LAMPIRAN

Lampiran 1. Pernyataan Selesai Revisi Proposal

FAKULTAS ILMU KESEHATAN DAN TEKNOLOGI
'AISYIYAH PALEMBANG
PROGRAM STUDI S1 FARMASI
Jl. Kol. H. Burlian –Lr. M. Husin No. 907 RT. 12/RW. 04 Kel. Karya Baru
Kec. Alang-alang LebarKM. 7,5 Palembang 30152 Telp. 0711-421981
www.unisa-palembang.ac.id farmasi.aisyiyah@gmail.com

بِسْمِ اللَّهِ الرَّحْمَٰنِ الرَّحِيمِ

FORMULIR
PERNYATAAN SELESAI REVISI PROPOSAL/ NASKAH SKRIPSI*)
(S-06)

Yang bertandatangan dibawah ini, tim penguji Skripsi 1/ Skripsi 2*):

Nama Mahasiswa : Novrina Nurhasanah

NIM : 2148201030l6

Judul Penelitian : Membangun Protokol Structure - Based Virtual Screening (SBVS) untuk Identifikasi Kandungan Ligan Anti-hipertensi

Pembimbing 1 : Gerry Nugraha, M.Sc., M.Farm

Pembimbing 2 : Suprayetno, S.Si., M.T

Tanggal Ujian : 11 Januari 2025

Menerangkan bahwa naskah Proposal/ ~~Skripsi~~*) telah selesai direvisi oleh tim penguji.

Nama	Tanda Tangan	Tanggal
1. Gerry Nugraha, M.Sc., M.Farm		14/01-2025
2. Suprayetno, S.Si., M.T		15/01-2025
3. Ade Oktasari, M.Sc		15/01-2025
4. Apt. Onny Indriani, M.Farm		14/01-2025

*) : Coret yang tidak perlu.

Lampiran 2. Surat Permohonan Izin Penelitian

	SURAT	No Dokumen	Form-A1
		Berlaku Sejak	
	PERMOHONAN IZIN PENELITIAN PROGRAM STUDI S-1 FARMASI UNIVERSITAS AISYIYAH PALEMBANG	Revisi	000

Hal : Permohonan Izin Penelitian

1	Skripsi
2	PKM/LKTI
3	Penelitian Dosen
4	Luar

Kepada Yth
Kabag Laboratorium Terpadu
Universitas 'Aisyiyah Palembang

Assalamualaikum Wr. Wb.
Sehubungan dengan penelitian kami dalam bidang KIMIA KOMPUTASI, dengan:
Judul Penelitian : Membangun Protokol Structure - Based Virtual Screening (SBVS) untuk Identifikasi Kandungan Ligan Anti-hipertensi
Nama Pembimbing : 1. Gerry Nugraha, M.Sc., M.Farm
2. Suprayetno, S.Si, M.T

No	Nama	NIM/NIP/NIK	No. HP
1	NOVITRIA NURHASANAH	21482010306	089626722068
2			
3			
4			
5			

Bermaksud mengajukan izin penelitian di Laboratorium*): **Farmasetika Dasar / Teknologi Farmasi / Kimia Farmasi / Biologi Farmasi / Farmakologi / Mikrobiologi / Komputasi**
Prodi S1 Farmasi Universitas 'Aisyiyah Palembang.
Penelitian tersebut akan kami laksanakan selama: ..... bulan,
yang terhitung dari : 19 | 03 | 2025 s.d 19 | 08 | 2025

Sebagai bahan pertimbangan, bersama ini dilampirkan lembar pengesahan proposal penelitian.
Demikian permohonan kami, atas perhatiannya diucapkan terima kasih.

Palembang, 19 Maret 2025

Mengetahui,
Dosen Pembimbing

Gerry Nugraha, M.Sc., M.Farm

Pemohon

Novitria Nurhasanah

Menyetujui,
Kabag Laboratorium Terpadu

Neni Riyanti, SKM., M.Kes

Kaprodi S1 Farmasi

Apt. Onny Indriani, M.Farm

Lembar Bimbingan

UNISA
UNIVERSITAS 'AISYIYAH PALEMBANG
FAKULTAS KESEHATAN DAN TEKNOLOGI (FKesT)
PROGRAM STUDI :
S1 FARMASI
Jl. Kol. H. Burlian – Lr. M. Husin KM. 7,5 No. 907 Kota Palembang, Kode Pos 30152, Telp (0711) 417135
Email: farmasi@unisa-palembang.ac.id

FORMULIR BIMBINGAN SKRIPSI

Nama : Novitria Nurhasanah
NIM : 214820103016
Nama Pembimbing : 1. Dr. Gerry Nugraha, M.Sc., M.Farm
2. Suprayetno, S.Si., M.T
Judul Skripsi : Membangun Protokol Structure-Based Virtual Screening (SBVS) Untuk Identifikasi Kandidat Ligan Anti-Hipertensi

No.	Tanggal Konsultasi	Keterangan	Paraf Pembimbing
1	23 Mei 2025	membahas mengenai isi pembahasan skripsi	
2	26 Mei 2025	cara mencari referensi jurnal untuk mempermudah mencari jurnal	
3	27 Mei 2025	Evaluasi penulisan BAB IV	
4	4 Juni 2025	Revisi format penulisan dan isi BAB IV	
5	6 Juni 2025	Revisi format penulisan dan isi BAB IV	
6	9 Juni 2025	Revisi gambar dan tabel BAB IV	
7	10 Juni 2025	Revisi BAB IV	
8	03 Juli 2025	Revisi lembar lampiran	
9	07 Juli 2025	Revisi BAB kesimpulan dan saran	
10	09 Juli 2025	Penyempurnaan isi pembahasan	
11	21 Juli 2025	Revisi BAB IV	
12	22 Juli 2025	Revisi gambar BAB IV	
13	24 Juli 2025	Membahas masalah struktur kimia	
14	25 Juli 2025	Revisi format penulisan	
15	26 Juli 2025	Revisi referensi jurnal	
16	28 Juli 2025	Revisi gambar ligan dan reseptor	
17	29 Juli 2025	Revisi struktur kimia	
18	30 Juli 2025	Membahas kesimpulan dan saran	
19	31 Juli 2025	Revisi lampiran	

Lampiran 3. Hasil data reseptor target pada obat hipertensi.

