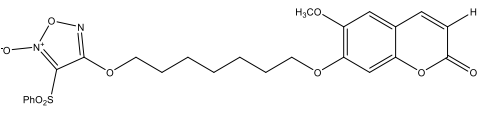
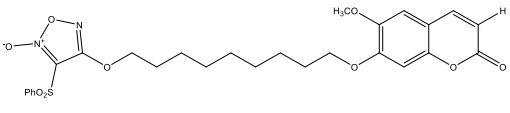
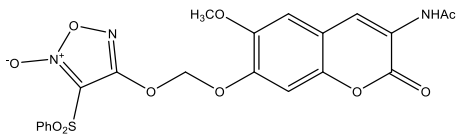
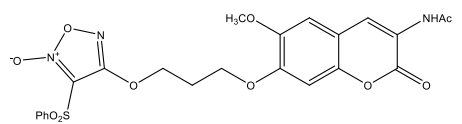
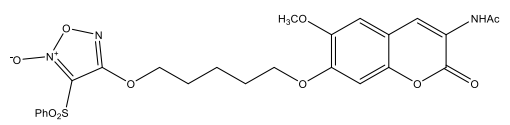
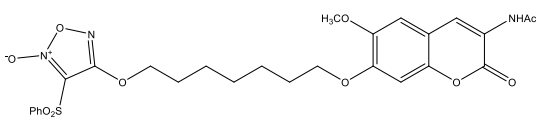
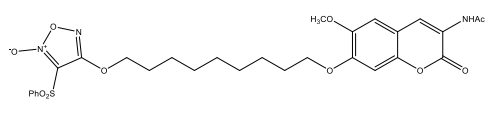
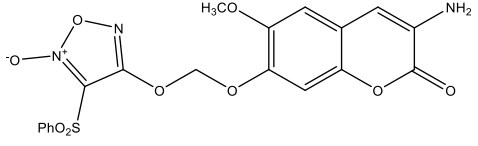
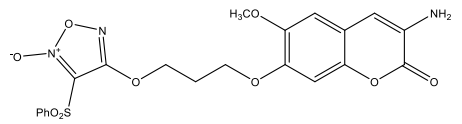
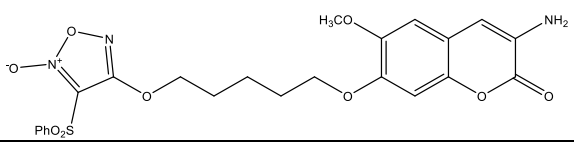
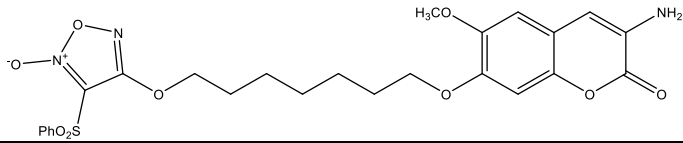
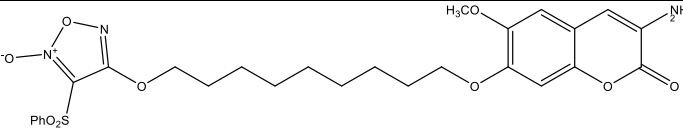


## LAMPIRAN

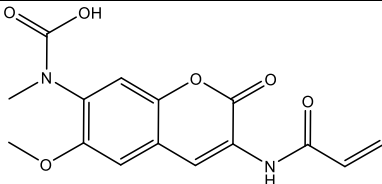
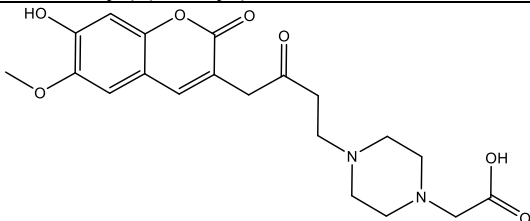
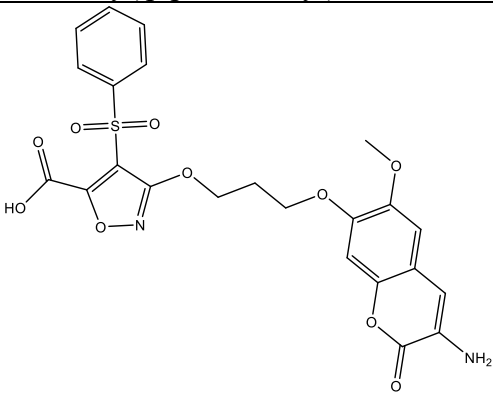
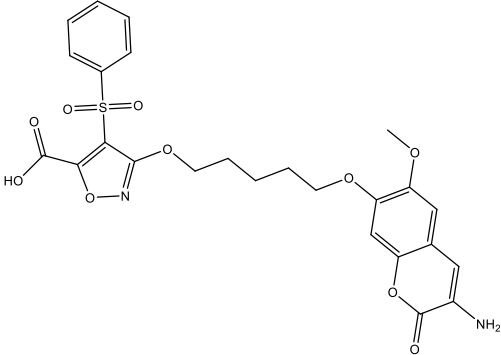
### Lampiran 1 Struktur lengkap 2D Senyawa Turunan Skopoletin

