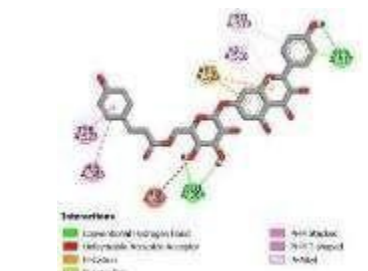
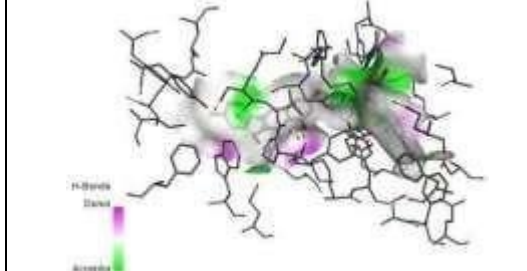
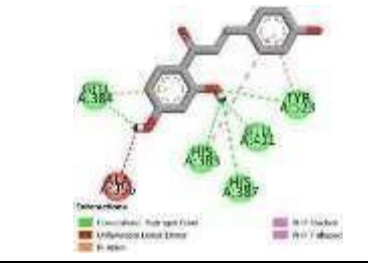
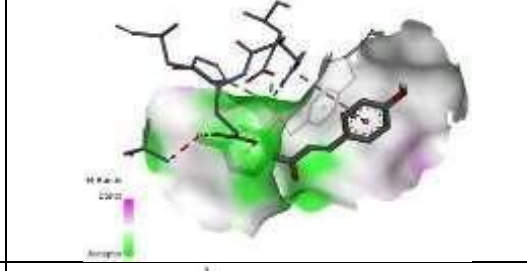
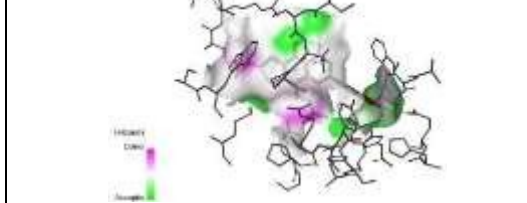
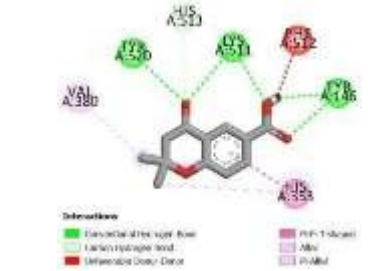
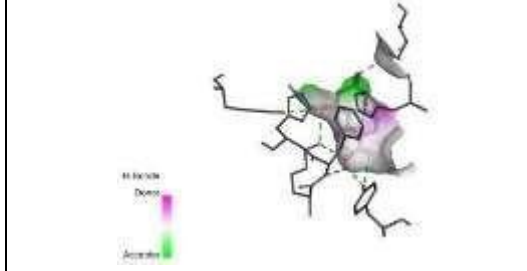
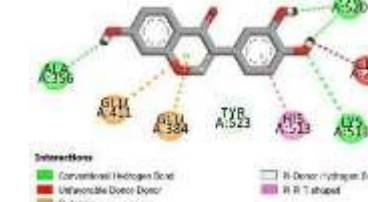
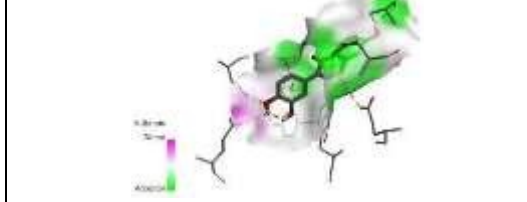




