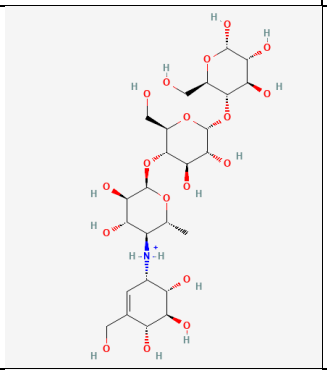
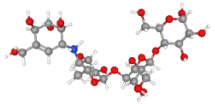
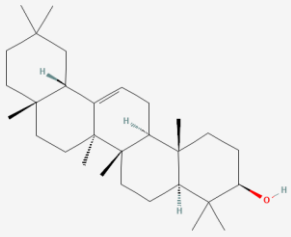
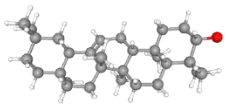
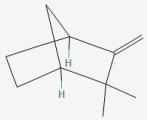
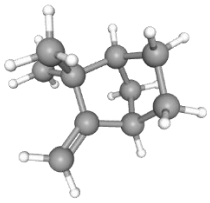
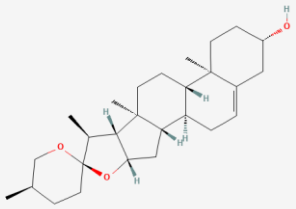
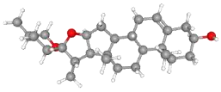
Lampiran 1 Daftar Ligan Uji dan Ligan Alami

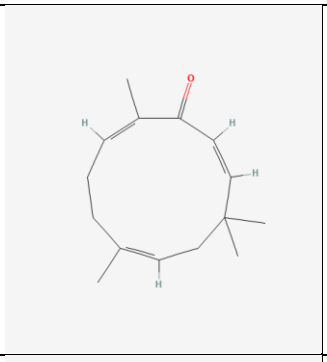
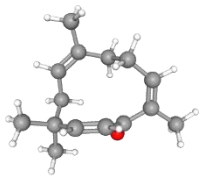
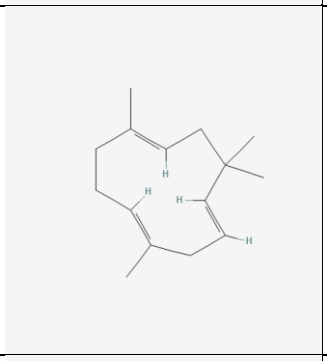
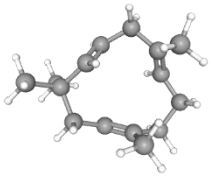
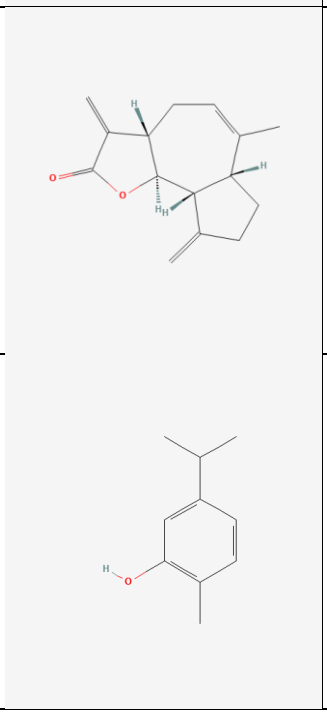
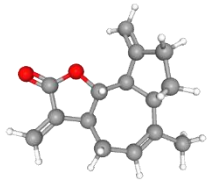
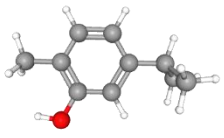
Kode senyawa	Nama Senyawa	Rumus senyawa	Smiles
Ligan alami	2QMJ	$C_{25}H_{44}NO_{18}$	C[C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)O[C@@H]2[C@H](O[C@@H]([C@@H]([C@H]2O)O)O[C@@H]3[C@H](O[C@@H]([C@@H]([C@H]3O)O)O)CO)CO)O)O)[NH2+][C@H]4C=C([C@H]([C@@H]([C@H]4O)O)O)CO
D2	Beta Amyrin	$C_{30}H_{50}O$	C[C@@]12CC[C@@]3(C(=CC[C@H]4[C@]3(CC[C@@H]5[C@@]4(CC[C@@H](C5(C)C)O)C)C)[C@@H]1CC(CC2)(C)C)C
D3	Camphene	$C_{10}H_{16}$	CC1(C2CCC(C2)C1=C)C
D4	Diosgenin	$C_{27}H_{42}O_3$	C[C@@H]1CC[C@@]2([C@H]([C@H]3[C@@H](O2)C[C@@H]4[C@@]3(CC[C@H]5[C@H]4CC=C6[C@@]5(CC[C@@H](C6)O)C)C)C)OC1
D5	Tetramethylcycloundeca	$C_{15}H_{22}O$	C/C/1=C/CC(/C=C\C(=O)/C(=C\CC1)/C)(C)C
D6	A-Humulene	$C_{15}H_{24}$	C/C/1=C\CC(/C=C/C/C(=C/CC1)/C)(C)C
D7	Eremanthin	$C_{15}H_{18}O_2$	CC1=CC[C@@H]2[C@@H]([C@@H]3[C@H]1CCC3=C)OC(=O)C2=C
D8	Carvacrol	$C_{10}H_{14}O$	CC1=C(C=C(C=C1)C(C)C)O
D9	pinocarveol	$C_{10}H_{16}O$	CC1(C2CC1C(=C)C(C2)O)C
D10	Cineol	$C_{10}H_{18}O$	CC1(C2CCC(O1)(CC2)C)C
D11	Cadinene	$C_{15}H_{26}$	C[C@H]1CC[C@H]([C@H]2[C@H]1C=C[C@@H](C2)C)C(C)C
D12	Reynosin	$C_{15}H_{20}O_3$	C[C@@]12CC[C@@H]3[C@@H]([C@H]1C(=C)CC[C@H]2O)OC(=O)C3=C
D13	Beta sitosterol	$C_{29}H_{50}O$	CC[C@H](CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)C(C)C
D14	Kaempferol	$C_{15}H_{10}O_6$	C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O

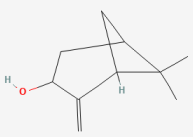
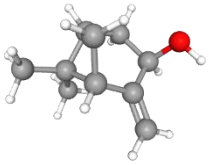
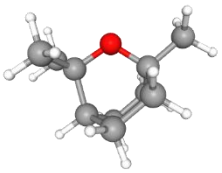
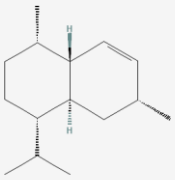
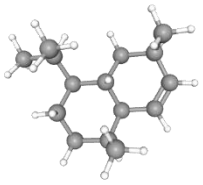
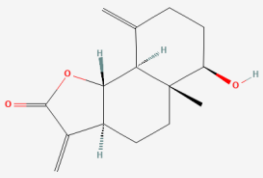
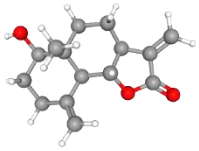
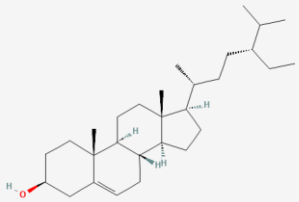
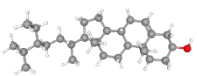
D15	Luteolin	$C_{15}H_{10}O_6$	C1=CC(=C(C=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O)O
D16	Apigenin	$C_{15}H_{10}O_5$	C1=CC(=CC=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O
D17	Rutin	$C_{27}H_{30}O_{16}$	C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)OC[C@@H]2[C@H]([C@@H]([C@H]([C@@H](O2)OC3=C(OC4=CC(=CC(=C4C3=O)O)O)C5=CC(=C(C=C5)O)O)O)O)O)O)O)O
D18	Naringenin	$C_{15}H_{12}O_5$	C1[C@H](OC2=CC(=CC(=C2C1=O)O)O)C3=CC=C(C=C3)O
D19	Hesperidin	$C_{28}H_{34}O_{15}$	C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)OC[C@@H]2[C@H]([C@@H]([C@H]([C@@H](O2)OC3=CC(=C4C(=O)C[C@H](OC4=C3)C5=CC(=C(C=C5)OC)O)O)O)O)O)O)O)O
D20	Myricetin	$C_{15}H_{10}O_8$	C1=C(C=C(C(=C1O)O)O)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O
D21	Isohamnetin	$C_{16}H_{12}O_{10}S$	COC1=C(C=CC(=C1)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)OS(=O)(=O)O)O
D22	Fisetin	$C_{15}H_{10}O_6$	C1=CC(=C(C=C1C2=C(C(=O)C3=C(O2)C=C(C=C3)O)O)O)O
D23	Baicalein	$C_{15}H_{10}O_5$	C1=CC=C(C=C1)C2=CC(=O)C3=C(O2)C=C(C(=C3O)O)O
D24	Chrysin	$C_{15}H_{10}O_4$	C1=CC=C(C=C1)C2=CC(=O)C3=C(C=C(C=C3O2)O)O
D25	Genistein	$C_{15}H_{10}O_5$	C1=CC(=CC=C1C2=COC3=CC(=CC(=C3C2=O)O)O)O
D26	Daidzein	$C_{15}H_{10}O_4$	C1=CC(=CC=C1C2=COC3=C(C2=O)C=CC(=C3)O)O
D27	Biochanin a	$C_{16}H_{12}O_5$	COC1=CC=C(C=C1)C2=COC3=CC(=CC(=C3C2=O)O)O
D28	Stigmasterol	$C_{29}H_{48}O$	CC[C@H](/C=C/[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)C(C)C
D29	Friedelin	$C_{30}H_{50}O$	C[C@H]1C(=O)CC[C@@H]2[C@@]1(CC[C@H]3[C@]2(CC[C@@]4([C@@]3(CC[C@@]5([C@H]4CC(CC5)(C)C)C)C)C)C)C