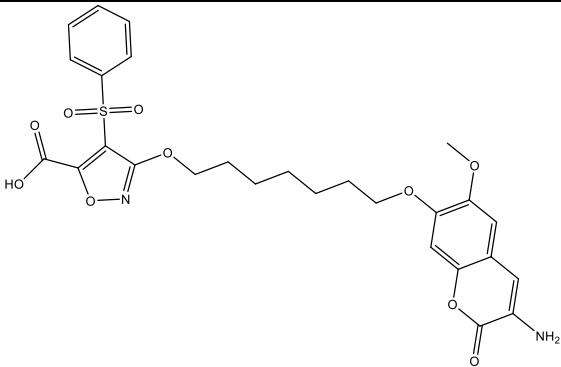
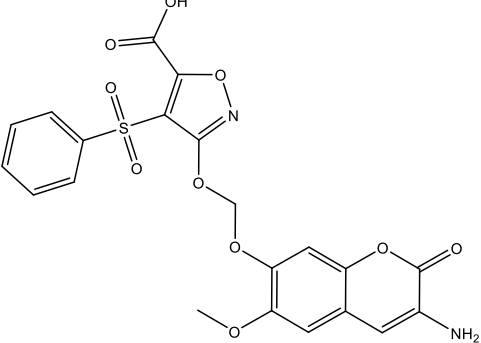
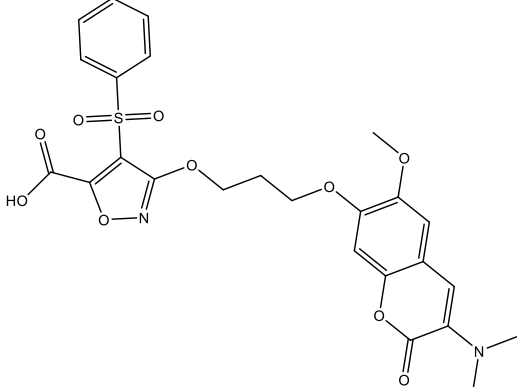
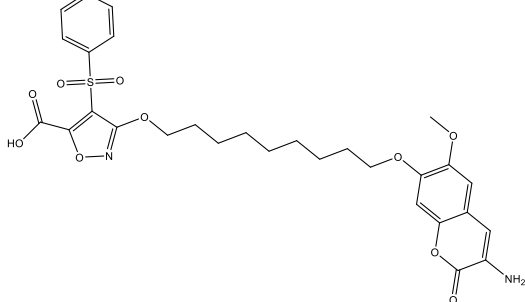
| Kode senyawa | Chem2d |
|--------------|--------|
| Sy1          |        |
| Sy2          |        |
| Sy3          |        |
| Sy4          |        |
| Sy5          |        |
| Sy6          |        |
| Sy7          |        |
| Sy8          |        |
| Sy9          |        |

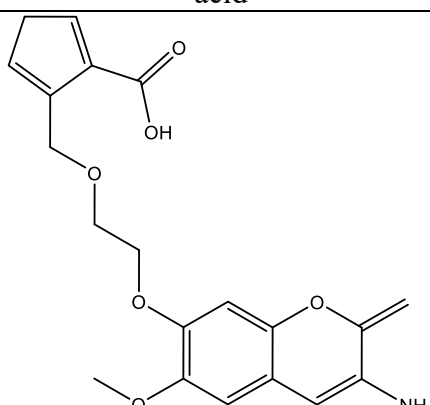
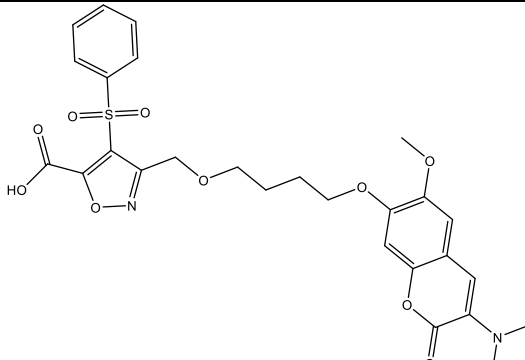
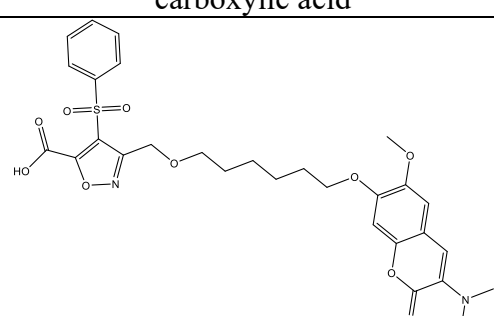
|      |                                                                                      |
|------|--------------------------------------------------------------------------------------|
| Sy10 |    |
| Sy11 |    |
| Sy12 |    |
| Sy13 |    |
| Sy14 |  |
| Sy15 |  |
| Sy16 |  |
| Sy17 |  |
| Sy18 |  |
| Sy19 |  |

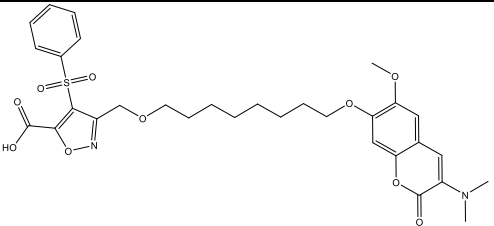
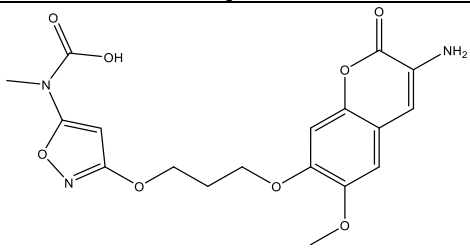
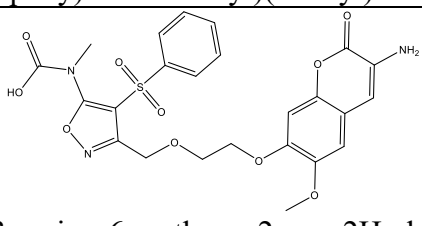
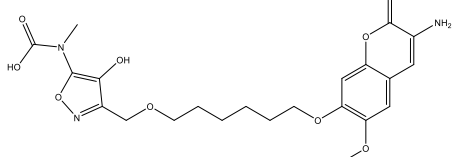
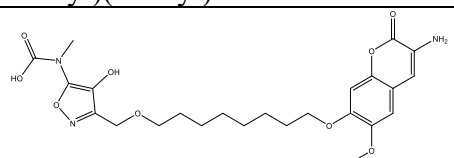
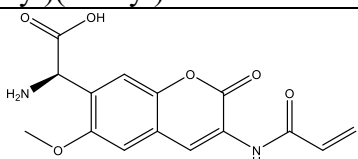
|      |                                                                                                                                                                 |
|------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Sy20 | <br><chem>OS(=O)(=O)c1c([N+]([O-])=O)nn1OCCCCCCCCCOc2c3c(ccc2O3)C(=O)N</chem> |
| Sy21 | <br><chem>OS(=O)(=O)c1c([N+]([O-])=O)nn1OCCCCCCCCCOc2c3c(ccc2O3)C(=O)N</chem> |