|      |                                                                                                                                                                                                                                                                                                                                             |                                                                                                                         |
|------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------|
| LU5  |  <p><b>Interactions:</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Unconventional Hydrogen Bond</li> <li>Pi-Pi Stacked</li> <li>Pi-Alkyne</li> <li>Pi-Hi Stacked</li> <li>Pi-Hi T-shaped</li> <li>Alkyne</li> </ul>   |  <p>Hydrogen Donor<br/>Acceptor</p>   |
| LU6  |  <p><b>Interactions:</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Unconventional Hydrogen Bond</li> <li>Pi-Pi Stacked</li> <li>Pi-Alkyne</li> <li>Pi-Hi Stacked</li> <li>Pi-Hi T-shaped</li> <li>Alkyne</li> </ul>   |  <p>Hydrogen Donor<br/>Acceptor</p>   |
| LU7  |  <p><b>Interactions:</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Unconventional Hydrogen Bond</li> <li>Pi-Pi Stacked</li> <li>Pi-Alkyne</li> <li>Pi-Hi Stacked</li> <li>Pi-Hi T-shaped</li> <li>Alkyne</li> </ul>  |  <p>Hydrogen Donor<br/>Acceptor</p>  |
| LU8  |  <p><b>Interactions:</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Unconventional Hydrogen Bond</li> <li>Pi-Pi Stacked</li> <li>Pi-Alkyne</li> <li>Pi-Hi Stacked</li> <li>Pi-Hi T-shaped</li> <li>Alkyne</li> </ul> |  <p>Hydrogen Donor<br/>Acceptor</p> |
| LU9  |  <p><b>Interactions:</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Unconventional Hydrogen Bond</li> <li>Pi-Pi Stacked</li> <li>Pi-Alkyne</li> <li>Pi-Hi Stacked</li> <li>Pi-Hi T-shaped</li> <li>Alkyne</li> </ul> |  <p>Hydrogen Donor<br/>Acceptor</p> |
| LU10 |  <p><b>Interactions:</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Unconventional Hydrogen Bond</li> <li>Pi-Pi Stacked</li> <li>Pi-Alkyne</li> <li>Pi-Hi Stacked</li> <li>Pi-Hi T-shaped</li> <li>Alkyne</li> </ul> |  <p>Hydrogen Donor<br/>Acceptor</p> |

|      |                                                                                                                                                                                 |                                       |
|------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------|
| LU11 | <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Pi-Stacked</li> <li>Pi-Alkyne</li> <li>Pi-Donor Hydrogen Bonds</li> </ul> | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |
| LU12 | <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Pi-Stacked</li> <li>Pi-Alkyne</li> <li>Pi-Donor Hydrogen Bonds</li> </ul> | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |
| LU13 | <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Pi-Stacked</li> <li>Pi-Alkyne</li> <li>Pi-Donor Hydrogen Bonds</li> </ul> | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |
| LU14 | <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Pi-Stacked</li> <li>Pi-Alkyne</li> <li>Pi-Donor Hydrogen Bonds</li> </ul> | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |
| LU15 | <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Pi-Stacked</li> <li>Pi-Alkyne</li> <li>Pi-Donor Hydrogen Bonds</li> </ul> | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |
| LU16 | <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Pi-Stacked</li> <li>Pi-Alkyne</li> <li>Pi-Donor Hydrogen Bonds</li> </ul> | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |

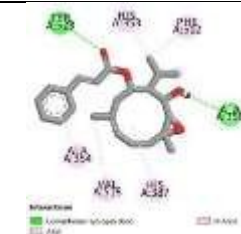
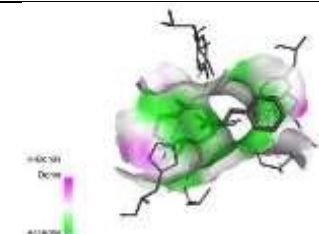
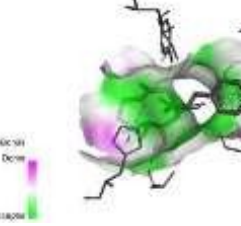
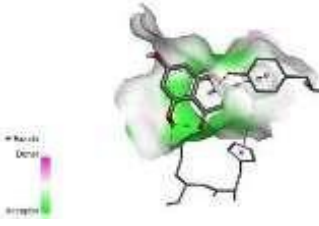
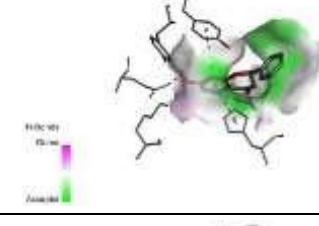
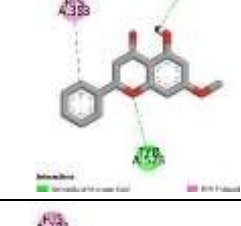
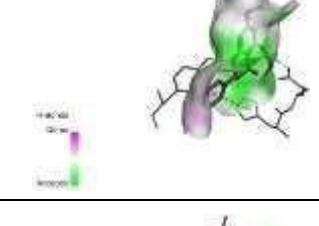
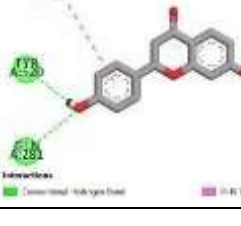
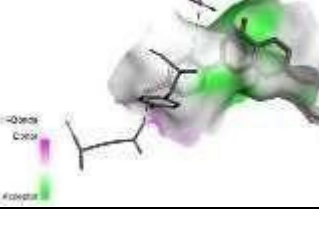


|      |                                                                                                                                                                                              |  |
|------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
| LU23 | <p>Interactions</p> <ul style="list-style-type: none"><li>Conventional Hydrogen Bond</li><li>Cation-Hydrogen Bond</li><li>Pi-Cation</li><li>Pi-Pi</li><li>Pi-Pi Stacked</li></ul>            |  |
| LU24 | <p>Interactions</p> <ul style="list-style-type: none"><li>Conventional Hydrogen Bond</li><li>Pi-Pi</li><li>Pi-Pi Stacked</li></ul>                                                           |  |
| LU25 | <p>Interactions</p> <ul style="list-style-type: none"><li>Conventional Hydrogen Bond</li><li>Pi-Pi</li><li>Pi-Pi Stacked</li></ul>                                                           |  |
| LU26 | <p>Interactions</p> <ul style="list-style-type: none"><li>Conventional Hydrogen Bond</li><li>Cation-Hydrogen Bond</li><li>Cation-Hydrogen Bond</li><li>Pi-Pi</li><li>Pi-Pi Stacked</li></ul> |  |
| LU27 | <p>Interactions</p> <ul style="list-style-type: none"><li>Conventional Hydrogen Bond</li><li>Cation-Hydrogen Bond</li><li>Pi-Pi</li></ul>                                                    |  |

