

## LAMPIRAN

### Lampiran 4. Senyawa kimia yang terkandung dalam alga cokelat.

| Kode Senyawa | Nama Senyawa                                                                                                                                                                | SMILES                                                                                                                                       |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------|
| S01          | Loliolide                                                                                                                                                                   | <chem>C[C@@]12C[C@H](CC(C1=CC(=O)O2)(C)C)O</chem>                                                                                            |
| S02          | Pachydictyol A                                                                                                                                                              | <chem>CC1=CC[C@@H]2[C@@H]1[C@@H]([C@@H](CCC2=C)[C@H](C)CCC=C(C)C)O</chem>                                                                    |
| S03          | 1H-Cyclopropa(3,4)cycloocta(1,2-c)furan-1-one, 4-((1R)-1,5-dimethyl-4-hexenyl)-3,4,5,6,7,7a,8,8a-octahydro-5-hydroxy-7-methyl-, (4S,5R,7R,7aS,8aS)-                         | <chem>C[C@@H]1C[C@H]([C@H](C2=C([C@@H]3[C@H]1C3)C(=O)OC2)[C@H](C)CCC=C(C)C)O</chem>                                                          |
| S04          | Dictyoxepin                                                                                                                                                                 | <chem>CC1=COC=C[C@]2([C@@H]1[C@@H]([C@@H](CC2)[C@H](C)CCC=C(C)C)O)C</chem>                                                                   |
| S05          | Verbascoside                                                                                                                                                                | <chem>C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)O[C@@H]2[C@H]([C@@H](O[C@@H]([C@H]2OC(=O)/C=C/C3=CC(=C(C=C3)O)O)CO)OCCC4=CC(=C(C=C4)O)O)O)O</chem> |
| S06          | Germacrene D                                                                                                                                                                | <chem>C/C1=C\CCCC(=C)/C=C/[C@@H](CC1)C(C)C</chem>                                                                                            |
| S07          | Gleenol                                                                                                                                                                     | <chem>C[C@@H]1CC[C@H]([C@H]([C@@]12CCC(=C2)C)O)C(C)C</chem>                                                                                  |
| S08          | [(2S,4S,5R,7R,8S)-5-methyl-8-[(2R)-6-methylhept-5-en-2-yl]-12-oxo-11-oxatricyclo[7.3.0.02,4]dodec-1(9)-en-7-yl] acetate                                                     | <chem>C[C@@H]1C[C@H]([C@H](C2=C([C@@H]3[C@H]1C3)C(=O)OC2)[C@H](C)CCC=C(C)C)OC(=O)C</chem>                                                    |
| S09          | 4-Hydroxydictyolactone                                                                                                                                                      | <chem>C/C1=C\C/C=C/2\ [C@@H](COC2=O)[C@@H]([C@@H](C1)O)[C@H](C)CCC=C(C)C</chem>                                                              |
| S10          | (R)-6-Butyl-1,4-cycloheptadiene                                                                                                                                             | <chem>CCCC[C@@H]1CC=CCC=C1</chem>                                                                                                            |
| S11          | (3S,8S,9S,10R,13R,14S,17R)-17-[(1R,4R)-4-hydroxy-4-isopropyl-1-methyl-hex-5-enyl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol | <chem>C[C@H](CC[C@](C=C)(C(C)C)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C</chem>                                    |
| S12          | 3-methyl-5-(6-methylhept-5-en-2-yl)-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol                                                                                    | <chem>CC1=CCC2C1C(C(CCC2=C)C(C)CCC=C(C)C)O</chem>                                                                                            |
| S13          | 3,8-dimethyl-5-(6-methylhept-5-en-2-yl)-3a,4,5,6,7,8a-hexahydro-1H-azulene-4,8-diol                                                                                         | <chem>CC1=CCC2C1C(C(CCC2(C)O)C(C)CCC=C(C)C)O</chem>                                                                                          |
| S14          | (3aS,4R,5S,8S,8aR)-3,8-dimethyl-5-[(2R)-6-methylhept-5-en-2-yl]-3a,4,5,6,7,8a-hexahydro-1H-azulene-4,8-diol                                                                 | <chem>CC1=CC[C@@H]2[C@@H]1[C@@H]([C@@H](CC[C@]2(C)O)[C@H](C)CCC=C(C)C)O</chem>                                                               |
| S15          | 2-[(1S,3aS,5E,9E,12aR)-3a,6,10-trimethyl-2,3,4,7,8,11,12,12a-octahydro-1H-                                                                                                  | <chem>C/C1=C\C/C=C/C[C@@]2(CC[C@@H]([C@H]2CC1)C(C)(C)O)C/C</chem>                                                                            |

| Kode Senyawa | Nama Senyawa                                                                                                                            | SMILES                                                                                  |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------|
|              | cyclopenta[11]annulen-1-yl]propan-2-ol                                                                                                  |                                                                                         |
| S16          | Bicyclosquisphellandrene                                                                                                                | <chem>C[C@@H]1CC[C@H](C2=CC(=C)CC[C@H]12)C(C)C</chem>                                   |
| S17          | 5-(2-hydroxy-6-methylhept-5-en-2-yl)-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol                                      | <chem>CC1=CCC2C1C(C(CCC2=C)C(C)(CCC=C(C)C)O)O</chem>                                    |
| S18          | (1S,6S,9R,10R)-9-hydroxy-6,10-dimethyl-2-methylidene-10-(4-methyl-3-oxopentyl)-12-oxatricyclo[7.2.1.0 <sup>1,6</sup> ]dodecan-5-one     | <chem>CC(C)C(=O)CC[C@@]1(C[C@]23C(=C)CCC(=O)[C@]2(CC[C@]1(O3)O)C)C</chem>               |
| S19          | (6R)-6-[(3aS,4R,5S,8aR)-4-hydroxy-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-5-yl]-2-methylheptan-3-one                   | <chem>CC1=CC[C@@H]2[C@@H]1[C@@H]([C@@H](CCC2=C)[C@H](C)CCC(=O)C(C)C)O</chem>            |
| S20          | Isopachydictyol A                                                                                                                       | <chem>CC1=CC[C@H]([C@H]([C@H]2[C@H]1CC=C2C)O)[C@H](C)CCC=C(C)C</chem>                   |
| S21          | (1S,2S,3aR,7S,8R,8aR)-1-methyl-7-[(2R)-6-methylhept-5-en-2-yl]-4-methylidene-2,3,3a,5,6,7,8,8a-octahydroazulene-1,2,8-triol             | <chem>C[C@H](CCC=C(C)C)[C@@H]1CCC(=C)[C@@H]2[C@@H]([C@@]([C@H]2[C@@H]1O)(C)O)O</chem>   |
| S22          | [(3R,3aS,5E,9E,11R,12aR)-10-formyl-6,12a-dimethyl-3-prop-1-en-2-yl-2,3,3a,4,7,8,11,12-octahydro-1H-cyclopenta[11]annulen-11-yl] acetate | <chem>C/C/1=C/C[C@H]2[C@@H](CC[C@@]2(C[C@H](/C(=C\CC1)/C=O)OC(=O)C)C(=C)C</chem>        |
| S23          | (1R,2E,5E,9R)-6-methyl-9-[(2S)-6-methylhept-5-en-2-yl]cyclonona-2,5-diene-1,2-dicarbaldehyde                                            | <chem>C/C/1=C\C/C=C(\[C@@H]([C@H](CC1)[C@@H](C)CCC=C(C)C)C=O)/C=O</chem>                |
| S24          | [(1R,3aS,4R,5S,8aR)-4-hydroxy-3-methyl-5-[(2R)-6-methylhept-5-en-2-yl]-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-1-yl] acetate    | <chem>CC1=C[C@H]([C@@H]2[C@@H]1[C@@H]([C@@H](C(C2=C)[C@H](C)CCC=C(C)C)O)OC(=O)C</chem>  |
| S25          | (1R,4S)-1,6-dimethyl-4-[(2R)-6-methylhept-5-en-2-yl]-1,2,3,4-tetrahydronaphthalene                                                      | <chem>C[C@@H]1CC[C@H](C2=C1C=CC(=C2)C)[C@H](C)CC=C(C)C</chem>                           |
| S26          | [(3aR,5S,7S,8R,8aS)-8-hydroxy-1-methyl-7-[(2R)-6-methylhept-5-en-2-yl]-4-methylidene-3a,5,6,7,8,8a-hexahydro-3H-azulen-5-yl] acetate    | <chem>CC1=CC[C@@H]2[C@@H]1[C@@H]([C@@H](C[C@@H](C2=C)OC(=O)C)[C@H](C)CCC=C(C)C)O</chem> |
| S27          | (1R,3aR,7S,8R,8aR)-1-methyl-7-[(2R)-6-methylhept-5-en-2-yl]-4-methylidene-3a,5,6,7,8,8a-hexahydroazulene-1,8-diol                       | <chem>C[C@H](CCC=C(C)C)[C@@H]1CCC(=C)[C@@H]2C=C[C@@]([C@H]2[C@@H]1O)(C)O</chem>         |
| S28          | (1S,3aS,5E,9E,12aR)-3a,6,10-trimethyl-1-prop-1-en-2-yl-1,2,4,7,8,11,12,12a-octahydrocyclopenta[11]annulen-3-one                         | <chem>C/C/1=C\CC/C(=C/C[C@]2([C@H](CC1)[C@H](CC2=O)C(=C)C)C)/C</chem>                   |

| Kode Senyawa | Nama Senyawa                                                                                                                                    | SMILES                                                                               |
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| S29          | [(1S,5R,6R,9R,10R)-9-hydroxy-6,10-dimethyl-2-methylidene-10-(4-methyl-3-oxopentyl)-12-oxatricyclo[7.2.1.0 <sup>1,6</sup> ]dodecan-5-yl] acetate | <chem>CC(C)C(=O)CC[C@@]1(C[C@]23C(=C)CC[C@H]([C@]2(CC[C@]1(O3)O)C)OC(=O)C)C</chem>   |
| S30          | (1R,2E,6E,10S)-3,7-dimethyl-10-[(2R)-6-methylhept-5-en-2-yl]cyclodeca-2,6-dien-1-ol                                                             | <chem>C/C1=C\CC/C=C/[C@@H]([C@@H](CC1)[C@H](C)CC=C(C)C)O)/C</chem>                   |
| S31          | (1R,4S,4aR,8aR)-1,6-dimethyl-4-[(2R)-6-methylhept-5-en-2-yl]-3,4,4a,7,8,8a-hexahydro-2H-naphthalen-1-ol                                         | <chem>CC1=C[C@H]2[C@@H](CC[C@@]([C@@H]2CC1)(C)O)[C@H](C)CCC=C(C)C</chem>             |
| S32          | (1S,4S,4aR,8aR)-1,6-dimethyl-4-[(2R)-6-methylhept-5-en-2-yl]-3,4,4a,7,8,8a-hexahydro-2H-naphthalen-1-ol                                         | <chem>CC1=C[C@H]2[C@@H](CC[C@]([C@@H]2CC1)(C)O)[C@H](C)CCC=C(C)C</chem>              |
| S33          | Hydroxyacetyldictyolal                                                                                                                          | <chem>C/C1=C\CC/C=C\([C@@H]([C@H]([C@H](C1)O)[C@@H](C)CCC=C(C)C)COC(=O)C)/C=O</chem> |
| S34          | (3aS,4R,5S,8aR)-5-[(2R,5R)-5-hydroxy-6-methylhept-6-en-2-yl]-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol                      | <chem>CC1=CC[C@@H]2[C@@H]1[C@@H]([C@@H](CCC2=C)[C@H](C)CC[C@H](C(=C)C)O)O</chem>     |
| S35          | (3aS,4R,5S,8aR)-5-[(2R,5S)-5-hydroxy-6-methylhept-6-en-2-yl]-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol                      | <chem>CC1=CC[C@@H]2[C@@H]1[C@@H]([C@@H](CCC2=C)[C@H](C)CC[C@H](C(=C)C)O)O</chem>     |
| S36          | (3aS,4R,5S,8aR)-5-[(2R)-4-[(2R)-3,3-dimethyloxiran-2-yl]butan-2-yl]-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol               | <chem>CC1=CC[C@@H]2[C@@H]1[C@@H]([C@@H](CCC2=C)[C@H](C)CC[C@H]3C(O3)(C)C)O</chem>    |
| S37          | (6E,10R)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-5,8,9,10-tetrahydro-4H-cyclonona[c]furan                                                     | <chem>C/C1=C\CCC2=COC=C2[C@H](CC1)[C@H](C)CCC=C(C)C</chem>                           |
| S38          | (6Z,10R)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-5,8,9,10-tetrahydro-4H-cyclonona[c]furan                                                     | <chem>C/C1=C/CCC2=COC=C2[C@H](CC1)[C@H](C)CCC=C(C)C</chem>                           |
| S39          | (3aS,5R,8aR)-3-methyl-5-[(2R)-6-methylhept-5-en-2-yl]-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulene                                          | <chem>CC1=CC[C@@H]2[C@@H]1C[C@@H](CCC2=C)[C@H](C)CCC=C(C)C</chem>                    |
| S40          | (3aR,5R)-3,8-dimethyl-5-[(2R)-6-methylhept-5-en-2-yl]-1,3a,4,5,6,7-hexahydroazulene                                                             | <chem>CC1=C2CC=C([C@H]2C[C@@H](CC1)[C@H](C)CCC=C(C)C)C</chem>                        |
| S41          | (3R,6R)-6-[(3aS,4R,5S,8aR)-4-hydroxy-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-5-yl]-2-methylheptane-2,3-diol                    | <chem>CC1=CC[C@@H]2[C@@H]1[C@@H]([C@@H](CCC2=C)[C@H](C)CC[C@H](C(C)(C)O)O)O</chem>   |

| Kode Senyawa | Nama Senyawa                                                                                                                             | SMILES                                                                                              |
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| S42          | [(1R,2E,5E,9R)-2-formyl-6-methyl-9-[(2S)-6-methylhept-5-en-2-yl]cyclonona-2,5-dien-1-yl]methyl acetate                                   | <chem>C/C1=C/C/C=C(\[C@@H]([C@H](CC1)[C@@H](C)CCC=C(C)C)COC(=O)C)/C=O</chem>                        |
| S43          | (1R,3aR,5E,9E,12S,12aS)-1-(2-hydroxypropan-2-yl)-3a,6,10-trimethyl-2,3,4,7,8,11,12,12a-octahydro-1H-cyclopenta[11]annulen-12-ol          | <chem>C/C1=C/C[C@]2(CC[C@H]([C@@H]2[C@H](C/C(=C/C1)C)O)C(C)(C)O)C</chem>                            |
| S44          | (6E)-7-methyl-10-(6-methylhept-5-en-2-yl)-3,3a,4,5,8,9,10,10a-octahydro-1H-cyclonona[c]furan-1-ol                                        | <chem>C/C1=C\CCCC2COC(C2C(CC1)C(C)CCC=C(C)C)O</chem>                                                |
| S45          | (3E,7E)-Dolabella-3,7-dien-18-ol                                                                                                         | <chem>C/C1=C\CC/C(=C/C[C@]2(CC[C@H]([C@@H]2CC1)C(C)(C)O)C)/C</chem>                                 |
| S46          | (1R,4R,7R,10S,15R)-7,10,15-trimethyl-4-propan-2-yl-14,16-dioxapentacyclo[8.4.2.01,9.03,7.013,15]hexadecan-4-ol                           | <chem>CC(C)[C@@]1(CC[C@]2(C1C[C@@]34C(C2)[C@@]5(CC[C@]3(O5)C)O4)C)C)O</chem>                        |
| S47          | 1-[(1S,6S,9R,10R,11S)-9,11-dihydroxy-6,10-dimethyl-2-methylidene-12-oxatricyclo[7.2.1.01,6]dodecan-10-yl]-4-methylpentan-3-one           | <chem>CC(C)C(=O)CC[C@@]1([C@@H]([C@]23C(=C)CCC[C@]2(CC[C@]1(O3)O)C)O)C</chem>                       |
| S48          | (10R)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-3,4,5,8,9,10-hexahydrocyclonona[c]furan-1-one                                            | <chem>CC1=C[C@H]([C@@H]2[C@@H]1[C@@H]([C@@H](C)CC2=C)[C@H](C)CCC=C(C)C)O)O</chem>                   |
| S49          | (1R,3aS,4R,5S,8aR)-3-methyl-5-[(2R)-6-methylhept-5-en-2-yl]-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulene-1,4-diol                    | <chem>CC1=C[C@H]([C@@H]2[C@@H]1[C@@H]([C@@H](C)CC2=C)[C@H](C)CCC=C(C)C)O)O</chem>                   |
| S50          | (4R,7R,8R,9S,12R)-9-[(2R)-6-methylhept-5-en-2-yl]-3-oxatricyclo[5.4.1.04,12]dodeca-1(11),5-dien-8-ol                                     | <chem>C[C@H](CCC=C(C)C)[C@@H]1CC=C2CO[C@H]3[C@@H]2[C@H]([C@@H]1O)C=C3</chem>                        |
| S51          | (1R,4S)-1,6-dimethyl-4-[(2S)-6-methylhept-5-en-2-yl]-1,2,3,4-tetrahydronaphthalene                                                       | <chem>C[C@@H]1CC[C@H](C2=C1C=CC(=C2)C)[C@@H](C)CCC=C(C)C</chem>                                     |
| S52          | [(2S,4S,5R,7R,8S,10R,12S)-10,12-dimethoxy-5-methyl-8-[(2R)-6-methylhept-5-en-2-yl]-11-oxatricyclo[7.3.0.02,4]dodec-1(9)-en-7-yl] acetate | <chem>C[C@@H]1C[C@H]([C@H](C2=C([C@@H]3[C@H]1C3)[C@H](O[C@H]2OC)OC)[C@H](C)CCC=C(C)C)OC(=O)C</chem> |
| S53          | (1S,4aS,5R,8S,8aR)-2,5-dimethyl-8-[(2R)-6-methylhept-5-en-2-yl]-4,4a,6,7,8,8a-hexahydro-1H-naphthalene-1,5-diol                          | <chem>CC1=CC[C@H]2[C@H]([C@@H]1O)[C@@H](CC[C@@]2(C)O)[C@H](C)CCC=C(C)C</chem>                       |
| S54          | [(2S,4S,5R,7R,8S)-8-[(E,2R)-6-hydroperoxy-6-methylhept-4-en-2-yl]-5-methyl-12-oxo-11-                                                    | <chem>C[C@@H]1C[C@H]([C@H](C2=C([C@@H]3[C@H]1C3)C(=O)OC2)[C@H](C)C/C=C/C(C)(C)OO)OC(=O)C</chem>     |

| Kode Senyawa | Nama Senyawa                                                                                                                                                                                                             | SMILES                                                                                                 |
|--------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|
| S55          | oxatricyclo[7.3.0.02,4]dodec-1(9)-en-7-yl] acetate<br>(3S,8S,9S,10R,13R,14S,17R)-17-((R,Z)-5-isopropylhept-5-en-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol | <chem>C/C=C(/CC[C@@H](C)[C@H]1CC[C@@H]2[C@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)\C(C)C</chem> |
| S56          | Dictyofuran C                                                                                                                                                                                                            | <chem>CC1=CC2=C(C=C(C=C2O1)O)C=O</chem>                                                                |
| S57          | (4R,5aR,6R,9aS,10aS)-4,6,9a-trihydroxy-5a,10a-dimethyl-9-methylidene-3-propan-2-yl-4,5,6,7,8,10-hexahydro-1H-benzo[f]azulen-2-one                                                                                        | <chem>CC(C)C1=C2[C@@H](C[C@@]3([C@@H](CCC(=C)[C@]3(C[C@]2(CC1=O)C)O)O)C)O</chem>                       |
| S58          | [(4R,5aS,6R,9aS,10aS)-4,6,9a-trihydroxy-10a-methyl-9-methylidene-2-oxo-3-propan-2-yl-4,5,6,7,8,10-hexahydro-1H-benzo[f]azulen-5a-yl]methyl acetate                                                                       | <chem>CC(C)C1=C2[C@@H](C[C@@]3([C@@H](CCC(=C)[C@]3(C[C@]2(CC1=O)C)O)O)COC(=O)C)O</chem>                |
| S59          | [(1S,3aR,4R,7aR)-7,7a-diformyl-3a-methyl-1-[(2S)-6-methylhept-5-en-2-yl]-2,3,4,5-tetrahydro-1H-inden-4-yl] acetate                                                                                                       | <chem>C[C@@H](CCC=C(C)C)[C@@H]1CC[C@@]2([C@]1(C(=CC[C@H]2OC(=O)C)C=O)C=O)C</chem>                      |
| S60          | [(3R,3aS,4S,6E,9R,10R,11E,12aR)-4-hydroxy-3-(2-hydroxypropan-2-yl)-6,10,12a-trimethyl-2,3,3a,4,5,8,9,10-octahydro-1H-cyclopenta[11]annulen-9-yl] acetate                                                                 | <chem>C[C@@H]1/C=C/[C@]2(CC[C@H]([C@@H]2[C@H](C/C=C/[C@H]1OC(=O)C)C)O)C(C)(C)O)C</chem>                |
| S61          | [(1R,3E,6E,8R,9R)-7,8-diformyl-3-methyl-9-[(2R)-6-methylhept-5-en-2-yl]cyclonona-3,6-dien-1-yl] acetate                                                                                                                  | <chem>C/C/1=C\C/C=C(\[C@@H]([C@H]([C@@H](C1)OC(=O)C)[C@H](C)CCC=C(C)C)C=O)/C=O</chem>                  |
| S62          | [(1R,2E,5E,9S)-2-formyl-6-methyl-9-[(2R)-6-methylhept-5-en-2-yl]cyclonona-2,5-dien-1-yl]methyl acetate                                                                                                                   | <chem>C/C/1=C\C/C=C(\[C@@H]([C@@H](CC1)[C@H](C)CCC=C(C)C)COC(=O)C)/C=O</chem>                          |
| S63          | [(3R,3aS,5E,9Z,11S,12aR)-10-formyl-6,12a-dimethyl-3-prop-1-en-2-yl-2,3,3a,4,7,8,11,12-octahydro-1H-cyclopenta[11]annulen-11-yl] acetate                                                                                  | <chem>C/C/1=C\C[C@H]2[C@@H](CC[C@@]2(C[C@@H]([C@@H]2C(=C/CC1)/C=O)OC(=O)C)C(=C)C</chem>                |
| S64          | 2-[(1R,3aR,4E,6S,9E,12S,12aS)-12-hydroxy-3a,6,10-trimethyl-2,3,6,7,8,11,12,12a-octahydro-1H-cyclopenta[11]annulen-1-yl]propan-2-yl acetate                                                                               | <chem>C[C@H]1CC/C=C(/C[C@@H]([C@H]2[C@@H](CC[C@@]2(/C=C1)C)C(C)(C)OC(=O)C)O)\C</chem>                  |
| S65          | (1R,3aE,6E,10R,10aR)-7-methyl-10-[(2S)-6-methylhept-5-en-2-yl]-3,5,8,9,10,10a-hexahydro-1H-cyclonona[c]furan-1-ol                                                                                                        | <chem>C/C/1=C\C/C=C/2CO[C@H]([C@@H]2[C@H](CC1)[C@@H](C)CCC=C(C)C)O</chem>                              |

| Kode Senyawa | Nama Senyawa                                                                                                                                | SMILES                                                                                          |
|--------------|---------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------|
| S66          | (1S,3aE,6Z,10S,10aR)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-3,5,8,9,10,10a-hexahydro-1H-cyclonona[c]furan-1-ol                           | <chem>C/C1=C/C/C=C\2/CO[C@@H]([C@@H]2[C@@H])(CC1)[C@H](C)CCC=C(C)C)O</chem>                     |
| S67          | (1S,3aE,6E,10S,10aS)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-3,5,8,9,10,10a-hexahydro-1H-cyclonona[c]furan-1-ol                           | <chem>C/C1=C\C/C/C=C\2/CO[C@@H]([C@H]2[C@@H])(CC1)[C@H](C)CCC=C(C)C)O</chem>                    |
| S68          | (3aR,4S,5R,8aS)-5-[(2S,5R)-6-chloro-5-hydroxy-6-methylheptan-2-yl]-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol            | <chem>CC1=CC[C@H]2[C@H]1[C@H]([C@H](CCC2=C)[C@@H](C)CC[C@H](C(C)(C)Cl)O)O</chem>                |
| S69          | (1S,3aS,4E,6R,9E,12R,12aR)-1-(2-hydroxypropan-2-yl)-3a,6,10-trimethyl-2,3,6,7,8,11,12,12a-octahydro-1H-cyclopenta[11]annulen-12-ol          | <chem>C[C@@H]\1CC/C=C(/C[C@H]([C@@H]2[C@H](CC[C@]2(/C=C1)C)C(C)(C)O)O)\C</chem>                 |
| S70          | (1R,3aR,4E,6S,9E,12S,12aS)-1-(2-hydroxypropan-2-yl)-3a,6,10-trimethyl-2,3,6,7,8,11,12,12a-octahydro-1H-cyclopenta[11]annulen-12-ol          | <chem>C[C@H]\1CC/C=C(/C[C@@H]([C@H]2[C@@H](CC[C@]2(/C=C1)C)C(C)(C)O)O)\C</chem>                 |
| S71          | (3aS,4S,5R,8aS)-5-[(2R)-2-hydroxy-6-methylhept-5-en-2-yl]-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol                     | <chem>CC1=CC[C@H]2[C@@H]1[C@@H]([C@@H](CCC2=C)[C@@](C)(CCC=C(C)C)O)O</chem>                     |
| S72          | (3aR,4S,5S,8aS)-5-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol                     | <chem>CC1=CC[C@H]2[C@H]1[C@@H]([C@H](CCC2=C)[C@](C)(CCC=C(C)C)O)O</chem>                        |
| S73          | (3aS,4S,5R,8aR)-5-[(2R)-2-hydroxy-6-methylhept-5-en-2-yl]-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol                     | <chem>CC1=CC[C@@H]2[C@@H]1[C@@H]([C@@H](CCC2=C)[C@@](C)(CCC=C(C)C)O)O</chem>                    |
| S74          | (4R,7S,8R,9S,12R)-6-methyl-9-[(2R)-6-methylhept-5-en-2-yl]-3-oxatricyclo[5.4.1.0 <sup>4,12</sup> ]dodeca-1(11),5-dien-8-ol                  | <chem>CC1=C[C@@H]2[C@@H]3[C@@H]1[C@@H]([C@@H](CC=C3CO2)[C@H](C)CCC=C(C)C)O</chem>               |
| S75          | (4R,7R,8S,9S,12R)-6-methyl-9-[(2R)-6-methylhept-5-en-2-yl]-3-oxatricyclo[5.4.1.0 <sup>4,12</sup> ]dodeca-1(11),5-dien-8-ol                  | <chem>CC1=C[C@@H]2[C@@H]3[C@H]1[C@H]([C@@H](CC=C3CO2)[C@H](C)CCC=C(C)C)O</chem>                 |
| S76          | (2S,4S,5R,7R,8S,10S,12R)-10,12-dimethoxy-5-methyl-8-[(2R)-6-methylhept-5-en-2-yl]-11-oxatricyclo[7.3.0.0 <sup>2,4</sup> ]dodec-1(9)-en-7-ol | <chem>C[C@@H]1C[C@H]([C@H](C2=C([C@@H]3[C@H]1C3)[C@@H](O[C@@H]2OC)OC)[C@H](C)CCC=C(C)C)O</chem> |

| Kode Senyawa | Nama Senyawa                                                                                                                                                      | SMILES                                                                                                         |
|--------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------|
| S77          | [(4S,5S,6R)-6-[(2R,3aR,4S,5R,7S,8aS)-2,4,7-trihydroxy-3,8-dimethylidene-1,2,3a,4,5,6,7,8a-octahydroazulen-5-yl]-5-acetyloxy-2-methylhept-2-en-4-yl] acetate       | <chem>C[C@H]([C@H]1C[C@@H](C(=C)[C@H]2C[C@H](C(=C)[C@@H]2[C@H]1O)O)[C@@H]([C@H](C=C(C)C)OC(=O)C)OC(=O)C</chem> |
| S78          | (1S,3R,5S,8E,12R,13S)-1,5,9-trimethyl-13-prop-1-en-2-yl-4-oxatricyclo[10.3.0.03,5]pentadec-8-en-15-one                                                            | <chem>C/C1=C\CC[C@]2([C@H](O2)C[C@]3([C@H](CC1)[C@H](CC3=O)C(=C)C)C)C</chem>                                   |
| S79          | (3aR,4R,5S,8S,8aR)-3,8-dimethyl-5-[(2R)-6-methylhept-5-en-2-yl]-3a,4,5,6,7,8a-hexahydro-1H-azulene-4,8-diol                                                       | <chem>CC1=CC[C@@H]2[C@H]1[C@@H]([C@@H](CC[C@]2(C)O)[C@H](C)CCC=C(C)C)O</chem>                                  |
| S80          | (1R,5E,8R,11S)-6-methyl-11-[(2S)-6-methylhept-5-en-2-yl]-9-oxabicyclo[6.2.1]undec-5-ene-2,10-dione                                                                | <chem>C/C1=C\CCC(=O)[C@H]2[C@@H]([C@@H](C1)OC2=O)[C@@H](C)CCC=C(C)C</chem>                                     |
| S81          | [(3aR,7S,8R,8aS)-8-hydroxy-1-methyl-7-[(2R)-6-methylhept-5-en-2-yl]-3,3a,6,7,8,8a-hexahydroazulen-4-yl]methyl acetate                                             | <chem>CC1=CC[C@@H]2[C@@H]1[C@@H]([C@@H](CC=C2COC(=O)C)[C@H](C)CCC=C(C)C)O</chem>                               |
| S82          | [(3R,3aS,4S,6E,8R,9R,10R,11E,12aR)-8,9-diacetyloxy-3-(2-hydroxypropan-2-yl)-6,10,12a-trimethyl-2,3,3a,4,5,8,9,10-octahydro-1H-cyclopenta[11]annulen-4-yl] acetate | <chem>C[C@@H]1/C=C/[C@]2(CC[C@H]([C@@H]2[C@H](C/C(=C/[C@H]([C@@H]1OC(=O)C)OC(=O)C/C)OC(=O)C)C(C)C)O)C</chem>   |
| S83          | (1S,3R,5S,8E,12R,13S)-1,5,9-trimethyl-13-prop-1-en-2-yl-4-oxatricyclo[10.3.0.03,5]pentadec-8-ene                                                                  | <chem>C/C1=C\CC[C@]2([C@H](O2)C[C@@]3(CC[C@@H]([C@H]3CC1)C(=C)C)C)C</chem>                                     |
| S84          | (3R,3aS,4S,5R,8aS)-5-[(2S,5R)-6-chloro-5-hydroxy-6-methylheptan-2-yl]-3-hydroperoxy-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydroazulen-4-ol                     | <chem>C[C@@H](CC[C@H](C(C)(C)Cl)O)[C@H]1CCC(=C)[C@H]2C=C[C@@]([C@@H]2[C@H]1O)(C)OO</chem>                      |
| S85          | [(4R,6R)-6-[(3S,3aR,4S,5R,8aS)-3,4-dihydroxy-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydroazulen-5-yl]-2-methylhept-2-en-4-yl] acetate                           | <chem>C[C@H](C[C@H](C=C(C)C)OC(=O)C)[C@H]1CCC(=C)[C@H]2C=C[C@]([C@H]2[C@H]1O)(C)O</chem>                       |
| S86          | [(2S,3S)-2-[(2R,3aR,4S,5R,7S,8aS)-2,4,7-trihydroxy-3,8-dimethylidene-1,2,3a,4,5,6,7,8a-octahydroazulen-5-yl]-6-methylhept-5-en-3-yl] acetate                      | <chem>C[C@@H]([C@H]1C[C@@H](C(=C)[C@H]2C[C@H](C(=C)[C@@H]2[C@H]1O)O)[C@H](CC=C(C)C)OC(=O)C</chem>              |
| S87          | [(2S,4R,5S,7R,8S)-5-methyl-8-[(2S)-6-methylhept-5-en-2-yl]-12-oxo-11-oxatricyclo[7.3.0.02,4]dodec-1(9)-en-7-yl] acetate                                           | <chem>C[C@H]1C[C@H]([C@H](C2=C([C@@H]3[C@@H]1C3)C(=O)OC2)[C@@H](C)CCC=C(C)C)OC(=O)C</chem>                     |