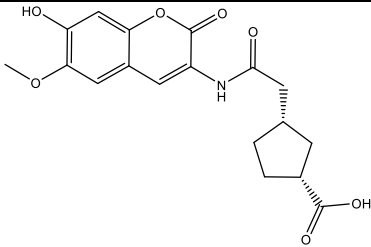
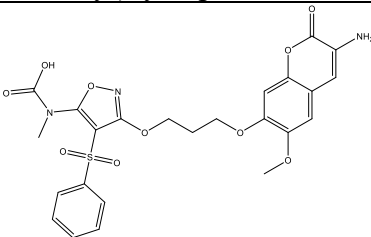
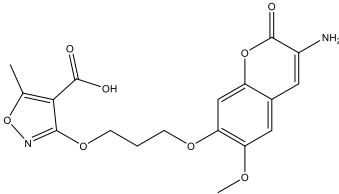
## Lampiran 2 Struktur 2D Senyawa Turunan Baru

| Kode Senyawa Baru | Struktur                                                                                                                                                                                                  |
|-------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| S1                |  <p>(3-acrylamido-6-methoxy-2-oxo-2H-chromen-7-yl)(methyl)carbamic acid</p>                                             |
| S2                |  <p>2-(4-(4-(7-hydroxy-6-methoxy-2-oxo-2H-chromen-3-yl)-3-oxobutyl)piperazin-1-yl)acetic acid</p>                       |
| S3                |  <p>3-((3-((3-amino-6-methoxy-2-oxo-2H-chromen-7-yl)oxy)propoxy)-4-(phenylsulfonyl)isoxazole-5-carboxylic acid</p>    |
| S4                |  <p>3-((5-((3-amino-6-methoxy-2-oxo-2H-chromen-7-yl)oxy)pentyl)oxy)-4-(phenylsulfonyl)isoxazole-5-carboxylic acid</p> |

|    |                                                                                                                                                                                                                 |
|----|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| S5 |  <p>3-((7-((3-amino-6-methoxy-2-oxo-2H-chromen-7-yl)oxy)heptyl)oxy)-4-(phenylsulfonyl)isoxazole-5-carboxylic acid</p>         |
| S6 |  <p>3-(((3-amino-6-methoxy-2-oxo-2H-chromen-7-yl)oxy)methoxy)-4-(phenylsulfonyl)isoxazole-5-carboxylic acid</p>              |
| S7 |  <p>3-(3-((3-(dimethylamino)-6-methoxy-2-oxo-2H-chromen-7-yl)oxy)propoxy)-4-(phenylsulfonyl)isoxazole-5-carboxylic acid</p> |
| S8 |                                                                                                                             |

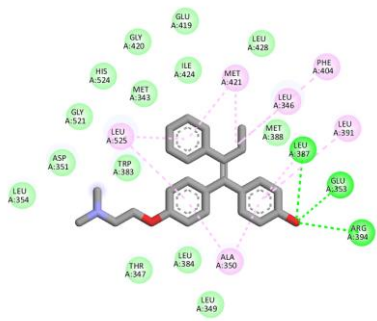
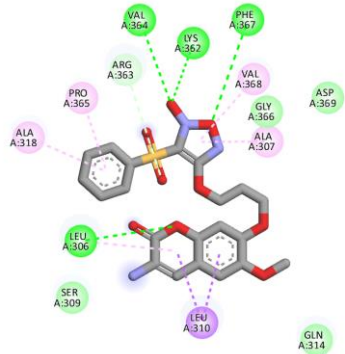
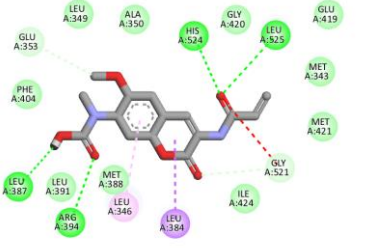
|     |                                                                                                                                                                                                                            |
|-----|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|     | 3-((9-((3-amino-6-methoxy-2-oxo-2H-chromen-7-yl)oxy)nonyl)oxy)-4-(phenylsulfonyl)isoxazole-5-carboxylic acid                                                                                                               |
| S9  |  <p>5-((2-((3-amino-6-methoxy-2-methylene-2H-chromen-7-yl)oxy)ethoxy)methyl)cyclopenta-1,4-diene-1-carboxylic acid</p>                   |
| S10 |  <p>3-(((4-((3-(dimethylamino)-6-methoxy-2-oxo-2H-chromen-7-yl)oxy)butoxy)methyl)-4-(phenylsulfonyl)isoxazole-5-carboxylic acid</p>     |
| S11 |  <p>3-(((6-((3-(dimethylamino)-6-methoxy-2-oxo-2H-chromen-7-yl)oxy)hexyl)oxy)methyl)-4-(phenylsulfonyl)isoxazole-5-carboxylic acid</p> |