Nama obat	Common name	Probability
Amlodipin	ADRA2A	1
	ADRA2C	1
	ADRA1D	1
	ADRA1A	1
	KCNK2	1
	ADRA1B	1
	SLC6A3	1
	HTR6	1
	PYGL	0.164912113
	PYGM	0.115736675
	NR1H4	0.115736675
	ADORA3	0.115736675
	CYP2C9	0.115736675
	ADORA2A	0.115736675
	CACNA1B	0.115736675
	F2	0.115736675
	PGR	0.115736675
	SLC6A2	0.115736675
	DRD3	0.115736675
	AR	0.115736675
	SIGMAR1	0.115736675
	PIM1	0.115736675
	PIM2	0.115736675
	MAPK14	0.115736675
	CHRM2	0.115736675
	CHRM1	0.115736675
	CHRM3	0.115736675
	NR3C1	0.115736675
	REN	0.115736675
	EGFR	0.115736675
	TAAR1	0.115736675
	CDK9	0.115736675
	FLT3	0.115736675
	CDK2 CCNA1 CCNA2	0.115736675
	JAK1	0.115736675
	JAK2	0.115736675
	TYK2	0.115736675
	GHSR	0.115736675
	BRD4	0.115736675
	BRD2	0.115736675
	BRD3	0.115736675
	ATAD2	0.115736675
	OPRK1	0.115736675
	ADRB2	0.115736675
	HTR2A	0.115736675
	CCNE2 CDK2 CCNE1	0.115736675
	OPRM1	0.115736675

	OPRD1	0.115736675
	RAF1	0.115736675
	MAPK8	0.115736675
	SLC6A4	0.115736675
	KDR	0.115736675
	MAPK9	0.115736675
	PIM3	0.115736675
	HRH1	0.115736675
	KCNH2	0.115736675
	XIAP	0.115736675
	ERBB2	0.115736675
	SRC	0.115736675
	SPHK1	0.115736675
	BACE1	0.115736675
	PTGER1	0.115736675
	CCNT1	0.115736675
	PRKCI	0.115736675
	ADRB1	0.115736675
	SYK	0.115736675
	ADORA1	0.115736675
	CACNA1D	0.115736675
	PRCP	0.115736675
	MTOR	0.115736675
	TERT	0.115736675
	NOS1	0.115736675
	PIK3CA	0.115736675
	NOS2	0.115736675
	NOS3	0.115736675
	CCNB3 CDK1 CCNB1 CCNB2	0.115736675
	CSF1R	0.115736675
	DPP4	0.115736675
	TRPV3	0.115736675
	EPHX2	0.115736675
	F10	0.115736675
	PRKCB	0.115736675
	LRRK2	0.115736675
	JAK3	0.115736675
	CHEK1	0.115736675
	ABCB1	0.115736675
	ACHE	0.115736675
	ADRB3	0.115736675
	GSK3B	0.115736675
	HSP90AB1	0.115736675
	KIF11	0.115736675
	MAP3K12	0.115736675
	BACE2	0.115736675
	CCR3	0.115736675
	CHRNA4 CHRNB2	0.115736675
	CHRNB3 CHRNA6 CHRNB2 CHRNA3	0.115736675
	MCHR1	0.115736675

	MDM2	0.115736675
	DYRK1A	0.115736675
	PARP1	0.115736675
Lisinopril	ACE	0.982335522
	REN	0.192104608
	XPNPEP1	0.13952343
	XPNPEP2	0.13952343
	MMP2	0.095663487
	MMP8	0.095663487
	ANPEP	0.095663487
	BACE1	0.095663487
	OPRM1	0.095663487
Captopril	ACE	0.956908465
	F2	0.956908465
	REN	0.956908465
	LTA4H	0.956908465
	MME	0.14375215
	XIAP	0.041470299
	SLC5A1	0.031226558
	ACE2	0.031226558
	PLA2G5	0.031226558
	ITGA2B ITGB3	0.031226558
	FNTA FNTB	0.031226558
	CPA3	0.031226558
	HLA-A	0.031226558
	AKR1B1	0.031226558
	SLC22A12	0.031226558
	NOTUM	0.031226558
	TBXAS1	0.031226558
	GSTK1	0.031226558
	MMP13	0.031226558
	MMP12	0.031226558
	DPP4	0.031226558
	BCAT2	0.031226558
	KMO	0.031226558
	PTGS2	0.031226558
	PARP1	0.031226558
	PARP2	0.031226558
	LAP3	0.031226558
	PTGDR2	0.031226558
	CXCL8	0.031226558
	GRM4	0.031226558
	PDE5A	0.031226558
	KDM6B	0.031226558
	PDE9A	0.031226558
	KDM4D	0.031226558
	KDM4C	0.031226558
	APEX1	0.031226558
	AKR1B10	0.031226558
	EDNRA	0.031226558

	HSPA1A	0.031226558
	ITGAL ICAM1 ITGB2	0.031226558
	PTGDR	0.031226558
	KDM4E	0.031226558
	SLCO1B1	0.031226558
	MIF	0.031226558
	KDM5C	0.031226558
	MAPK10	0.031226558
	SORT1	0.031226558
	KDM4A	0.031226558
	ABCC1	0.031226558
	EGLN3	0.031226558
	EDNRB	0.031226558
	ITGAV	0.031226558
	ECE1	0.031226558
	CDC25B	0.031226558
	HSP90AA1	0.031226558
	NR1H4	0.031226558
	AKR1C3	0.031226558
Furosemid	GPR35	0.999621429
	CA2	0.999621429
	CA7	0.999621429
	CA1	0.999621429
	CA6	0.999621429
	CA12	0.999621429
	CA14	0.999621429
	CA9	0.999621429
	CA4	0.999621429
	CA13	0.999621429
	CA5B	0.999621429
	HSD11B1	0.999621429
	CA5A	0.999621429
	CPB2	0.097874534
	KDM5A	0.097874534
	KDM5B	0.097874534
	AKR1C2	0.097874534
	PARP15	0.097874534
	PARP1	0.097874534
	ITGAL ICAM1 ITGB2	0.097874534
	SORT1	0.097874534
	PTGDR2	0.097874534
	CPB1	0.097874534
	GRIK1	0.097874534
	PDPK1	0.097874534
	PTGS2	0.097874534
	DUSP3	0.097874534
	DHODH	0.097874534
	FOLH1	0.097874534
	PARP10	0.097874534
	CPA1	0.097874534

