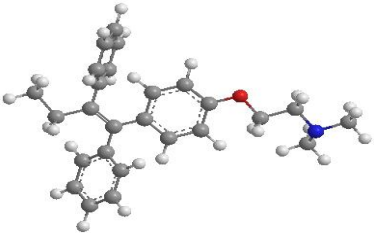
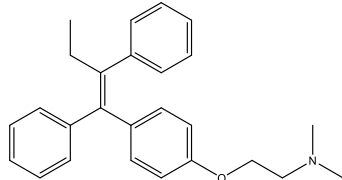
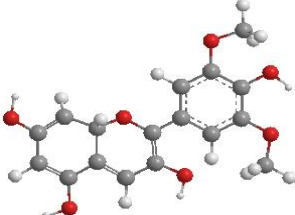
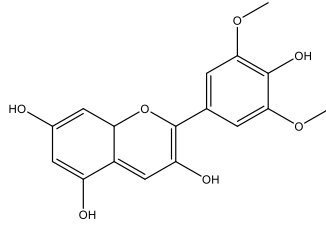
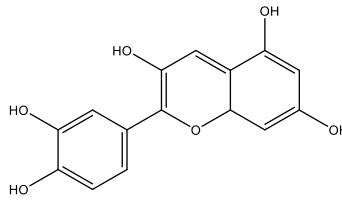
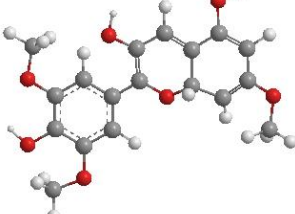
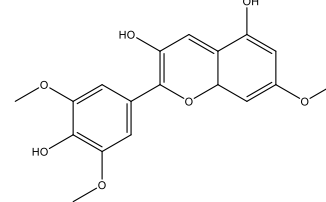
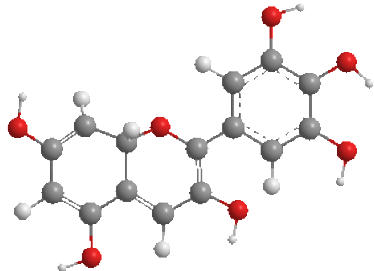
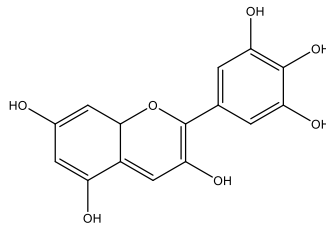
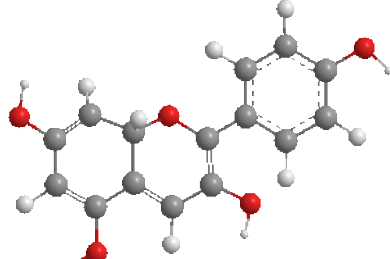
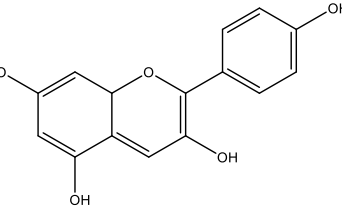
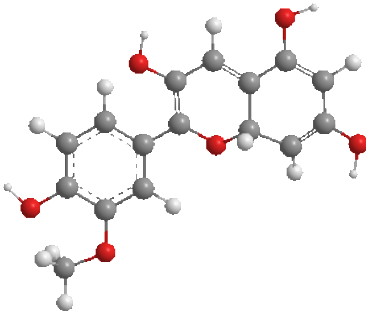
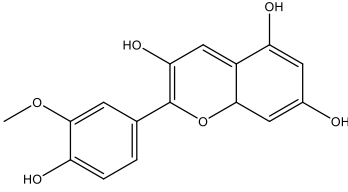
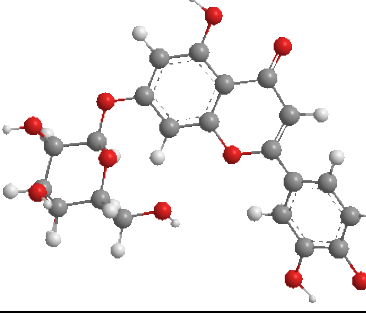
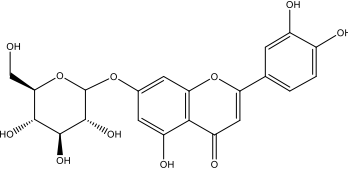
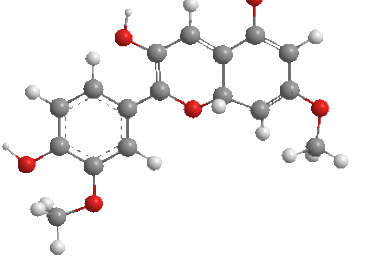
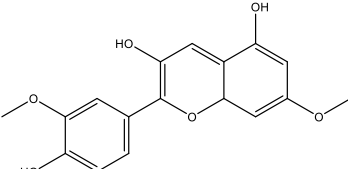
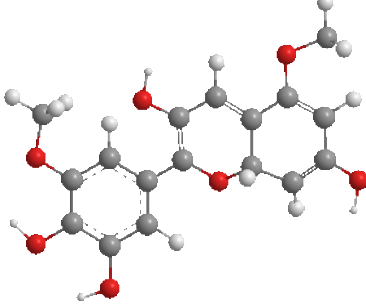
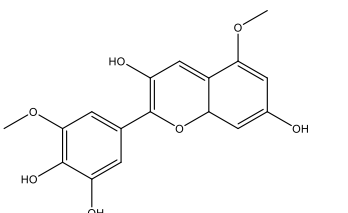
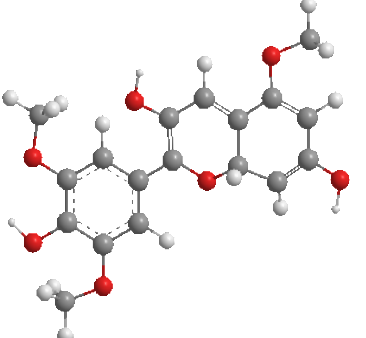
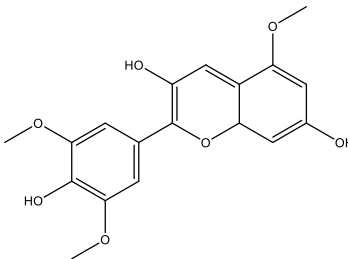
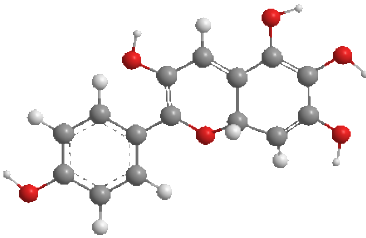
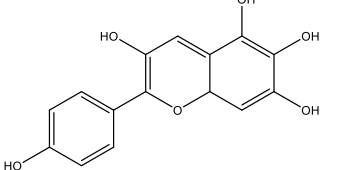
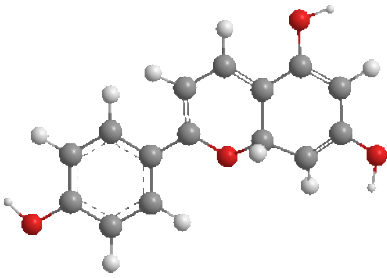
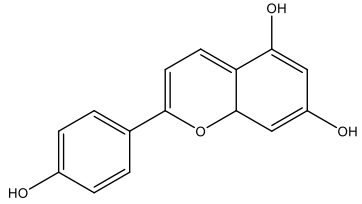
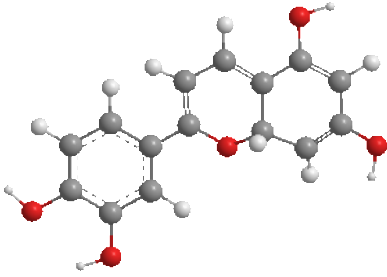
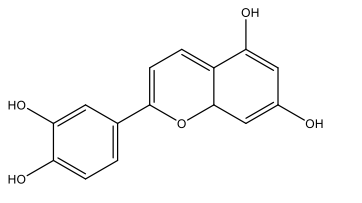
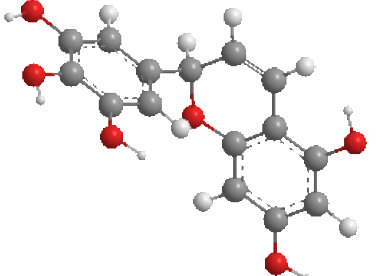
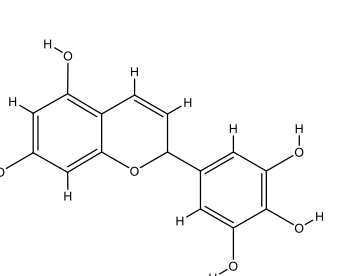
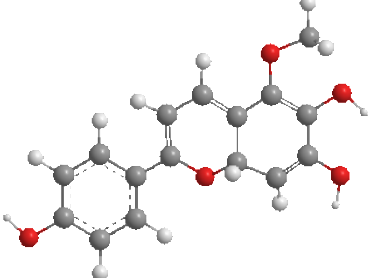
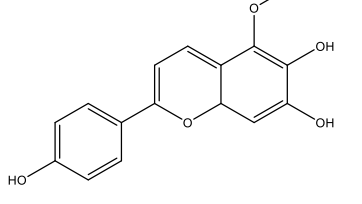
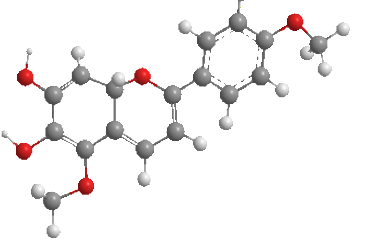
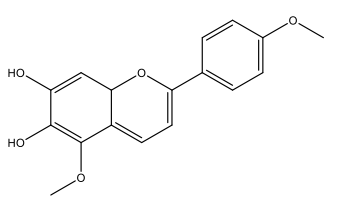


