


## LAMPIRAN

### Lampiran 1. Surat izin penelitian

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

Hal : Permohonan Izin Penelitian

Kepada Yth  
Kabag Laboratorium Terpadu  
Universitas 'Aisyiyah Palembang

1	Skripsi
2	PKM/LKTI
3	Penelitian Dosen
4	Luar

Assalamualaikum Wr. Wb.

Sehubungan dengan penelitian kami dalam bidang Kimia Komputasi, dengan:

Judul Penelitian : Membangun Protokol Structure-Based Virtual  
Screening (SBVS) Untuk Identifikasi Kandidat Ligan  
Anti-Asma

Nama Pembimbing : 1. Gerry Nugraha, M.Sc., M.Farm  
2. Suprayatno, S.Si., M.T.

No	Nama	NIM/NIP/NIK	No. HP
1	<u>Risna Pinitia</u>	<u>214820103023</u>	<u>0831 4291 0131</u>
2			
3			
4			
5			

Bermaksud mengajukan izin penelitian di Laboratorium<sup>\*)</sup>: **Farmasetika Dasar / Teknologi Farmasi / Kimia Farmasi / Biologi Farmasi / Farmakologi / Mikrobiologi / Komputasi Prodi S1 Farmasi Universitas 'Aisyiyah Palembang.**

Penelitian tersebut akan kami laksanakan selama: 6 bulan,  
yang terhitung dari : 

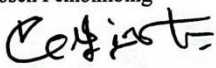
19	03	2024
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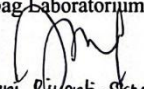
 s.d 


19	08	2025
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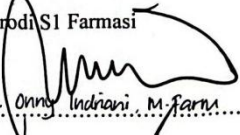
Sebagai bahan pertimbangan, bersama ini dilampirkan lembar pengesahan proposal penelitian. Demikian permohonan kami, atas perhatiannya diucapkan terima kasih.

Palembang, 19 Maret 2025

Mengetahui,  
Dosen Pembimbing  
  
Gerry Nugraha, M.Sc., M.Farm

Menyetujui,  
Kabag Laboratorium Terpadu  
  
Neni Riyanti, S.Kn., M.Kes

Pemohon  
  
Risna Pinitia

Kaprodi S1 Farmasi  
  
Art. Onno Indriani, M.Farm

## Lampiran 2. Lembar bimbingan skripsi



**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 : Risna Pinisia  
NIM : 214820103023  
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-Asma

No.	Tanggal Konsultasi	Keterangan	Paraf Pembimbing
1	25 Mei 2025	Revisi Judul	
2	26 Mei 2025	Revisi tata cara pembuatan latar belakang	
3	28 Mei 2025	Revisi BAB Pendahuluan	
4	05 Juni 2025	Revisi BAB I	
5	06 Juni 2025	Revisi BAB II	
6	08 Juni 2025	Revisi BAB II	
7	18 Juni 2025	Revisi BAB II	
8	20 Juni 2025	Revisi BAB III	
9	20 Juni 2025	Acc proposal	
10	29 Juni 2025	Revisi BAB III	
11	28 Agustus 2025	Revisi sempro	
12	03 september 2025	Revisi sempro	
	05 september 2025	Revisi BAB IV	
	07 september 2025	Revisi BAB IV	
	14 september 2025	Revisi BAB V & 5	
	16 september 2025	Revisi BAB V & 5	
	20 september 2025	Revisi lampiran & dapus	
	22 september 2025	Revisi dapus	
	23 september 2025	Acc skripsi	