	HAO2	0.097874534
	ADAMTS5	0.097874534
	PYGL	0.097874534
	PYGM	0.097874534
	EDNRA	0.097874534
	MMP3	0.097874534
	MMP9	0.097874534
	PTPN1	0.097874534
	KDM6B	0.097874534
	CASP1	0.097874534
	EGFR	0.097874534
	ADORA1	0.097874534
	PDE4B	0.097874534
	APEX1	0.097874534
	MAP2K1	0.097874534
	GSTP1	0.097874534
	GSTM2	0.097874534
	ECE1	0.097874534
	DAO	0.097874534
	SCN9A	0.097874534
	SLC22A12	0.097874534
	PLEC	0.097874534
	FBP1	0.097874534
	METAP2	0.097874534
	MME	0.097874534
	MIF	0.097874534
	PDE8B	0.097874534
	SLCO1B1	0.097874534
Nifedipin	CACNA1C	1
	HTR2C	1
	ADORA1	1
	MYLK	1
	ADORA3	1
	CYP1A2	1
	CCR2	1
	CACNA1D	1
	KCNA5	1
	ADORA2A	0.256161866
	CYP2C9	0.122339194
	CYP2C19	0.122339194
	AR	0.10560828
	NR3C1	0.10560828
	PGR	0.10560828
	CNR1	0.097239989
	NR1H4	0.097239989
	ADRA1A	0.097239989
	ABCB1	0.097239989
	ALOX15	0.097239989
	VCAM1	0.097239989
	NR1I2	0.097239989

	ADRA1D	0.097239989
	EGFR	0.097239989
	PDE5A	0.097239989
	MAOB	0.097239989
	ADRA1B	0.097239989
	TSPO	0.097239989
	JAK3	0.097239989
	JAK2	0.097239989
	FBP1	0.097239989
	GABRA1	0.097239989
	GABRB3 GABRA3 GABRG2	0.097239989
	GABRB3 GABRG2 GABRA1	0.097239989
	GABRB3 GABRG2 GABRA5	0.097239989
	GABRA2 GABRB3 GABRG2	0.097239989
	GABRA1 GABRB2 GABRG2	0.097239989
	GABRA5	0.097239989
	ALOX5	0.097239989
	PIK3CA	0.097239989
	KDR	0.097239989
	PLCG2	0.097239989
	FLT3	0.097239989
	MAPK8	0.097239989
	ESR2	0.097239989
	MAPK10	0.097239989
	MAPK9	0.097239989
	ADRA2A	0.097239989
	ADRA2C	0.097239989
	ADRA2B	0.097239989
	STK33	0.097239989
	DRD2	0.097239989
	MKNK1	0.097239989
	TERT	0.097239989
	PPME1	0.097239989
	RET	0.097239989
	CTSK	0.097239989
	GUSB	0.097239989
	GRM5	0.097239989
	SCN9A	0.097239989
	BRAF	0.097239989
	TNNI3K	0.097239989
	ALPL	0.097239989
	CBFB	0.097239989
	CDK5R1 CDK5	0.097239989
	CCNE1 CDK2	0.097239989
	ACHE	0.097239989
	BCHE	0.097239989
	CES1	0.097239989
	GSK3B	0.097239989
	TLR4	0.097239989
	APP	0.097239989

	GCK	0.097239989
	GRM1	0.097239989
	ABCG2	0.097239989
	ABL1	0.097239989
	DAPK3	0.097239989
	SRC	0.097239989
	PTK2	0.097239989
	EPHB2	0.097239989
	MKNK2	0.097239989
	AKT1	0.097239989
	LRRK2	0.097239989
	CYP19A1	0.097239989
	ELANE	0.097239989
	PTGS2	0.097239989
	LCK	0.097239989
	MAPK14	0.097239989
	PIK3CD	0.097239989
	CYP17A1	0.097239989
	CRHR1	0.097239989
	CDK2 CCNA1 CCNA2	0.097239989
	METAP1	0.097239989
	CDK2	0.097239989
	CA14	0.097239989
	NAAA	0.097239989
	FLT1	0.097239989
	TYMS	0.097239989
	CCNB3 CDK1 CCNB1 CCNB2	0.097239989
	FGFR1	0.097239989