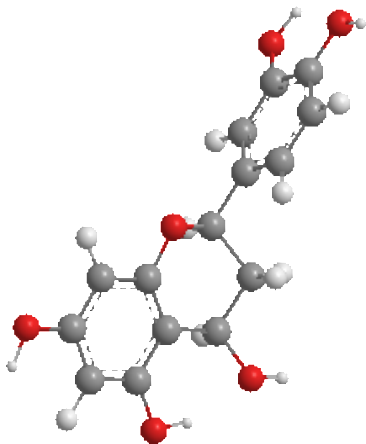
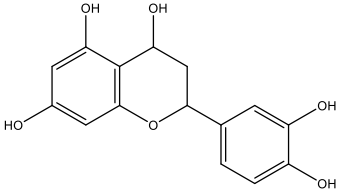
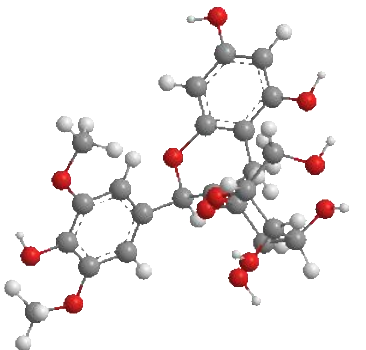
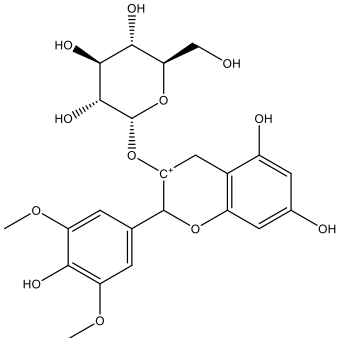
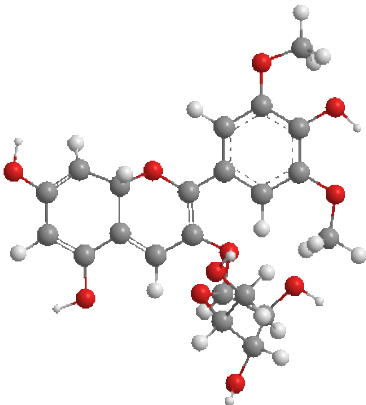
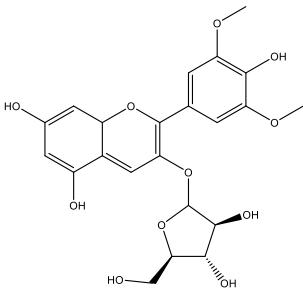
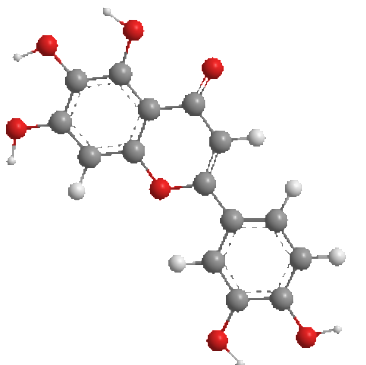
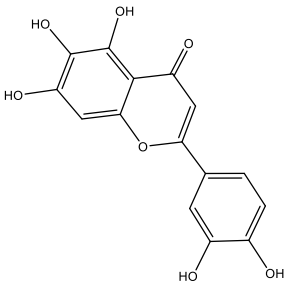
LAMPIRAN

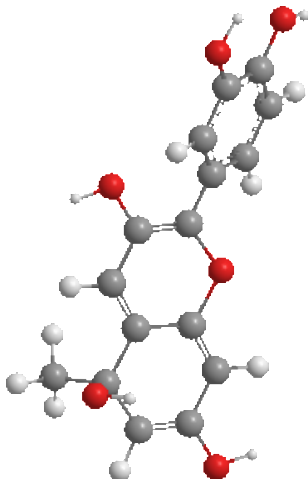
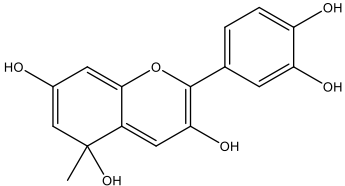
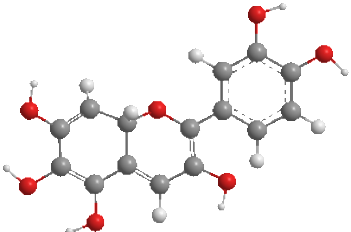
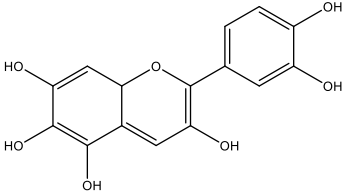
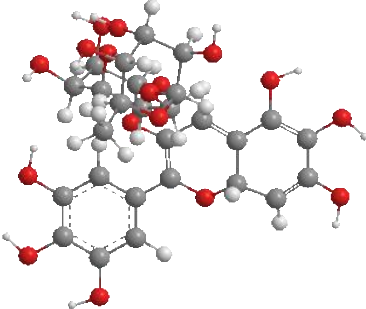
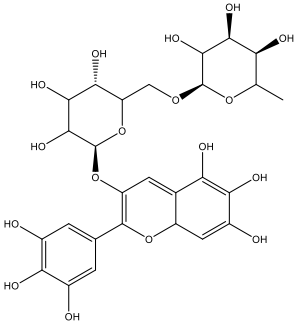
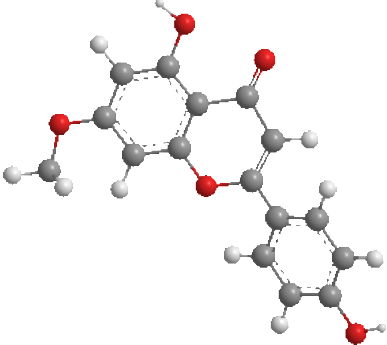
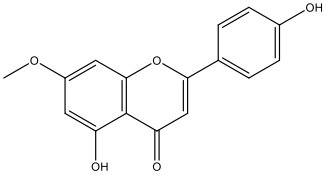
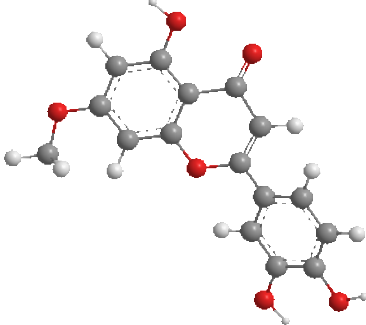
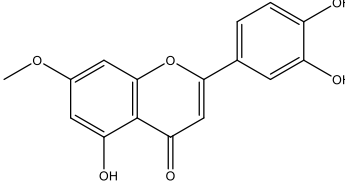
Lampiran 1 Visualisasi Struktur 2D dan 3D Ligan Uji

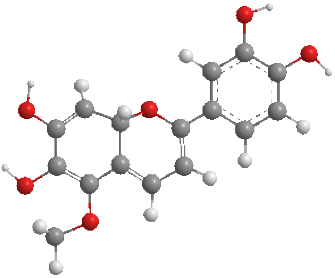
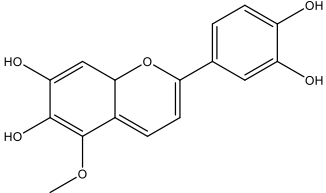
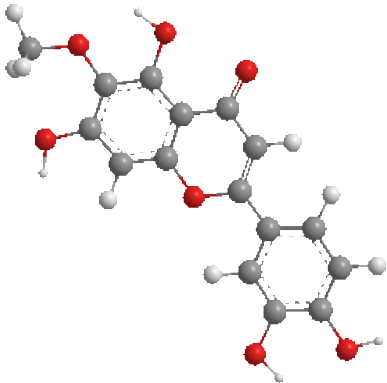
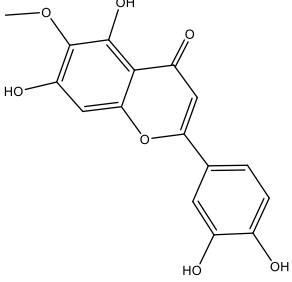
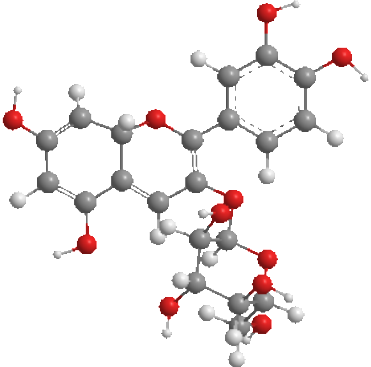
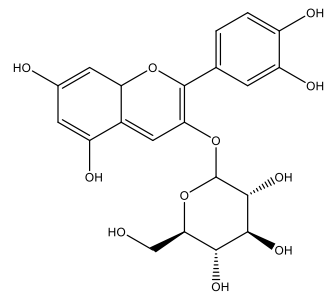
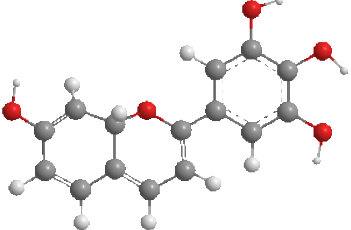
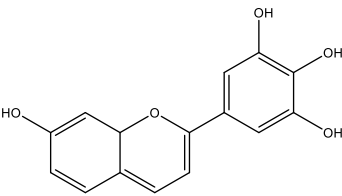
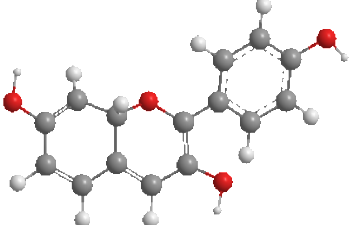
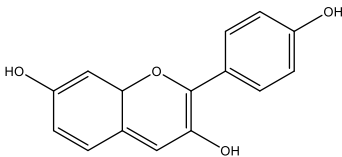
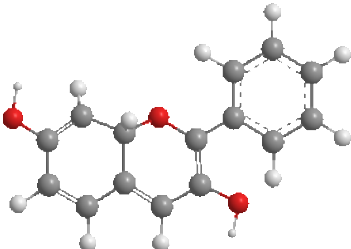
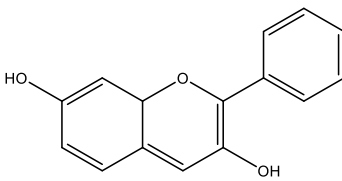
Kode Ligan	Nama Senyawa	Struktur 3D	Struktur 2D
A1	Tamoxifen		
A2	Malvidin		
A3	sianidin		
A4	hirsutinidin		
A5	delphinidin		
A6	pelargonidin		