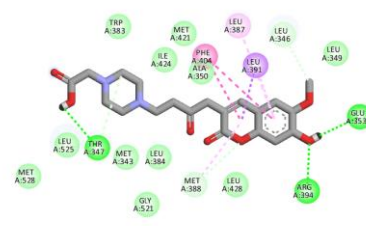
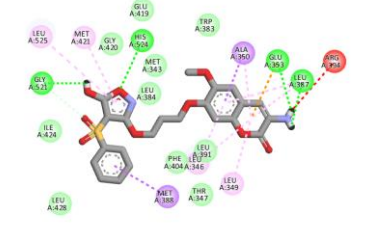
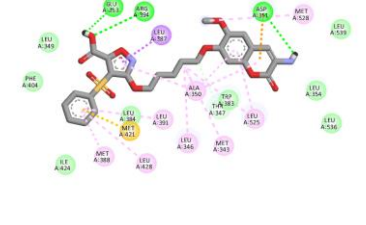
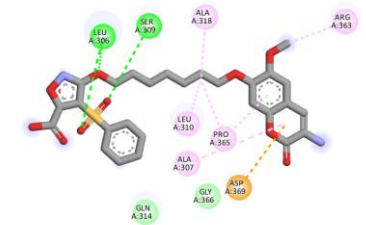
|     |                                                                                                                                                                                                                          |
|-----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| S12 |  <p>3-(((8-((3-(dimethylamino)-6-methoxy-2-oxo-2H-chromen-7-yl)oxy)octyl)oxy)methyl)-4-(phenylsulfonyl)isoxazole-5-carboxylic acid</p> |
| S13 |  <p>(3-(3-((3-amino-6-methoxy-2-oxo-2H-chromen-7-yl)oxy)propoxy)isoxazol-5-yl)(methyl)carbamic acid</p>                                |
| S14 |  <p>(3-((2-((3-amino-6-methoxy-2-oxo-2H-chromen-7-yl)oxy)ethoxy)methyl)-4-(phenylsulfonyl)isoxazol-5-yl)(methyl)carbamic acid</p>     |
| S15 |  <p>(3-(((6-((3-amino-6-methoxy-2-oxo-2H-chromen-7-yl)oxy)hexyl)oxy)methyl)-4-hydroxyisoxazol-5-yl)(methyl)carbamic acid</p>         |
| S16 |  <p>(3-(((8-((3-amino-6-methoxy-2-oxo-2H-chromen-7-yl)oxy)octyl)oxy)methyl)-4-hydroxyisoxazol-5-yl)(methyl)carbamic acid</p>         |
| S17 |                                                                                                                                      |

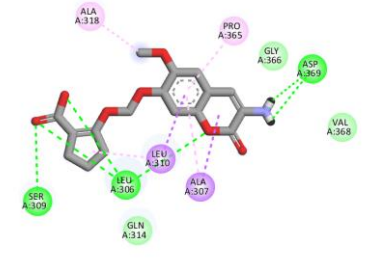
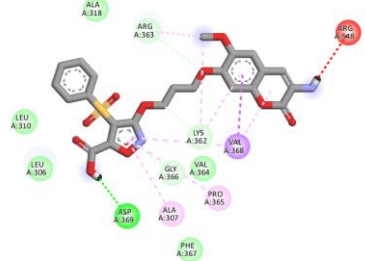
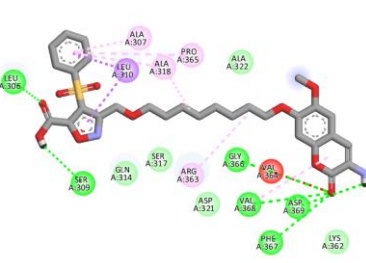
|     |                                                                                                                                                                                                              |
|-----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|     | (R)-2-(3-acrylamido-6-methoxy-2-oxo-2H-chromen-7-yl)-2-aminoacetic acid                                                                                                                                      |
| S18 |  <p>(1R,3S)-3-(2-((7-hydroxy-6-methoxy-2-oxo-2H-chromen-3-yl)amino)-2-oxoethyl)cyclopentane-1-carboxylic acid</p>          |
| S19 |  <p>(3-(3-((3-amino-6-methoxy-2-oxo-2H-chromen-7-yl)oxy)propoxy)-4-(phenylsulfonyl)isoxazol-5-yl)(methyl)carbamic acid</p> |
| S20 |  <p>3-(3-((3-amino-6-methoxy-2-oxo-2H-chromen-7-yl)oxy)propoxy)-5-methylisoxazole-4-carboxylic acid</p>                  |

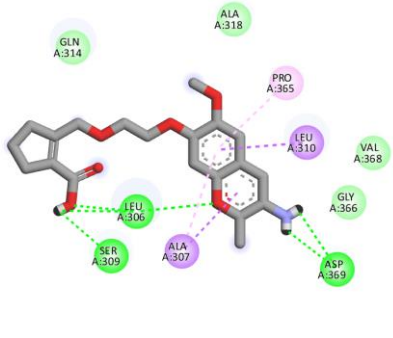
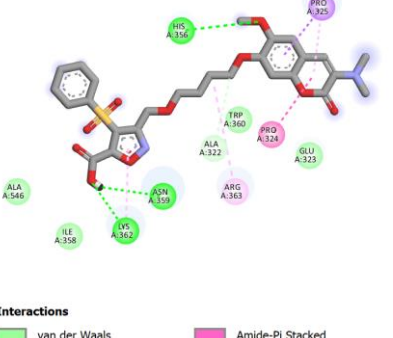
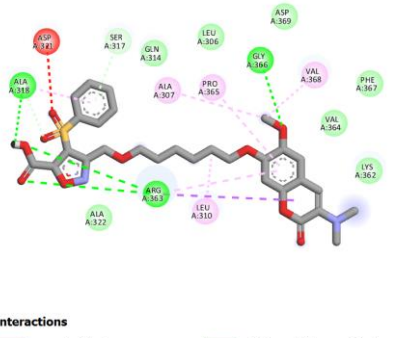


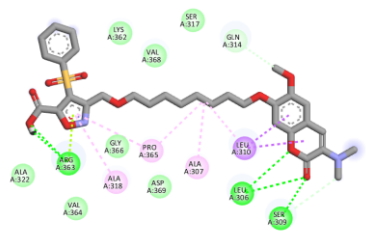
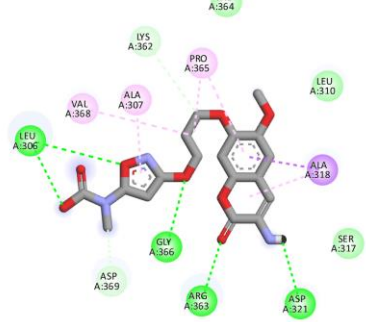
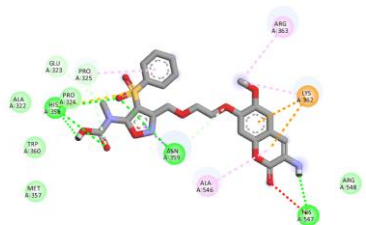
### Lampiran 3 Visualisasi Interaksi hasil Penambatan Molekul ligan uji