### Lampiran 3. Data hasil *swissargetprediction*

A	B	C	D	E	F	G	H
Nama Obat	Target	Common Name	Uniprot ID	CHEMBL ID	Target Class	Probability*	Known actives (%)
1	salbutamol	Adrenergic receptor beta	ADRB2	P07550	CHEMBL210	Family A G protein-coupled receptor	1 70 / 101
2		Mu opioid receptor	OPRM1	P35372	CHEMBL233	Family A G protein-coupled receptor	0,068975016 86 / 140
3		Beta-1 adrenergic receptor	ADRB1	P08588	CHEMBL213	Family A G protein-coupled receptor	0,057956876 58 / 50
4		Dopamine D4 receptor	DRD4	P21917	CHEMBL219	Family A G protein-coupled receptor	0,057956876 14 / 27
5		Dopamine D3 receptor	DRD3	P35462	CHEMBL234	Family A G protein-coupled receptor	0,057956876 17 / 65
6		Beta-3 adrenergic receptor	ADRB3	P13945	CHEMBL246	Family A G protein-coupled receptor	0,057956876 18 / 25
7		Dopamine D2 receptor	DRD2	P14416	CHEMBL217	Family A G protein-coupled receptor	0,057956876 36 / 142
8		Neurexin-1 receptor 2	NMUR2	Q9GZQ4	CHEMBL1075144	Family A G protein-coupled receptor	0,057956876 1 / 1
9		Alpha-1d adrenergic receptor	ADRA1D	P25100	CHEMBL223	Family A G protein-coupled receptor	0,048952898 5 / 6
10		Alpha-L-fucosidase I	FUCA1	P04066	CHEMBL4176	Enzyme	0,048952898 41 / 0
11		Alpha-2a adrenergic receptor	ADRA2A	P08913	CHEMBL1867	Family A G protein-coupled receptor	0,048952898 6 / 6
12		Alpha-1a adrenergic receptor	ADRA1A	P35348	CHEMBL229	Family A G protein-coupled receptor	0,048952898 11 / 17
13		Purine nucleoside phosphorylase	PNP	P00491	CHEMBL4338	Enzyme	0,048952898 84 / 0
14		S-methyl-5-thioadenosine phosphorylase	MTAP	Q13126	CHEMBL4941	Enzyme	0,048952898 54 / 0
15		Adrenergic receptor alpha-2	ADRA2C	P18825	CHEMBL1916	Family A G protein-coupled receptor	0,048952898 2 / 4
16		Alpha-2b adrenergic receptor	ADRA2B	P18089	CHEMBL1942	Family A G protein-coupled receptor	0,048952898 5 / 7
17		Endoplasmic reticulum mannose-oligosaccharide 1,2-alpha-mannosidase	MAN1B1	Q8UKM7	CHEMBL2308	Enzyme	0,048952898 9 / 0
18		Dipeptidyl peptidase IV	DPP4	P27487	CHEMBL284	Protease	0,048952898 95 / 0
19		Melatonin receptor 1A	MTNR1A	P48039	CHEMBL1945	Family A G protein-coupled receptor	0,048952898 0 / 97
20		Alpha-1b adrenergic receptor	ADRA1B	P35368	CHEMBL232	Family A G protein-coupled receptor	0,048952898 4 / 4
21		Beta-galactosidase	GLB1	P16278	CHEMBL2522	Glycosylase	0,048952898 6 / 0
22		Liver glycogen phosphorylase	PYGL	P06737	CHEMBL2568	Enzyme	0,048952898 57 / 0
23		Serine/threonine-protein kinase PIM1	PIM1	P11309	CHEMBL2147	Kinase	0,048952898 9 / 0
24		Glutathione reductase	GSR	P00390	CHEMBL2755	Oxidoreductase	0,048952898 1 / 0
25		CDC7/DBF4 (Cell division cycle 7-related protein kinase/Activator of S CDC7	O00311	CHEMBL5443	Kinase	0,048952898 2 / 0	
26		Histamine H1 receptor	HRH1	P35367	CHEMBL231	Family A G protein-coupled receptor	0,048952898 14 / 4
27		Dopamine transporter (by homology)	SLC6A3	Q01959	CHEMBL238	Electrochemical transporter	0,048952898 69 / 71
28		Protein kinase C iota	PKCI	P41743	CHEMBL2598	Kinase	0,048952898 1 / 0
29		Lysosomal alpha-glucosidase (by homology)	GAA	P10253	CHEMBL2608	Hydrolase	0,048952898 6 / 0
30		Beta-glucosidase	GBA2	Q9HCG7	CHEMBL3761	Enzyme	0,048952898 22 / 0
31		Delta opioid receptor	OPRD1	P41143	CHEMBL236	Family A G protein-coupled receptor	0,048952898 83 / 48
32							
53	terbutaline	Adrenergic receptor beta	ADRB2	P07550	CHEMBL210	Family A G protein-coupled receptor	0,98024389 85 / 91
54		Beta-1 adrenergic receptor	ADRB1	P08588	CHEMBL213	Family A G protein-coupled receptor	0,337919226 67 / 49
55		Dopamine D4 receptor	DRD4	P21917	CHEMBL219	Family A G protein-coupled receptor	0,29462222 27 / 40
56		Dopamine D3 receptor	DRD3	P35462	CHEMBL234	Family A G protein-coupled receptor	0,29462222 39 / 112
57		Beta-3 adrenergic receptor	ADRB3	P13945	CHEMBL246	Family A G protein-coupled receptor	0,29462222 31 / 17
58		Alpha-1a adrenergic receptor	ADRA1A	P35348	CHEMBL229	Family A G protein-coupled receptor	0,184442068 28 / 117
59		Mu opioid receptor	OPRM1	P35372	CHEMBL233	Family A G protein-coupled receptor	0,129815191 132 / 256
60		Alpha-1b adrenergic receptor	ADRA1B	P35368	CHEMBL232	Family A G protein-coupled receptor	0,121096795 12 / 4
61		Dopamine D2 receptor	DRD2	P14416	CHEMBL217	Family A G protein-coupled receptor	0,095125689 76 / 222
62		Alpha-2a adrenergic receptor	ADRA2A	P08913	CHEMBL1867	Family A G protein-coupled receptor	0,08642693 9 / 8
63		Alpha-2b adrenergic receptor	ADRA2B	P18089	CHEMBL1942	Family A G protein-coupled receptor	0,08642693 5 / 9
64		Alpha-1d adrenergic receptor	ADRA1D	P25100	CHEMBL223	Family A G protein-coupled receptor	0,077758326 12 / 6
65		Delta opioid receptor	OPRD1	P41143	CHEMBL236	Family A G protein-coupled receptor	0,077758326 134 / 105
66		Kappa Opioid receptor	OPRK1	P41145	CHEMBL237	Family A G protein-coupled receptor	0,077758326 88 / 110
67		Serotonin 2a (5-HT2a) receptor (by homology)	HTR2A	P28223	CHEMBL224	Family A G protein-coupled receptor	0,069097444 74 / 80