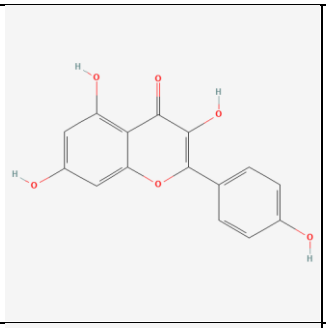
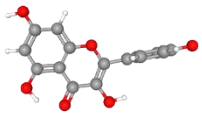
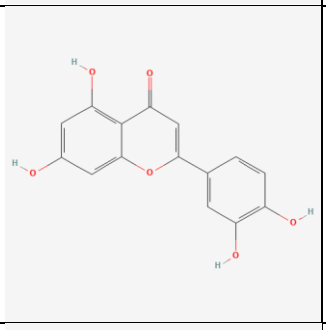
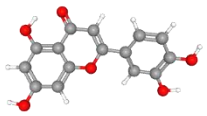
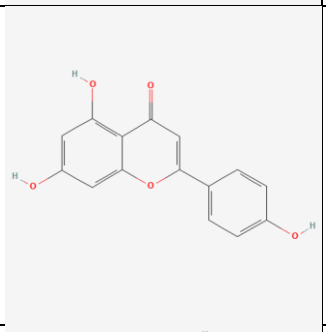
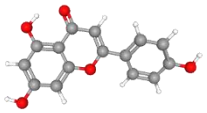
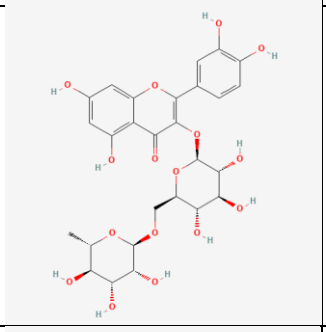
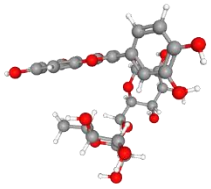
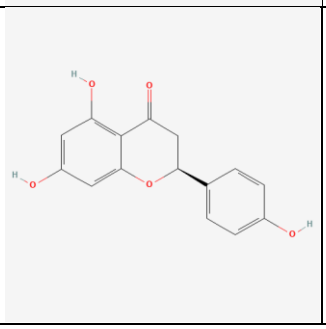
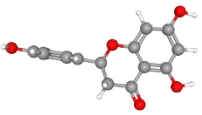
D30	Lanosterol	$C_{30}H_{50}O$	C[C@H](CCC=C(C)C)[C@H]1CC[C@@]2([C@@]1(CCC3=C2CC[C@@H]4[C@@]3(CC[C@@H](C4(C)C)O)C)C)C
D31	Cycloartenol	$C_{30}H_{50}O$	C[C@H](CCC=C(C)C)[C@H]1CC[C@@]2([C@@]1(CC[C@]34[C@H]2CC[C@@H]5[C@]3(C4)CC[C@@H](C5(C)C)O)C)C
D32	Fucosterol	$C_{29}H_{48}O$	C/C=C(\CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)/C(C)C
D33	Botulin		
D34	Uvaol	$C_{30}H_{50}O_2$	C[C@@H]1CC[C@@]2(CC[C@@]3(C(=CC[C@H]4[C@]3(CC[C@@H]5[C@@]4(CC[C@@H](C5(C)C)O)C)C)[C@@H]2[C@H]1C)C)CO
D35	Geraniol	$C_{10}H_{18}O$	CC(=CCC/C(=C/CO)/C)C
D36	Myrcene	$C_{10}H_{16}$	CC(=CCCC(=C)C=C)C
D37	Caryophyllene	$C_{15}H_{24}$	C/C/1=C\CCC(=C)[C@H]2CC([C@@H]2CC1)(C)C
D38	Sabinene	$C_{10}H_{16}$	CC(C)C12CCC(=C)C1C2
D39	Bisabolol	$C_{15}H_{26}O$	CC1=CC[C@@H](CC1)[C@@](C)(CCC=C(C)C)O
D40	Farnesol	$C_{15}H_{26}O$	CC(=CCCC(=CCCC(=CCO)C)C)C
D41	nerol	$C_{10}H_{18}O$	CC(=CCC/C(=C\CO)/C)C

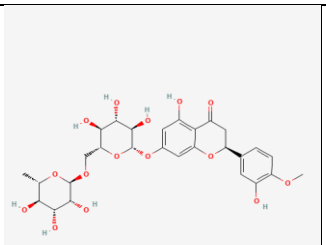
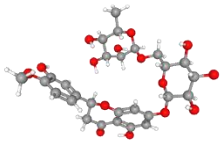
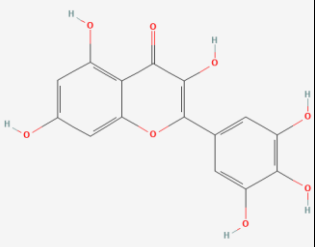
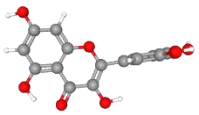
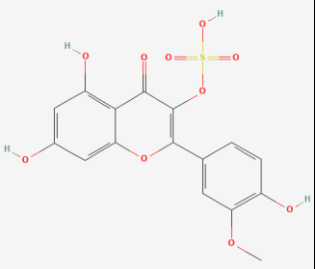
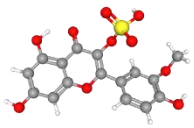
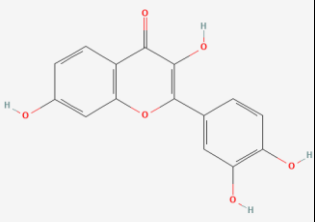
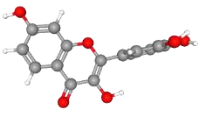
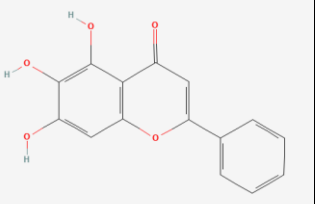
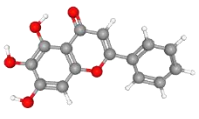
Lampiran 2 Struktur 2D dan 3D Ligan Uji dan Ligan Alami

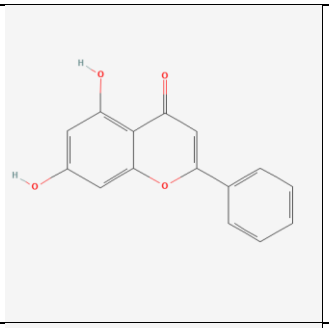
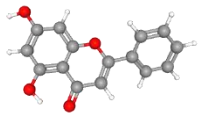
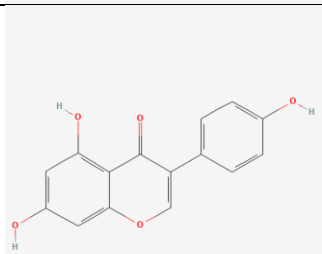
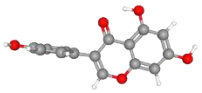
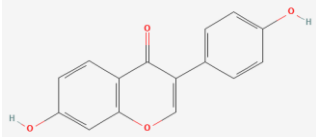
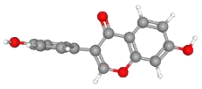
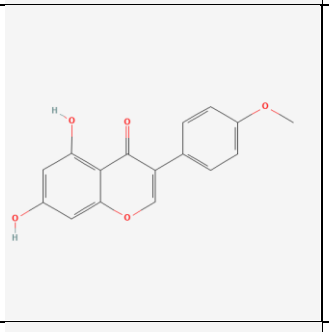
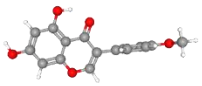
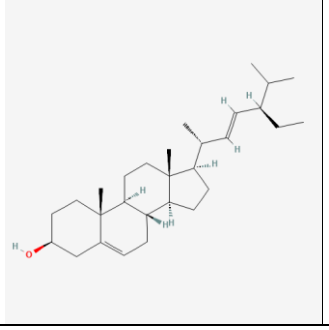
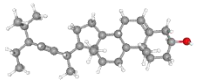
Kode senyawa	Struktur 2D	Rumus senyawa
Ligan alami		
D2		
D3		
D4		

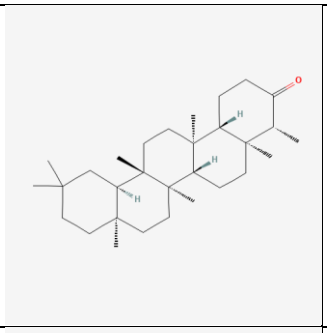
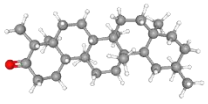
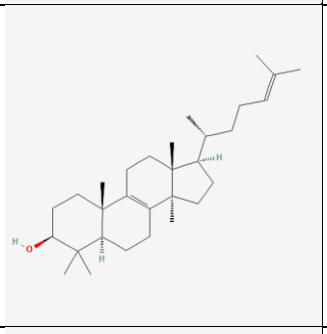
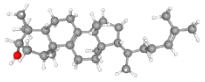
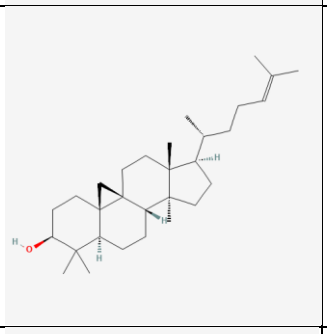
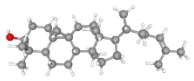
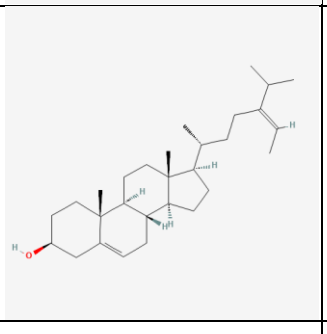
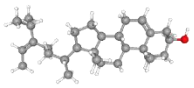
D5		
D6		
D7		
D8		

D9		
D10		
D11		
D12		
D13		

D14		
D15		
D16		
D17		
D18		

D19		
D20		
D21		
D22		
D23		

D24		
D25		
D26		
D27		
D28		

D29		
D30		
D31		
D32		
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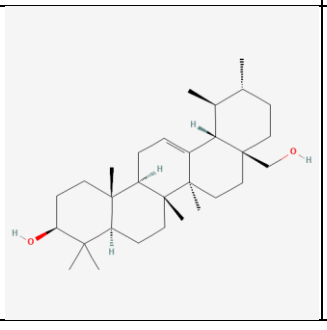
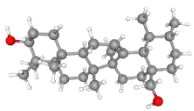
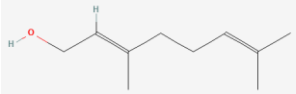
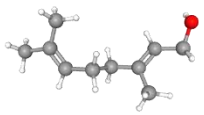
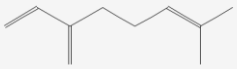
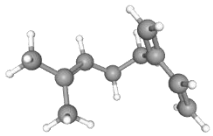
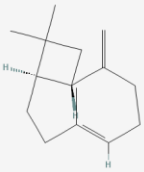
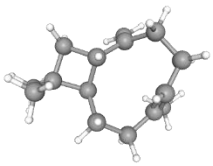
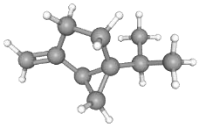
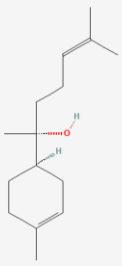
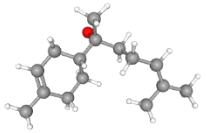
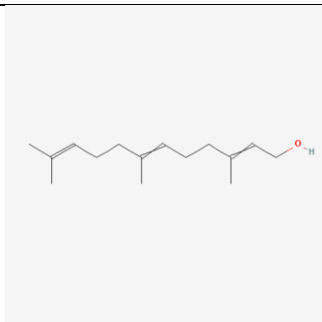
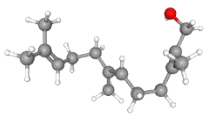
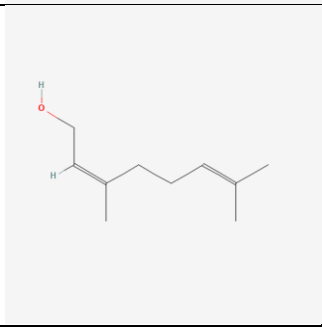
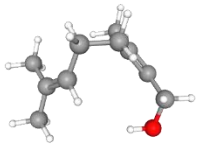
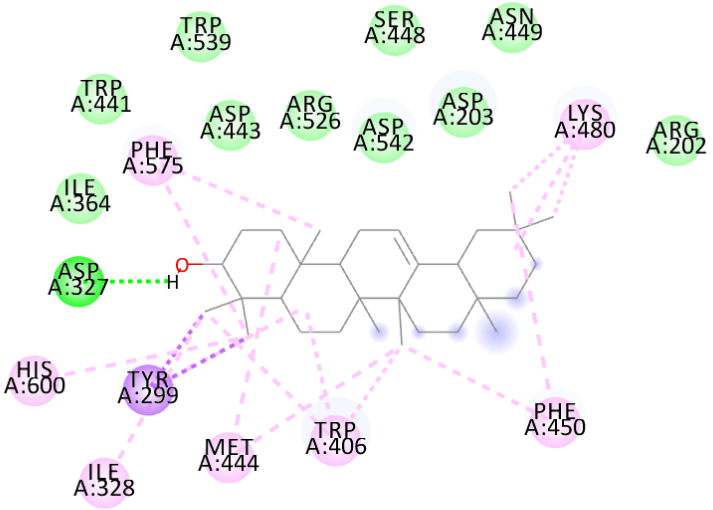
D34		

