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LAMPIRAN

Lampiran 1 Perhitungan Kromatografi Kolom Klasik

- Perhitungan Adsorben

πr2t x 0,62(density silica gel 60) = 3,14 x 0,852 x 20 x 0,62 = 28,13 gram

- Perhitungan Sample

Perbandingan sampel dengan adsorben adalah maksimal 1:20. Maka jumlah sampel fraksi yang disiapkan sebanyak = 28.130 mg/20 = 1.407 mg. Karena total bobot fraksi yang ada adalah 870 mg maka fraksi yang digunakan setengahnya = 435 mg.

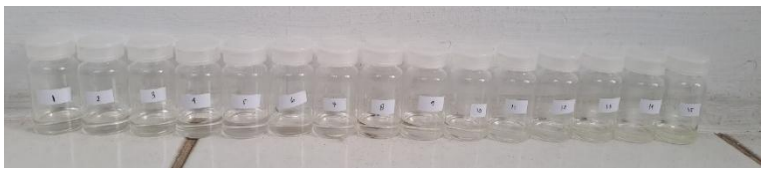
- Perhitungan Eluen

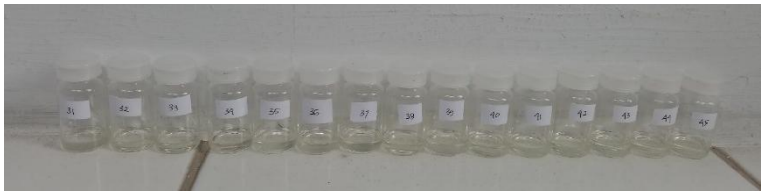
Kloroform-etil asetat (7:3) dibuat 1000 ml :