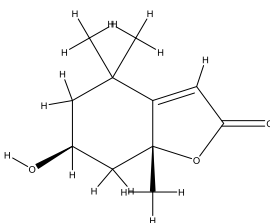
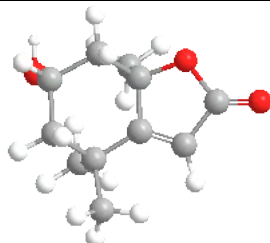
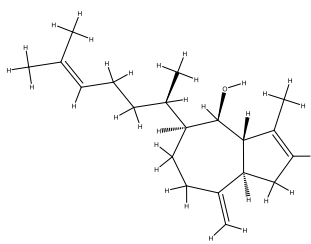
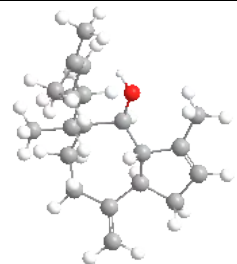
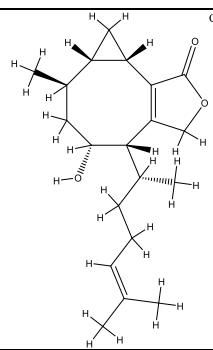
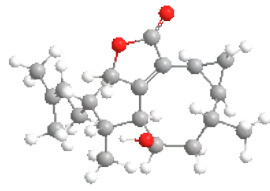
| Kode Senyawa | Nama Senyawa                                                                                                                                                 | SMILES                                                                                                             |
|--------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|
| S88          | [(1S,3aS,4E,6R,9E,12R,12aR)-1-(2-hydroxypropan-2-yl)-3a,6,10-trimethyl-2,3,6,7,8,11,12,12a-octahydro-1H-cyclopenta[11]annulen-12-yl] acetate                 | <chem>C[C@@H]\1CC/C=C/C[C@H]([C@@H]2[C@H](CC[C@]2(/C=C1)C)C(C)(C)O)OC(=O)C\C</chem>                                |
| S89          | [(1R,3aR,4E,6S,9E,12S,12aS)-1-(2-hydroxypropan-2-yl)-3a,6,10-trimethyl-2,3,6,7,8,11,12,12a-octahydro-1H-cyclopenta[11]annulen-12-yl] acetate                 | <chem>C[C@H]\1CC/C=C/C[C@@H]([C@H]2[C@@H](CC[C@]2(/C=C1)C)C(C)(C)O)OC(=O)C\C</chem>                                |
| S90          | (1S,5R,6S,10S)-10-hydroxy-5-[(2R)-6-methylhept-5-en-2-yl]-2-methylidenebicyclo[4.3.1]dec-7-ene-7-carbaldehyde                                                | <chem>C[C@H](CCC=C(C)C)[C@H]1CCC(=C)[C@@H]2CC=C([C@H]1[C@H]2O)C=O</chem>                                           |
| S91          | (1R,2S,6S,7S,8S)-1,3-dimethyl-8-[(2R)-6-methylhept-5-en-2-yl]tricyclo[4.4.0.02,7]dec-3-ene                                                                   | <chem>CC1=CC[C@H]2[C@H]3[C@@H]1[C@@]2(CC[C@H]3[C@H](C)CCC=C(C)C)C</chem>                                           |
| S92          | (1S,2S,6S,7S,8S)-1,3-dimethyl-8-[(2S)-6-methylhept-5-en-2-yl]tricyclo[4.4.0.02,7]dec-3-ene                                                                   | <chem>CC1=CC[C@H]2[C@H]3[C@@H]1[C@]2(CC[C@H]3[C@@H](C)CCC=C(C)C)C</chem>                                           |
| S93          | (3aR,7S,8R,8aS)-8-hydroxy-1-methyl-7-[(2R)-6-methylhept-5-en-2-yl]-3,3a,6,7,8,8a-hexahydroazulene-4-carbaldehyde                                             | <chem>CC1=CC[C@@H]2[C@@H]1[C@@H]([C@@H](CC=C2C=O)[C@H](C)CCC=C(C)C)O</chem>                                        |
| S94          | (3aS,7R,8S,8aR)-8-hydroxy-1-methyl-7-[(2R)-6-methylhept-5-en-2-yl]-3,3a,6,7,8,8a-hexahydroazulene-4-carbaldehyde                                             | <chem>CC1=CC[C@H]2[C@H]1[C@H]([C@H](CC=C2C=O)[C@@H](C)CCC=C(C)C)O</chem>                                           |
| S95          | 2-[(3R,3aS,5E,9S,10E,12aR)-5,9,12a-trimethyl-2,3,3a,4,7,8,9,12-octahydro-1H-cyclopenta[11]annulen-3-yl]propan-2-ol                                           | <chem>C[C@H]\1CC/C=C/C[C@H]2[C@@H](CC[C@@]2(/C=C1)C)C(C)(C)O\C</chem>                                              |
| S96          | [(4S,5S,6R)-6-[(3R,3aS,4R,5S,7R,8aR)-3,4,7-trihydroxy-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydroazulen-5-yl]-5-acetyloxy-2-methylhept-2-en-4-yl] acetate | <chem>C[C@H]([C@@H]1C[C@H](C(=C)[C@@H]2C=C[C@@]([C@@H]2[C@@H]1O)(C)O)O)[C@@H]([C@H](C=C(C)C)OC(=O)C)OC(=O)C</chem> |
| S97          | 2-[(1S,3aS,4E,6R,9E,12aR)-3a,6,10-trimethyl-2,3,6,7,8,11,12,12a-octahydro-1H-cyclopenta[11]annulen-1-yl]propan-2-yl acetate                                  | <chem>C[C@@H]\1CC/C=C/CC[C@@H]2[C@H](CC[C@]2(/C=C1)C)C(C)(C)OC(=O)C\C</chem>                                       |
| S98          | [(2S,3S,5R)-2-[(3aR,4S,5R,7S,8aS)-4,7-dihydroxy-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-5-yl]-5-                                            | <chem>CC1=CC[C@H]2[C@H]1[C@H]([C@H](C[C@@H](C2=C)O)[C@H](C)[C@H](C[C@H](C(=C)C)O)OC(=O)C)O</chem>                  |

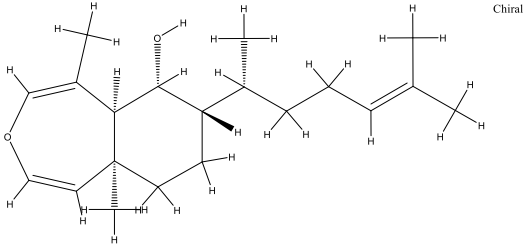
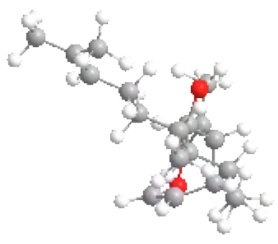
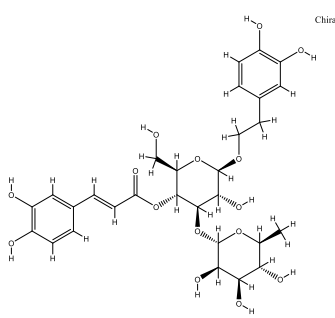
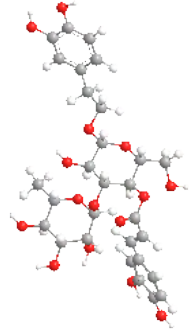
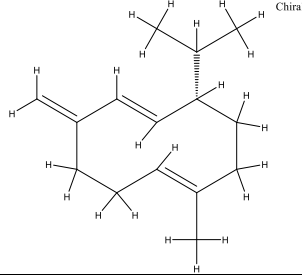
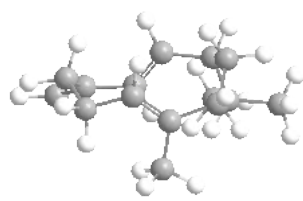
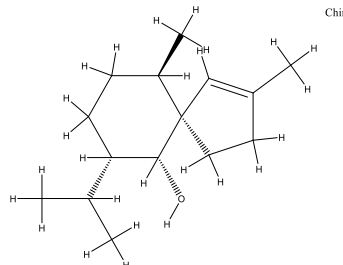
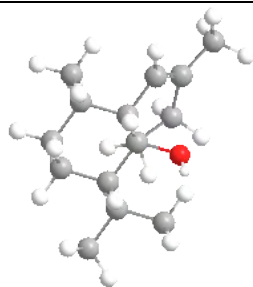
| Kode Senyawa | Nama Senyawa                                                                                                                                                            | SMILES                                                                                                   |
|--------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------|
| S99          | hydroxy-6-methylhept-6-en-3-yl] acetate<br>[(1R,2E,6E,10S)-3,7-dimethyl-10-[(2R)-6-methylhept-5-en-2-yl]cyclodeca-2,6-dien-1-yl] acetate                                | <chem>C/C1=C\CC/C(=C/[C@@H]([C@@H](CC1)[C@H](C)CC=C(C)C)OC(=O)C)/C</chem>                                |
| S100         | [(Z)-[(1S,3Z,5E,8S,11R)-6-methyl-11-[(2S)-6-methylhept-5-en-2-yl]-10-oxo-9-oxabicyclo[6.2.1]undeca-3,5-dien-2-ylidene)methyl] acetate                                   | <chem>C/C1=C\C=C/C(=C/OC(=O)C)/[C@@H]2[C@H]([C@H](C1)OC2=O)[C@@H](C)CCC=C(C)C</chem>                     |
| S101         | [(1R,5R,8S,9S)-1,2-diethyl-5-methyl-8-[(2R)-6-methylhept-5-en-2-yl]-9-bicyclo[3.3.1]non-2-enyl] acetate                                                                 | <chem>C[C@H](CCC=C(C)C)[C@@H]1CC[C@@]2(CC=C([C@]1([C@H]2)OC(=O)C)C=O)C=O)C</chem>                        |
| S102         | [(3R,3aS,4S,6E,8R,9R,10R,11E,12aR)-9-acetyloxy-4-hydroxy-3-(2-hydroxypropan-2-yl)-6,10,12a-trimethyl-2,3,3a,4,5,8,9,10-octahydro-1H-cyclopenta[11]annulen-8-yl] acetate | <chem>C[C@@H]1/C=C/[C@]2(CC[C@H]([C@@H]2[C@H](C/C(=C/[C@H]([C@@H]1OC(=O)C)OC(=O)C)/C)O)C(C)(C)O)C</chem> |
| S103         | (3aS,4R,5S,8S,8aR)-3,8-dimethyl-5-[(2R)-6-methylhept-6-en-2-yl]-3a,4,5,6,7,8a-hexahydro-1H-azulene-4,8-diol                                                             | <chem>CC1=CC[C@@H]2[C@@H]1[C@@H]([C@@H](CC[C@]2(C)O)[C@H](C)CCCC(=C)C)O</chem>                           |
| S104         | (3aS,4R,5S,8aR)-3-methyl-5-[(2R)-6-methylhept-6-en-2-yl]-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol                                                           | <chem>CC1=CC[C@@H]2[C@@H]1[C@@H]([C@@H](CCC2=C)[C@H](C)CCCC(=C)C)O</chem>                                |
| S105         | [(2S,3S)-2-[(3aS,4R,5S,7R,8aR)-4,7-dihydroxy-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-5-yl]-6-methylhept-6-en-3-yl] acetate                             | <chem>CC1=CC[C@@H]2[C@@H]1[C@@H]([C@@H](C[C@H](C2=C)O)[C@H](C)[C@H](CCC(=C)C)OC(=O)C)O</chem>            |
| S106         | (1R,5R,8S,9S)-9-hydroxy-5-methyl-8-[(2R)-6-methylhept-5-en-2-yl]bicyclo[3.3.1]non-2-ene-1,2-dicarbaldehyde                                                              | <chem>C[C@H](CCC=C(C)C)[C@@H]1CC[C@@]2(CC=C([C@]1([C@H]2)O)C=O)C=O)C</chem>                              |
| S107         | (3aS,5R,8S,8aR)-8-methoxy-3,8-dimethyl-5-[(2R)-6-methylhept-5-en-2-yl]-3a,4,5,6,7,8a-hexahydro-1H-azulene                                                               | <chem>CC1=CC[C@@H]2[C@@H]1C[C@@H](CC[C@]2(C)OC)[C@H](C)CCC=C(C)C</chem>                                  |
| S108         | [(1Z,5E,8R,11S)-6-methyl-11-[(2S)-6-methylhept-5-en-2-yl]-10-oxo-9-oxabicyclo[6.2.1]undeca-1,5-dien-2-yl]methyl acetate                                                 | <chem>C/C1=C\CC/C(=C/2[C@@H]([C@@H](C1)OC2=O)[C@@H](C)CCC=C(C)C)/COC(=O)C</chem>                         |
| S109         | (3aE,6E,10R,10aR)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-1,5,8,9,10,10a-hexahydrocyclonona[c]furan-3-one                                                             | <chem>C/C1=C\C/C=C/2[C@H](COC2=O)[C@H](CC1)[C@H](C)CCC=C(C)C</chem>                                      |
| S110         | (3aE,6E,10S,10aS)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-                                                                                                            | <chem>C/C1=C\C/C=C/2[C@@H](COC2=O)[C@@H](CC1)[C@H](C)CCC=C(C)C</chem>                                    |

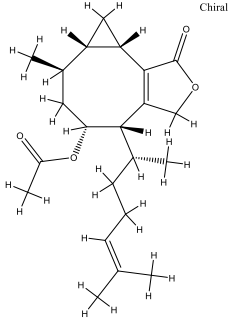
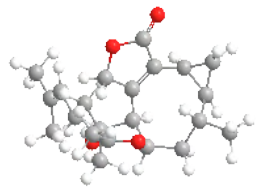
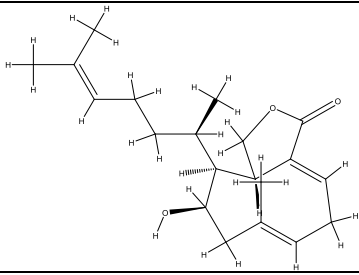
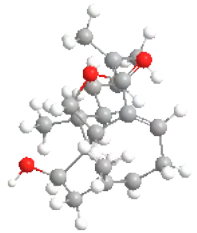
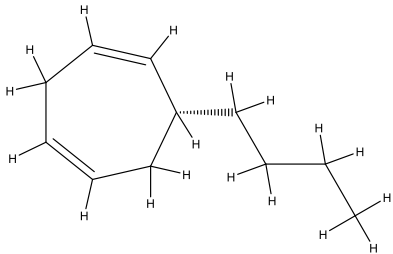
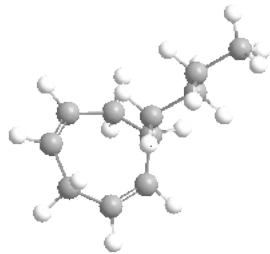
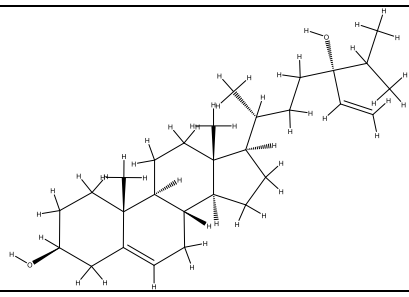
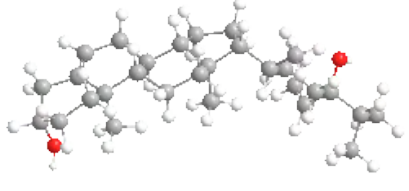
| Kode Senyawa | Nama Senyawa                                                                                                                                                                                    | SMILES                                                                                                      |
|--------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------|
| S111         | 1,5,8,9,10,10a-hexahydrocyclonona[c]furan-3-one [(1R,3R,3aE,6E,9S,10R,10aR)-1,3-dimethoxy-7-methyl-10-[(2S)-6-methylhept-5-en-2-yl]-3,5,8,9,10,10a-hexahydro-1H-cyclonona[c]furan-9-yl] acetate | <chem>C/C1=C/C/C=C/2\ [C@@H]([C@H]([C@H](C1)OC(=O)C)[C@@H](C)CCC=C(C)C)[C@@H](O[C@H]2OC)OC</chem>           |
| S112         | [(3R,3aS,4S,6E,8R,9R,10R,11E,12aR)-9-acetyloxy-3-(2-acetyloxypropan-2-yl)-4-hydroxy-6,10,12a-trimethyl-2,3,3a,4,5,8,9,10-octahydro-1H-cyclopenta[11]annulen-8-yl] acetate                       | <chem>C[C@@H]1/C=C/[C@]2(CC[C@H]([C@@H]2[C@H](C/C=C/[C@H]([C@@H]1OC(=O)C)OC(=O)C)/C)O)C(C)(C)OC(=O)C</chem> |
| S113         | (6E,10S)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-3,4,5,8,9,10-hexahydrocyclonona[c]furan-1-one                                                                                                | <chem>C/C1=C\CCC2=C([C@@H](CC1)[C@H](C)CCC=C(C)C)C(=O)OC2</chem>                                            |
| S114         | (1S,3R,5S,8E,12R,13S,15R)-1,5,9-trimethyl-13-prop-1-en-2-yl-4-oxatricyclo[10.3.0.03,5]pentadec-8-en-15-ol                                                                                       | <chem>C/C1=C\CC[C@]2([C@H](O2)C[C@]3([C@H](CC1)[C@H](C[C@H]3O)C(=C)C)C)C</chem>                             |
| S115         | [(1S,2E,5E,8R,9R)-2-formyl-8-hydroxy-6-methyl-9-[(2R)-6-methylhept-5-en-2-yl]cyclonona-2,5-dien-1-yl]methyl acetate                                                                             | <chem>C/C1=C\C/C=C([C@H]([C@H]([C@@H](C1)O)[C@H](C)CCC=C(C)C)COC(=O)C)/C=O</chem>                           |
| S116         | [(3aE,6E,9R,10S,10aS)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-3-oxo-1,5,8,9,10,10a-hexahydrocyclonona[c]furan-9-yl] acetate                                                                   | <chem>C/C1=C\C/C=C/2\ [C@@H](COC2=O)[C@@H]([C@@H](C1)OC(=O)C)[C@H](C)CCC=C(C)C</chem>                       |
| S117         | (1S,3aE,6E,10R,10aR)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-3,5,8,9,10,10a-hexahydro-1H-cyclonona[c]furan-1-ol                                                                               | <chem>C/C1=C\C/C=C/2\CO[C@@H]([C@@H]2[C@H](CC1)[C@H](C)CCC=C(C)C)O</chem>                                   |
| S118         | (1S,10R,10aR)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-3,5,8,9,10,10a-hexahydro-1H-cyclonona[c]furan-1-ol                                                                                      | <chem>CC1=CCC=C2CO[C@@H]([C@@H]2[C@H](CC1)[C@H](C)CCC=C(C)C)O</chem>                                        |
| S119         | (3R,3aS,7R,7aS)-7-hydroxy-7a-methyl-3-[(2S)-6-methylhept-5-en-2-yl]-2,3,6,7-tetrahydro-1H-indene-3a,4-dicarbaldehyde                                                                            | <chem>C[C@@H](CCC=C(C)C)[C@H]1CC[C@]2([C@@]1(C(=CC[C@H]2O)C=O)C=O)C</chem>                                  |
| S120         | (1R,2S,5E,8R,11S)-6-methyl-11-[(2S)-6-methylhept-5-en-2-yl]-10-oxo-9-oxabicyclo[6.2.1]undec-5-ene-2-carbaldehyde                                                                                | <chem>C/C1=C\CC[C@@H]([C@H]2[C@@H]([C@@H](C1)OC2=O)[C@@H](C)CCC=C(C)C)C=O</chem>                            |
| S121         | 2-[(1S,3aS,4E,6R,9E,12aR)-3a,6,10-trimethyl-2,3,6,7,8,11,12,12a-octahydro-1H-                                                                                                                   | <chem>C[C@@H]\1CC/C=C/CC[C@@H]2[C@H](CC[C@]2(/C=C1)C)C(C)(C)O)\C</chem>                                     |

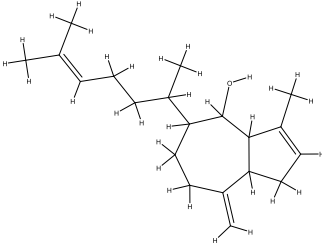
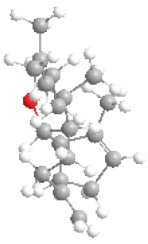
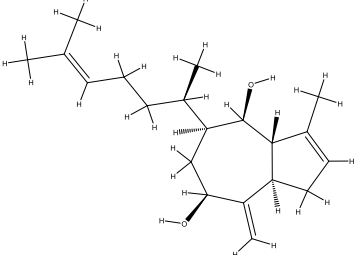
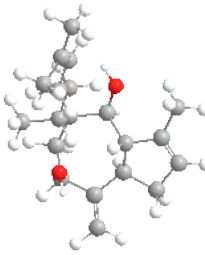
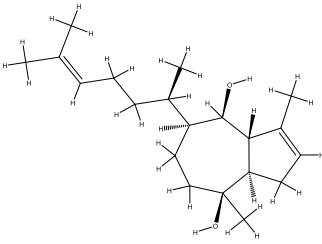
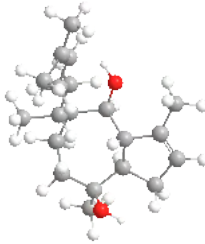
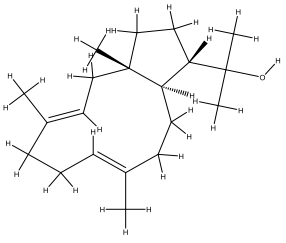
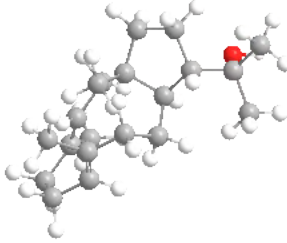
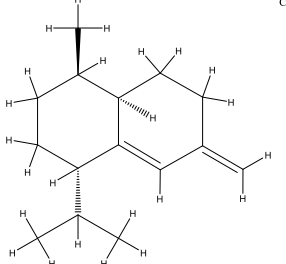
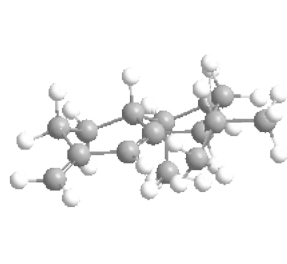
| Kode Senyawa | Nama Senyawa                                                                                                                                            | SMILES                                                                         |
|--------------|---------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------|
| S122         | cyclopenta[11]annulen-1-yl]propan-2-ol<br>[(1R,8S,9R)-2-formyl-8-hydroxy-6-methyl-9-[(2S)-6-methylhept-5-en-2-yl]cyclonona-2,5-dien-1-yl]methyl acetate | <chem>CC1=CCC=C([C@@H]([C@H]([C@H](C1)O)[C@@H](C)CCC=C(C)C)COC(=O)C)C=O</chem> |

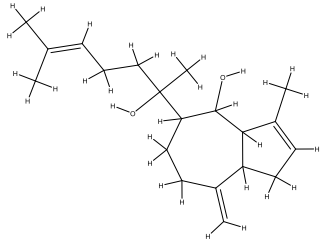
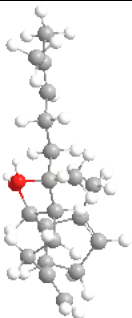
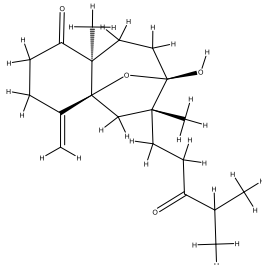
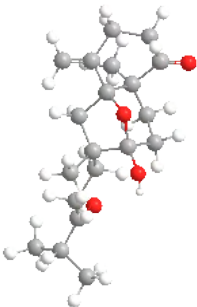
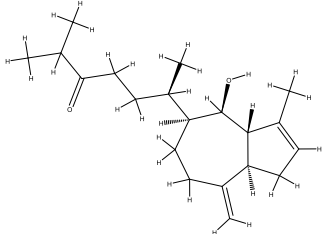
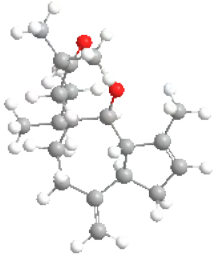
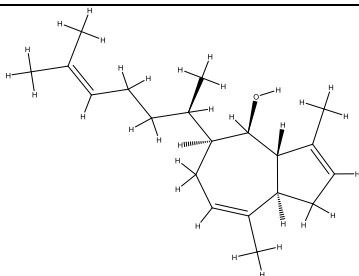
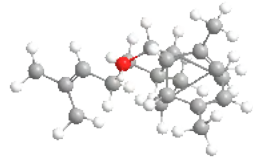
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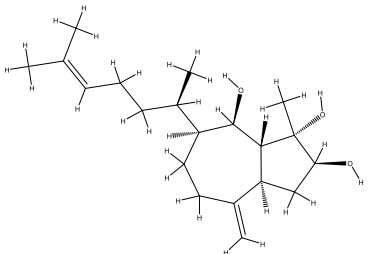
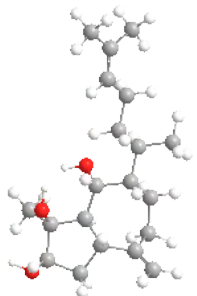
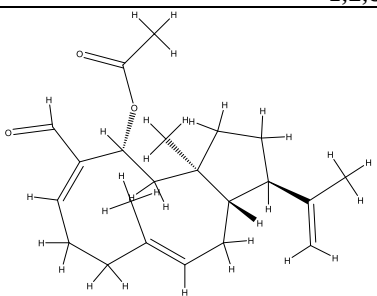
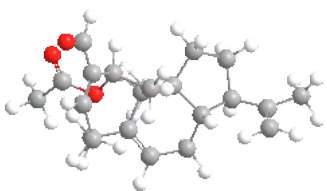
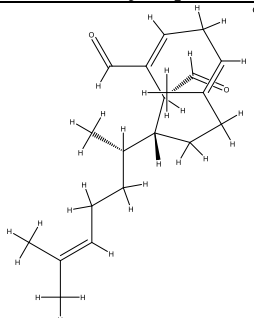
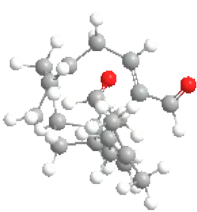
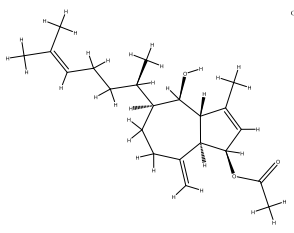
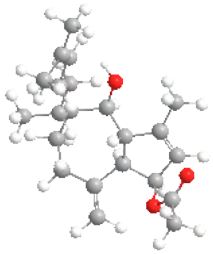
| Kode Senyawa                                                                                                                                        | Struktur 2D                                                                                       | Struktur 3D                                                                           |
|-----------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S01                                                                                                                                                 |  <p>Chiral</p>   |    |
| Loliolide                                                                                                                                           |                                                                                                   |                                                                                       |
| S02                                                                                                                                                 |  <p>Chiral</p> |  |
| Pachydictyol A                                                                                                                                      |                                                                                                   |                                                                                       |
| S03                                                                                                                                                 |  <p>Chiral</p> |  |
| 1H-Cyclopropa(3,4)cycloocta(1,2-c)furan-1-one, 4-((1R)-1,5-dimethyl-4-hexenyl)-3,4,5,6,7,7a,8,8a-octahydro-5-hydroxy-7-methyl-, (4S,5R,7R,7aS,8aS)- |                                                                                                   |                                                                                       |