D35		
D36		
D37		
D38		
D39		

D40		
D41		

Lampiran 3 Visualisasi Hasil Penambatan Molekul Ligan Uji



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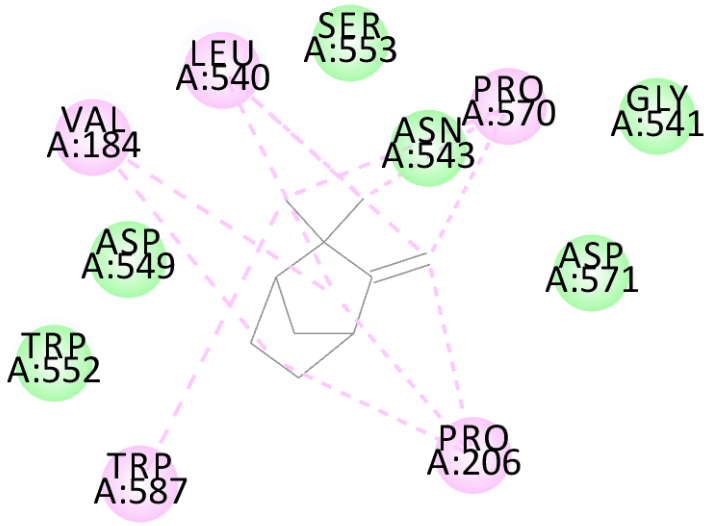

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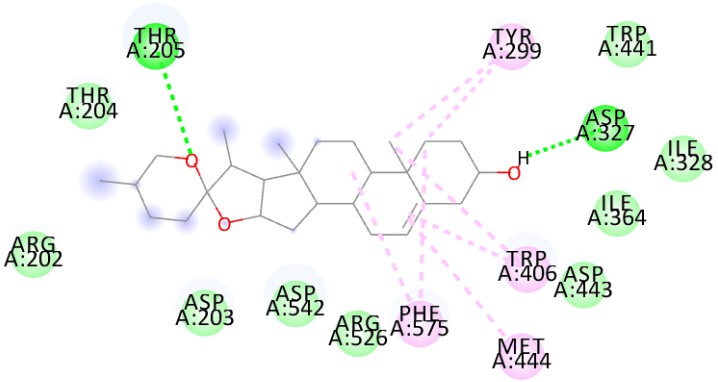
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ILE
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ILE
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ARG
A:202
TRP
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PHE
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MET
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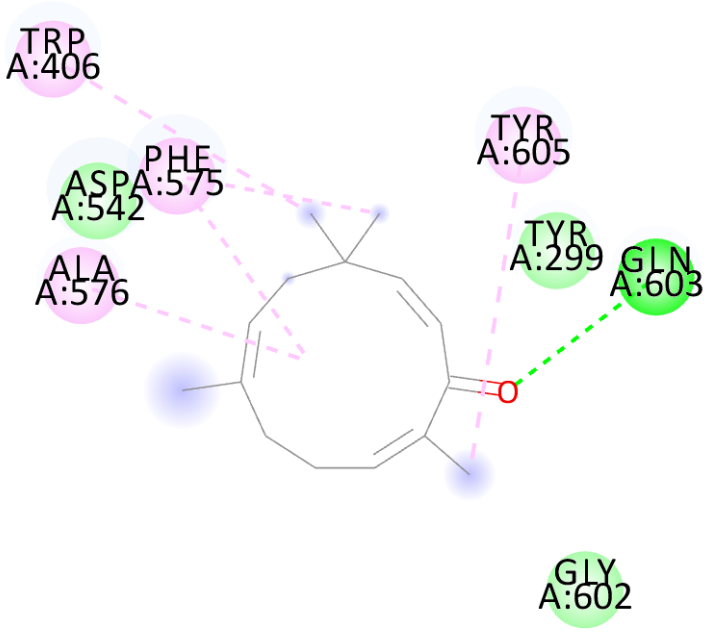
D4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GLY
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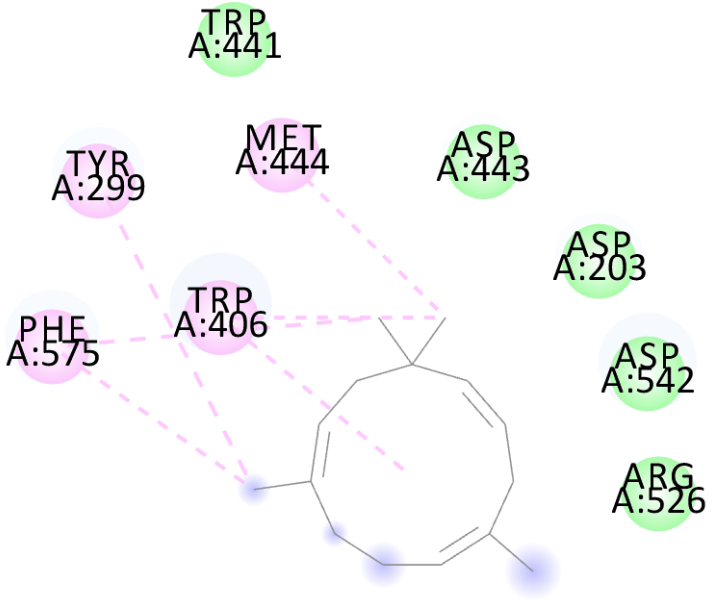
D5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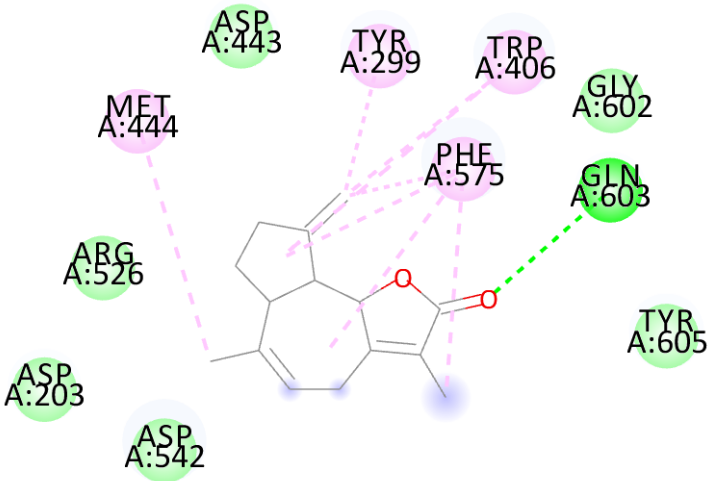
D6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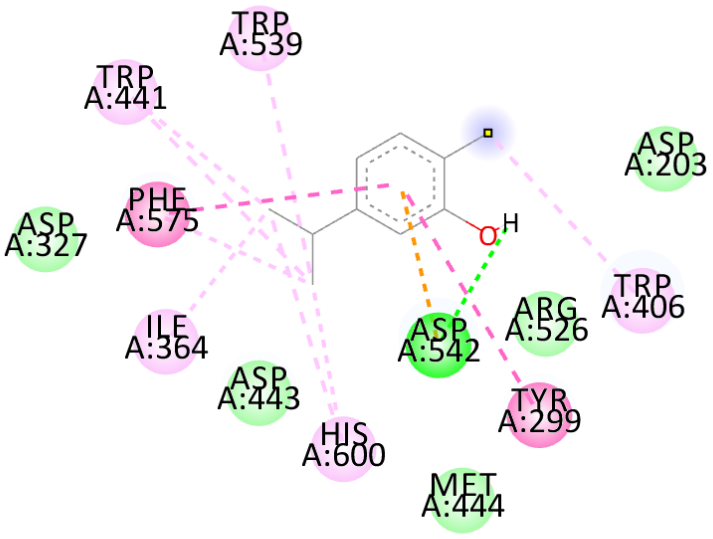
D7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H
O
TRP
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ASP
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HIS
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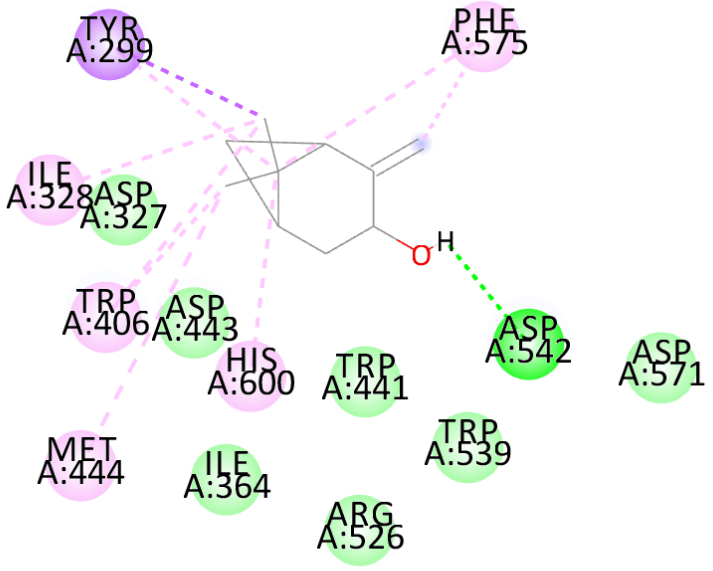
MET
A:444

