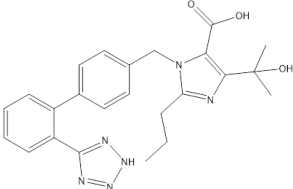
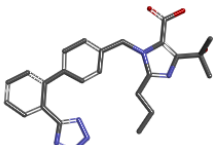
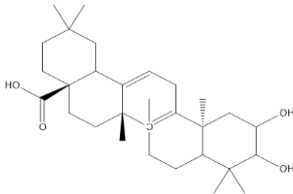
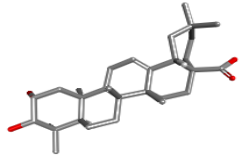
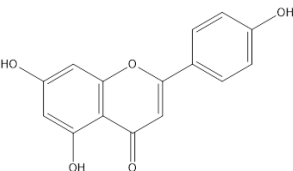
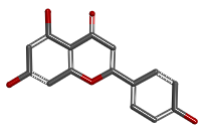
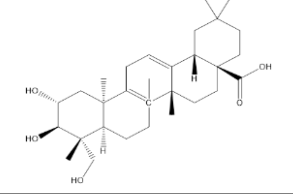
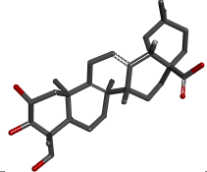
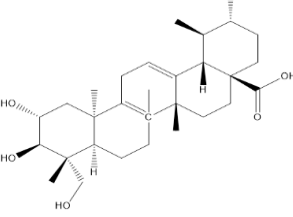
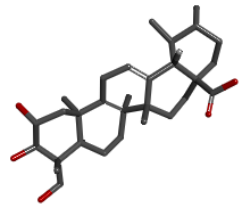
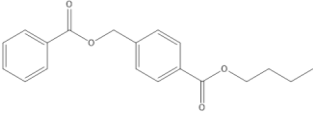
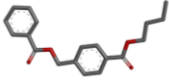
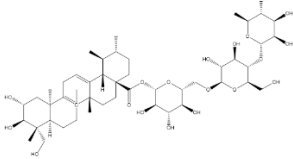
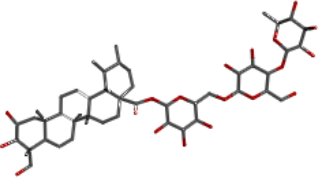
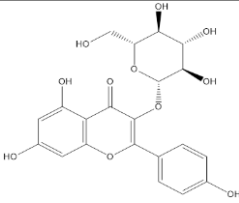
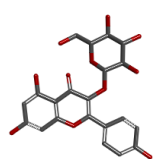
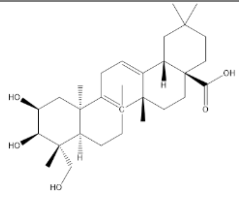
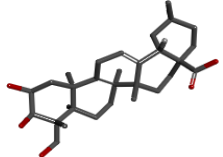
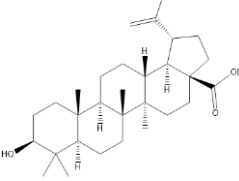
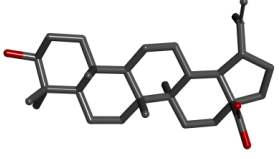
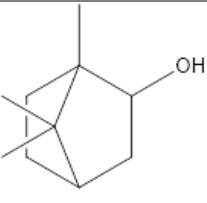
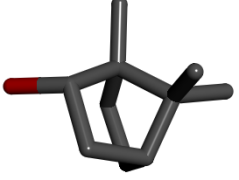
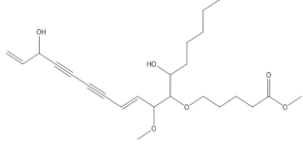
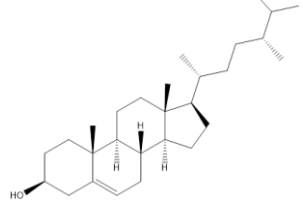
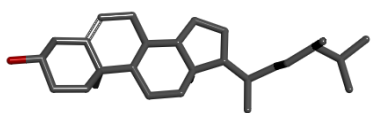
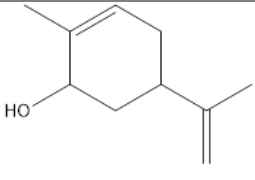
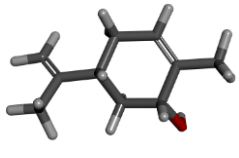
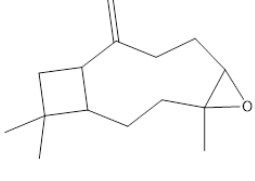
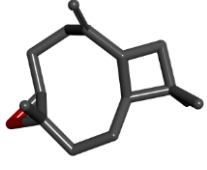
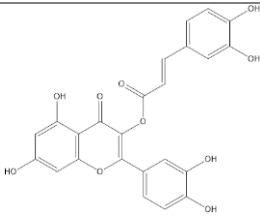
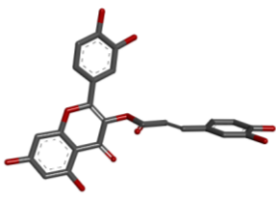
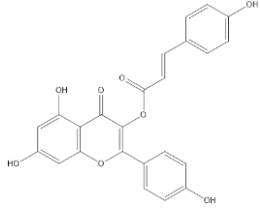
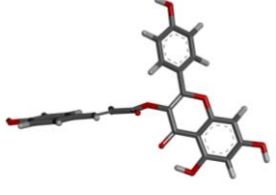
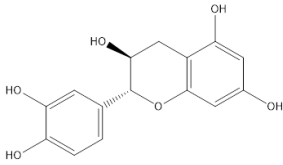
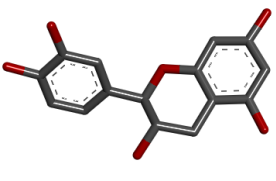
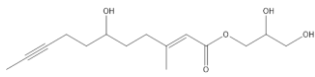
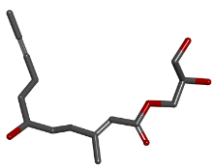
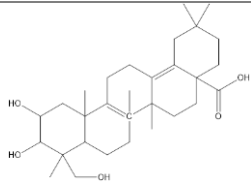
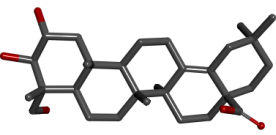
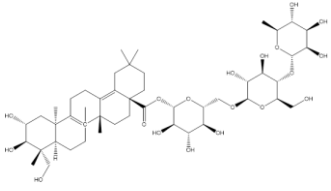
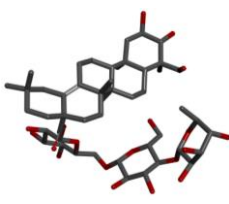
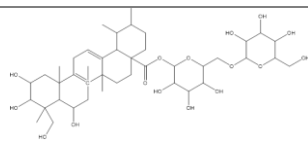
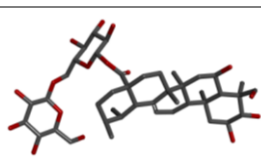
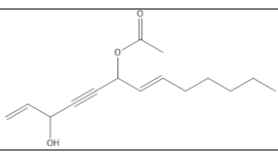
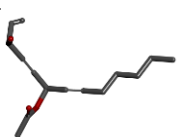
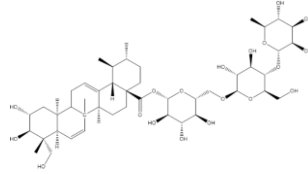
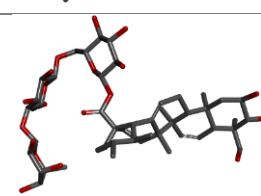


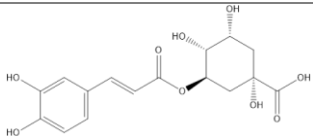
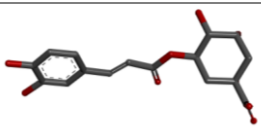
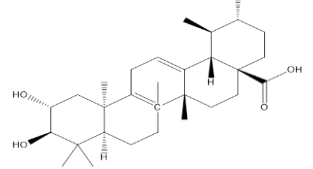
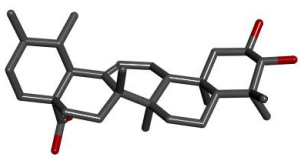
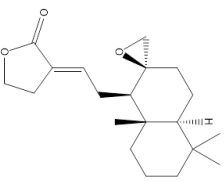
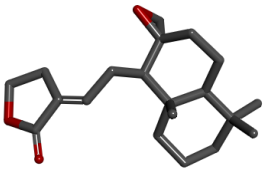
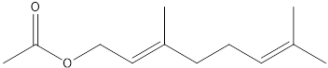
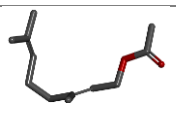
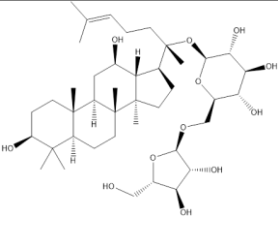
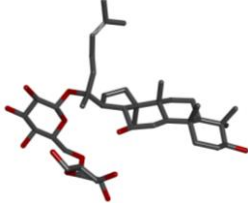
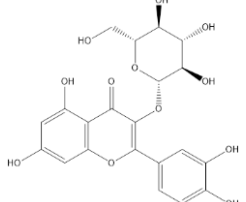
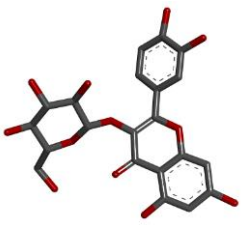
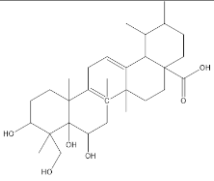
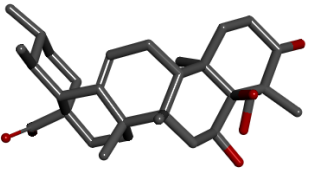
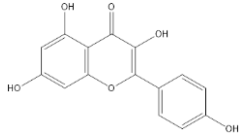
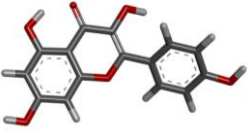
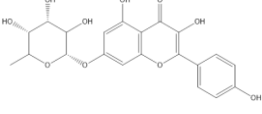
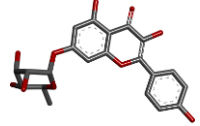
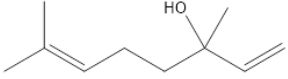
## LAMPIRAN

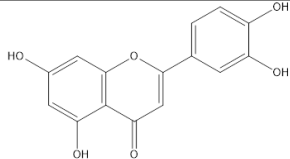
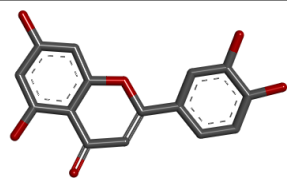
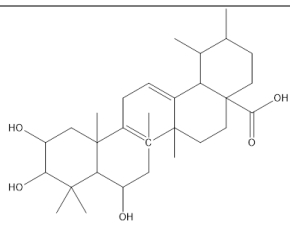
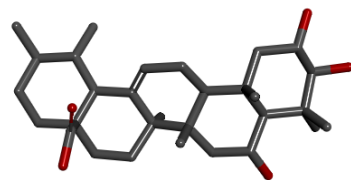
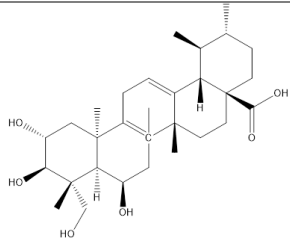
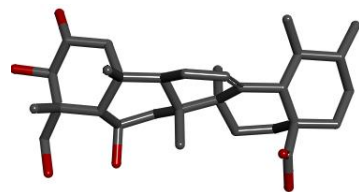
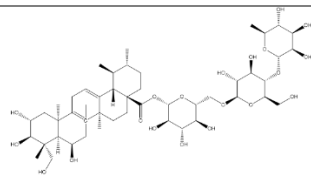
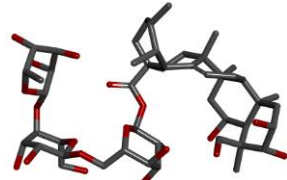
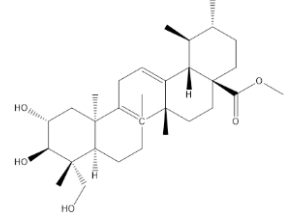
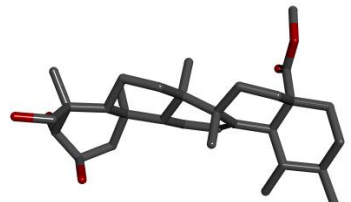
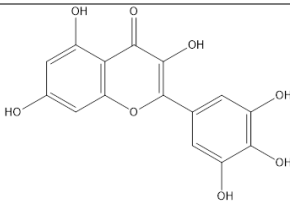
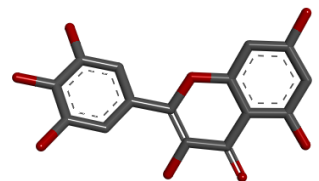
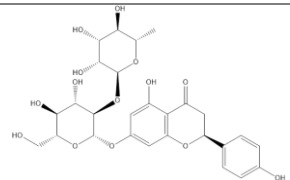
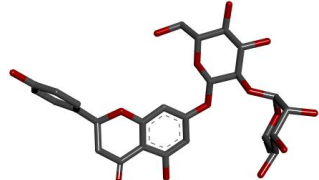
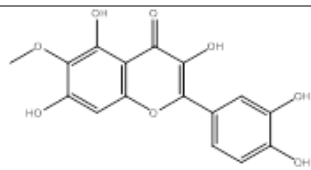
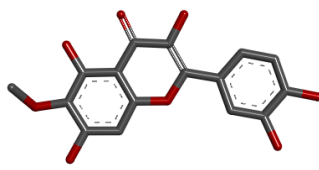
## Lampiran 1 Daftar Senyawa Uji yang Digunakan

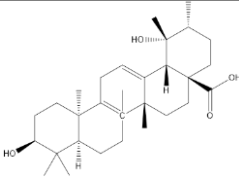
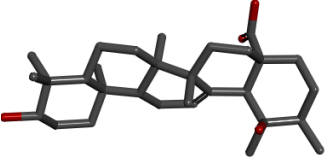
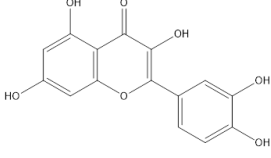
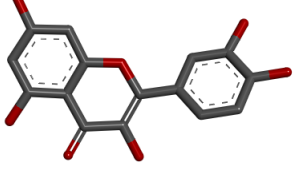
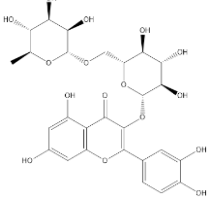
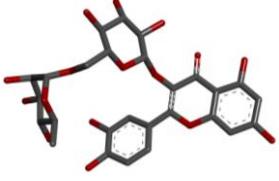
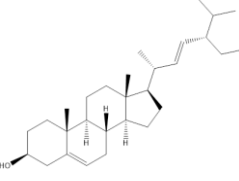
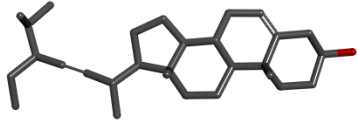
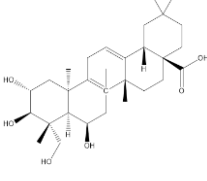
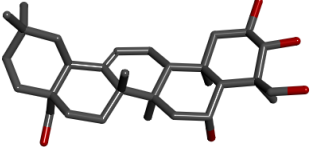
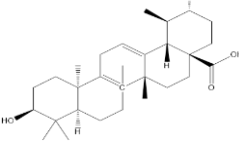
| Kode Ligan | Rumus Kimia          | Struktur 2D                                                                         | Struktur 3D                                                                           |
|------------|----------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| Olmesartan | $C_{30}H_{53}N_3O_6$ |    |    |
| L1         | $C_{30}H_{48}O_4$    |    |    |
| L2         | $C_{15}H_{10}O_5$    |   |   |
| L3         | $C_{30}H_{48}O_5$    |  |  |
| L4         | $C_{30}H_{48}O_5$    |  |  |
| L5         | $C_{19}H_{20}O_4$    |  |  |
| L6         | $C_{48}H_{78}O_{19}$ |  |  |

|     |                      |                                                                                     |                                                                                       |
|-----|----------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| L7  | $C_{21}H_{20}O_{11}$ |    |    |
| L8  | $C_{30}H_{48}O_5$    |    |    |
| L9  | $C_{30}H_{48}O_3$    |    |    |
| L10 | $C_{10}H_{18}O$      |   |   |
| L11 | $C_{24}H_{36}O_6$    |  |  |
| L12 | $C_{28}H_{48}O$      |  |  |
| L13 | $C_{10}H_{16}O$      |  |  |
| L14 | $C_{15}H_{24}O$      |  |  |

|     |                      |                                                                                     |                                                                                       |
|-----|----------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| L15 | $C_{24}H_{16}O_{10}$ |    |    |
| L16 | $C_{24}H_{16}O_8$    |    |    |
| L17 | $C_{15}H_{14}O_6$    |    |    |
| L18 | $C_{15}H_{24}O_5$    |   |   |
| L19 | $C_{30}H_{48}O_5$    |  |  |
| L20 | $C_{48}H_{78}O_{19}$ |  |  |
| L21 | $C_{42}H_{68}O_{16}$ |  |  |
| L22 | $C_{15}H_{22}O_3$    |  |  |
| L23 | $C_{48}H_{76}O_{19}$ |  |  |

|     |                      |                                                                                     |                                                                                       |
|-----|----------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| L24 | $C_{16}H_{18}O_9$    |    |    |
| L25 | $C_{30}H_{48}O_4$    |    |    |
| L26 | $C_{20}H_{30}O_3$    |    |    |
| L27 | $C_{12}H_{20}O_2$    |    |    |
| L28 | $C_{41}H_{70}O_{12}$ |   |   |
| L29 | $C_{21}H_{20}O_{12}$ |  |  |
| L30 | $C_{30}H_{48}O_6$    |  |  |
| L31 | $C_{15}H_{10}O_6$    |  |  |
| L32 | $C_{21}H_{20}O_{10}$ |  |  |
| L33 | $C_{10}H_{18}O$      |  |  |

|     |                      |                                                                                     |                                                                                       |
|-----|----------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| L34 | $C_{15}H_{10}O_6$    |    |    |
| L35 | $C_{30}H_{48}O_5$    |    |    |
| L36 | $C_{30}H_{48}O_6$    |    |    |
| L37 | $C_{48}H_{78}O_{20}$ |   |   |
| L38 | $C_{31}H_{50}O_5$    |  |  |
| L39 | $C_{15}H_{10}O_8$    |  |  |
| L40 | $C_{27}H_{32}O_{14}$ |  |  |
| L41 | $C_{16}H_{12}O_8$    |  |  |

|     |                      |                                                                                     |                                                                                       |
|-----|----------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| L42 | $C_{30}H_{48}O_4$    |    |    |
| L43 | $C_{15}H_{10}O_7$    |    |    |
| L44 | $C_{27}H_{30}O_{16}$ |    |    |
| L45 | $C_{29}H_{48}O$      |   |   |
| L46 | $C_{30}H_{48}O_6$    |  |  |
| L47 | $C_{30}H_{48}O_3$    |  |  |