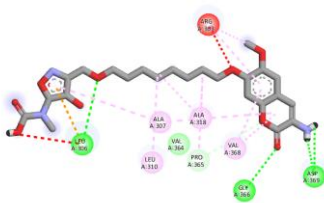
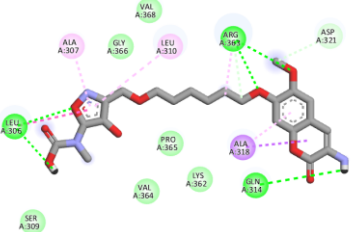
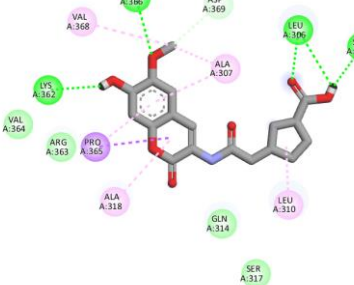
| Kode Ligan  | VISUALISASI 2D                                                                                                                                                                                                                                                                                                              | Residu Asam Amino                                                                                                                                                                                          |
|-------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Ligan Alami |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Alkyl</li> <li>Pi-Alkyl</li> </ul>                                                                           | <p>THR347 LEU384 ALA350<br/> LEU349 ARG394 GLU353<br/> LEU387 LEU391 MET388<br/> LEU346 PHE404 LEU428<br/> MET421 ILE424 GLU419<br/> MET343 GLY420 HIS524<br/> LEU525 TRP383 GLY521 ASP351<br/> LEU354</p> |
| Acuan       |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Carbon Hydrogen Bond</li> <li>Pi-Sigma</li> <li>Pi-Alkyl</li> </ul>                                         | <p>LEU306 SER309 LEU310<br/> GLN314 ALA307 ASP369<br/> GLY366 VAL368 PHE367<br/> LYS362 VAL364 ARG363<br/> PRO365 ALA318</p>                                                                               |
| S1          |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Carbon Hydrogen Bond</li> <li>Unfavorable Acceptor-Acceptor</li> <li>Pi-Sigma</li> <li>Pi-Alkyl</li> </ul> | <p>PHE404 LEU387 LEU391<br/> ARG394 MET388 LEU346<br/> LEU384 ILE424 GLY521 MET421<br/> MET343 GLU419 LEU525<br/> GLY420 HIS524 ALA350 LEU349<br/> GLU353</p>                                              |

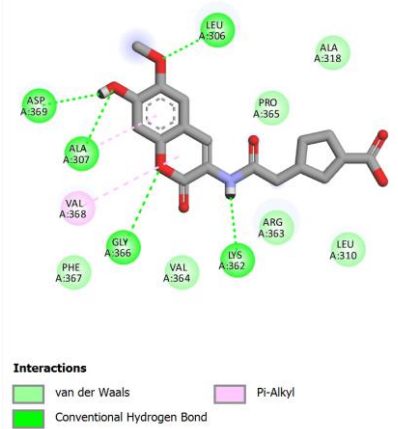
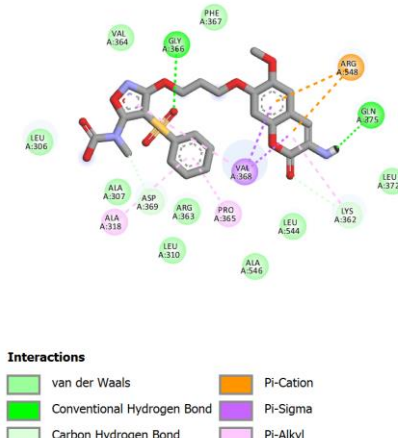
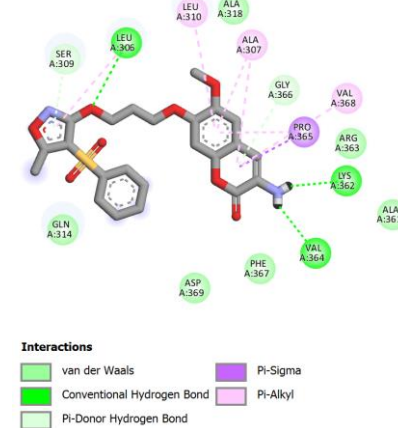
|    |                                                                                                                                                                                                                                                                                                                                          |                                                                                                                                                                                          |
|----|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| S2 |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Carbon Hydrogen Bond</li> <li>Pi-Sigma</li> <li>Pi-Pi T-shaped</li> <li>Pi-Alkyl</li> </ul>                               | <p>MET528 LEU525 THR347<br/>MET343 LEU384 GLY521<br/>MET388 LEU428 ARG394<br/>GLU353 LEU349 LEU346<br/>LEU391 LEU387 LEU404<br/>ALA350 ILE424 TRP383</p>                                 |
| S3 |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Carbon Hydrogen Bond</li> <li>Unfavorable Donor-Donor</li> <li>Pi-Anion</li> <li>Pi-Sigma</li> <li>Pi-Alkyl</li> </ul>    | <p>GLY521 ILE424 LEU428 MET388<br/>PHE404 LEU346 THR347<br/>LEU391 LEU349 ARG394<br/>LEU387 GLU353 ALA350<br/>TRP383 LEU384 MET343 HIS524<br/>GLU419 GLY420 MET421<br/>LEU525</p>        |
| S4 |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Carbon Hydrogen Bond</li> <li>Pi-Anion</li> <li>Pi-Sigma</li> <li>Pi-Sulfur</li> <li>Alkyl</li> <li>Pi-Alkyl</li> </ul> | <p>LEU349 PHE404 ILE42 MET388<br/>LEU384 MET421 LEU428<br/>LEU391 ALA350 LEU346<br/>MET343 THR347 TRP383<br/>LEU525 LEU356 LEU354<br/>LEU539 MET 528 ASP351<br/>LEU387 ARG394 GLU353</p> |
| S5 |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Pi-Anion</li> <li>Alkyl</li> <li>Pi-Alkyl</li> </ul>                                                                    | <p>GLN314 LEU310 ALA307<br/>GLY366 PRO365 ASP369<br/>ARG363 ALA318 SER309<br/>LEU306</p>                                                                                                 |