D8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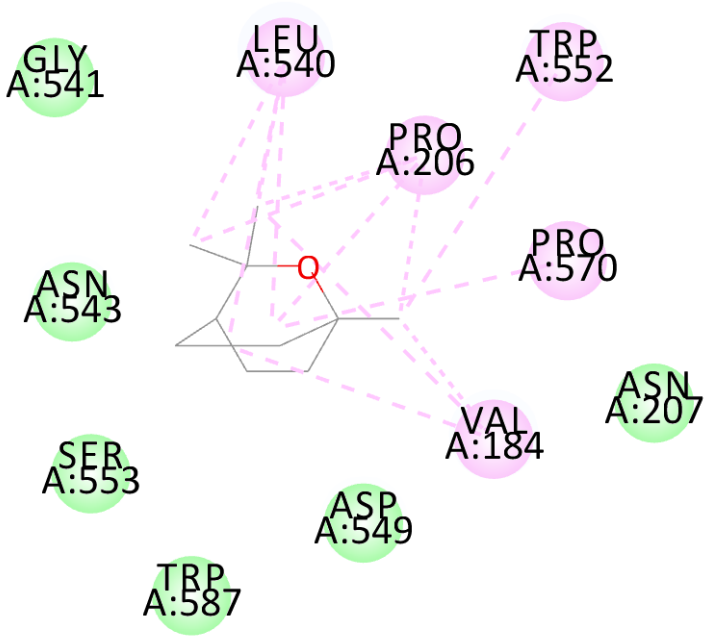
D9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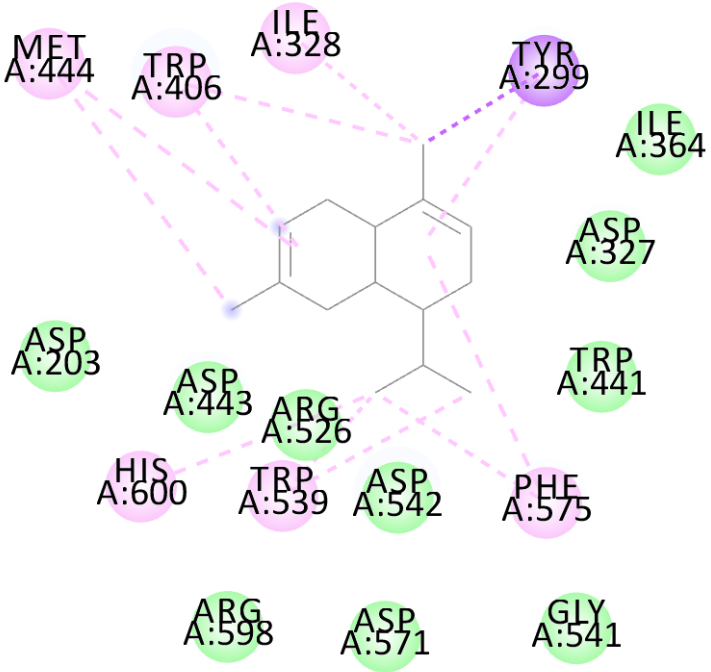
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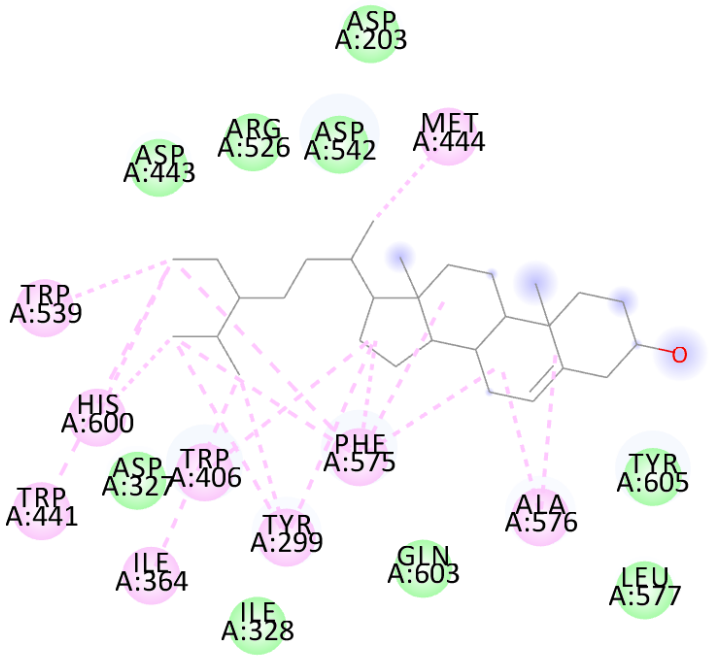
D11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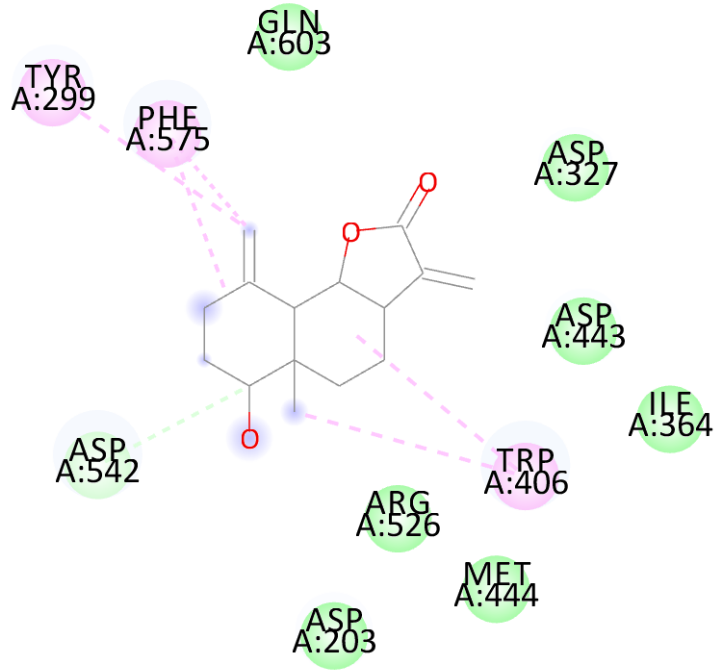
D12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ASP
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ASP
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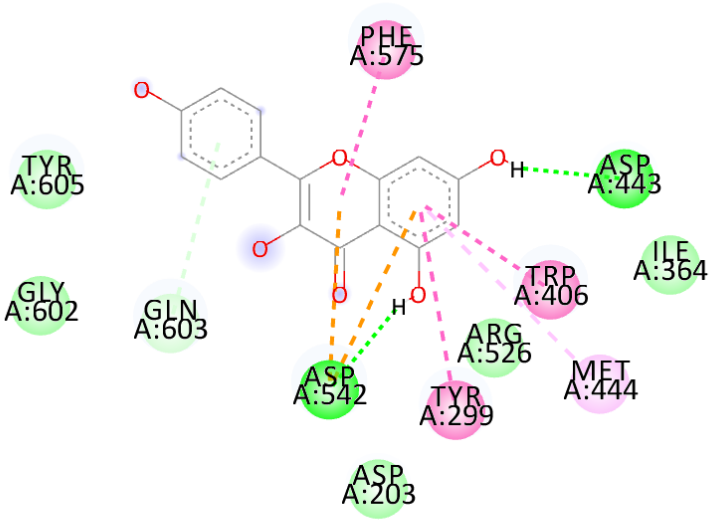
D13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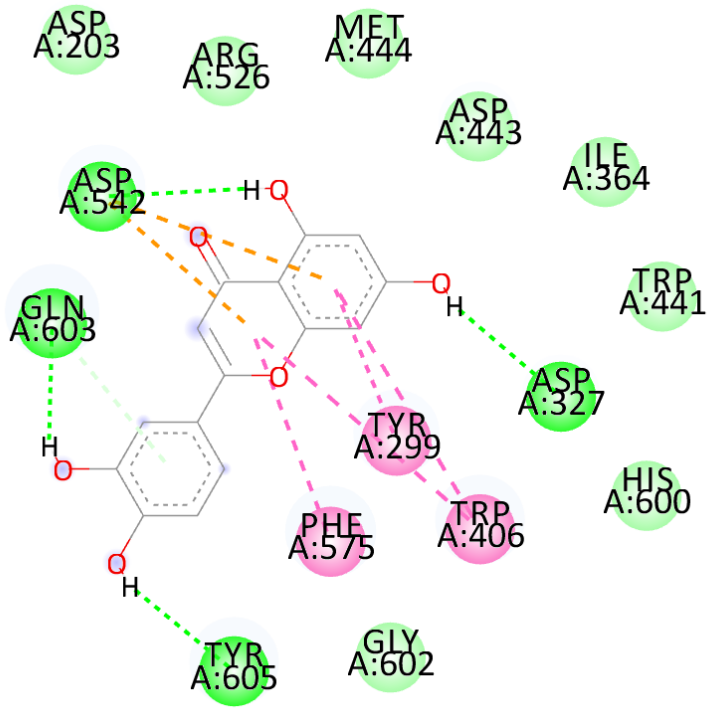
D14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GLY
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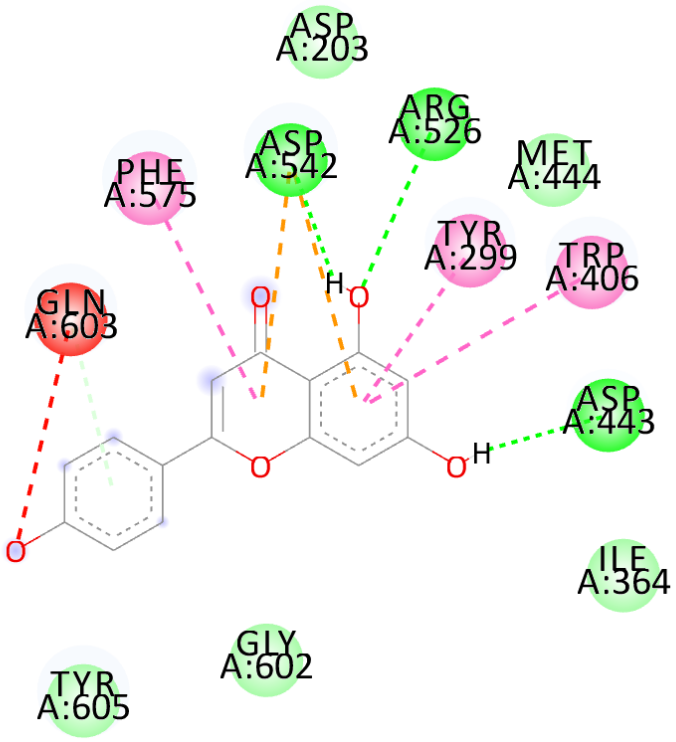
D15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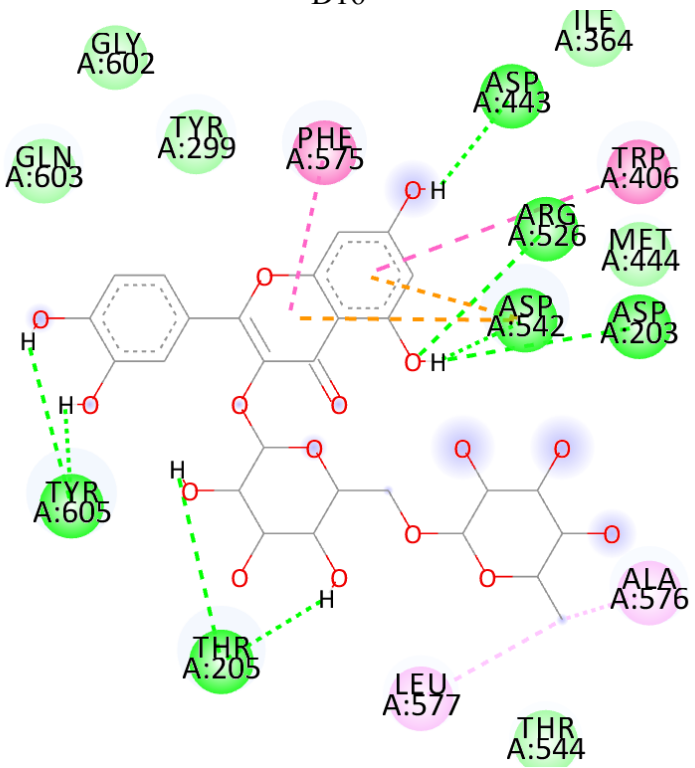
D16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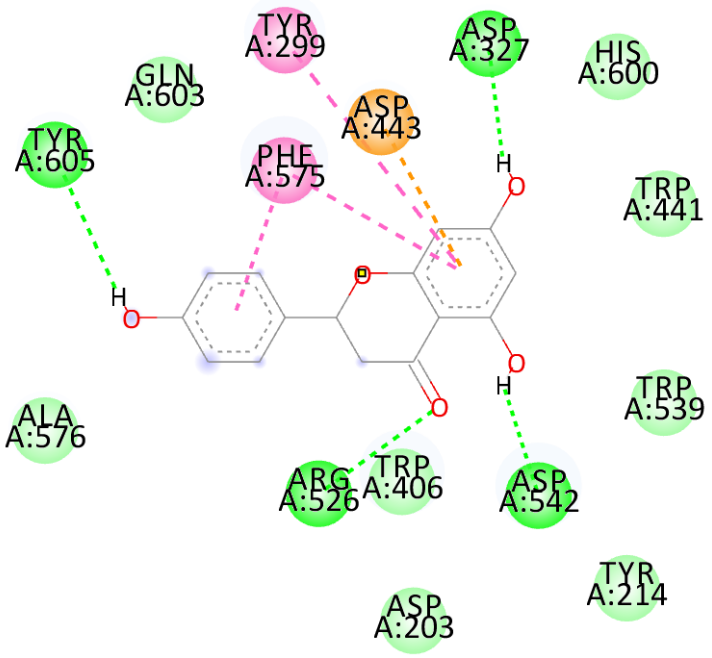
D17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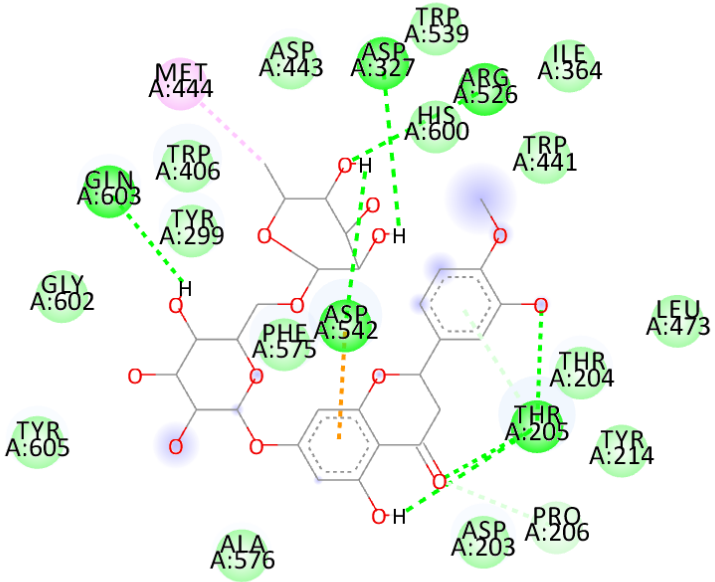
D18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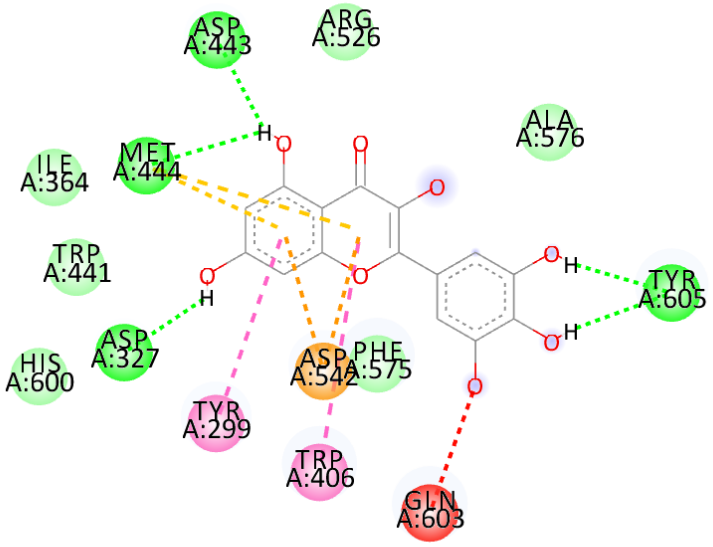
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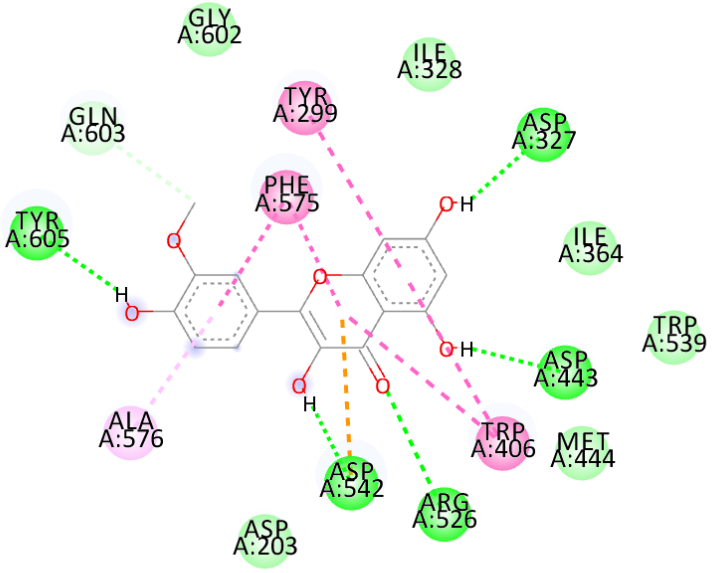
D20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ASP A:327
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ASP A:443
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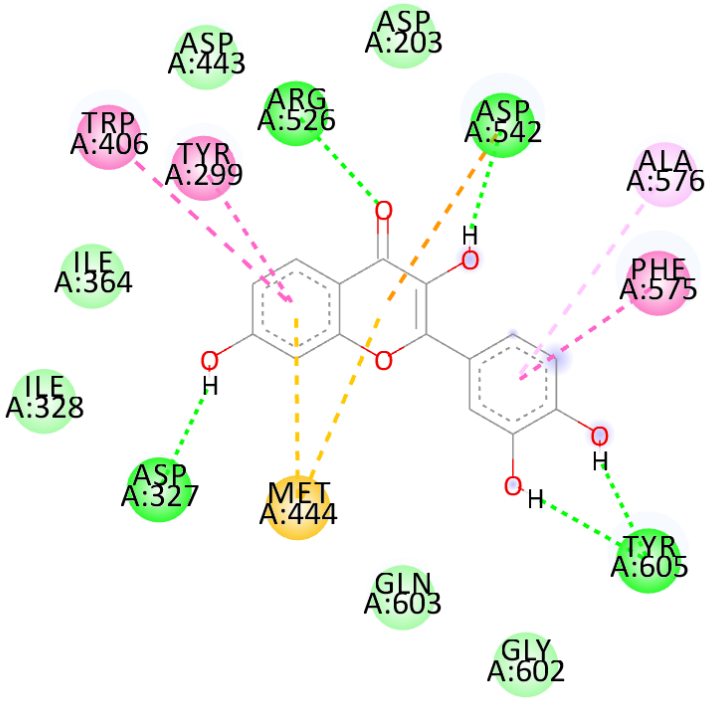
ASP A:203