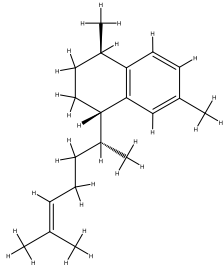
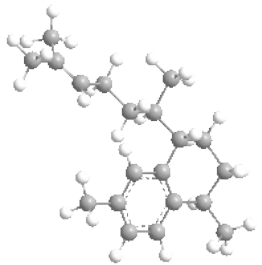
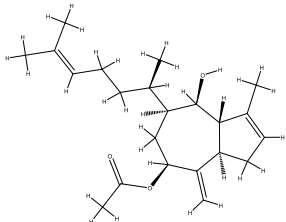
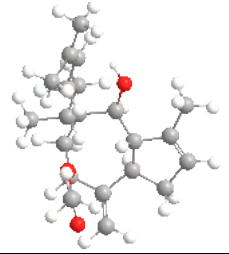
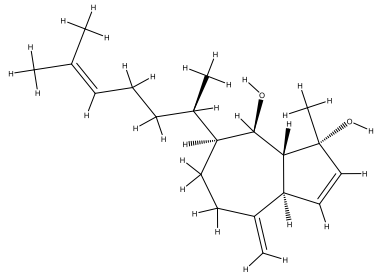
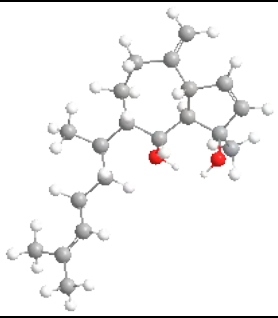
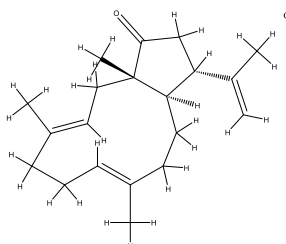
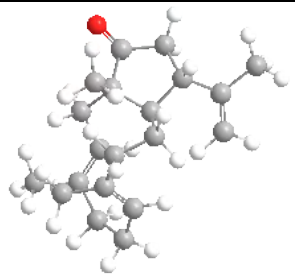
| Kode Senyawa | Struktur 2D                                                                                                                                                                                                     | Struktur 3D                                                                           |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S04          | <br><chem>C[C@H]1C[C@@H]2C[C@H](C1)O[C@H]2C=C</chem><br>Chiral                                                                 |    |
| Dictyoxepin  |                                                                                                                                                                                                                 |                                                                                       |
| S05          | <br><chem>COc1cc(OC)c(O)c(O)c1OC(=O)C[C@H]2O[C@H](C[C@@H]3O[C@H](CO)[C@H](O)[C@@H]3O)[C@H](O)[C@@H](O)[C@H]2O</chem><br>Chiral |   |
| Verbascoside |                                                                                                                                                                                                                 |                                                                                       |
| S06          | <br><chem>C[C@H]1C[C@@H]2C[C@H](C1)C=C2</chem><br>Chiral                                                                     |  |
| Germacrene D |                                                                                                                                                                                                                 |                                                                                       |
| S07          | <br><chem>C[C@H]1C[C@@H]2C[C@H](C1)C=C2</chem><br>Chiral                                                                     |  |
| Gleenol      |                                                                                                                                                                                                                 |                                                                                       |

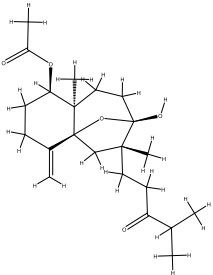
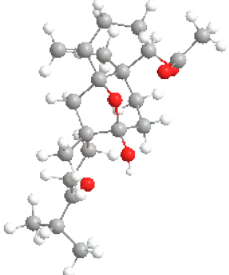
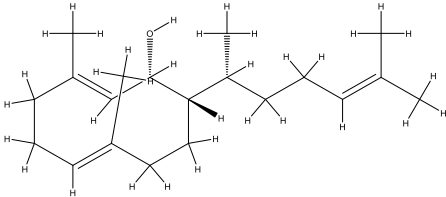
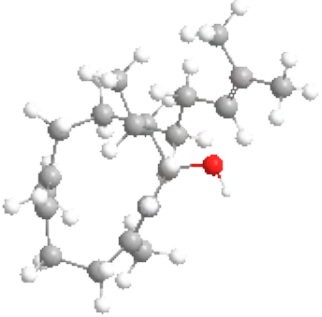
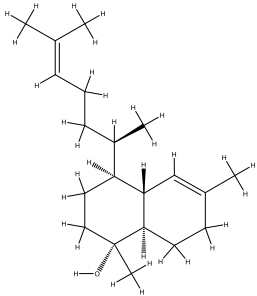
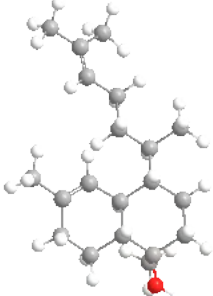
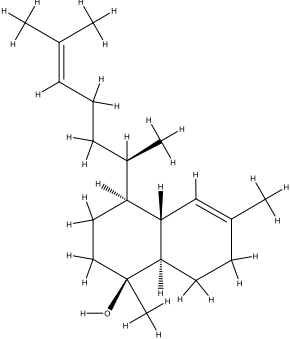
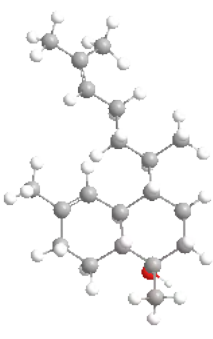
| Kode Senyawa                                                                                                                                                                | Struktur 2D                                                                         | Struktur 3D                                                                           |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S08                                                                                                                                                                         |    |    |
| [(2S,4S,5R,7R,8S)-5-methyl-8-[(2R)-6-methylhept-5-en-2-yl]-12-oxo-11-oxatricyclo[7.3.0.02,4]dodec-1(9)-en-7-yl] acetate                                                     |                                                                                     |                                                                                       |
| S09                                                                                                                                                                         |   |   |
| 4-Hydroxydictyolactone                                                                                                                                                      |                                                                                     |                                                                                       |
| S10                                                                                                                                                                         |  |  |
| (R)-6-Butyl-1,4-cycloheptadiene                                                                                                                                             |                                                                                     |                                                                                       |
| S11                                                                                                                                                                         |  |  |
| (3S,8S,9S,10R,13R,14S,17R)-17-[(1R,4R)-4-hydroxy-4-isopropyl-1-methyl-hex-5-enyl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol |                                                                                     |                                                                                       |

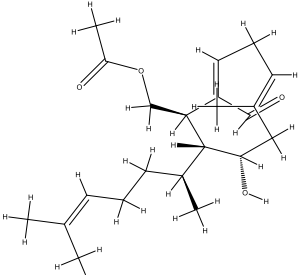
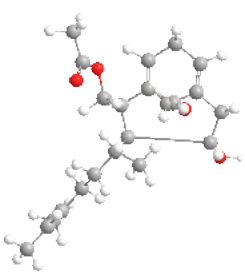
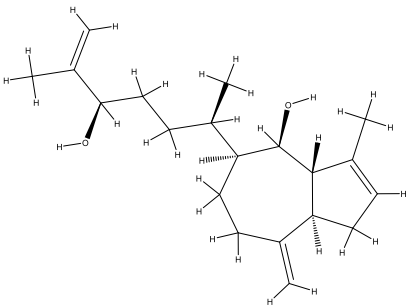
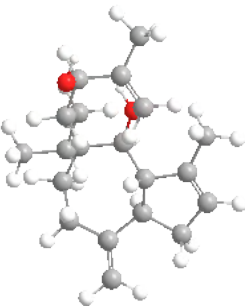
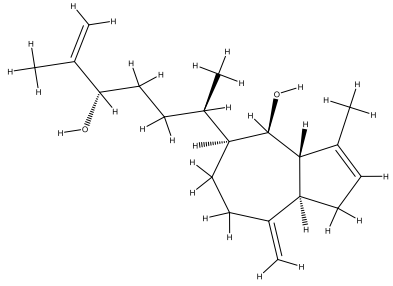
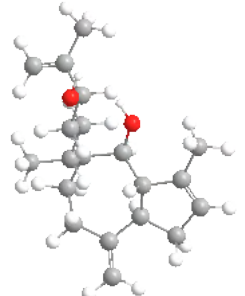
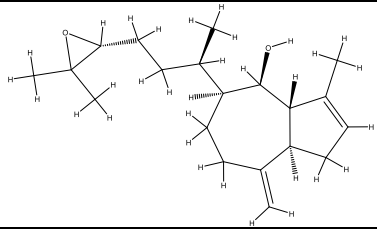
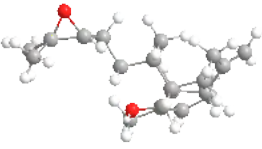
| Kode Senyawa                                                                                                     | Struktur 2D                                                                                       | Struktur 3D                                                                           |
|------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S12                                                                                                              |  <p>Chiral</p>   |    |
| 3-methyl-5-(6-methylhept-5-en-2-yl)-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol                         |                                                                                                   |                                                                                       |
| S13                                                                                                              |  <p>Chiral</p>   |    |
| 3,8-dimethyl-5-(6-methylhept-5-en-2-yl)-3a,4,5,6,7,8a-hexahydro-1H-azulene-4,8-diol                              |                                                                                                   |                                                                                       |
| S14                                                                                                              |  <p>Chiral</p>  |   |
| (3aS,4R,5S,8S,8aR)-3,8-dimethyl-5-[(2R)-6-methylhept-5-en-2-yl]-3a,4,5,6,7,8a-hexahydro-1H-azulene-4,8-diol      |                                                                                                   |                                                                                       |
| S15                                                                                                              |  <p>Chiral</p> |  |
| 2-[(1S,3aS,5E,9E,12aR)-3a,6,10-trimethyl-2,3,4,7,8,11,12,12a-octahydro-1H-cyclopenta[11]annulen-1-yl]propan-2-ol |                                                                                                   |                                                                                       |
| S16                                                                                                              |  <p>Chiral</p> |  |

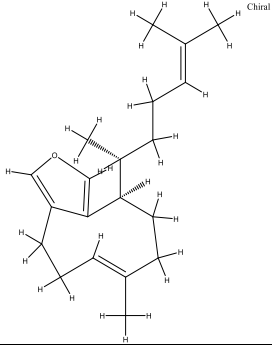
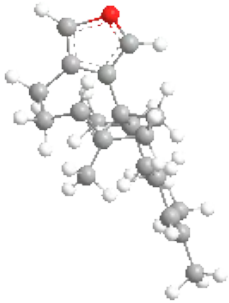
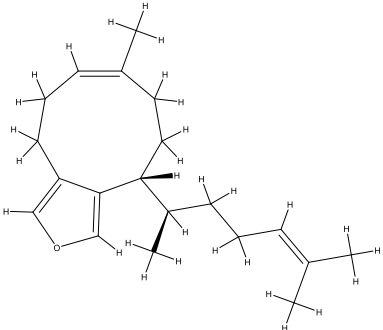
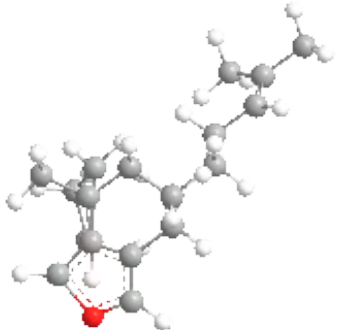
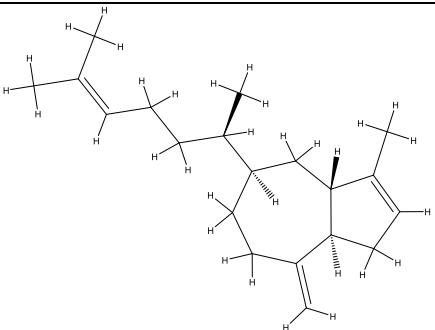
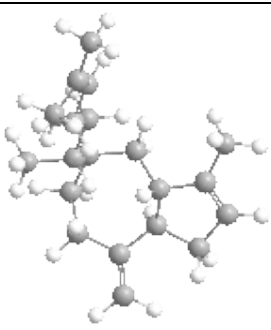
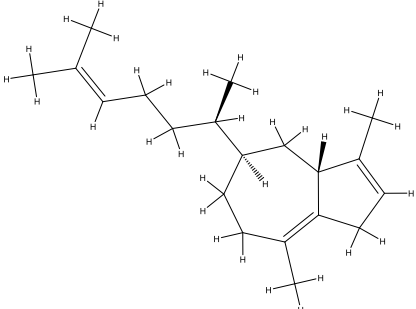
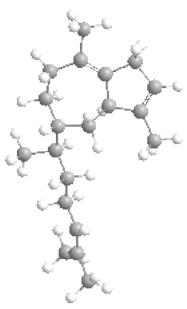
| Kode Senyawa                                                                                                           | Struktur 2D                                                                                       | Struktur 3D                                                                           |
|------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| Bicyclosesquiphellandrene                                                                                              |                                                                                                   |                                                                                       |
| S17                                                                                                                    |  <p>Chiral</p>   |    |
| 5-(2-hydroxy-6-methylhept-5-en-2-yl)-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol                     |                                                                                                   |                                                                                       |
| S18                                                                                                                    |  <p>Chiral</p>  |   |
| (1S,6S,9R,10R)-9-hydroxy-6,10-dimethyl-2-methylidene-10-(4-methyl-3-oxopentyl)-12-oxatricyclo[7.2.1.01,6]dodecan-5-one |                                                                                                   |                                                                                       |
| S19                                                                                                                    |  <p>Chiral</p> |  |
| (6R)-6-[(3aS,4R,5S,8aR)-4-hydroxy-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-5-yl]-2-methylheptan-3-one  |                                                                                                   |                                                                                       |
| S20                                                                                                                    |  <p>Chiral</p> |  |
| Isopachydictyol A                                                                                                      |                                                                                                   |                                                                                       |

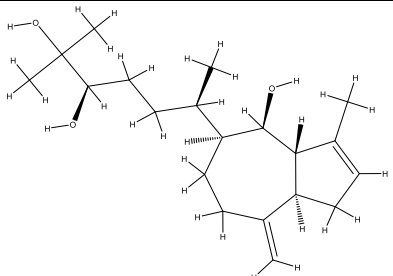
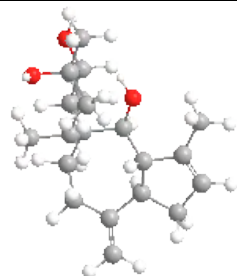
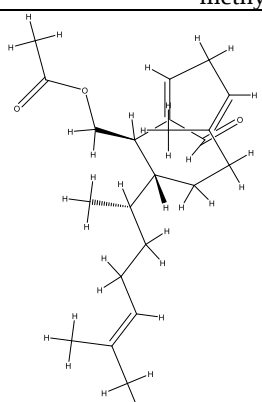
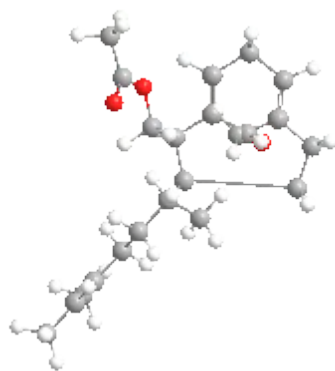
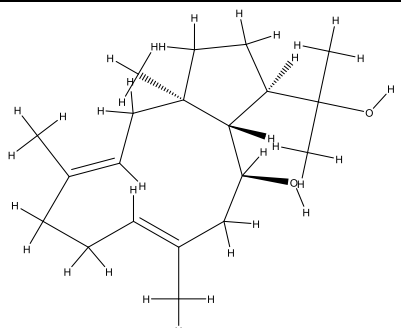
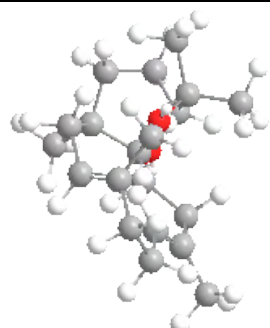
| Kode Senyawa                                                                                                                            | Struktur 2D                                                                         | Struktur 3D                                                                           |
|-----------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S21                                                                                                                                     |    |    |
| (1S,2S,3aR,7S,8R,8aR)-1-methyl-7-[(2R)-6-methylhept-5-en-2-yl]-4-methylidene-2,3,3a,5,6,7,8,8a-octahydroazulene-1,2,8-triol             |                                                                                     |                                                                                       |
| S22                                                                                                                                     |   |    |
| [(3R,3aS,5E,9E,11R,12aR)-10-formyl-6,12a-dimethyl-3-prop-1-en-2-yl-2,3,3a,4,7,8,11,12-octahydro-1H-cyclopenta[11]annulen-11-yl] acetate |                                                                                     |                                                                                       |
| S23                                                                                                                                     |  |  |
| (1R,2E,5E,9R)-6-methyl-9-[(2S)-6-methylhept-5-en-2-yl]cyclonona-2,5-diene-1,2-dicarbaldehyde                                            |                                                                                     |                                                                                       |
| S24                                                                                                                                     |  |  |
| [(1R,3aS,4R,5S,8aR)-4-hydroxy-3-methyl-5-[(2R)-6-methylhept-5-en-2-yl]-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-1-yl] acetate    |                                                                                     |                                                                                       |

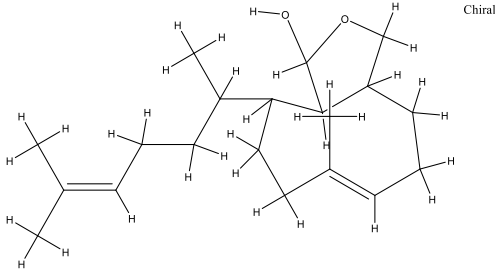
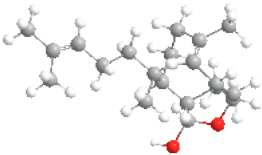
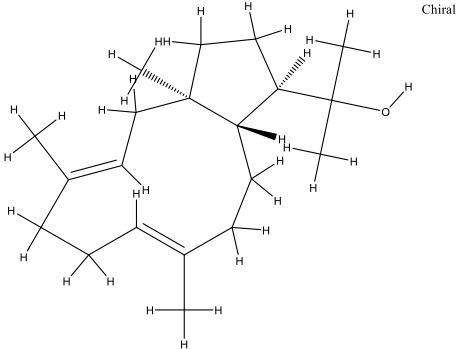
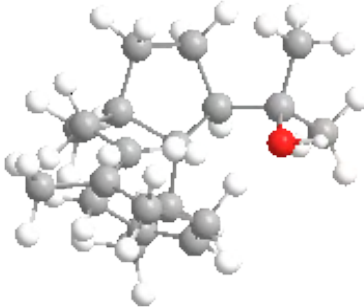
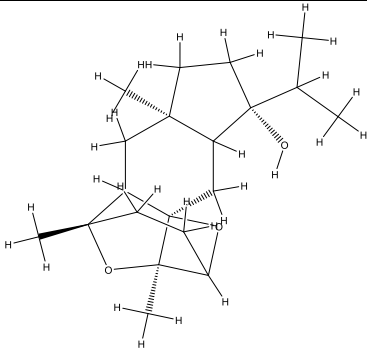
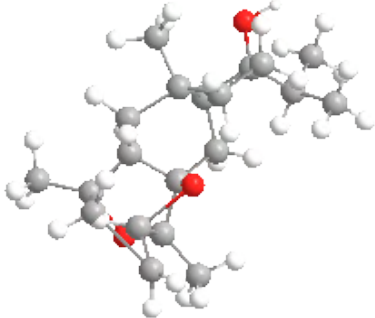
| Kode Senyawa                                                                                                                         | Struktur 2D                                                                                       | Struktur 3D                                                                           |
|--------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S25                                                                                                                                  |  <p>Chiral</p>   |    |
| (1R,4S)-1,6-dimethyl-4-[(2R)-6-methylhept-5-en-2-yl]-1,2,3,4-tetrahydronaphthalene                                                   |                                                                                                   |                                                                                       |
| S26                                                                                                                                  |  <p>Chiral</p>   |    |
| [(3aR,5S,7S,8R,8aS)-8-hydroxy-1-methyl-7-[(2R)-6-methylhept-5-en-2-yl]-4-methylidene-3a,5,6,7,8,8a-hexahydro-3H-azulen-5-yl] acetate |                                                                                                   |                                                                                       |
| S27                                                                                                                                  |  <p>Chiral</p> |  |
| (1R,3aR,7S,8R,8aR)-1-methyl-7-[(2R)-6-methylhept-5-en-2-yl]-4-methylidene-3a,5,6,7,8,8a-hexahydroazulene-1,8-diol                    |                                                                                                   |                                                                                       |
| S28                                                                                                                                  |  <p>Chiral</p> |  |
| (1S,3aS,5E,9E,12aR)-3a,6,10-trimethyl-1-prop-1-en-2-yl-1,2,4,7,8,11,12,12a-octahydrocyclopenta[11]annulen-3-one                      |                                                                                                   |                                                                                       |

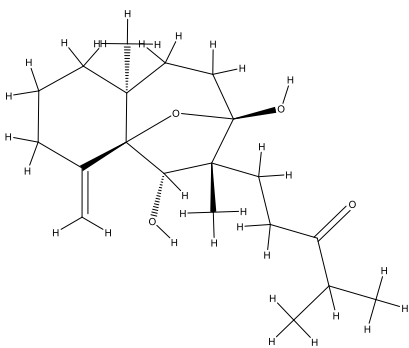
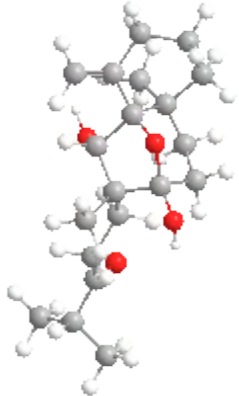
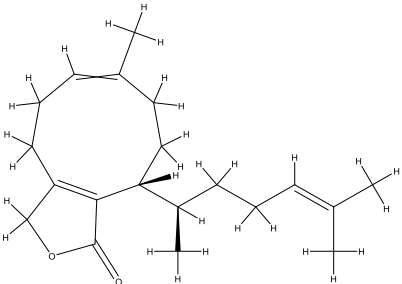
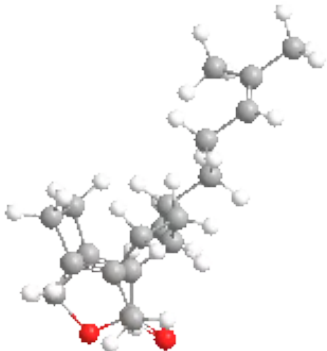
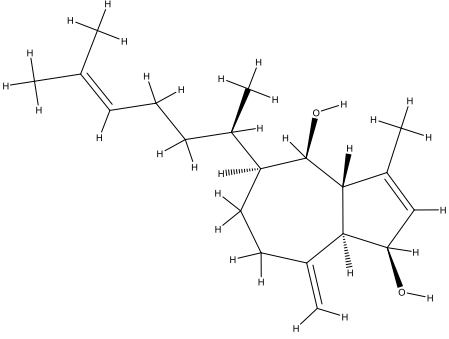
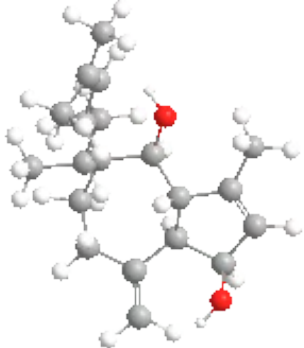
| Kode Senyawa                                                                                                    | Struktur 2D                                                                         | Struktur 3D                                                                           |
|-----------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S29                                                                                                             |    |    |
| (1S,3aS,5E,9E,12aR)-3a,6,10-trimethyl-1-prop-1-en-2-yl-1,2,4,7,8,11,12,12a-octahydrocyclopenta[11]annulen-3-one |                                                                                     |                                                                                       |
| S30                                                                                                             |    |   |
| (1R,2E,6E,10S)-3,7-dimethyl-10-[(2R)-6-methylhept-5-en-2-yl]cyclodeca-2,6-dien-1-ol                             |                                                                                     |                                                                                       |
| S31                                                                                                             |  |  |
| (1R,4S,4aR,8aR)-1,6-dimethyl-4-[(2R)-6-methylhept-5-en-2-yl]-3,4,4a,7,8,8a-hexahydro-2H-naphthalen-1-ol         |                                                                                     |                                                                                       |
| S32                                                                                                             |  |  |
| (1S,4S,4aR,8aR)-1,6-dimethyl-4-[(2R)-6-methylhept-5-en-2-yl]-3,4,4a,7,8,8a-hexahydro-2H-naphthalen-1-ol         |                                                                                     |                                                                                       |

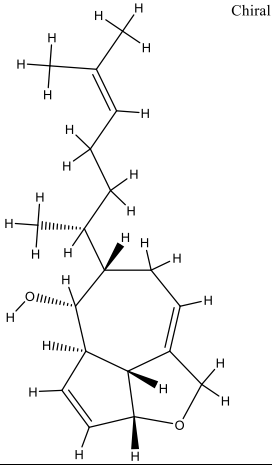
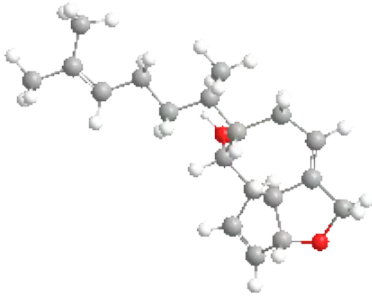
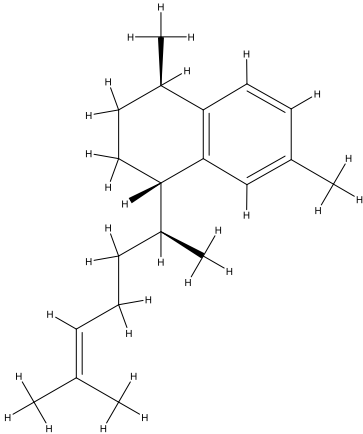
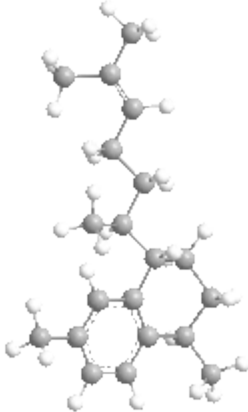
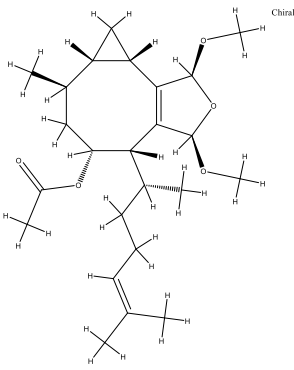
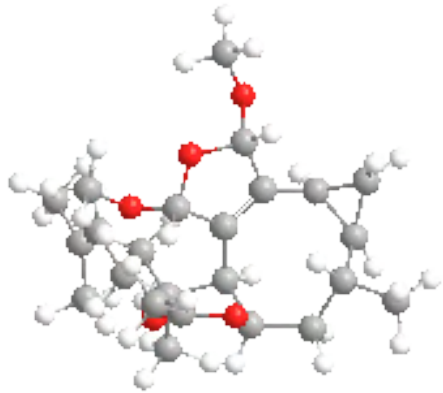
| Kode Senyawa                                                                                                                      | Struktur 2D                                                                         | Struktur 3D                                                                           |
|-----------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S33                                                                                                                               |    |    |
| Hydroxyacetyldictyolal                                                                                                            |                                                                                     |                                                                                       |
| S34                                                                                                                               |   |   |
| (3aS,4R,5S,8aR)-5-[(2R,5R)-5-hydroxy-6-methylhept-6-en-2-yl]-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol        |                                                                                     |                                                                                       |
| S35                                                                                                                               |  |  |
| (3aS,4R,5S,8aR)-5-[(2R,5S)-5-hydroxy-6-methylhept-6-en-2-yl]-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol        |                                                                                     |                                                                                       |
| S36                                                                                                                               |  |  |
| (3aS,4R,5S,8aR)-5-[(2R)-4-[(2R)-3,3-dimethyloxiran-2-yl]butan-2-yl]-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol |                                                                                     |                                                                                       |