## Lampiran 2 Interaksi Hasil Penambatan Molekul Ligan Uji

| Kode Ligan | Interaksi                                                                                                                                             | Jarak Ikatan | Residu asam amino                                                                                                                                |
|------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|--------------|--------------------------------------------------------------------------------------------------------------------------------------------------|
| L1         | Ikatan Hidrogen                                                                                                                                       |              |                                                                                                                                                  |
|            | NH1 - Arg167:O                                                                                                                                        | 3,0152       |                                                                                                                                                  |
|            | NH2 - Arg167:O                                                                                                                                        | 2,98735      |                                                                                                                                                  |
|            | H - Asp263:O                                                                                                                                          | 1,86536      | Gln15, Asp263, Arg167, Leu3, Ser5, Tyr184, Phe A:182, Ala 181, Cys180, Ser105, Tyr87, Trp84, Ile288, Tyr35, Tyr92, Pro285, Thr88, Met284, Gln267 |
| L2         | Ikatan Hidrofobik                                                                                                                                     |              |                                                                                                                                                  |
|            | • $\pi$ - Alkyl: Leu3, Ser5, Tyr184, Phe A:182, Ala181, Cys180, Ser105                                                                                |              |                                                                                                                                                  |
|            | Interaksi Van der Waals                                                                                                                               |              |                                                                                                                                                  |
|            | Tyr87, Trp84, Ile288, Tyr35, Tyr92, Pro285, Thr88, Met284, Gln267                                                                                     |              |                                                                                                                                                  |
| L3         | Ikatan Hidrogen                                                                                                                                       |              |                                                                                                                                                  |
|            | NH1 - Arg167:O3                                                                                                                                       | 2,95387      |                                                                                                                                                  |
|            | H30 - Pro285:O                                                                                                                                        | 2,10048      |                                                                                                                                                  |
|            | H28 - Cys180:O                                                                                                                                        | 1,99665      | Ile286, Cys289, Thr88, Tyr35, Trp84, Arg67, Cys180, Tyr87, Tyr92, Val79, Ile31, Ile288, Val179                                                   |
| L4         | Ikatan Hidrofobik                                                                                                                                     |              |                                                                                                                                                  |
|            | • $\pi$ - Alkyl: Ile31, Ile288, Val179                                                                                                                |              |                                                                                                                                                  |
|            | • $\pi$ - $\pi$ T-Shaped: Tyr92, Val179                                                                                                               |              |                                                                                                                                                  |
|            | • $\pi$ - donor Hydrogen bond: Tyr87                                                                                                                  |              |                                                                                                                                                  |
| L5         | Interaksi Van der Waals                                                                                                                               |              |                                                                                                                                                  |
|            | Ile286, Cys89, Thr88, Tyr35, Trp84                                                                                                                    |              |                                                                                                                                                  |
|            | Ikatan Hidrogen                                                                                                                                       |              |                                                                                                                                                  |
|            | NH2 - Arg167:O5                                                                                                                                       | 2,60357      |                                                                                                                                                  |
| L6         | H74 - Ala21:O                                                                                                                                         | 2,07938      |                                                                                                                                                  |
|            | Ikatan Hidrofobik                                                                                                                                     |              |                                                                                                                                                  |
|            | • $\pi$ - Alkyl: Ile28, Tyr5, Trp84, Pro285, Tyr85, Tyr92                                                                                             |              |                                                                                                                                                  |
|            | • $\pi$ - Sigma: Trp84                                                                                                                                |              |                                                                                                                                                  |
| L7         | Interaksi Van der Waals                                                                                                                               |              |                                                                                                                                                  |
|            | Val108, Tyr35, Ile288, Met284, Pro285, Thr282, Asp281, Ile27, Arg23, Gly22, Tyr92, Val179, Tyr87, Arg167, Ala121, Trp84, Ile28, Pro285, Tyr85, Tyr 92 |              |                                                                                                                                                  |
|            | Ikatan Hidrogen                                                                                                                                       |              |                                                                                                                                                  |
|            | N - Gln267:O                                                                                                                                          | 2,84661      |                                                                                                                                                  |
| L8         | H - Tyr184: OH                                                                                                                                        | 1,8891       |                                                                                                                                                  |
|            | H - Phe182:O                                                                                                                                          | 2,77139      |                                                                                                                                                  |
|            | H - Thr88:O                                                                                                                                           | 2,00778      |                                                                                                                                                  |
|            | Ikatan Hidrofobik                                                                                                                                     |              |                                                                                                                                                  |
| L9         | • $\pi$ - Alkyl: Ala181, Ile288, Val108                                                                                                               |              |                                                                                                                                                  |
|            | • $\pi$ -Sigma: Trp84                                                                                                                                 |              |                                                                                                                                                  |
|            | Interaksi Van der Waals                                                                                                                               |              |                                                                                                                                                  |
|            | Leu3, Val179, Cys180, Arg167, Ser109, Tyr99, Tyr92, Tyr87, Met284, Pro289, Asp263, Phe182, Tyr184, Gln267, Thr88, Trp84, Ala181, Ile288, Val108       |              |                                                                                                                                                  |
| L10        | Ikatan Hidrogen                                                                                                                                       |              |                                                                                                                                                  |
|            | OH - Tyr35:O                                                                                                                                          | 2,9532       |                                                                                                                                                  |
|            | NH1 - Arg167:O                                                                                                                                        | 2,96678      |                                                                                                                                                  |
|            |                                                                                                                                                       |              | Thr88, Tyr92, Pro285, Cys289, Cys180, Arg167,                                                                                                    |

|    |                                                                                                                                                                                                                                                              |         |                               |                                           |
|----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------------------------------|-------------------------------------------|
|    | Ikatan Hidrofobik                                                                                                                                                                                                                                            |         |                               | Tyr35, Ile288, Tyr87, Trp84, Val81, Ile38 |
|    | <ul style="list-style-type: none"> <li>• <math>\pi</math> - Alkyl: Val81, Ile38</li> <li>• <math>\pi</math> - Sigma: Ile288</li> <li>• <math>\pi</math> - <math>\pi</math> Stacked dan <math>\pi</math> - <math>\pi</math> T-Shaped: Tyr87, Trp84</li> </ul> |         |                               |                                           |
|    | Ikatan Van der Waals                                                                                                                                                                                                                                         |         |                               |                                           |
|    | Thr88, Tyr92, Pro285, Cys289, Cys180                                                                                                                                                                                                                         |         |                               |                                           |
| L6 | Ikatan Hidrogen                                                                                                                                                                                                                                              |         |                               |                                           |
|    | O - Thr88:O                                                                                                                                                                                                                                                  | 3,13695 |                               |                                           |
|    | OH - Tyr113:O                                                                                                                                                                                                                                                | 2,77209 |                               |                                           |
|    | N - Ala163: O                                                                                                                                                                                                                                                | 2,58726 |                               |                                           |
|    | N - Lys199:O                                                                                                                                                                                                                                                 | 2,84569 | Gln267, Met284, Tyr87,        |                                           |
|    | H - Ala159:O                                                                                                                                                                                                                                                 | 2,36019 | Tyr92, Pro285, Ile31, Val108, |                                           |
|    | H - Tyr35:OH                                                                                                                                                                                                                                                 | 2,4064  | Ser105, Phe182, Ser109,       |                                           |
|    | H - AsP263:O2                                                                                                                                                                                                                                                | 2,12987 | Ala106, Ser160, Pro162,       |                                           |
|    | H - Thr88:OG1                                                                                                                                                                                                                                                | 1,94764 | Arg167, Ile288, Ala181,       |                                           |
|    | Ikatan Hidrofobik                                                                                                                                                                                                                                            |         | Cys180, Tyr292, His256,       |                                           |
|    | <ul style="list-style-type: none"> <li>• <math>\pi</math> - Alkyl: Pro162, Phe82, Ile288, Val108, Trp A84</li> <li>• <math>\pi</math> - Sigma: TRP A:84</li> </ul>                                                                                           |         | Val179, Gln15, Ala21          |                                           |
|    | Interaksi Van der Waals                                                                                                                                                                                                                                      |         | Asp281, Asp263, Thr88,        |                                           |
|    | Gln267, Met284, Tyr87, Tyr92, Pro285, Ile31, Val108, Ser105, Phe182, Ser109, Ala106, Ser160, Pro162, Arg167, Ile288, Ala181, Cys180, Tyr292, His256, Val179, Gln15, Ala21, Asp281                                                                            |         | Tyr35, Ala163, Ala159,        |                                           |
|    |                                                                                                                                                                                                                                                              |         | Tyr113, Lys199, Trp84,        |                                           |
|    |                                                                                                                                                                                                                                                              |         | Pro162, Phe82, Ile288,        |                                           |
|    |                                                                                                                                                                                                                                                              |         | Val108, Trp84                 |                                           |
| L7 | Ikatan Hidrogen                                                                                                                                                                                                                                              |         |                               |                                           |
|    | NH1 - Arg167: O                                                                                                                                                                                                                                              | 3,03026 |                               |                                           |
|    | NH2 - Arg167: O                                                                                                                                                                                                                                              | 2,95486 |                               |                                           |
|    | N - Phe182:O                                                                                                                                                                                                                                                 | 2,85927 |                               |                                           |
|    | H - Tyr184:OH                                                                                                                                                                                                                                                | 2,29853 |                               |                                           |
|    | H - Cys180:O                                                                                                                                                                                                                                                 | 2,14112 | Trp84, Tyr35, Val108, Ile288, |                                           |
|    | Ikatan Hidrofobik                                                                                                                                                                                                                                            |         | Pro285, Arg167, Cys180,       |                                           |
|    | <ul style="list-style-type: none"> <li>• <math>\pi</math> - Alkyl: Ile31, Ile288, Val179</li> <li>• <math>\pi</math> - <math>\pi</math> T-Shared: Tyr92</li> </ul>                                                                                           |         | Ala181, Tyr87, Tyr92, Ile31,  |                                           |
|    | Interaksi Van der Waals                                                                                                                                                                                                                                      |         | Ile288, Val179                |                                           |
|    | Trp84, Tyr35, Val108, Ile288                                                                                                                                                                                                                                 |         |                               |                                           |
| L8 | Ikatan Hidrogen                                                                                                                                                                                                                                              |         |                               |                                           |
|    | OH - Tyr92: O                                                                                                                                                                                                                                                | 3,04116 |                               |                                           |
|    | H - Thr88: O                                                                                                                                                                                                                                                 | 2,21364 |                               |                                           |
|    | Ikatan Hidrofobik                                                                                                                                                                                                                                            |         | Ile31, Tyr35, Trp84, Trp87,   |                                           |
|    | <ul style="list-style-type: none"> <li>• <math>\pi</math> - Alkyl: Trp253, Leu112, His256, Ile288, Met284, Pro285</li> </ul>                                                                                                                                 |         | Val108, Arg167, Ser105,       |                                           |
|    | Interaksi Van der Waals                                                                                                                                                                                                                                      |         | Ser109, Trp253, Leu112,       |                                           |
|    | Ile31, Tyr35, Trp84, Trp87, Val108, Arg167, Ser105, Ser109                                                                                                                                                                                                   |         | His256, Ile288, Met284,       |                                           |
|    |                                                                                                                                                                                                                                                              |         | Pro285, Thr88, Tyr92          |                                           |
|    |                                                                                                                                                                                                                                                              |         |                               |                                           |
|    |                                                                                                                                                                                                                                                              |         |                               |                                           |
| L9 | Ikatan Hidrogen                                                                                                                                                                                                                                              |         |                               |                                           |
|    | O - Thr88:O                                                                                                                                                                                                                                                  | 2,82621 | Ile31, Ile228, Arg167,        |                                           |
|    | N - Phe182:O                                                                                                                                                                                                                                                 | 2,8102  | Tyr184, Cys180, Ala181,       |                                           |
|    | Ikatan Hidrofobik                                                                                                                                                                                                                                            |         | Gln267, Gln15, Asp281,        |                                           |
|    | <ul style="list-style-type: none"> <li>• <math>\pi</math> - Alkyl: Tyr35, Trp84, Pro285, Tyr87,</li> </ul>                                                                                                                                                   |         | Asp263, Thr88, Phe182,        |                                           |
|    |                                                                                                                                                                                                                                                              |         | Tyr92, Tyr35, Trp84, Pro285,  |                                           |
|    |                                                                                                                                                                                                                                                              |         | Tyr87, Met284                 |                                           |
|    |                                                                                                                                                                                                                                                              |         |                               |                                           |
|    |                                                                                                                                                                                                                                                              |         |                               |                                           |
|    |                                                                                                                                                                                                                                                              |         |                               |                                           |



|     |                                                                                                                                                                         |         |                                                                                                                                     |
|-----|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------------------------------------------------------------------------------------------------------------------------------------|
|     | Met284                                                                                                                                                                  |         |                                                                                                                                     |
|     | • $\pi$ - Sigma: Tyr92                                                                                                                                                  |         |                                                                                                                                     |
|     | Interaksi Van der Waals<br>Ile31, Ile228, Arg167, Tyr184, Cys180, Ala181,<br>Gln267, Gln15, Asp281, Asp263                                                              |         |                                                                                                                                     |
|     | Ikatan Hidrogen<br>H - Tyr35:OH                                                                                                                                         | 1,81695 |                                                                                                                                     |
| L10 | Ikatan Hidrofobik<br>• $\pi$ - Alkyl: Trp84, Ile288                                                                                                                     |         | Thr88, Tyr87, Pro285, Tyr92,<br>Ile31, Tyr35, Trp84, Ile288                                                                         |
|     | Interaksi Van der Waals<br>Thr88, Tyr87, Pro285, Tyr92, Ile31                                                                                                           |         |                                                                                                                                     |
|     | Ikatan Hidrogen<br>O - Thr88:O                                                                                                                                          | 2,95748 |                                                                                                                                     |
|     | OH - Tyr92:O                                                                                                                                                            | 3,01738 |                                                                                                                                     |
|     | NH2 - Arg167:O                                                                                                                                                          | 2,81455 | Val179, Cys180, Phe182,                                                                                                             |
|     | H - Tyr292:O                                                                                                                                                            | 2,07923 | Tyr87, Ile31, Ile27, Pro285,<br>Trp84, Ile288, Tyr35,                                                                               |
| L11 | Ikatan Hidrofobik<br>• $\pi$ - Alkyl: Ala A:181                                                                                                                         |         | Cys289, Ile38, Asn295,<br>Phe293, Phe77, Leu81,<br>Val108, Ser105, Arg167,<br>Thr88, Tyr92, Tyr292                                  |
|     | Interaksi Van der Waals<br>Val179, Cys180, Phe182, Tyr87, Ile31, Ile27,<br>Pro285, Trp84, Ile288, Tyr35, Cys289, Ile38,<br>Asn295, Phe293, Phe77, Leu81, Val108, Ser105 |         |                                                                                                                                     |
|     | Ikatan Hidrogen<br>C - Tyr87:OH                                                                                                                                         | 3,66144 |                                                                                                                                     |
| L12 | Ikatan Hidrofobik<br>• $\pi$ - Alkyl: Ile38, Leu 81, Phe77, Trp84, Val108<br>• $\pi$ - Sigma: Tys292, Tyr35, Tyr92                                                      |         | Phe293, Cys289, Thr88,<br>Ile288, Arg167, Cys180,<br>Ser105, Tyr87, Tys292,<br>Tyr35, Tyr92, Ile38, Leu 81,<br>Phe77, Trp84, Val108 |
|     | Interaksi Van der Waals<br>Phe293, Cys289, Thr88, Ile288, Arg167, Cys180,<br>Ser105                                                                                     |         |                                                                                                                                     |
|     | Ikatan Hidrogen<br>H - Thr88:O                                                                                                                                          | 1,79439 |                                                                                                                                     |
| L13 | Ikatan Hidrofobik<br>• $\pi$ -Alkyl: Val108, Tyr35, Tyr92, Pro285, Ile31,<br>Ile288<br>• $\pi$ -Sigma: Trp84                                                            |         | Tyr87, Thr88, Trp84, Val108,<br>Tyr35, Tyr92, Pro285, Ile31,<br>Ile288                                                              |
|     | Interaksi Van der Waals<br>Tyr87                                                                                                                                        |         |                                                                                                                                     |
| L14 | Ikatan Hidrofobik<br>• $\pi$ - Alkyl: Tyr92, Ile31, Thr88, Arg167                                                                                                       |         | Arg167, Tyr92, Ile31, Thr88,                                                                                                        |
|     | Interaksi Van der Waals<br>Arg167, Tyr92, Ile31, Thr88                                                                                                                  |         |                                                                                                                                     |
|     | Ikatan Hidrogen<br>NH1 - Arg167:O                                                                                                                                       | 2,91246 | Tyr92, Ile31, Thr88, Trp84,<br>Phe77, Leu81, Phe182,                                                                                |
|     | NH2 - Arg167:O                                                                                                                                                          | 2,68134 | Cys180, Arg167, Tyr82,                                                                                                              |
| L15 | H - Cys180:O                                                                                                                                                            | 2,14465 | Tyr292, Tyr35, Ala181,                                                                                                              |
|     | OH - Tyr35: N                                                                                                                                                           | 3,58444 | Val179, Pro285, Ile288,                                                                                                             |
|     | OH - Tyr87: N                                                                                                                                                           | 3,67897 | Val108                                                                                                                              |

