 ,909
3	Muricin B	-7 ,7	3 ,789	1 ,535
4	Muricin B	-7 ,6	4 ,19	2 ,158
5	Muricin B	-7 ,2	10 ,392	1 ,777
6	Muricin B	-7 ,2	3 ,777	2 ,191
7	Muricin B	-7 ,2	2 ,823	1 ,23
8	Muricin B	-6 ,9	5 ,169	2 ,74
9	Muricin B	-6 ,8	4 ,584	2 ,58

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin C	-8 ,1	0	0
2	Muricin C	-7 ,9	10 ,253	3 ,053
3	Muricin C	-7 ,7	2 ,43	1 ,738
4	Muricin C	-7 ,2	3 ,424	1 ,873
5	Muricin C	-7 ,1	9 ,672	3 ,306
6	Muricin C	-6 ,9	8 ,831	2 ,898
7	Muricin C	-6 ,9	9 ,051	3 ,18
8	Muricin C	-6 ,8	6 ,721	3 ,254
9	Muricin C	-6 ,8	8 ,604	1 ,865

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin D	-8	0	0
2	Muricin D	-7 ,9	5 ,771	3 ,13
3	Muricin D	-7 ,8	4 ,091	2 ,096
4	Muricin D	-7 ,5	3 ,858	1 ,682
5	Muricin D	-7 ,5	3 ,382	1 ,676
6	Muricin D	-7 ,4	4 ,709	1 ,833
7	Muricin D	-7 ,3	6 ,859	4 ,06
8	Muricin D	-7	6 ,567	3 ,937
9	Muricin D	-7	9 ,999	5 ,288

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin F	-7 ,3	0	0
2	Muricin F	-7 ,3	3 ,043	1 ,836
3	Muricin F	-7 ,2	10 ,995	1 ,859
4	Muricin F	-7 ,2	5 ,767	2 ,708
5	Muricin F	-7 ,1	11 ,365	1 ,89
6	Muricin F	-7	2 ,251	0 ,909
7	Muricin F	-6 ,9	10 ,115	2 ,776
8	Muricin F	-6 ,9	11 ,348	4 ,429
9	Muricin F	-6 ,9	6 ,836	3 ,254

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin H	-7 ,2	0	0
2	Muricin H	-7 ,2	3 ,694	1 ,968
3	Muricin H	-7	9 ,88	2 ,456
4	Muricin H	-7	4 ,421	2 ,034
5	Muricin H	-7	9 ,992	2 ,285
6	Muricin H	-6 ,7	5 ,172	2 ,261
7	Muricin H	-6 ,7	5 ,365	2 ,397
8	Muricin H	-6 ,7	2 ,907	1 ,787
9	Muricin H	-6 ,6	8 ,356	4 ,836

Mode	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
1	Muricin I	-7 ,4	0	0
2	Muricin I	-7 ,2	10 ,888	2 ,271
3	Muricin I	-7 ,1	9 ,417	4 ,643
4	Muricin I	-6 ,9	9 ,662	4 ,878
5	Muricin I	-6 ,8	9 ,414	2 ,852
6	Muricin I	-6 ,8	8 ,431	4 ,064
7	Muricin I	-6 ,8	6 ,929	3 ,662
8	Muricin I	-6 ,8	9 ,591	4 ,979
9	Muricin I	-6 ,8	11 ,161	4 ,518