A7	peonidin		
A8	Petunidin		
A9	rosinidin		
A11	Europinidin		
A12	capensidin		
A13	Aurantidin		

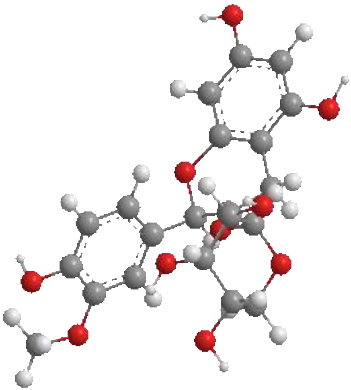
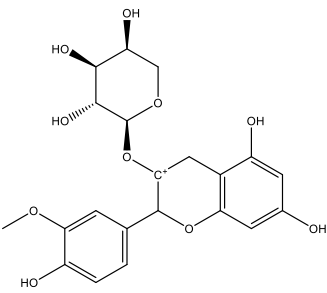
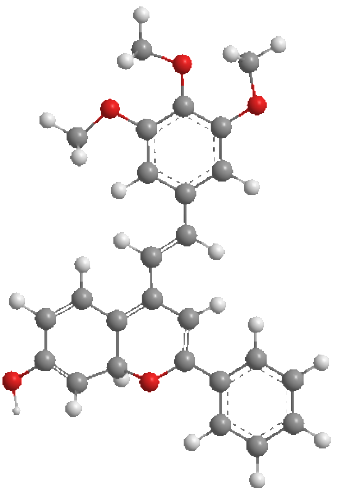
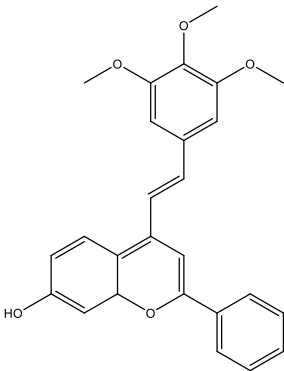
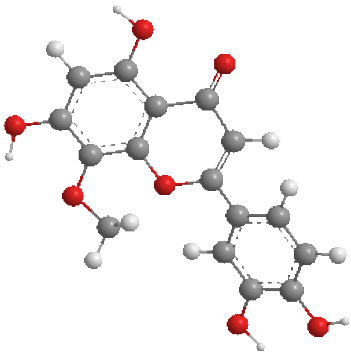
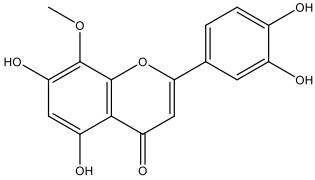
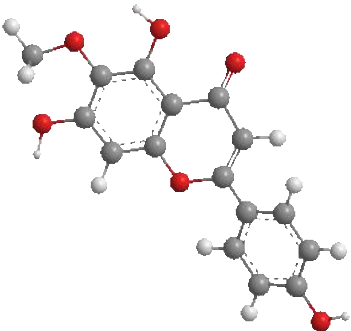
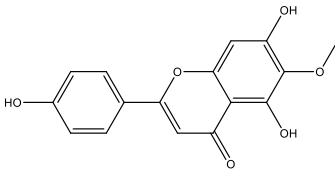
A14	Apigenidin		
A15	luteolinidin		
A16	tricetinidin		
A17	Carajurone		
A18	Carajurin		

A19	luteoforol		
A20	Oenin		
A21	Malvidin 3-arabinoside		
A22	6-Hydroxyluteolin		

A23	5-Methylcyanidin		
A24	6-Hydroxycyanidin		
A25	6-Hydroxydelphinidin 3-rutinoside		
A26	Genkwanin		
A27	7-O-Methylfluteolin		

A28	5-Methyl-6-hydroxyluteolinidin		
A29	6-Methoxyluteolin		
A30	Cyanidin 3-O-glucoside		
A31	3',4',5',7-Tetrahydroxyflavylium		
A32	3,4',7-Trihydroxyflavylium		
A33	3,7-Dihydroxyflavylium		

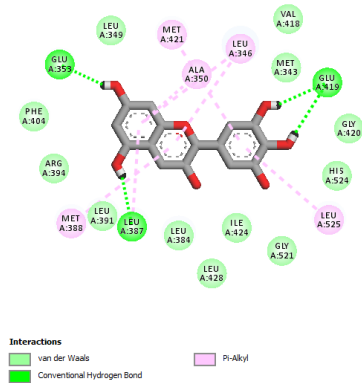
A34	3',4'-Dihydroxyflavylium		
A35	5,7-Dihydroxyflavylium		
A36	3,4'-Dihydroxy-8-methoxyflavylium		
A37	6-Hydroxyflavylium		
A38	7-Hydroxyflavylium		
A39	4-Hydroxyflavylium		

A40	Peonidin 3-arabinoside		
A41	4-(3,4,5-Trimethoxystyryl) anthocyanidin-7-ol		
A42	8-Methoxyluteolin		
A43	Hispidulin / 6-O-Methylapigenin		

Lampiran 2 Interaksi Ligan 3ERT Hasil Penambatan Molekul

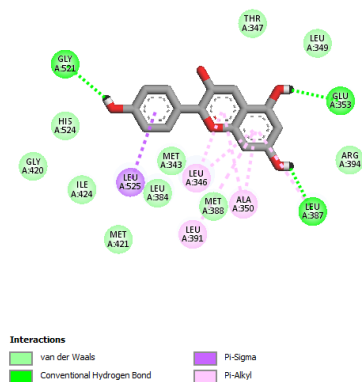
Kode Ligan	VISUALISASI 2D	Residu Asam Amino
A1	Interactions - van der Waals - Conventional Hydrogen Bond - Carbon Hydrogen Bond - Pi-Sulfur - Alkyl - Pi-Alkyl	MET388 MET421 ILE424 LEU428 LEU387 LEU391 LEU346 ALA350 LEU525 AGR394 GLU353 THR347 THR347 MET343 ASP351 LEU354 LEU349 GLY521 HIS524 GLY420 PHE404 GLU419 LEU384 TRP383
A2	Interactions - van der Waals - Conventional Hydrogen Bond - Carbon Hydrogen Bond - Pi-Anion - Pi-Sigma - Pi-Alkyl	AGR396 GLU353 TRP393 PRO324 ILE326 GLU323 AGR94 LYS449, MET357, ILE386, LEU387, LEU327, HIS356, PRO325, PHE445
A3	Interactions - van der Waals - Conventional Hydrogen Bond - Carbon Hydrogen Bond - Pi-Sigma - Pi-Alkyl	GLU353 GLU419 LEU387 LEU346 MET388 LEU346 ALA350 LEU387 LEU391 MET421 ILE424 LEU525, GLY521, LEU428, LEU384, PHE404, AGR394, LEU349, VAL418, MET343, GLY420, HIS524
A4	Interactions - van der Waals - Conventional Hydrogen Bond - Carbon Hydrogen Bond - Pi-Anion - Pi-Sigma - Pi-Alkyl	GLU353 TRP393 AGR394 PRO324 PRO324 GLU323 GLY442, PHE445, VAL446, LYS449, TRP360, MET357, ILE386, GLY390, LEU391, ILE326, PRO325

A5



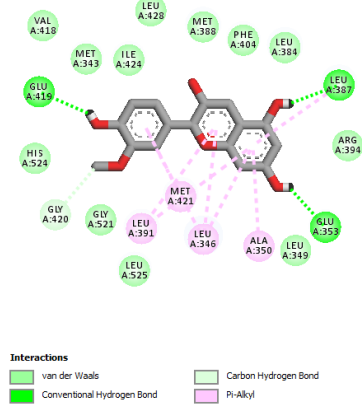
GLU353 GLU419 GLU419
LEU387 LEU346 MET388
LEU346 ALA350 LEU387
MET421 LEU525 LEU349,
VAL418, MET343, GLY420,
HIS524, GLY521, ILE424,
LEU428, LEU384, LEU391,
AGR394, PHE404

A6



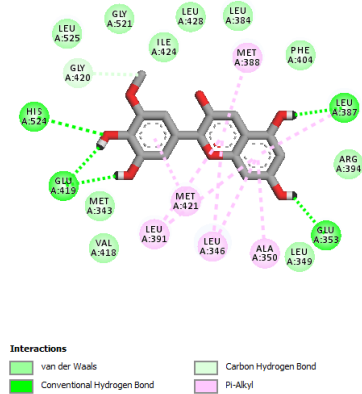
GLU353 LEU387 GLY521
LEU346 ALA350 LEU346
ALA350 LEU387 LEU391
LEU525 THR347, LEU349,
AGR394, MET388, MET343,
LEU384, MET421, ILE424,
GLY420, HIS424