|                                                                                                                    |                                                                                                                                                                                                                         |         |                                                                                                                                |
|--------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|--------------------------------------------------------------------------------------------------------------------------------|
| Ikatan Hidrofobik                                                                                                  |                                                                                                                                                                                                                         |         |                                                                                                                                |
| <ul style="list-style-type: none"> <li><math>\pi</math> - Alkyl: Ala181, Val179, Pro285, Ile288, Val108</li> </ul> |                                                                                                                                                                                                                         |         |                                                                                                                                |
| Interaksi Van der Waals                                                                                            |                                                                                                                                                                                                                         |         |                                                                                                                                |
| Tyr92, Ile31, Thr88, Trp84, Phe77, Leu81, Phe182                                                                   |                                                                                                                                                                                                                         |         |                                                                                                                                |
| L16                                                                                                                | Ikatan Hidrogen                                                                                                                                                                                                         |         |                                                                                                                                |
|                                                                                                                    | NH1 - Arg167:O                                                                                                                                                                                                          | 2,83453 |                                                                                                                                |
|                                                                                                                    | NH2 - Arg167:O                                                                                                                                                                                                          | 2,77759 |                                                                                                                                |
|                                                                                                                    | H - Cys180:O                                                                                                                                                                                                            | 2,22155 |                                                                                                                                |
|                                                                                                                    | OH - Tyr35:N                                                                                                                                                                                                            | 3,58316 |                                                                                                                                |
|                                                                                                                    | OH - Tyr87:N                                                                                                                                                                                                            | 3,61    | Leu81, Phe77, Tyr292, Phe182, Tyr92, Ile31, Thr88, Arg167, Cys180, Tyr87, Tyr35, Trp84, Ile288, Val108, Pro285, Ala181, Val179 |
|                                                                                                                    | Ikatan Hidrofobik                                                                                                                                                                                                       |         |                                                                                                                                |
|                                                                                                                    | <ul style="list-style-type: none"> <li><math>\pi</math> - Alkyl: Ile288, Val108, Pro285, Ala181, Val179</li> <li><math>\pi</math> - Sigma: Trp84</li> <li><math>\pi</math>- <math>\pi</math> T-shaped: Trp84</li> </ul> |         |                                                                                                                                |
|                                                                                                                    | Interaksi Van der Waals                                                                                                                                                                                                 |         |                                                                                                                                |
|                                                                                                                    | Phe77, Tyr292, Phe182, Tyr92, Ile31, Thr88                                                                                                                                                                              |         |                                                                                                                                |
| L17                                                                                                                | Ikatan Hidrogen                                                                                                                                                                                                         |         |                                                                                                                                |
|                                                                                                                    | H - Ala21:O                                                                                                                                                                                                             | 1,94354 |                                                                                                                                |
|                                                                                                                    | H - Asp281:O                                                                                                                                                                                                            | 2,49868 |                                                                                                                                |
|                                                                                                                    | H - Tyr35:OH                                                                                                                                                                                                            | 2,0261  |                                                                                                                                |
|                                                                                                                    | H - Trp84:O                                                                                                                                                                                                             | 2,28839 |                                                                                                                                |
|                                                                                                                    | H - Thr88:O                                                                                                                                                                                                             | 2,11386 |                                                                                                                                |
|                                                                                                                    | C - Pro285:O                                                                                                                                                                                                            | 3,65978 | Met284, Ile288, Gly22, Arg23, Tyr87, Thr88, Trp84, Ala21, Asp281, Tyr35, Pro285, Tyr92, Pro285                                 |
|                                                                                                                    | Ikatan Hidrofobik                                                                                                                                                                                                       |         |                                                                                                                                |
|                                                                                                                    | <ul style="list-style-type: none"> <li><math>\pi</math>- <math>\pi</math> Stacked: Tyr92</li> <li><math>\pi</math>- Alkyl: Pro285</li> </ul>                                                                            |         |                                                                                                                                |
|                                                                                                                    | Interaksi Van der Waals                                                                                                                                                                                                 |         |                                                                                                                                |
|                                                                                                                    | Met284, Ile288, Gly22, Arg23, Tyr87                                                                                                                                                                                     |         |                                                                                                                                |
| L18                                                                                                                | Ikatan Hidrogen                                                                                                                                                                                                         |         |                                                                                                                                |
|                                                                                                                    | OH - Tyr92:O                                                                                                                                                                                                            | 2,79463 |                                                                                                                                |
|                                                                                                                    | H - Asp281:O                                                                                                                                                                                                            | 2,11912 |                                                                                                                                |
|                                                                                                                    | H - Tyr92:OH                                                                                                                                                                                                            | 2,05522 |                                                                                                                                |
|                                                                                                                    | H - Tyr35:OH                                                                                                                                                                                                            | 2,02489 |                                                                                                                                |
|                                                                                                                    | Ikatan Hidrofobik                                                                                                                                                                                                       |         |                                                                                                                                |
|                                                                                                                    | <ul style="list-style-type: none"> <li><math>\pi</math> - Alkyl: Tyr87, Trp84</li> <li><math>\pi</math> - Sigma: Tyr35</li> </ul>                                                                                       |         |                                                                                                                                |
|                                                                                                                    | Interaksi Van der Waals                                                                                                                                                                                                 |         |                                                                                                                                |
|                                                                                                                    | Met284, Pro285, Ile31, Thr88, Ile288, Val108, Phe77, Leu81, Tyr292, Cys289                                                                                                                                              |         |                                                                                                                                |
|                                                                                                                    | Ikatan Hidrogen                                                                                                                                                                                                         |         |                                                                                                                                |
| L19                                                                                                                | NH2 - Arg167:O                                                                                                                                                                                                          | 2,63754 |                                                                                                                                |
|                                                                                                                    | H - Ala21:O                                                                                                                                                                                                             | 2,49078 | Gln15, Asp281, Ile27, Thr282, Ala21, Tyr92, Arg167, Gly22, Val108, Ile288, Tyr35, Met284, Trp84, Pro285, Tyr87                 |
|                                                                                                                    | H - Ala21:O                                                                                                                                                                                                             | 1,99593 |                                                                                                                                |
|                                                                                                                    | H - Tyr92:OH                                                                                                                                                                                                            | 1,83263 |                                                                                                                                |
|                                                                                                                    | C - Gly22:O                                                                                                                                                                                                             | 2,88754 |                                                                                                                                |
|                                                                                                                    | Ikatan Hidrofobik                                                                                                                                                                                                       |         |                                                                                                                                |
|                                                                                                                    | <ul style="list-style-type: none"> <li><math>\pi</math> - Alkyl: Val108, Ile288, Tyr35, Met284,</li> </ul>                                                                                                              |         |                                                                                                                                |

|                                                         |                                                                                                                                                            |         |
|---------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|
| Trp84, Pro285, Tyr87                                    |                                                                                                                                                            |         |
| Interaksi Van der Waals<br>Gln15, Asp281, Ile27, Thr282 |                                                                                                                                                            |         |
| L20                                                     | Ikatan Hidrogen                                                                                                                                            |         |
|                                                         | O - Ser109:O                                                                                                                                               | 3,25887 |
|                                                         | NH2 - Arg167:O                                                                                                                                             | 3,39257 |
|                                                         | H - Phe182:O                                                                                                                                               | 1,91486 |
|                                                         | H - Tyr184:OH                                                                                                                                              | 2,04824 |
|                                                         | H - Thr260:O                                                                                                                                               | 1,92387 |
|                                                         | H - Ser109:O                                                                                                                                               | 2,09414 |
|                                                         | Ikatan Hidrofobik                                                                                                                                          |         |
|                                                         | <ul style="list-style-type: none"> <li><math>\pi</math> - Alkyl: Met284, Tyr92, Ile91, Tyr39, Pro289, Ile288, Val264, Trp84, Try87</li> </ul>              |         |
|                                                         | Interaksi Van der Waals<br>Leu3, Ser9, Gln15, Thr88, Ser109, His256, Gln267, Lys199, Tyr292, Cys180, Ala181, His183, Asp263                                |         |
| L21                                                     | Ikatan Hidrogen                                                                                                                                            |         |
|                                                         | NH1 - Arg167:O                                                                                                                                             | 2,87977 |
|                                                         | N - Phe182: O                                                                                                                                              | 3,00584 |
|                                                         | H - Asp263:O                                                                                                                                               | 1,98431 |
|                                                         | H - Tyr87:OH                                                                                                                                               | 2,45882 |
|                                                         | H - Ser109:O                                                                                                                                               | 1,97387 |
|                                                         | Ikatan Hidrofobik                                                                                                                                          |         |
|                                                         | <ul style="list-style-type: none"> <li><math>\pi</math> - Alkyl: Lys199, Val108, Ile288, Pro285, Trp84</li> <li><math>\pi</math> - Sigma: Trp84</li> </ul> |         |
|                                                         | Interaksi Van der Waals<br>Cys180, Val179, Tyr92, Thr88, Ile31, Tyr35, His256, Thr260, Trp253, Leu112, Tyr113, Met284, Ala18                               |         |
|                                                         |                                                                                                                                                            |         |
| L22                                                     | Ikatan Hidrogen                                                                                                                                            |         |
|                                                         | NH2 - Arg167:O                                                                                                                                             | 2,82358 |
|                                                         | H - Thr88:O                                                                                                                                                | 1,81815 |
|                                                         | Ikatan Hidrofobik                                                                                                                                          |         |
|                                                         | <ul style="list-style-type: none"> <li><math>\pi</math> - Sigma: Trp84</li> <li><math>\pi</math> - Alkyl: Ile38, Cys289, Tyr35</li> </ul>                  |         |
|                                                         | Interaksi Van der Waals<br>Ser105, Tyr87, Tyr92, Pro285, Ile31, Phe293, Tyr292, Leu81, Phe77, Ile288, Val108                                               |         |
|                                                         |                                                                                                                                                            |         |
|                                                         | Ikatan Hidrogen                                                                                                                                            |         |
|                                                         | OH - Tyr92:O                                                                                                                                               | 2,52583 |
|                                                         | NH2 - Arg167:O                                                                                                                                             | 2,74996 |
| L23                                                     | N - Phe182:O                                                                                                                                               | 2,95957 |
|                                                         | OH - Tyr184:O                                                                                                                                              | 2,93692 |
|                                                         | H - Thr88:O                                                                                                                                                | 2,81375 |
|                                                         | H - Tyr92:OH                                                                                                                                               | 2,34146 |
|                                                         | H - Asp263:O                                                                                                                                               | 1,78614 |
|                                                         | C - Tyr35:OH                                                                                                                                               | 2,65523 |
|                                                         | Ikatan Hidrofobik                                                                                                                                          |         |
|                                                         | <ul style="list-style-type: none"> <li><math>\pi</math> - Alkyl: Trp84, Tyr 87, Ile288, Val108,</li> </ul>                                                 |         |
|                                                         |                                                                                                                                                            |         |
|                                                         |                                                                                                                                                            |         |

|     |                                                                                                                                                                                                                                              |                                                     |                                                                                                                                                                                                                  |
|-----|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|     | His256, Leu 112, Trp253                                                                                                                                                                                                                      |                                                     |                                                                                                                                                                                                                  |
|     | Interaksi Van der Waals<br>Ile31, Tyr35, Pro285, Ser105, Ala181, Asp281,<br>Met284, Gln267, Gln15, Thr260, Ser109, Tyr292                                                                                                                    |                                                     |                                                                                                                                                                                                                  |
| L24 | Ikatan Hidrogen<br>NH2 - Arg167:O<br>H - Trp84:O<br>H - Hr88:O<br>H - Ser105:O<br>H - Ser109:O<br><br>Ikatan Hidrofobik<br>• $\pi$ - $\pi$ Stacked: Trp84                                                                                    | 2,71303<br>2,25724<br>2,06149<br>2,39794<br>2,02865 | Tyr87, Try92, Ile288, Tyr292,<br>Trp253, His256, Leu112,<br>Tyr35, Phe77, Val108,<br>Ala163, Phe 182, Thr88,<br>Trp84, Ser105, Arg167,<br>Ser109                                                                 |
|     | Interaksi Van der Waals<br>Tyr87, Try92, Ile288, Tyr292, Trp253, His256,<br>Leu112, Tyr35, Phe77, Val108, Ala163, Phe 182                                                                                                                    |                                                     |                                                                                                                                                                                                                  |
| L25 | Ikatan Hidrogen<br>NH2 - Arg167:O<br>H - Gly22:O<br>H - Ala21:O<br><br>Ikatan Hidrofobik<br>• $\pi$ - Alkyl: Pro285, Ile288, Tyr35, Tyr87, Tyr92<br>• $\pi$ -Pigma: Trp84                                                                    | 2,60298<br>2,14345<br>2,01451                       | Ile27, Thr282, Asp281,<br>Met284, Val108, Ala21,<br>Gly22, Arg167, Trp84,<br>Pro285, Ile288, Tyr35, Tyr87,<br>Tyr92                                                                                              |
|     | Interaksi Van der Waals:<br>Ile27, Thr282, Asp281, Met284, Val108, Ala21,<br>Gly22, Arg167                                                                                                                                                   |                                                     |                                                                                                                                                                                                                  |
| L26 | Ikatan Hidrogen<br>NH1 - Arg167:O<br><br>Ikatan Hidrofobik<br>• $\pi$ - Alkyl: Tyr292, Val108, Ile288, Pro285,<br>Met284, Trp84<br>• $\pi$ - Sigma: Tyr92                                                                                    | 2,62483                                             | Phe77, Tyr35, Thr88, Ile31,<br>Try87, Ser105, Cys180,<br>Leu81, Arg167, Tyr92,<br>Tyr292, Val108, Ile288,<br>Pro285, Met284, Trp84                                                                               |
|     | Interaksi Van der Waals<br>Phe77, Tyr35, Thr88, Ile31, Try87, Ser105,<br>Cys180, Leu81                                                                                                                                                       |                                                     |                                                                                                                                                                                                                  |
| L27 | Ikatan Hidrofobik<br>• $\pi$ -Alkyl: Val108, Phe77, Leu81, Cys289, Ile3<br>• $\pi$ - Pigma: Tyr35, Trp84<br><br>Interaksi Van der Waals<br>Tyr292, Ile288, Phe293, Tyr87, Thr88                                                              |                                                     | Tyr292, Ile288, Phe293,<br>Tyr87, Thr88, Tyr35, Trp84,<br>Val108, Phe77, Leu81,<br>Cys289, Ile38                                                                                                                 |
| L28 | Ikatan Hidrogen<br>NH2 - Arg167:O<br>N - Phe182: O<br>H - Cys180:O<br>H - Gln257:O<br><br>Ikatan Hidrofobik<br>• $\pi$ - Alkyl: Val108, Tyr35, His256, Ile288,<br>Tyr292, Lys199, Trp253, Phe204, Leu112,<br>Met284<br>• $\pi$ -Sigma: Trp84 | 2,59744<br>2,95423<br>2,04486<br>2,17955            | Tyr184, Gln267, Thr260,<br>Asn200, Ser109, Tyr87,<br>Val179, Asp263, Ala181,<br>Phe182, Gln257, Arg167,<br>Cys180, Trp84, Val108,<br>Tyr35, His256, Ile288,<br>Tyr292, Lys199, Trp253,<br>Phe204, Leu112, Met284 |