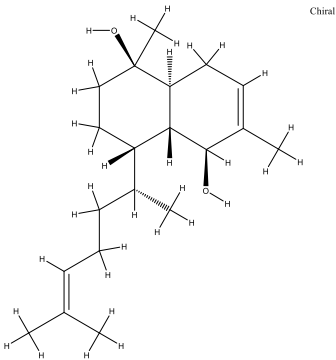
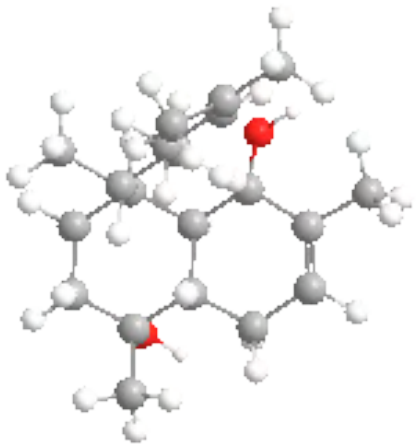
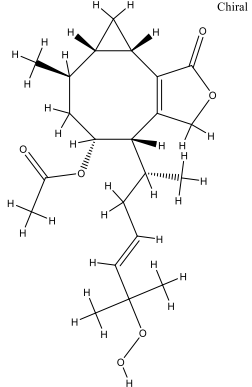
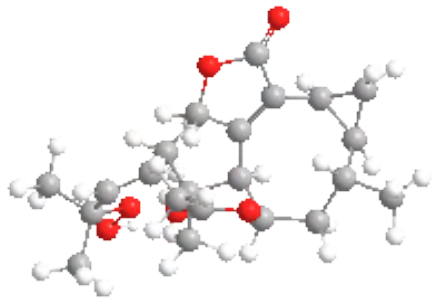
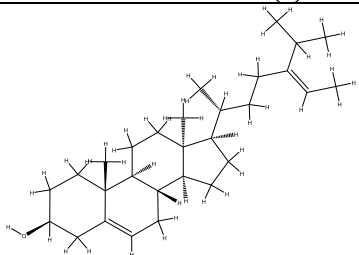
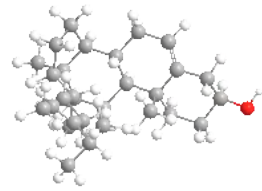
| Kode Senyawa                                                                                           | Struktur 2D                                                                         | Struktur 3D                                                                           |
|--------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S37                                                                                                    |    |    |
| (6E,10R)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-5,8,9,10-tetrahydro-4H-cyclonona[c]furan            |                                                                                     |                                                                                       |
| S38                                                                                                    |   |   |
| (6Z,10R)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-5,8,9,10-tetrahydro-4H-cyclonona[c]furan            |                                                                                     |                                                                                       |
| S39                                                                                                    |  |  |
| (3aS,5R,8aR)-3-methyl-5-[(2R)-6-methylhept-5-en-2-yl]-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulene |                                                                                     |                                                                                       |
| S40                                                                                                    |  |  |

| Kode Senyawa | Struktur 2D                                                                                                                                                                                                            | Struktur 3D                                                                           |
|--------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S41          | <p>(3aR,5R)-3,8-dimethyl-5-[(2R)-6-methylhept-5-en-2-yl]-1,3a,4,5,6,7-hexahydroazulene</p>                                            |    |
| S42          | <p>(3R,6R)-6-[(3aS,4R,5S,8aR)-4-hydroxy-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-5-yl]-2-methylheptane-2,3-diol</p>  |   |
| S43          | <p>[(1R,2E,5E,9R)-2-formyl-6-methyl-9-[(2S)-6-methylhept-5-en-2-yl]cyclonona-2,5-dien-1-yl]methyl acetate</p>                       |  |
|              | <p>(1R,3aR,5E,9E,12S,12aS)-1-(2-hydroxypropan-2-yl)-3a,6,10-trimethyl-2,3,4,7,8,11,12,12a-octahydro-1H-cyclopenta[11]annulen-12-ol</p>                                                                                 |                                                                                       |

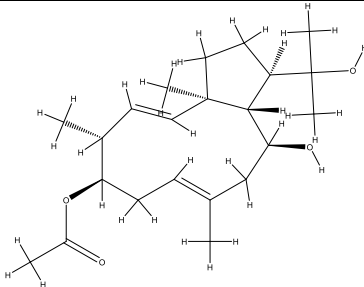
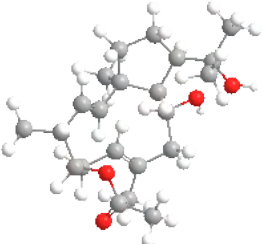
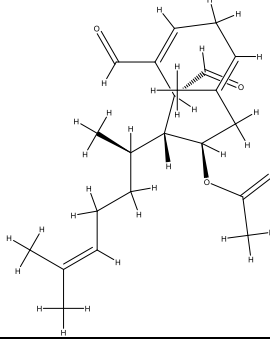
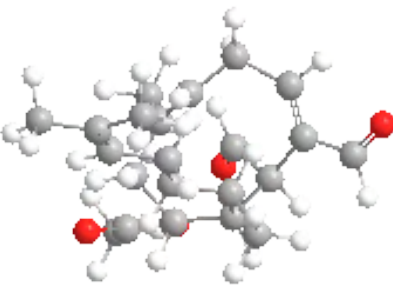
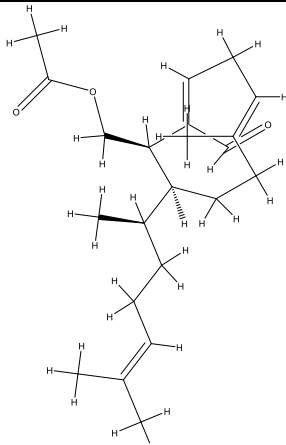
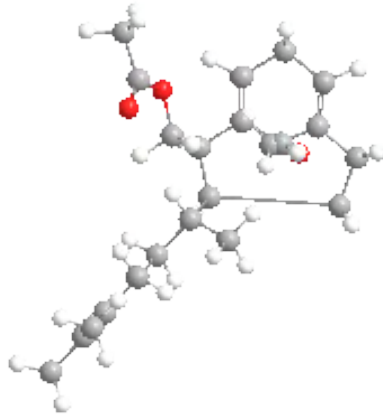
| Kode Senyawa                                                                                                   | Struktur 2D                                                                         | Struktur 3D                                                                           |
|----------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S44                                                                                                            |    |    |
| (6E)-7-methyl-10-(6-methylhept-5-en-2-yl)-3,3a,4,5,8,9,10,10a-octahydro-1H-cyclonona[c]furan-1-ol              |                                                                                     |                                                                                       |
| S45                                                                                                            |   |   |
| (3E,7E)-Dolabella-3,7-dien-18-ol                                                                               |                                                                                     |                                                                                       |
| S46/66                                                                                                         |  |  |
| (1R,4R,7R,10S,15R)-7,10,15-trimethyl-4-propan-2-yl-14,16-dioxapentacyclo[8.4.2.01,9.03,7.013,15]hexadecan-4-ol |                                                                                     |                                                                                       |

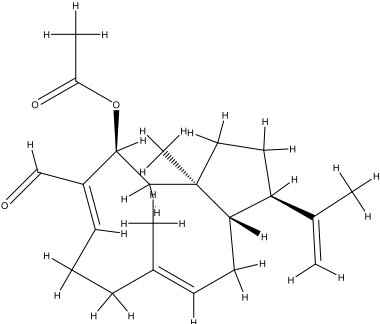
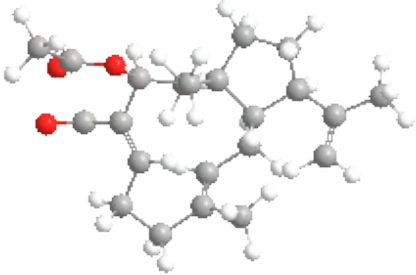
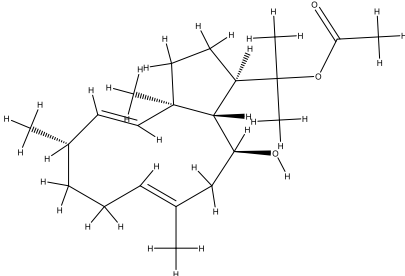
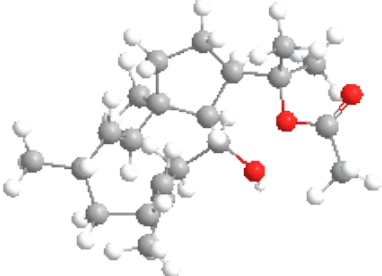
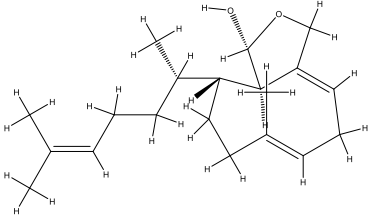
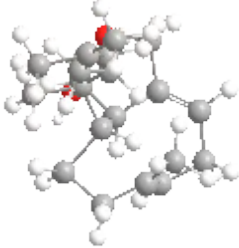
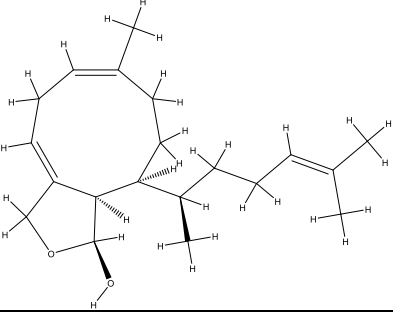
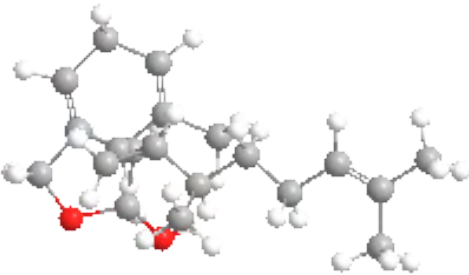
| Kode Senyawa                                                                                                                   | Struktur 2D                                                                                       | Struktur 3D                                                                           |
|--------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S47                                                                                                                            | <p>Chiral</p>    |    |
| 1-[(1S,6S,9R,10R,11S)-9,11-dihydroxy-6,10-dimethyl-2-methylidene-12-oxatricyclo[7.2.1.01,6]dodecan-10-yl]-4-methylpentan-3-one |                                                                                                   |                                                                                       |
| S48                                                                                                                            | <p>Chiral</p>   |   |
| (10R)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-3,4,5,8,9,10-hexahydrocyclonona[c]furan-1-one                                  |                                                                                                   |                                                                                       |
| S49                                                                                                                            | <p>Chiral</p>  |  |
| (1R,3aS,4R,5S,8aR)-3-methyl-5-[(2R)-6-methylhept-5-en-2-yl]-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulene-1,4-diol          |                                                                                                   |                                                                                       |

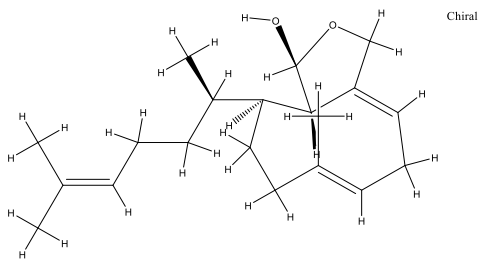
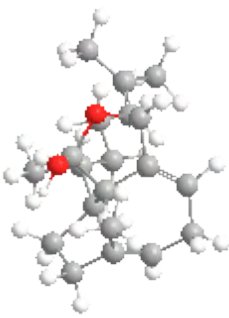
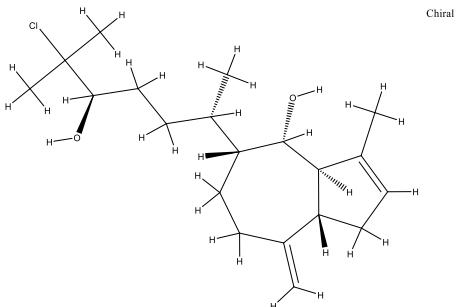
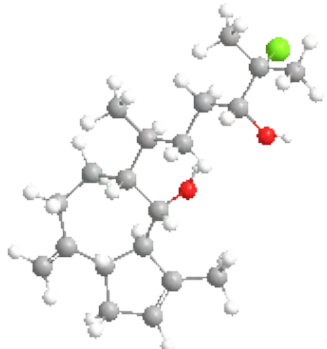
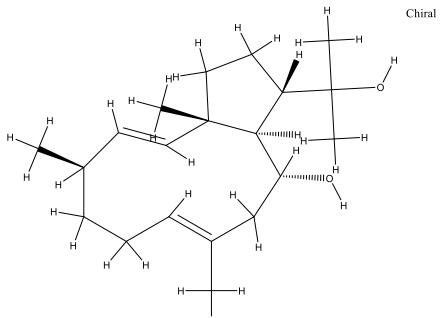
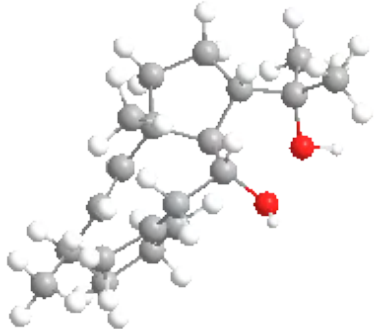
| Kode Senyawa | Struktur 2D                                                                                                                              | Struktur 3D                                                                           |
|--------------|------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S50          |  <p>Chiral</p>                                          |    |
|              | (1R,3aS,4R,5S,8aR)-3-methyl-5-[(2R)-6-methylhept-5-en-2-yl]-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulene-1,4-diol                    |                                                                                       |
| S51          |  <p>Chiral</p>                                         |   |
|              | (1R,4S)-1,6-dimethyl-4-[(2S)-6-methylhept-5-en-2-yl]-1,2,3,4-tetrahydronaphthalene                                                       |                                                                                       |
| S52          |  <p>Chiral</p>                                        |  |
|              | [(2S,4S,5R,7R,8S,10R,12S)-10,12-dimethoxy-5-methyl-8-[(2R)-6-methylhept-5-en-2-yl]-11-oxatricyclo[7.3.0.02,4]dodec-1(9)-en-7-yl] acetate |                                                                                       |

| Kode Senyawa | Struktur 2D                                                                         | Struktur 3D                                                                           |
|--------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S53          |    |    |
| S54          |   |   |
| S55          |  |  |

| Kode Senyawa                                                                                                                                       | Struktur 2D | Struktur 3D |
|----------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-------------|
| S56                                                                                                                                                |             |             |
| Dictyofuran C                                                                                                                                      |             |             |
| S57                                                                                                                                                |             |             |
| (4R,5aR,6R,9aS,10aS)-4,6,9a-trihydroxy-5a,10a-dimethyl-9-methylidene-3-propan-2-yl-4,5,6,7,8,10-hexahydro-1H-benzo[f]azulen-2-one                  |             |             |
| S58                                                                                                                                                |             |             |
| [(4R,5aS,6R,9aS,10aS)-4,6,9a-trihydroxy-10a-methyl-9-methylidene-2-oxo-3-propan-2-yl-4,5,6,7,8,10-hexahydro-1H-benzo[f]azulen-5a-yl]methyl acetate |             |             |
| S59                                                                                                                                                |             |             |

| Kode Senyawa | Struktur 2D                                                                                                                                                                                                                                        | Struktur 3D                                                                           |
|--------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S60          | <p>[(1S,3aR,4R,7aR)-7,7a-diformyl-3a-methyl-1-[(2S)-6-methylhept-5-en-2-yl]-2,3,4,5-tetrahydro-1H-inden-4-yl] acetate</p>                                         |    |
| S61          | <p>[(3R,3aS,4S,6E,9R,10R,11E,12aR)-4-hydroxy-3-(2-hydroxypropan-2-yl)-6,10,12a-trimethyl-2,3,3a,4,5,8,9,10-octahydro-1H-cyclopenta[11]annulen-9-yl] acetate</p>  |   |
| S62          | <p>[(1R,3E,6E,8R,9R)-7,8-diformyl-3-methyl-9-[(2R)-6-methylhept-5-en-2-yl]cyclonona-3,6-dien-1-yl] acetate</p>                                                  |  |
|              | <p>[(1R,2E,5E,9S)-2-formyl-6-methyl-9-[(2R)-6-methylhept-5-en-2-yl]cyclonona-2,5-dien-1-yl]methyl acetate</p>                                                                                                                                      |                                                                                       |

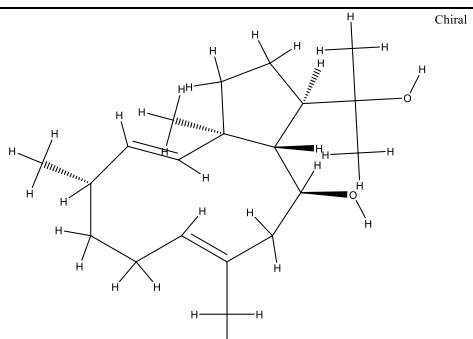
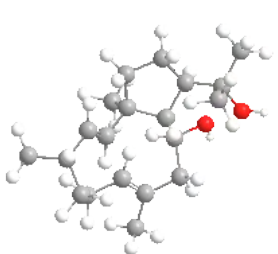
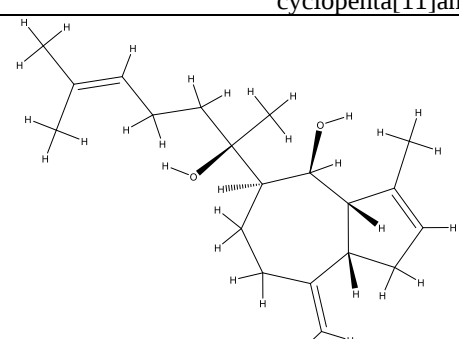
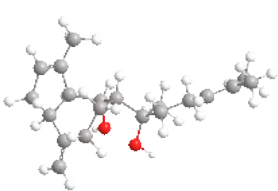
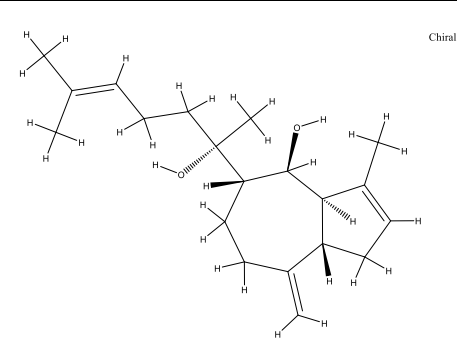
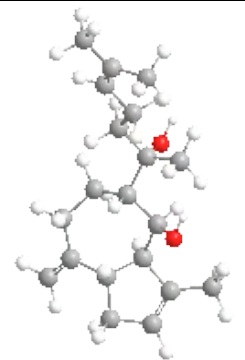
| Kode Senyawa | Struktur 2D                                                                                                                                | Struktur 3D                                                                           |
|--------------|--------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S63          |  <p>Chiral</p>                                            |    |
|              | [(3R,3aS,5E,9Z,11S,12aR)-10-formyl-6,12a-dimethyl-3-prop-1-en-2-yl-2,3,3a,4,7,8,11,12-octahydro-1H-cyclopenta[11]annulen-11-yl] acetate    |                                                                                       |
| S64          |  <p>Chiral</p>                                           |   |
|              | 2-[(1R,3aR,4E,6S,9E,12S,12aS)-12-hydroxy-3a,6,10-trimethyl-2,3,6,7,8,11,12,12a-octahydro-1H-cyclopenta[11]annulen-1-yl]propan-2-yl acetate |                                                                                       |
| S65          |  <p>Chiral</p>                                          |  |
|              | (1R,3aE,6E,10R,10aR)-7-methyl-10-[(2S)-6-methylhept-5-en-2-yl]-3,5,8,9,10,10a-hexahydro-1H-cyclonona[c]furan-1-ol                          |                                                                                       |
| S66          |  <p>Chiral</p>                                          |   |
|              | (1S,3aE,6Z,10S,10aR)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-3,5,8,9,10,10a-hexahydro-1H-cyclonona[c]furan-1-ol                          |                                                                                       |

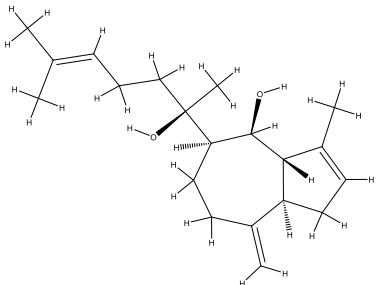
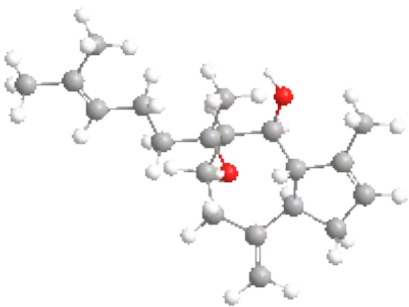
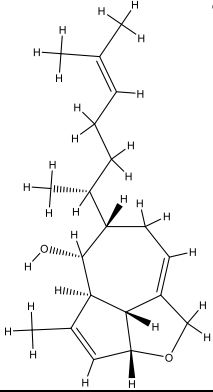
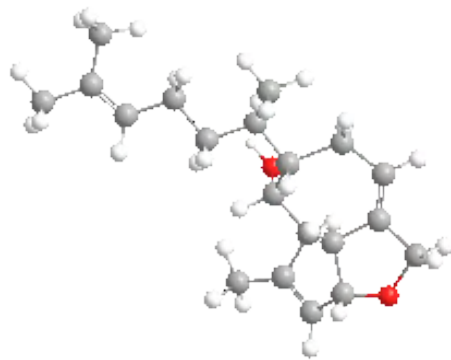
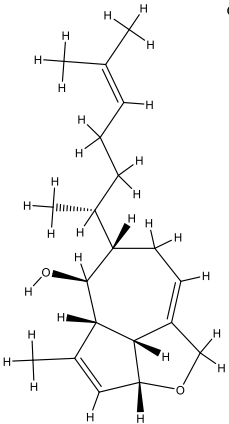
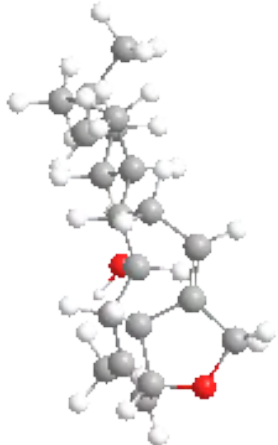
| Kode Senyawa | Struktur 2D                                                                                       | Struktur 3D                                                                           |
|--------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S67          |  <p>Chiral</p>   |    |
| S68          |  <p>Chiral</p>  |   |
| S69          |  <p>Chiral</p> |  |

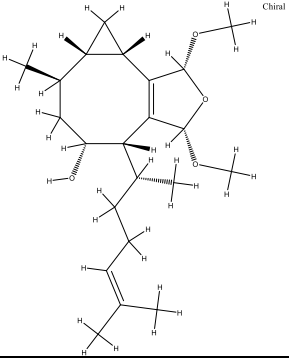
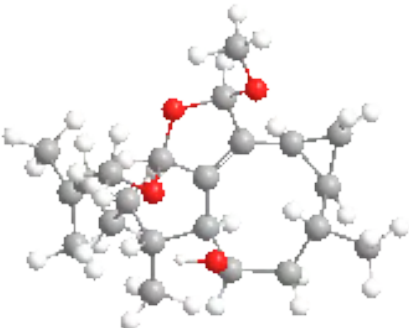
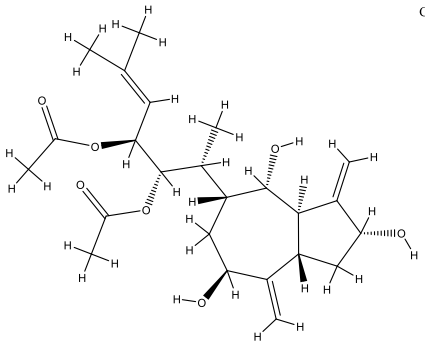
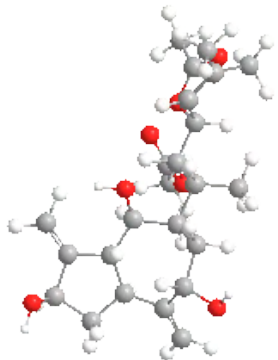
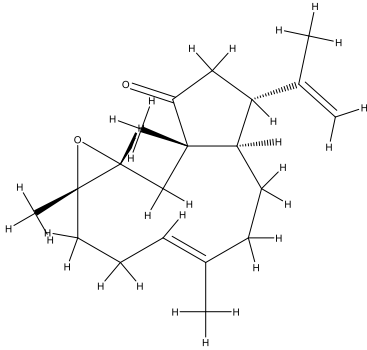
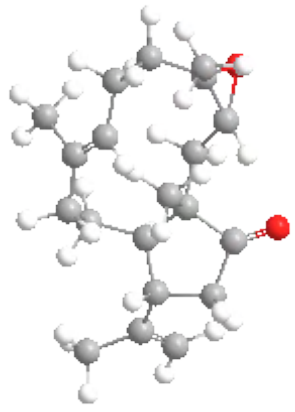
(1S,3aE,6Z,10S,10aR)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-3,5,8,9,10,10a-hexahydro-1H-cyclonona[c]furan-1-ol

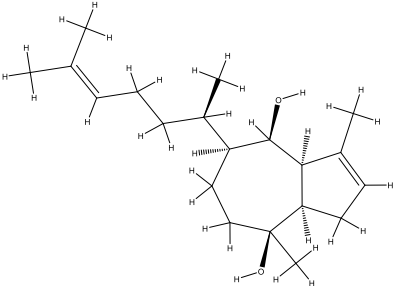
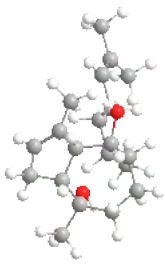
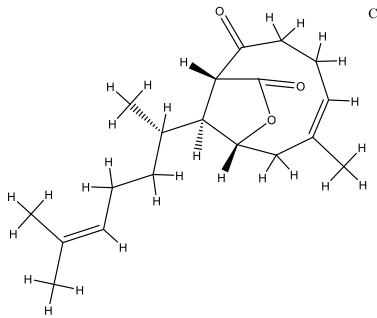
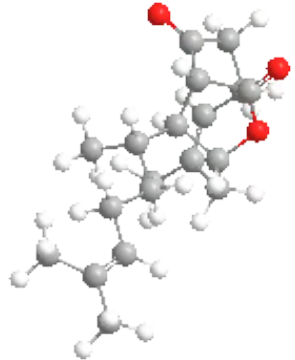
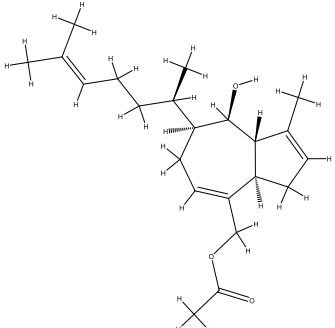
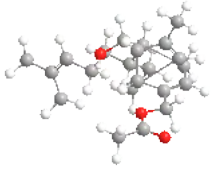
(3aR,4S,5R,8aS)-5-[(2S,5R)-6-chloro-5-hydroxy-6-methylheptan-2-yl]-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol

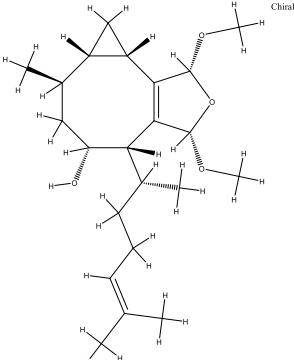
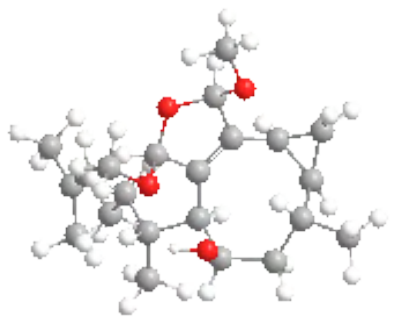
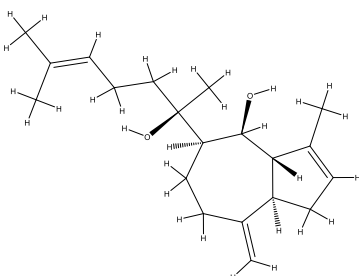
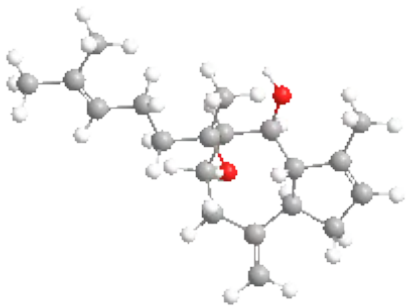
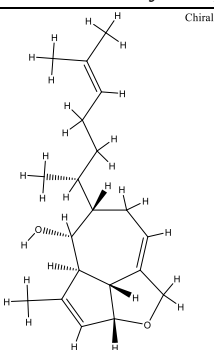
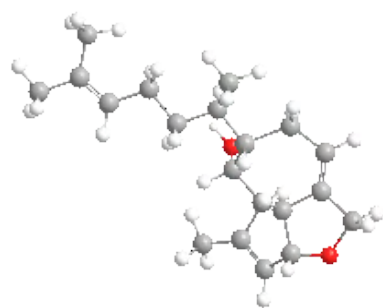
(1S,3aS,4E,6R,9E,12R,12aR)-1-(2-hydroxypropan-2-yl)-3a,6,10-trimethyl-2,3,6,7,8,11,12,12a-octahydro-1H-cyclopenta[11]annulen-12-ol