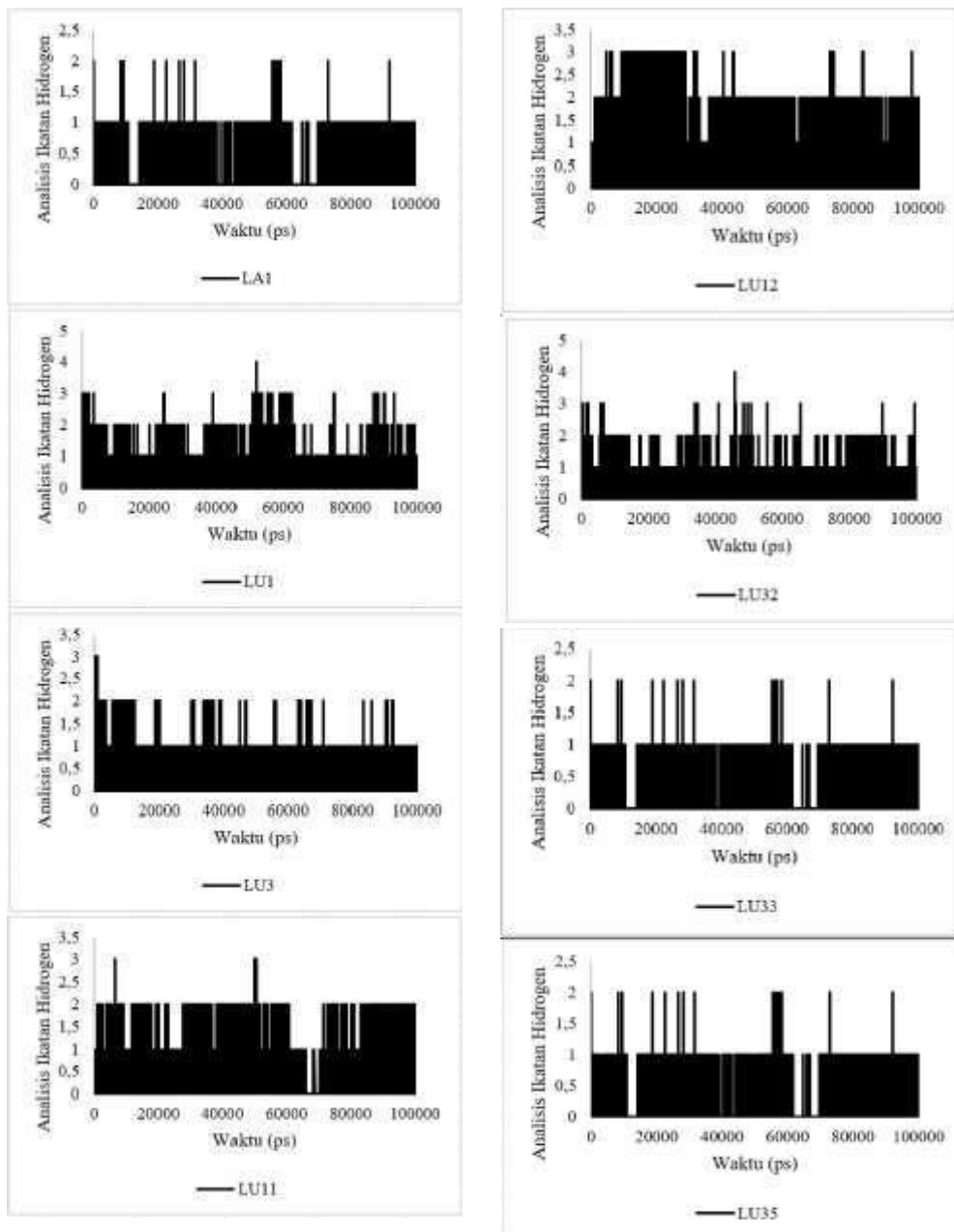
|      |                                                                                                                                                                                                                                                                                |                                       |
|------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------|
| LU28 | <p>Interactions:<br/> <span style="color: green;">■</span> Conventional Hydrogen Bond<br/> <span style="color: grey;">■</span> Cation-Hydrogen Bond</p>                                                                                                                        | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |
| LU29 | <p>Interactions:<br/> <span style="color: green;">■</span> Conventional Hydrogen Bond<br/> <span style="color: grey;">■</span> Cation-Hydrogen Bond</p>                                                                                                                        | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |
| LU30 | <p>Interactions:<br/> <span style="color: green;">■</span> Conventional Hydrogen Bond<br/> <span style="color: grey;">■</span> Cation-Hydrogen Bond<br/> <span style="color: red;">■</span> Aromatic-π Interaction<br/> <span style="color: purple;">■</span> π-π Stacking</p> | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |
| LU31 | <p>Interactions:<br/> <span style="color: green;">■</span> Conventional Hydrogen Bond<br/> <span style="color: grey;">■</span> Cation-Hydrogen Bond<br/> <span style="color: red;">■</span> Aromatic-π Interaction<br/> <span style="color: purple;">■</span> π-π Stacking</p> | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |
| LU32 | <p>Interactions:<br/> <span style="color: green;">■</span> Conventional Hydrogen Bond<br/> <span style="color: grey;">■</span> Cation-Hydrogen Bond<br/> <span style="color: red;">■</span> Aromatic-π Interaction<br/> <span style="color: purple;">■</span> π-π Stacking</p> | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |

|      |                                                                                                                                                                                                                                                                                                              |                                       |
|------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------|
| LU33 | <p><b>Interactions:</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Unconventional Hydrogen Bond</li> <li>Hydrophobic Interaction</li> <li>H-Donor...H-Acceptor Bond</li> <li>H-Donor...H-Donor</li> <li>H-Acceptor...H-Acceptor</li> <li>H-Donor...H-Acceptor</li> </ul> | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |
| LU34 | <p><b>Interactions:</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Unconventional Hydrogen Bond</li> <li>Hydrophobic Interaction</li> <li>H-Donor...H-Acceptor Bond</li> <li>H-Donor...H-Donor</li> <li>H-Acceptor...H-Acceptor</li> <li>H-Donor...H-Acceptor</li> </ul> | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |
| LU35 | <p><b>Interactions:</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Unconventional Hydrogen Bond</li> <li>Hydrophobic Interaction</li> <li>H-Donor...H-Acceptor Bond</li> <li>H-Donor...H-Donor</li> <li>H-Acceptor...H-Acceptor</li> <li>H-Donor...H-Acceptor</li> </ul> | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |
| LU36 | <p><b>Interactions:</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Unconventional Hydrogen Bond</li> <li>Hydrophobic Interaction</li> <li>H-Donor...H-Acceptor Bond</li> <li>H-Donor...H-Donor</li> <li>H-Acceptor...H-Acceptor</li> <li>H-Donor...H-Acceptor</li> </ul> | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |
| LU37 | <p><b>Interactions:</b></p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Unconventional Hydrogen Bond</li> <li>Hydrophobic Interaction</li> <li>H-Donor...H-Acceptor Bond</li> <li>H-Donor...H-Donor</li> <li>H-Acceptor...H-Acceptor</li> <li>H-Donor...H-Acceptor</li> </ul> | <p>H-Bonds<br/>Donor<br/>Acceptor</p> |

|      |                                                                                                                                                                                                    |                                      |
|------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------|
| LU38 | <p>Interactions:</p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Hydrophobic Donor-Donor</li> <li>H-bond</li> <li>Pi-Pi Stacked</li> <li>Pi-Pi T-Stacked</li> </ul> | <p>H-Bonds Donor</p> <p>Acceptor</p> |
| LU39 | <p>Interactions:</p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Hydrophobic Donor-Donor</li> <li>H-bond</li> <li>Pi-Pi Stacked</li> <li>Pi-Pi T-Stacked</li> </ul> | <p>H-Bonds Donor</p> <p>Acceptor</p> |
| LU40 | <p>Interactions:</p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Hydrophobic Donor-Donor</li> <li>H-bond</li> <li>Pi-Pi Stacked</li> <li>Pi-Pi T-Stacked</li> </ul> | <p>H-Bonds Donor</p> <p>Acceptor</p> |
| LU41 | <p>Interactions:</p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Hydrophobic Donor-Donor</li> <li>H-bond</li> <li>Pi-Pi Stacked</li> <li>Pi-Pi T-Stacked</li> </ul> | <p>H-Bonds Donor</p> <p>Acceptor</p> |
| LU42 | <p>Interactions:</p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Hydrophobic Donor-Donor</li> <li>H-bond</li> <li>Pi-Pi Stacked</li> <li>Pi-Pi T-Stacked</li> </ul> | <p>H-Bonds Donor</p> <p>Acceptor</p> |
| LU43 | <p>Interactions:</p> <ul style="list-style-type: none"> <li>Conventional Hydrogen Bond</li> <li>Hydrophobic Donor-Donor</li> <li>H-bond</li> <li>Pi-Pi Stacked</li> <li>Pi-Pi T-Stacked</li> </ul> | <p>H-Bonds Donor</p> <p>Acceptor</p> |