|                                                                                                     |                                                                                                                                                                                                                                                    |         |
|-----------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|
| Interaksi Van der Waals<br>Tyr184, Gln267, Thr260, Asn200, Ser109, Tyr87,<br>Val179, Asp263, Ala181 |                                                                                                                                                                                                                                                    |         |
| L29                                                                                                 | Ikatan Hidrogen                                                                                                                                                                                                                                    |         |
|                                                                                                     | NH1 - Arg167:O                                                                                                                                                                                                                                     | 2,7454  |
|                                                                                                     | N - Phe182:O                                                                                                                                                                                                                                       | 2,89047 |
|                                                                                                     | H - Tyr184:OH                                                                                                                                                                                                                                      | 2,16846 |
|                                                                                                     | H - Cys180:O                                                                                                                                                                                                                                       | 2,1202  |
|                                                                                                     | H - Tyr87:OH                                                                                                                                                                                                                                       | 1,95223 |
|                                                                                                     | H - Tyr35:OH                                                                                                                                                                                                                                       | 2,04364 |
|                                                                                                     | Ikatan Hidrofobik                                                                                                                                                                                                                                  |         |
|                                                                                                     | <ul style="list-style-type: none"> <li>• <math>\pi</math>-Alkyl: Val108</li> <li>• <math>\pi</math>-Lone Pair: Tyr92</li> <li>• <math>\pi</math>- <math>\pi</math> Stacked: Trp84, Tyr92</li> </ul>                                                |         |
|                                                                                                     | Interaksi Van der Waals<br>Phe77, Leu81, Ile288, Pro285, Val179, Ala181,<br>Gln267, Met284, Ser105                                                                                                                                                 |         |
| L30                                                                                                 | Ikatan Hidrogen                                                                                                                                                                                                                                    |         |
|                                                                                                     | OH - Tyr184:O                                                                                                                                                                                                                                      | 3,00453 |
|                                                                                                     | H - Asp263:O                                                                                                                                                                                                                                       | 2,1524  |
|                                                                                                     | H - Tyr35:OH                                                                                                                                                                                                                                       | 2,27733 |
|                                                                                                     | Ikatan Hidrofobik                                                                                                                                                                                                                                  |         |
|                                                                                                     | <ul style="list-style-type: none"> <li>• <math>\pi</math> - Alkyl: Met284, Tyr92, Tyr87, Ile31, Ala181, Pro285, Ile188, Val179, Trp84</li> </ul>                                                                                                   |         |
|                                                                                                     | Interaksi Van der Waals<br>Phe182, Arg167, Cys180, Val108, Thr88                                                                                                                                                                                   |         |
|                                                                                                     | Ikatan Hidrogen                                                                                                                                                                                                                                    |         |
|                                                                                                     | O - Thr88:O                                                                                                                                                                                                                                        | 3,28215 |
|                                                                                                     | H - Tyr35:OH                                                                                                                                                                                                                                       | 1,78089 |
| L31                                                                                                 | Ikatan Hidrofobik                                                                                                                                                                                                                                  |         |
|                                                                                                     | <ul style="list-style-type: none"> <li>• <math>\pi</math>-Alkyl: Val108</li> <li>• <math>\pi</math>-Sigma: Ile288</li> <li>• <math>\pi</math>- <math>\pi</math> Stacked &amp; <math>\pi</math>- <math>\pi</math> T-shaped: Trp84, Tyr87</li> </ul> |         |
|                                                                                                     | Interaksi Van der Waals<br>Tyr92, Ile31, Leu811, Phe77, Tyr292, Arg167,<br>Ala181, Phe182                                                                                                                                                          |         |
|                                                                                                     | Ikatan Hidrogen                                                                                                                                                                                                                                    |         |
|                                                                                                     | OH - Tyr35:O                                                                                                                                                                                                                                       | 2,80065 |
|                                                                                                     | O - Thr88:O                                                                                                                                                                                                                                        | 3,17478 |
|                                                                                                     | H - Tyr87:OH                                                                                                                                                                                                                                       | 1,91336 |
|                                                                                                     | H - Tyr35:OH                                                                                                                                                                                                                                       | 1,94934 |
|                                                                                                     | H - Ser105:O                                                                                                                                                                                                                                       | 2,78903 |
|                                                                                                     | H - Ser109:O                                                                                                                                                                                                                                       | 2,08522 |
| L32                                                                                                 | Ikatan Hidrofobik                                                                                                                                                                                                                                  |         |
|                                                                                                     | <ul style="list-style-type: none"> <li>• <math>\pi</math> - Cation: Arg167</li> <li>• <math>\pi</math> - <math>\pi</math> Stacked &amp; <math>\pi</math>- <math>\pi</math> T-shaped: Trp84</li> </ul>                                              |         |
|                                                                                                     | Interaksi Van der Waals<br>Cys180, Val179, Ala181, Ala163, Ile288, Ile31,<br>Tyr92                                                                                                                                                                 |         |
|                                                                                                     | Ikatan Hidrogen                                                                                                                                                                                                                                    |         |
|                                                                                                     | Phe293, Ile38, Leu81, Phe77,                                                                                                                                                                                                                       |         |
|                                                                                                     |                                                                                                                                                                                                                                                    |         |
|                                                                                                     |                                                                                                                                                                                                                                                    |         |
|                                                                                                     |                                                                                                                                                                                                                                                    |         |
|                                                                                                     |                                                                                                                                                                                                                                                    |         |
|                                                                                                     |                                                                                                                                                                                                                                                    |         |
| L33                                                                                                 | Ikatan Hidrogen                                                                                                                                                                                                                                    |         |
|                                                                                                     |                                                                                                                                                                                                                                                    |         |
|                                                                                                     |                                                                                                                                                                                                                                                    |         |
|                                                                                                     |                                                                                                                                                                                                                                                    |         |
|                                                                                                     |                                                                                                                                                                                                                                                    |         |
|                                                                                                     |                                                                                                                                                                                                                                                    |         |
|                                                                                                     |                                                                                                                                                                                                                                                    |         |
|                                                                                                     |                                                                                                                                                                                                                                                    |         |
|                                                                                                     |                                                                                                                                                                                                                                                    |         |
|                                                                                                     |                                                                                                                                                                                                                                                    |         |

|     |                                                                                                                                                                |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|-----|----------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|--------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|     | H - Cys289:O                                                                                                                                                   | 1,98974 | Asn295, Val108, Trp84                                                                                                                | Cys289, Tyr292, Ile288,                                                                            | Tyr35, Ile288,                                                                       |
|     | Ikatan Hidrofobik                                                                                                                                              |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | <ul style="list-style-type: none"> <li><math>\pi</math> - Alkyl: Tyr35, Val108, Tyr292, Ile288, Trp84</li> </ul>                                               |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | Interaksi Van der Waals                                                                                                                                        |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | Phe293, Ile38, Leu81, Phe77, Asn295                                                                                                                            |         |                                                                                                                                      |                                                                                                    |                                                                                      |
| L34 | Ikatan Hidrogen                                                                                                                                                |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | NH - Arg167:O                                                                                                                                                  | 2,91639 |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | H - Pro285:O                                                                                                                                                   | 2,14023 |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | H - Cys180:O                                                                                                                                                   | 2,04375 |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | C - Ala181:O                                                                                                                                                   | 3,40483 | Met284, Thr88, Pro285, Tyr35, Tyr87, Ala181, Ile31, Ile288, Pro285                                                                   | Cys289, Val179, Arg167, Tyr87, Ala181, Tyr92, Pro285                                               | Ile286, Trp84, Cys180, Tyr92, Pro285                                                 |
|     | Ikatan Hidrofobik                                                                                                                                              |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | <ul style="list-style-type: none"> <li><math>\pi</math> - Alkyl: Ile31, Ile288, Pro285</li> <li><math>\pi</math>- <math>\pi</math>: T-shaped: Tyr92</li> </ul> |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | Interaksi Van der Waals                                                                                                                                        |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | Met284, Cys289, Ile286, Thr88, Val179, Trp84                                                                                                                   |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | Ikatan Hidrogen                                                                                                                                                |         |                                                                                                                                      |                                                                                                    |                                                                                      |
| L35 | NE2 - Gln15:O                                                                                                                                                  | 2,74438 |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | O - Thr88:O                                                                                                                                                    | 3,1867  |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | H - Asp263:O                                                                                                                                                   | 1,80065 |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | C - Pro285:O                                                                                                                                                   | 3,72515 | Gln267, Tyr35, Gln15, Thr88, Met284, Trp84, Tyr87                                                                                    | Asp281, Arg167, Ile288, Val108,                                                                    | Ile31, Asp263, Tyr92, Pro285, Tyr92, Val108,                                         |
|     | Ikatan Hidrofobik                                                                                                                                              |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | <ul style="list-style-type: none"> <li><math>\pi</math> - Alkyl: Met284, Ile288, Val108, Trp84, Tyr87</li> <li><math>\pi</math> - Sigma: Tyr92</li> </ul>      |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | Interaksi Van der Waals                                                                                                                                        |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | Gln267, Asp281, Ile31, Tyr35, Arg167                                                                                                                           |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | Ikatan Hidrogen                                                                                                                                                |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | O -Thr88:O                                                                                                                                                     | 3,09575 |                                                                                                                                      |                                                                                                    |                                                                                      |
| L36 | H - Ala21:O                                                                                                                                                    | 2,15941 |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | H - Tyr35:OH                                                                                                                                                   | 1,84533 |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | C - Asp281:O                                                                                                                                                   | 3,30549 | Met284, Arg167, Tyr35, Gln15, Trp84, Ile288, Pro285, Tyr87                                                                           | Gly22, Ser105, Ala21, Tyr92, Val108,                                                               | Arg23, Thr88, Asp281, Val108,                                                        |
|     | Ikatan Hidrofobik                                                                                                                                              |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | <ul style="list-style-type: none"> <li><math>\pi</math> - Alkyl: Val108, Ile288, Pro285, Tyr87</li> <li><math>\pi</math> - Sigma: Trp84, Tyr92</li> </ul>      |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | Interaksi Van der Waals                                                                                                                                        |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | Met284, Gly22, Arg23, Arg167, Ser105                                                                                                                           |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | Ikatan Hidrogen                                                                                                                                                |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | O - Ser109:O                                                                                                                                                   | 2,62646 | Ala181, Tyr113, Ala163, Trp253, Asp281, Ser109, Ile288, Thr260, Phe182, Tyr92, Met284, Tyr184, Phe182, Tyr92, Met284, Tyr92, Met284, | Val108, Ala159, Pro162, Thr88, Leu3, Asr263, Arg167, Ser109, His256, Tyr184, Tyr92, Pro285, Tyr87, | Tyr292, Ser160, Leu112, Val179, Gln15, Gln267, His256, Tyr184, Tyr92, Pro285, Tyr87, |
|     | NH2 - Arg167:O                                                                                                                                                 | 2,83525 |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | O - Thr260:O                                                                                                                                                   | 2,87648 |                                                                                                                                      |                                                                                                    |                                                                                      |
| L37 | H - Asp263:O                                                                                                                                                   | 1,9542  |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | H - His256:N                                                                                                                                                   | 2,45996 |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | C - Ser109:O                                                                                                                                                   | 3,57351 |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | Ikatan Hidrofobik                                                                                                                                              |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | <ul style="list-style-type: none"> <li><math>\pi</math> - Alkyl: Pro285, Tyr184, Phe182, Tyr87, Tyr92, Met284, Trp84</li> </ul>                                |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | Interaksi Van der Waals                                                                                                                                        |         |                                                                                                                                      |                                                                                                    |                                                                                      |
|     | Ala181, Val108, Tyr292, Tyr113, Ala159, Ser160,                                                                                                                |         |                                                                                                                                      |                                                                                                    |                                                                                      |

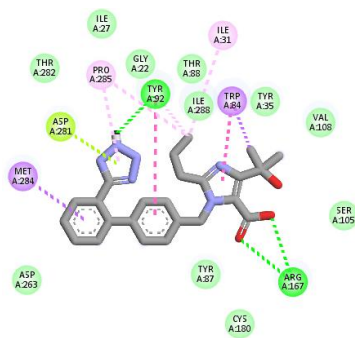
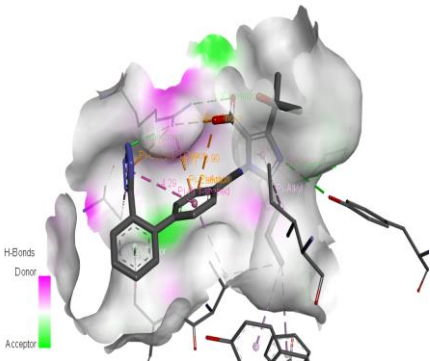
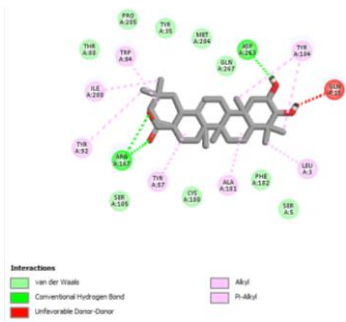
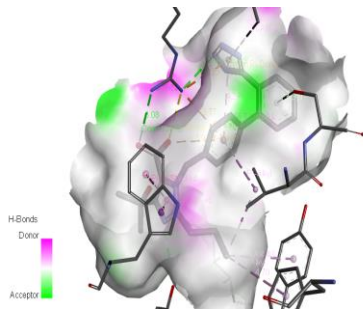
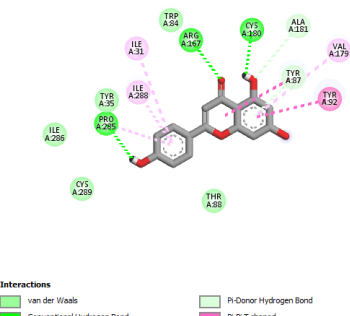
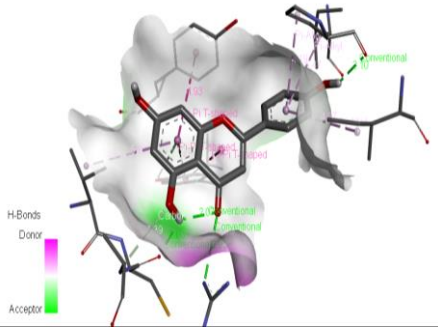
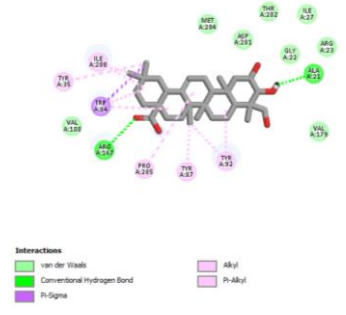
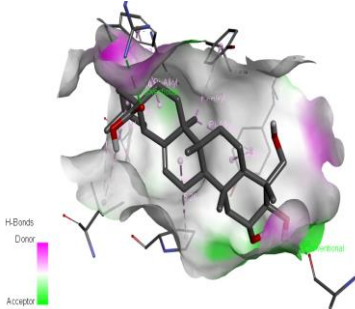
|     |                                                                                                                                                                                                                                                                                                                                        |         |                                                                                                                                                                                         |
|-----|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|     | Ala163, Pro162, Leu112, Trp253, Thr88, Val179, Asp281, Leu3, Gln15                                                                                                                                                                                                                                                                     |         |                                                                                                                                                                                         |
|     | Ikatan Hidrogen                                                                                                                                                                                                                                                                                                                        |         |                                                                                                                                                                                         |
|     | O - Thr88:O                                                                                                                                                                                                                                                                                                                            | 2,77171 |                                                                                                                                                                                         |
|     | H - Tyr184:OH                                                                                                                                                                                                                                                                                                                          | 2,01535 |                                                                                                                                                                                         |
| L38 | Ikatan Hidrofobik <ul style="list-style-type: none"> <li>• <math>\pi</math> - Alkyl: Ala181, Ile288, Val108</li> <li>• <math>\pi</math> - Sigma: Trp84</li> </ul> Interaksi Van der Waals<br>Leu3, Asp263, Gln267, Met284, Tyr87, Pro285, Tyr92, Ile31, Tyr35, Ser105, Arg167, Cys180, Phe182                                          |         | Leu3, Asp263, Gln267, Met284, Tyr87, Pro285, Tyr92, Ile31, Tyr35, Ser105, Arg167, Cys180, Phe182, Tyr184, Thr88, Trp84, Ala181, Ile288, Val108                                          |
|     | Ikatan Hidrogen                                                                                                                                                                                                                                                                                                                        |         |                                                                                                                                                                                         |
|     | O - Thr88:O                                                                                                                                                                                                                                                                                                                            | 3,13635 |                                                                                                                                                                                         |
|     | NH - Arg167:O                                                                                                                                                                                                                                                                                                                          | 2,88028 |                                                                                                                                                                                         |
|     | H - Thr88:O                                                                                                                                                                                                                                                                                                                            | 2,05173 |                                                                                                                                                                                         |
|     | H - Tyr35:OH                                                                                                                                                                                                                                                                                                                           | 2,06966 |                                                                                                                                                                                         |
|     | H - Cys180:O                                                                                                                                                                                                                                                                                                                           | 1,91765 |                                                                                                                                                                                         |
|     | H - Asp263:O                                                                                                                                                                                                                                                                                                                           | 2,16142 |                                                                                                                                                                                         |
| L39 | C - Ala181:O                                                                                                                                                                                                                                                                                                                           | 2,95165 | Gln267, Met284, Ile228, Ile31, Tyr92, Tyr87, Phe182, Tyr184, Asp263, Tyr35, Thr88, Cys180, Ala181, Arg167, Trp84                                                                        |
|     | Ikatan Hidrofobik <ul style="list-style-type: none"> <li>• <math>\pi</math> - Cation: Arg167</li> <li>• <math>\pi</math> - <math>\pi</math> Stacked: Trp84</li> </ul> Interaksi Van der Waals<br>Gln267, Met284, Ile228, Ile31, Tyr92, Tyr87, Phe182, Tyr184                                                                           |         |                                                                                                                                                                                         |
|     | Ikatan Hidrogen                                                                                                                                                                                                                                                                                                                        |         |                                                                                                                                                                                         |
|     | OH - Tyr35:O                                                                                                                                                                                                                                                                                                                           | 3,18586 |                                                                                                                                                                                         |
|     | O - Thr88: O                                                                                                                                                                                                                                                                                                                           | 2,95627 |                                                                                                                                                                                         |
|     | OH - Tyr92:O                                                                                                                                                                                                                                                                                                                           | 2,83607 |                                                                                                                                                                                         |
|     | NH1 - Arg167:O                                                                                                                                                                                                                                                                                                                         | 2,83824 |                                                                                                                                                                                         |
|     | N - Phe182: O                                                                                                                                                                                                                                                                                                                          | 2,83097 |                                                                                                                                                                                         |
|     | H - Tyr35:OH                                                                                                                                                                                                                                                                                                                           | 1,98646 |                                                                                                                                                                                         |
|     | H - Cys180:O                                                                                                                                                                                                                                                                                                                           | 2,36532 |                                                                                                                                                                                         |
|     | H - Tyr87:OH                                                                                                                                                                                                                                                                                                                           | 2,17552 |                                                                                                                                                                                         |
| L40 | OH - Tyr292:N                                                                                                                                                                                                                                                                                                                          | 4,04742 | Ser109, Leu112, Lys199, Thr260, His256, Ile31, Ile288, Val179, Ala181, Phe77, Tyr92, Thr88, Tyr35, Tyr87, Phe182, Cys180, Ala181, Arg167, Tyr292, Trp253, Trp 84, Val108, Pro285, Tyr92 |
|     | Ikatan Hidrofobik <ul style="list-style-type: none"> <li>• <math>\pi</math> - Alkyl:Val108, Pro285, Tyr92</li> <li>• <math>\pi</math> - Sigma: Trp253</li> <li>• <math>\pi</math>- <math>\pi</math> T-shaped: Trp84</li> </ul> Interaksi Van der Waals<br>Ser109, Leu112, Lys199, Thr260, His256, Ile31, Ile288, Val179, Ala181, Phe77 |         |                                                                                                                                                                                         |
|     | Ikatan Hidrogen                                                                                                                                                                                                                                                                                                                        |         |                                                                                                                                                                                         |
|     | OH - Tyr87:O                                                                                                                                                                                                                                                                                                                           | 2,93861 |                                                                                                                                                                                         |
|     | N - Phe182: O                                                                                                                                                                                                                                                                                                                          | 2,90518 |                                                                                                                                                                                         |
|     | H - Tyr35:OH                                                                                                                                                                                                                                                                                                                           | 1,95836 |                                                                                                                                                                                         |
| L41 | Ikatan Hidrofobik <ul style="list-style-type: none"> <li>• <math>\pi</math> - Alkyl: Ala181, Pro285</li> <li>• <math>\pi</math> - Cation: Arg167</li> </ul> Interaksi Van der Waals                                                                                                                                                    |         | Trp84, Tyr184, Val179, Tyr92, Thr88, Ile31, Tyr35, Phe182, Tyr87, Arg167, Ala181, Pro285                                                                                                |