68		Adrenergic receptor alpha-2	ADRA2C	P18825	CHEMBL1916	Family A G protein-coupled receptor	0,069097444 2 / 8
69		Neurexin-1 receptor 2	NMUR2	Q9GZQ4	CHEMBL1075144	Family A G protein-coupled receptor	0,060424588 1 / 1
70		Purine nucleoside phosphorylase	PNP	P00491	CHEMBL4338	Enzyme	0,060424588 50 / 0
71		Serotonin transporter	SLC6A4	P31645	CHEMBL228	Electrochemical transporter	0,060424588 230 / 96
72		Serotonin 3a (5-HT3a) receptor	HTR3A	P46098	CHEMBL1899	Ligand-gated ion channel	0,060424588 11 / 1
73		S-methyl-5-thioadenosine phosphorylase	MTAP	Q13126	CHEMBL4941	Enzyme	0,060424588 46 / 0
74		Transient receptor potential cation channel subfamily V member 3	TRPV3	Q8NET8	CHEMBL5522	Voltage-gated ion channel	0,060424588 33 / 0
75		Glutathione reductase	GSR	P00390	CHEMBL2755	Oxidoreductase	0,060424588 1 / 8
76		Dipeptidyl peptidase IV	DPP4	P27487	CHEMBL284	Protease	0,060424588 95 / 0
77		Metastin receptor	KISS1R	Q969F8	CHEMBL5413	Family A G protein-coupled receptor	0,060424588 4 / 0
78		Nitric oxide synthase, inducible (by homology)	NOS2	P35228	CHEMBL4481	Enzyme	0,060424588 9 / 0
79		Uridine phosphorylase 1	UPP1	Q16831	CHEMBL4811	Enzyme	0,060424588 3 / 0
80		Serotonin 1a (5-HT1a) receptor	HTR1A	P08908	CHEMBL214	Family A G protein-coupled receptor	0,060424588 40 / 13
81		Indoleamine 2,3-dioxygenase	IDO1	P14902	CHEMBL4685	Enzyme	0,060424588 4 / 0
82		Dopamine D1 receptor	DRD1	P21728	CHEMBL2056	Family A G protein-coupled receptor	0,060424588 17 / 72
83		Neuronal acetylcholine receptor protein alpha-4 subunit	CHRNA4	P43681	CHEMBL1882	Ligand-gated ion channel	0,060424588 21 / 0
84		Protein kinase C iota	PKCI	P41743	CHEMBL2598	Kinase	0,060424588 1 / 0
87	fenoterol	Adrenergic receptor beta	ADRB2	P07550	CHEMBL210	Family A G protein-coupled receptor	1 96 / 115
88		Beta-1 adrenergic receptor	ADRB1	P08588	CHEMBL213	Family A G protein-coupled receptor	0,324775887 57 / 56
89		Dopamine D2 receptor	DRD2	P14416	CHEMBL217	Family A G protein-coupled receptor	0,111501865 30 / 393
90		Beta-3 adrenergic receptor	ADRB3	P13945	CHEMBL246	Family A G protein-coupled receptor	0,111501865 51 / 41
91		Mu opioid receptor	OPRM1	P35372	CHEMBL233	Family A G protein-coupled receptor	0,111501865 131 / 512
92		Dopamine D4 receptor	DRD4	P21917	CHEMBL219	Family A G protein-coupled receptor	0,111501865 3 / 70
93		Dopamine D3 receptor	DRD3	P35462	CHEMBL234	Family A G protein-coupled receptor	0,111501865 8 / 185
94		Glutamate NMDA receptor; GRIN1/GRIN2B	GRIN1	Q05586	Q1	Ligand-gated ion channel	0,111501865 5 / 21
95		Glutamate [NMDA] receptor subunit epsilon 2	GRIN2B	Q13224	CHEMBL1904	Ligand-gated ion channel	0,111501865 0 / 8
96		Anti-estrogen binding site (AEBS)	EBP	Q15125	CHEMBL4931	Enzyme	0,111501865 0 / 11
97		Serotonin 1a (5-HT1a) receptor	HTR1A	P08908	CHEMBL214	Family A G protein-coupled receptor	0,111501865 35 / 53
98		Neurexin-1 receptor 2	NMUR2	Q9GZQ4	CHEMBL1075144	Family A G protein-coupled receptor	0,111501865 0 / 1
99		Alpha-2a adrenergic receptor	ADRA2A	P08913	CHEMBL1867	Family A G protein-coupled receptor	0,111501865 8 / 11
100		Adrenergic receptor alpha-2	ADRA2C	P18825	CHEMBL1916	Family A G protein-coupled receptor	0,111501865 5 / 12
101		Alpha-2b adrenergic receptor	ADRA2B	P18089	CHEMBL1942	Family A G protein-coupled receptor	0,111501865 3 / 10
102		Alpha-1a adrenergic receptor	ADRA1A	P35348	CHEMBL229	Family A G protein-coupled receptor	0,111501865 14 / 28
103		Alpha-1d adrenergic receptor	ADRA1D	P25100	CHEMBL223	Family A G protein-coupled receptor	0,111501865 10 / 8
104		Alpha-1b adrenergic receptor	ADRA1B	P35368	CHEMBL232	Family A G protein-coupled receptor	0,111501865 10 / 6
105		Serotonin transporter	SLC6A4	P31645	CHEMBL228	Electrochemical transporter	0,111501865 96 / 238
106		Metabotropic glutamate receptor 5	GRM5	P41594	CHEMBL3227	Family C G protein-coupled receptor	0,111501865 0 / 1
107		Histamine H1 receptor	HRH1	P35367	CHEMBL231	Family A G protein-coupled receptor	0,111501865 4 / 18
108		HERG	KCNH2	Q12809	CHEMBL240	Voltage-gated ion channel	0,111501865 35 / 20
109		Dopamine transporter (by homology)	SLC6A3	Q01959	CHEMBL238	Electrochemical transporter	0,111501865 58 / 236
110		Serotonin 2a (5-HT2a) receptor	HTR2A	P28223	CHEMBL224	Family A G protein-coupled receptor	0,111501865 40 / 129
111		Sigma opioid receptor	SIGMAR1	Q99720	CHEMBL287	Membrane receptor	0,111501865 8 / 324
112		Tyrosine-protein kinase FYN	FYN	P06241	CHEMBL1841	Kinase	0,111501865 0 / 7
113		Delta opioid receptor	OPRD1	P41143	CHEMBL236	Family A G protein-coupled receptor	0,111501865 101 / 298
114		Kappa Opioid receptor	OPRK1	P41145	CHEMBL237	Family A G protein-coupled receptor	0,111501865 101 / 233
115		Cannabinoid receptor 1	CNR1	P21554	CHEMBL218	Family A G protein-coupled receptor	0,111501865 0 / 18
116		Serotonin 5a (5-HT5a) receptor (by homology)	HTR5A	P47898	CHEMBL3426	Family A G protein-coupled receptor	0,111501865 0 / 15