|    |                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                |
|----|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| S6 |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Pi-Sigma</li> <li>Alkyl</li> <li>Pi-Alkyl</li> </ul>                                                                                                 | <p>SER309 LEU306 GLN314<br/>         LEU310 ALA307 VAL368<br/>         ASP369 GLY366 PRO365<br/>         ALA318</p>                                                                            |
| S7 |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Carbon Hydrogen Bond</li> <li>Unfavorable Donor-Donor</li> <li>Pi-Donor Hydrogen Bond</li> <li>Pi-Sigma</li> <li>Alkyl</li> <li>Pi-Alkyl</li> </ul> | <p>LEU310 LEU306 ASP369<br/>         ALA307 GLY366 PHE367<br/>         PRO365 VAL364 LYS362<br/>         VAL368 ARG548 ARG363<br/>         ALA318</p>                                          |
| S8 |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Unfavorable Acceptor-Acceptor</li> <li>Pi-Sigma</li> <li>Alkyl</li> <li>Pi-Alkyl</li> </ul>                                                        | <p>LEU306 SER309 GLN314 SER317<br/>         ARG363 ASP321 GLY366<br/>         VAL368 PHE367 ASP369<br/>         VAL364 LYS362 ALA322<br/>         PRO365 ALA318 LEU310<br/>         ALA307</p> |

|     |                                                                                                                                                                                                                                                                                                                                                                            |                                                                                                                             |
|-----|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------|
| S9  |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Pi-Sigma</li> <li>Pi-Alkyl</li> </ul>                                                                                                                       | SER309 LEU306 ALA307 ASP369<br>GLY366 VAL368 LEU310<br>PRO365 ALA318 GLN314                                                 |
| S10 |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Carbon Hydrogen Bond</li> <li>Pi-Sigma</li> <li>Amide-Pi Stacked</li> <li>Alkyl</li> <li>Pi-Alkyl</li> </ul>                                               | ALA546 ILE358 LYS362 ASN359<br>ALA322 ARG363 TRP369<br>PRO324 GLU323 PRO325 HIS356                                          |
| S11 |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Carbon Hydrogen Bond</li> <li>Unfavorable Acceptor-Acceptor</li> <li>Pi-Donor Hydrogen Bond</li> <li>Pi-Sigma</li> <li>Alkyl</li> <li>Pi-Alkyl</li> </ul> | ALA318 ALA322 ARG363<br>LEU310 LYS362 VAL364<br>PHE367 VAL368 ASP369<br>GLY366 PRO365 LEU 306<br>ALA307 GLN314 SER317 ASP21 |

|     |                                                                                                                                                                                                                                                                                                                                                                                  |                                                                                                                                                                     |
|-----|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| S12 |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Carbon Hydrogen Bond</li> <li>Pi-Sigma</li> <li>Pi-Lone Pair</li> <li>Alkyl</li> <li>Pi-Alkyl</li> </ul>                                                          | <p>ALA322 ARG363 VAL364<br/>         ALA318 GLY366 PRO365<br/>         ASP369 ALA307 LEU310<br/>         LEU306 SER309 GLN314 SER317<br/>         VAL368 LYS362</p> |
| S13 |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Carbon Hydrogen Bond</li> <li>Pi-Sigma</li> <li>Alkyl</li> <li>Pi-Alkyl</li> </ul>                                                                               | <p>LEU306 ASP369 GLY366<br/>         ARG363 ASP321 SER317<br/>         ALA318 LEU310 VAL364<br/>         PRO365 LYS362 ALA307<br/>         VAL368</p>               |
| S14 |  <p><b>Interactions</b></p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Carbon Hydrogen Bond</li> <li>Unfavorable Acceptor-Acceptor</li> <li>Pi-Cation</li> <li>Pi-Sigma</li> <li>Pi-Sulfur</li> <li>Alkyl</li> <li>Pi-Alkyl</li> </ul> | <p>ALA322 TRP360 MET357<br/>         ASN359 ALA546 HIS547<br/>         ARG548 LYS362 ARG363<br/>         PRO325 GLU323 PRO324 HIS356</p>                            |