Lampiran 4.Hasil prediksi reseptor pada penyakit anti-hipertensi

Reseptor Penyakit Hipertensi					
1	BMPR2	122.868	127	BMPR1B	15.12088
2	AGTR1	67.25175	128	HMOX1	14.84815
3	ACE	64.7554	129	MTX2	14.6865
4	AGT	64.58568	130	LINC00963	14.67147
5	TBX4	54.03925	131	F5	14.66659
6	NR3C2	53.93244	132	CASC2	14.66227
7	NOS3	52.6247	133	KNG1	14.65848
8	KCNK3	48.75474	134	HOTAIR	14.58992
9	ACVRL1	44.38021	135	PLAT	14.56073
10	SMAD9	44.18044	136	PIEZO2	14.50459
11	CPS1	42.717	137	LOC106627981	14.48066
12	GNB3	41.94118	138	LPL	14.46873
13	SARS2	41.55809	139	MIR759	14.45312
14	ENG	37.51498	140	PAXIP1-DT	14.4144
15	ATP13A3	36.78733	141	SELP	14.33637
16	CAV1	36.52058	142	LOC129992813	14.20886
17	ADD1	36.18692	143	ABCC8	14.19945
18	REN	34.30341	144	ADRB1	14.12067
19	CYP11B2	33.94545	145	PKD1-AS1	14.11045
20	EIF2AK4	33.0291	146	ACE2	14.08222
21	HYT4	32.54431	147	INSR	14.03907
22	HYT3	32.4819	148	PGR-AS1	13.96212
23	HYT1	32.39532	149	ELN	13.94324
24	PDE3A	32.17579	150	CACNA1H	13.93192
25	PTGIS	32.0968	151	CBS	13.90396
26	HSD11B2	30.01178	152	AGTR2	13.89495
27	NOS2	29.88957	153	F2	13.79352
28	HYT2	29.41568	154	SOD1	13.64694
29	HYT5	29.30778	155	PKHD1	13.60213
30	HYT6	29.30778	156	ACSM3	13.58983
31	SOX17	28.44073	157	ADRB3	13.44489
32	SELE	28.17325	158	FN1	13.40013
33	DGUOK	27.82704	159	STK39	13.29425
34	CORIN	27.66121	160	CLCNKB	13.26705
35	EDN1	27.49101	161	FBN1	13.25469
36	NPPA	27.45892	162	COMT	13.208
37	WNK4	26.51029	163	XDH	13.16657
38	ECE1	26.41057	164	CACNA1D	13.10147
39	CYP3A5	26.3938	165	HIF1A	13.00141
40	CYP11B1	26.2356	166	VEGFA	12.99669

41	SCNN1B	26.11124	167	SLC12A1	12.97297
42	BMPR1A	25.81672	168	FGA	12.92488
43	INS	25.42436	169	RET	12.9011
44	WNK1	25.40674	170	NOTCH1	12.87446
45	PKD1	24.92489	171	CCL2	12.85159
46	FLT1	24.78344	172	LOC129934096	12.78916
47	MIR21	24.76971	173	G6PC3	12.68547
48	KCNA5	23.82595	174	APOA1-AS	12.68206
49	GDF2	23.3629	175	SNHG7	12.6398
50	GIMAP5	23.05255	176	MMP2	12.62043
51	KLHL3	22.95292	177	SNHG14	12.61892
52	H19	22.7748	178	IL1B	12.60139
53	PNMT	22.51741	179	MIR503HG	12.59006
54	MALAT1	22.45936	180	NF1	12.56391
55	MIR17	22.42276	181	IL10	12.46166
56	CDCA3	22.11492	182	JAK2	12.36602
57	ALB	21.95797	183	PGF	12.24501
58	SCNN1G	21.75787	184	NPR3	12.23405
59	LOC102723566	21.72371	185	IGF1	12.20644
60	HYT8	21.45844	186	KCNIP1	12.17811
61	CRP	21.2929	187	CYBA	12.14585
62	MTHFR	21.25066	188	UTS2	12.10794
63	MIAT	21.19805	189	UCA1	12.10585
64	NPPB	20.71773	190	LEPR	12.09356
65	PPARG	20.68644	191	DLX6-AS1	12.06424
66	IL6	20.37082	192	MMP9	11.96114
67	MIR204	19.9564	193	HLA-B	11.95238
68	SFTA3	19.87355	194	SFTPC	11.86794
69	RFH1	19.86273	195	ICAM1	11.84809
70	RGS5	19.85037	196	ZEB2-AS1	11.80785
71	TGFB1	19.80522	197	GRK4	11.79921
72	PVT1	19.7827	198	ENPP1	11.78085
73	HYT7	19.75435	199	BMP6	11.68065
74	SCNN1A	19.70086	200	POMC	11.66527
75	CUL3	19.66972	201	DANCR	11.65613
76	ATP1B1	19.57286	202	CCAT1	11.65613
77	MYH9	19.15067	203	SGK1	11.65516
78	PKD2	18.95068	204	BDKRB2	11.58119
79	GBA1	18.94906	205	GATA3-AS1	11.55077
80	APOE	18.92896	206	PON1	11.53078
81	TNF	18.71746	207	GLA	11.52491
82	SERPINE1	18.71131	208	AKT1	11.52268

83	COL4A4	18.56211	209	LOC110673972	11.51935
84	MEN1	18.45985	210	MT-TI	11.50657
85	ADRB2	18.43175	211	CHGA	11.49654
86	ADIPOQ	18.21725	212	ADD2	11.43639
87	LOC106799833	18.05441	213	ENPEP	11.4343
88	FOXF1	17.81757	214	EDNRB	11.42683
89	PAH	17.77695	215	TP53	11.3814
90	KCNJ5	17.63795	216	SMAD3	11.36942
91	MT-CO2	17.4238	217	SHBG	11.36194
92	GIMAP1-GIMAP5	17.35846	218	GPT	11.34028
93	LEP	17.31962	219	NPY	11.3147
94	COL4A5	17.30416	220	CST3	11.29491
95	MIR20A	17.10816	221	BMP2	11.27812
96	CELA2A	17.08053	222	EPO	11.24214
97	THBD	16.92142	223	TMEM67	11.23714
98	CAPNS1	16.91866	224	SLC6A4	11.20644
99	CTEPH1	16.91329	225	BBS2	11.1816
100	CYP17A1	16.89782	226	NAGLU	11.15487
101	VHL	16.77219	227	APLN	11.15387
102	APOB	16.74844	228	LDLR	11.15341
103	EPHX1	16.64305	229	NEDD4L	11.13326
104	NR3C1	16.5669	230	CASR	11.10368
105	UMOD	16.54744	231	SST	11.08569
106	MIR451A	16.53934	232	VCAM1	11.06772
107	DGUOK-AS1	16.50065	233	BMP4	10.96504
108	RPL5	16.45296	234	CETP	10.95221
109	APOA1	16.44136	235	TH	10.92527
110	F12	16.30016	236	KCNJ1	10.88282
111	SLC12A3	16.17356	237	ALDH2	10.85259
112	MIR155	16.15967	238	ACTA2	10.83829
113	INF2	16.00457	239	BBS5	10.81892
114	MIR22	15.9776	240	ENSG00000230926	10.73895
115	SMAD4	15.75201	241	F3	10.69541
116	EDNRA	15.68078	242	CCN2	10.69051
117	ADM	15.60205	243	PDE5A	10.67208
118	DARS2	15.56291	244	GATA4	10.65835
119	STOX1	15.39475	245	TAC3	10.65302
120	NOTCH3	15.38971	246	SPP1	10.65192
121	NSD1	15.28745	247	SOD2-OT1	10.6304
122	DIPK1A	15.27746	248	NFU1	10.52834
123	VWF	15.24569	249	PRKAR1A	10.50373
124	RETN	15.22394	250	RNLS	10.4781