118	procaterol	Adrenergic receptor beta	ADRB2	P07550	CHEMBL210	Family A G protein-coupled receptor	1 93 / 151
119		Beta-1 adrenergic receptor	ADRB1	P08588	CHEMBL213	Family A G protein-coupled receptor	0,196657136 72 / 102
120		Dopamine D3 receptor	DRD3	P35462	CHEMBL234	Family A G protein-coupled receptor	0,147256737 115 / 78
121		Dopamine D4 receptor	DRD4	P21917	CHEMBL219	Family A G protein-coupled receptor	0,108099949 67 / 10
122		Dopamine D2 receptor	DRD2	P14416	CHEMBL217	Family A G protein-coupled receptor	0,108099949 211 / 115
123		Muscarinic acetylcholine receptor M3	CHRM3	P20309	CHEMBL245	Family A G protein-coupled receptor	0,097874534 69 / 133
124		Dopamine D1 receptor	DRD1	P21728	CHEMBL2058	Family A G protein-coupled receptor	0,097874534 35 / 4
125		Muscarinic acetylcholine receptor M2	CHRM2	P08172	CHEMBL211	Family A G protein-coupled receptor	0,097874534 84 / 3
126		Alpha-1d adrenergic receptor	ADRA1D	P25100	CHEMBL223	Family A G protein-coupled receptor	0,097874534 22 / 26
127		Troponin, cardiac muscle	TNNC1 TNNT2 TNI	P63316 P45	CHEMBL2095202	Unclassified protein	0,097874534 1 / 0
128		Phosphodiesterase 11A	PDE11A	Q9HCR9	CHEMBL2717	Phosphodiesterase	0,097874534 5 / 0
129		Dipeptidyl peptidase IV	DPP4	P27487	CHEMBL284	Protease	0,097874534 135 / 0
130		Metastin receptor	KISS1R	Q969F8	CHEMBL5413	Family A G protein-coupled receptor	0,097874534 4 / 0
131		Neuronal acetylcholine receptor; alpha3/alpha6/beta2/beta3	CHRN3 CHRNA6	Q05901 Q1	CHEMBL2109233	Ligand-gated ion channel	0,097874534 4 / 0
132		Carbonic anhydrase II	CA2	P00918	CHEMBL205	Lyase	0,097874534 47 / 0
133		Carbonic anhydrase I	CA1	P00915	CHEMBL261	Lyase	0,097874534 37 / 0
134		Monoamine oxidase A	MAOA	P21397	CHEMBL1951	Oxidoreductase	0,097874534 6 / 4
135		Glycine transporter 1	SLC6A9	P48067	CHEMBL2337	Electrochemical transporter	0,097874534 35 / 0
136		Serotonin transporter	SLC6A4	P31645	CHEMBL228	Electrochemical transporter	0,097874534 519 / 75
137		Transient receptor potential cation channel subfamily V member 3	TRPV3	Q8NET8	CHEMBL5522	Voltage-gated ion channel	0,097874534 55 / 0
138		HERG	KCNH2	Q12809	CHEMBL240	Voltage-gated ion channel	0,097874534 85 / 29
139		Voltage-gated potassium channel subunit Kv1.5	KCNA5	P22460	CHEMBL4306	Voltage-gated ion channel	0,097874534 18 / 3
140		S-methyl-S-thioadenosine phosphorylase	MTAP	Q13126	CHEMBL4941	Enzyme	0,097874534 29 / 0
141		Rho-associated protein kinase	ROCK2 ROCK1	O75116 Q1	CHEMBL2111459	Kinase	0,097874534 2 / 0
142		Tyrosine-protein kinase JAK1	JAK1	P23458	CHEMBL2835	Kinase	0,097874534 58 / 0
143		Dipeptidyl peptidase II	DPP7	Q9UHL4	CHEMBL3976	Protease	0,097874534 23 / 0
144		Neuronal acetylcholine receptor; alpha2/beta4	CHRN4 CHRNA2	P30926 Q11	CHEMBL2109230	Ligand-gated ion channel	0,097874534 2 / 0
145		Neuronal acetylcholine receptor; alpha3/beta2	CHRN3 CHRNB2	P32297 P17	CHEMBL2109234	Ligand-gated ion channel	0,097874534 1 / 0
146		Nicotinic acetylcholine receptor alpha4/beta2/alpha5	CHRNA5 CHRNB2	P30532 P17	CHEMBL3038461	Ligand-gated ion channel	0,097874534 1 / 0
147		P-glycoprotein 1	ABCB1	P08183	CHEMBL4302	Primary active transporter	0,097874534 61 / 9
148		Fibroblast activation protein alpha	FAP	Q12884	CHEMBL4683	Protease	0,097874534 2 / 0
149		Cytochrome P450 1A2	CYP1A2	P05177	CHEMBL3356	Cytochrome P450	0,097874534 1 / 0