|                                                                                                       |                                                                                                   |                                                            |                                  |  |                                                                                                                                                                           |  |  |
|-------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|------------------------------------------------------------|----------------------------------|--|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|--|
| Trp84, Tyr184, Val179, Tyr92, Thr88, Ile31                                                            |                                                                                                   |                                                            |                                  |  |                                                                                                                                                                           |  |  |
| L42                                                                                                   | Ikatan Hidrogen                                                                                   |                                                            |                                  |  |                                                                                                                                                                           |  |  |
|                                                                                                       | NH2 - Arg167: O                                                                                   |                                                            | 2,59013                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | H - Ala21:O                                                                                       |                                                            | 1,73344                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | Ikatan Hidrofobik                                                                                 |                                                            |                                  |  | Asp281, Arg23, Gly22, Ile288, Val108, Ala21, Arg167, Trp84, Tyr92, Pro285, Tyr87, Tyr35, Met284                                                                           |  |  |
|                                                                                                       |                                                                                                   | • $\pi$ -Alkyl: Tyr92, Pro285, Tyr87, Trp84, Tyr35, Met284 |                                  |  |                                                                                                                                                                           |  |  |
|                                                                                                       |                                                                                                   | • $\pi$ -Sigma: Trp84                                      |                                  |  |                                                                                                                                                                           |  |  |
| Interaksi Van der Waals                                                                               |                                                                                                   |                                                            |                                  |  |                                                                                                                                                                           |  |  |
| Asp281, Arg23, Gly22, Ile288, Val108                                                                  |                                                                                                   |                                                            |                                  |  |                                                                                                                                                                           |  |  |
| L43                                                                                                   | Ikatan Hidrogen                                                                                   |                                                            |                                  |  |                                                                                                                                                                           |  |  |
|                                                                                                       | O - Thr88: O                                                                                      |                                                            | 3,24463                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | NH - Arg167:O                                                                                     |                                                            | 2,83517                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | JH - Tyr35:OH                                                                                     |                                                            | 2,02937                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | H - Cys180:O                                                                                      |                                                            | 1,89134                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | H - Asp263:O                                                                                      |                                                            | 2,11876                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | C - Ala181:O                                                                                      |                                                            | 2,96633                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | Ikatan Hidrofobik                                                                                 |                                                            |                                  |  | Gln267, Met284, Tyr87, Tyr92, Ile31, Ile288, Phe182, Tyr184, Asp263, Thr88, Tyr35, Cys180, Arg167, Ala181, Trp84                                                          |  |  |
|                                                                                                       |                                                                                                   |                                                            | • $\pi$ -Cation: Arg167          |  |                                                                                                                                                                           |  |  |
|                                                                                                       |                                                                                                   |                                                            | • $\pi$ - $\pi$ - Stacked: Trp84 |  |                                                                                                                                                                           |  |  |
| Interaksi Van der Waals:                                                                              |                                                                                                   |                                                            |                                  |  |                                                                                                                                                                           |  |  |
| Gln267, Met284, Tyr87, Tyr92, Ile31, Ile288, Phe182, Tyr184                                           |                                                                                                   |                                                            |                                  |  |                                                                                                                                                                           |  |  |
| L44                                                                                                   | Ikatan Hidrogen:                                                                                  |                                                            |                                  |  |                                                                                                                                                                           |  |  |
|                                                                                                       | NH1 - Arg167:O                                                                                    |                                                            | 2,65549                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | NH2 - Arg167:O                                                                                    |                                                            | 2,86348                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | N - Phe182:O                                                                                      |                                                            | 2,78437                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | H - Tyr87:OH                                                                                      |                                                            | 2,27882                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | H - Tyr35:OH                                                                                      |                                                            | 1,79154                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | H - Cys180:O                                                                                      |                                                            | 2,092                            |  |                                                                                                                                                                           |  |  |
|                                                                                                       | H - Tyr184:OH                                                                                     |                                                            | 2,21519                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | Ikatan Hidrofobik                                                                                 |                                                            |                                  |  | His256, Ser109, Met284, Gln267, Ala181, Val179, Pro285, Phe77, Leu81, Ala104, Tyr292, His256, Ser105, Tyr184, Phe182, Cys180, Tyr87, Tyr35, Arg167, Trp84, Ile288, Val108 |  |  |
|                                                                                                       |                                                                                                   |                                                            | • $\pi$ -Alkyl: Ile288, Val108   |  |                                                                                                                                                                           |  |  |
|                                                                                                       |                                                                                                   | • $\pi$ - $\pi$ Stacked: Trp84                             |                                  |  |                                                                                                                                                                           |  |  |
| Interaksi Van der Waals                                                                               |                                                                                                   |                                                            |                                  |  |                                                                                                                                                                           |  |  |
| His256, Ser109, Met284, Gln267, Ala181, Val179, Pro285, Phe77, Leu 81, Ala104, Tyr292, His256, Ser105 |                                                                                                   |                                                            |                                  |  |                                                                                                                                                                           |  |  |
| L45                                                                                                   | Ikatan Hidrogen                                                                                   |                                                            |                                  |  |                                                                                                                                                                           |  |  |
|                                                                                                       | H - Asp263:O                                                                                      |                                                            | 1,9447                           |  |                                                                                                                                                                           |  |  |
|                                                                                                       | Ikatan Hidrofobik                                                                                 |                                                            |                                  |  |                                                                                                                                                                           |  |  |
|                                                                                                       | • $\pi$ - Alkyl: Tyr35, Leu81, Ile288, Phe77, Val108, Tyr292, Met284, Pro285, Tyr87, Ile31, Tyr92 |                                                            |                                  |  | Arg167, Gln267, Asp281, Thr88, Asp263, Trp84, Tyr35, Leu81, Ile288, Phe77, Val108, Tyr292, Met284, Pro285, Tyr87, Ile31, Tyr92                                            |  |  |
|                                                                                                       |                                                                                                   | • $\pi$ - Sigma: Trp84                                     |                                  |  |                                                                                                                                                                           |  |  |
| Interaksi Van der Waals                                                                               |                                                                                                   |                                                            |                                  |  |                                                                                                                                                                           |  |  |
| Arg167, Gln267, Asp281, Thr88                                                                         |                                                                                                   |                                                            |                                  |  |                                                                                                                                                                           |  |  |
| L46                                                                                                   | Ikatan Hidrogen                                                                                   |                                                            |                                  |  |                                                                                                                                                                           |  |  |
|                                                                                                       | O - Thr88: O                                                                                      |                                                            | 3,20622                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | NH2 - Arg167:O                                                                                    |                                                            | 2,77386                          |  |                                                                                                                                                                           |  |  |
|                                                                                                       | H - Tyr92:OH                                                                                      |                                                            | 1,81982                          |  |                                                                                                                                                                           |  |  |

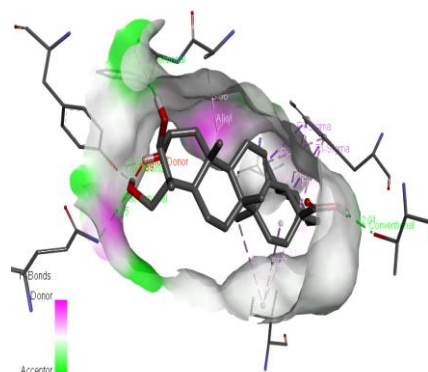
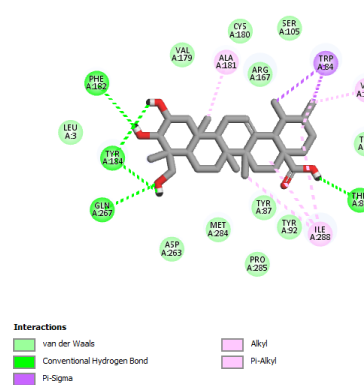


|     |                                                                                                                                                               |         |                               |
|-----|---------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------------------------------|
|     | H - Ser105:O                                                                                                                                                  | 2,91026 | Tyr87, Trp84, Ile288, His256, |
|     | H - Ser109:O                                                                                                                                                  | 2,24941 | Val108                        |
|     | C - Tyr35:OH                                                                                                                                                  | 3,45404 |                               |
|     | Ikatan Hidrofobik                                                                                                                                             |         |                               |
|     | <ul style="list-style-type: none"> <li>• <math>\pi</math> - Alkyl: Tyr87, Trp84, Ile288, His256, Val108</li> </ul>                                            |         |                               |
|     | Interaksi Van der Waals                                                                                                                                       |         |                               |
|     | Pro285, Ile31, Ala163, Phe182, Lys199, Tyr184                                                                                                                 |         |                               |
|     | Ikatan Hidrogen                                                                                                                                               |         |                               |
|     | NH2 - Arg167:O                                                                                                                                                | 2,65206 |                               |
|     | H - Ala21:O                                                                                                                                                   | 1,80701 |                               |
| L47 | Ikatan Hidrofobik                                                                                                                                             |         |                               |
|     | <ul style="list-style-type: none"> <li>• <math>\pi</math> - Alkyl: Tyr92, Tyr87, Ile288, Tyr35, Pro285</li> <li>• <math>\pi</math>-Sigma: TRP A:84</li> </ul> |         |                               |
|     | Arg23, Gly22, Asp281, Met284, Thr88, Val108, Ala21, Arg167, Trp84, Tyr92, Tyr87, Ile288, Tyr35, Pro285                                                        |         |                               |
|     | Interaksi Van der Waals                                                                                                                                       |         |                               |
|     | Arg23, Gly22, Asp281, Met284, Thr88, Val108                                                                                                                   |         |                               |

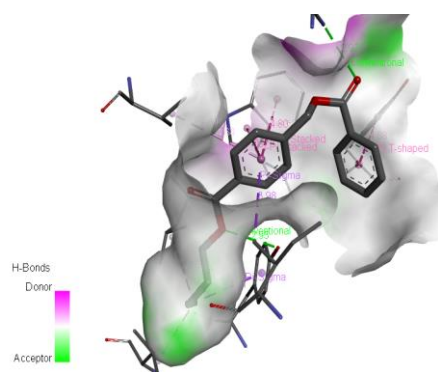
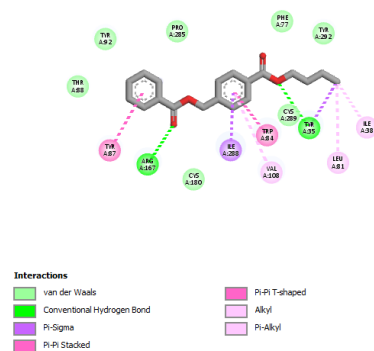
### Lampiran 3 Visualisasi 2D dan 3D Interaksi Penambatan Molekul Ligan Uji

| Kode Ligan | 2D                                                                                                                                                                                                                                                                                                                  | 3D                                                                                   |
|------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
| Ligan A1   |                                                                                                                                                                                                                                    |    |
| L1         |  <p>Interactions</p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Unfavorable Donor-Donor</li> <li>Alkyl</li> <li>Alkyl</li> </ul>                                           |   |
| L2         |  <p>Interactions</p> <ul style="list-style-type: none"> <li>van der Waals</li> <li>Conventional Hydrogen Bond</li> <li>Carbon Hydrogen Bond</li> <li>Pi-Donor Hydrogen Bond</li> <li>Pi-Pi T-shaped</li> <li>Pi-Alkyl</li> </ul> |  |
| L3         |  <p>Interactions</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>Alkyl</li> </ul>                                                         |  |

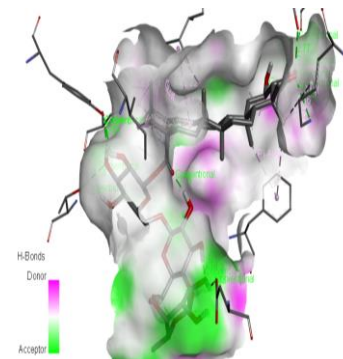
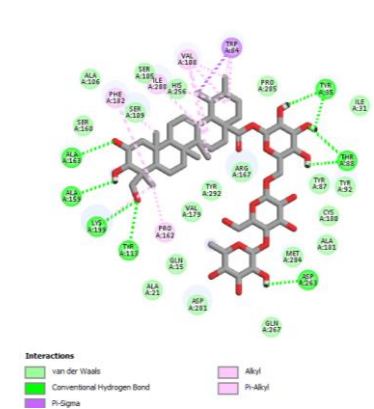
L4



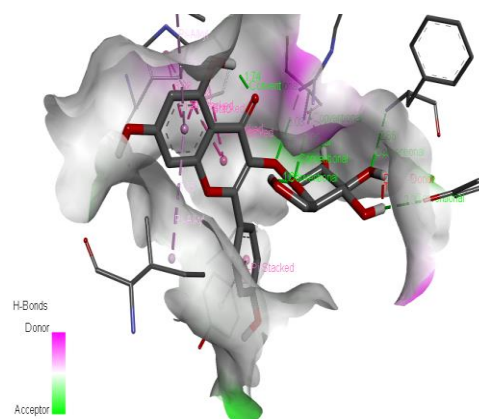
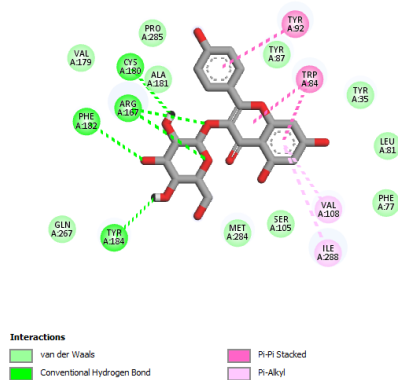
L5



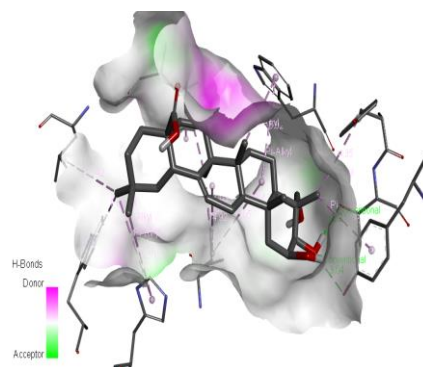
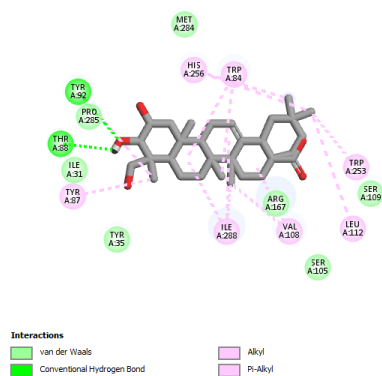
L6



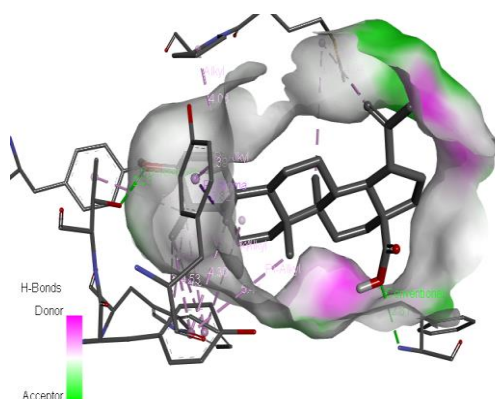
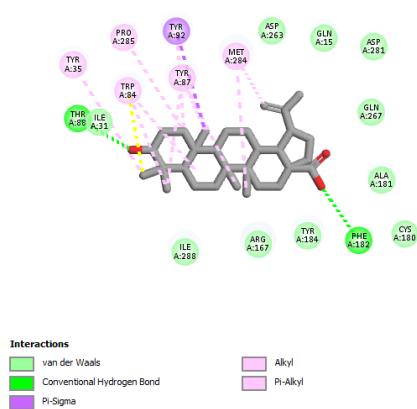
L7



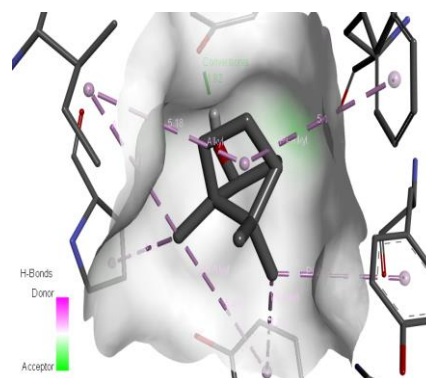
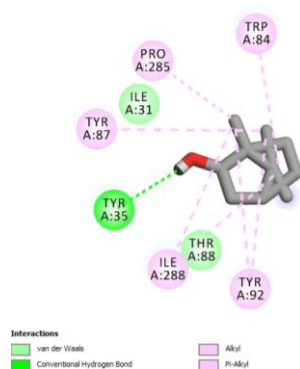
L8



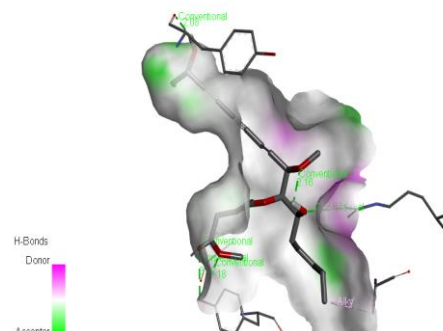
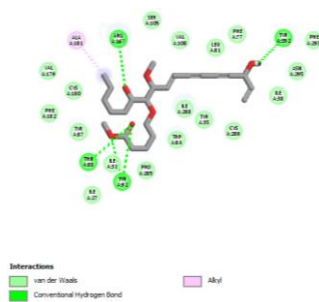
L9