D21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GLY
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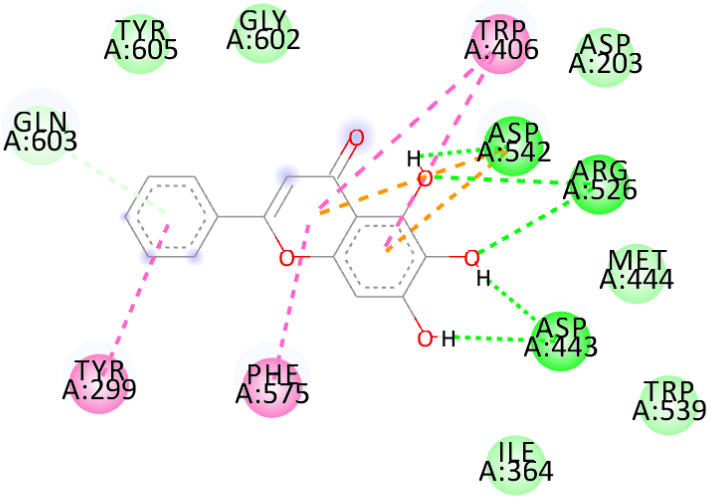
D22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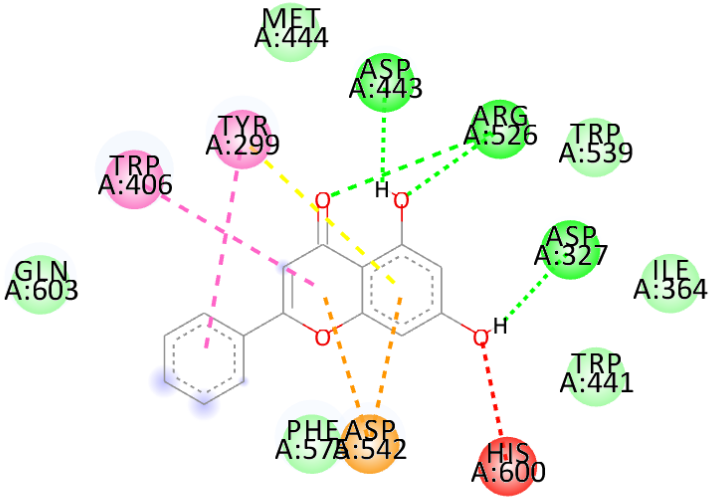
D23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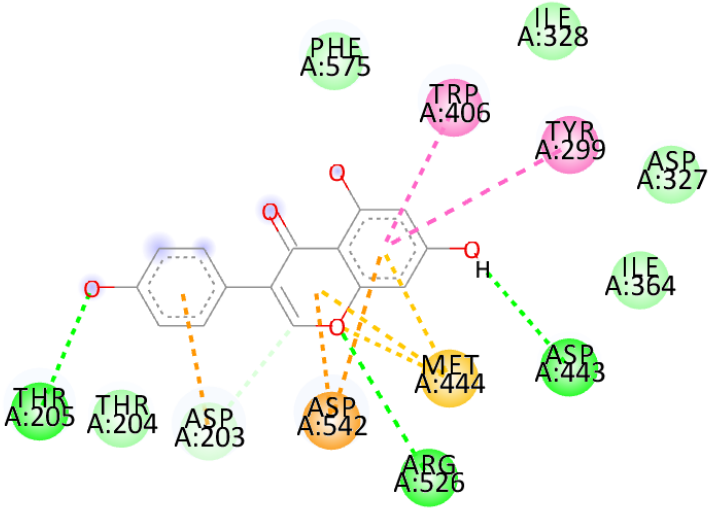
D24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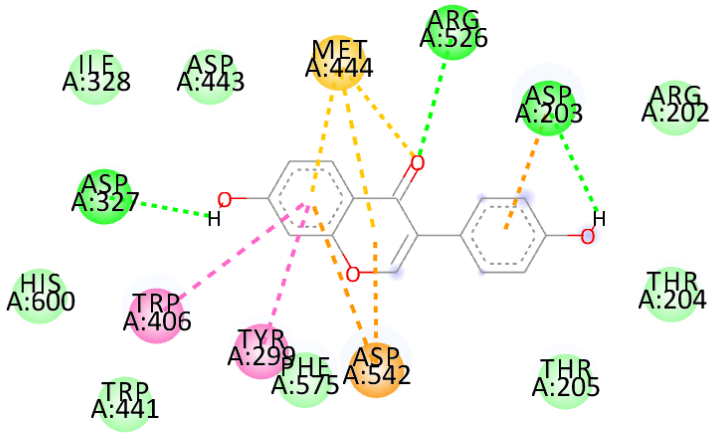
D25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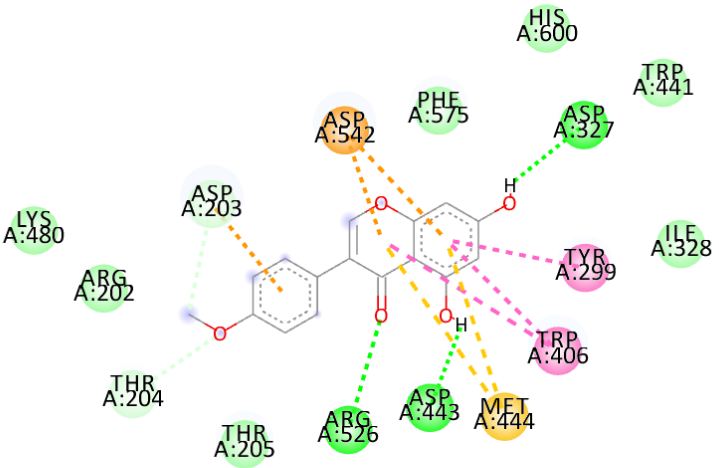
D26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ASP
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ARG
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THR
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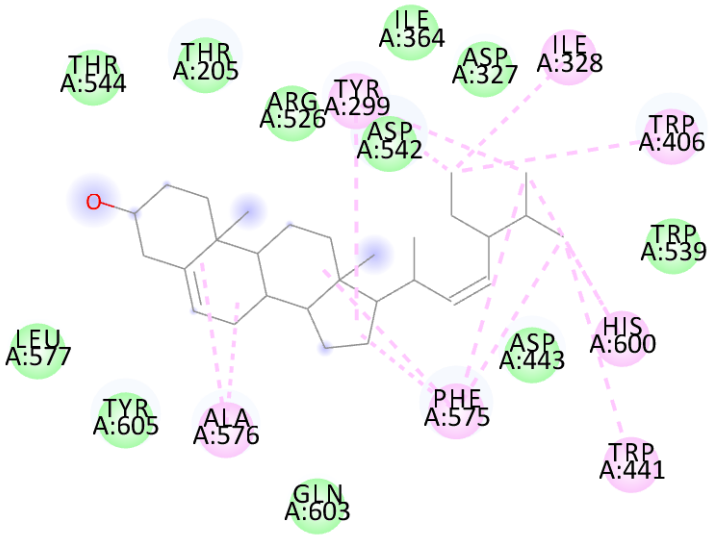
D27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A:577
HIS
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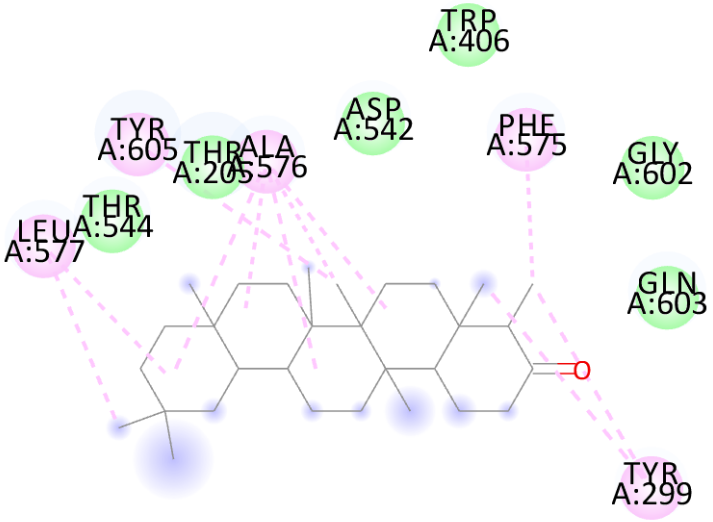
D28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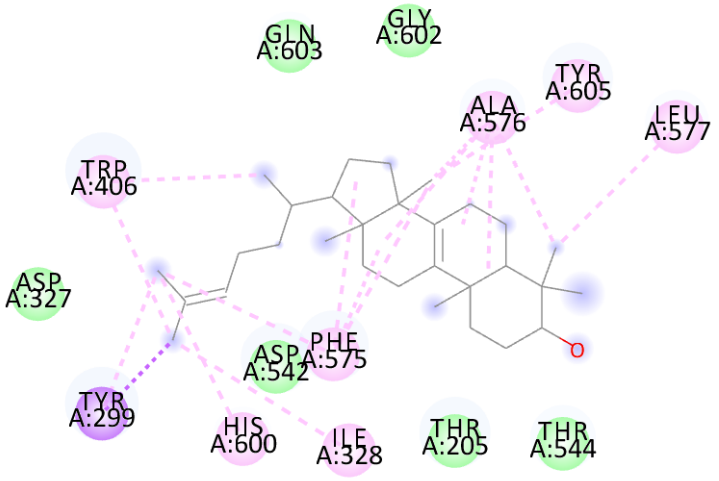
D29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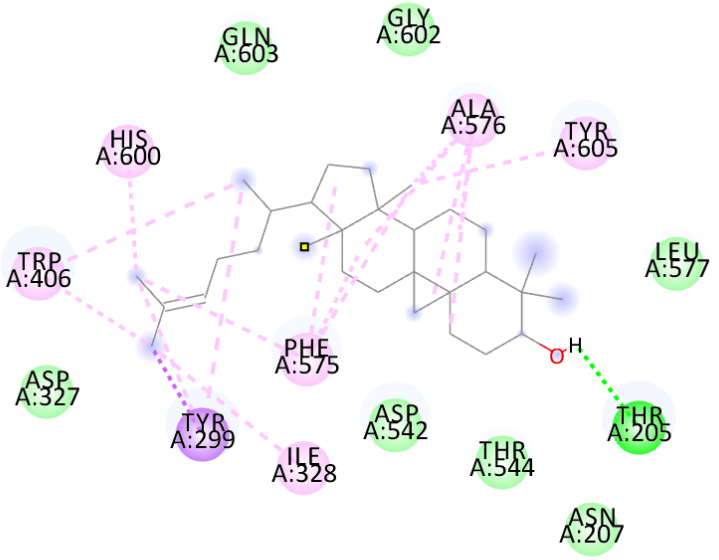
D30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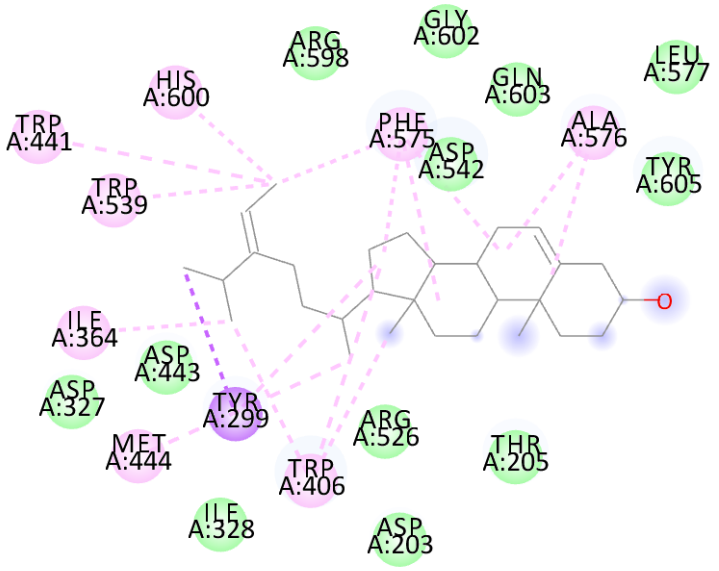
D31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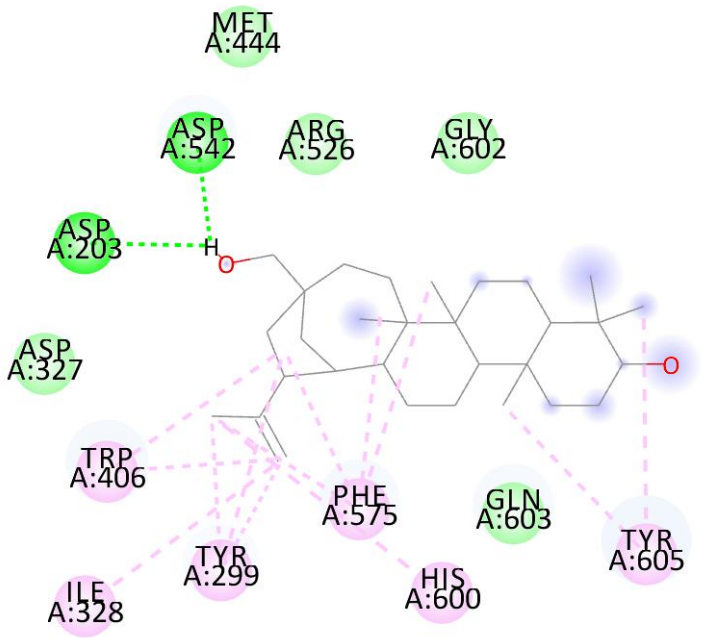
D32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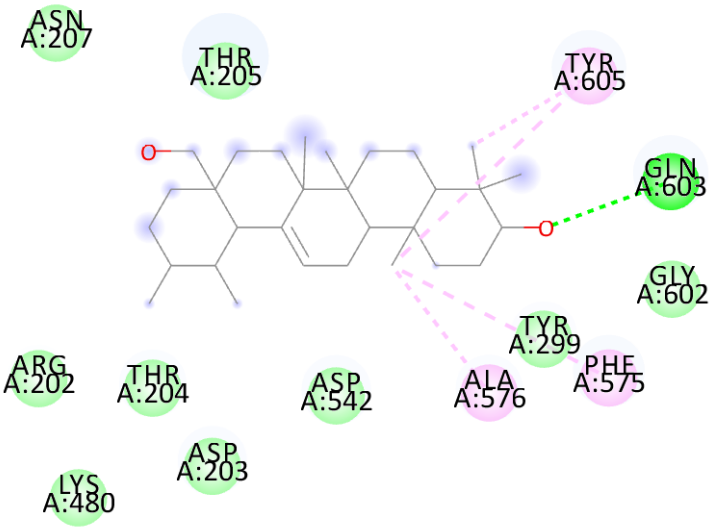
D33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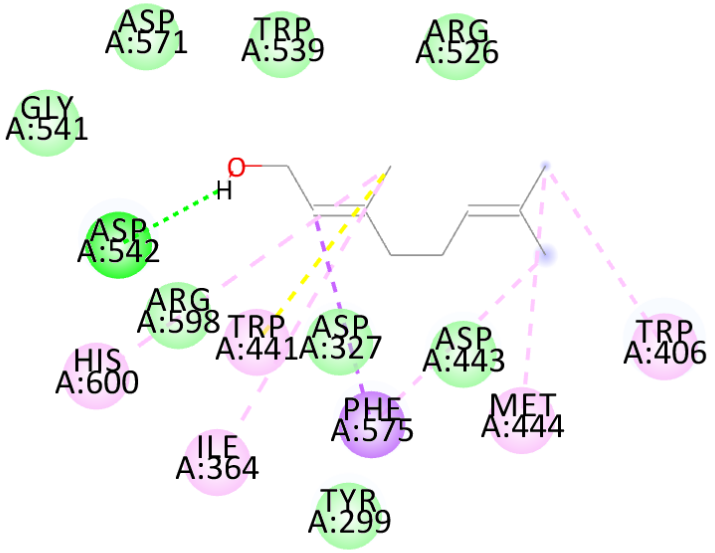
D34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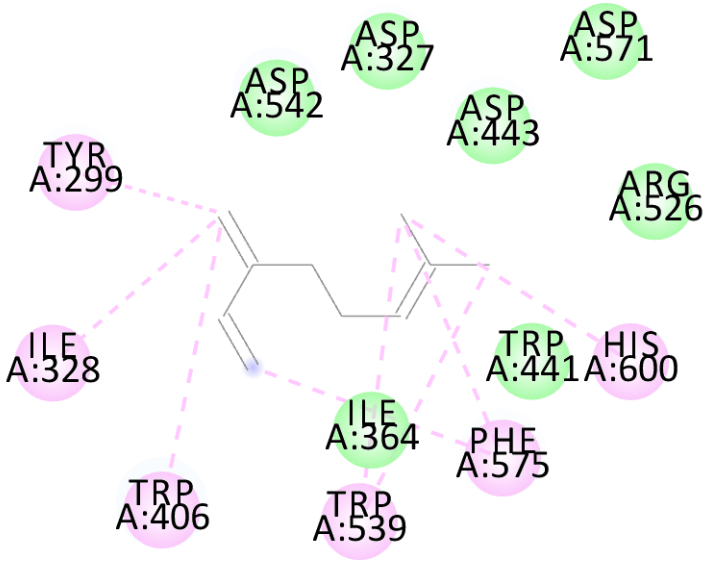
D35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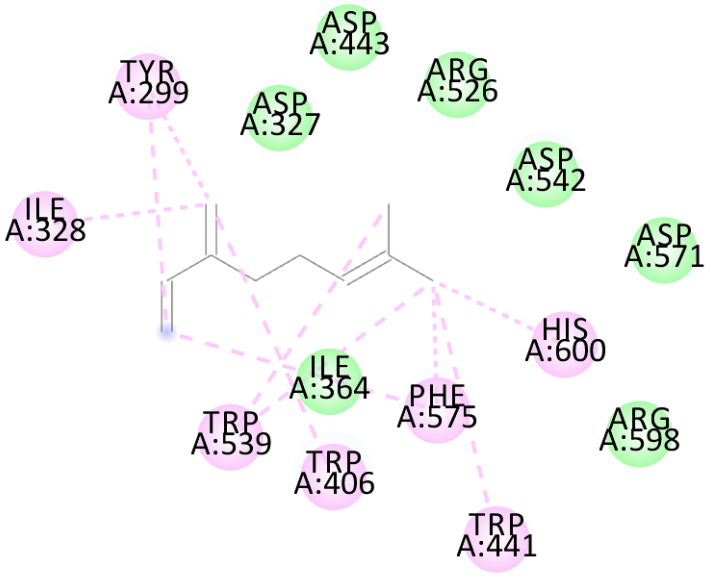
D36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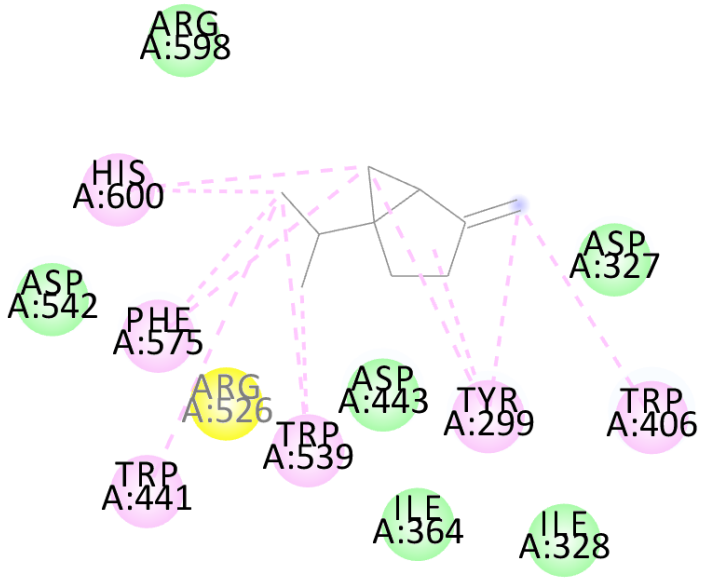
D37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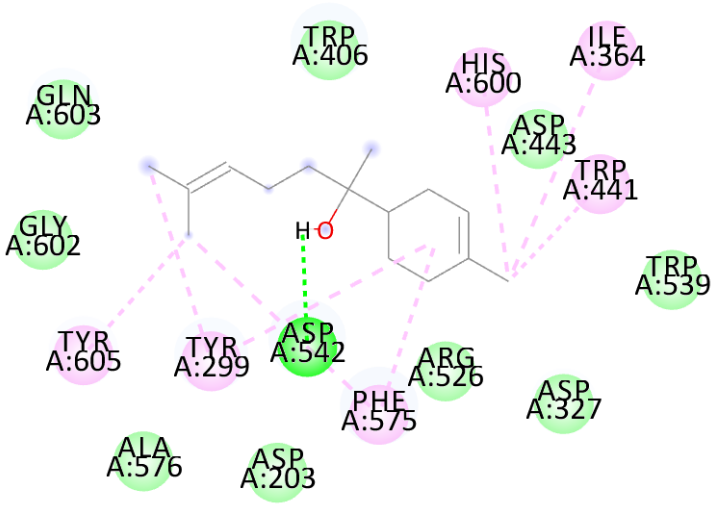
D38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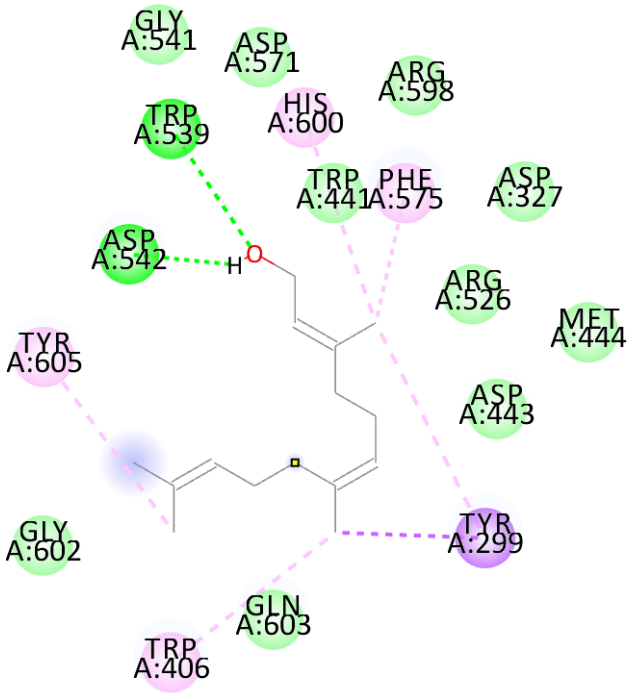
D39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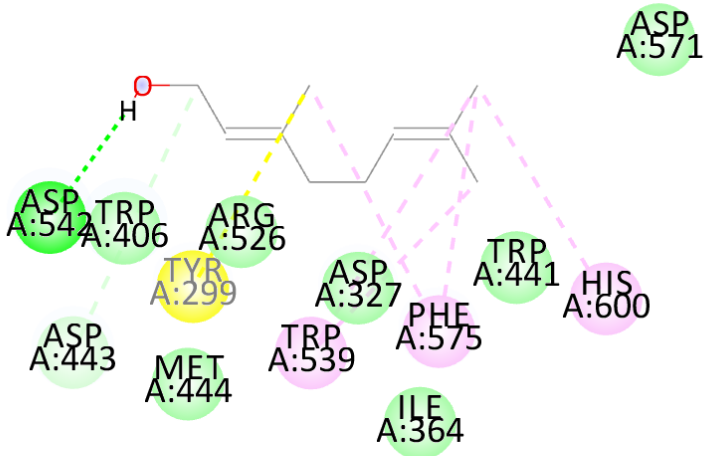
D40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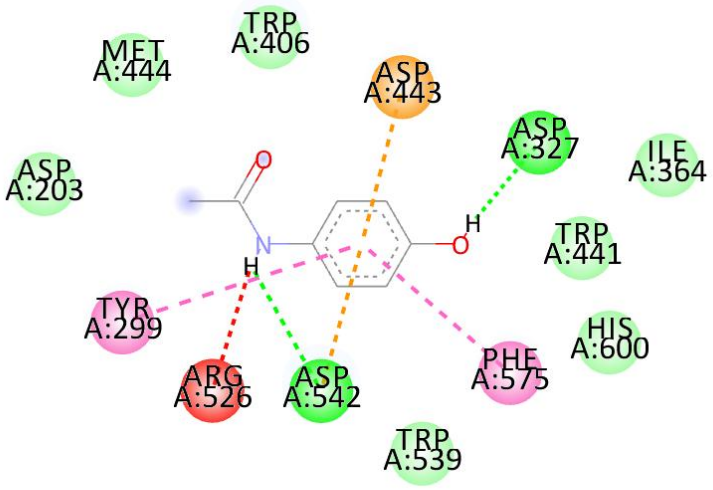
D41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D42