## Lampiran 4. Data 177 gen atau protein yang terkait dengan penyakit asma pada laman *GeneCards*

	Symbol ▲	Description	Category ▲	UniProt ID	GIFTS ▲	GC id ▲	Score ▼
1	IL13	Interleukin 13	Protein Coding	P35225	57	GC05P132656	65.52
2	ADRB2	Adrenoceptor Beta 2	Protein Coding	P07550	62	GC05P159202	53.14
3	TNF	Tumor Necrosis Factor	Protein Coding	P01375	65	GC06P181893	50.92
4	CCL11	C-C Motif Chemokine Ligand 11	Protein Coding	P51671	58	GC17P034285	50.67
5	ALOX5	Arachidonate 5-Lipoxygenase	Protein Coding	P09917	62	GC10P045374	49.30
6	SCGB1A1	Secretoglobin Family 1A Member 1	Protein Coding	P11684	54	GC11P062405	45.25
7	TBX21	T-Box Transcription Factor 21	Protein Coding	Q9JUL17	59	GC17P047733	40.47
8	NPSR1	Neuropeptide S Receptor 1	Protein Coding	Q6W5P4	52	GC07P034658	38.87
9	HNMT	Histamine N-Methyltransferase	Protein Coding	P50135	58	GC02P137964	37.53
10	PHF11	PHD Finger Protein 11	Protein Coding	Q9JUL8	46	GC13P049495	37.51
11	IL12B	Interleukin 12B	Protein Coding	P29460	57	GC05M159314	37.30
12	SCGB3A2	Secretoglobin Family 3A Member 2	Protein Coding	Q96PL1	50	GC05P147870	35.60
13	MUC7	Mucin 7, Secreted	Protein Coding	Q8TAX7	47	GC04P070430	34.83
14	IL4R	Interleukin 4 Receptor	Protein Coding	P24394	60	GC16P120788	34.11
15	HLA-G	Major Histocompatibility Complex, Class I, G	Protein Coding	P17693	57	GC06P181845	33.08
16	PTGER2	Prostaglandin E Receptor 2	Protein Coding	P43116	61	GC14P052314	32.22
17	CARD11	Caspase Recruitment Domain Family Member 11	Protein Coding	Q9BXL7	59	GC07M002906	32.17
18	IL4	Interleukin 4	Protein Coding	P05112	59	GC05P132673	32.00
19	IL5	Interleukin 5	Protein Coding	P05113	58	GC05M132541	31.80
20	PLA2G7	Phospholipase A2 Group VII	Protein Coding	Q13093	63	GC06M046704	30.96
21	RNASE3	Ribonuclease A Family Member 3	Protein Coding	P12724	52	GC14P020891	30.81
22	MIR126	MicroRNA 126	RNA Gene (miRNA)		31	GC09P136670	30.51
23	PVT1	Pvt1 Oncogene	RNA Gene (lncRNA)		33	GC08P128394	30.36
24	FKBP5	FKBP Prolyl Isomerase 5	Protein Coding	Q13451	62	GC06M106625	29.54
25	CHI3L1	Chitinase 3 Like 1	Protein Coding	P36222	59	GC01M203148	29.17
26	IGHE	Immunoglobulin Heavy Constant Epsilon	Protein Coding	P01854	42	GC14M124465	29.09
27	ASRT4	Asthma-Related Traits, Susceptibility To, 4	Genetic Locus		7	GC01U902370	28.18
28	PTGDR	Prostaglandin D2 Receptor	Protein Coding	Q13258	58	GC14P052267	28.03
29	BRCA2	BRCA2 DNA Repair Associated	Protein Coding	P51587	61	GC13P032315	27.94
30	CARD11-AS1	CARD11 Antisense RNA 1	RNA Gene (lncRNA)		20	GC07P018918	27.81
31	IRAK3	Interleukin 1 Receptor Associated Kinase 3	Protein Coding	Q9Y616	58	GC12P075754	27.09
32	ODAD3	Outer Dynein Arm Docking Complex Subunit 3	Protein Coding	A5D8V7	47	GC19M108144	26.85
33	MIR152	MicroRNA 152	RNA Gene (miRNA)		30	GC17M048037	26.74
34	MIR148B	MicroRNA 148b	RNA Gene (miRNA)		30	GC12P054337	26.64
35	ASRT3	Asthma-Related Traits, Susceptibility To, 3	Genetic Locus		7	GC02U901663	26.63
36	ASRT6	Asthma-Related Traits, Susceptibility To, 6	Genetic Locus		7	GC17U901148	26.63
37	MIR148A	MicroRNA 148a	RNA Gene (miRNA)		29	GC07M025950	26.26