|                                                                 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                    |                                                                  |                                                                 |                                                      |                                                           |                                              |                                                                                                               |                                              |                                                                                                               |
|-----------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------|------------------------------------------------------------------|-----------------------------------------------------------------|------------------------------------------------------|-----------------------------------------------------------|----------------------------------------------|---------------------------------------------------------------------------------------------------------------|----------------------------------------------|---------------------------------------------------------------------------------------------------------------|
| S15                                                             |  <p><b>Interactions</b></p> <table><tr><td><span style="color: green;">■</span> van der Waals</td><td><span style="color: red;">■</span> Unfavorable Acceptor-Acceptor</td></tr><tr><td><span style="color: green;">■</span> Conventional Hydrogen Bond</td><td><span style="color: orange;">■</span> Pi-Cation</td></tr><tr><td><span style="color: green;">■</span> Carbon Hydrogen Bond</td><td><span style="color: pink;">■</span> Alkyl</td></tr><tr><td><span style="color: red;">■</span> Unfavorable Donor-Donor</td><td><span style="color: pink;">■</span> Pi-Alkyl</td></tr></table> | <span style="color: green;">■</span> van der Waals | <span style="color: red;">■</span> Unfavorable Acceptor-Acceptor | <span style="color: green;">■</span> Conventional Hydrogen Bond | <span style="color: orange;">■</span> Pi-Cation      | <span style="color: green;">■</span> Carbon Hydrogen Bond | <span style="color: pink;">■</span> Alkyl    | <span style="color: red;">■</span> Unfavorable Donor-Donor                                                    | <span style="color: pink;">■</span> Pi-Alkyl | LEU306 LEU310 ALA307<br>VAL364 ALA 318 VAL368<br>GLY366 ASP369 ARG303                                         |
| <span style="color: green;">■</span> van der Waals              | <span style="color: red;">■</span> Unfavorable Acceptor-Acceptor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                    |                                                                  |                                                                 |                                                      |                                                           |                                              |                                                                                                               |                                              |                                                                                                               |
| <span style="color: green;">■</span> Conventional Hydrogen Bond | <span style="color: orange;">■</span> Pi-Cation                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                    |                                                                  |                                                                 |                                                      |                                                           |                                              |                                                                                                               |                                              |                                                                                                               |
| <span style="color: green;">■</span> Carbon Hydrogen Bond       | <span style="color: pink;">■</span> Alkyl                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                    |                                                                  |                                                                 |                                                      |                                                           |                                              |                                                                                                               |                                              |                                                                                                               |
| <span style="color: red;">■</span> Unfavorable Donor-Donor      | <span style="color: pink;">■</span> Pi-Alkyl                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                    |                                                                  |                                                                 |                                                      |                                                           |                                              |                                                                                                               |                                              |                                                                                                               |
| S16                                                             |  <p><b>Interactions</b></p> <table><tr><td><span style="color: green;">■</span> van der Waals</td><td><span style="color: purple;">■</span> Pi-Sigma</td></tr><tr><td><span style="color: green;">■</span> Conventional Hydrogen Bond</td><td><span style="color: pink;">■</span> Amide-Pi Stacked</td></tr><tr><td><span style="color: green;">■</span> Carbon Hydrogen Bond</td><td><span style="color: pink;">■</span> Alkyl</td></tr><tr><td><span style="color: red;">■</span> Unfavorable Donor-Donor</td><td><span style="color: pink;">■</span> Pi-Alkyl</td></tr></table>             | <span style="color: green;">■</span> van der Waals | <span style="color: purple;">■</span> Pi-Sigma                   | <span style="color: green;">■</span> Conventional Hydrogen Bond | <span style="color: pink;">■</span> Amide-Pi Stacked | <span style="color: green;">■</span> Carbon Hydrogen Bond | <span style="color: pink;">■</span> Alkyl    | <span style="color: red;">■</span> Unfavorable Donor-Donor                                                    | <span style="color: pink;">■</span> Pi-Alkyl | LEU306 SER309 VAL364<br>PRO365 LYS362 ALA318<br>GLN314 SER317 ASP321<br>ARG363 LEU310 VAL368<br>GLY366 ALA307 |
| <span style="color: green;">■</span> van der Waals              | <span style="color: purple;">■</span> Pi-Sigma                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                                                    |                                                                  |                                                                 |                                                      |                                                           |                                              |                                                                                                               |                                              |                                                                                                               |
| <span style="color: green;">■</span> Conventional Hydrogen Bond | <span style="color: pink;">■</span> Amide-Pi Stacked                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                                                    |                                                                  |                                                                 |                                                      |                                                           |                                              |                                                                                                               |                                              |                                                                                                               |
| <span style="color: green;">■</span> Carbon Hydrogen Bond       | <span style="color: pink;">■</span> Alkyl                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                    |                                                                  |                                                                 |                                                      |                                                           |                                              |                                                                                                               |                                              |                                                                                                               |
| <span style="color: red;">■</span> Unfavorable Donor-Donor      | <span style="color: pink;">■</span> Pi-Alkyl                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                    |                                                                  |                                                                 |                                                      |                                                           |                                              |                                                                                                               |                                              |                                                                                                               |
| S17                                                             |  <p><b>Interactions</b></p> <table><tr><td><span style="color: green;">■</span> van der Waals</td><td><span style="color: purple;">■</span> Pi-Sigma</td></tr><tr><td><span style="color: green;">■</span> Conventional Hydrogen Bond</td><td><span style="color: pink;">■</span> Alkyl</td></tr><tr><td><span style="color: green;">■</span> Carbon Hydrogen Bond</td><td><span style="color: pink;">■</span> Pi-Alkyl</td></tr></table>                                                                                                                                                     | <span style="color: green;">■</span> van der Waals | <span style="color: purple;">■</span> Pi-Sigma                   | <span style="color: green;">■</span> Conventional Hydrogen Bond | <span style="color: pink;">■</span> Alkyl            | <span style="color: green;">■</span> Carbon Hydrogen Bond | <span style="color: pink;">■</span> Pi-Alkyl | VAL364 ARG363 PRO365<br>ALA318 GLN314 SER317<br>LEU310 SER309 LEU306<br>ALA307 ASP369 GLY366<br>VAL368 LYS362 |                                              |                                                                                                               |
| <span style="color: green;">■</span> van der Waals              | <span style="color: purple;">■</span> Pi-Sigma                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                                                    |                                                                  |                                                                 |                                                      |                                                           |                                              |                                                                                                               |                                              |                                                                                                               |
| <span style="color: green;">■</span> Conventional Hydrogen Bond | <span style="color: pink;">■</span> Alkyl                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                    |                                                                  |                                                                 |                                                      |                                                           |                                              |                                                                                                               |                                              |                                                                                                               |
| <span style="color: green;">■</span> Carbon Hydrogen Bond       | <span style="color: pink;">■</span> Pi-Alkyl                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                    |                                                                  |                                                                 |                                                      |                                                           |                                              |                                                                                                               |                                              |                                                                                                               |

|     |                                                                                                                                                                                                                                                                                                 |                                                                                                                                       |
|-----|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------|
| S18 |  <p><b>Interactions</b></p> <ul style="list-style-type: none"><li>van der Waals</li><li>Conventional Hydrogen Bond</li><li>Pi-Alkyl</li></ul>                                                                  | ASP369 ALA307 VAL368<br>PHE367 GLY366 VAL364<br>LYS362 ARG363 LEU310<br>ALA318 PRO365 LEU306                                          |
| S19 |  <p><b>Interactions</b></p> <ul style="list-style-type: none"><li>van der Waals</li><li>Conventional Hydrogen Bond</li><li>Carbon Hydrogen Bond</li><li>Pi-Cation</li><li>Pi-Sigma</li><li>Pi-Alkyl</li></ul> | LEU306 ALA307 ALA318<br>ASP369 ARG363 LEU310<br>PRO365 ALA546 VAL368<br>LEU544 LYS362 LEU372<br>GLN375 ARG548 PHE367<br>GLY366 VAL364 |
| S20 |  <p><b>Interactions</b></p> <ul style="list-style-type: none"><li>van der Waals</li><li>Conventional Hydrogen Bond</li><li>Pi-Donor Hydrogen Bond</li><li>Pi-Sigma</li><li>Pi-Alkyl</li></ul>                | GLN314 ASP369 PHE367<br>VAL364 ALA361 LYS362<br>ARG363 VAL368 PRO365<br>GLY366 ALA307 ALA318<br>LEU310 LEU306 SER309                  |