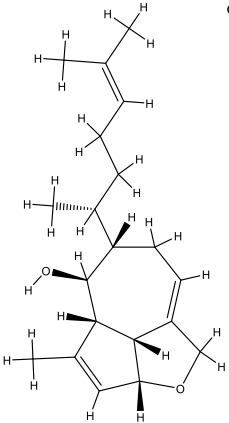
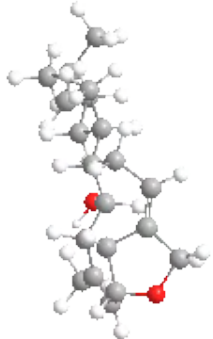
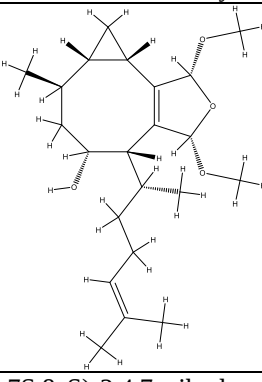
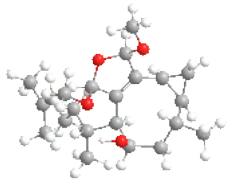
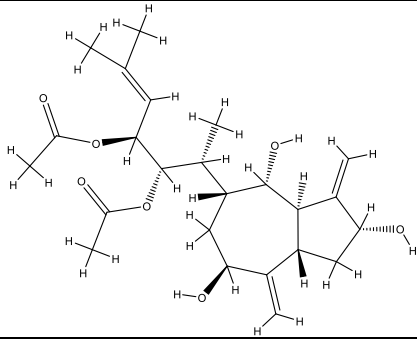
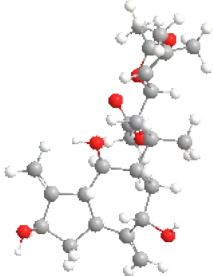
| Kode Senyawa | Struktur 2D                                                                                                                                                                                                                 | Struktur 3D                                                                           |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S70          |  <p>(1R,3aR,4E,6S,9E,12S,12aS)-1-(2-hydroxypropan-2-yl)-3a,6,10-trimethyl-2,3,6,7,8,11,12,12a-octahydro-1H-cyclopenta[11]annulen-12-ol</p> |    |
| S71          |  <p>(3aS,4S,5R,8aS)-5-[(2R)-2-hydroxy-6-methylhept-5-en-2-yl]-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol</p>           |   |
| S72          |  <p>(3aR,4S,5S,8aS)-5-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol</p>          |  |

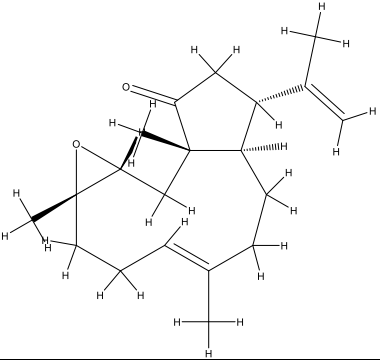
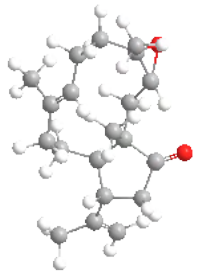
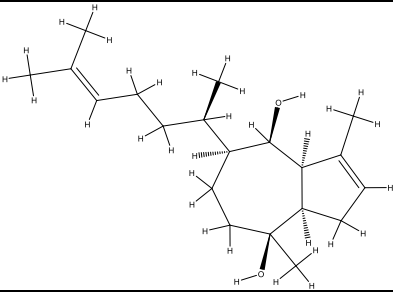
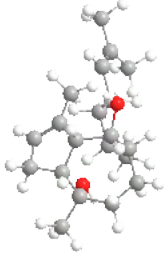
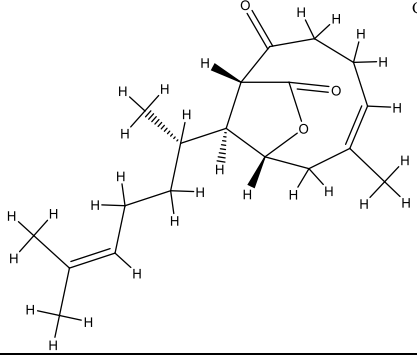
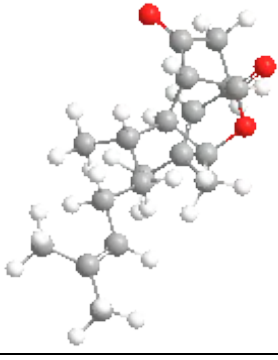
| Kode Senyawa | Struktur 2D                                                                                                             | Struktur 3D                                                                           |
|--------------|-------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S73          |  <p>Chiral</p>                         |    |
|              | (3aS,4S,5R,8aR)-5-[(2R)-2-hydroxy-6-methylhept-5-en-2-yl]-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol |                                                                                       |
| S74          |  <p>Chiral</p>                        |    |
|              | (4R,7S,8R,9S,12R)-6-methyl-9-[(2R)-6-methylhept-5-en-2-yl]-3-oxatricyclo[5.4.1.0.4,12]dodeca-1(11),5-dien-8-ol          |                                                                                       |
| S75          |  <p>Chiral</p>                       |  |
|              | (4R,7R,8S,9S,12R)-6-methyl-9-[(2R)-6-methylhept-5-en-2-yl]-3-oxatricyclo[5.4.1.0.4,12]dodeca-1(11),5-dien-8-ol          |                                                                                       |

| Kode Senyawa                                                                                                                                                | Struktur 2D                                                                         | Struktur 3D                                                                           |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S76                                                                                                                                                         |    |    |
| (2S,4S,5R,7R,8S,10S,12R)-10,12-dimethoxy-5-methyl-8-[(2R)-6-methylhept-5-en-2-yl]-11-oxatricyclo[7.3.0.02,4]dodec-1(9)-en-7-ol                              |                                                                                     |                                                                                       |
| S77                                                                                                                                                         |   |   |
| [(4S,5S,6R)-6-[(2R,3aR,4S,5R,7S,8aS)-2,4,7-trihydroxy-3,8-dimethylidene-1,2,3a,4,5,6,7,8a-octahydroazulen-5-yl]-5-acetyloxy-2-methylhept-2-en-4-yl] acetate |                                                                                     |                                                                                       |
| S78                                                                                                                                                         |  |  |
| (1S,3R,5S,8E,12R,13S)-1,5,9-trimethyl-13-prop-1-en-2-yl-4-oxatricyclo[10.3.0.03,5]pentadec-8-en-15-one                                                      |                                                                                     |                                                                                       |

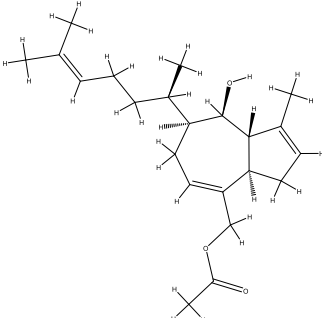
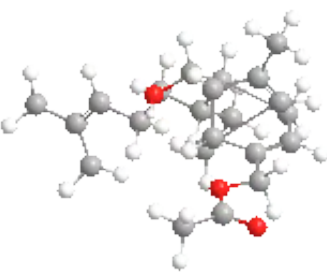
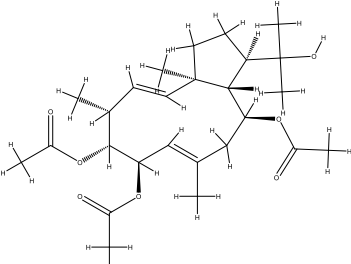
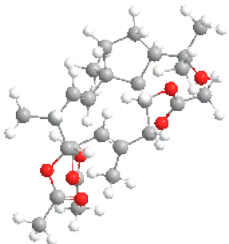
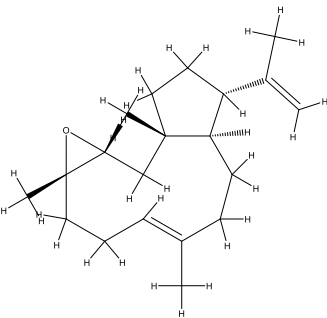
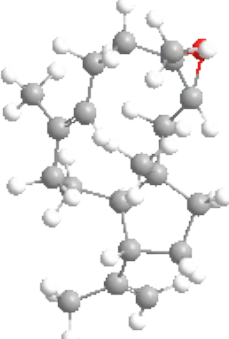
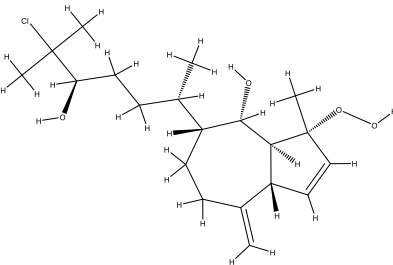
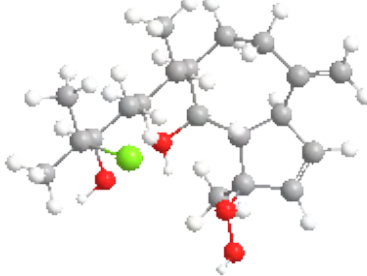
| Kode Senyawa | Struktur 2D                                                                                                           | Struktur 3D                                                                           |
|--------------|-----------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S79          |                                      |    |
|              | (3aR,4R,5S,8S,8aR)-3,8-dimethyl-5-[(2R)-6-methylhept-5-en-2-yl]-3a,4,5,6,7,8a-hexahydro-1H-azulene-4,8-diol           |                                                                                       |
| S80          |                                     |   |
|              | (1R,5E,8R,11S)-6-methyl-11-[(2S)-6-methylhept-5-en-2-yl]-9-oxabicyclo[6.2.1]undec-5-ene-2,10-dione                    |                                                                                       |
| S81          |                                    |  |
|              | [(3aR,7S,8R,8aS)-8-hydroxy-1-methyl-7-[(2R)-6-methylhept-5-en-2-yl]-3,3a,6,7,8,8a-hexahydroazulen-4-yl]methyl acetate |                                                                                       |

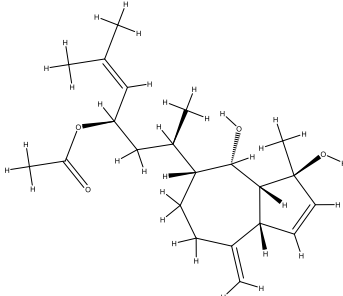
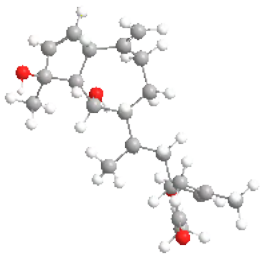
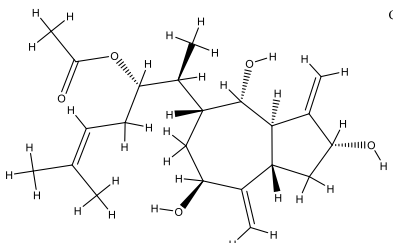
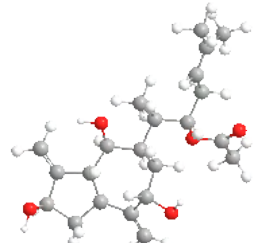
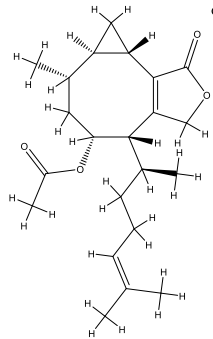
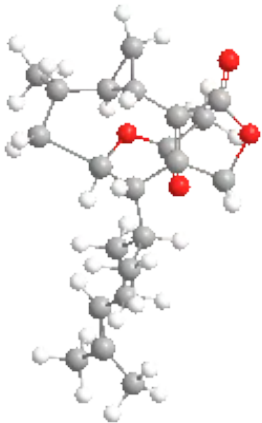
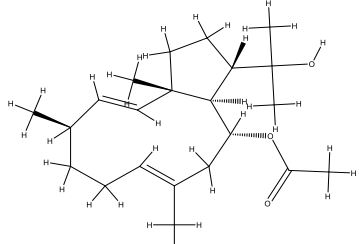
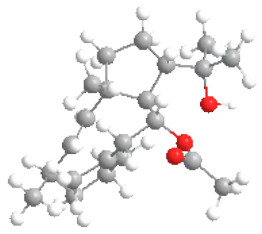
| Kode Senyawa                                                                                                                                                      | Struktur 2D                                                                         | Struktur 3D                                                                           |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S82                                                                                                                                                               |    |    |
| [(3R,3aS,4S,6E,8R,9R,10R,11E,12aR)-8,9-diacetyloxy-3-(2-hydroxypropan-2-yl)-6,10,12a-trimethyl-2,3,3a,4,5,8,9,10-octahydro-1H-cyclopenta[11]annulen-4-yl] acetate |                                                                                     |                                                                                       |
| S83                                                                                                                                                               |   |   |
| (1S,3R,5S,8E,12R,13S)-1,5,9-trimethyl-13-prop-1-en-2-yl-4-oxatricyclo[10.3.0.03,5]pentadec-8-ene                                                                  |                                                                                     |                                                                                       |
| S84                                                                                                                                                               |  |  |
| (3R,3aS,4S,5R,8aS)-5-[(2S,5R)-6-chloro-5-hydroxy-6-methylheptan-2-yl]-3-hydroperoxy-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydroazulen-4-ol                     |                                                                                     |                                                                                       |

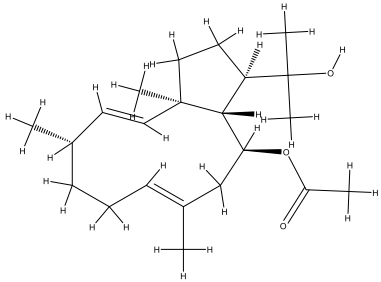
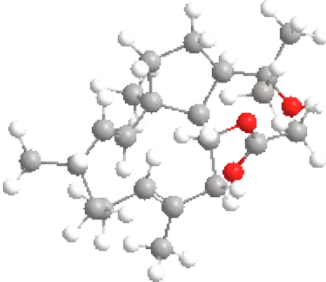
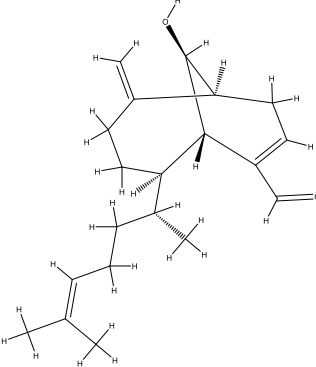
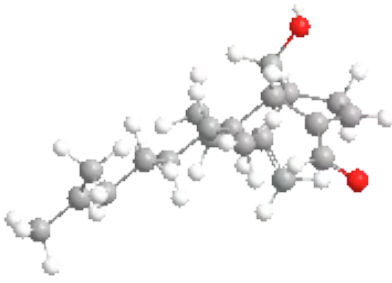
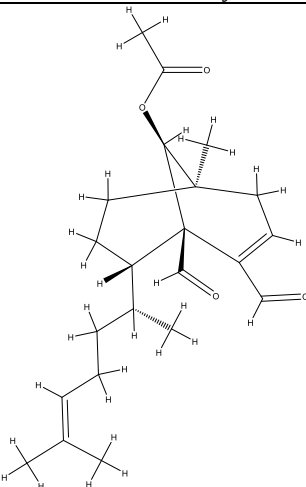
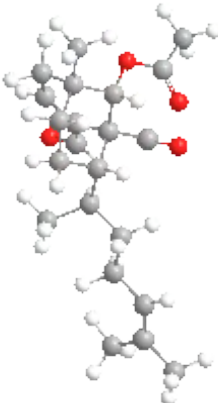
| Kode Senyawa                                                                                                                                        | Struktur 2D                                                                         | Struktur 3D                                                                           |
|-----------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S85                                                                                                                                                 |    |    |
| <p>[(4R,6R)-6-[(3S,3aR,4S,5R,8aS)-3,4-dihydroxy-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydroazulen-5-yl]-2-methylhept-2-en-4-yl] acetate</p>      |                                                                                     |                                                                                       |
| S86                                                                                                                                                 |   |   |
| <p>[(2S,3S)-2-[(2R,3aR,4S,5R,7S,8aS)-2,4,7-trihydroxy-3,8-dimethylidene-1,2,3a,4,5,6,7,8a-octahydroazulen-5-yl]-6-methylhept-5-en-3-yl] acetate</p> |                                                                                     |                                                                                       |
| S87                                                                                                                                                 |  |  |
| <p>[(2S,4R,5S,7R,8S)-5-methyl-8-[(2S)-6-methylhept-5-en-2-yl]-12-oxo-11-oxatricyclo[7.3.0.02,4]dodec-1(9)-en-7-yl] acetate</p>                      |                                                                                     |                                                                                       |

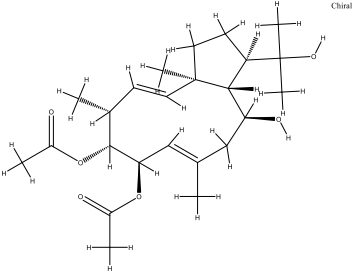
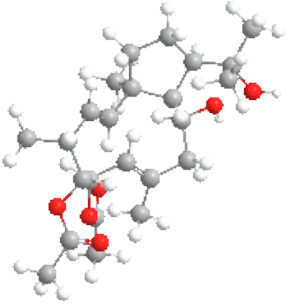
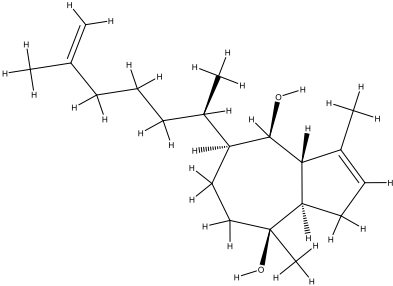
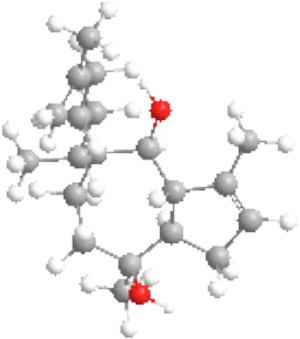
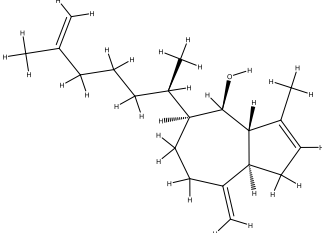
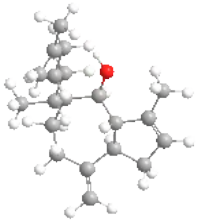
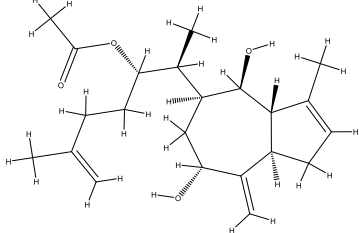
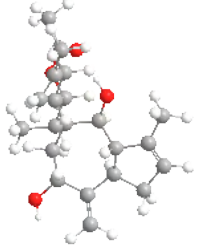
| Kode Senyawa | Struktur 2D                                                                                       | Struktur 3D                                                                           |
|--------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S88          |  <p>Chiral</p>   |    |
| S89          |  <p>Chiral</p>  |   |
| S90          |  <p>Chiral</p> |  |

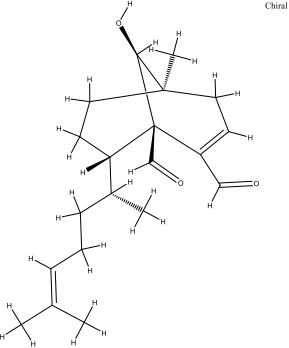
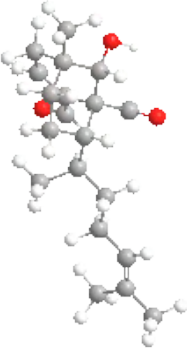
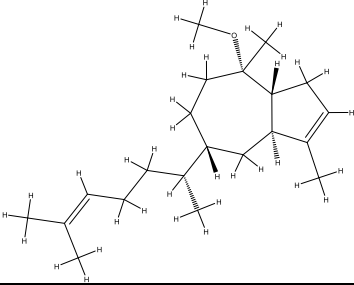
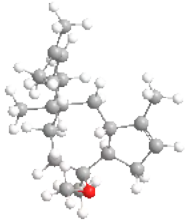
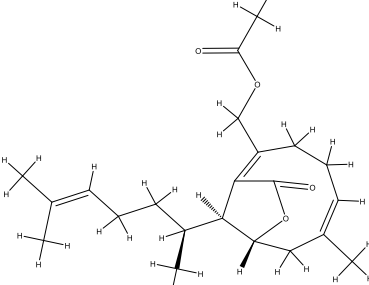
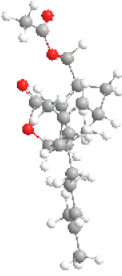
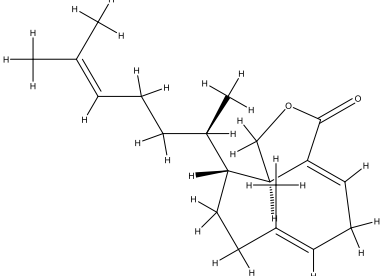
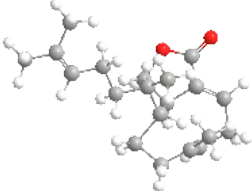
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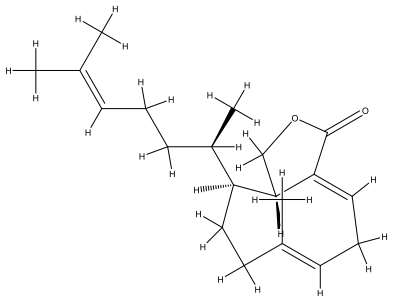
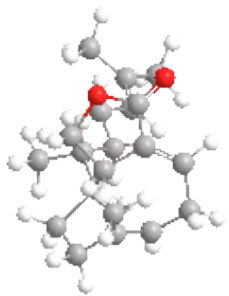
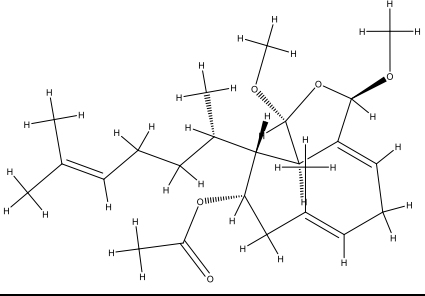
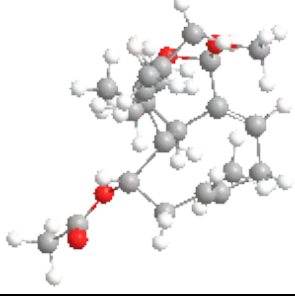
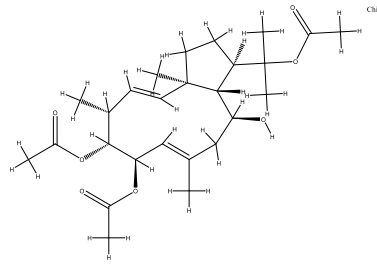
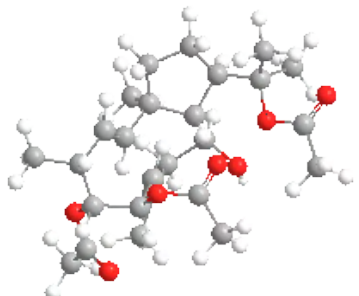
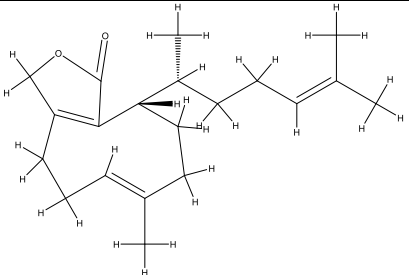
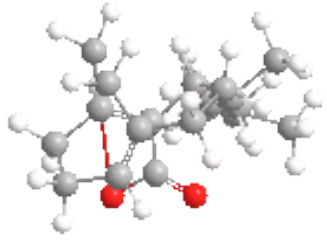
| Kode Senyawa                                                                                                     | Struktur 2D                                                                         | Struktur 3D                                                                           |
|------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S91                                                                                                              |    |    |
| (1R,2S,6S,7S,8S)-1,3-dimethyl-8-[(2R)-6-methylhept-5-en-2-yl]tricyclo[4.4.0.0.2,7]dec-3-ene                      |                                                                                     |                                                                                       |
| S92                                                                                                              |   |   |
| (1S,2S,6S,7S,8S)-1,3-dimethyl-8-[(2S)-6-methylhept-5-en-2-yl]tricyclo[4.4.0.0.2,7]dec-3-ene                      |                                                                                     |                                                                                       |
| S93                                                                                                              |  |  |
| (3aR,7S,8R,8aS)-8-hydroxy-1-methyl-7-[(2R)-6-methylhept-5-en-2-yl]-3,3a,6,7,8,8a-hexahydroazulene-4-carbaldehyde |                                                                                     |                                                                                       |
| S94                                                                                                              |  |  |
| (3aS,7R,8S,8aR)-8-hydroxy-1-methyl-7-[(2R)-6-methylhept-5-en-2-yl]-3,3a,6,7,8,8a-hexahydroazulene-4-carbaldehyde |                                                                                     |                                                                                       |

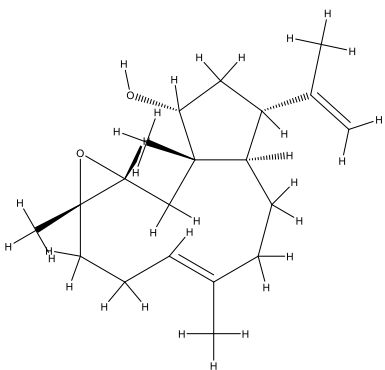
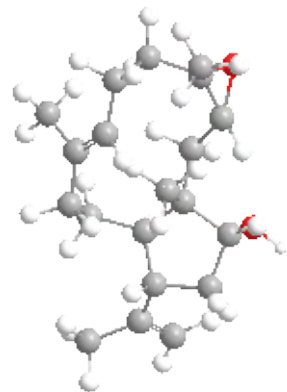
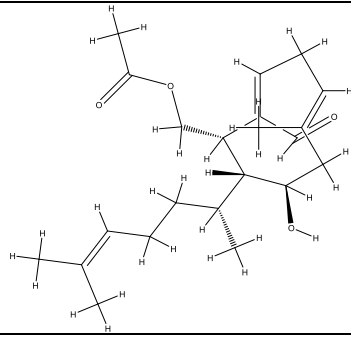
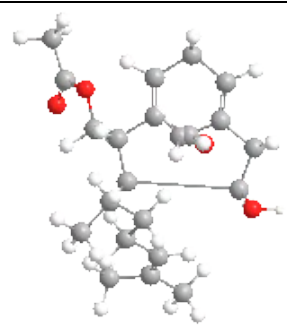
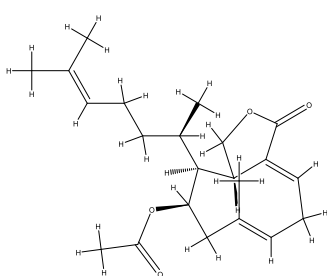
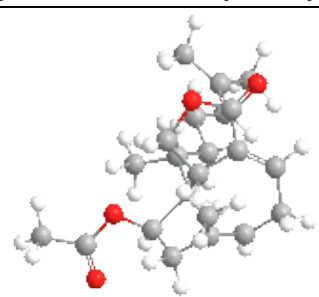
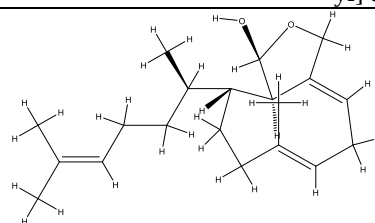
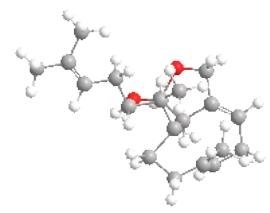
| Kode Senyawa | Struktur 2D                                                                                       | Struktur 3D                                                                           |
|--------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S95          |  <p>Chiral</p>   |    |
| S96          |  <p>Chiral</p>   |    |
| S97          |  <p>Chiral</p> |  |
| S98          |  <p>Chiral</p> |  |