A7



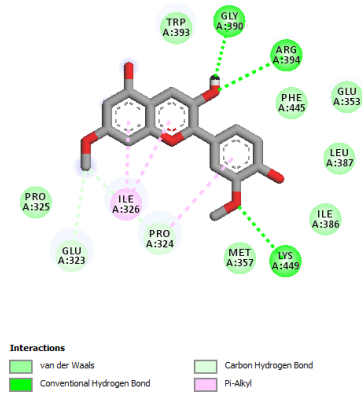
GLU353 GLU419 LEU387
GLY420 LEU346 LEU391
LEU346 ALA350 LEU387
LEU391 LEU346 MET421
VAL418, MET343, ILE424,
LEU428, MET388, PHE404,
LEU384, ARG394, LEU349,
LEU525, GLY521, HIS524

A8



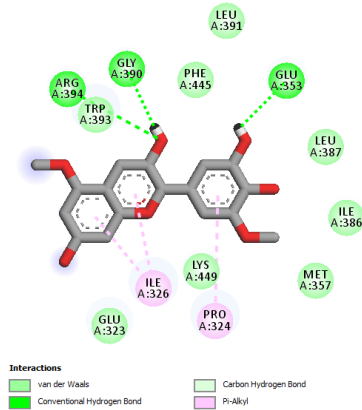
HIS524 GLU419 GLU419
LEU387 GLU353 GLY420
LEU346 MET388 LEU391
LEU346 ALA350 LEU387
LEU391 MET421 LEU525,
GLY521, ILE424, LEU428,
LEU384, PHE404, ARG394,
LEU349, MET343, VAL418

A9



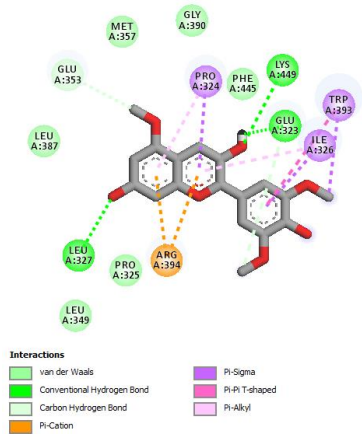
ARG394 LYS449 GLY390
ARG394 GLU323 PRO324
ILE326 ILE326 PRO324
TRP393, PHE445, GLUE353,
LEU387, ILE386, MET357,

A11



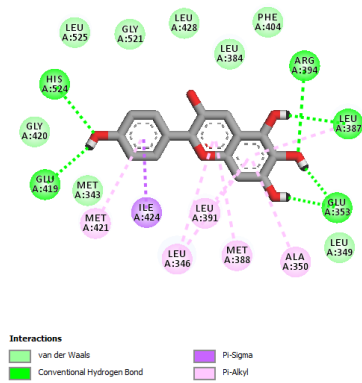
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ARG394 PRO324 ILE326
TRP393, PHE445, GLUE353,
LEU387, ILE386, MET357,
LYS449, GLU323

A12



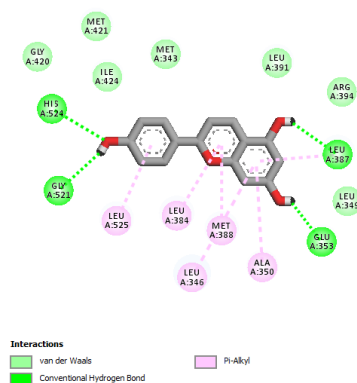
LEU327 LYS449 GLU323
GLU353 ARG394 PRO324
ILE326 TRP393 ILE326
PRO324 LEU387, MET357,
GLY390, PHE445, PRO325,
LEU349

A13



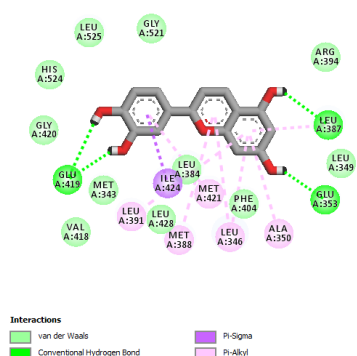
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LEU346 MET388 LEU346
ALA350 LEU387 LEU391
MET421

A14



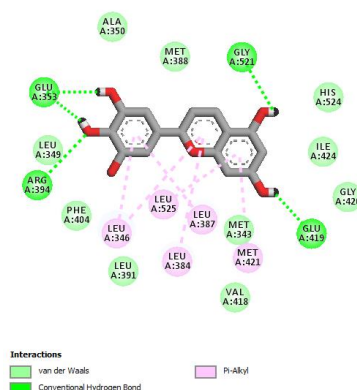
HIS524 GLY521 LEU387
 GLU353 LEU384 MET388
 LEU346 ALA350 LEU387
 LEU525 GLY420 MET421
 OLE424 MET343 LEU391
 ARG394 LEU349

A15



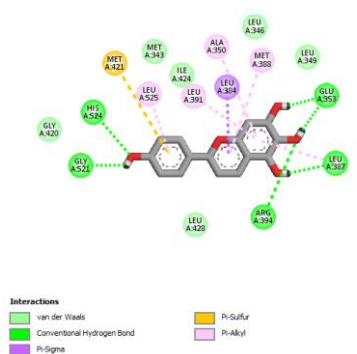
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 GLU353 ILE424 MET388
 LEU346 ALA350 LEU387
 LEU391 MET421 GLY420
 HIS524 LEU525 GLY521
 ARG394 LEU349 PHE404
 LEU384 LEU428 MET343
 VAL418

A16

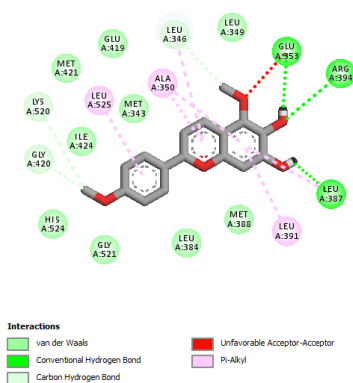


ARG394 GLU353 GLY521
 GLU419 GLU353 LEU346
 LEU384 MET421 LEU525
 LEU346 LEU387 ALA350,
 MET388, HIS524, ILE424,
 GLY420, MET343, VAL418,
 LEU391, PHE404, LEU349

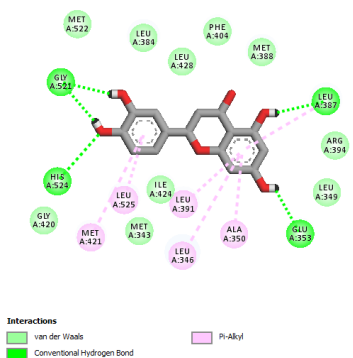
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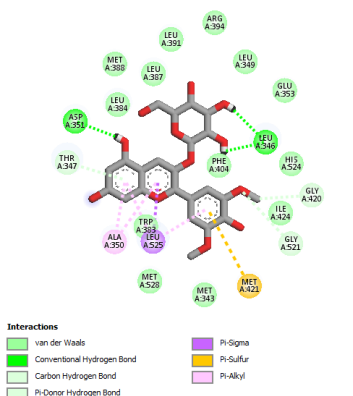
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 LEU387 LEU391 LEU525
 GLY420, MET343, LEU346,
 ILE424, LEU349, LEU428



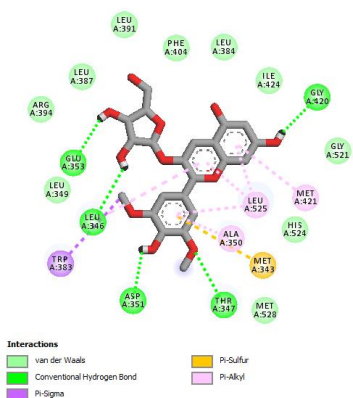
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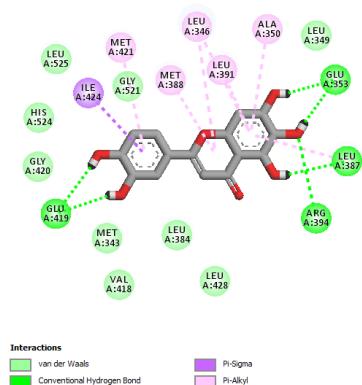
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A21

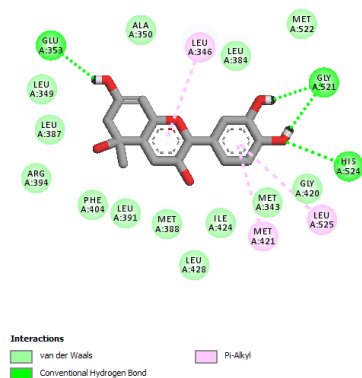


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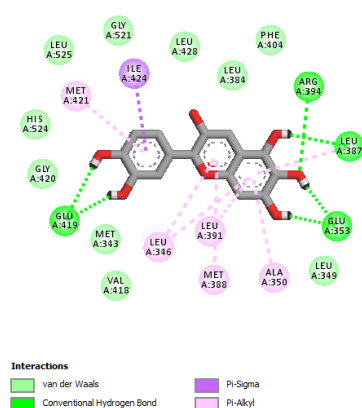
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 ILE424 LEU346 LEU346 ALA350
 LEU387 LEU391 MET421 GLY420,
 HIS524, LEU525, GLY521, LEU349,
 LEU428, LEU384, VAL418, MET343