## Lampiran 4. Hasil Cek Plagiarisme

|                                         |                                                                                                                                                                                                                                                                     |              |                |
|-----------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------|----------------|
| Skripsi_SITI AL HUMAIROH 211FF03132.pdf |                                                                                                                                                                                                                                                                     |              |                |
| ORIGINALITY REPORT                      |                                                                                                                                                                                                                                                                     |              |                |
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| 1                                       | text-id.123dok.com<br>Internet Source                                                                                                                                                                                                                               | 3%           |                |
| 2                                       | Zhixian Shi, Na Li, Cheng Chen, Yujin Wang, Zhichao Lei, Li Chen, Jianbo Sun. "Novel NO-releasing scopoletin derivatives induce cell death via mitochondrial apoptosis pathway and cell cycle arrest", European Journal of Medicinal Chemistry, 2020<br>Publication | 1%           |                |
| 3                                       | positori.uin-alauddin.ac.id<br>Internet Source                                                                                                                                                                                                                      | 1%           |                |
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## Lampiran 5. Kartu Bimbingan

|               |                                    |                   |                                                                                      |
|---------------|------------------------------------|-------------------|--------------------------------------------------------------------------------------|
| NIM           | 211FF03132                         | Nama Mahasiswa    | SITI AL HUMAIROH                                                                     |
| Program Studi | SI Farmasi                         | Jenis TA          | Skripsi                                                                              |
| Periode Mulai | 2024 Ganjil                        | SKS Lulus         | 149 SKS                                                                              |
| Tgl. Mulai    | 4 Maret 2025                       | Judul Tugas Akhir | Hubungan Kuantitatif Struktur Aktifitas Turunan Skopoletin Sebagai Antiproliferative |
| Tahap         | Sidang Akhir/ Komprehensif (Ujian) | Status            | Selesai                                                                              |

| No | Tanggal          | Dosen Pembimbing                     | Topik                                                                  | Disetujui | Aksi                                                                                                                                                                        |
|----|------------------|--------------------------------------|------------------------------------------------------------------------|-----------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1  | 13 Maret 2025    | Dr. apt. Fauzan Zein Muttaqin, M.Si. | pelatihan penelitian                                                   |           |       |
| 1  | 21 Februari 2025 | apt. Purwaniati, M.Si.               | Prosedur penelitian secara lengkap                                     | ✓         |       |
| 2  | 3 Mei 2025       | Dr. apt. Fauzan Zein Muttaqin, M.Si. | Presentasi                                                             |           |       |
| 2  | 6 Mei 2025       | apt. Purwaniati, M.Si.               | Bimbingan hasil Optimasi                                               | ✓         |       |
| 3  | 5 Mei 2025       | Dr. apt. Fauzan Zein Muttaqin, M.Si. | pemilihan dan kombinasi deskriptor                                     |           |       |
| 3  | 16 Mei 2025      | apt. Purwaniati, M.Si.               | Bimbingan hasil perhitungan deskriptor dan pembuatan model persamaan   | ✓         |       |
| 4  | 27 Mei 2025      | Dr. apt. Fauzan Zein Muttaqin, M.Si. | Bimbingan hasil perhitungan deskriptor dan model persamaan yang dibuat |           |       |
| 4  | 13 Juni 2025     | apt. Purwaniati, M.Si.               | Bimbingan Hasil desain senyawa baru                                    | ✓         |       |
| 5  | 6 Mei 2025       | Dr. apt. Fauzan Zein Muttaqin, M.Si. | bimbingan hasil perhitungan deskriptor                                 |           |       |
| 5  | 30 Juni 2025     | apt. Purwaniati, M.Si.               | laporan hasil docking                                                  | ✓         |       |
| 6  | 7 Juli 2025      | apt. Purwaniati, M.Si.               | laporan draft skripsi                                                  | ✓         |       |
| 6  | 16 Mei 2025      | Dr. apt. Fauzan Zein Muttaqin, M.Si. | pembuatan model HKSA                                                   |           |       |
| 7  | 10 Juli 2025     | apt. Purwaniati, M.Si.               | revisi draft skripsi                                                   | ✓         |     |
| 7  | 13 Juni 2025     | Dr. apt. Fauzan Zein Muttaqin, M.Si. | laporan hasil desain senyawa turunan baru                              |           |   |
| 8  | 1 Juli 2025      | apt. Purwaniati, M.Si.               | membahas hasil penambatan molekul                                      | ✓         |   |
| 8  | 11 Juli 2025     | Dr. apt. Fauzan Zein Muttaqin, M.Si. | laporan hasil dan pembahasan penelitian yang telah dilakukan           |           |   |

**Lampiran 6. Daftar Riwayat Hidup****RIWAYAT HIDUP***Curriculum Vitae***Data Pribadi/ Personal Details**

Nama / Name : Siti Al Humairoh

Tanggal Lahir / Place, Date of Birth : Bandung 12 Juni 2002

Alamat / Address : Kp. Cijolang Rt04/Rw 09 Desa. Ciaro,  
Kec. Nagreg, Kab. Bandung

Kode Pos / Postal Code : 40215

Jenis Kelamin / Gender : Perempuan

Negara / Nationality : Indonesia

Agama / Religion : Islam

**Riwayat Pendidikan**

| <b>Periode</b> | <b>Sekolah/Institusi/Universitas</b>   | <b>Jenjang</b> |
|----------------|----------------------------------------|----------------|
| 2008-2009      | TK Al-Munawaroh                        | TK             |
| 2009-2015      | Komplek SDN Ciaro 2                    | SD             |
| 2015-2018      | SMP IT Daarul Anba Tasikmalaya         | SMP            |
| 2018-2021      | SMK Kesehatan Bhakti Kencana Limbangan | SMK            |
| 2021-2025      | Universitas Bhakti Kencana Bandung     | S1             |