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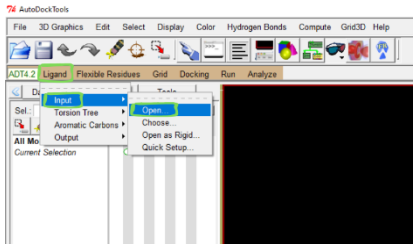
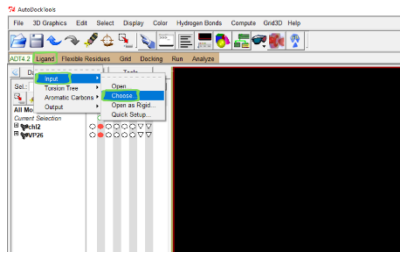
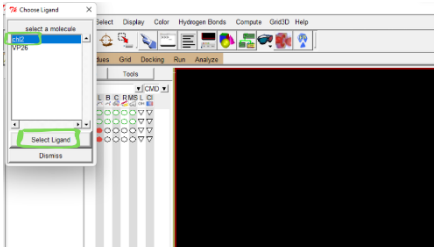
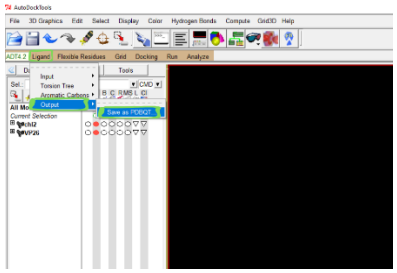
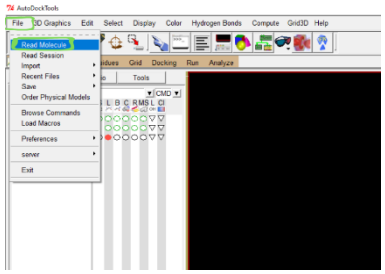
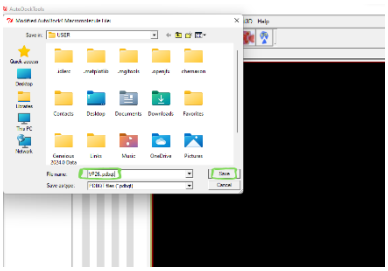
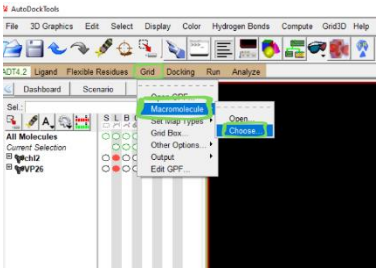
LAMPIRAN

Lampiran 1. *Prosedur* molecular docking

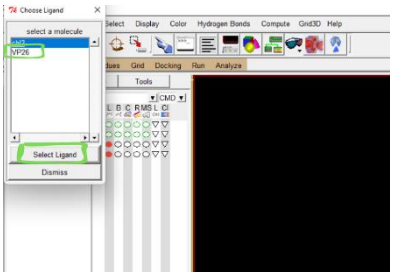
No	Gambar	Keterangan
1.		Buka aplikasi autodock tools kemudian klik icon ligand pilih input kemudian open untuk memasukkan file ligan yang telah di preparasi.
2.		Setelah file ligan telah masuk klik kembali icon ligand pilih input kemudian choose.
3.		Kemudian akan muncul pop up box dan pilih file ligan kemudian klik select.
4.		Setelah ligan dipilih klik icon ligand pilih output kemudian save as pdbqt. Simpan ke dalam folder yang diinginkan dengan format “nama file.pdbqt”.
5.		Untuk memasukkan file protein klik icon file pilih read molecule dan pilih file protein yang telah di preparasi.

6. 

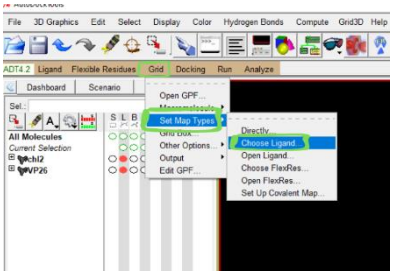
Akan muncul pop up box untuk menyimpan protein dengan format “nama file.pdbqt”.

7. 