38	+	NPSR1-AS1	NPSR1 Antisense RNA 1	RNA Gene (lncRNA)		28	GC07M034287	25.54
39	+	FLG	Filaggrin	Protein Coding	P20930	54	GC01M167330	24.38
40	+	LOC109286563	TBX21 Promoter Region	Functional Element		5	GC17P047731	24.07
41	+	ADAM33	ADAM Metallopeptidase Domain 33	Protein Coding	Q9BZ11	50	GC20M004356	23.96
42	+	MS4A2	Membrane Spanning 4-Domains A2	Protein Coding	Q01362	51	GC11P060088	23.45
43	+	CYSLTR1	Cysteinyl Leukotriene Receptor 1	Protein Coding	Q9Y271	55	GC0XM078271	22.98
44	+	ASRT8	Asthma-Related Traits, Susceptibility To, 8	Genetic Locus		7	GC09U901396	22.98
45	+	STAT6	Signal Transducer And Activator Of Transcription 6	Protein Coding	P42226	64	GC12M057095	22.91
46	+	TSLP	Thymic Stromal Lymphopoietin	Protein Coding	Q969D9	52	GC05P111070	22.42
47	+	IL10	Interleukin 10	Protein Coding	P22301	60	GC01M206767	22.37
48	+	IFNG	Interferon Gamma	Protein Coding	P01579	63	GC12M068154	22.17
49	+	LTC4S	Leukotriene C4 Synthase	Protein Coding	Q16873	56	GC05P179793	21.74
50	+	CXCL8	C-X-C Motif Chemokine Ligand 8	Protein Coding	P10145	57	GC04P073740	21.73
51	+	SPINK5	Serine Peptidase Inhibitor Kazal Type 5	Protein Coding	Q9NQ38	53	GC05P148025	21.57
52	+	HAVCR1	Hepatitis A Virus Cellular Receptor 1	Protein Coding	Q96D42	55	GC05M157028	21.29
53	+	TGFB1	Transforming Growth Factor Beta 1	Protein Coding	P01137	65	GC19M041301	20.62
54	+	ORMDL3	ORMDL Sphingolipid Biosynthesis Regulator 3	Protein Coding	Q8N138	49	GC17M039921	19.29
55	+	CCL5	C-C Motif Chemokine Ligand 5	Protein Coding	P13501	56	GC17M035871	19.23
56	+	IL17A	Interleukin 17A	Protein Coding	Q16552	55	GC06P052186	18.71
57	+	IL9	Interleukin 9	Protein Coding	P15248	56	GC05M135891	18.61
58	+	IL33	Interleukin 33	Protein Coding	O95760	53	GC09P010645	17.93
59	+	IL6	Interleukin 6	Protein Coding	P05231	64	GC07P022725	17.91
60	+	TLR4	Toll Like Receptor 4	Protein Coding	O00206	64	GC09P117704	17.88
61	+	GSTM1	Glutathione S-Transferase Mu 1	Protein Coding	P09488	55	GC01P109687	17.82
62	+	CD14	CD14 Molecule	Protein Coding	P08571	58	GC05M140631	17.81
63	+	GSTP1	Glutathione S-Transferase Pi 1	Protein Coding	P09211	62	GC11P067583	17.10
64	+	EPX	Eosinophil Peroxidase	Protein Coding	P11678	57	GC17P058192	16.62
65	+	CFTR	CF Transmembrane Conductance Regulator	Protein Coding	P13569	66	GC07P117287	16.55
66	+	IL3	Interleukin 3	Protein Coding	P08700	57	GC05P132060	16.35
67	+	SELP	Selectin P	Protein Coding	P16109	59	GC01M169558	16.25
68	+	IL1B	Interleukin 1 Beta	Protein Coding	P01584	60	GC02M112829	16.04
69	+	TBXA2R	Thromboxane A2 Receptor	Protein Coding	P21731	63	GC19M003594	16.03
70	+	CTLA4	Cytotoxic T-Lymphocyte Associated Protein 4	Protein Coding	P16410	61	GC02P204860	15.77
71	+	TLR2	Toll Like Receptor 2	Protein Coding	O60603	65	GC04P153684	15.39
72	+	IL1RL1	Interleukin 1 Receptor Like 1	Protein Coding	Q01638	54	GC02P102294	15.32
73	+	IL18	Interleukin 18	Protein Coding	Q14116	57	GC11M112143	15.31
74	+	HLA-DRB1	Major Histocompatibility Complex, Class II, DR Beta 1	Protein Coding	P01911	60	GC06M106528	15.15
75	+	CSF2	Colony Stimulating Factor 2	Protein Coding	P04141	58	GC05P132073	15.10
76	+	NR3C1	Nuclear Receptor Subfamily 3 Group C Member 1	Protein Coding	P04150	62	GC05M143277	14.95