A23



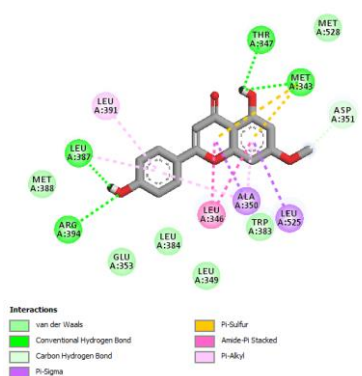
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 MET421 LEU525 ALA250 LEU384
 MET522 GLY420 MET343 ILE424
 LEU428 MET388 LEU391 PHE404
 ARG394 LEU387 LEU349

A24



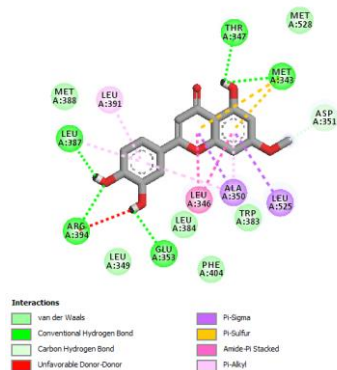
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 LEU346 ALA350 LEU387
 LEU391 MET421 GLY420 HIS 524
 LEU525 GLY521 LEU428 LEU384
 PHE404 LEU349 VAL418 MET343

A26



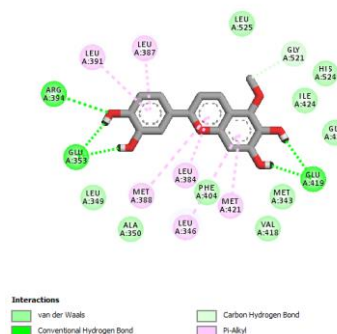
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 ALA350 LEU525 LEU346 LEU346
 ALA350 LEU387 LEU391
 MET343 MET388 MET528 TRP383
 LEU439 LEU384 GLU353

A27



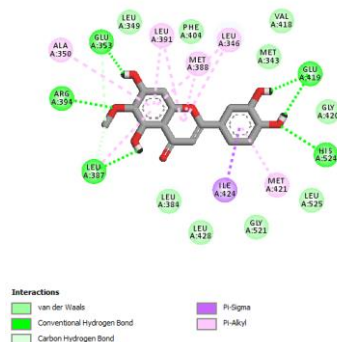
ARG394 GLU353 LEU387 MET343
 THR347 ASP351 ALA350 LEU525
 LEU346 THR347 LEU346 ALA350
 LEU387 LEU391 MET388 MET528
 TRP383 PHE404 LEU384 LEU349

A28



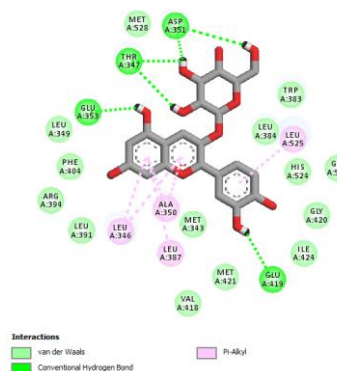
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 LEU525 HIS524 ILE424 GLY420
 MET343 VAL418 PHE404 ALA350
 LEU349

A29



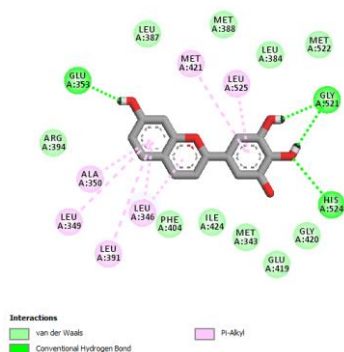
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 LEU387 GLU353 LEU387 ILE424
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 VAL418 GLY420 LEU525 GLY521
 LEU428 LEU384

A30



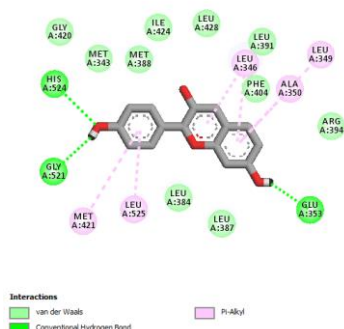
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 LEU346 ALA350 LEU346
 ALA350 LEU387 LEU525 LEU391
 ARG394 PHE404 LEU349 MET528
 LEU384 TRP383 HIS524 GLY521
 GLY420 ILE424 MET421 VAL418
 MET343

A31



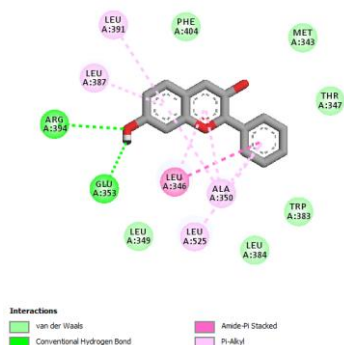
GLY521 LEU346 LEU349
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 LEU384 MET522 GLY420 GLU419
 MET343 ILE424 PHE404

A32



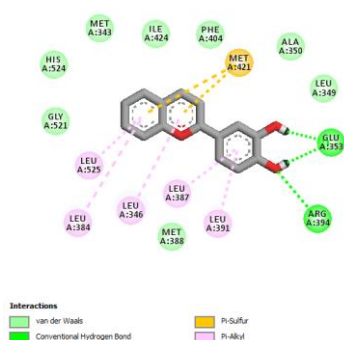
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 ALA350 MET421 LEU525
 GLY420 MET343 ILE424 LEU428
 LEU391 PHE404 ARG394 LEU387
 LEU384

A33

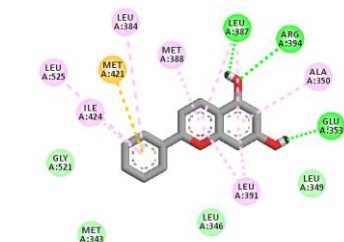


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 ALA350 LEU387 LEU391
 LEU525 LEU346 THR347

A34



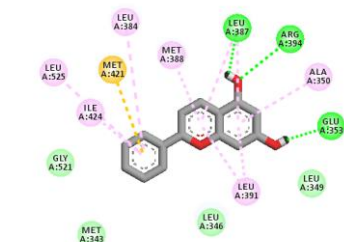
ARG394 GLU353 MET421 LEU346
 LEU525 LEU387 LEU391 GLY521
 HIS524 MET343 ILE424 PHE404
 ALA350 LEU349 MET388

A35

Interactions

van der Waals
Conventional Hydrogen Bond
Pi-Sulfur
Pi-Alkyl

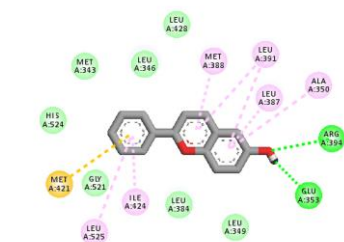
ARG394 LEU387 GLU353 MET421
LEU387 MET388 LEU391
ALA350 LEU387 LEU391
LEU384 ILE424 LEU525 GLY521
MET343 LEU346 LEU349

A36

Interactions

van der Waals
Conventional Hydrogen Bond
Pi-Sulfur
Pi-Alkyl

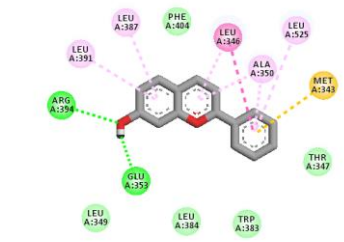
ARG394 LEU387 GLU353 MET421
LEU387 MET388 LEU391
ALA350 LEU387 LEU391
ILE424 LEU525 ILE424 GLY521
MET343 LEU346 LEU349

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Interactions

van der Waals
Conventional Hydrogen Bond
Pi-Sulfur
Pi-Alkyl

ARG394 GLU353 MET421 MET388
LEU391 ALA350 LEU387
LEU391 ILE424 LEU525 HIS524
MET343 LEU346 LEU428 LEU349
LEU384 GLY512

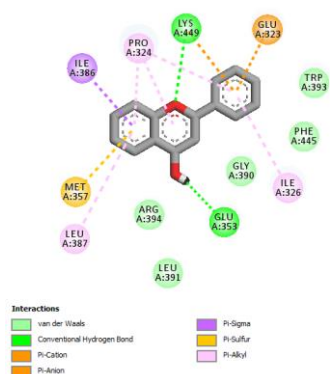
A38

Interactions

van der Waals
Conventional Hydrogen Bond
Pi-Sulfur
Amide-Pi Stacked
Pi-Alkyl

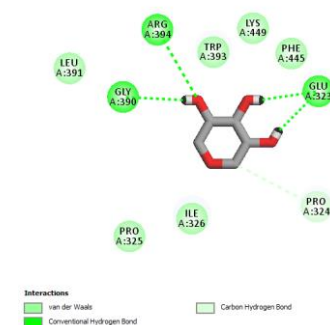
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LEU391 ALA350 LEU525 PHE404
THR347 TRP383 LEU384 LEU349

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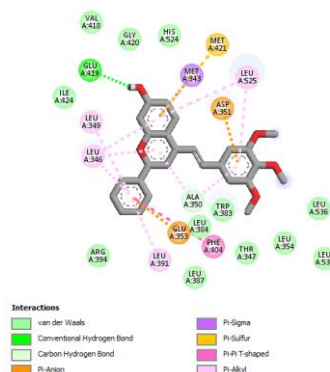
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 LEU391 GLY390 PHE445 TRP393