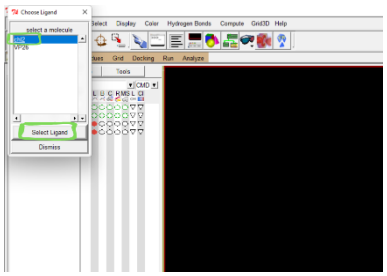
Klik icon grid pilih macromolecule dan choose.

8. 

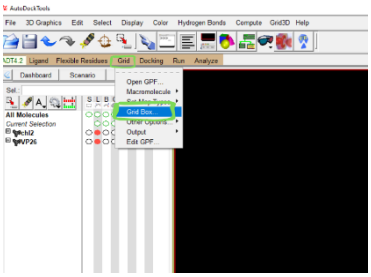
Kemudian akan muncul pop up box dan pilih file protein kemudian klik select.

9. 

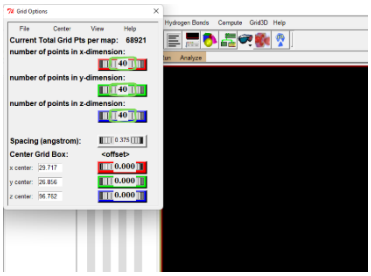
Klik icon grid pilih set map types dan choose ligand.

10. 

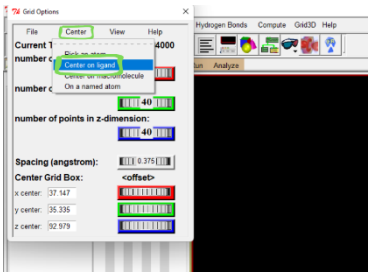
Kemudian akan muncul pop up box dan pilih file ligan kemudian klik select.

11. 

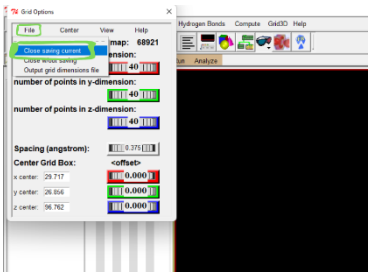
Klik icon grid dan pilih grid box.

12. 

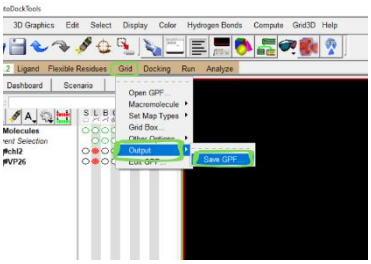
Muncul pop up box untuk mengatur ukuran box. Atar ukuran box pada ukuran 40x40x40.

13. 

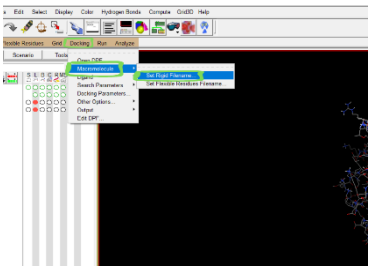
Klik icon center dan pilih center on ligand.

14. 

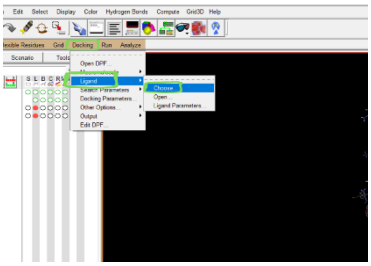
Klik icon file dan pilih close saving curren dan kemudian tutup pop up box tersebut.

15. 

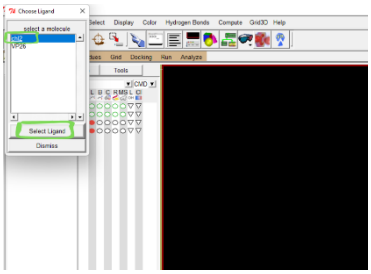
Klik icon grid pilih output kemudian save gpf. Lalu simpan dengan format “nama file.gpf”

16. 

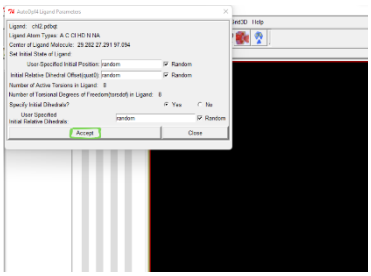
Klik icon docking pilih macromolecule dan set rigid file name. Kemudian pilih file yang telah di save dengan format ".pdbqt".