|      |                                                                                                                                                                                                                 |                                                                                                                                                                    |
|------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| LU44 |  <p>Hydrophobic<br/>Hydrophobic-Hydrogen Bond<br/>H-Bond<br/>H-Bond-Hydrogen Bond<br/>H-Bond-Hydrogen Bond-Hydrogen Bond</p>   |  <p>H-Bond<br/>H-Bond-Hydrogen Bond<br/>H-Bond-Hydrogen Bond-Hydrogen Bond</p>   |
| LU45 |  <p>Hydrophobic<br/>Hydrophobic-Hydrogen Bond<br/>H-Bond<br/>H-Bond-Hydrogen Bond<br/>H-Bond-Hydrogen Bond-Hydrogen Bond</p>   |  <p>H-Bond<br/>H-Bond-Hydrogen Bond<br/>H-Bond-Hydrogen Bond-Hydrogen Bond</p>   |
| LU46 |  <p>Hydrophobic<br/>Hydrophobic-Hydrogen Bond<br/>H-Bond<br/>H-Bond-Hydrogen Bond<br/>H-Bond-Hydrogen Bond-Hydrogen Bond</p>  |  <p>H-Bond<br/>H-Bond-Hydrogen Bond<br/>H-Bond-Hydrogen Bond-Hydrogen Bond</p>  |
| LU47 |  <p>Hydrophobic<br/>Hydrophobic-Hydrogen Bond<br/>H-Bond<br/>H-Bond-Hydrogen Bond<br/>H-Bond-Hydrogen Bond-Hydrogen Bond</p> |  <p>H-Bond<br/>H-Bond-Hydrogen Bond<br/>H-Bond-Hydrogen Bond-Hydrogen Bond</p> |
| LU48 |  <p>Hydrophobic<br/>Hydrophobic-Hydrogen Bond<br/>H-Bond<br/>H-Bond-Hydrogen Bond<br/>H-Bond-Hydrogen Bond-Hydrogen Bond</p> |  <p>H-Bond<br/>H-Bond-Hydrogen Bond<br/>H-Bond-Hydrogen Bond-Hydrogen Bond</p> |
| LU49 |  <p>Hydrophobic<br/>Hydrophobic-Hydrogen Bond<br/>H-Bond<br/>H-Bond-Hydrogen Bond<br/>H-Bond-Hydrogen Bond-Hydrogen Bond</p> |  <p>H-Bond<br/>H-Bond-Hydrogen Bond<br/>H-Bond-Hydrogen Bond-Hydrogen Bond</p> |
| LU50 |  <p>Hydrophobic<br/>Hydrophobic-Hydrogen Bond<br/>H-Bond<br/>H-Bond-Hydrogen Bond<br/>H-Bond-Hydrogen Bond-Hydrogen Bond</p> |  <p>H-Bond<br/>H-Bond-Hydrogen Bond<br/>H-Bond-Hydrogen Bond-Hydrogen Bond</p> |