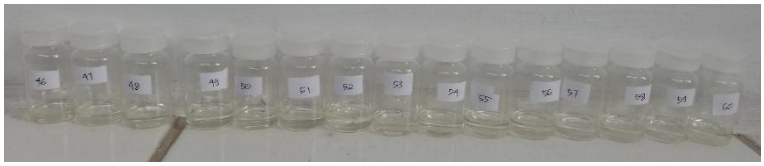
Kloroform : 700 mL

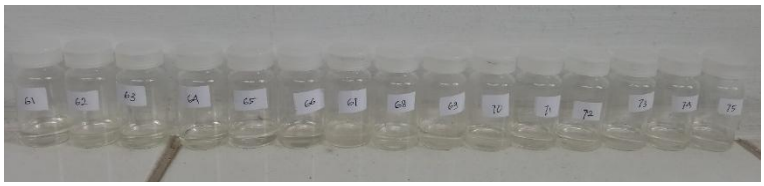
Etil Asetat : 300 mL

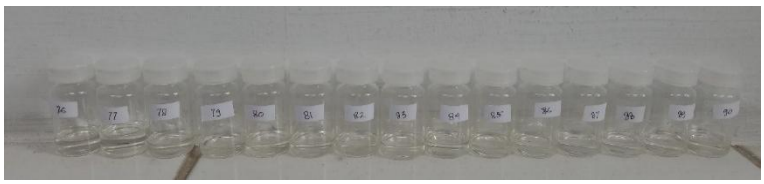
Lampiran 2 Hasil Subfraksinasi

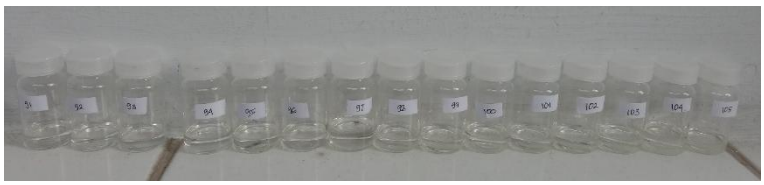


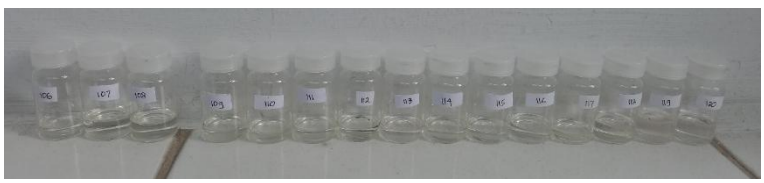


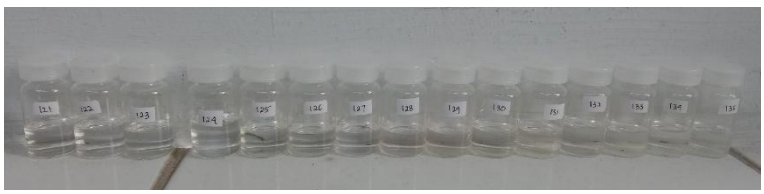


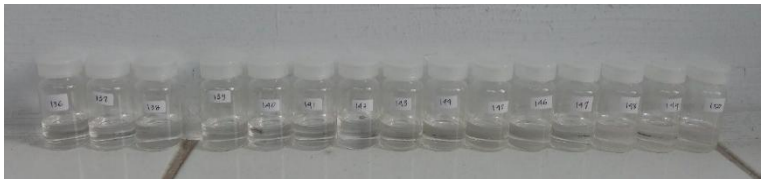


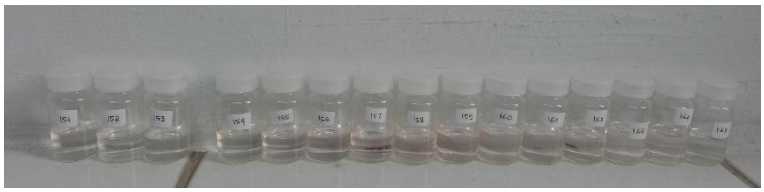


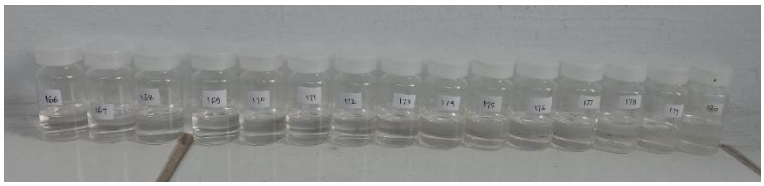


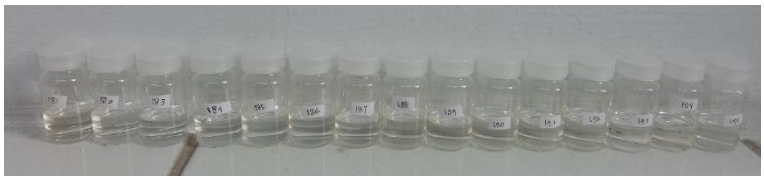


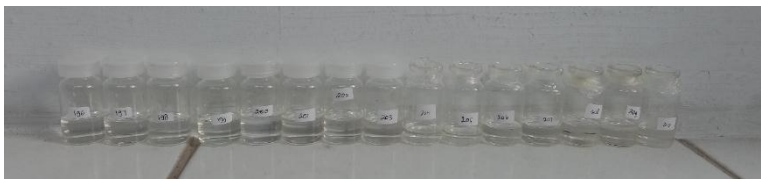


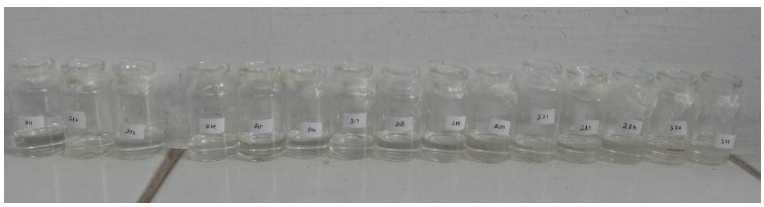


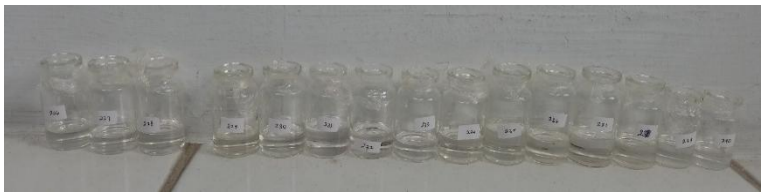


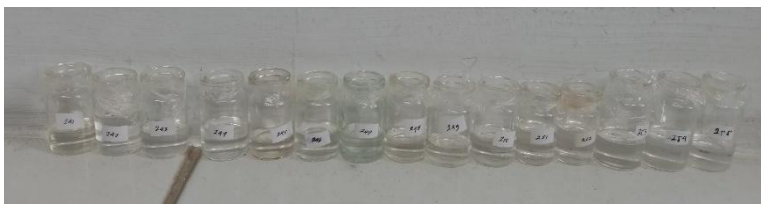


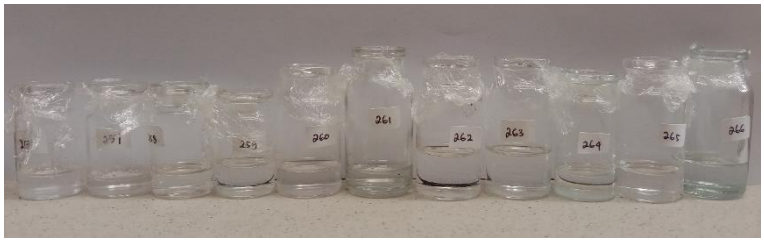








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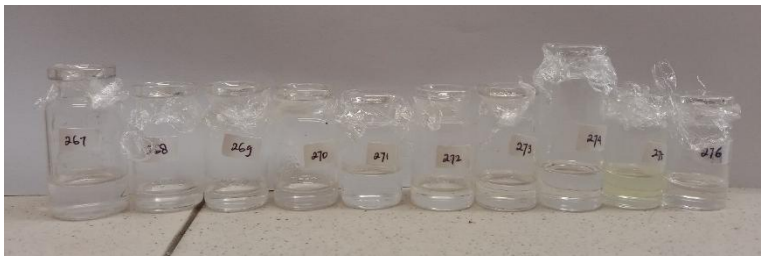
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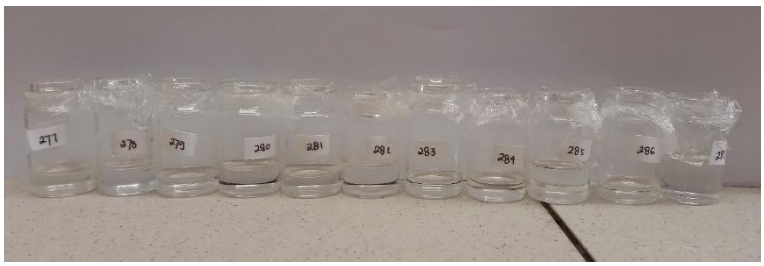
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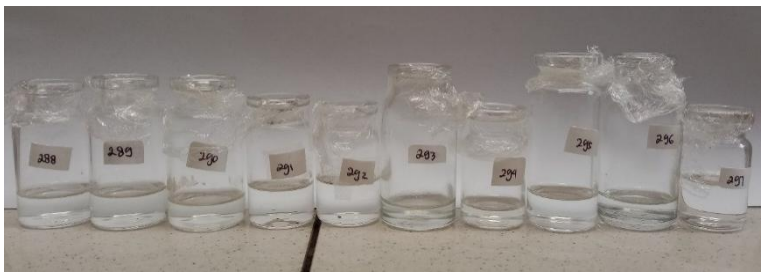
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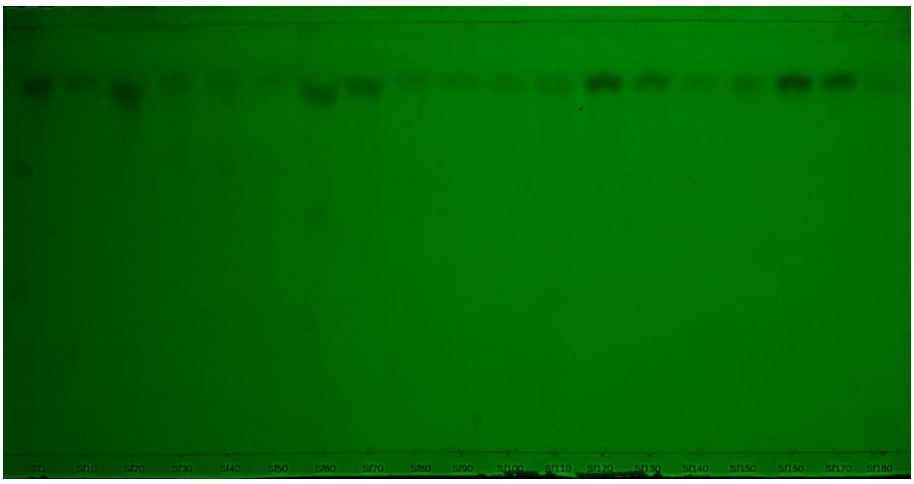
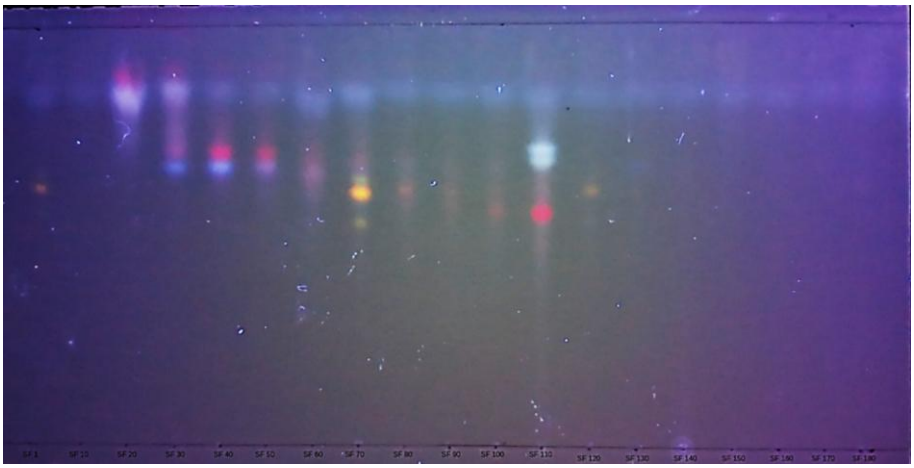
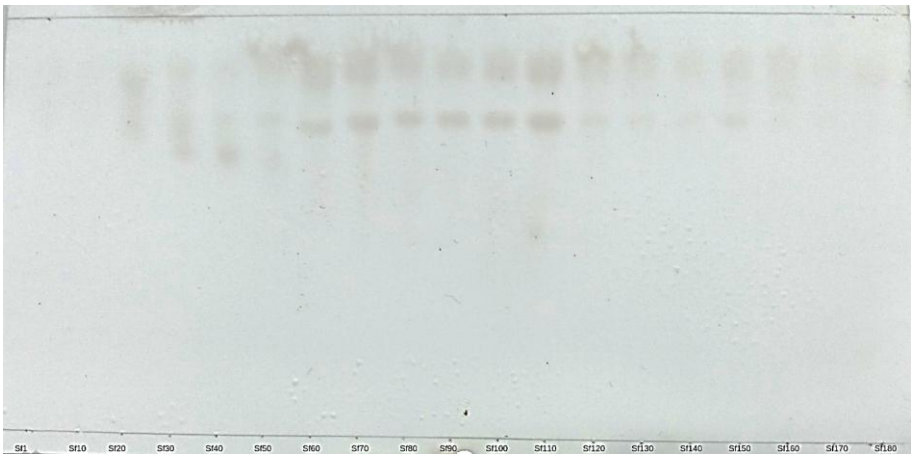
Lampiran 3 Hasil Komatografi Lapis Tipis



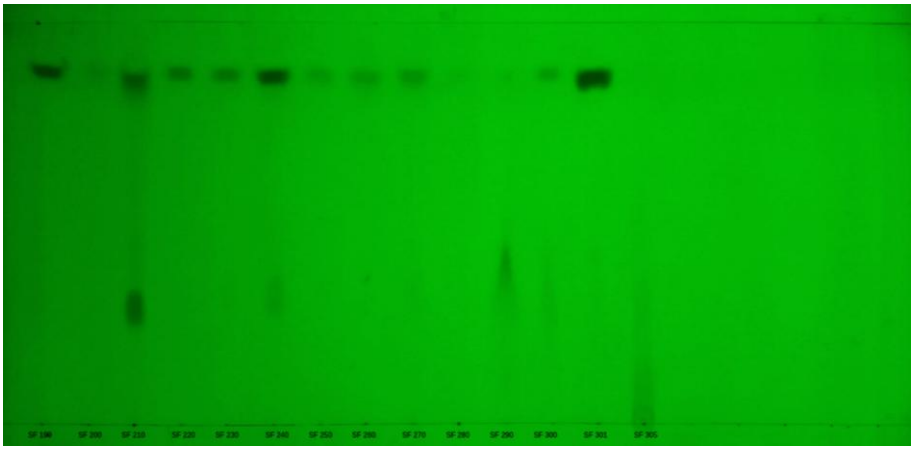
Subfraksi 1-180 pada UV 254 nm



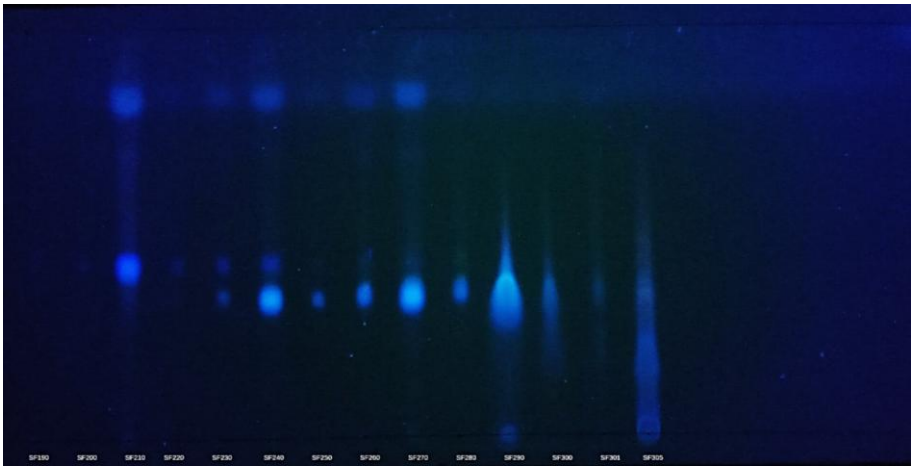
Subfraksi 1-180 pada UV 366 nm



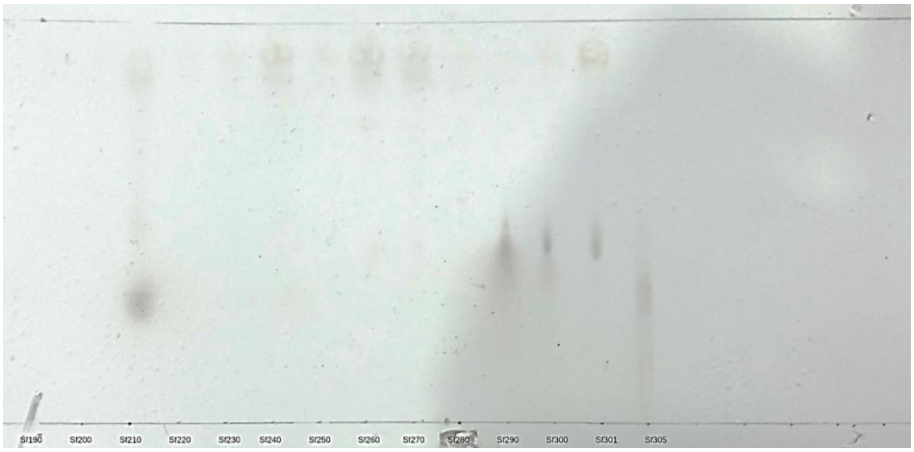
Subfraksi 1-180 dengan penampak bercak H_2SO_4