17. 

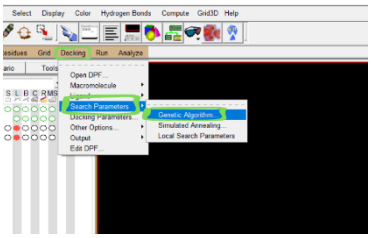
Klik icon docking pilih ligand dan choose.

18. 

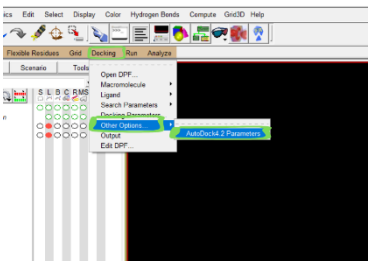
Kemudian akan muncul pop up box dan pilih file ligan kemudian klik select.

19. 

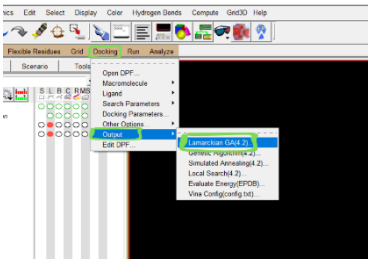
Kemudian akan muncul pop up box dan klik accept.

20. 

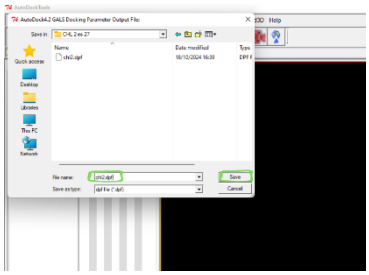
Klik icon docking pilih search parameters dan pilih genetic alhorithm. K Kemudian akan muncul pop up box dan klik accept.Kemudian akan muncul pop up box dan klik accept.

21. 

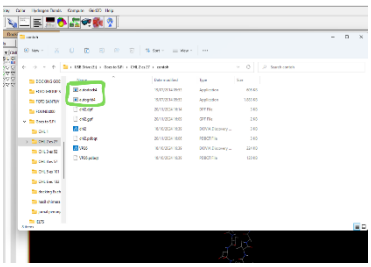
Klik icon docking pilih other option dan autodock4.2 parameters. Kemudian akan muncul 2 pop up box secara berurutan dan klik accept pada keduanya.

22. 

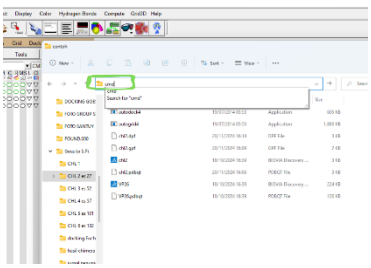
Klik icon docking pilih output dan lamarckian GA(4.2).

23. 

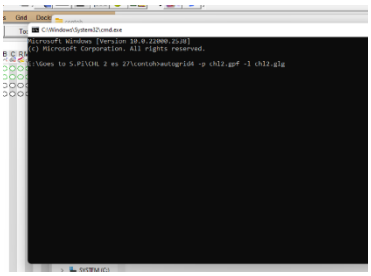
Simpan pada folder penelitian dengan fromat “nama file.dpf”.

24. 

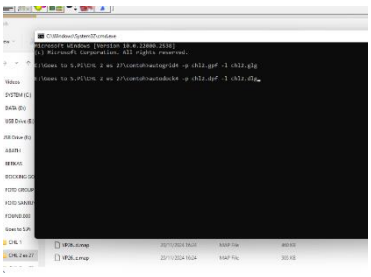
Buka folder pebelitian dan pastikan sudah terdapat software autodock4.

25. 

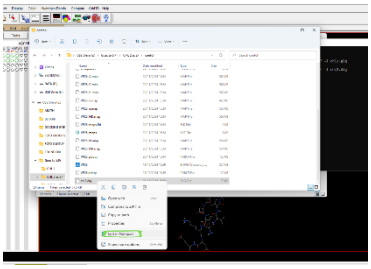
Ketik cmd pada bagian atas seperti pada gambar.

26. 