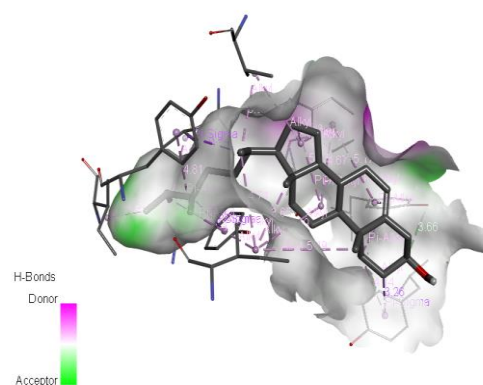
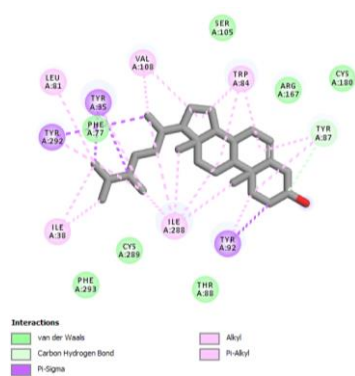
L10



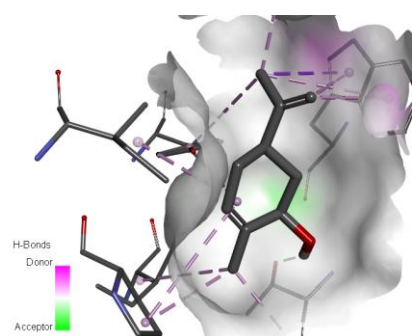
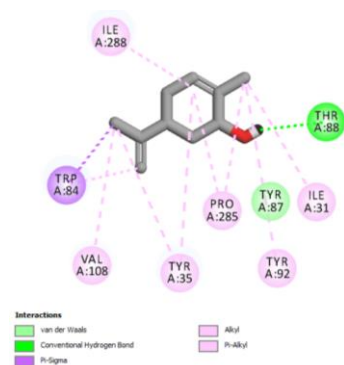
L11



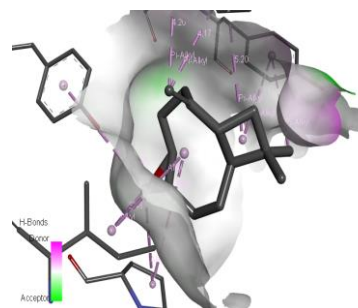
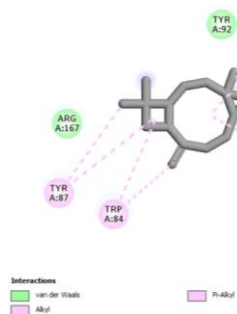
L12



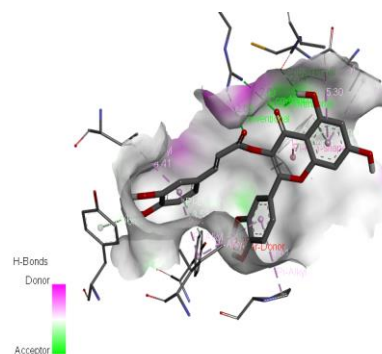
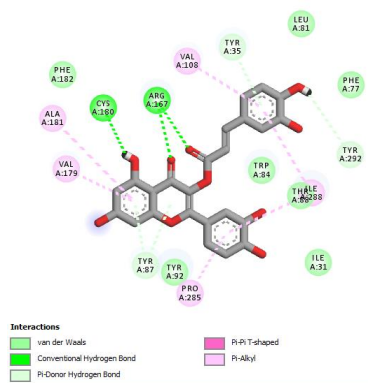
L13



L14

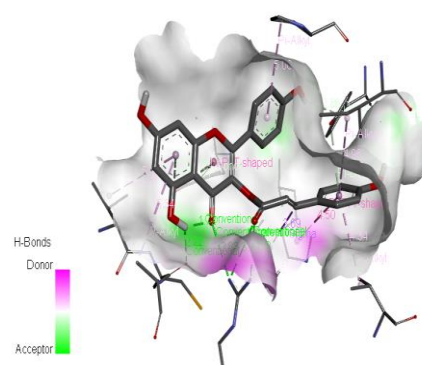
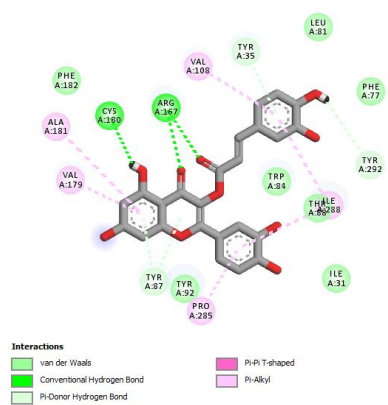


L15

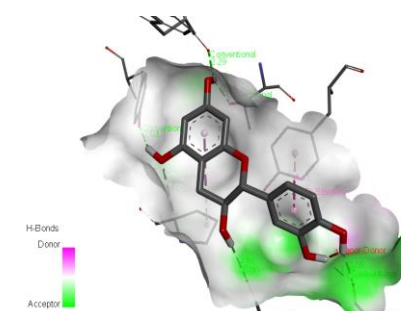
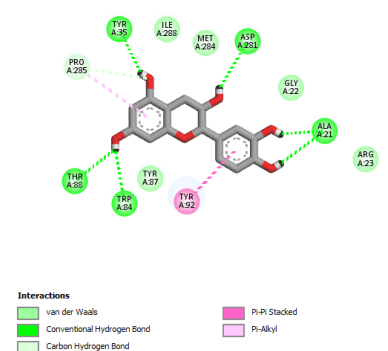




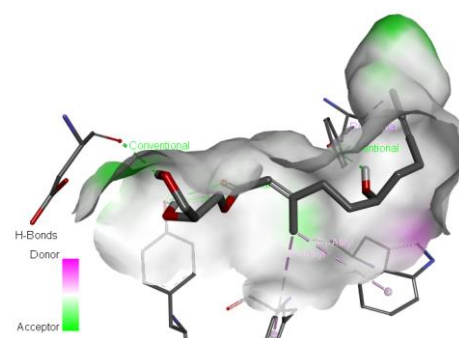
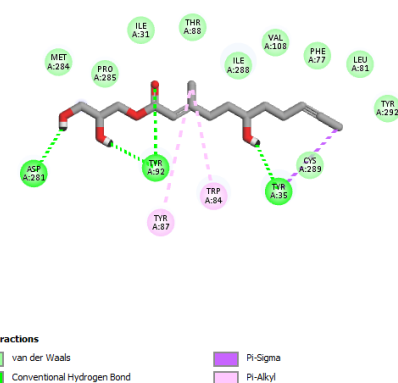
L16



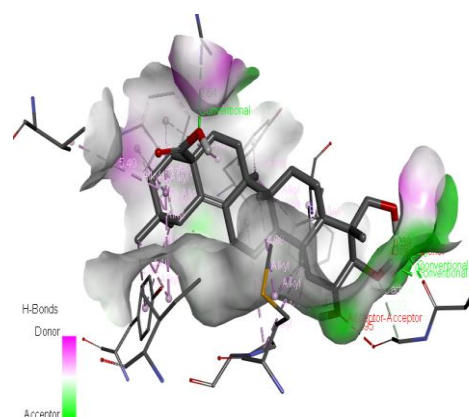
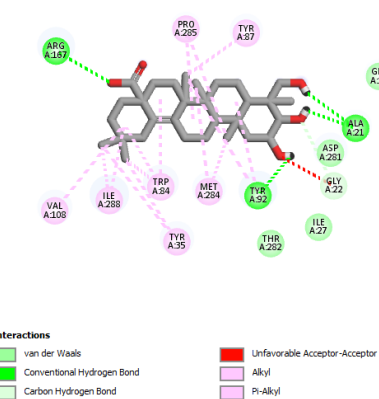
L17



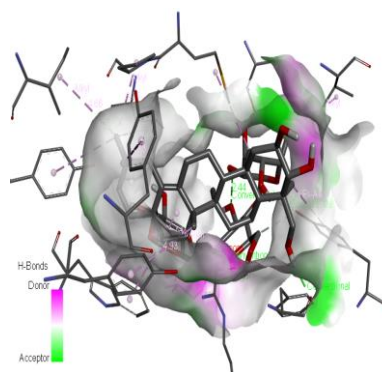
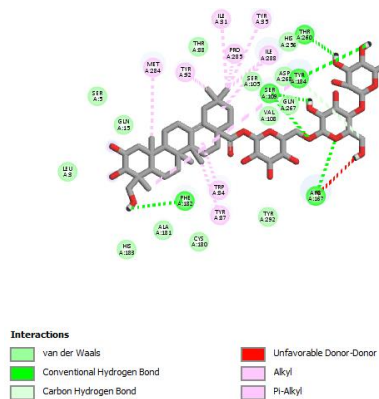
L18



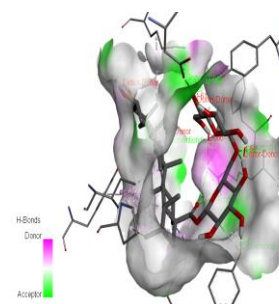
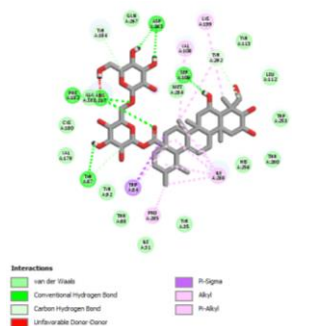
L19



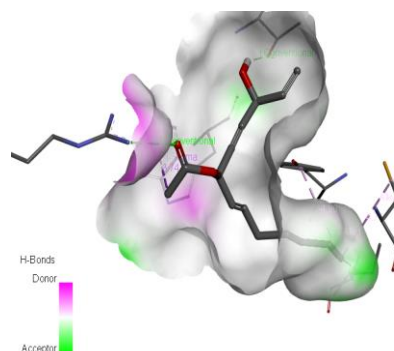
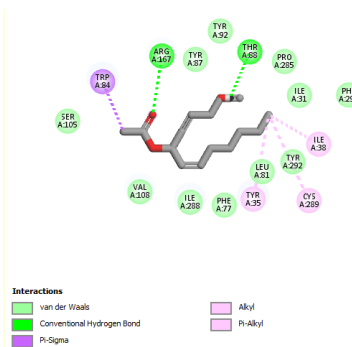
L20



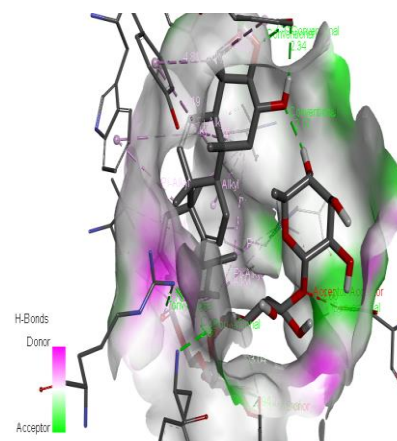
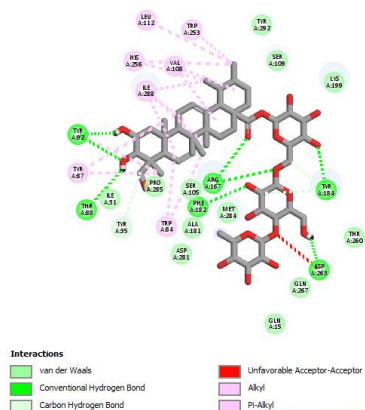
L21



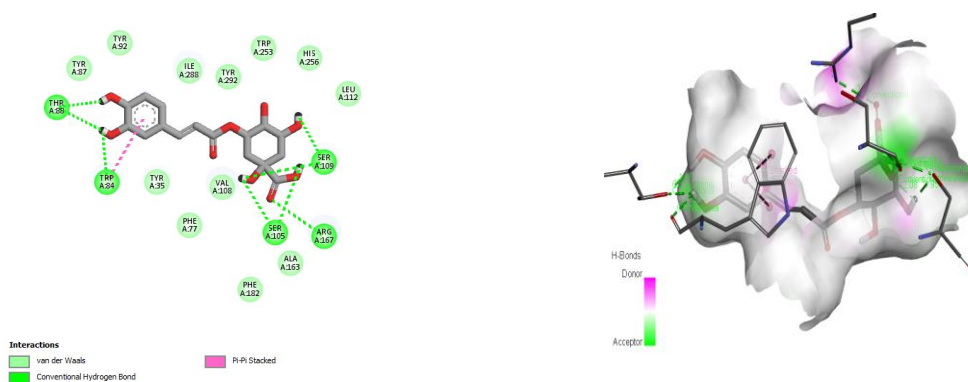
L22



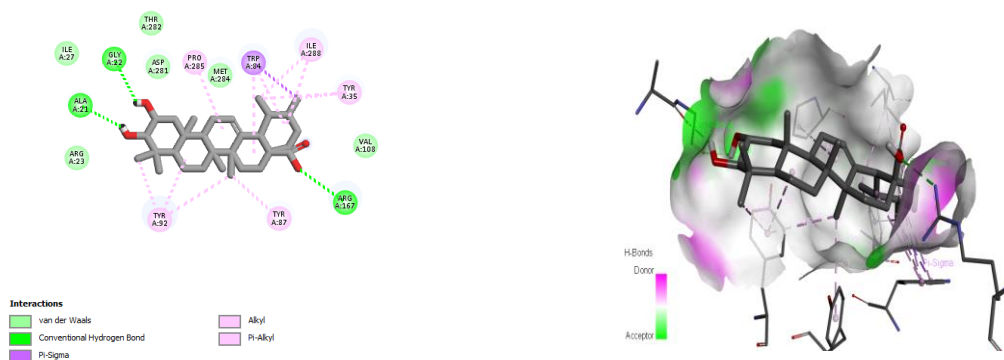
L23



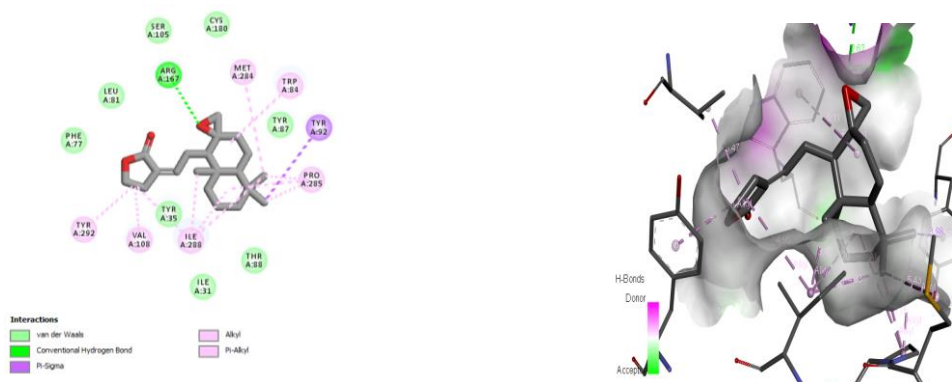
L24



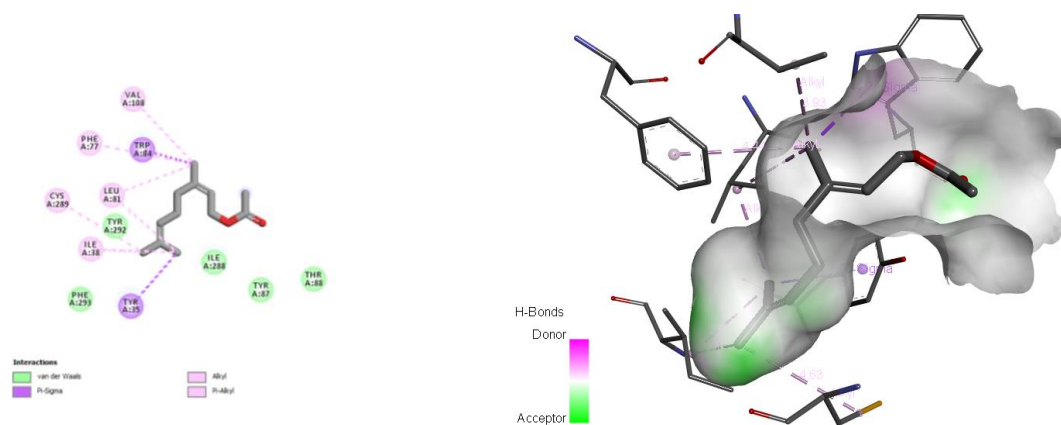
L25



L26

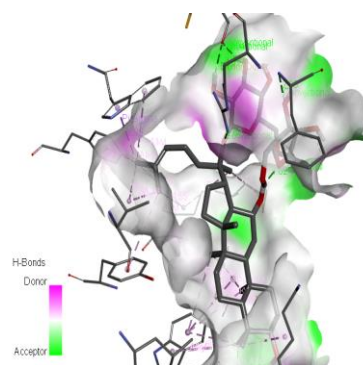
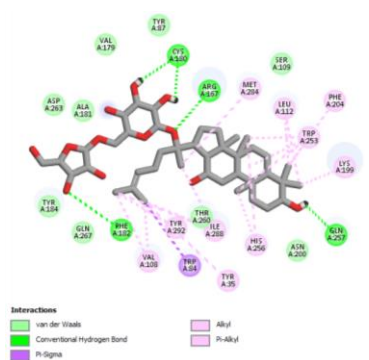


L27

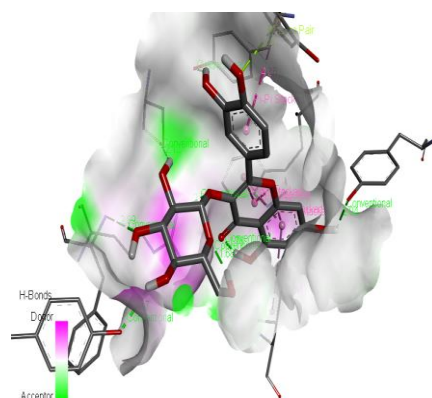
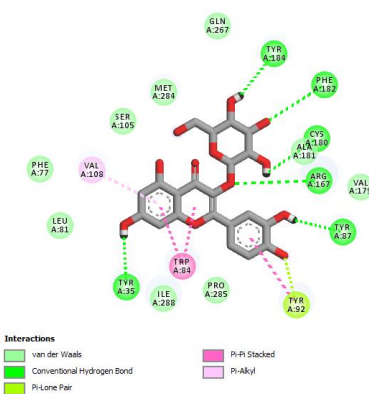