A40



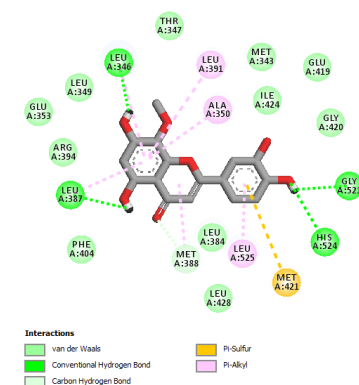
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 LEU391 TRP393 LYS449 PHE445
 ILE326 PRO325

A41

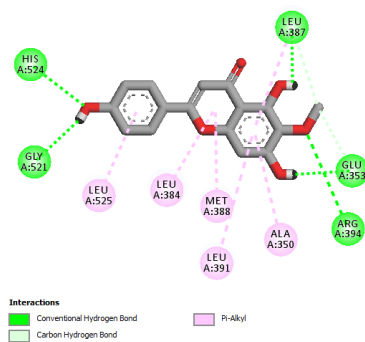


GLU419 ALA350 ASP351 GLU353
 MET343 PHE404 LEU346
 ALA350
 LEU346
 LEU525 ALA350 LEU525
 LEU346 LEU349 ILE424 VAL418
 GLY420 HIS524 LEU536 LEU539
 LEU354 THR347 TRP383 LEU384
 LEU387 ARG394

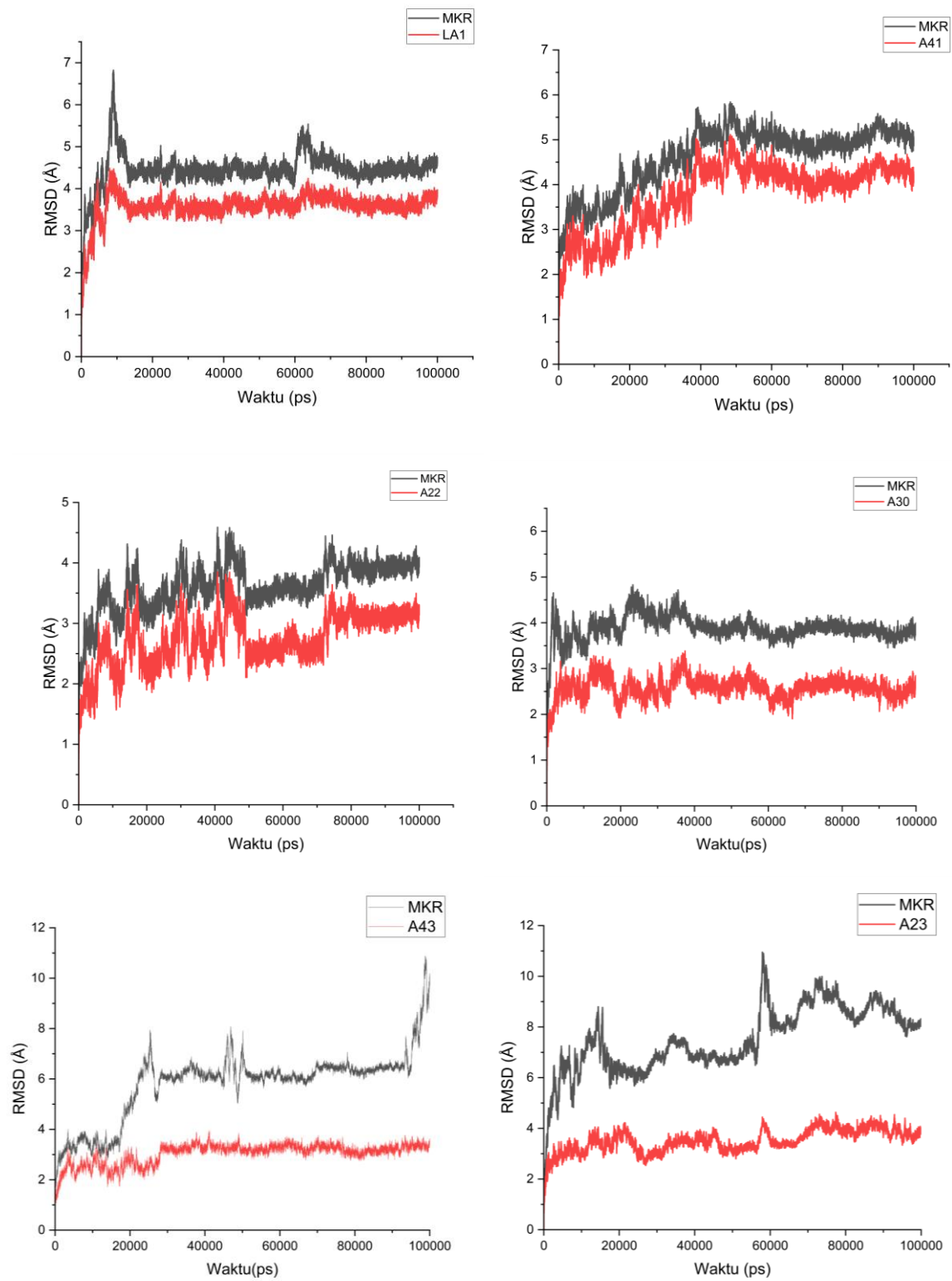
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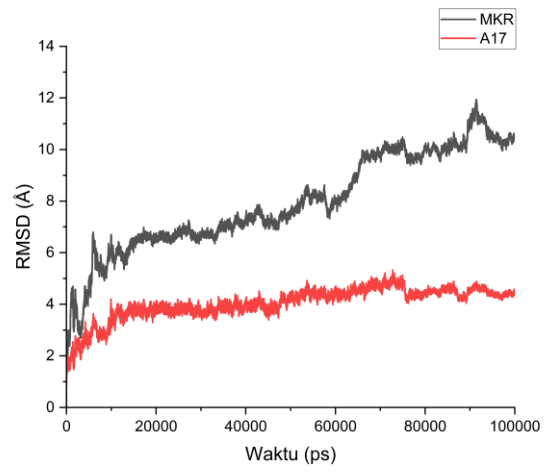


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 MET388 MET421 MET388
 LEU391 LEU525 GLU353, LEU349,
 THR347 MET343 IL3424 GLU419
 GLY420 LEU428 LEU382

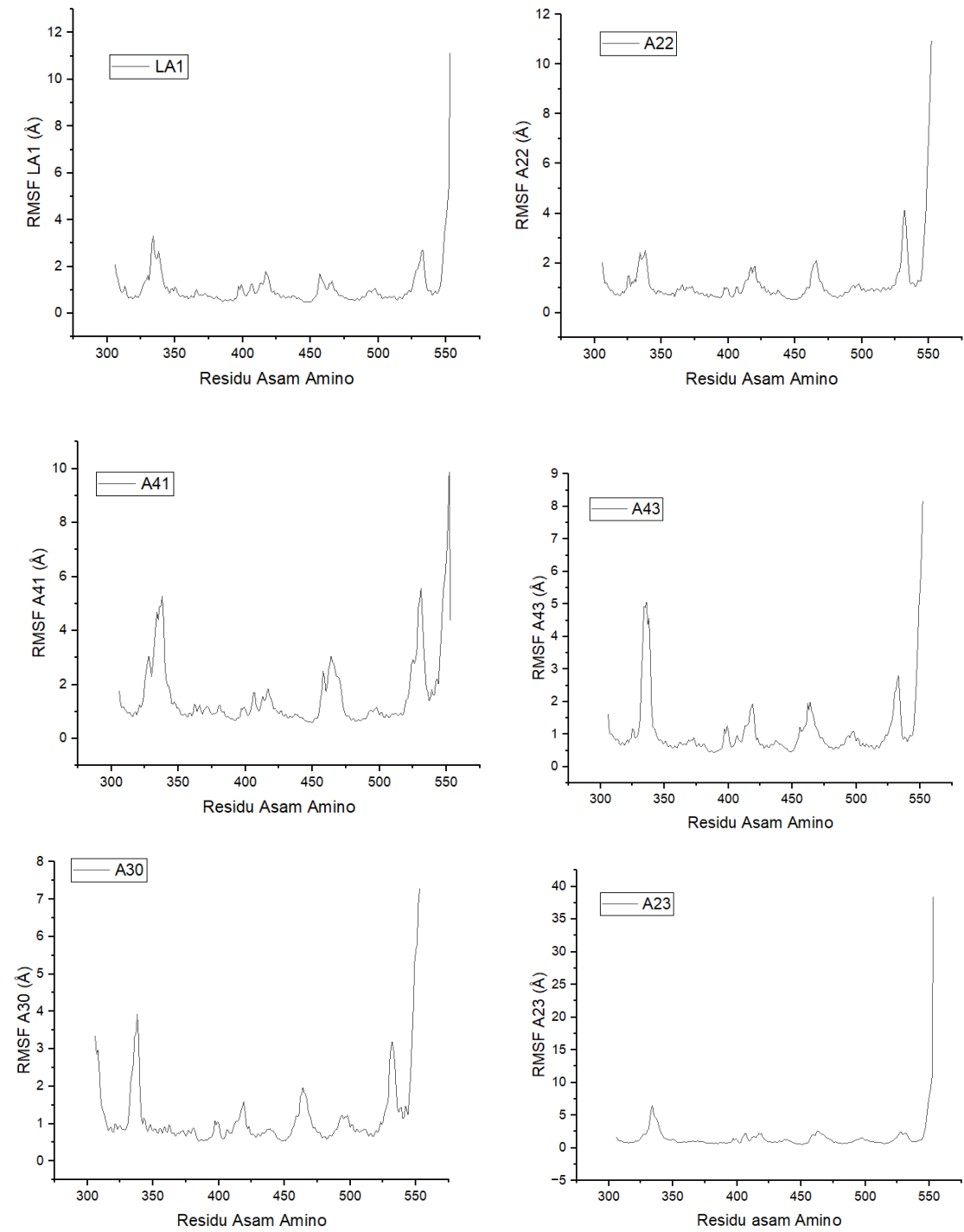
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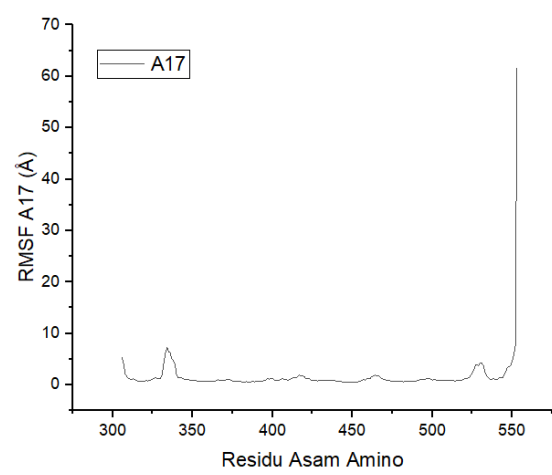
ARG394 HIS524 LEU387 GLU353
LEU387 LEU384 MET388
LEU387 LEU391 LEU525
GLY420, MET343 MET421 ILE424
LEU428 LEU349 LEU346