77	+	ICAM1	Intercellular Adhesion Molecule 1	Protein Coding	P05362	63	GC19P151796	14.88
78	+	IGES	Immunoglobulin E Concentration, Serum	Genetic Locus		11	GC05U990033	14.86
79	+	CHIA	Chitinase Acidic	Protein Coding	Q9BZP6	53	GC01P112030	14.76
80	+	IL2	Interleukin 2	Protein Coding	P60568	58	GC04M122451	14.57
81	+	DPP10	Dipeptidyl Peptidase Like 10	Protein Coding	Q8N608	55	GC02P114442	14.55
82	+	CYSLTR2	Cysteinyl Leukotriene Receptor 2	Protein Coding	Q9NS75	58	GC13P048653	14.49
83	+	LTA	Lymphotoxin Alpha	Protein Coding	P01374	55	GC06P181891	14.40
84	+	GSDMB	Gasdermin B	Protein Coding	Q8TAX9	44	GC17M039904	14.33
85	+	GATA3	GATA Binding Protein 3	Protein Coding	P23771	63	GC10P008045	14.31
86	+	ALOX5AP	Arachidonate 5-Lipoxygenase Activating Protein	Protein Coding	P20292	56	GC13P030713	13.88
87	+	VCAM1	Vascular Cell Adhesion Molecule 1	Protein Coding	P19320	58	GC01P100719	13.85
88	+	NOS2	Nitric Oxide Synthase 2	Protein Coding	P35228	62	GC17M027756	13.80
89	+	MIR155	MicroRNA 155	RNA Gene (miRNA)		30	GC21P025573	13.62
90	+	HLA-DQB1	Major Histocompatibility Complex, Class II, DQ Beta 1	Protein Coding	P01920	57	GC06M106540	13.60
91	+	MPO	Myeloperoxidase	Protein Coding	P05164	65	GC17M058269	13.47
92	+	MMP9	Matrix Metalloproteinase 9	Protein Coding	P14780	66	GC20P046008	13.45
93	+	CCL2	C-C Motif Chemokine Ligand 2	Protein Coding	P13500	62	GC17P034255	13.25
94	+	IL5RA	Interleukin 5 Receptor Subunit Alpha	Protein Coding	Q01344	58	GC03M003066	13.21
95	+	CCL17	C-C Motif Chemokine Ligand 17	Protein Coding	Q92583	52	GC16P121634	13.19
96	+	JAK1	Janus Kinase 1	Protein Coding	P23458	66	GC01M064833	13.14
97	+	CCL24	C-C Motif Chemokine Ligand 24	Protein Coding	O00175	50	GC07M081059	13.13
98	+	CCR3	C-C Motif Chemokine Receptor 3	Protein Coding	P51677	59	GC03P064845	13.08
99	+	CCL26	C-C Motif Chemokine Ligand 26	Protein Coding	Q9Y258	50	GC07M075769	13.06
100	+	POSTN	Periostin	Protein Coding	Q15063	55	GC13M037562	13.06
101	+	SMAD3	SMAD Family Member 3	Protein Coding	P84022	66	GC15P067063	13.02
102	+	IL6R	Interleukin 6 Receptor	Protein Coding	P08887	63	GC01P154405	12.97
103	+	NOD2	Nucleotide Binding Oligomerization Domain Containing 2	Protein Coding	Q9HC29	61	GC16P050693	12.88
104	+	IL16	Interleukin 16	Protein Coding	Q14005	54	GC15P081159	12.85
105	+	ACE	Angiotensin I Converting Enzyme	Protein Coding	P12821	64	GC17P063477	12.84
106	+	IL2RA	Interleukin 2 Receptor Subunit Alpha	Protein Coding	P01589	63	GC10M006010	12.83
107	+	MYLK	Myosin Light Chain Kinase	Protein Coding	Q15746	65	GC03M123610	12.80
108	+	PTGDR2	Prostaglandin D2 Receptor 2	Protein Coding	Q9Y5Y4	55	GC11M060850	12.78
109	+	BDNF	Brain Derived Neurotrophic Factor	Protein Coding	P23560	62	GC11M027654	12.64
110	+	PTGS2	Prostaglandin-Endoperoxide Synthase 2	Protein Coding	P35354	62	GC01M186671	12.53
111	+	HRH1	Histamine Receptor H1	Protein Coding	P35367	58	GC03P027032	12.47
112	+	CDHR3	Cadherin Related Family Member 3	Protein Coding	Q6ZTQ4	47	GC07P105876	12.39
113	+	TLR6	Toll Like Receptor 6	Protein Coding	Q9Y2C9	57	GC04M038828	12.16
114	+	MUC5AC	Mucin 5AC, Oligomeric Mucus/Gel-Forming	Protein Coding	P98088	51	GC11P020281	12.13
115	+	FOXP3	Forkhead Box P3	Protein Coding	Q9BZS1	59	GC0XM049250	12.11