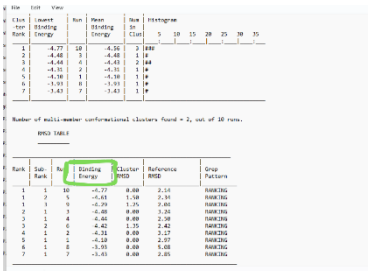
Setelah muncul pop up box dari cmd ketik “autogrid4 -p nama file.gpf -l nama file.glg”.

27. 

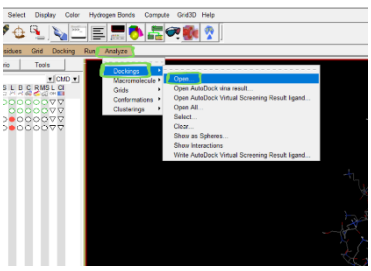
Setelah selesai berproses ketik “autodock4 -p nama file.dpf -l namafile.dlg”.

28. 

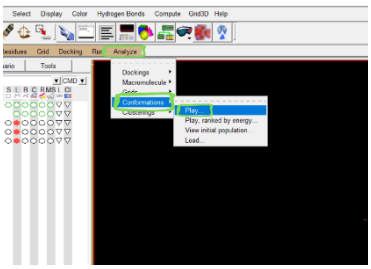
Setelah autodock selesai akan muncul file dengan format “.dlg”. Klik kanan pada file tersebut dan pilih edit in notepad.

29. 

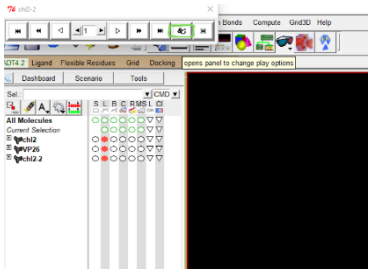
Pada notepad akan ada tabel binding affinity yang didapatkan.

30. 

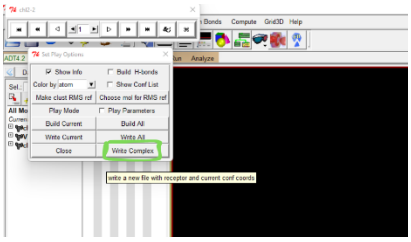
Kembali buka aplikasi autodock tools klik icon analyze pilih dockings dan open. Kemudian pilih file dengan format “.dlg”

31. 

Klik icon analyze pilih conformation dan play.

32. 

Kemudian akan muncul pop up box dan klik icon seperti pada gambar.

33. 

Kemudian akan muncul pop up box lain dan pilih write complex dan simpan pada folder dengan format “.pdb”

Lampiran 2. Senyawa Rumput Laut *Glacilaria changii*

No	Senyawa	Area %	Berat Molekul (MW)	Smiles	PubChem ID
1	*Hexadecylmethylglycerol*	0.02	330	CCCCCCCCCCCCCCCCOC[C@H](CO)OC	10936445
2	*Methyl ester of 3-hydroxydecanoic acid*	0.02			
3	*3-PYRIDINAMINE*	0.05			
4	*1H-Pyrrole, 3-methyl- (CAS)*	0.04			
5	*2-Pentanone, 4,4-dimethyl- (CAS)*	0.01			
6	*2-FURANMETHANOL*	0.01			
7	*N-(2-Methylbutylidene)isobutylami*	0.00			
8	*PYRAZINE, 2,6-DIMETHYL-*	0.01			
9	*1,8-Nonadien-3-ol*	0.00			
10	*NICKEL 1-AMINO-1,9-DIISOTHIOCIPNO-4,8-DI-AZAUNDECAMINE*	0.00			
11	*Cyclohexane, 1,3-dimethoxy-5-methyl-, stereoisomer*	0.00			