Lampiran 3 Grafik RMSD Hasil Simulasi Dinamika Molekul Selama 100 ns

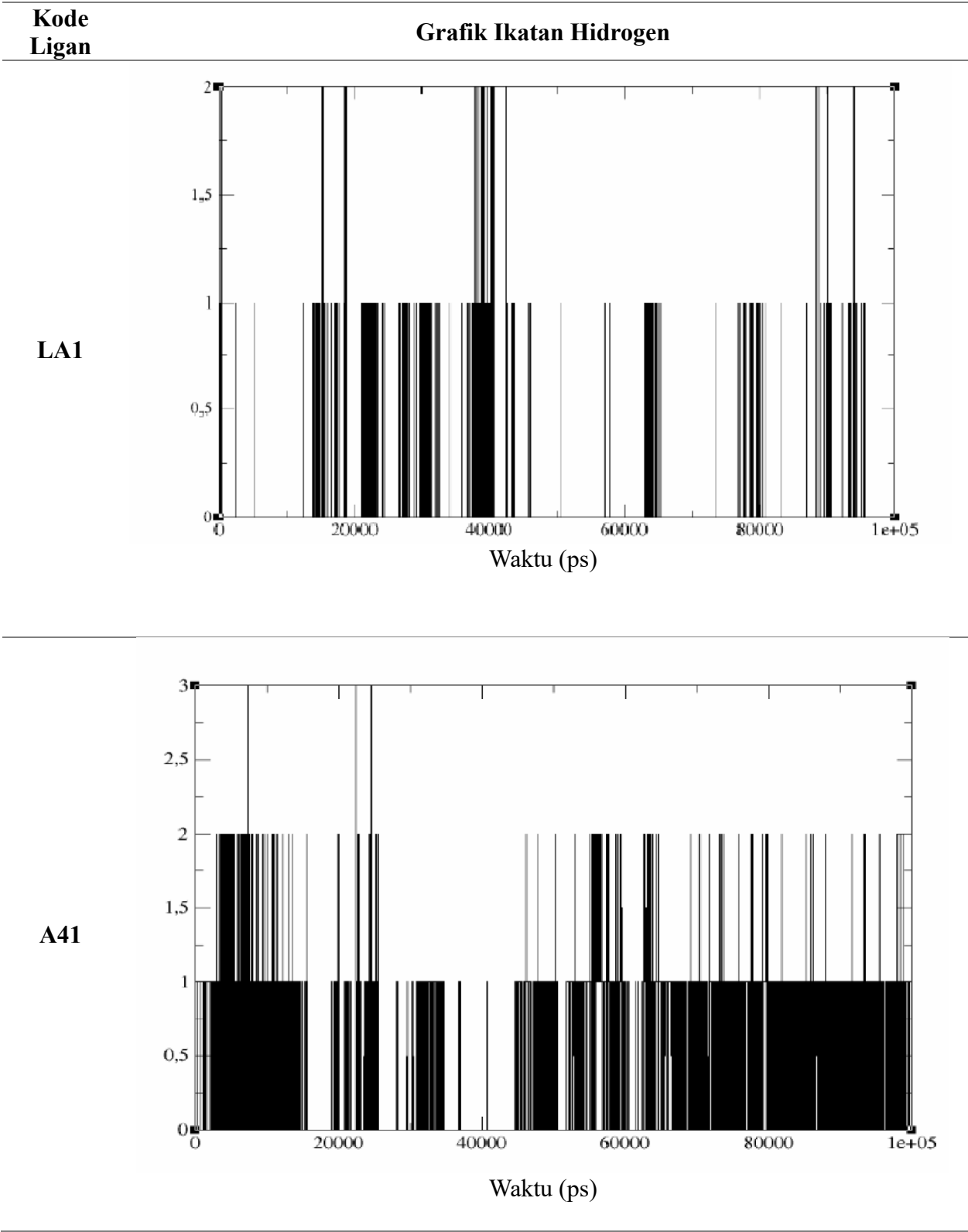


Lampiran 4 Grafik RMSF

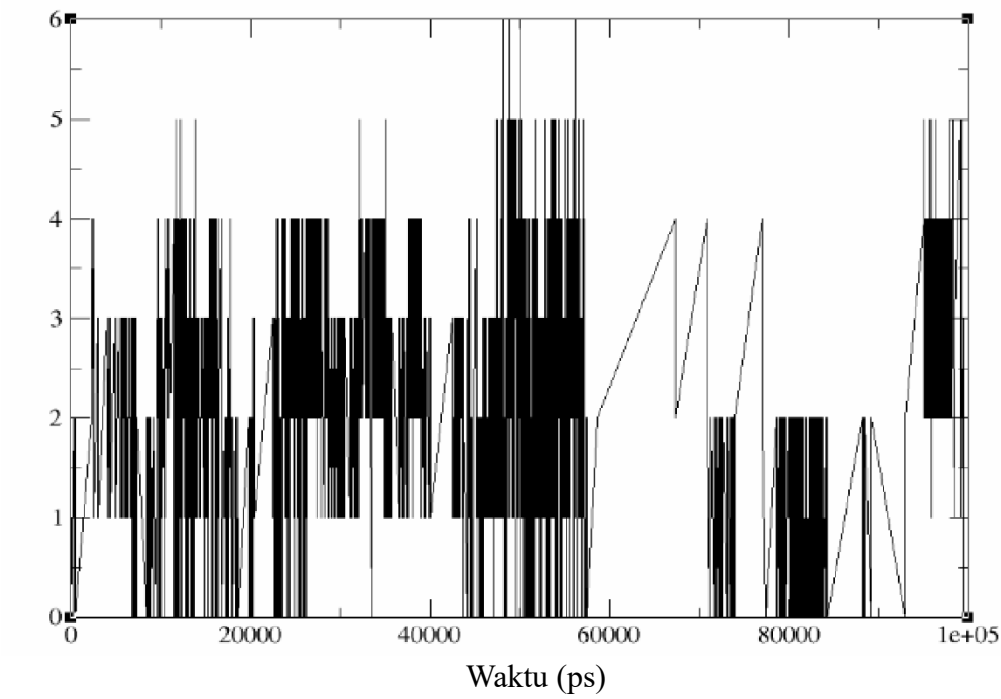




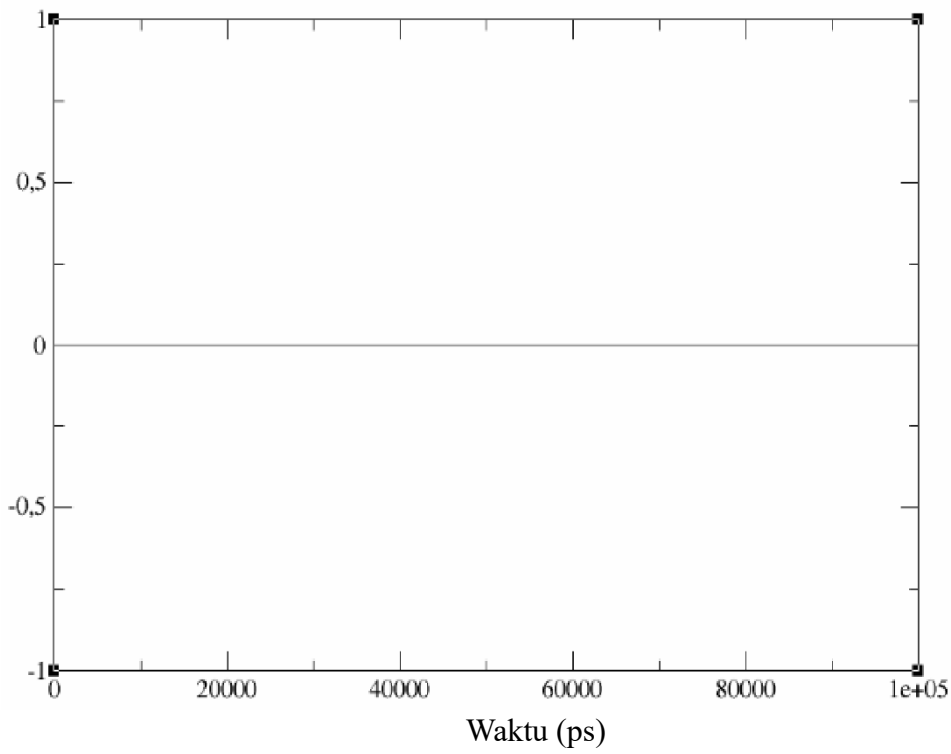
Lampiran 5 Grafik Analisis Ikatan Hidrogen Selama 100ns