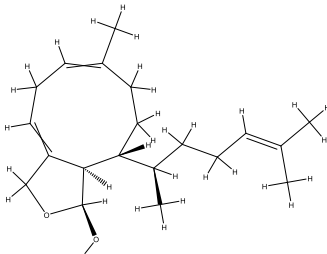
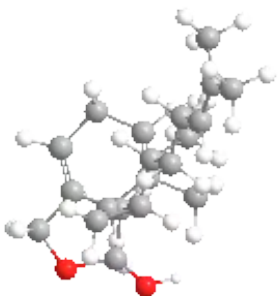
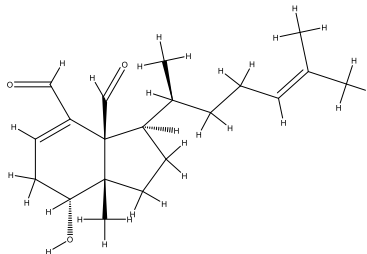
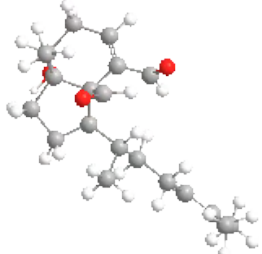
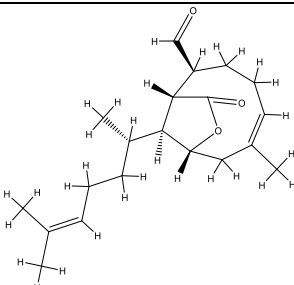
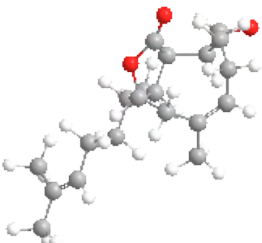
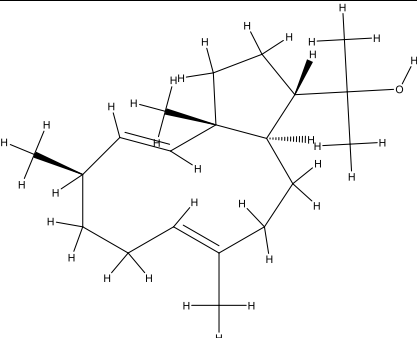
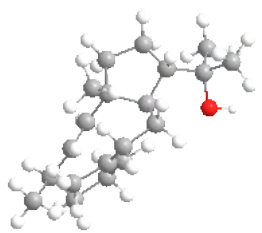
| Kode Senyawa                                                                                                                          | Struktur 2D                                                                                       | Struktur 3D                                                                           |
|---------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S99                                                                                                                                   |  <p>Chiral</p>   |    |
| [(1R,2E,6E,10S)-3,7-dimethyl-10-[(2R)-6-methylhept-5-en-2-yl]cyclodeca-2,6-dien-1-yl] acetate                                         |                                                                                                   |                                                                                       |
| S100                                                                                                                                  |  <p>Chiral</p>  |   |
| [(Z)-[(1S,3Z,5E,8S,11R)-6-methyl-11-[(2S)-6-methylhept-5-en-2-yl]-10-oxo-9-oxabicyclo[6.2.1]undeca-3,5-dien-2-ylidene]methyl] acetate |                                                                                                   |                                                                                       |
| S101                                                                                                                                  |  <p>Chiral</p> |  |
| [(1R,5R,8S,9S)-1,2-diformyl-5-methyl-8-[(2R)-6-methylhept-5-en-2-yl]-9-bicyclo[3.3.1]non-2-enyl] acetate                              |                                                                                                   |                                                                                       |

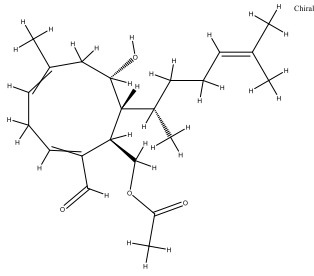
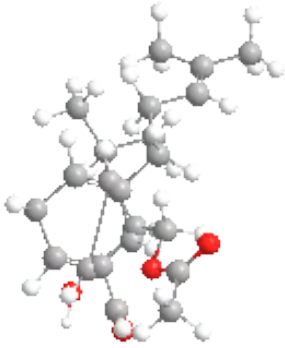
| Kode Senyawa                                                                                                                                                            | Struktur 2D                                                                         | Struktur 3D                                                                           |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S102                                                                                                                                                                    |    |    |
| [(3R,3aS,4S,6E,8R,9R,10R,11E,12aR)-9-acetyloxy-4-hydroxy-3-(2-hydroxypropan-2-yl)-6,10,12a-trimethyl-2,3,3a,4,5,8,9,10-octahydro-1H-cyclopenta[11]annulen-8-yl] acetate |                                                                                     |                                                                                       |
| S103                                                                                                                                                                    |   |   |
| (3aS,4R,5S,8S,8aR)-3,8-dimethyl-5-[(2R)-6-methylhept-6-en-2-yl]-3a,4,5,6,7,8a-hexahydro-1H-azulene-4,8-diol                                                             |                                                                                     |                                                                                       |
| S104                                                                                                                                                                    |  |  |
| (3aS,4R,5S,8aR)-3-methyl-5-[(2R)-6-methylhept-6-en-2-yl]-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-4-ol                                                           |                                                                                     |                                                                                       |
| S105                                                                                                                                                                    |  |  |
| [(2S,3S)-2-[(3aS,4R,5S,7R,8aR)-4,7-dihydroxy-3-methyl-8-methylidene-3a,4,5,6,7,8a-hexahydro-1H-azulen-5-yl]-6-methylhept-6-en-3-yl] acetate                             |                                                                                     |                                                                                       |

| Kode Senyawa                                                                                                            | Struktur 2D                                                                         | Struktur 3D                                                                           |
|-------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S106                                                                                                                    |    |    |
| (1R,5R,8S,9S)-9-hydroxy-5-methyl-8-[(2R)-6-methylhept-5-en-2-yl]bicyclo[3.3.1]non-2-ene-1,2-dicarbaldehyde              |                                                                                     |                                                                                       |
| S107                                                                                                                    |   |   |
| (3aS,5R,8S,8aR)-8-methoxy-3,8-dimethyl-5-[(2R)-6-methylhept-5-en-2-yl]-3a,4,5,6,7,8a-hexahydro-1H-azulene               |                                                                                     |                                                                                       |
| S108                                                                                                                    |  |  |
| [(1Z,5E,8R,11S)-6-methyl-11-[(2S)-6-methylhept-5-en-2-yl]-10-oxo-9-oxabicyclo[6.2.1]undeca-1,5-dien-2-yl]methyl acetate |                                                                                     |                                                                                       |
| S109                                                                                                                    |  |  |
| (3aE,6E,10R,10aR)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-1,5,8,9,10,10a-hexahydrocyclonona[c]furan-3-one             |                                                                                     |                                                                                       |

| Kode Senyawa                                                                                                                                                              | Struktur 2D                                                                         | Struktur 3D                                                                           |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S110                                                                                                                                                                      |    |    |
| (3aE,6E,10S,10aS)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-1,5,8,9,10,10a-hexahydrocyclonona[c]furan-3-one                                                               |                                                                                     |                                                                                       |
| S111                                                                                                                                                                      |   |   |
| [(1R,3R,3aE,6E,9S,10R,10aR)-1,3-dimethoxy-7-methyl-10-[(2S)-6-methylhept-5-en-2-yl]-3,5,8,9,10,10a-hexahydro-1H-cyclonona[c]furan-9-yl] acetate                           |                                                                                     |                                                                                       |
| S112                                                                                                                                                                      |  |  |
| [(3R,3aS,4S,6E,8R,9R,10R,11E,12aR)-9-acetyloxy-3-(2-acetyloxypropan-2-yl)-4-hydroxy-6,10,12a-trimethyl-2,3,3a,4,5,8,9,10-octahydro-1H-cyclopenta[11]annulen-8-yl] acetate |                                                                                     |                                                                                       |
| S113                                                                                                                                                                      |  |  |
| (6E,10S)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-3,4,5,8,9,10-hexahydrocyclonona[c]furan-1-one                                                                          |                                                                                     |                                                                                       |

| Kode Senyawa                                                                                                                  | Struktur 2D                                                                                       | Struktur 3D                                                                           |
|-------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S114                                                                                                                          |  <p>Chiral</p>   |    |
| (1S,3R,5S,8E,12R,13S,15R)-1,5,9-trimethyl-13-prop-1-en-2-yl-4-oxatricyclo[10.3.0.03,5]pentadec-8-en-15-ol                     |                                                                                                   |                                                                                       |
| S115                                                                                                                          |  <p>Chiral</p>  |   |
| [(1S,2E,5E,8R,9R)-2-formyl-8-hydroxy-6-methyl-9-[(2R)-6-methylhept-5-en-2-yl]cyclonona-2,5-dien-1-yl]methyl acetate           |                                                                                                   |                                                                                       |
| S116                                                                                                                          |  <p>Chiral</p> |  |
| [(3aE,6E,9R,10S,10aS)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-3-oxo-1,5,8,9,10,10a-hexahydrocyclonona[c]furan-9-yl] acetate |                                                                                                   |                                                                                       |
| S117                                                                                                                          |  <p>Chiral</p> |  |
| (1S,3aE,6E,10R,10aR)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-3,5,8,9,10,10a-hexahydro-1H-cyclonona[c]furan-1-ol             |                                                                                                   |                                                                                       |

| Kode Senyawa                                                                                                         | Struktur 2D                                                                                       | Struktur 3D                                                                           |
|----------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| S118                                                                                                                 |  <p>Chiral</p>   |    |
| (1S,10R,10aR)-7-methyl-10-[(2R)-6-methylhept-5-en-2-yl]-3,5,8,9,10,10a-hexahydro-1H-cyclonona[c]furan-1-ol           |                                                                                                   |                                                                                       |
| S119                                                                                                                 |  <p>Chiral</p>   |    |
| (3R,3aS,7R,7aS)-7-hydroxy-7a-methyl-3-[(2S)-6-methylhept-5-en-2-yl]-2,3,6,7-tetrahydro-1H-indene-3a,4-dicarbaldehyde |                                                                                                   |                                                                                       |
| S120                                                                                                                 |  <p>Chiral</p> |  |
| (1R,2S,5E,8R,11S)-6-methyl-11-[(2S)-6-methylhept-5-en-2-yl]-10-oxo-9-oxabicyclo[6.2.1]undec-5-ene-2-carbaldehyde     |                                                                                                   |                                                                                       |
| S121                                                                                                                 |  <p>Chiral</p> |  |
| 2-[(1S,3aS,4E,6R,9E,12aR)-3a,6,10-trimethyl-2,3,6,7,8,11,12,12a-octahydro-1H-cyclopenta[11]annulen-1-yl]propan-2-ol  |                                                                                                   |                                                                                       |

| Kode Senyawa                                                                                                  | Struktur 2D                                                                       | Struktur 3D                                                                         |
|---------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
| S122                                                                                                          |  |  |
| [(1R,8S,9R)-2-formyl-8-hydroxy-6-methyl-9-[(2S)-6-methylhept-5-en-2-yl]cyclonona-2,5-dien-1-yl]methyl acetate |                                                                                   |                                                                                     |

**Lampiran 6.** Hasil penambatan Molekul Ligan Uji.

| Kode Senyawa | $\Delta G$ (kcal/mol) | Ki (nM) | Ikatan Hidrogen |                           | Ikatan Hidrofobik |                                                                                          | Golongan Senyawa        |
|--------------|-----------------------|---------|-----------------|---------------------------|-------------------|------------------------------------------------------------------------------------------|-------------------------|
|              |                       |         | Jumlah          | Residu Asam Amino         | Jumlah            | Residu Asam Amino                                                                        |                         |
| R18          | -12,00                | 1,6     | 3               | Thr 877, Asn 705, Arg 752 | 2                 | Leu 704, Met 745                                                                         |                         |
| S01          | -7,17                 | 5530    | 3               | Met 742, Arg 752, Gln 711 | 1                 | Phe 764                                                                                  | Monoterpenoid lakton    |
| S03          | -10,06                | 42,5    | 3               | Leu 704, Gln 711, Arg 752 | 6                 | Met 749, Val 746, Phe 764, Met 745, Met 742, Trp 741                                     | Diterpenoid lakton      |
| S06          | -8,28                 | 854,62  |                 |                           | 3                 | Met 745, Leu 704, Phe 764                                                                | Seskuiterpenoid         |
| S07          | -7,7                  | 2260    | 1               | Asn 705                   | 5                 | Leu 873, Phe 876, Met 780, Phe 764, Leu 704                                              | Seskuiterpenoid alkohol |
| S08          | -9,94                 | 51,72   | 1               | Gln 711                   | 5                 | Met 749, Phe 764, Val 746, Met 745, Met 742                                              | Diterpenoid asetat      |
| S09          | -10,67                | 14,99   | 1               | Leu 704                   | 6                 | Met 745, Phe 764, Leu 707, Phe 876, Leu 701, Leu 880                                     | Diterpenoid lakton      |
| S10          | -6,04                 | 37070   |                 |                           | 8                 | Leu 873, Met 754, Val 746, Met 780, Leu 707, Met 787, Phe 764, Met 742                   | Seskuiterpenoid alkohol |
| S12          | -9,99                 | 47,58   |                 |                           | 10                | Leu 707, Leu 704, Met 745, Met 749, Phe 764, Val 746, Phe 876, Leu 873, Leu 880, Met 780 | Hidrokarbon siklik      |
| S13          | -9,66                 | 83,68   | 2               | Leu 704, Met 742          | 7                 | Met 749, Met 745, Phe 764, Met 780, Leu 873, Leu 880, Leu 701                            | Seskuiterpenoid alkohol |
| S14          | -9,75                 | 71,33   | 2               | Asn 705, Leu 873          | 9                 | Met 780, Phe 876, Leu 701, Met 745, Phe 764, Leu 704, Val 746, Met 749, Met 787          | Seskuiterpenoid diol    |
| S15          | -8,94                 | 281,82  |                 |                           | 4                 | Met 745, Phe 764, Met 749, Leu 704                                                       | Seskuiterpenoid diol    |
| S16          | -8,58                 | 517,20  |                 |                           | 8                 | Met 780, Leu 704, Met 787, Phe 764, Leu 873, Leu 707, Met 749, Met 745                   | Seskuiterpenoid diol    |
| S17          | -9,82                 | 63,66   | 1               | Asn 705                   | 4                 | Met 745, Phe 764, Leu 707, Phe 876                                                       | Diterpenoid alkohol     |
| S18          | -10,39                | 24,04   | 1               | Arg 752                   |                   |                                                                                          | Seskuiterpenoid         |

| Kode Senyawa | $\Delta G$ (kcal/mol) | Ki (nM) | Ikatan Hidrogen |                                  | Ikatan Hidrofobik |                                                                               | Golongan Senyawa              |
|--------------|-----------------------|---------|-----------------|----------------------------------|-------------------|-------------------------------------------------------------------------------|-------------------------------|
|              |                       |         | Jumlah          | Residu Asam Amino                | Jumlah            | Residu Asam Amino                                                             |                               |
| S19          | -10,25                | 30,55   | 1               | Leu 704                          | 3                 | <b>Met 745, Met 749, Phe 764</b>                                              | Seskuiterpenoid alkohol       |
| S20          | -10,22                | 32,08   | 1               | Leu 704                          | 6                 | <b>Met 780, Phe 876, Leu 873, Phe 764, Met 749, Met 745</b>                   | Diterpenoid lakton            |
| S21          | -9,75                 | 71,26   | 3               | <b>Met 742, Asn 705, Thr 877</b> | 4                 | <b>Met 745, Leu 707, Phe 764, Met 749</b>                                     | Diterpenoid keton             |
| S22          | -9,72                 | 75,58   |                 |                                  | 2                 | <b>Phe 764, Leu 704</b>                                                       | Diterpenoid                   |
| S23          | -10,03                | 44,54   |                 |                                  | 4                 | <b>Leu 873, Met 742, Met 745, Phe 764</b>                                     | Seskuiterpenoid triol         |
| S24          | -10,84                | 11,28   | 1               | <b>Met 742</b>                   | 4                 | <b>Phe 876, Met 780, Leu 704, Leu 873</b>                                     | Diterpenoid asetat            |
| S26          | -10,36                | 25,33   | 2               | <b>Arg 752, Gln 746</b>          | 4                 | <b>Phe 876, Leu 873, Met 742, Leu 704</b>                                     | Diterpenoid dialdehida        |
| S27          | -9,74                 | 72,41   | 2               | Leu 701, <b>Asn 705</b>          | 8                 | <b>Phe 876, Met 780, Met 787, Val 746, Leu 704, Met 749, Met 754, Phe 764</b> | Seskuiterpenoid asetat        |
| S28          | -9,98                 | 79,52   | 3               | <b>Arg 752, Gln 711, Met 742</b> | 2                 | <b>Met 749, Met 745</b>                                                       | Seskuiterpenoid asetat        |
| S29          | -11,03                | 8,19    | 1               | <b>Arg 752</b>                   |                   |                                                                               | Seskuiterpenoid diol          |
| S33          | -9,56                 | 98,02   | 1               | <b>Thr 877</b>                   | 2                 | <b>Met 745, Leu 707</b>                                                       | Diterpenoid keton             |
| S34          | -9,97                 | 48,93   | 3               | <b>Asn 705, Thr 877, Leu 704</b> | 5                 | <b>Met 780, Phe 876, Met 749, Phe 764, Met 745</b>                            | Diterpenoid asetat            |
| S35          | -10,34                | 26,47   | 2               | <b>Gln 711, Arg 752</b>          | 1                 | <b>Leu 873</b>                                                                | Diterpenoid hidroksi-aldehida |
| S36          | -10,29                | 28,62   | 1               | Leu 704                          | 3                 | <b>Phe 764, Met 749, Met 745</b>                                              | Seskuiterpenoid alkohol       |
| S41          | -10,15                | 36,08   | 3               | <b>Arg 752, Met 745, Asn 705</b> | 5                 | <b>Leu 701, Leu 704, Phe 876, Met 780, Leu 880</b>                            | Seskuiterpenoid alkohol       |
| S43          | -8,46                 | 624,27  | 2               | Met 780, <b>Thr 877</b>          | 1                 | Leu 704                                                                       | Seskuiterpenoid epoksida      |
| S45          | -9,04                 | 236,58  | 1               | Leu 704                          |                   |                                                                               | Seskuiterpenoid diol          |
| S46          | -9,96                 | 50,20   | 1               | <b>Asn 705</b>                   | 5                 | <b>Met 749, Val 746, Met 745, Phe 764, Met 787</b>                            | Diterpenoid alkohol           |
| S47          | -9,89                 | 56,25   |                 |                                  | 6                 | <b>Leu 880, Met 780, Phe 876, Leu 873, Met 745, Phe 764</b>                   | Diterpenoid alkohol           |
| S48          | -10,12                | 38,47   |                 |                                  | 6                 | <b>Phe 764, Met 745, Leu 873, Phe 876, Met 780, Leu 880</b>                   | Seskuiterpenoid lakton        |

| Kode Senyawa | $\Delta G$ (kcal/mol) | Ki (nM) | Ikatan Hidrogen |                                 | Ikatan Hidrofobik |                                                                                                 | Golongan Senyawa           |
|--------------|-----------------------|---------|-----------------|---------------------------------|-------------------|-------------------------------------------------------------------------------------------------|----------------------------|
|              |                       |         | Jumlah          | Residu Asam Amino               | Jumlah            | Residu Asam Amino                                                                               |                            |
| S49          | -10,03                | 44,34   | 1               | Leu 704                         | 3                 | <b>Leu 873, Phe 876, Met 780</b>                                                                | Diterpenoid aldehida       |
| S50          | -10,17                | 35,19   | 1               | Leu 704                         | 2                 | <b>Met 749, Phe 764</b>                                                                         | Diterpenoid polioksigenasi |
| S52          | -10,67                | 15,14   |                 |                                 | 2                 | Leu 704, Met 780                                                                                | Diterpenoid alkohol-keton  |
| S53          | -9,79                 | 66,66   | 1               | Leu 704                         | 6                 | <b>Phe 891, Leu 880, Leu 873, Met 745, Phe 764, Met 749</b>                                     | Diterpenoid keton          |
| S54          | -10,33                | 26,80   | 1               | <b>Gln 711</b>                  | 4                 | <b>Met 749, Val 746, Phe 764, Met 745</b>                                                       | Seskuiterpenoid diol       |
| S56          | -6,92                 | 8410    |                 |                                 |                   |                                                                                                 | Seskuiterpenoid trisiklik  |
| S57          | -9,7                  | 77,76   | 3               | <b>Leu 873, Met742, Gly 708</b> | 2                 | <b>Met 780, Phe 876</b>                                                                         | Seskuiterpenoid asetat     |
| S58          | -9,15                 | 195,01  | 2               | <b>Met 742, Leu 873</b>         | 3                 | <b>Met 780, Phe 876, Phe 764</b>                                                                | Seskuiterpenoid diol       |
| S59          | -10,15                | 36,57   |                 |                                 | 4                 | <b>Leu 873, Met 742, Met 745, Val 746</b>                                                       | Seskuiterpenoid peroksida  |
| S60          | -10,33                | 26,90   | 2               | <b>Gln 711, Thr 877</b>         | 1                 | Leu 704                                                                                         | Diterpenoid furan          |
| S61          | -9,67                 | 81,33   | 1               | <b>Val 746</b>                  | 5                 | <b>Leu 873, Met 742, Leu 707, Met 745, Leu 704</b>                                              | Seskuiterpenoid oksigenasi |
| S63          | -9,59                 | 93,85   |                 |                                 | 5                 | <b>Met 742, Phe 876, Leu 704, Met 787, Phe 764</b>                                              | Seskuiterpenoid asetat     |
| S64          | -10,55                | 18,44   | 1               | <b>Arg 752</b>                  | 4                 | <b>Met 780, Phe 876, Leu 880, Leu 704</b>                                                       | Seskuiterpenoid aldehida   |
| S65          | -10,02                | 45,54   |                 |                                 | 3                 | <b>Met 742, Met 745, Phe 764</b>                                                                | Diterpenoid asetat         |
| S66          | -9,6                  | 91,10   | 1               | Leu 704                         | 6                 | <b>Leu 704, Met 745, Met 742, Met 895, Trp 741, Phe 764</b>                                     | Diterpenoid asetat         |
| S67          | -10,38                | 24,71   | 1               | <b>Met 742</b>                  | 8                 | <b>Met 780, Leu 873, Phe 876, Leu 880, Met 745, Phe 764, Leu 707, Leu 704</b>                   | Seskuiterpenoid aldehida   |
| S68          | -10,42                | 23,07   | 2               | Leu 701, <b>Asn 705</b>         | 10                | <b>Met 745, Leu 704, Leu 707, Phe 764, Met 787, Met 749, Val 746, Phe 876, Met 780, Leu 880</b> | Seskuiterpenoid            |
| S69          | -9,65                 | 84,99   |                 |                                 | 3                 | <b>Met 745, Leu 704, Leu 707</b>                                                                | Seskuiterpenoid            |
| S70          | -10,02                | 44,86   | 1               | Gln711                          | 3                 | <b>Leu 704, Leu 873, Met 742</b>                                                                | Seskuiterpenoid            |

| Kode Senyawa | $\Delta G$ (kcal/mol) | Ki (nM) | Ikatan Hidrogen |                                   | Ikatan Hidrofobik |                                                                              | Golongan Senyawa             |
|--------------|-----------------------|---------|-----------------|-----------------------------------|-------------------|------------------------------------------------------------------------------|------------------------------|
|              |                       |         | Jumlah          | Residu Asam Amino                 | Jumlah            | Residu Asam Amino                                                            |                              |
| S71          | -9,69                 | 78,99   | 1               | Asn 705                           | 7                 | Met 780, <b>Leu 873, Phe 876</b> , Leu 704, <b>Met 749, Phe 764, Met 745</b> | Seskuiterpenoid              |
| S72          | -10,27                | 29,69   | 2               | Leu 704, Met 780                  | 4                 | <b>Met 749, Met 745, Phe 764, Val 746</b>                                    | Diterpenoid alkohol          |
| S73          | -9,85                 | 60,37   | 2               | Leu 704                           | 3                 | <b>Met 745, Met 749, Phe 764</b>                                             | Seskuiterpenoid asetat       |
| S74          | -10,45                | 21,85   | 1               | Leu 704                           | 3                 | <b>Phe 876, Leu 873</b> , Met 780                                            | Diterpenoid lakton keton     |
| S75          | -10,3                 | 28,38   | 1               | Leu 704                           | 1                 | Leu 704                                                                      | Seskuiterpenoid diol         |
| S76          | -9,52                 | 102,02  | 1               | Leu 704                           | 7                 | Met 743, <b>Leu 873, Met 745, Met 749</b> , Met 787, <b>Val 746, Phe 764</b> | Diterpenoid lakton dione     |
| S77*         | -10,89                | 10,39   | 3               | <b>Thr 877, Arg 752, Gln 711</b>  | 3                 | <b>Leu 873, Phe 876</b> , Met 780                                            | Seskuiterpenoid asetat       |
| S78          | -9,96                 | 50,09   |                 |                                   | 3                 | Leu 704, Leu 707, <b>Met 745</b>                                             | Diterpenoid asetat           |
| S79          | -9,48                 | 112,40  | 1               | Asn 705                           | 4                 | <b>Leu 873, Phe 764, Met 745</b> , Leu 707                                   | Diterpenoid alkohol          |
| S80          | -9,97                 | 48,87   |                 |                                   | 5                 | <b>Met 745, Phe 764</b> , Met 787, <b>Val 746, Met 749</b>                   | Seskuiterpenoid hidroperoksi |
| S81          | -9,77                 | 68,41   |                 |                                   | 6                 | <b>Met 749, Met 745, Val 746, Leu 873</b> , Met 780, <b>Phe 876</b>          | Seskuiterpenoid asetat       |
| S82          | -9,69                 | 79,34   | 3               | <b>Thr 877, Gly 708, Met 745</b>  | 1                 | <b>Phe 764</b>                                                               | Seskuiterpenoid asetat       |
| S84          | -10,12                | 38,14   | 2               | Leu 704, <b>Leu 873</b>           | 5                 | Leu 707, <b>Phe 764, Met 745, Phe 876, Leu 880</b>                           | Seskuiterpenoid asetat       |
| S85          | -10,41                | 23,23   | 2               | <b>Arg 752, Gln 711, Asn 705</b>  | 5                 | <b>Met 742, Phe 764, Met 749, Met 745, Val 746</b>                           | Diterpenoid asetat           |
| S86          | -10,27                | 29,84   | 3               | <b>Phe 764, Gln 711</b> , Leu 704 | 3                 | <b>Phe 876, Leu 873</b> , Met 780                                            | Diterpenoid asetat           |
| S87          | -10,19                | 34,13   |                 |                                   | 5                 | <b>Leu 873, Met 742, Met 895, Trp 741</b> , Ile 899                          | Diterpenoid asetat           |
| S88          | -10,87                | 10,81   |                 |                                   | 3                 | Leu 704, <b>Met 745</b> , Leu 707                                            | Seskuiterpenoid diol         |
| S89          | -10,1                 | 39,79   |                 |                                   | 5                 | Leu 704, Met 780, Leu 701, <b>Phe 876, Leu 880</b>                           | Seskuiterpenoid              |