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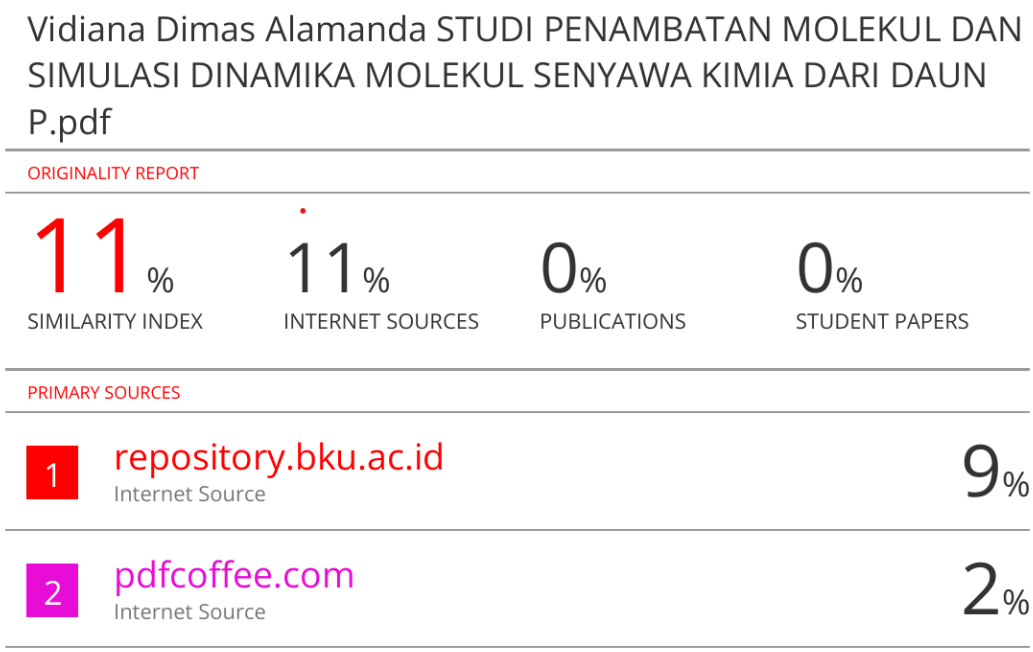