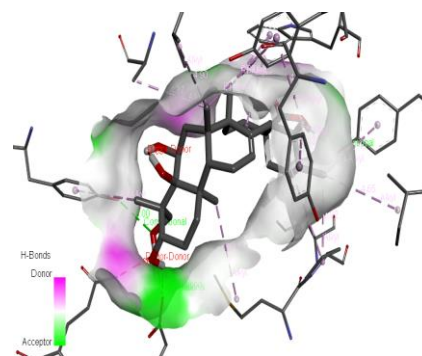
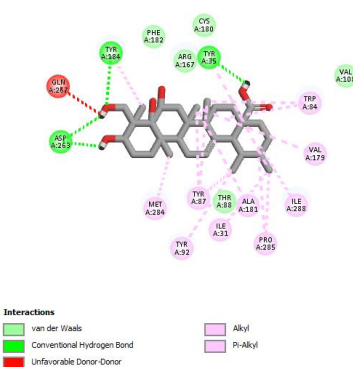
L28



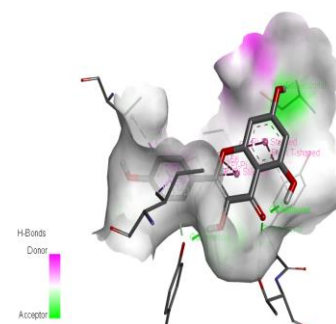
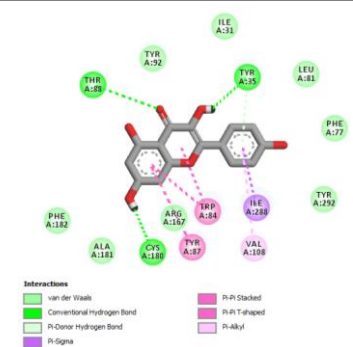
L29



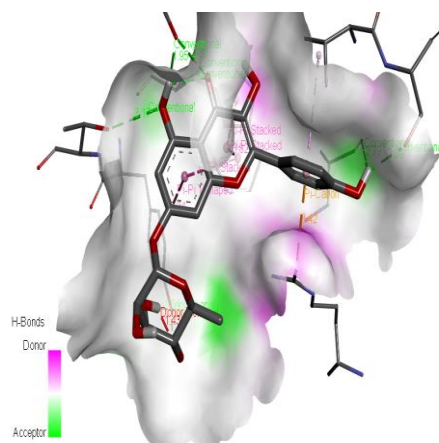
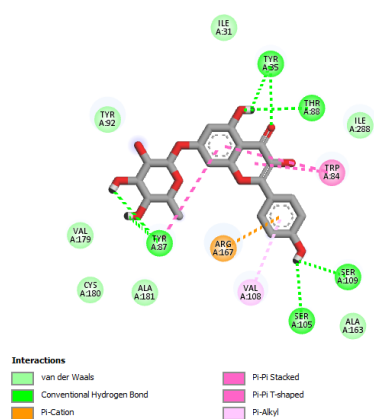
L30



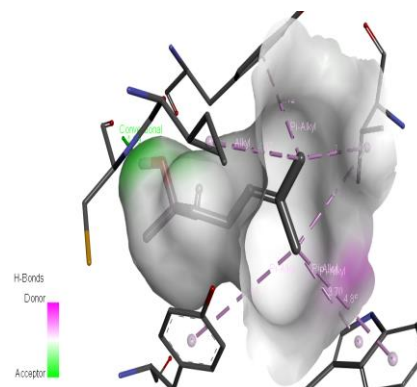
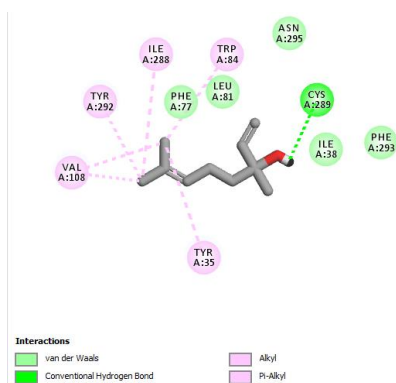
L31



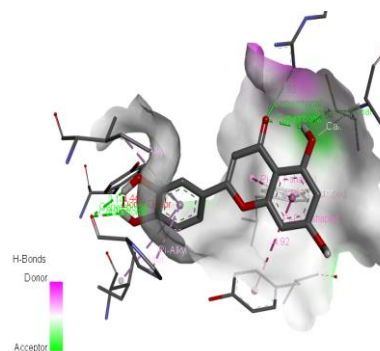
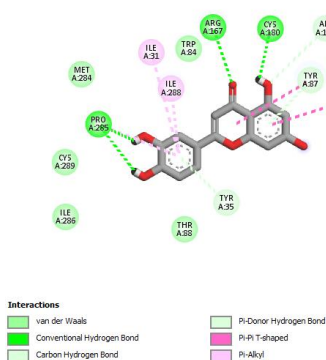
L32



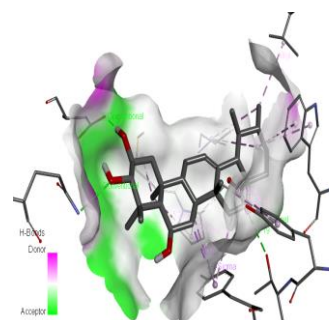
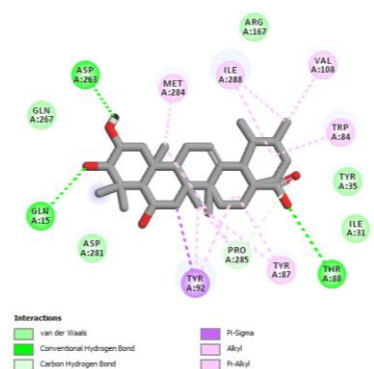
L33



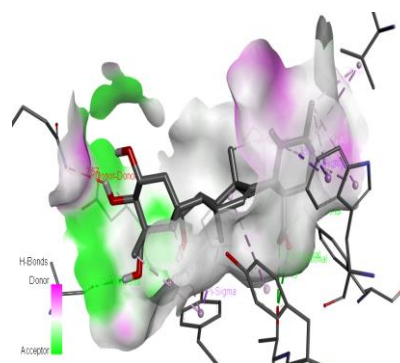
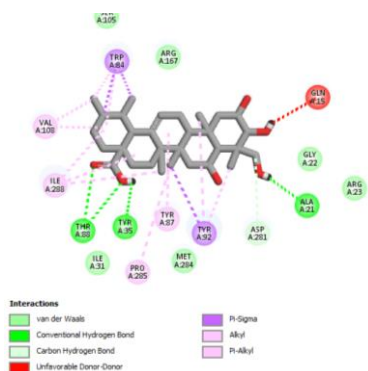
L34



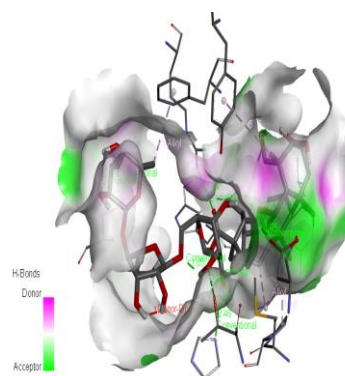
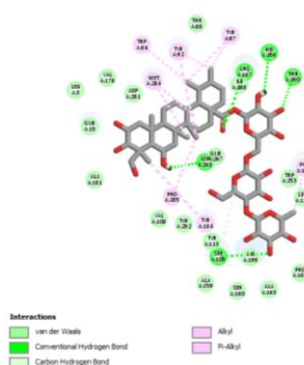
L35



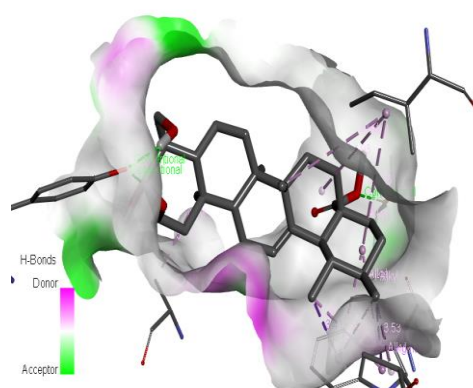
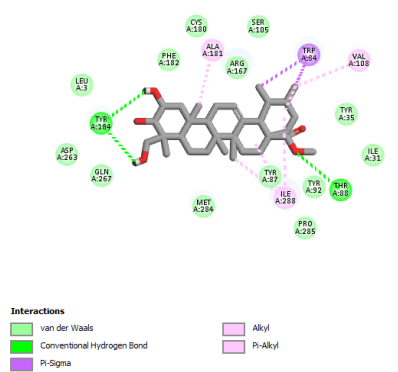
L36



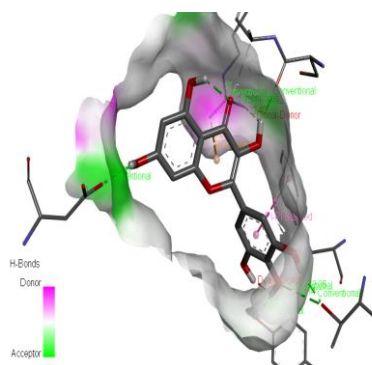
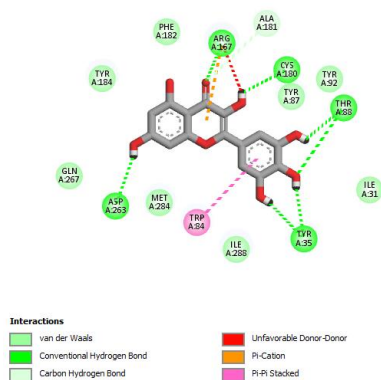
L37



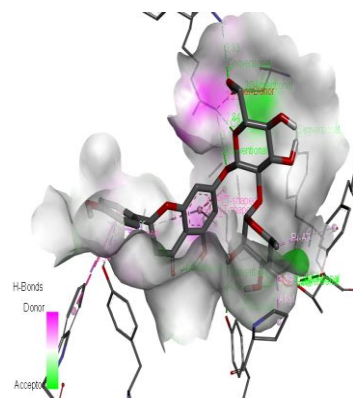
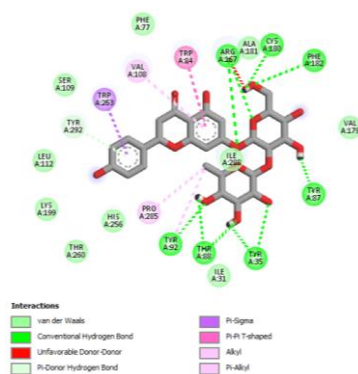
L38



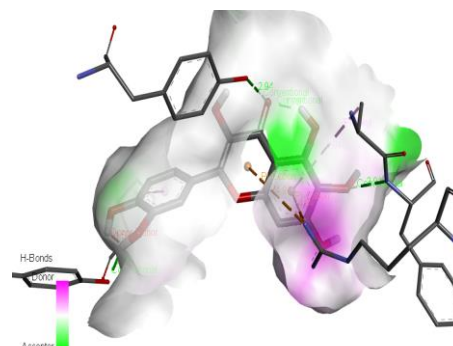
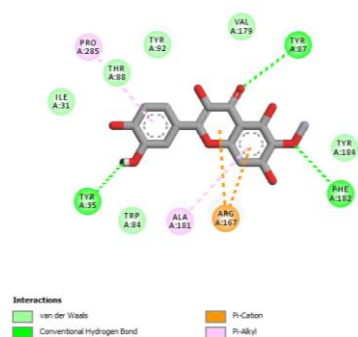
L39



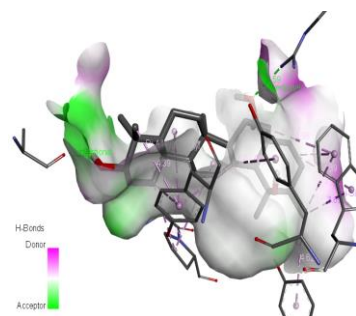
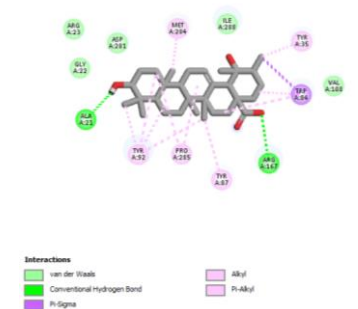
L40



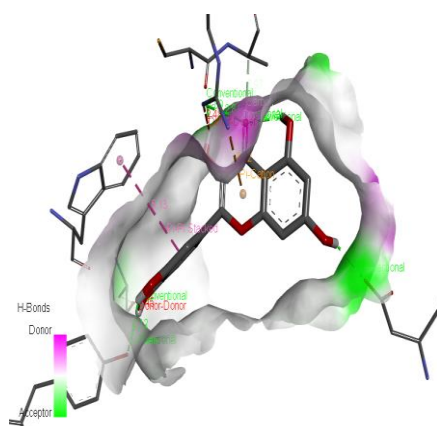
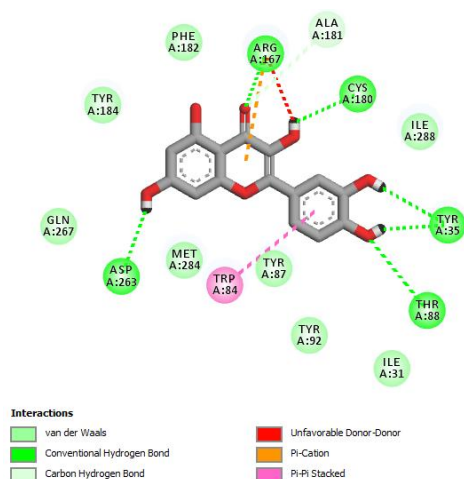
L41



L42

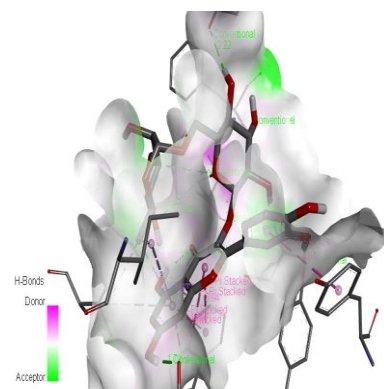
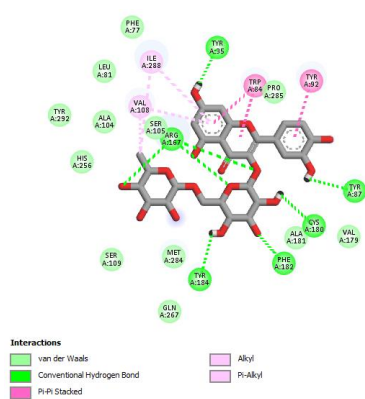


L43

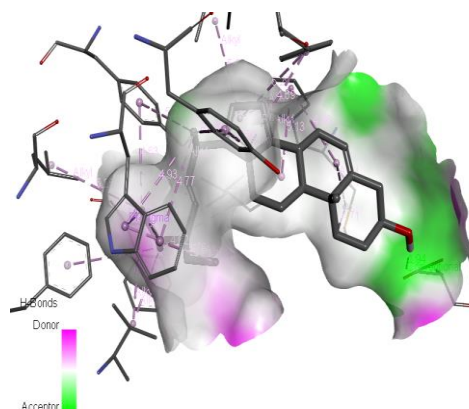
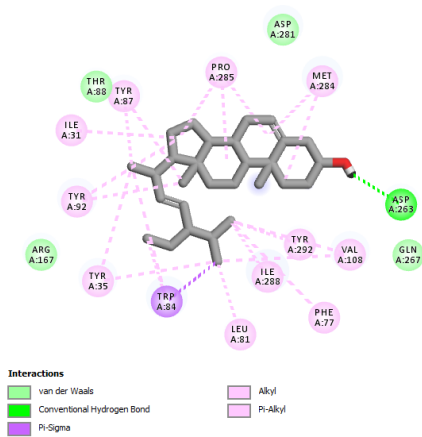




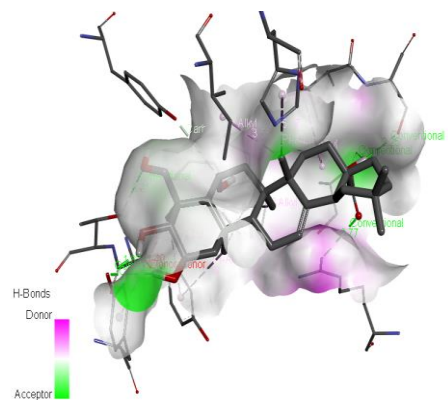
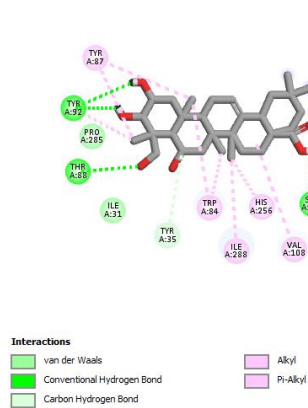
L44



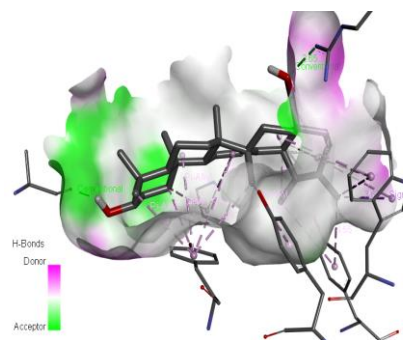
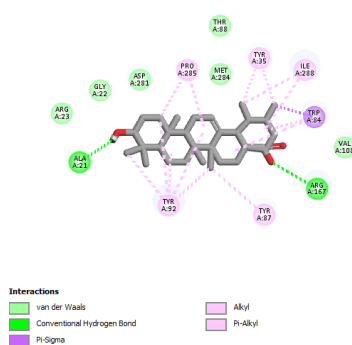
L45