125	GNAS	15.16932	251	DBH	10.46508
126	KCNMB1	15.16432	252	NKX2-5	10.37721

Lampiran 5. Perintah docking pada YASARA

```
# YASARA MACRO
# TOPIC: 5. Structure prediction
# TITLE: Docking a ligand to a receptor
# REQUIRES: Structure
# AUTHOR: Elmar Krieger
# LICENSE: GPL
# DESCRIPTION: This macro runs VINA or AutoDock to predict the structure of
a ligand-receptor complex. It can also continue a docking run that got interrupted.
An analysis log file is written at the end.

# Parameter section - adjust as needed, but NOTE that some changes only take
effect
# if you start an entirely new docking job, not if you continue an existing one.
#
=============================================================
Processors 10
Processors GPU=1
Antialias 0
Console Off

# You can either set the target structure by clicking on Options > Macro > Set
target,
# by providing it as command line argument (see docs at Essentials > The
command line),
# or by uncommenting the line below and specifying it directly.
#MacroTarget '/home/myname/projects/docking/1sdf'

# Docking method, either VINA (CPU only) or AutoDockLGA (runs on the GPU
if enabled at Options > Processors > Set compute GPU)
method='AutoDockLGA'

# Number of docking runs (maximally 999, each run can take up to an hour)
runs=100

# Docking results usually cluster around certain hot spot conformations,
# and the lowest energy complex in each cluster is saved. Two complexes belong
to
# different clusters if the ligand RMSD is larger than this minimum [A]:
rmsdmin=5.0

# Set to 1 to keep the ligand completely rigid (alternatively you can provide
# the ligand as a *.yob file and fix certain dihedral angles only).
rigid=0
```

Lampiran 6. Perintah md_runmembrane

```
# YASARA MACRO
# TOPIC: 3. Molecular Dynamics
# TITLE: Running a molecular dynamics simulation of a membrane protein with normal or fast
speed
# REQUIRES: Dynamics
# AUTHOR: Elmar Krieger
# LICENSE: GPL
# DESCRIPTION: This macro sets up and runs a simulation of a membrane protein. It scans the
protein for secondary structure elements with hydrophobic surface residues, orients it accordingly
and embeds it in a membrane of adjustable lipid composition. Finally a 250 ps restrained
equilibration simulation is run, which ensures that the membrane can adapt to the newly embedded
protein. Then the real simulation starts.

# Include library functions
include md_library

# Parameter section - adjust as needed, but NOTE that some changes only take
# effect if you start an entirely new simulation, not if you continue an existing one.
#
==========================================================================
==============

#nice -n 20 /home/al/yasara/yasara -txt "/home/al/yasara/2021/ovi/03_md/md_runmembrane.mcr"

Processors CPUThreads=50,GPU=1
Antialias 0
Console Off

# The structure to simulate must be present with a .pdb or .sce extension.
# If a .sce (=YASARA scene) file is present, the membrane and cell must have been added.
# You can either set the target structure by clicking on Options > Macro > Set target,
# by providing it as command line argument (see docs at Essentials > The command line),
# or by uncommenting the line below and specifying it directly.
#MacroTarget 'c:\MyProject\1crn'
MacroTarget /home/al/yasara/2021/ovi /03_md/1o86.yob,Remove=Extension
# Extension of the cell on each side of the protein in the membrane plane (=XZ plane)
# '15' means that the membrane will be 30 A larger than the protein
memextension=15

# Extension of the cell on each side of the protein along the third (water) axis (=Y-axis)
# '10' means that the cell will be 20 A higher than the protein
waterextension=10

# Flag to use a square membrane. This makes sure that also elongated proteins
# embedded in the membrane can rotate freely during very long simulations. If
# only a short simulation is planned, it can be speeded up by setting the flag
# to 0, creating a rectangular membrane that fits the solute more tightly.
square=1

# Membrane composition: The three letter names of phosphatidyl-ethanolamine (PEA),
# phosphatidyl-choline (PCH, also known as POPC), phosphatidyl-serine (PSE), phosphatidyl-
glycerol (PGL),
# cholesterol (CLR) and cardiolipin (CDL) are each followed by the mass percentage for
# each membrane side, and must sum up to 100. CDL conntent cannot exceed 30%.
```

```
# All lipids are 1-palmitoyl, 2-oleoyl by default, except CDL with four 18:2 tails.
# The first percentage is for the bottom side of the membrane, the second is for the top side.
# When YASARA shows you the suggested membrane embedding, you need to check that the
protein
# orientation matches the membrane composition. If not, flip first and second percentages below
and
# rerun the macro. Note that PCH has a large headgroup which cannot form hydrogen bonds, and
# thus reduces membrane stability. PEA is the most stable membrane lipid.
memcomplist()='PEA',100,100,'PCH',0,0,'PSE',0,0,'PGL',0,0,'CLR',0,0,'CDL',0,0
# Or uncomment below to use your own membrane template with 10x10 lipids on each side,
# see membrane simulation recipes for details. In this case, 'memcomplist' will be ignored.
# The 'usermemlist' contains the name of your membrane template followed by its X and Z size.
# If your membrane template name is 'YourChoice', it must be saved as
yasara/yob/membrane_YourChoice.yob
usermemlist()='' # Default
#usermemlist()='YourChoice',77.21,73.24 # Example: Use own membrane 'YourChoice' of 77.21
x 73.24 A size
# pH at which the simulation should be run, by default physiological pH 7.4.
ph=7.4
# The ion concentration as a mass fraction, here we use 0.9% NaCl (physiological solution)
ions='Na,Cl,0.9'
# Forcefield to use (this is a YASARA command, so no '=' used)
ForceField AMBER14
# Simulation temperature, which also serves as the random number seed (see Temp command).
# If you increase the temperature significantly by X%, you also need to reduce the timestep by X%
# by changing the 'tslist' that matches your speed below.
temperature='310'
# Pressure at which the simulation should be run [bar].
pressure=1
# Cutoff
cutoff=8
# Equilibration period in picoseconds:
# During this initial equilibration phase, the membrane is artificially stabilized
# so that it can repack and cover the solute, while solvent molecules are kept outside.
equiperiod=250
# Delay for animations, 1=maximum speed
delay=100
# The format used to save the trajectories: YASARA 'sim', GROMACS 'xtc' or AMBER 'mdcrd'.
# If you don't pick 'sim', a single *.sim restart file will be saved too, since the other
# two formats don't contain velocities, only positions.
format='sim'
# Duration of the complete simulation, must be longer than equiperiod above.
# Alternatively use e.g. duration=5000 to simulate for 5000 picoseconds
# 'if !count duration' simply checks if variable 'duration' as been defined previously (e.g. by an
including macro)
if !count duration
 duration=20000
```