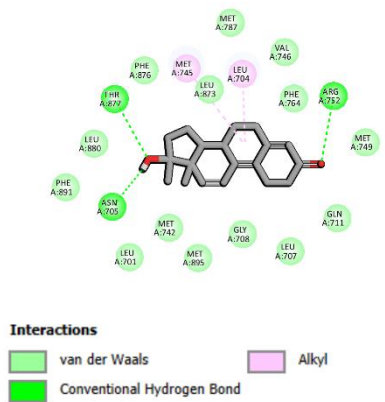
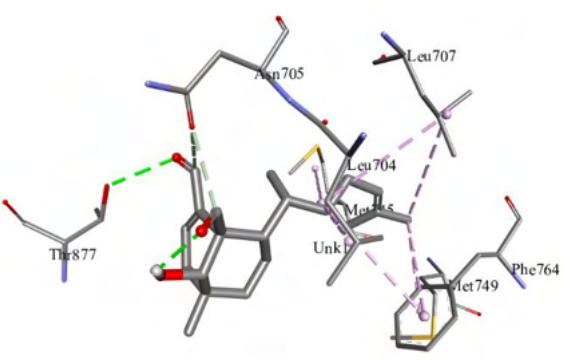
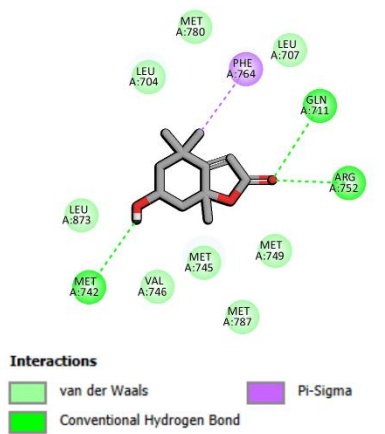
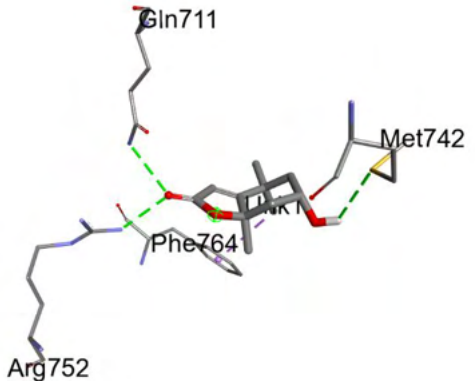
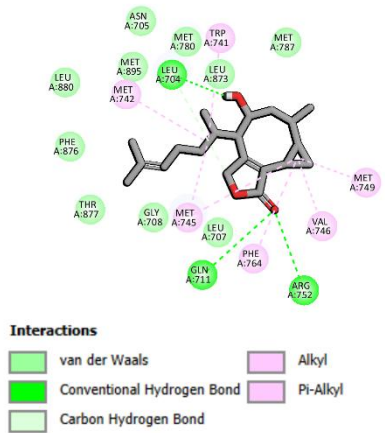
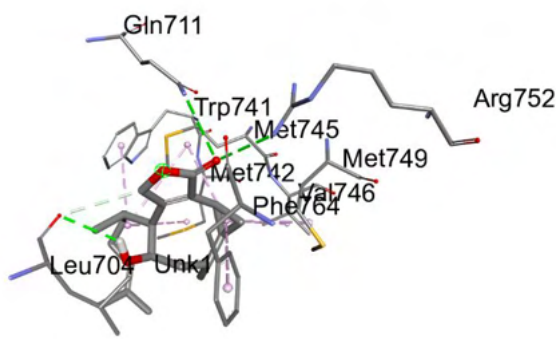
| Kode Senyawa | $\Delta G$ (kcal/mol) | Ki (nM) | Ikatan Hidrogen |                           | Ikatan Hidrofobik |                                                                        | Golongan Senyawa         |
|--------------|-----------------------|---------|-----------------|---------------------------|-------------------|------------------------------------------------------------------------|--------------------------|
|              |                       |         | Jumlah          | Residu Asam Amino         | Jumlah            | Residu Asam Amino                                                      |                          |
| S90          | -9,61                 | 90,88   | 2               | Arg 752, Leu 704          | 5                 | Leu 704, Phe 764, Met 780, Phe 891, Leu 880                            | Seskuiterpenoid aldehida |
| S93          | -10,13                | 37,79   | 2               | Arg 752, Met 742          | 5                 | Met 745, Met 749, Phe 764, Val 746, Leu 704                            | Diterpenoid keton lakton |
| S94          | -10,61                | 16,71   | 1               | Arg 752                   | 5                 | Met 749, Phe 764, Val 746, Met 745, Trp 741                            | Diterpenoid asetat       |
| S96          | -10,65                | 15,65   | 2               | Gln 711, Met 742          | 3                 | Leu 880, Leu 701, Leu 704                                              | Seskuiterpenoid asetat   |
| S98          | -9,75                 | 70,73   | 3               | Leu 701, Asn 705, Met 742 | 4                 | Phe 764, Leu 707, Met 749, Met 745                                     | Seskuiterpenoid asetat   |
| S100*        | -11,04                | 8,11    |                 |                           | 3                 | Leu 704, Leu 707, Met 745                                              | Seskuiterpenoid aldehida |
| S101         | -9,7                  | 76,98   |                 |                           | 4                 | Phe 764, Met 745, Leu 704, Met 749                                     | Diterpenoid alkohol      |
| S102         | -8,74                 | 390,31  | 1               | Thr 877                   | 1                 | Phe 764                                                                | Seskuiterpenoid asetat   |
| S103         | -9,36                 | 138,39  | 2               | Met 742, Gln 711          | 6                 | Met 745, Leu 707, Val 746, Met 749, Leu 704, Phe 764                   | Seskuiterpenoid aldehida |
| S105         | -10,28                | 28,98   | 1               | Leu 704                   | 6                 | Met 780, Leu 880, Phe 891, Met 749, Phe 764, Met 745                   | Seskuiterpenoid asetat   |
| S106         | -9,68                 | 80,59   | 1               | Thr 877                   | 5                 | Phe 764, Met 745, Leu 707, Met 749, Leu 704                            | Seskuiterpenoid asetat   |
| S111         | -8,52                 | 564,41  | 2               | Leu 701, Asn 705          | 5                 | Met 742, Leu 873, Met 745, Leu 704, Leu 707                            | Seskuiterpenoid diol     |
| S112         | -9,78                 | 68,22   | 2               | Arg 752, Thr 877          | 1                 | Phe 764                                                                | Seskuiterpenoid asetat   |
| S113         | -9,87                 | 58,62   | 1               | Leu 873                   | 8                 | Leu 707, Met 749, Met 742, Met 745, Leu 704, Leu 873, Phe 764, Val 746 | Seskuiterpenoid diol     |
| S114         | -9,78                 | 68,12   | 2               | Asn 705, Leu 704          | 4                 | Leu 704, Leu 873, Met 745, Met 742                                     | Seskuiterpenoid asetat   |
| S115         | -9,56                 | 98,07   | 1               | Thr 877                   | 3                 | Met 745, Met 749, Phe 764                                              | Seskuiterpenoid asetat   |
| S116*        | -11,55                | 3,40    | 1               | Thr 877                   | 5                 | Leu 704, Leu 707, Met 780, Met 745, Phe 764                            | Diterpenoid triol        |
| S117         | -10,23                | 31,60   | 1               | Leu 704                   | 3                 | Leu 704, Met 745, Phe 764                                              | Diterpenoid triol        |
| S118         | -9,82                 | 62,67   |                 |                           | 4                 | Leu 707, Met 745, Met 749, Phe 764                                     | Diterpenoid tetraol      |

| Kode Senyawa      | $\Delta G$ (kcal/mol) | Ki (nM) | Ikatan Hidrogen |                                  | Ikatan Hidrofobik |                                                                      | Golongan Senyawa  |
|-------------------|-----------------------|---------|-----------------|----------------------------------|-------------------|----------------------------------------------------------------------|-------------------|
|                   |                       |         | Jumlah          | Residu Asam Amino                | Jumlah            | Residu Asam Amino                                                    |                   |
| S119              | -9,52                 | 105,07  | 1               | <b>Thr 877</b>                   | 4                 | Leu 704, Leu 707, <b>Met 745, Met 749</b>                            | Diterpenoid diol  |
| S120              | -9,65                 | 83,74   |                 |                                  | 9                 | Leu 707, <b>Met 745, Met 749, Phe 764, Val 746</b>                   | Diterpenoid diol  |
| S122              | -10,01                | 46,02   | 1               | Leu 704                          | 10                | Leu 701, Leu 707, <b>Leu 880, Met 707, Met 745, Met 780, Phe 764</b> | Diterpenoid triol |
| Bicalutam<br>ide* | -10,36                | 25,43   | 3               | <b>Arg 752, Leu 704, Asn 705</b> | 5                 | Leu 707, <b>Leu 873, Met 780, Val 746, Met 749</b>                   |                   |
| Flutamide         | -8,1                  | 1150    | 3               | <b>Arg 752, Gln 711, Met 742</b> | 4                 | <b>Met 745, Met 749</b>                                              |                   |

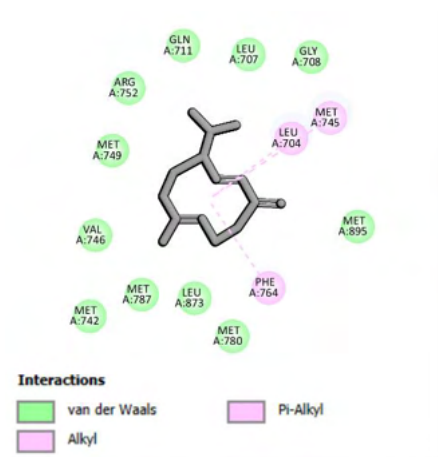
Keterangan:

\*: Senyawa yang masuk ke tahap simulasi dinamika molekul

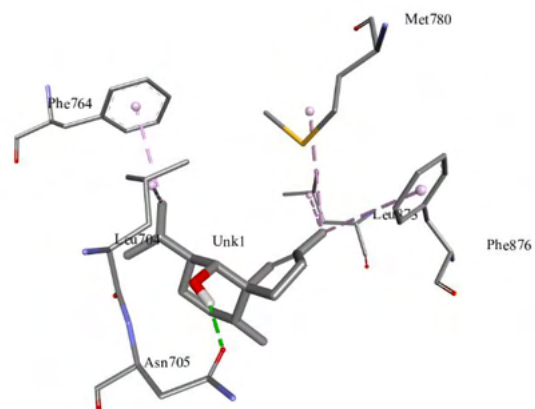
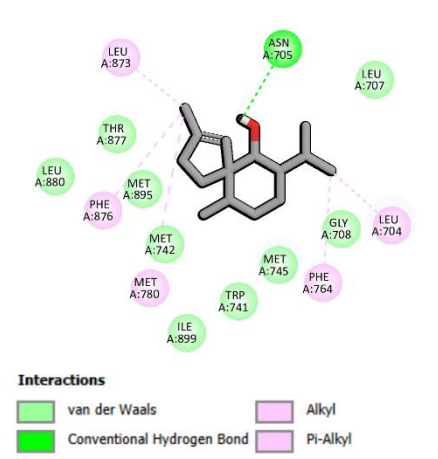
Lampiran 7. Visualisasi hasil penambatan molekul 2D dan 3D.

| Kode Ligan | 2D                                                                                                                                                                                                                                                                   | 3D                                                                                   |
|------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
| R18        |  <p>Interactions</p> <ul style="list-style-type: none"><li>van der Waals</li><li>Conventional Hydrogen Bond</li><li>Alkyl</li></ul>                                                 |    |
| S01        |  <p>Interactions</p> <ul style="list-style-type: none"><li>van der Waals</li><li>Conventional Hydrogen Bond</li><li>Pi-Sigma</li></ul>                                             |   |
| S03        |  <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>Alkyl</li><li>Pi-Alkyl</li></ul> |  |

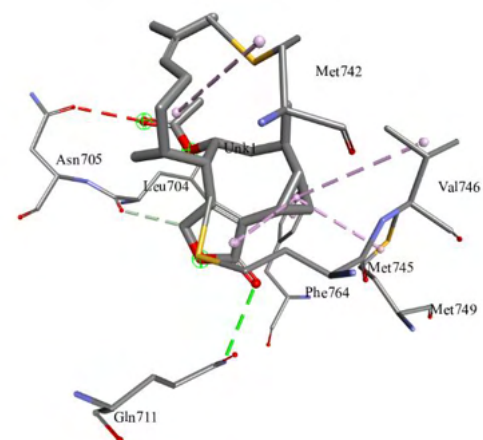
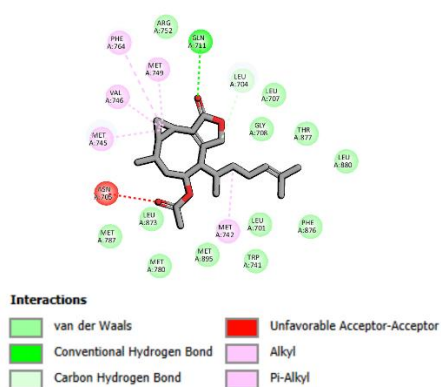
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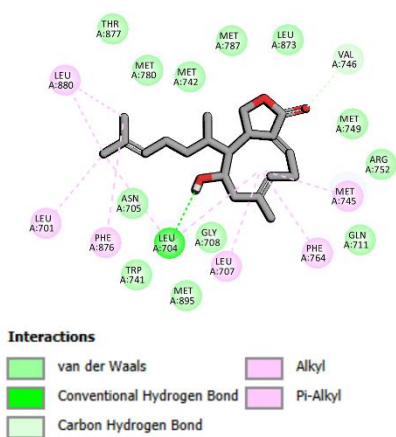
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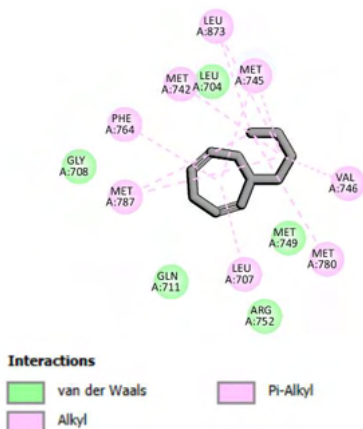
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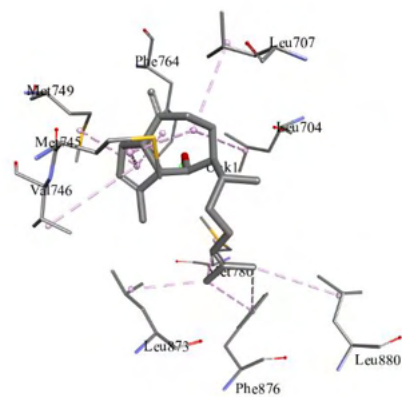
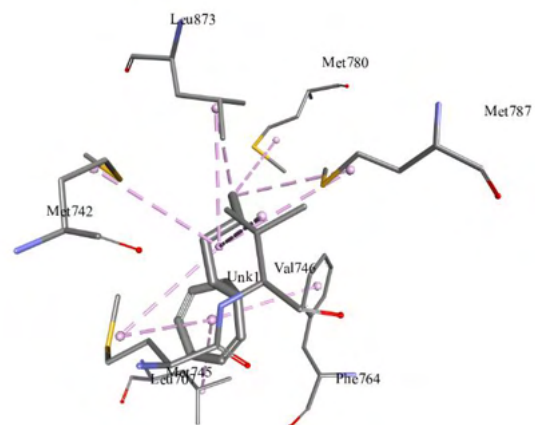
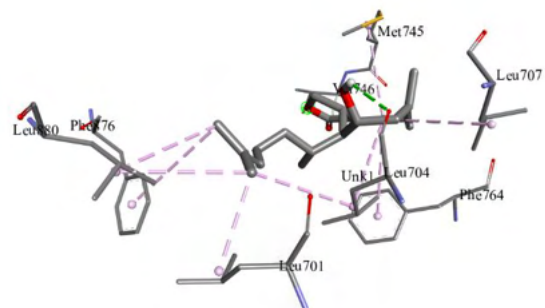
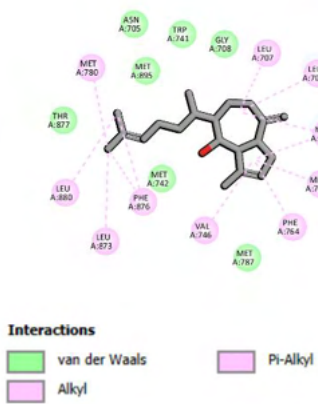
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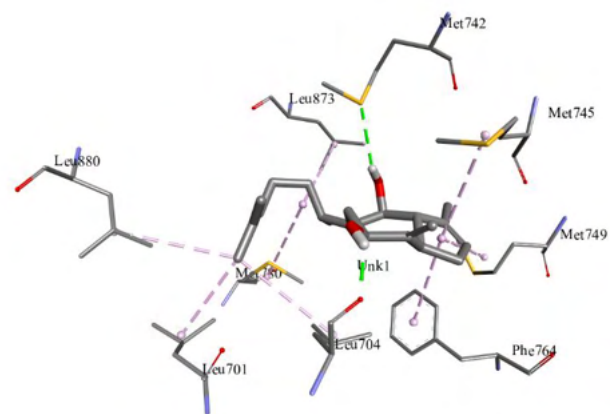
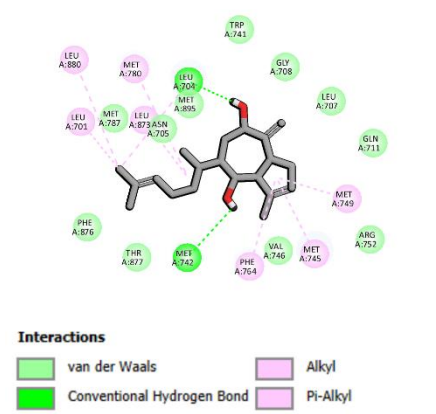
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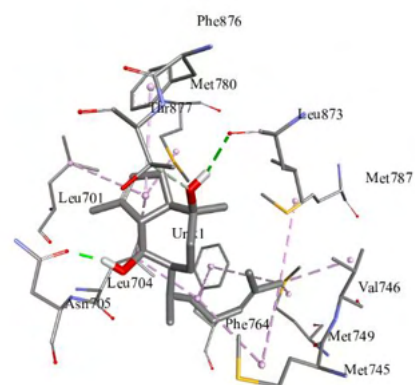
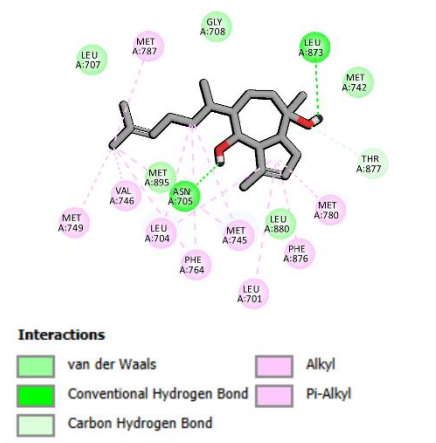
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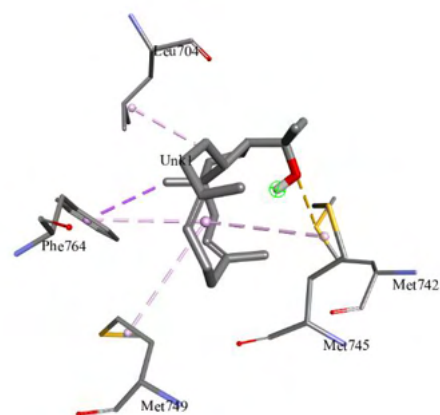
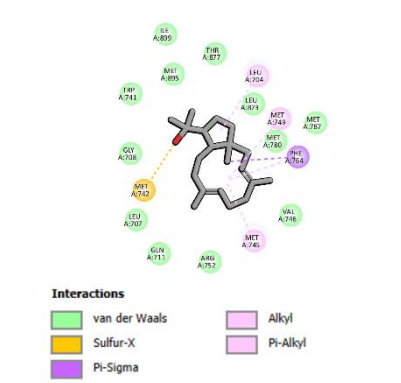
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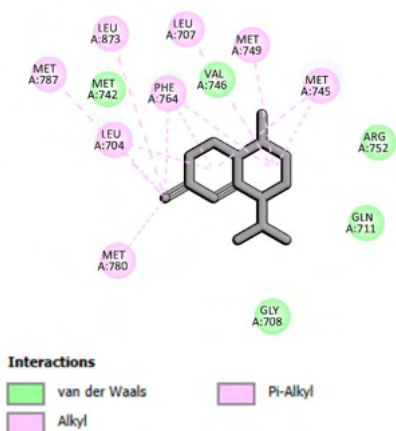
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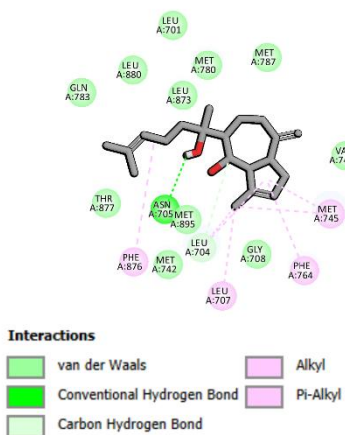
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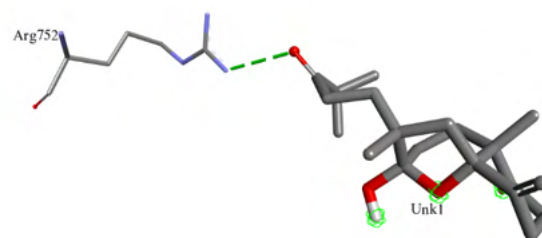
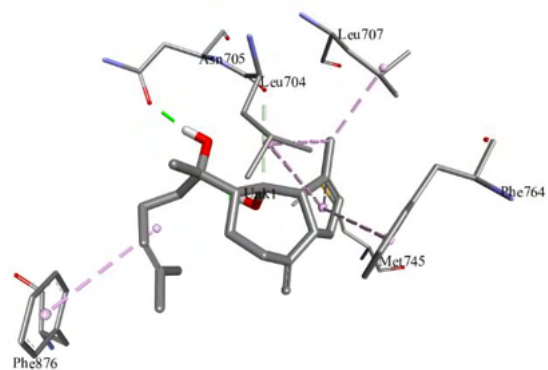
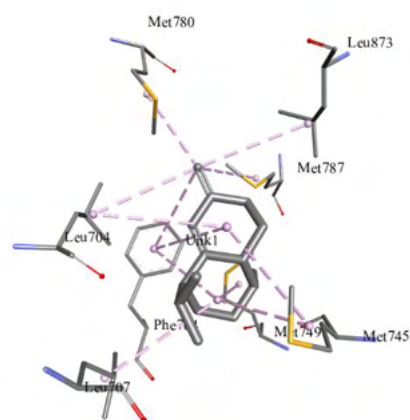
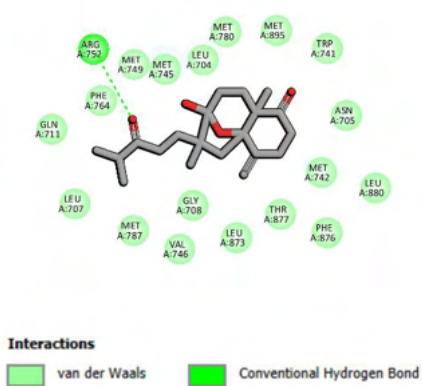
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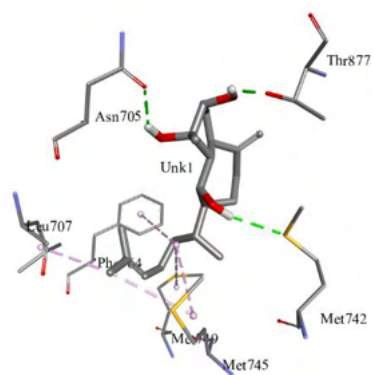
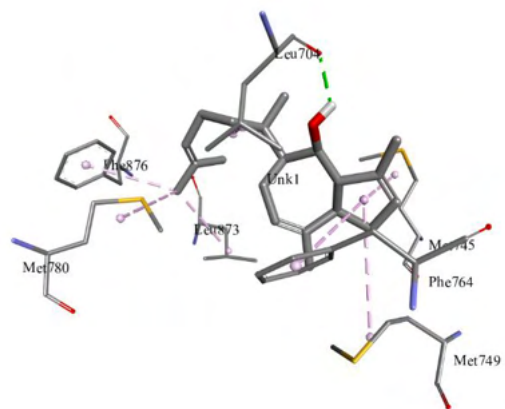
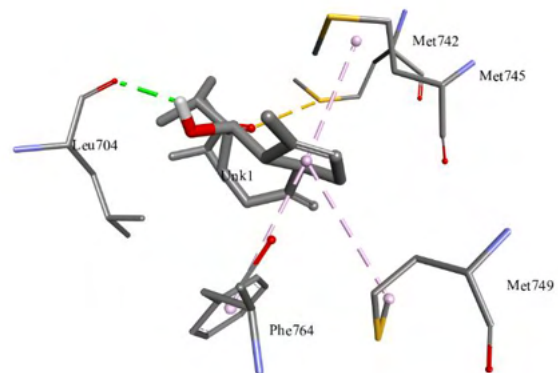


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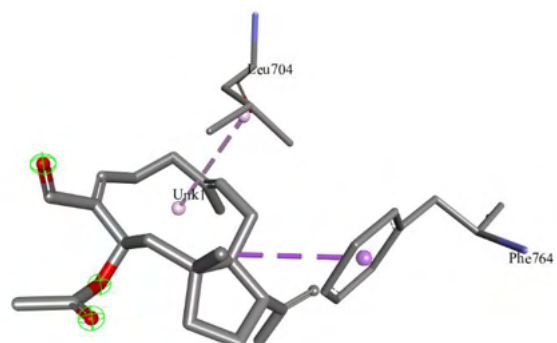
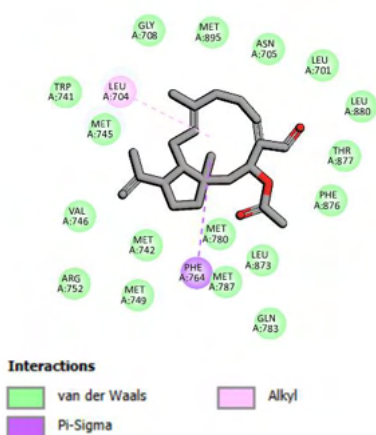


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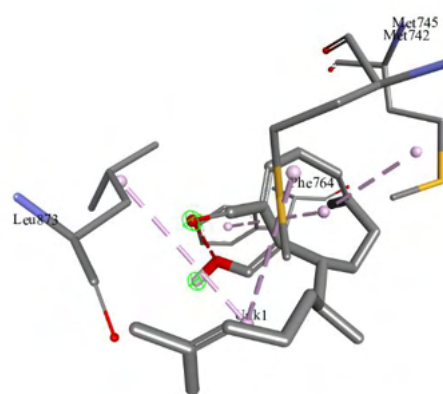
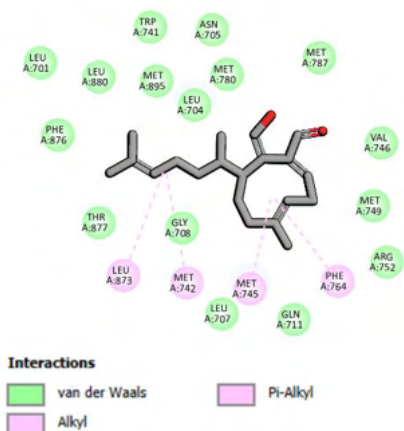