116	+	IL18R1	Interleukin 18 Receptor 1	Protein Coding	Q13478	56	GC02P102311	12.11
117	+	IL1RN	Interleukin 1 Receptor Antagonist	Protein Coding	P18510	62	GC02P154111	12.00
118	+	CAT	Catalase	Protein Coding	P04040	64	GC11P034460	11.99
119	+	TLR9	Toll Like Receptor 9	Protein Coding	Q9NR96	58	GC03M054885	11.98
120	+	CCR5	C-C Motif Chemokine Receptor 5	Protein Coding	P51681	60	GC03P064850	11.90
121	+	MBL2	Mannose Binding Lectin 2	Protein Coding	P11226	60	GC10M052760	11.75
122	+	IL17F	Interleukin 17F	Protein Coding	Q96PD4	54	GC06M106847	11.55
123	+	FCER2	Fc Epsilon Receptor II	Protein Coding	P06734	56	GC19M108008	11.50
124	+	STAT5B	Signal Transducer And Activator Of Transcription 5B	Protein Coding	P51692	62	GC17M042199	11.47
125	+	ASOBS	Asthma And Obesity Susceptibility, Chromosome 16p11 Inversion Related	Genetic Locus		1	GC16U901990	11.46
126	+	IL1A	Interleukin 1 Alpha	Protein Coding	P01583	58	GC02M112773	11.45
127	+	ADA	Adenosine Deaminase	Protein Coding	P00813	64	GC20M044620	11.44
128	+	LEP	Leptin	Protein Coding	P41159	59	GC07P128241	11.43
129	+	SERPINE1	Serpin Family E Member 1	Protein Coding	P05121	63	GC07P101127	11.42
130	+	TAC1	Tachykinin Precursor 1	Protein Coding	P20366	54	GC07P097734	11.41
131	+	NAT2	N-Acetyltransferase 2	Protein Coding	P11245	57	GC08P018391	11.40
132	+	SMAD2	SMAD Family Member 2	Protein Coding	Q15796	65	GC18M047809	11.36
133	+	SERPINA1	Serpin Family A Member 1	Protein Coding	P01009	62	GC14M094376	11.31
134	+	IRF1	Interferon Regulatory Factor 1	Protein Coding	P10914	60	GC05M132440	11.30
135	+	KNG1	Kininogen 1	Protein Coding	P01042	61	GC03P186717	11.30
154	+	NLRP3	NLR Family Pyrin Domain Containing 3	Protein Coding	Q96P20	62	GC01P247632	10.68
155	+	CXCR3	C-X-C Motif Chemokine Receptor 3	Protein Coding	P49682	58	GC0XM071615	10.66
156	+	CD69	CD69 Molecule	Protein Coding	Q07108	54	GC12M035789	10.66
157	+	TRPA1	Transient Receptor Potential Cation Channel Subfamily A Member 1	Protein Coding	O75762	60	GC08M072019	10.65
158	+	LTA4H	Leukotriene A4 Hydrolase	Protein Coding	P09960	56	GC12M096000	10.62
159	+	TIMP1	TIMP Metallopeptidase Inhibitor 1	Protein Coding	P01033	57	GC0XP060812	10.58
160	+	ARG1	Arginase 1	Protein Coding	P05089	62	GC06P183096	10.54
161	+	TLR10	Toll Like Receptor 10	Protein Coding	Q9BXR5	50	GC04M038773	10.52
162	+	EDN1	Endothelin 1	Protein Coding	P05305	61	GC06P012910	10.50
163	+	FCER1A	Fc Epsilon Receptor Ia	Protein Coding	P12319	54	GC01P159283	10.44
164	+	GLCC1	Glucocorticoid Induced 1	Protein Coding	Q86VQ1	47	GC07P019110	10.43
165	+	MIR146A	MicroRNA 146a	RNA Gene (miRNA)		31	GC05P160485	10.36
166	+	GSDMA	Gasdermin A	Protein Coding	Q96QA5	47	GC17P154759	10.29
167	+	DENND1B	DENN Domain Containing 1B	Protein Coding	Q6P351	45	GC01M197473	10.28
168	+	MIF	Macrophage Migration Inhibitory Factor	Protein Coding	P14174	61	GC22P023894	10.28
169	+	IL9R	Interleukin 9 Receptor	Protein Coding	Q01113	47	GC0XP155997	10.25
170	+	CCL3	C-C Motif Chemokine Ligand 3	Protein Coding	P10147	54	GC17M036088	10.18
171	+	CSAR1	Complement C5a Receptor 1	Protein Coding	P21730	58	GC19P047290	10.18
172	+	C3	Complement C3	Protein Coding	P01024	62	GC19M006677	10.17
173	+	CXCL10	C-X-C Motif Chemokine Ligand 10	Protein Coding	P02778	57	GC04M076021	10.16
174	+	CRP	C-Reactive Protein	Protein Coding	P02741	58	GC01M167583	10.16
175	+	AQP5	Aquaporin 5	Protein Coding	P55064	60	GC12P049961	10.16
176	+	HAVCR2	Hepatitis A Virus Cellular Receptor 2	Protein Coding	Q8TDQ0	58	GC05M157063	10.10
177	+	SFTPD	Surfactant Protein D	Protein Coding	P35247	57	GC10M079937	10.04
178	+	ITGA4	Integrin Subunit Alpha 4	Protein Coding	P13612	62	GC02P181501	10.02
179	+	KITLG	KIT Ligand	Protein Coding	P21583	60	GC12M088492	10.00
180	+	ITGAL	Integrin Subunit Alpha L	Protein Coding	P20701	60	GC16P030472	10.00

## Lampiran 5. Perintah docking pada YASARA-Structure

```

# 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/1.sdf'

# 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 *.job 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/desti/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\lcrn'
MacroTarget /home/al/yasara/2021/desti/03_md/1hwl.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 content 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 'timestep' 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\1cm'
#MacroTarget /home/gerry/pafr/2_md/5zkg.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 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)\1hwl(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)\1hwl(k)_complex.sce
  Clear
#Calculation
method = 'VINALS'
runs = 1
rmsdmin = 5.0
rigid = 1
for j=00001 to 00200
  LoadSce (MacroDir)\1hwl(j)_complex.sce
  NameObj 1,receptor
  NameObj 2,ligand
  ForceField AMBER03
  Boundary Wall
  Longrange None
```

## Lampiran 9. 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\lcrn'
# 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'
```