Subfraksi 190-305 pada UV 254 nm

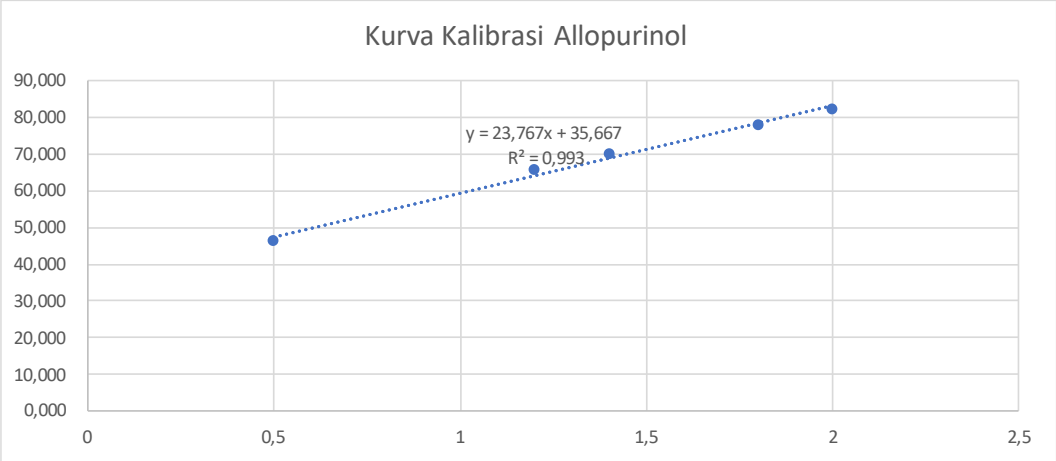


Subfraksi 190-305 pada UV 366 nm



Subfraksi 190-305 dengan penampak bercak H_2SO_4

Lampiran 4 Hasil Kurva Kalibrasi Standar Allopurinol

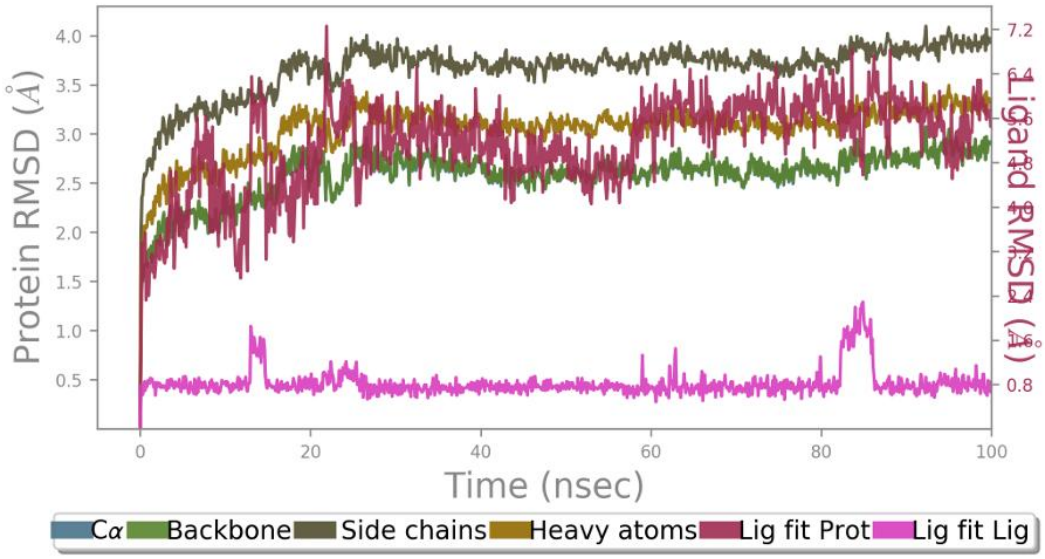


Lampiran 5 Hasil Identifikasi LC-MS/MS

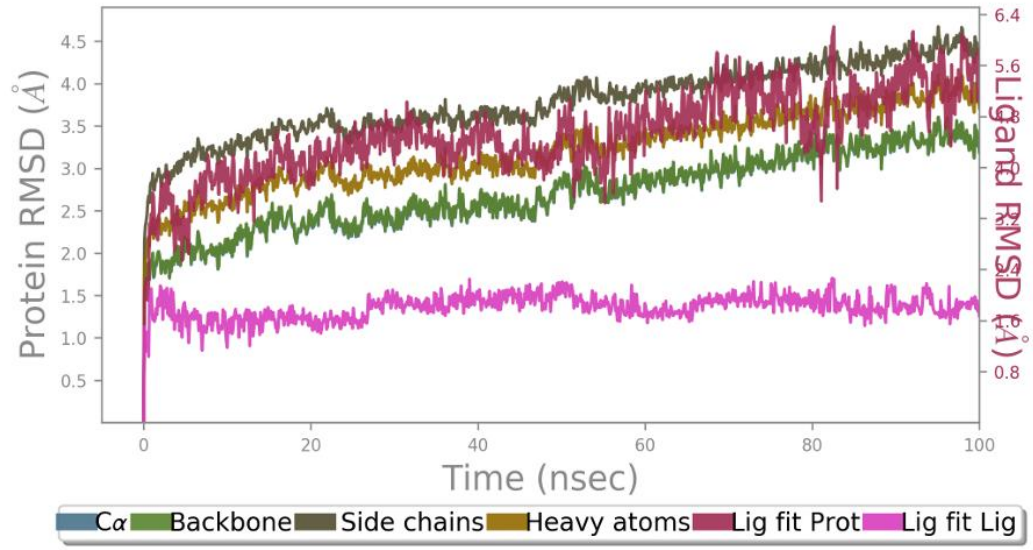
no.	Senyawa	Golongan	Golongan senyawa metabolit sekunder	Similaraty	Aktivitas antioksidan
1	Bis(2-ethylhexyl)adipate	Ester	fatty acid esters/diester (plasticizer)	99,5	
2	Bis(2-ethylhexyl) phthalate	Ester	diethylhexyl phthalate(DEHP)/phthalates (plasticizer)	99,8	ada
3	Oleamide	Asam lemak amida	fatty amides	99,2	
4	Bis(3,5,5-trimethylhexyl) phthalate	Ester	benzoate ester	98,4	
5	Stearamide	Asam lemak amida	primary fatty acid amide	99,5	
6	Phthalic acid	Asam dikarboksilat aromatik	aromatic dicarboxylic acid	98,5	
7	1-Stearoylglycerol	ester	glycerolipids	96,2	
8	Tri-o-Cresyl phosphate	organophosphate	organophosphorus ester	95,4	ada
9	3,5-di-tert-Butyl-4-hydroxybenzaldehyde	Aldehida	hydroxybenzaldehyde	97,2	
10	4-Methoxycinnamic acid	Asam karboksilat	Phenolic	95,7	
11	Decanamide	Amida	fatty amides	98	
12	Adipic acid	Asam karboksilat	dicarboxylic acid	98,3	
13	Monolaurin	ester	mono ester	<90	ada
14	Avobenzone	Benzene tersubstitusi	Flavonoids	95,6	ada
15	Bis(2-ethylhexyl) terephthalate	ester	DEHT (Dioctyl terephthalate or DOTP)/phthalates (plasticizer)	93,6	
16	Diethyl phthalate	ester	esters of phthalic acid	99,1	
17	Methyl palmitate	ester	fatty acid methyl ester	98,9	ada
18	Bis(7-methyloctyl) adipate	ester	Adipic acid	<90	
19	Dibutyl hexanedioate	ester	Adipic acid	98,6	
20	12-oxo Phytodienoic Acid	asam karboksilat	carbocyclic fatty acid	92,6	ada
21	9-Oxo-10(E),12(E)-octadecadienoic acid	asam karboksilat	fatty acid	97,8	ada
22	2,3-dihydroxypropyl 12-methyltridecanoate	ester	mehyl ester	94,6	
23	Bis(methylbenzylidene)sorbitol	acetal	carbohydrate	99,9	
24	Bis(2-ethylhexyl) sebacate	ester	ester	<90	
25	Alverine	senyawa heterosiklik	senyawa heterosiklik	<90	
26	Monoolein	alkohol	alkohol	98,9	
27	Triethylene glycol monobutyl ether	alkohol	alkohol	98,7	
28	Cholest-4-en-3-one	keton	steroid	91,8	
29	Ethyl palmitoleate	ester	fatty acid	<90	
30	α-Linolenic acid	asam karboksilat	fatty acid	99,3	ada
31	Galaxolidone	keton	isochromenes	92,3	
32	Diisobutyl adipate	ester	fatty acid	<90	ada
33	Perillartine	oxime	monoterpenoids	<90	
34	Dihomo-γ-linolenic acid ethyl ester	ester	fatty acid	92,9	
35	α-Eleostearic acid	asam karboksilat	fatty acid	99,1	ada
36	1-Linoleoyl glycerol	alkohol	alkohol	96,3	
37	Benzophenone	benzena tersubstitusi	Phenolic	99,4	ada
38	Octocrylene	ester sinamat	ester sinamat	91,3	
39	1,2-Cyclohexane dicarboxylic acid diisononyl ester	ester	ester	93,2	
40	Hexadecanamide	amida	fatty acid amide	96,6	
41	Tributyl citrate	ester	ester	98,8	
42	Palmitoleic acid	asam karboksilat	fatty acid	99,1	ada
43	Guanine	nukloebasa	purine nucleobase	99,2	
44	Vitamin E Acetate	ester	Phenolic	<90	ada
45	Tridemorph	senyawa alifatik	Oxazinanes	98,1	
46	8-{3-Oxo-2-[(2E)-2-penten-1-yl]-1-cyclopenten-1-yl}octanoic acid	asam karboksilat	fatty acid	<90	
47	2-(Methylthio)benzothiazole	senyawa heterosiklik	heterocyclic compounds	99,3	
48	2,6-Di-tert-butyl-1,4-benzoquinone	keton	Quinones	94,1	ada
49	Adenine	senawa heterosiklik	purine nucleobase	99	
50	Diphenylamine	senyawa organonitrogen	aromatic amine	99,9	ada
51	Celecoxib	senyawa heterosiklik	NSAIDs	97,9	ada
52	Ethyl oleate	ester	fatty acid	98,4	
53	α-Pyrrolidinopropiophenone	senyawa heterosiklik	senyawa heterosiklik	92,4	
54	3,5-di-tert-Butyl-4-hydroxybenzoic acid	Asam karboksilat	flavonoids	96,1	
55	Octhilinone (OIT)	senyawa heterosiklik	senyawa heterosiklik	90,2	
56	droxy-6-[2-(2-methyl-1,2,4a,5,6,7,8,8a octahydronaphthalen-1-yl)ethyl]oxan-2	lakton	Sesquiterpene	93	ada
57	Dibenzylamine	senyawa organonitrogen	aromatic amine	100	
58	Bicine	asam amino	amino acids	99	
59	Oxybenzone	senyawa fenol	Phenolic	97,8	
60	cis-12-Octadecenoic acid methyl ester	ester	fatty acid	95,8	
61	3-[3-(1,3-dimethyl-1H-pyrazol-4-yl)-1H-1,2,4-triazol-1-yl]-5- methylisoxazole	senyawa heterosiklik	senyawa heterosiklik	<90	
62	(+)-ar-Turmerone	senyawa terpen	sesquiterpenoid	99,3	ada
63	Ricinine	senyawa heterosiklik	Alkaloids	91,5	
64	N-Octyl-2-pyrrolidone	senyawa heterosiklik	senyawa heterosiklik	<90	
65	acridine-9(10H)-thione	senyawa heterosiklik	senyawa heterosiklik	96,6	
66	Trimellitic anhydride	Senyawa anhydrida	dicarboxylic anhydride	99,6	
67	Triphenyl phosphate	senyawa organofosfor	ester	90,8	ada
68	4-Methylbenzophenone	benzena tersubstitusi	Phenolic	93,8	
69	NP-019374			<90	
70	Dodecylamine	senyawa organonitrogen	aliphatic amine	97	
71	Tangeritin	senyawa heterosiklik	Flavonoids	94,9	ada
72	NP-001798			96	
73	Methyl yellow	senyawa pewarna	senyawa pewarna	<90	
74	hyl-9-oxo-7-(propan-2-yl)-1,2,3,4,4a,9,10,10a octahydrophenanthrene-1-carbo	Asam karboksilat terpenoid	Terpenoids	<90	

Keterangan: yang diberi highlight kuning = similarity<90%, yang diberi highlight hijau = metabolit sekunder

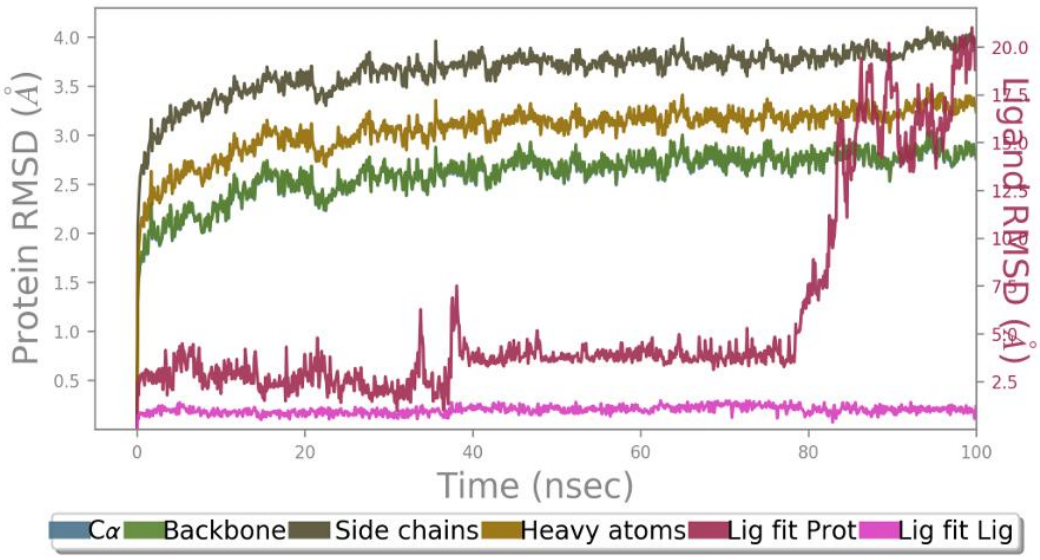
Lampiran 6 RMSD Protein-Ligan



Cholest-4-en-3-one



4-hydroxy-6-[2-(2-methyl-1,2,4a,5,6,7,8,8a-octahydronaphthalen-1-yl)ethyl]oxan-2-one