12	*Benzeneethanamine, 4-chloro-.alpha.,.alpha.-dimethyl- (CAS)*	0.00			
13	*Cyclohexanone, 3,5-dimethoxy-, trans-*	0.00			
14	*(trans)-2-Azidocyclohexan-1-ol*	0.00			
15	*1,2,3-CYCLOHEXANETRIOL-O,O',O''-D3*	0.02			
16	*1,2-Propanediol, 3-chloro-*	0.03			
17	*CYCLOHEXANONE, 4-HYDROXY-*	0.03			
18	*Cyclopropaneacetic acid, 2-hexyl-*	0.02			
19	*1,4-DIAZABICYCLO[2.2.2]OCTANE*	0.08			
20	*Cyclopropanecarboxamide, N-hept-2-yl-*	0.01			
21	*N,N-Diethylpiperidine-4-carboxamide*	0.00			
22	*Dipropargyl sulfide*	0.00			
23	*Butyric acid, 3-amino-4-methoxy*	0.01			

24	*Acetic acid, fluoro-, ethyl ester*	0.01			
25	*6,8-DIOXABICYCLO(3.2.1)OCTAN-3L-OL-3-D1*	0.19	131		
26	*1,2,3-Propanetriol (CAS)*	1.65			
27	*Bicyclo[10.1.0]tridec-1-ene*	0.00			
28	*2-Phenylethylsilane*	0.08			
29	*1,5-Anhydro-2-O-acetyl-3,4,6-tri-O-methyl-D-glucitol*	0.05			
30	*Butyric acid, dodecyl ester*	0.27			
31	*Naphthalene, 1,2-dihydro-1,1,6-trimethyl-*	0.09			
32	*TRICYCLO[4.3.0.03,8]NONAN-2-ONE*	0.08			
33	*1-Hydroxysulfonyl-3,4,4-trimethyl-2-azetidinone*	0.46			
34	*6,7-Epoxyoctadecanoic acid methyl ester*	0.08	312	CCCCCCCCCCCCC1C(O1)CCCCC(=O)OC	537043
35	*Propanedioic acid, hexyl-, diethyl*	0.02			

	ester (CAS)				
36	*BENZENE, 1-HEPTENYL-*	0.02			
37	*2-Tridecyne*	0.07			
38	*Phenol, 2,4-bis(1,1-dimethylethyl)-(CAS)*	0.07	206	CC(C)(C)C1=CC(=C(C=C1)O)C(C)(C)C	7311
39	*1-Chloroundecane*	0.03	190	CCCCCCCCCCCCl	17186
40	*Formic acid, decyl ester*	0.06	186	CCCCCCCCCCOC=O	79541
41	*trans-.beta.-Ionone*	0.11	192	CC1=C(C(CCC1)(C)C)/C=C/C(=O)C	638014
42	*2,4-Difluorobenzoic acid, 2-formyl-4,6-dichlorophenyl ester*	0.16	330	C1=CC(=C(C=C1F)F)C(=O)OC2=C(C=C(C=C2Cl)Cl)C=O	91717056
43	*Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl- (CAS)*	0.11	220	CC1=CC(=C(C(=C1)C(C)(C)C)O)C(C)(C)C	31404
44	*PHENOL, 2,4-BIS(1,1-DIMETHYLETHYL)-*	0.52	206	CC(C)(C)C1=CC(=C(C=C1)O)C(C)(C)C	7311
45	*1,6-Anhydro-.beta.-d-talopyranose*	1.82	162.14	C1[C@@H]2[C@@H]([C@@H]([C@@H]([C@H](O1)O2)O)O)O	1777528
46	*Dodecanoic acid (CAS)*				
47	*Fumaric acid, ethyl 2-methylallyl*	0.27	198.22	CCOC(=O)/C=C/C(=O)OCC(=C)C	5461492

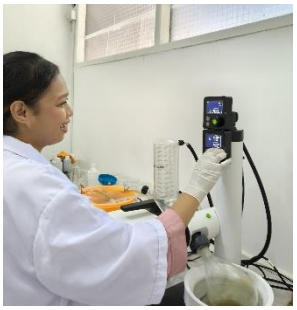
	ester				
48	*9-OXABICYCLO[3.3.1]NONAN-2-ONE-3,3-D2, 6-HYDROXY-, ENDO-*	0.41			
49	*Heptadecane*	0.55			
50	*Heptadecanenitrile (CAS)*	0.10	251	CCCCCCCCCCCCCCCCC#N	79388
51	*9-Tetradecenal, (Z)-*	0.09			
52	*Tetradecanoic acid*	1.43	228	CCCCCCCCCCCCCC(=O)O	11005
53	*6-Hydroxy-4,4,7a-trimethyl-5,6,7,7a-tetrahydrobenzofuran-2(4H)-one*	0.22	196	CC1(CC(CC2(C1=CC(=O)O2)C)O)C	14334
54	*2-Pentadecanone, 6,10,14-trimethyl-*	0.27			
55	*Neophytadiene*	0.06	278	CC(C)CCCC(C)CCCC(C)CCCC(=C)C=C	10446
56	*Pentadecanoic acid*	0.31	242	CCCCCCCCCCCCCCC(=O)O	13849
57	*Dispiro[5.2.5.2]hexadecan-1-one*	1.73	234	C1CCC2(CC1)CCC3(CCCCC3=O)CC2	616403
58	*HEXADECANOIC ACID, METHYL ESTER*	1.76	270	CCCCCCCCCCCCCCCC(=O)OC	8181