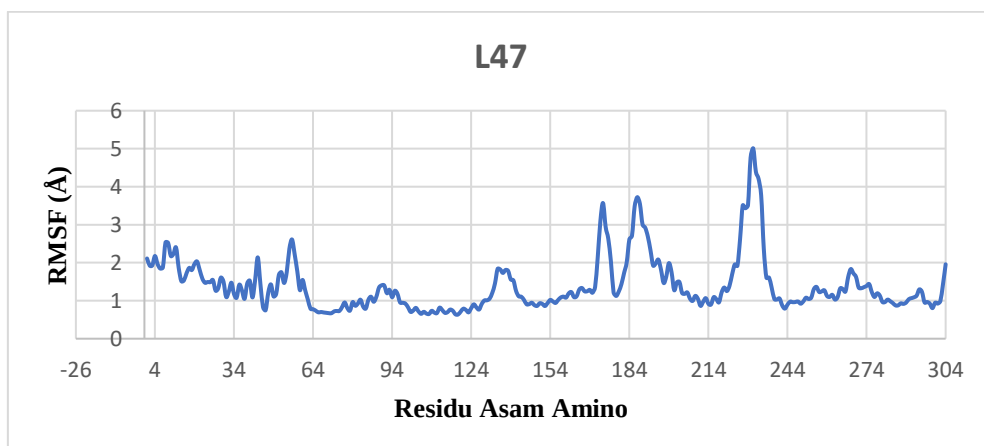
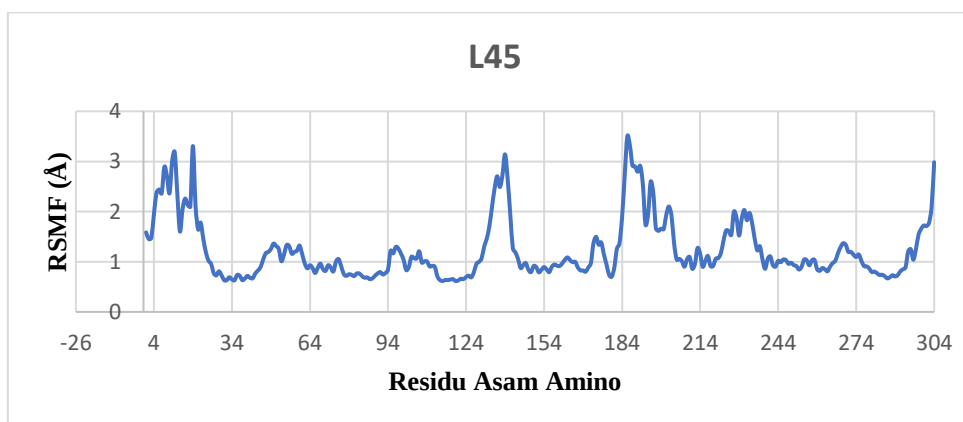
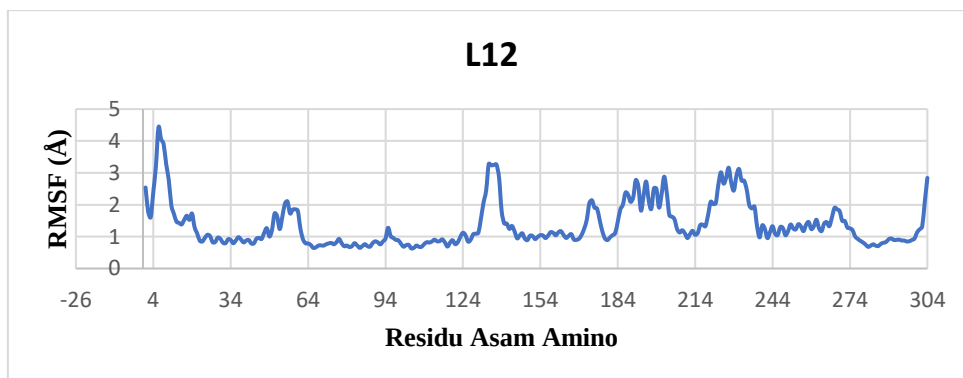
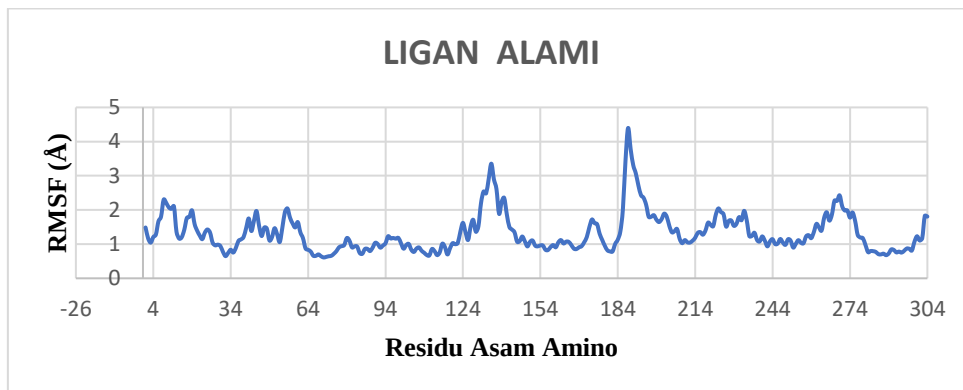


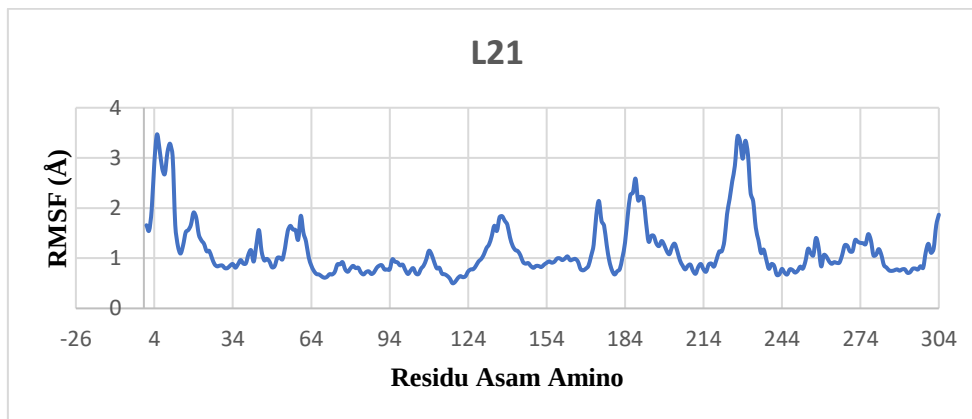
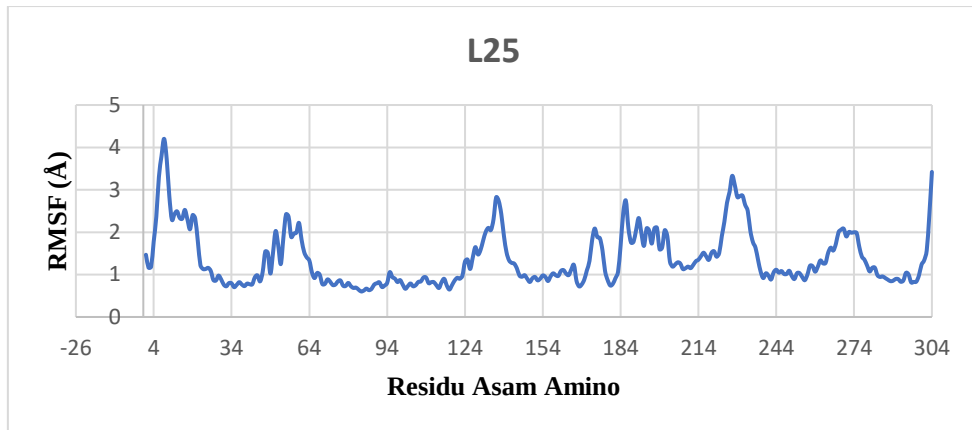
L46



L47



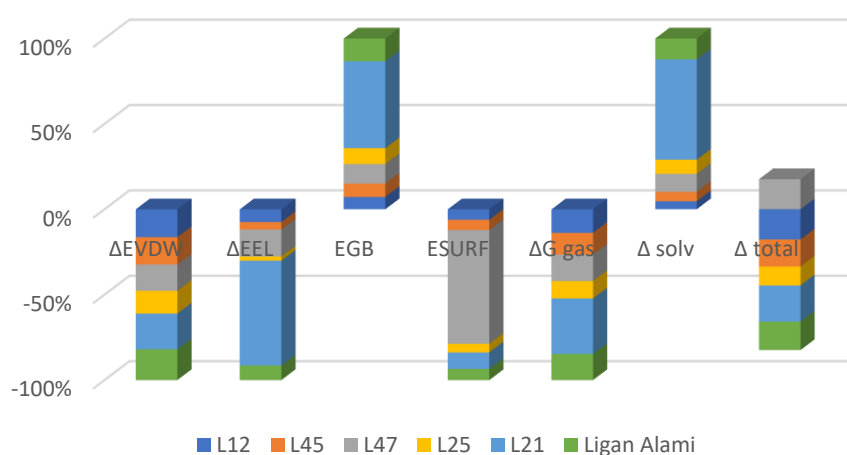
**Lampiran 4 Fluktuasi Residu di sekitar Atom Pengikatan**



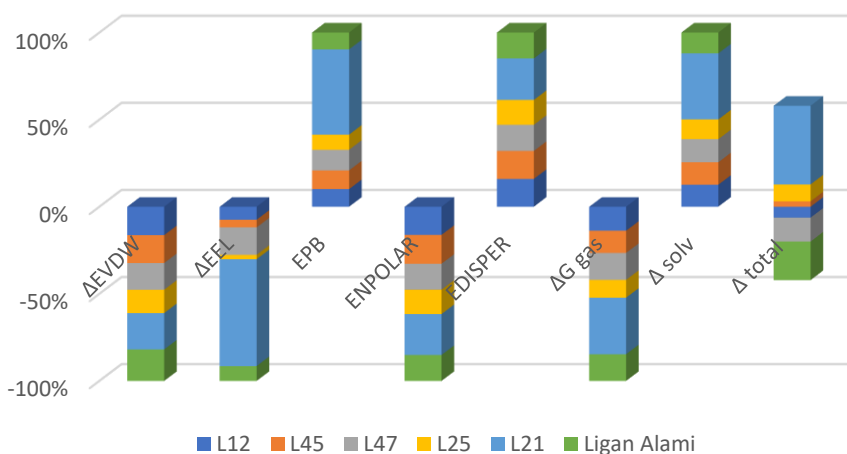
### Lampiran 5 MMPBSA dan MMGBSA

| Hasil Perhitungan MMPBSA   |               |              |          |          |          |                  |               |                |
|----------------------------|---------------|--------------|----------|----------|----------|------------------|---------------|----------------|
| Komponen Energi (kkal/mol) |               |              |          |          |          |                  |               |                |
| Kode Ligan                 | $\Delta EVDW$ | $\Delta EEL$ | EPB      | ENPOLAR  | EDISPER  | $\Delta G_{gas}$ | $\Delta solv$ | $\Delta total$ |
| L12                        | -56,0453      | -10,2312     | 27,594   | -38,3390 | 72,8314  | -66,2765         | 62,0865       | -4,1900        |
| L45                        | -55,3038      | -6,0002      | 29,3317  | -39,41   | 73,6181  | -61,4799         | 63,5398       | 2,06           |
| L47                        | -52,8469      | -21,6945     | 32,2484  | -35,3396 | 68,3891  | -74,5414         | 65,2979       | -9,2435        |
| L25                        | -45,9543      | -3,3898      | 23,7239  | -33,2949 | 65,448   | -49,3441         | 55,8737       | 6,5296         |
| L21                        | -72,0485      | -84,361      | 133,6296 | -55,6983 | 108,8499 | -156,4094        | 186,7813      | 30,3718        |
| Ligan Alami                | -62,2177      | -11,7117     | 26,4383  | -35,4742 | 68,0887  | -73,9294         | 59,0528       | -14,8767       |

**Grafik Komponen Energi MMGBSA**

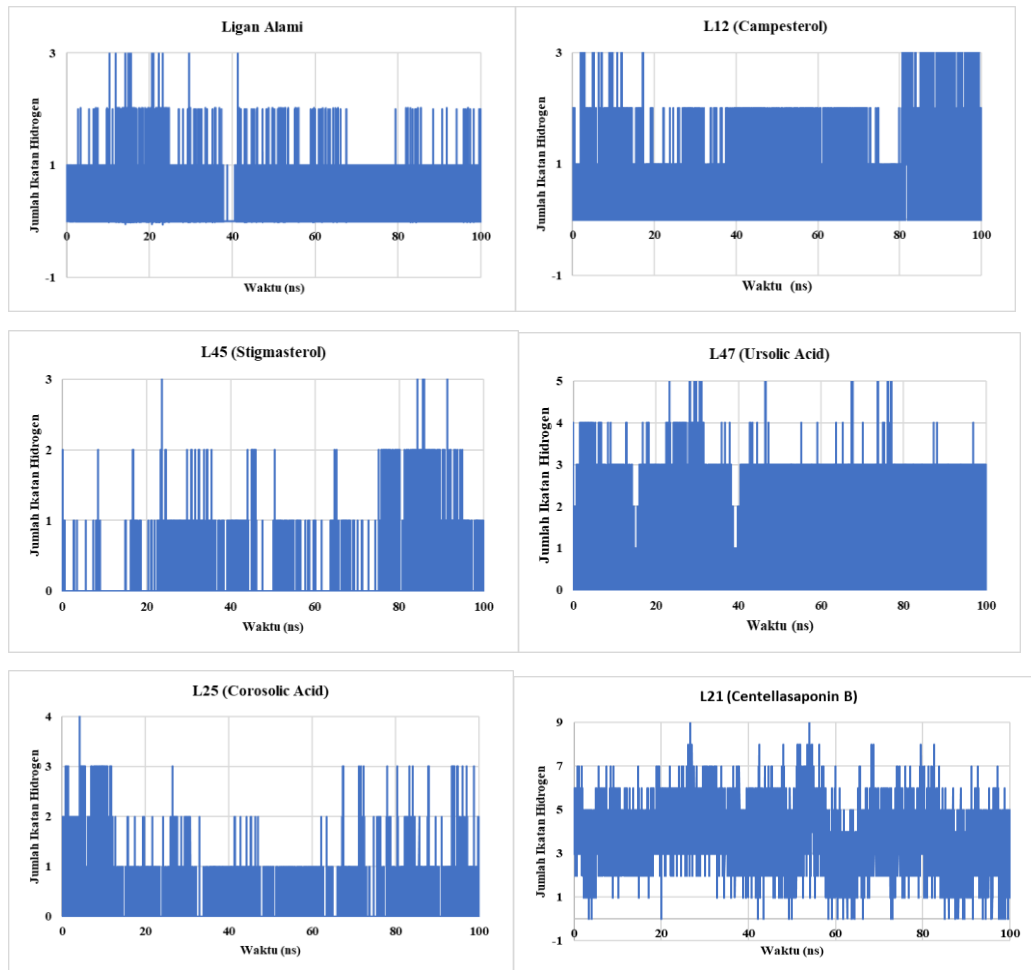


**Grafik Komponen Energi MMPBSA**





## Lampiran 6 Ikatan Hidrogen





## SURAT PERNYATAAN

Yang bertanda tangan di bawah ini,

Nama : Margareta Isa Peni

N P M : 11181245

adalah mahasiswa Fakultas Farmasi, Universitas Bhakti Kencana, menyatakan dengan sesungguhnya bahwa Naskah Tugas Akhir/Skripsi yang saya tulis dengan judul:

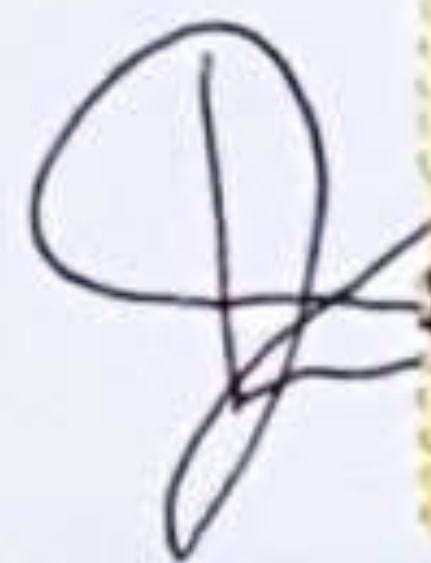
**PENAMBATAN MOLEKUL DAN DINAMIKA MOLEKUL SENYAWA  
PEGAGAN (*Centella asiatica* L.) TERHADAP RESEPTOR ANGIOTENSIN II  
TIPE 1 SEBAGAI ANTIHIPERTENSI**

*adalah benar-benar merupakan hasil karya saya sendiri. Apabila di kemudian hari diketahui bahwa isi Naskah Skripsi ini merupakan hasil plagiasi, maka saya bersedia menerima sanksi berupa pembatalan kelulusan dan atau pencabutan gelar yang saya peroleh.*

Demikian surat pernyataan ini saya buat untuk dapat dipergunakan sebagaimana mestinya.

Bandung, 9 Agustus 2022

Yang membuat pernyataan,

Margareta Isa Peni

NPM 11181245



## **SURAT PERNYATAAN**

Yang bertanda tangan di bawah ini,

Nama : Margareta Isa Peni

N P M : 11181245

Menyatakan bahwa demi kepentingan perkembangan ilmu pengetahuan, saya menyetujui abstrak Skripsi yang saya tulis dengan judul:

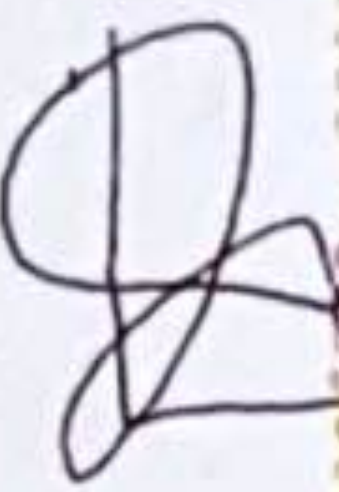
### **PENAMBATAN MOLEKUL DAN DINAMIKA MOLEKUL SENYAWA PEGAGAN (*Centella asiatica* L.) TERHADAP RESEPTOR ANGIOTENSIN II TIPE 1 SEBAGAI ANTIHIPERTENSI**

Untuk dipublikasikan atau ditampilkan di internet atau media lain yaitu Digital Library Perpustakaan Universitas Bhakti Kencana untuk kepentingan akademik, sebatas sesuai dengan Undang-Undang Hak Cipta.

Demikian surat pernyataan ini saya buat untuk dapat dipergunakan sebagaimana mestinya.

Bandung, 9 Agustus 2022

Yang membuat pernyataan,

Margareta Isa Peni

NPM 11181245