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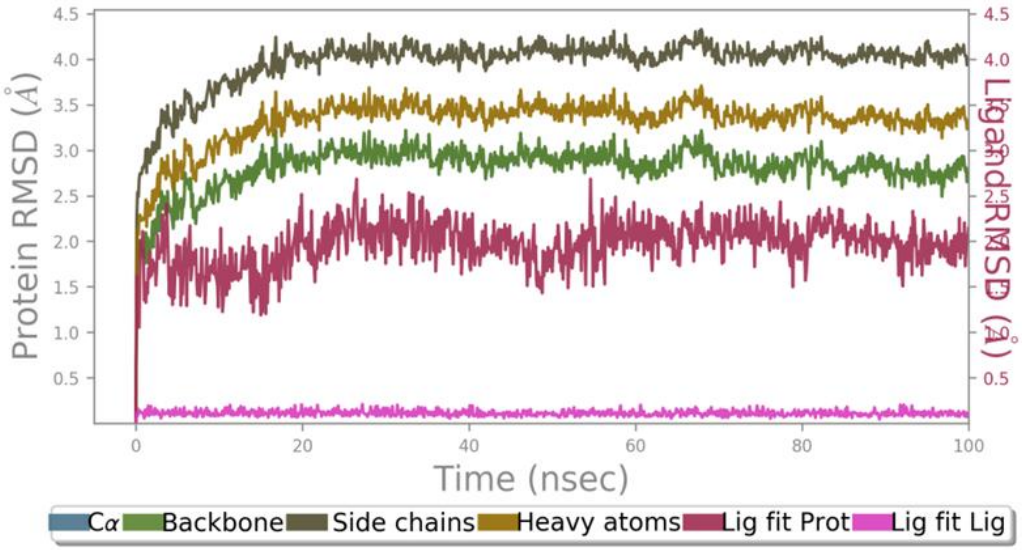
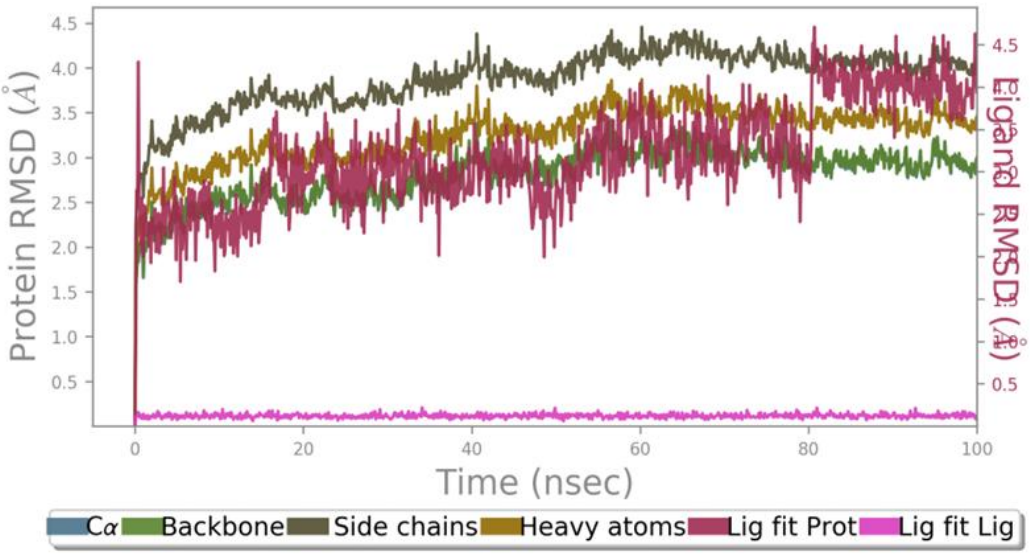


Allopurinol



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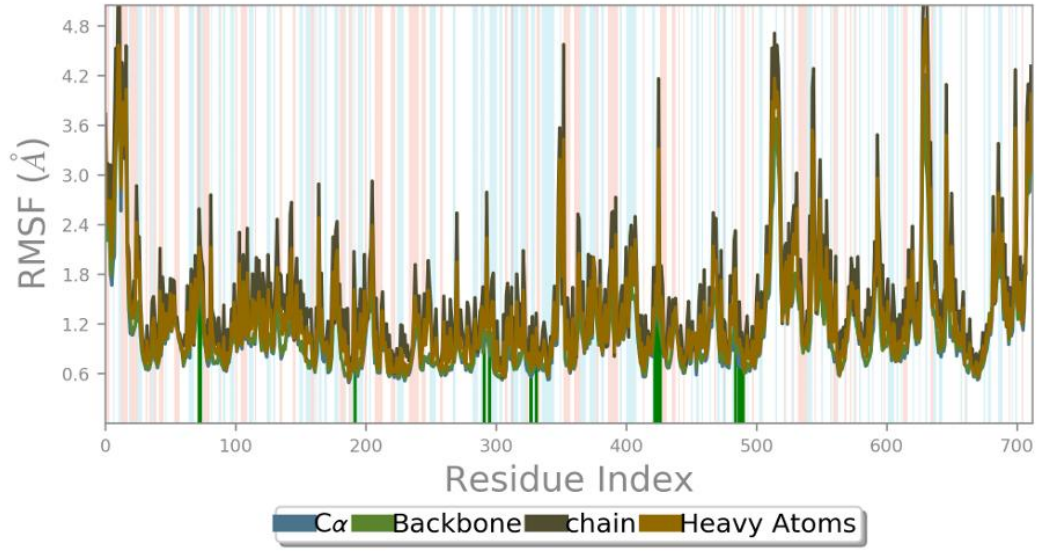
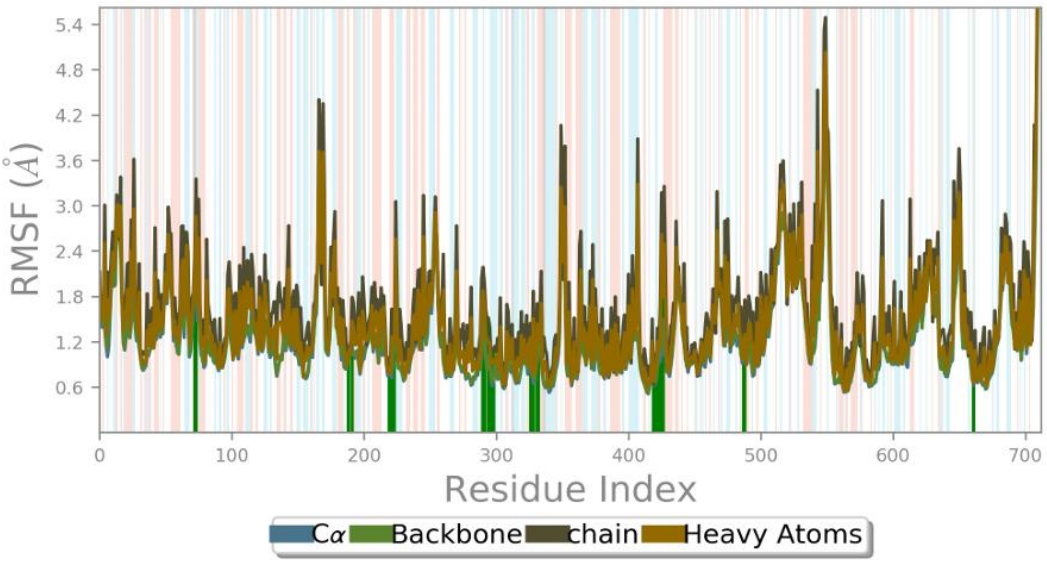
Lampiran 7 RMSF Protein



Cholest-4-en-3-one



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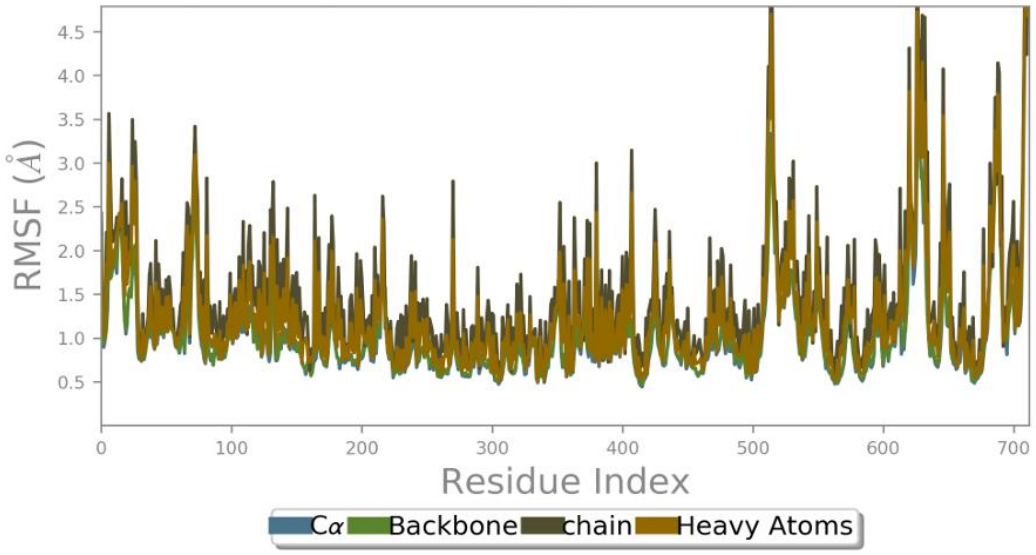

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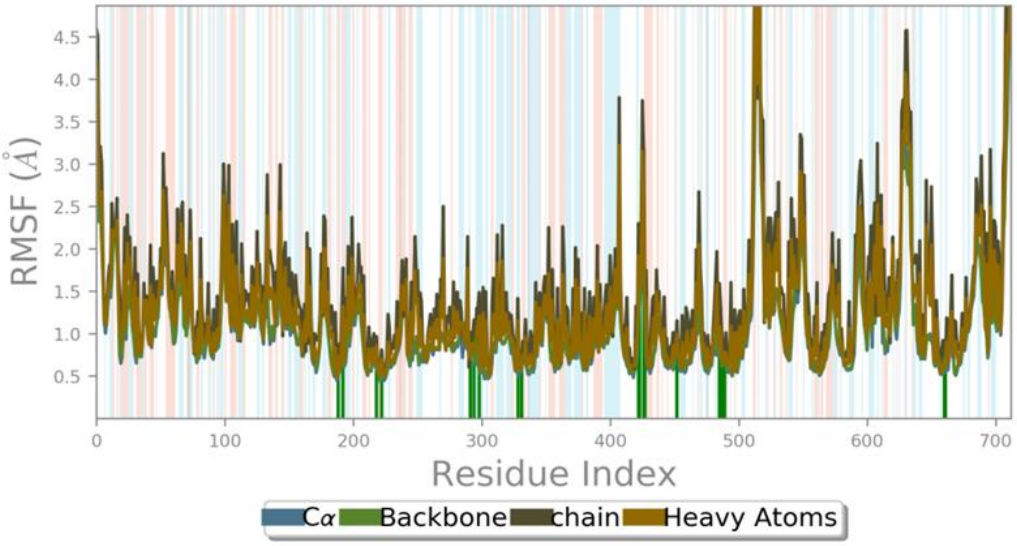