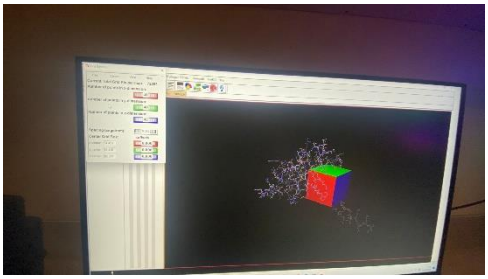
59	*n-Hexadecanoic acid*	0.06	256	CCCCCCCCCCCCCCCC(=O)O	985
60	*n-Hexadecanoic acid*	37.21			
61	*9-Octadecenoic acid (Z)- (CAS)*	1.84	282	CCCCCCCC/C=C\CCCCCCCC(=O)O	445639
62	*9-Octadecenoic acid (Z)-, methyl ester*	1.44	296	CCCCCCCC/C=C\CCCCCCCC(=O)OC	5364509
63	*OCTADEC-9-ENOIC ACID*	5.99	282	CCCCCCCCC=CCCCCCCCC(=O)O	965
64	*2-dodecenoic acid (CAS)*	0.02			
65	*5,8,11,14-Eicosatetraenoic acid, methyl ester, (all-Z)-*	1.58	318	CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)OC	6421258
66	*Dimethylaminoethyl palmitate*	0.66	327	CCCCCCCCCCCCCCCC(=O)OCCN(C)C	3075922
67	*Arachidonic acid*	17.41	304	CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)O	444899
68	*Perilla alcohol angelate*	0.09			
69	*2,6,6,9,2',6',6',9'-OCTAMETHYL-[8,8']BI[TRICYCLO[5.4.0.0 2,9]UNDECYL]*	2.29			
70	*Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester*	3.02	330	CCCCCCCCCCCCCCCC(=O)OC(CO)CO	123409
71	*3-Cyclopentylpropionic acid, 2-*	0.56	213	CN(C)CCOC(=O)CCC1CCCC1	91693811

	dimethylaminoethyl ester				
72	*Arachidonic acid*	0.58			
73	*Oleoyl chloride*	0.37			
74	*9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester*	0.77	356	CCCCCCCC/C=C\CCCCCCCC(=O)OCC(CO)O	5283468
75	*Cyclohexanol, 4-(1,1-dimethylethyl)-1-(2-propenyl)-*	0.53			
76	*9-Octadecenamide, (Z)- (CAS)*	0.67			
77	*5,8,11,14-Eicosatetraenoic acid, ethyl ester, (all-Z)-*	0.58	332	CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)OCC	5367369
78	*5,8,11,14-EICOSATETRAENOIC ACID, ETHYL ESTER, (ALL-Z)-*	1.62			
79	*Heptafluorobutanamide, N-(2-phenylethyl)-N-hexadecyl-*	0.53			
80	*CHOLEST-5-EN-3-OL (3.BETA.)-*	7.89	386	C[C@H](CCCC(C)C)[C@H]1CC [C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4 [C@@]3(CC[C@@H](C4)O)C)C	5997

Lampiran 3. Dokumentasi Kegiatan

No	Dokumentasi	Keterangan
1.		Pencucian rumput laut
2.		Pengeringan rumput laut
3.		Menghaluskan rumput laut yang sudah kering

4.		Proses maserasi
5.		Penyaringan ekstrak sampel
6.		Rotary evaporator
7.		Proses GC-MS

8.		Proses docking