## Lampiran 2 Analisis Ikatan Hidrogen selama 100 ns (100000 ps)



### Lampiran 3 Kartu Bimbingan

|   |                  |                                      |                                                     |   |                                                                                                                                                                             |
|---|------------------|--------------------------------------|-----------------------------------------------------|---|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1 | 23 Oktober 2024  | Dr. apt. FAUZAN ZEIN MUTTAQIN, M.Si. | Bimbingan Mengenai Penelitian                       | ✓ |       |
| 1 | 23 Oktober 2024  | ANNE YULIANTINI                      | Bimbingan Mengenai Penelitian                       | ✓ |       |
| 2 | 24 Oktober 2024  | ANNE YULIANTINI                      | Bimbingan Mengenai Senyawa Uji                      | ✓ |       |
| 2 | 1 November 2024  | Dr. apt. FAUZAN ZEIN MUTTAQIN, M.Si. | Bimbingan mengenai kode PDB dan Ligan Uji           | ✓ |       |
| 3 | 29 November 2024 | Dr. apt. FAUZAN ZEIN MUTTAQIN, M.Si. | konfirmasi hasil Nilai RMSD                         | ✓ |       |
| 3 | 8 November 2024  | ANNE YULIANTINI                      | Bimbingan mengenai laporan kemajuan 1               | ✓ |       |
| 4 | 29 November 2024 | ANNE YULIANTINI                      | konfirmasi hasil nilai RMSD                         | ✓ |       |
| 4 | 3 Desember 2024  | Dr. apt. FAUZAN ZEIN MUTTAQIN, M.Si. | mengkonfirmasi file hasil docking dan hidrogennya   | ✓ |       |
| 5 | 7 Desember 2024  | Dr. apt. FAUZAN ZEIN MUTTAQIN, M.Si. | Menentukan senyawa uji yang akan di simulasi MD     | ✓ |       |
| 5 | 3 Desember 2024  | ANNE YULIANTINI                      | mengkonfirmasi file hasil docking dan hidrogennya   | ✓ |       |
| 6 | 17 Desember 2024 | Dr. apt. FAUZAN ZEIN MUTTAQIN, M.Si. | Bimbingan mengenai preparasi ligan dan MD           | ✓ |       |
| 6 | 20 Desember 2024 | ANNE YULIANTINI                      | bimbingan kemajuan 2 dan melakukan presentasi       | ✓ |     |
| 7 | 2 Januari 2025   | ANNE YULIANTINI                      | konfirmasi pustaka tentang nilai konstanta inhibisi | ✓ |   |
| 7 | 20 Desember 2024 | Dr. apt. FAUZAN ZEIN MUTTAQIN, M.Si. | Mengkonfirmasi hasil laporan kemajuan 2             | ✓ |   |
| 8 | 6 Desember 2024  | Dr. apt. FAUZAN ZEIN MUTTAQIN, M.Si. | Mengkonfirmasi hasil docking                        | ✓ |   |
| 8 | 7 Januari 2025   | ANNE YULIANTINI                      | Mengkonfirmasi hasil MD                             | ✓ |   |
| 9 | 13 Januari 2025  | ANNE YULIANTINI                      | Hadit analisis MD                                   | ✓ |   |
| 9 | 13 Januari 2025  | Dr. apt. FAUZAN ZEIN MUTTAQIN, M.Si. | Mengkonfirmasi analisis hasil MD                    | ✓ |   |
| 9 | 13 Januari 2025  | Dr. apt. FAUZAN ZEIN MUTTAQIN, M.Si. | Mengkonfirmasi analisis hasil MD                    | ✓ |   |

## Lampiran 4 Plagiarisme



**Lampiran 5 Daftar Riwayat Hidup****DAFTAR RIWAYAT HIDUP**

Nama Lengkap : Karmilah

Tempat, Tanggal Lahir : Cianjur, 29 juli 2002

Alamat : Kp. Ciwaru RT/RW 003/007, Desa Babakan Caringin,  
Kecamatan Karang tengah, Kabupaten Cianjur,  
Provinsi Jawa Barat

Status : Belum Menikah

Agama : Islam

Nomor Hp : 0877-2597-9696

Alamat email : [karmilahk620@gmail.com](mailto:karmilahk620@gmail.com)

Pendidikan : 2009 – 2014 SDN Selajambe2  
2014 – 2017 MTS Nurul Islam  
2017 – 2020 SMK Kesehatan Bhakti Medica  
2020 – 2025 Universitas Bhakti Kencana