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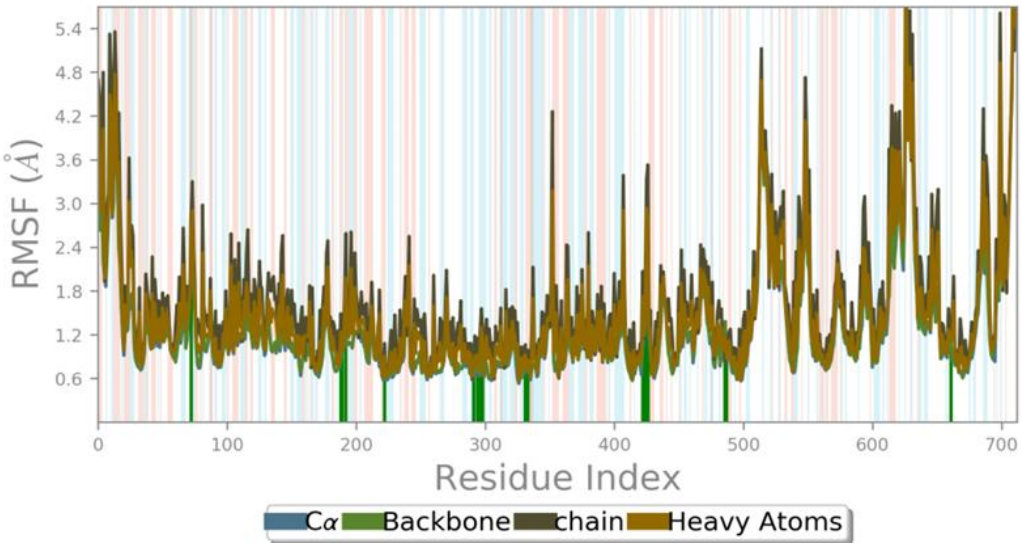

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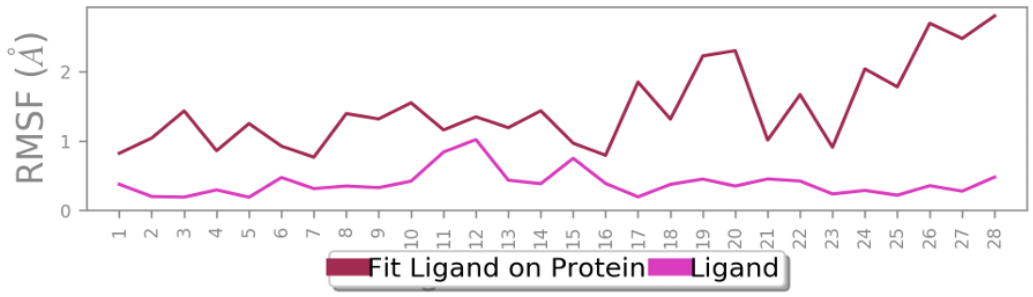
Lampiran 8 RMSF Ligan



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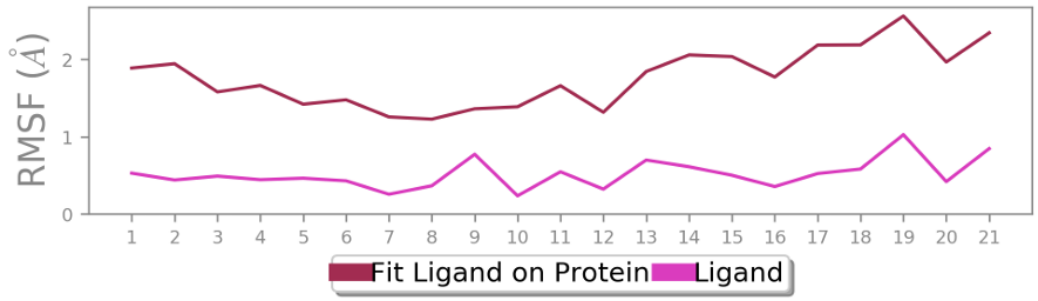
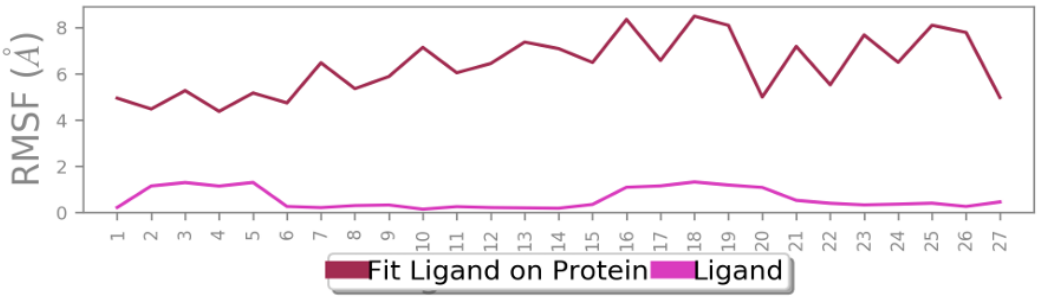


4-hydroxy-6-[2-(2-methyl-1,2,4a,5,6,7,8,8a-octahydronaphthalen-1-yl)ethyl]oxan-2-one



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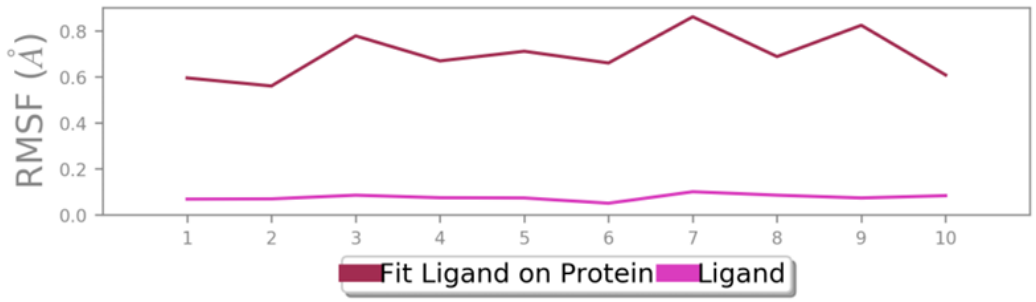
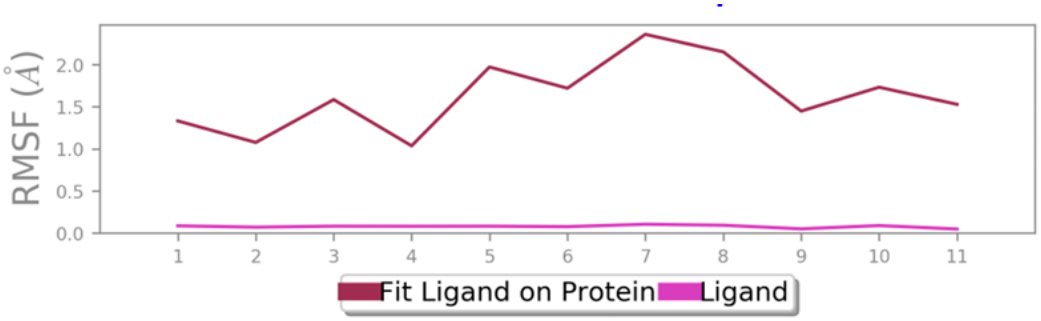


Allopurinol



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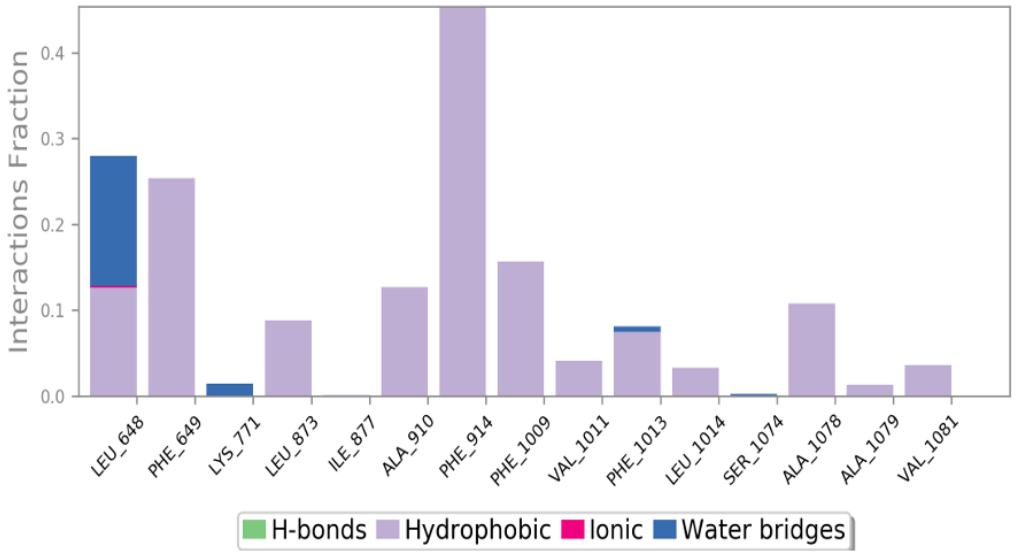
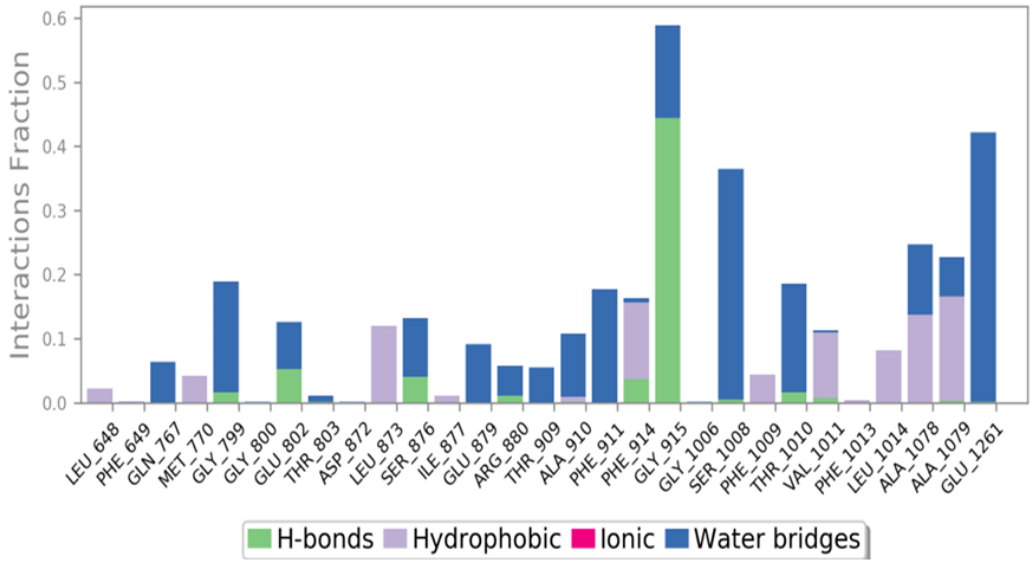
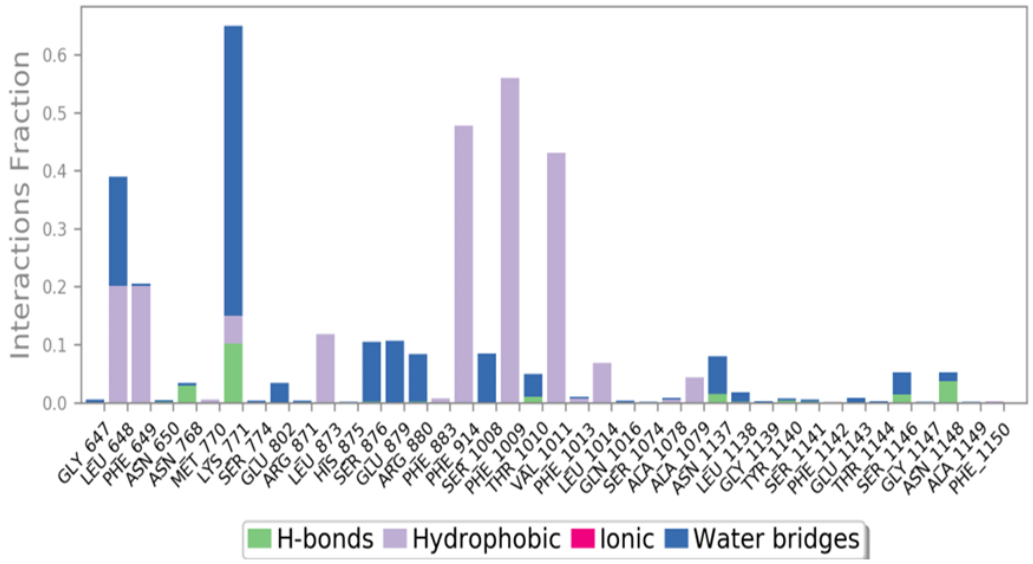
Lampiran 9 Kontak Protein-Ligan