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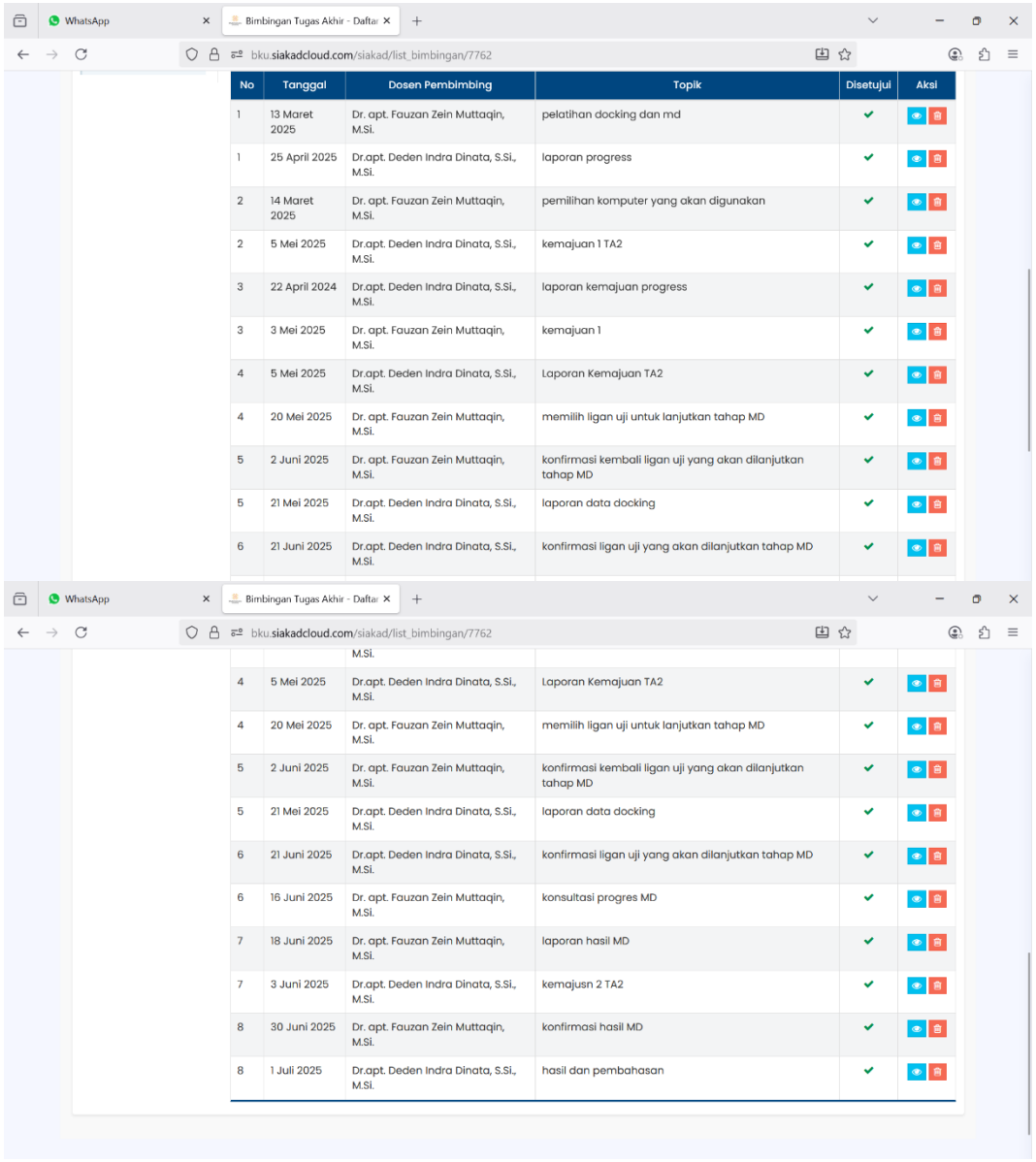
Lampiran 5 kartu bimbingan