Lampiran 7. perintah md_convert-sim2pdb.mcr

```
# YASARA MACRO
# TOPIC: 3. Molecular Dynamics
# TITLE: Convert between Sim, XTC, MDCrd and PDB simulation trajectories
# REQUIRES: Dynamics 9.5.10
# AUTHOR: Elmar Krieger
# LICENSE: GPL
# DESCRIPTION: This macro converts an existing MD trajectory between various formats.
Supported are conversions between YASARA Sim, GROMACS XTC and AMBER MDCrd
trajectories, as well as conversion to PDB files
# Parameter section - adjust as needed
# ====================================
Antialias 0
Console Off
Processors cputhreads=1, gpu=0
#nice -n 20 /home/gerry/yasara/yasara -txt "/home/gerry/pafr/2_md/md_convert-sim2pdb.mcr"
# The trajectory to convert must be present with a .sim, .xtc or .mdcrd extension.
# The starting scene *_water.sce is also required.
# You can either set the target by clicking on Options > Macro > Set target,
# by providing it as command line argument (see docs at Essentials > The command line),
# or by uncommenting the line below and specifying it directly.
#MacroTarget = 'c:\MyProject\1crn'
#MacroTarget /home/gerry/pafr/2_md/5zkp.sce,Remove=Extension
# Source format (srcformat) can be 'sim' (see SaveSim/LoadSim), 'xtc' (see SaveXTC/LoadXTC)
# or 'mdcrd' (see SaveMDCrd/LoadMDCrd).
# Destination format (dstformat) can be 'sim', 'xtc', 'mdcrd', 'pdb' (a series of PDB files)
# or 'pdbw' (a series of wrapped PDB files, where all atoms are inside the cell
# and potentially wrapped around periodic boundaries (i.e. broken molecules)).
# If one is left empty, YASARA will ask for the formats interactively.
srcformat='sim'
dstformat='pdb'
# Flag if water object should be included (1) or not (0)
waterincluded=0
# Forcefield to use
ForceField AMBER14
```

Lampiran 8. perintah md_analyze.mcr

```
# YASARA MACRO
# TOPIC: 3. Molecular Dynamics
# TITLE: Analyzing a molecular dynamics trajectory
# REQUIRES: Dynamics
# AUTHOR: Elmar Krieger and Kornel Ozvoldik
# LICENSE: GPL
# DESCRIPTION: This macro analyzes a simulation and creates a detailed report with a large
number of plots, e.g. energies, RMSDs, hydrogen bonds. It also tries to identify the main ligand
and provides ligand-specific data. All results are additionally written to a simple text table, which
can be imported into your favorite spreadsheet program. Your own analysis can often be added
with just one line of code, search for 'Example:'.
RequireVersion 20.1.1
# MD report initialization parameters and flags
# ========================================
# The structure to analyze must be present with a .sce extension.
# You can either set the target structure by clicking on Options > Macro > Set target,
# by providing it as command line argument (see docs at Essentials > The command line),
# or by uncommenting the line below (=remove the '#') and specifying it directly.
#MacroTarget 'c:\MyProject\1crn'
# Set common beginning for all result filenames. By default,
# this is the same as the macro target, but you can change
# it to run multiple analyses at the same time.
resultbase=MacroTarget # Default
#resultbase='(MacroTarget)_run1' # Example
# Forcefield to use for analysis, should be the same as the one used to run the simulation
ForceField AMBER14,SetPar=Yes # Default
#ForceField YASARA2,SetPar=Yes # Example: Add a quality Z-score in YASARA Structure
# Number of the solute object whose RMSDs from the starting conformation will be calculated
# If the protein is an oligomer, check the documentation of the 'Sup' command at 'analyzing a
simulation' to avoid pitfalls.
soluteobj=1
# Flag to convert the entire trajectory to PDB format (solute object only)
pdbsaved=0
# The B-factors calculated from the root-mean-square fluctuations can be too large to fit them
# into the PDB file's B-factor column. Replace e.g. 1.0 with 0.1 to scale them down to 10%
bfactorscale=1.0
# Trajectory block to be analyzed. The 'if not count block' skips this part if this macro is included
# by the md_analyzeblock macro, that analyzes the trajectory in blocks (see 'Analyzing a
trajectory' in the docs).
if not count block
 # First snapshot to be analyzed, increase number to ignore an equilibration period.
 firstsnapshot=0
 # Number of snapshots to be analyzed
 snapshots='all'
```