Cholest-4-en-3-one



4-hydroxy-6-[2-(2-methyl-1,2,4a,5,6,7,8,8a-octahydronaphthalen-1-yl)ethyl]oxan-2-one



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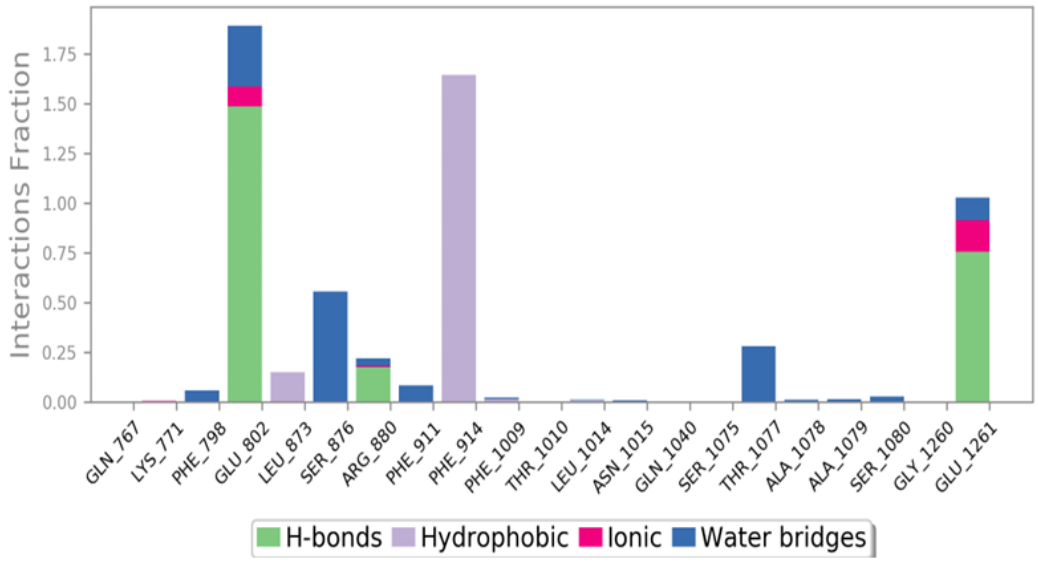
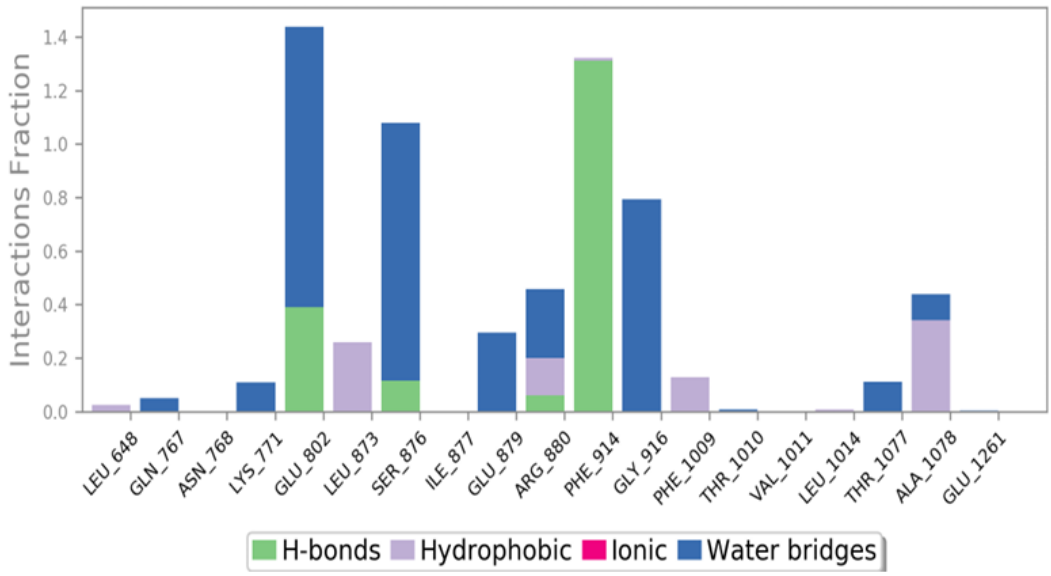


Allopurinol



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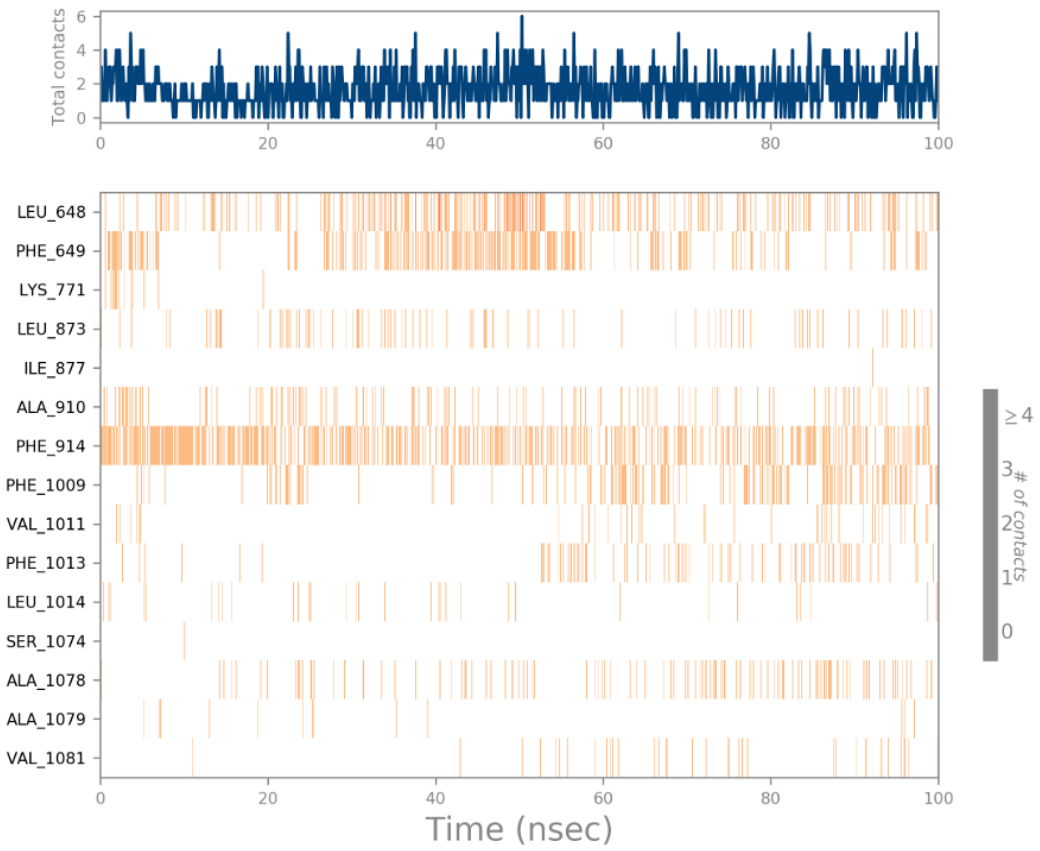
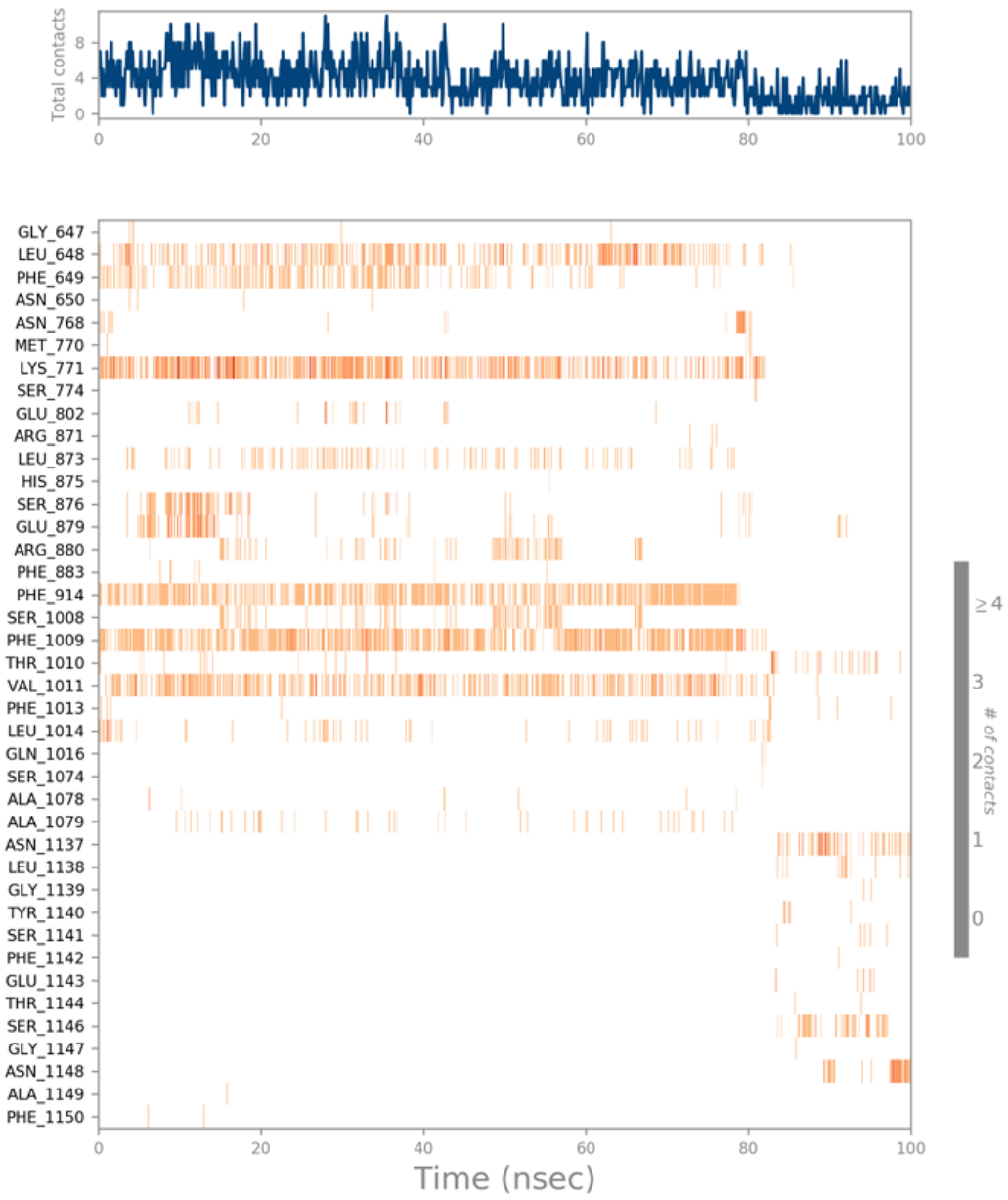
Lampiran 10 Kontak Lanjutan Protein-Ligan