No	Tanggal	Dosen Pembimbing	Topik	Disetujui	Aksi
1	13 Maret 2025	Dr. apt. Fauzan Zein Muttaqin, M.Si.	pelatihan docking dan md	✔	
1	25 April 2025	Dr.apt. Deden Indra Dinata, S.Si., M.Si.	laporan progress	✔	
2	14 Maret 2025	Dr. apt. Fauzan Zein Muttaqin, M.Si.	pemilihan komputer yang akan digunakan	✔	
2	5 Mei 2025	Dr.apt. Deden Indra Dinata, S.Si., M.Si.	kemajuan 1 TA2	✔	
3	22 April 2024	Dr.apt. Deden Indra Dinata, S.Si., M.Si.	laporan kemajuan progress	✔	
3	3 Mei 2025	Dr. apt. Fauzan Zein Muttaqin, M.Si.	kemajuan 1	✔	
4	5 Mei 2025	Dr.apt. Deden Indra Dinata, S.Si., M.Si.	Laporan Kemajuan TA2	✔	
4	20 Mei 2025	Dr. apt. Fauzan Zein Muttaqin, M.Si.	memilih ligan uji untuk lanjutkan tahap MD	✔	
5	2 Juni 2025	Dr. apt. Fauzan Zein Muttaqin, M.Si.	konfirmasi kembali ligan uji yang akan dilanjutkan tahap MD	✔	
5	21 Mei 2025	Dr.apt. Deden Indra Dinata, S.Si., M.Si.	laporan data docking	✔	
6	21 Juni 2025	Dr.apt. Deden Indra Dinata, S.Si., M.Si.	konfirmasi ligan uji yang akan dilanjutkan tahap MD	✔	
6	16 Juni 2025	Dr. apt. Fauzan Zein Muttaqin, M.Si.	konsultasi progres MD	✔	
7	18 Juni 2025	Dr. apt. Fauzan Zein Muttaqin, M.Si.	laporan hasil MD	✔	
7	3 Juni 2025	Dr.apt. Deden Indra Dinata, S.Si., M.Si.	kemajusn 2 TA2	✔	
8	30 Juni 2025	Dr. apt. Fauzan Zein Muttaqin, M.Si.	konfirmasi hasil MD	✔	
8	1 Juli 2025	Dr.apt. Deden Indra Dinata, S.Si., M.Si.	hasil dan pembahasan	✔	

Lampiran 6 Curriculum vitae

VIDIANA DIMAS ALAMANDA

FARMASI

KONTAK

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Jl.Karang Asih No.35

https://www.instagram.com/dimassssal

PENDIDIKAN

2018-2021
SMK CIPTA SKILL

- Jurusan Farmasi

2021-2025
UNIVERSITAS BHAKTI KENCANA

- Sarjana Farmasi
- GPA: 3.12 / 4.0

SKILLS

- Peracikan Obat
- Pemahaman Dasar Kefarmasian
- Pelayanan Resep Dokter
- Manajemen Penyetokan Obat
- Komunikasi
- Kerjasama Tim
- Manajemen Waktu

PROFILE

Saya adalah lulusan Sarjana Farmasi Universitas Bhakti Kencana (2025) dengan IPK 3.12. Memiliki pengalaman magang di Puskesmas Puter dalam bidang pelayanan kefarmasian, edukasi pasien, dan pengelolaan obat. Aktif dalam kegiatan penelitian dan kewirausahaan dengan prestasi Juara 1 Lomba Program Kreativitas Mahasiswa (PKM) serta berhasil lolos pendanaan Program Pembinaan Mahasiswa Wirausaha (P2MW) melalui inovasi pupuk cair organik dari sampah sisa makanan.

Memiliki ketertarikan pada bidang farmasi, pelayanan kesehatan, serta pengembangan produk berbasis penelitian. Terbiasa bekerja secara tim maupun individu, mampu berkomunikasi dengan baik, serta memiliki semangat belajar dan beradaptasi dengan lingkungan kerja baru.

PENGALAMAN

Magang di puskesmas 2020

UPT puskesmas puter

- Menerima resep dari dokter
- Skrining resep
- Penyiapan resep
- PIO
- Stock of name

Juara 1 Lomba PKM 2023

PROGRAM KREATIF MAHASISWA

- Mengolah sampah sisa makanan menjadi pupuk cair organik
- Mengurangi limbah sampah sisa makanan
- Menjadikan sampah organik berguna bagi masyarakat

Lolos Pendanaan P2MW 2023

PROGRAM PEMBINAAN MAHASISWA WIRAUSAHA

- Berhasil mengembangkan produk pupuk cair organik hasil penelitian PKM menjadi program wirausaha dengan potensi komersial.