Lampiran 9. perintah BEcalculation.mcr

```
Antialias 0
Console Off
Processors cputhreads=1, gpu=0
#nice -n 20 /home/gerry/yasara/yasara -txt "/home/gerry/2_H2R/7_sce/BEcalculation.mcr"
#konversi pdb ke sce
for k=00001 to 00200
 LoadPDB (MacroDir)\1o86 (k).pdb,Center=No,Correct=No
 SplitObj 1
 DelObj 3
 NiceOriAll
 Cell Auto,Extension=5,Shape=Cuboid,Obj 2
 FixAll
 ForceField NOVA,SetPar=Yes
 Boundary Wall
 SaveSce (MacroDir)\1o86 (k)_complex.sce
 Clear
#Calculation
method = 'VINALS'
runs = 1
rmsdmin = 5.0
rigid = 1
for j=00001 to 00200
 LoadSce (MacroDir)\1o86 (j)_complex.sce
 NameObj 1,receptor
 NameObj 2,ligand
 ForceField AMBER03
 Boundary Wall
 Longrange None
```

Lampiran 10. Mengambil nilai terendah dengan ubuntu
Open terminal
Grep 001 *.log > grep_log
Ambil kolom ketiga awk ‘{print $3}’ grep_log > awk_log
Mengurutkan nilai sort awk_log > spasi sort_awk
Mencari data yang terdapat nilai terendah grep 13.7870 *.log

Lampiran 11. Nilai *free binding energy* selama simulasi dinamika sebanyak 200 snapshoot yang sudah diurutkan dengan bantuan Ubuntu

	Nilai *free binding energy*				
1	-10.6800	68	-12.2070	135	-12.6000
2	-10.8540	69	-12.2080	136	-12.6080
3	-11.0320	70	-12.2120	137	-12.6190
4	-11.1080	71	-12.2170	138	-12.6220
5	-11.1680	72	-12.2180	139	-12.6320
6	-11.1710	73	-12.2240	140	-12.6510
7	-11.2050	74	-12.2240	141	-12.6560
8	-11.2130	75	-12.2270	142	-12.6610
9	-11.2250	76	-12.2290	143	-12.6830
10	-11.2270	77	-12.2430	144	-12.6890
11	-11.2600	78	-12.2570	145	-12.7170
12	-11.2810	79	-12.2570	146	-12.7170
13	-11.2920	80	-12.2610	147	-12.7230
14	-11.3010	81	-12.2620	148	-12.7330
15	-11.3150	82	-12.2620	149	-12.7470
16	-11.3540	83	-12.2660	150	-12.7590
17	-11.3710	84	-12.2700	151	-12.7610
18	-11.4480	85	-12.2920	152	-12.7640
19	-11.4800	86	-12.3040	153	-12.7650
20	-11.4950	87	-12.3090	154	-12.7660
21	-11.5420	88	-12.3110	155	-12.7680
22	-11.5460	89	-12.3150	156	-12.7740
23	-11.5630	90	-12.3220	157	-12.7830
24	-11.5950	91	-12.3260	158	-12.8040
25	-11.5950	92	-12.3290	159	-12.8070
26	-11.6080	93	-12.3320	160	-12.8410
27	-11.6570	94	-12.3430	161	-12.8560
28	-11.6630	95	-12.3520	162	-12.8590
29	-11.6920	96	-12.3650	163	-12.8650
30	-11.7060	97	-12.3710	164	-12.8730
31	-11.7200	98	-12.3800	165	-12.8780
32	-11.7330	99	-12.3810	166	-12.8860
33	-11.7360	100	-12.3960	167	-12.9010
34	-11.7390	101	-12.4000	168	-12.9080
35	-11.7960	102	-12.4000	169	-12.9230
36	-11.8080	103	-12.4010	170	-12.9390
37	-11.8100	104	-12.4050	171	-12.9540
38	-11.8170	105	-12.4110	172	-12.9550

39	-11.8660	106	-12.4160	173	-12.9690
40	-11.8730	107	-12.4210	174	-12.9890
41	-11.8760	108	-12.4240	175	-13.0080
42	-11.8910	109	-12.4330	176	-13.0210
43	-11.9160	110	-12.4330	177	-13.0330
44	-11.9250	111	-12.4400	178	-13.0340
45	-11.9310	112	-12.4460	179	-13.0590
46	-11.9560	113	-12.4520	180	-13.0730
47	-11.9890	114	-12.4580	181	-13.0770
48	-12.0300	115	-12.4640	182	-13.080
49	-12.0460	116	-12.4750	183	-13.0990
50	-12.0560	117	-12.4780	184	-13.1250
51	-12.0570	118	-12.4810	185	-13.1270
52	-12.0600	119	-12.4850	186	-13.1420
53	-12.0660	120	-12.5060	187	-13.1660
54	-12.0720	121	-12.5080	188	-13.1980
55	-12.0850	122	-12.5140	189	-13.2050
56	-12.0890	123	-12.5190	190	-13.2210
57	-12.0920	124	-12.5210	191	-13.2220
58	-12.0960	125	-12.5230	192	-13.2260
59	-12.1230	126	-12.5440	193	-13.2290
60	-12.1360	127	-12.5530	194	-13.2300
61	-12.1470	128	-12.5550	195	-13.2840
62	-12.1570	129	-12.5670	196	-13.3010
63	-12.1800	130	-12.5900	197	-13.4410
64	-12.1800	131	-12.5910	198	-13.4910
65	-12.1850	132	-12.5920	199	-13.5130
66	-12.1870	133	-12.5980	200	-13.7870
67	-12.2000	134	-12.5980		