Cholest-4-en-3-one

4-hydroxy-6-[2-(2-methyl-1,2,4a,5,6,7,8,8a-octahydronaphthalen-1-yl)ethyl]oxan-2-one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0
20
40
60
80
100
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LEU_648
PHE_649
ASN_650
ASN_768
MET_770
LYS_771
SER_774
GLU_802
ARG_871
LEU_873
HIS_875
SER_876
GLU_879
ARG_880
PHE_883
PHE_914
SER_1008
PHE_1009
THR_1010
VAL_1011
PHE_1013
LEU_1014
GLN_1016
SER_1074
ALA_1078
ALA_1079
ASN_1137
LEU_1138
GLY_1139
TYR_1140
SER_1141
PHE_1142
GLU_1143
THR_1144
SER_1146
GLY_1147
ASN_1148
ALA_1149
PHE_1150
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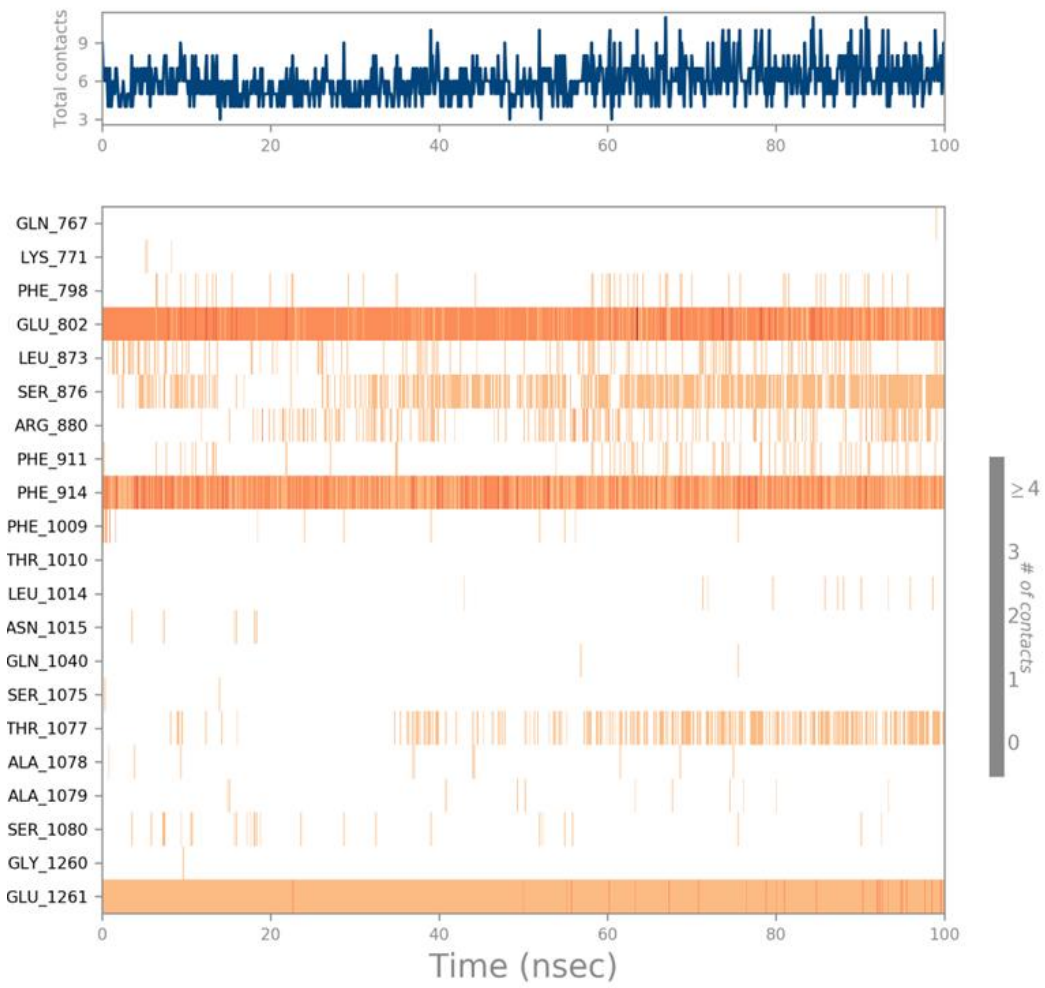
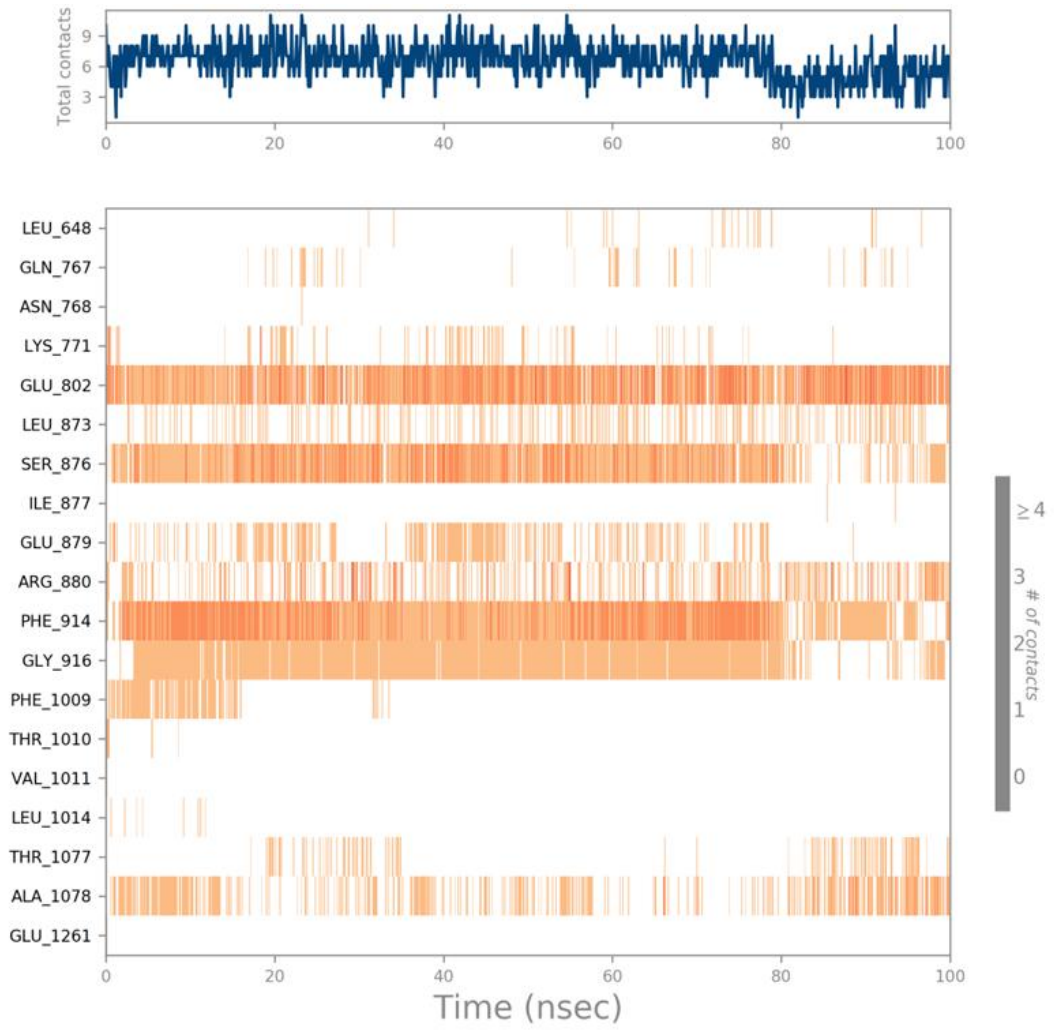
20
40
60
80
100
Time (nsec)
≥ 4
3
2
1
0
# of contacts