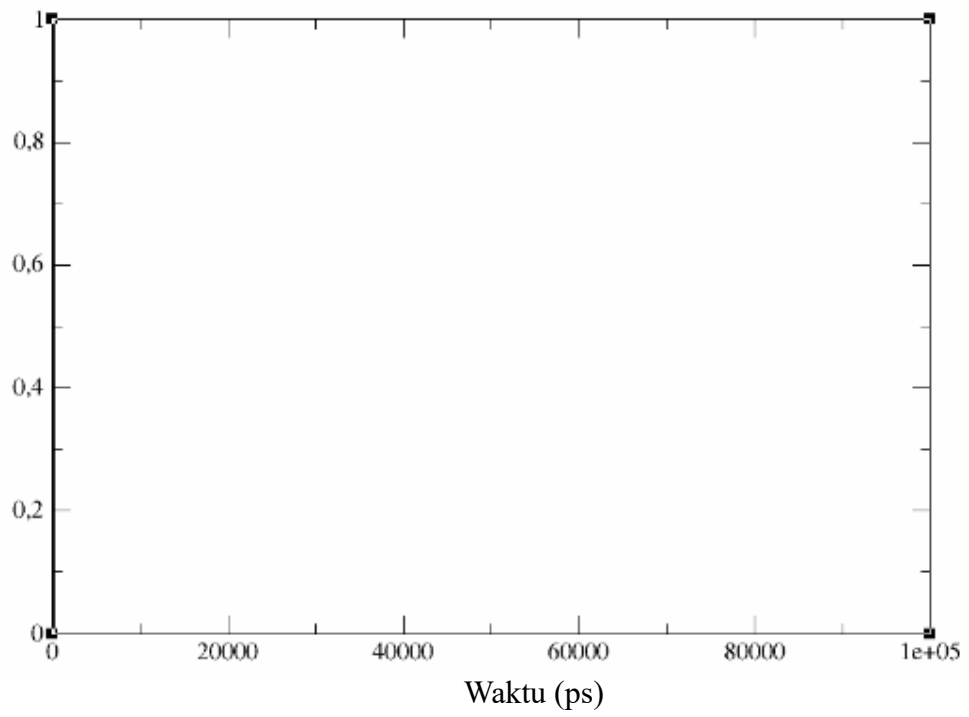
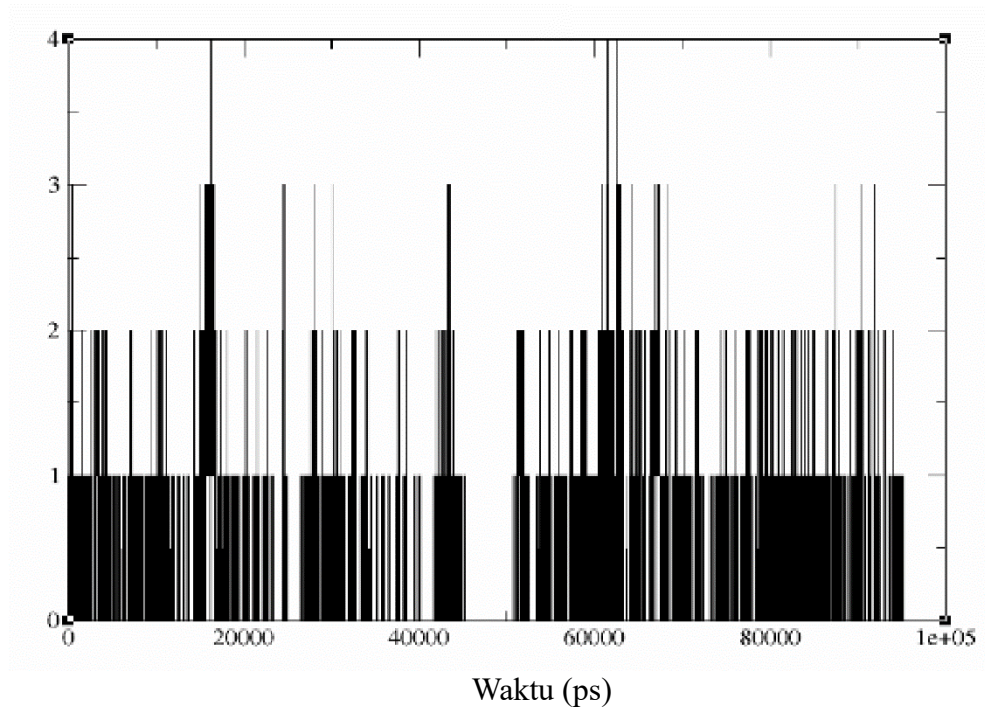


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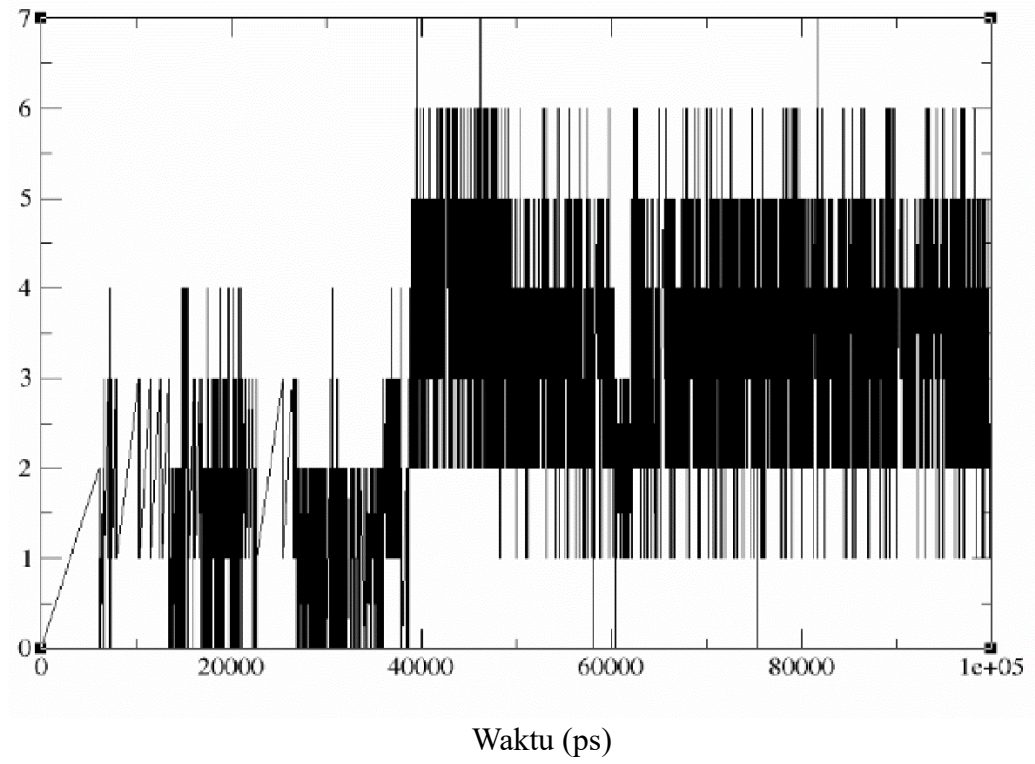


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Lampiran 6 Daftar Riwayat Hidup

RIWAYAT HIDUP



Nama	: Anisa Nursafitri Chaniago
Tempat, Tanggal Lahir	: Bandung, 25 Oktober 1999
Jenis Kelamin	: Perempuan
Anak Ke	: 1 (Tunggal)
Nama Ayah	: Junaedi Chaniago
Nama Ibu	: Yeyen Yeni Yulianti
Alamat	: Kp. Warung Peuteuy Rt/Rw: 06/07 Desa Panenjoan, Kec. Cicalengka Kab. Bandung, Jawa Barat (40395)
Riwayat Pendidikan	: SDN Panenjoan SMP Ma'arif Cicalengka SMK Guna Dharma Nusantara Universitas Bhakti Kencana Bandung
Alamat Email	: anisa.anc77@gmail.com
Status Mahasiswa	: Reguler
Jalur Pendaftaran	: Seleksi Mandiri

36. Anisa Nursafitri Chaniago_191FF03007

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Pembimbing Utama	: Apt. Purwaniati, M. Si
Nama Mahasiswa	: Anisa Nursafitri Chaniago
NPM	: 191FF03007
Bidang Ilmu	: Analisis Farmasi dan Kimia Medisinal

No	Hari/Tanggal	Waktu	Tempat	Materi	Paraf Dosen
1	2 Februari 2023	10.45	UBK	Acc Proposal dan laporan Progres Penelitian	
2.	3 Maret 2023	13.30	UBK	Diskusi Progres Penelitian dan kendala Penelitian	
3	6 April 2023	10.30	WA	Laporan Progres penelitian dan Diskusi kendala	
4.	8 Mei 2023	13.00	UBK	Diskusi dan laporan progres penelitian	
5	11 Mei 2023	12.00	WA	Diskusi hasil Validasi Docking	
6	14. Juni 2023	08.00	WA	Diskusi hasil Docking untuk MD	
7	16. Juni 2023	15.00	UBK	Diskusi terkait MD	
8.	5 Juli 2023	10.00	UBK	Draft laporan Penelitian dan Diskusi Penelitian.	

Catatan : Kartu ini harus dibawa setiap kali melakukan bimbingan dan harus diisi oleh dosen pembimbing.

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