Lampiran 12. Nilai RMSD bb

1.722	1.711	1.64	1.66	1.646	1.643	1.538	1.489
1.78	1.685	1.636	1.636	1.671	1.634	1.631	1.508
1.547	1.71	1.659	1.691	1.675	1.633	1.64	1.457
1.546	1.659	1.728	1.755	1.621	1.6	1.624	1.371
1.525	1.687	1.738	1.646	1.723	1.634	1.634	1.453
1.502	1.706	1.77	1.66	1.839	1.664	1.546	1.451
1.56	1.703	1.784	1.74	1.785	1.693	1.531	1.484
1.607	1.636	1.668	1.616	1.669	1.763	1.501	1.418
1.631	1.727	1.675	1.627	1.776	1.676	1.456	1.561
1.521	1.701	1.649	1.645	1.692	1.634	1.589	1.546
1.655	1.689	1.624	1.796	1.629	1.775	1.527	1.5
1.679	1.655	1.645	1.762	1.601	1.721	1.531	1.558
1.6	1.601	1.718	1.725	1.638	1.717	1.514	1.529
1.625	1.615	1.789	1.707	1.605	1.697	1.63	1.542
1.599	1.632	1.79	1.665	1.497	1.696	1.544	1.52
1.641	1.658	1.703	1.602	1.649	1.671	1.508	1.57
1.618	1.688	1.645	1.629	1.616	1.648	1.59	1.569
1.632	1.626	1.67	1.592	1.682	1.64	1.57	1.574
1.647	1.553	1.661	1.733	1.59	1.631	1.567	1.587
1.555	1.644	1.601	1.62	1.576	1.697	1.555	1.637
1.616	1.56	1.676	1.665	1.711	1.655	1.516	1.626
1.647	1.567	1.758	1.65	1.59	1.63	1.536	1.638
1.742	1.655	1.72	1.583	1.586	1.572	1.499	1.562
1.745	1.683	1.586	1.684	1.566	1.62	1.511	1.582
1.681	1.691	1.648	1.561	1.588	1.553	1.546	1.702

Lampiran 13. Nilai RMSD kompleks ligan-reseptor 1o86 selama simulasi *molecular dynamics*

Nilai RMSD kompleks ligan-reseptor 1o86 selama 20ns							
0.1		5.1	0.025	10.1	0.068	15.1	0.0448
0.2		5.2	0.0258	10.2	0.0864	15.2	0.0584
0.3		5.3	0.0348	10.3	0.0738	15.3	0.0592
0.4	0.099	5.4	0.0442	10.4	0.0462	15.4	0.0754
0.5	0.078	5.5	0.0702	10.5	0.0848	15.5	0.069
0.6	0.034	5.6	0.0768	10.6	0.1076	15.6	0.064
0.7	0.046	5.7	0.0696	10.7	0.1064	15.7	0.0662
0.8	0.063	5.8	0.059	10.8	0.0894	15.8	0.0776
0.9	0.0622	5.9	0.0602	10.9	0.0832	15.9	0.0686
1	0.0738	6	0.056	11	0.0812	16	0.0648
1.1	0.0976	6.1	0.0282	11.1	0.0724	16.1	0.0648
1.2	0.0962	6.2	0.0382	11.2	0.0662	16.2	0.0674
1.3	0.095	6.3	0.061	11.3	0.032	16.3	0.0442
1.4	0.0326	6.4	0.0892	11.4	0.097	16.4	0.0352
1.5	0.0298	6.5	0.084	11.5	0.101	16.5	0.0374
1.6	0.0176	6.6	0.084	11.6	0.104	16.6	0.0492
1.7	0.024	6.7	0.0744	11.7	0.1128	16.7	0.0604
1.8	0.0284	6.8	0.0488	11.8	0.1098	16.8	0.0478
1.9	0.0636	6.9	0.055	11.9	0.0466	16.9	0.05
2	0.0586	7	0.0496	12	0.059	17	0.0436
2.1	0.0644	7.1	0.0722	12.1	0.0538	17.1	0.0328
2.2	0.0864	7.2	0.0822	12.2	0.0346	17.2	0.0356
2.3	0.106	7.3	0.0822	12.3	0.0398	17.3	0.0244
2.4	0.0702	7.4	0.0916	12.4	0.0422	17.4	0.0226
2.5	0.0582	7.5	0.0884	12.5	0.0286	17.5	0.0272
2.6	0.0318	7.6	0.064	12.6	0.0374	17.6	0.0216
2.7	0.0254	7.7	0.0582	12.7	0.0468	17.7	0.0452
2.8	0.0302	7.8	0.042	12.8	0.0316	17.8	0.1032
2.9	0.0314	7.9	0.0416	12.9	0.0288	17.9	0.0846
3	0.0304	8	0.0416	13	0.033	18	0.077
3.1	0.034	8.1	0.0524	13.1	0.0448	18.1	0.0722
3.2	0.0422	8.2	0.0674	13.2	0.0708	18.2	0.0644
3.3	0.0558	8.3	0.0418	13.3	0.052	18.3	0.0554
3.4	0.0586	8.4	0.0416	13.4	0.052	18.4	0.074
3.5	0.0552	8.5	0.0688	13.5	0.0742	18.5	0.0838
3.6	0.0456	8.6	0.0732	13.6	0.0798	18.6	0.0986
3.7	0.0736	8.7	0.084	13.7	0.0706	18.7	0.0388
3.8	0.0512	8.8	0.082	13.8	0.0748	18.8	0.035
3.9	0.0374	8.9	0.066	13.9	0.0252	18.9	0.0298

4	0.0312	9	0.0902	14	0.0294	19	0.0238
4.1	0.0378	9.1	0.0636	14.1	0.0378	19.1	0.026
4.2	0.0288	9.2	0.047	14.2	0.0304	19.2	0.035
4.3	0.0784	9.3	0.0522	14.3	0.0262	19.3	0.044
4.4	0.0808	9.4	0.0432	14.4	0.0264	19.4	0.0184
4.5	0.0612	9.5	0.0558	14.5	0.0232	19.5	0.0296
4.6	0.037	9.6	0.06	14.6	0.0206	19.6	0.0384
4.7	0.0428	9.7	0.0672	14.7	0.065	19.7	0.048
4.8	0.0618	9.8	0.0574	14.8	0.0628	19.8	0.047
4.9	0.0712	9.9	0.0676	14.9	0.053	19.9	0.06
5	0.0802	10	0.0638	15	0.0446	20	0.06