Tangeritin



Allopurinol



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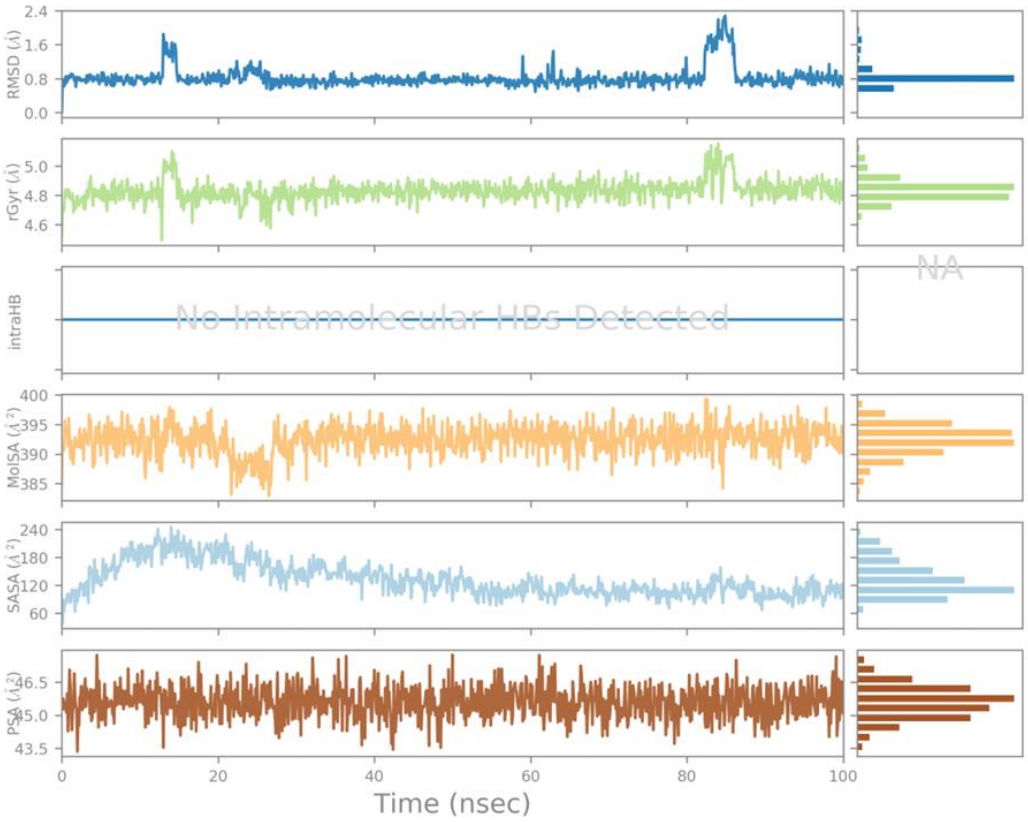
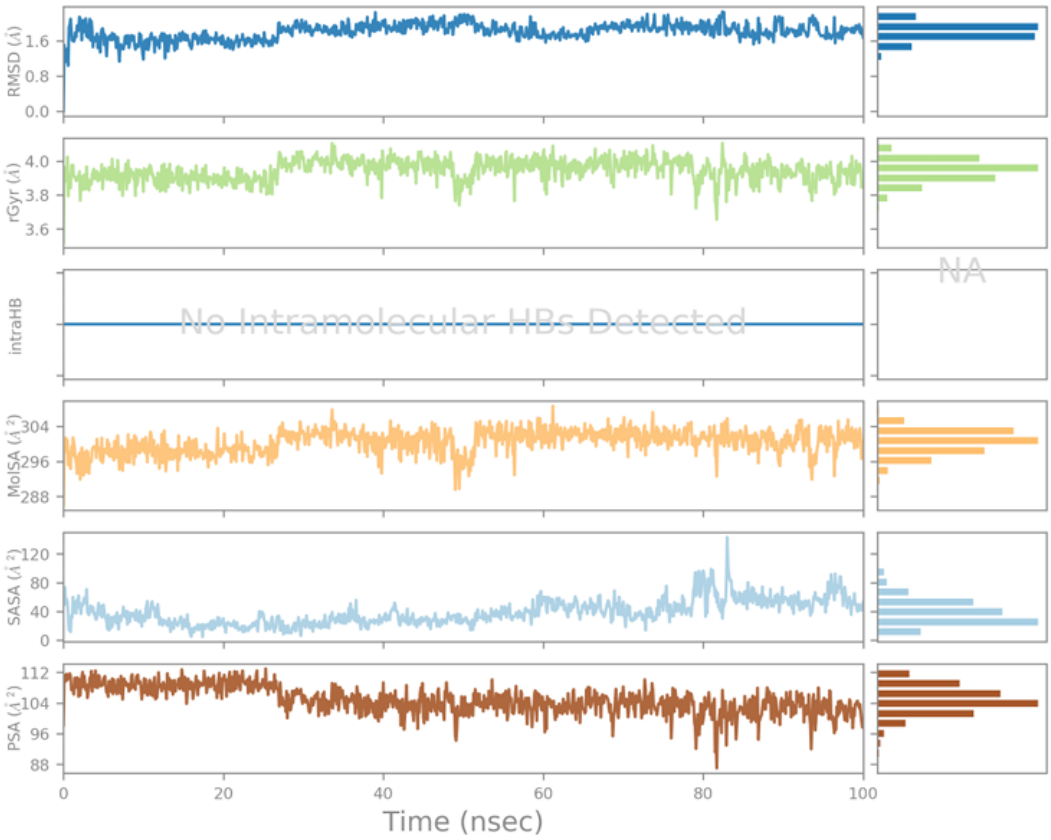
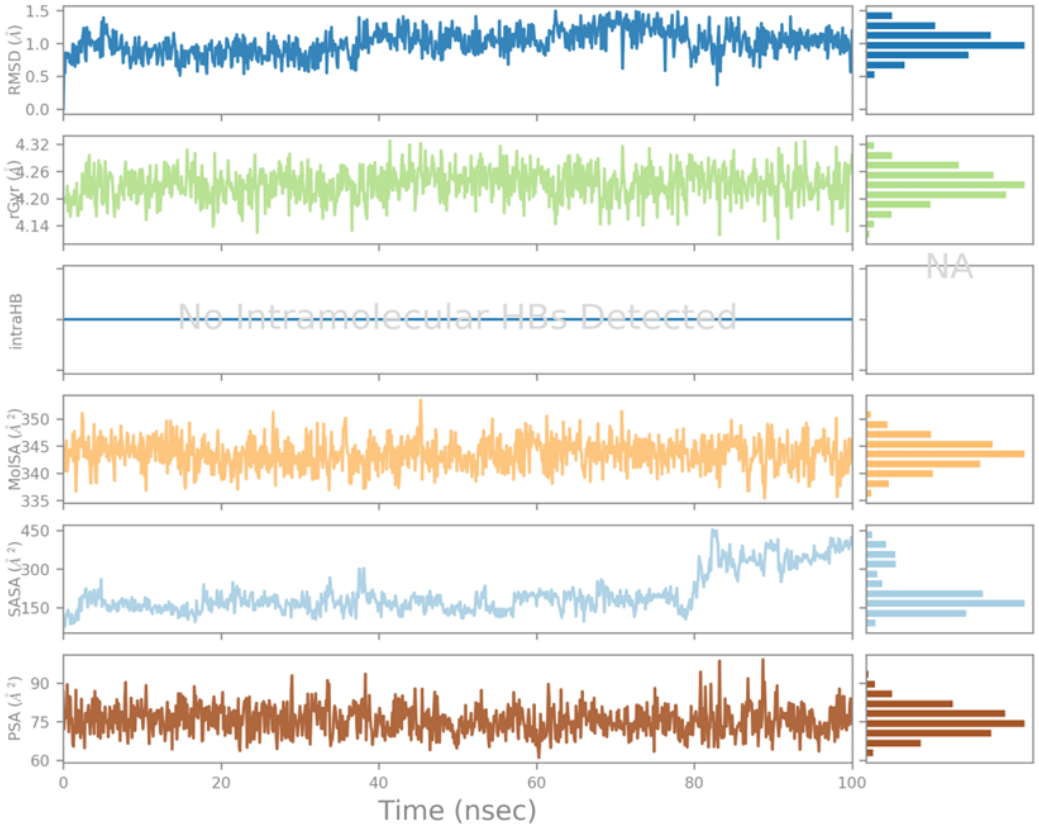
Lampiran 11 Karakteristik Ligan



Cholest-4-en-3-one



4-hydroxy-6-[2-(2-methyl-1,2,4a,5,6,7,8,8a-octahydronaphthalen-1-yl)ethyl]oxan-2-one


RMSD (Å)
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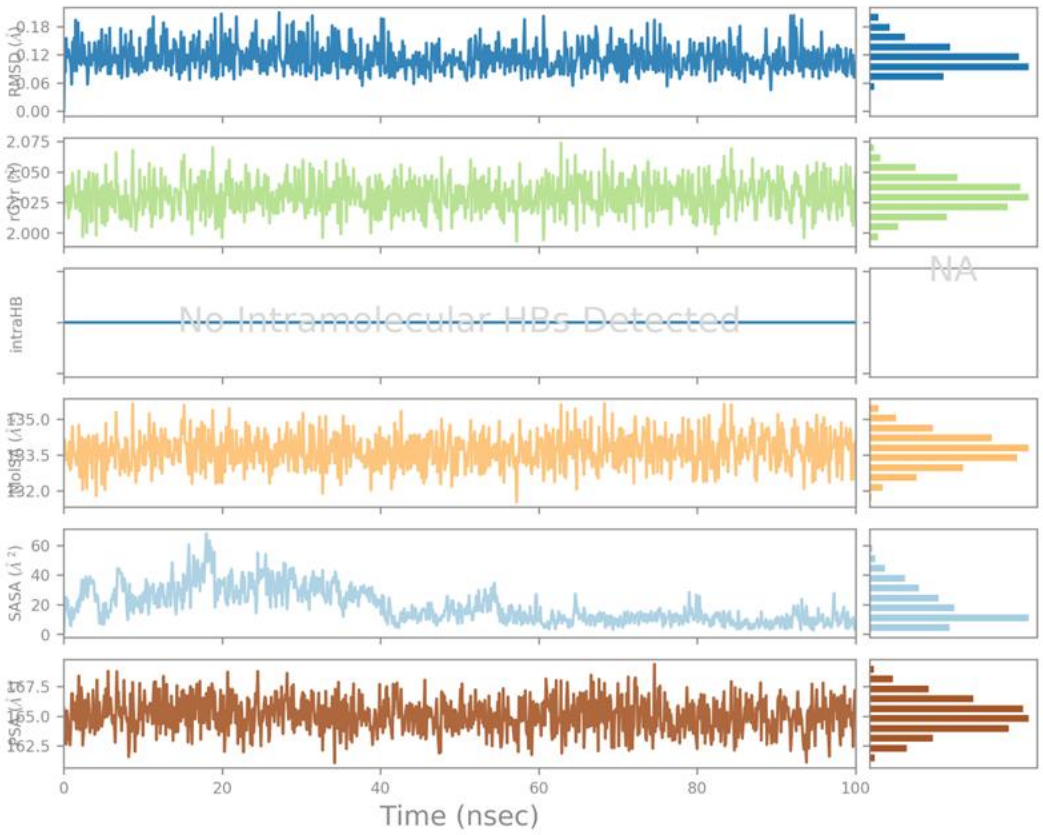
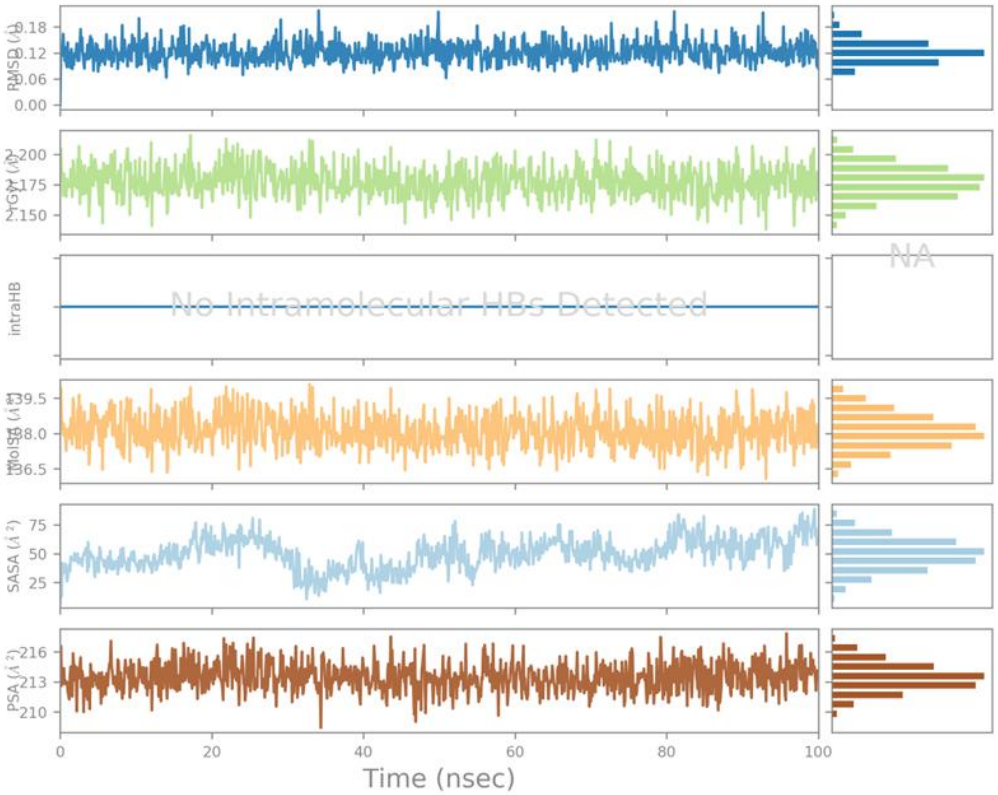
1.0
0.5
0.0
rGyr (Å)
4.32
4.26
4.20
4.14
intraHB
No Intramolecular HBs Detected
NA
MolSA (Å²)
350
345
340
335
SASA (Å²)
450
300
150
PSA (Å²)
90
75
60
0
20
40
60
80
100
Time (nsec)

Tangeritin



Allopurinol



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