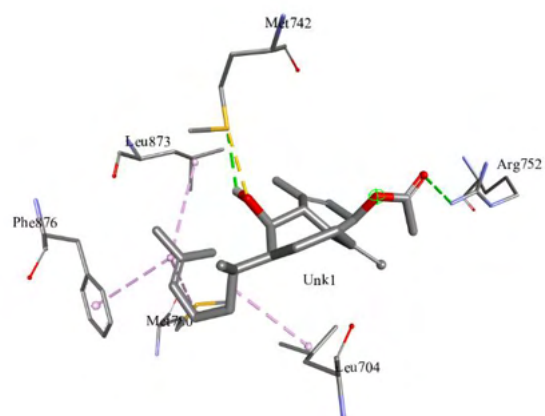
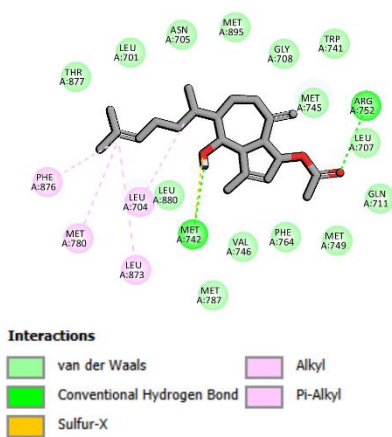
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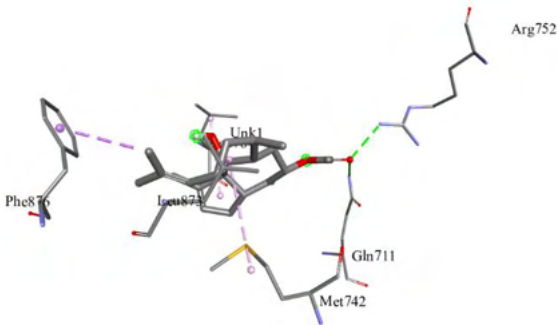
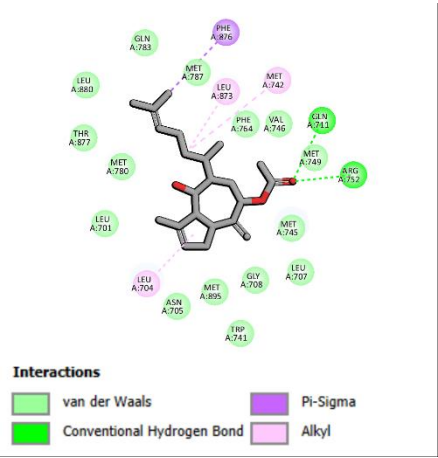
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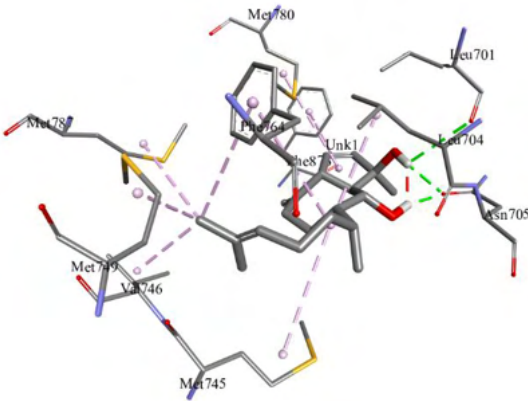
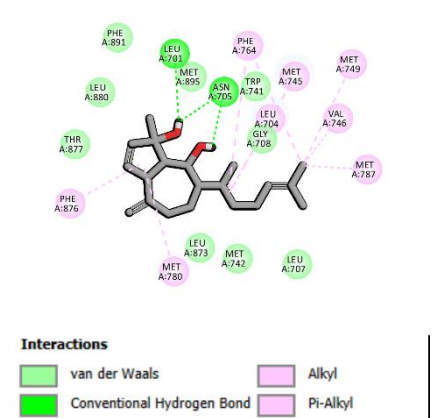
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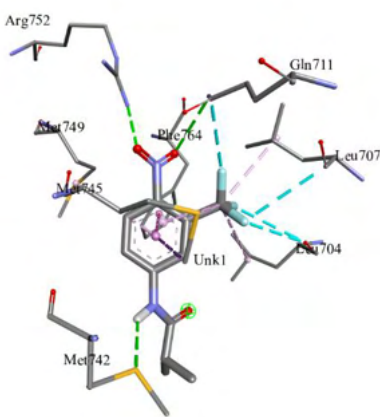
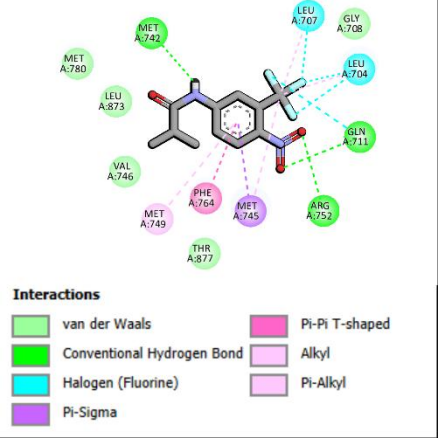
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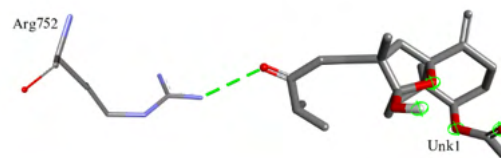
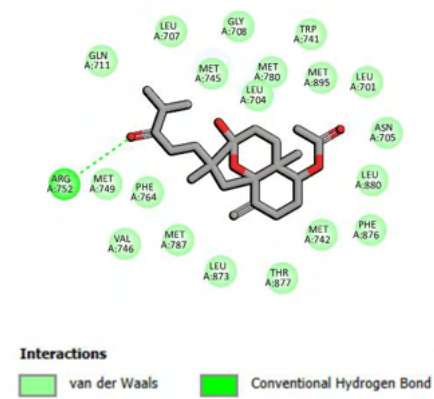
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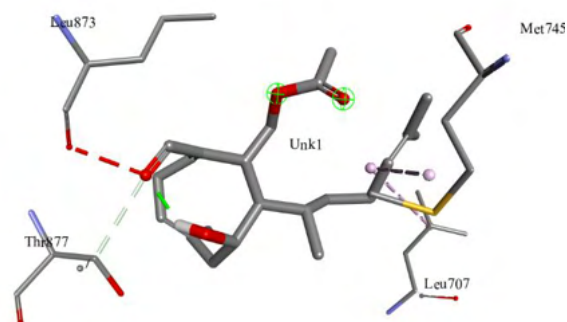
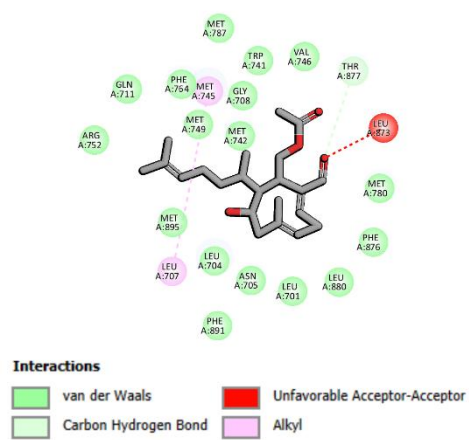
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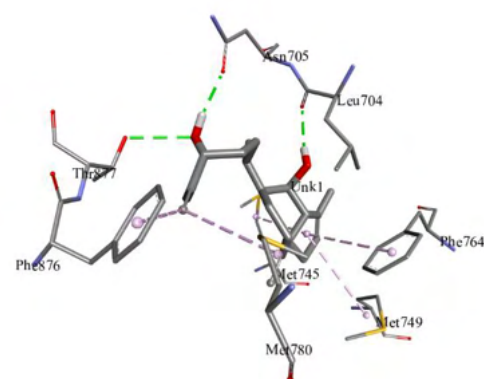
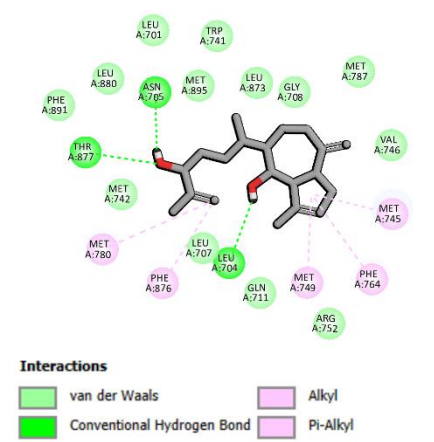
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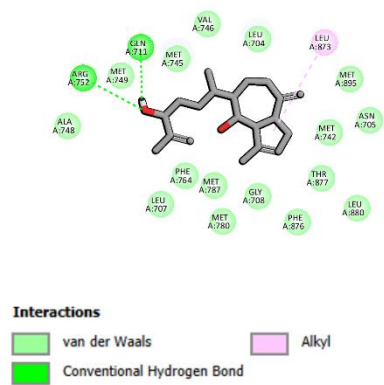
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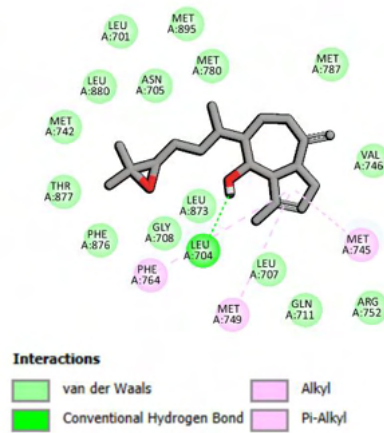
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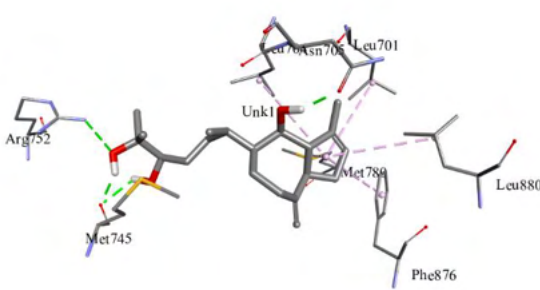
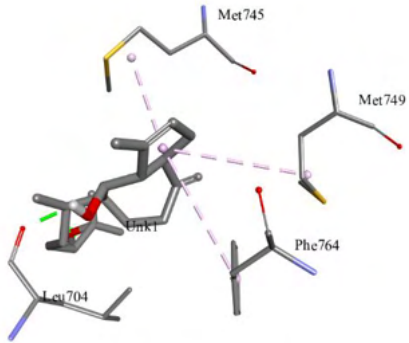
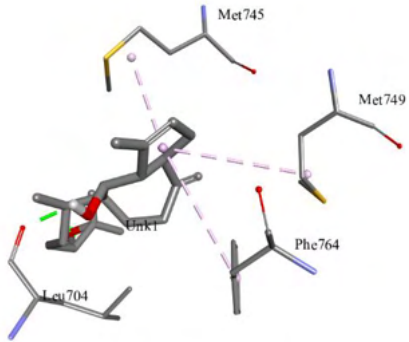
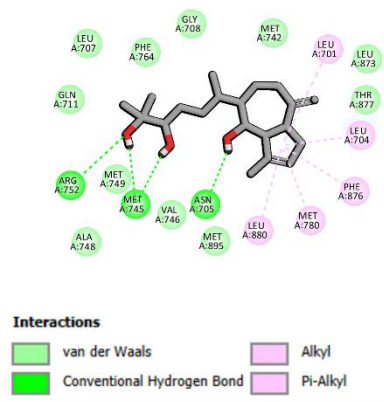
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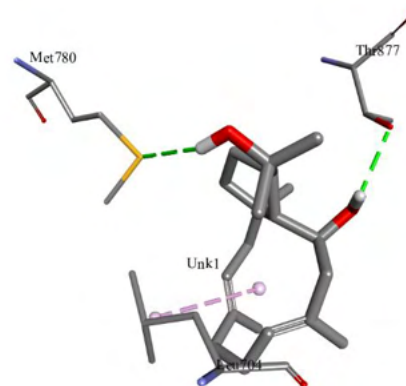
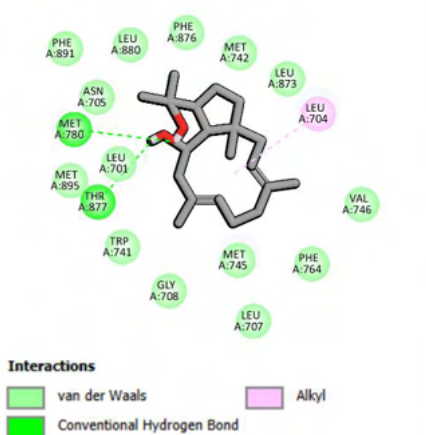
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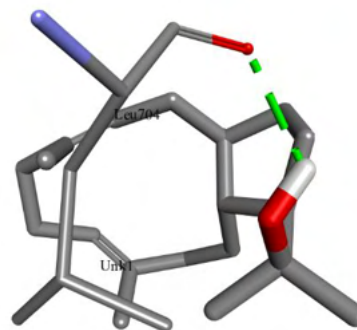
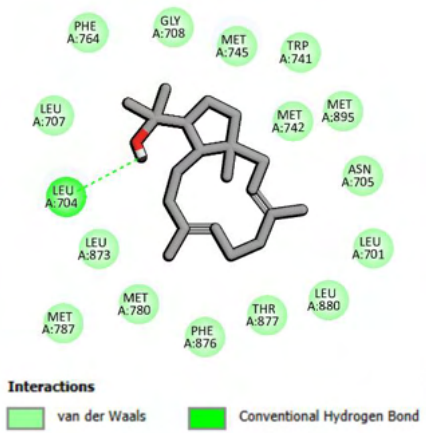
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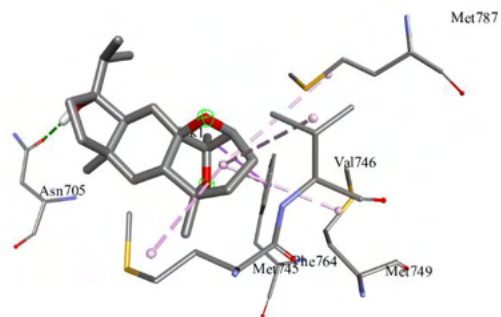
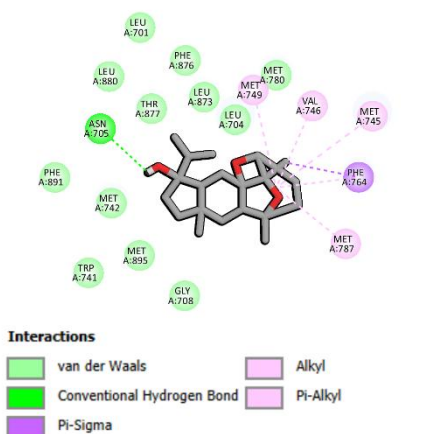
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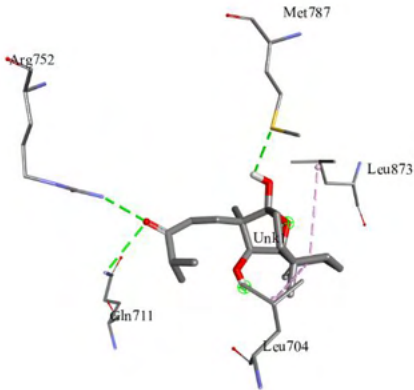
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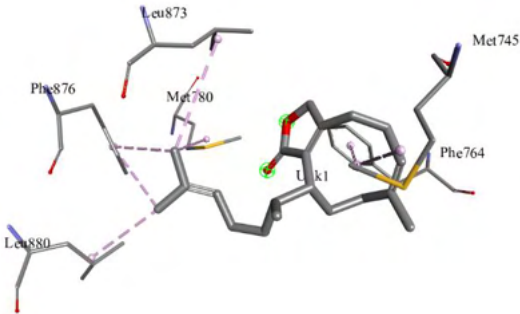
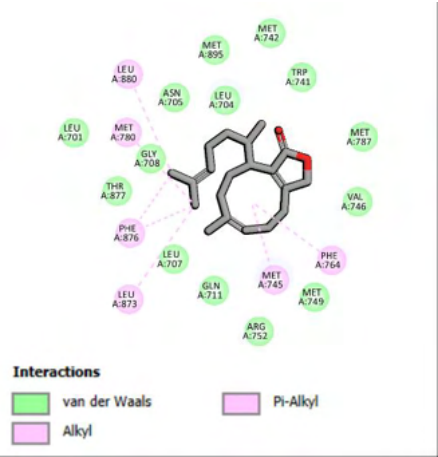
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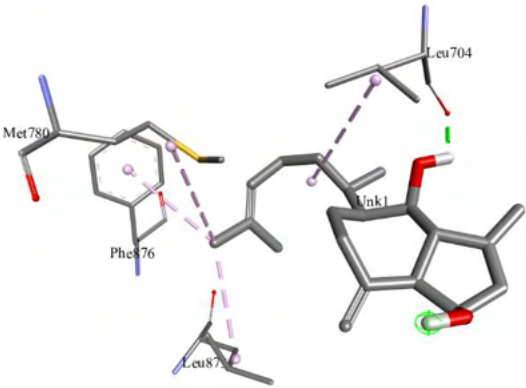
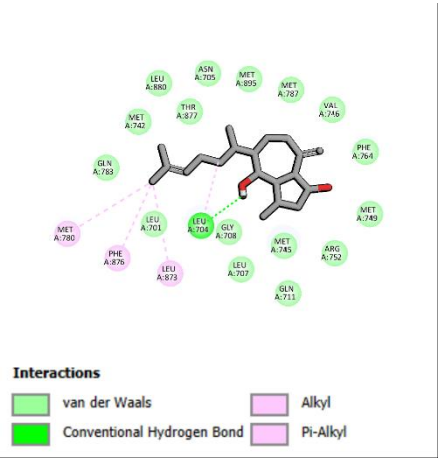
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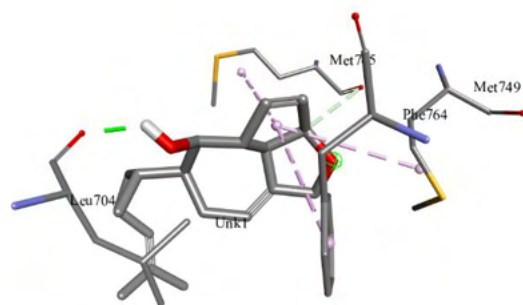
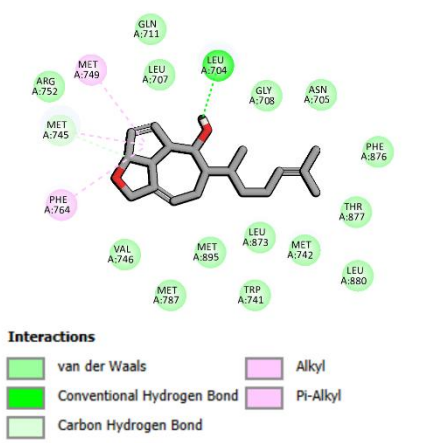
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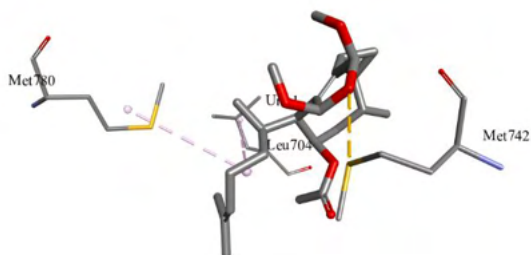
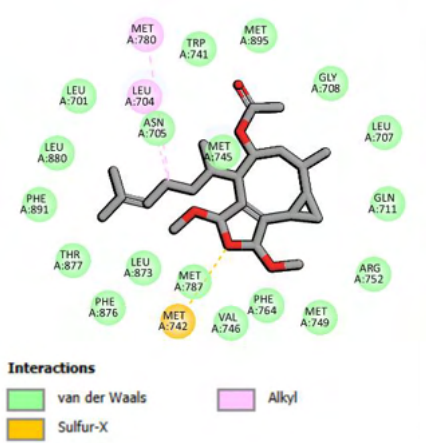
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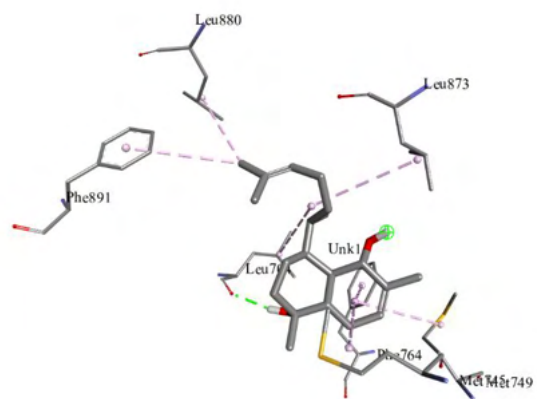
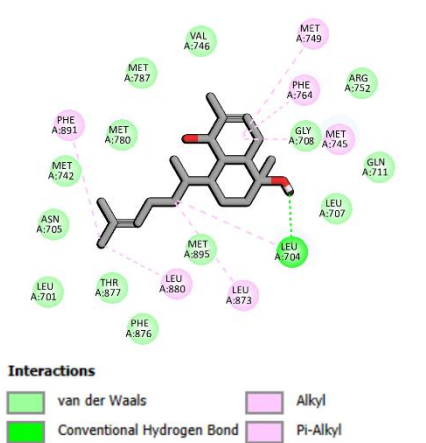
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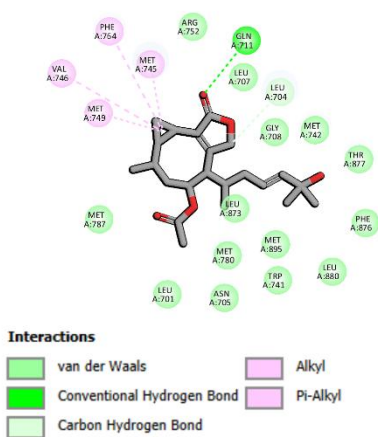
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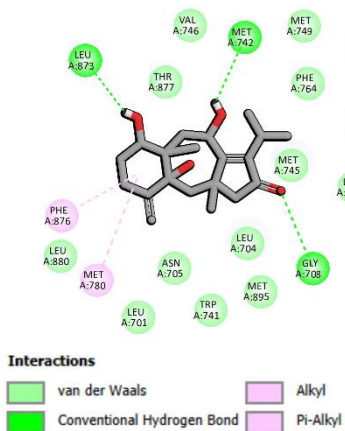
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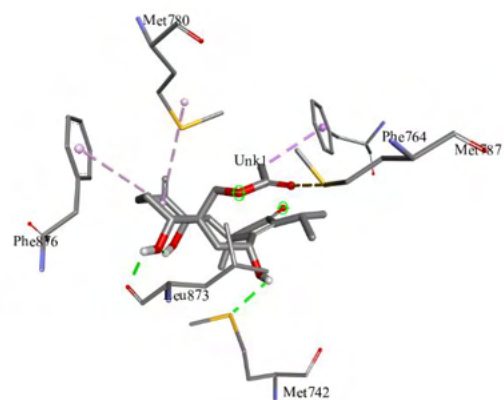
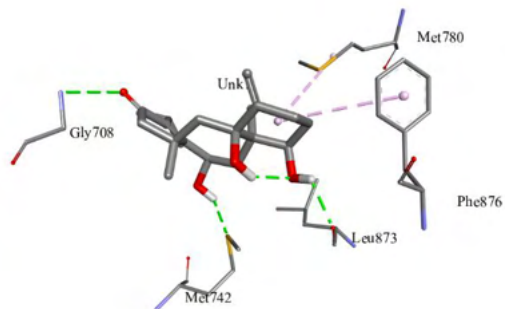
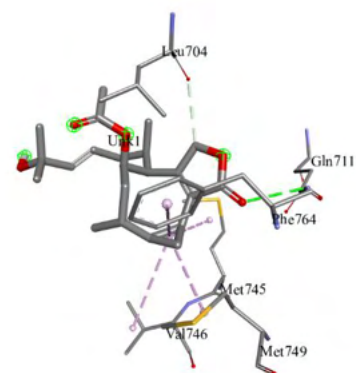
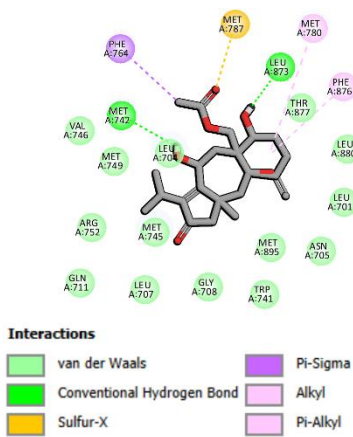
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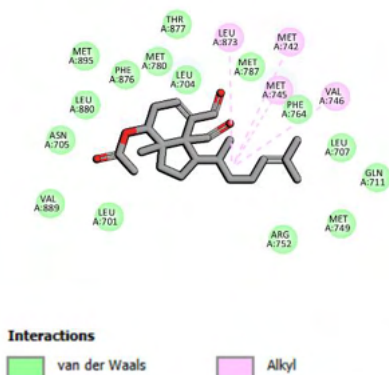
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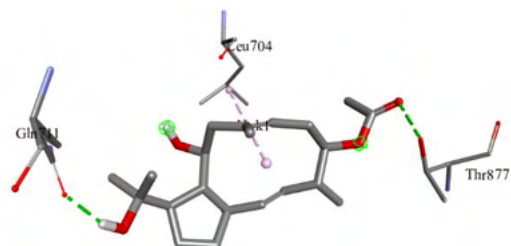
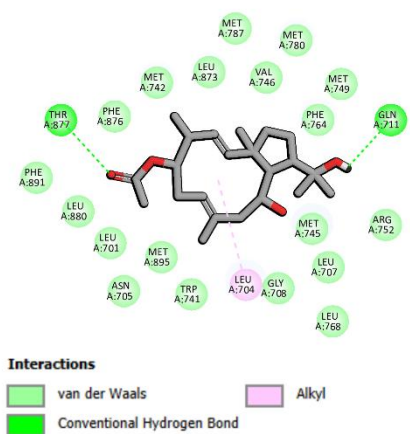
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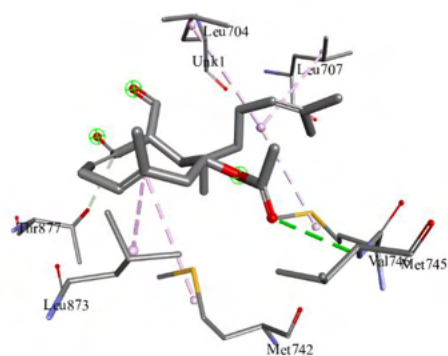
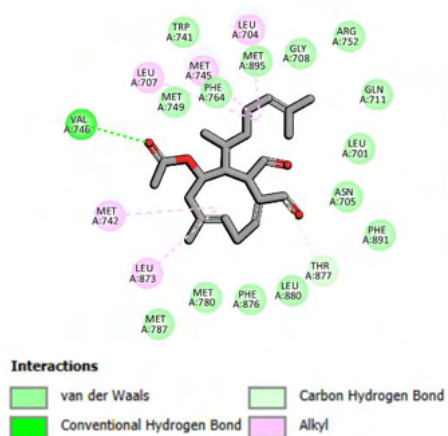
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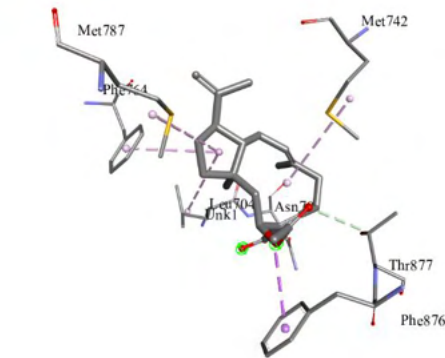
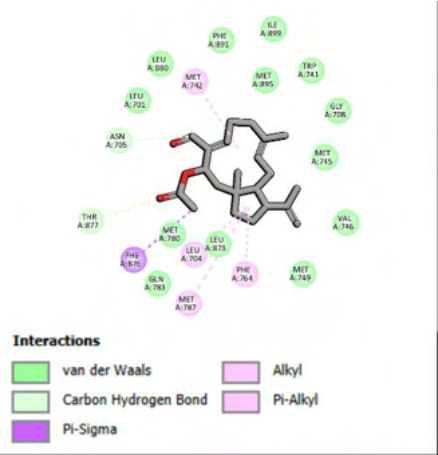
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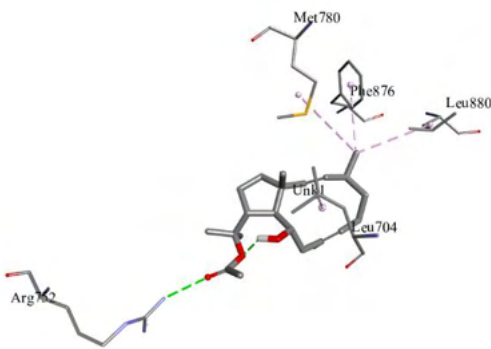
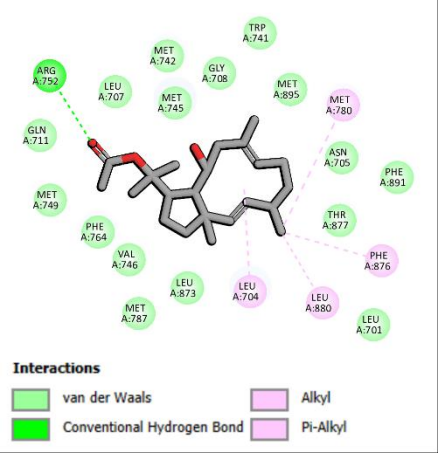
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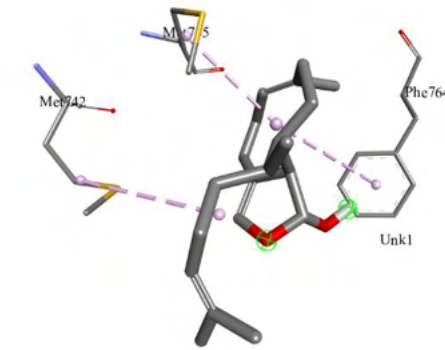
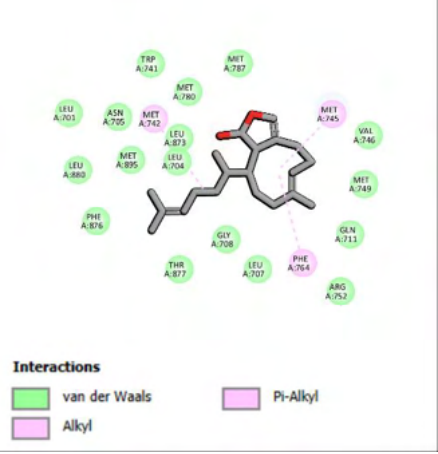
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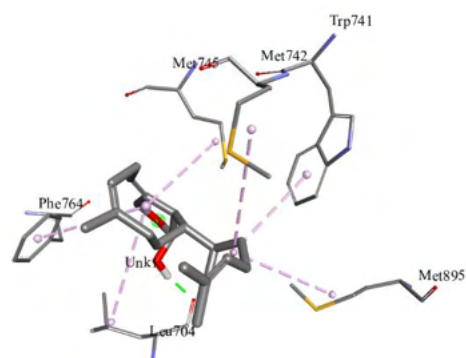
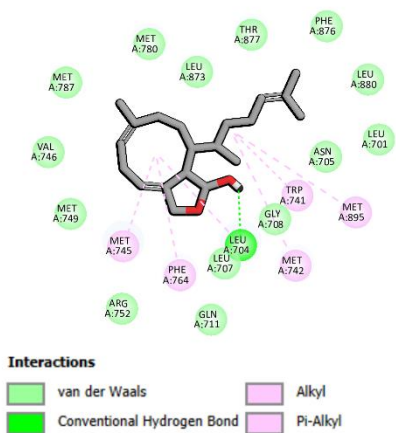
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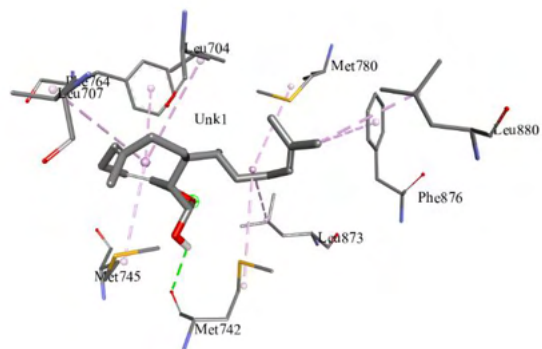
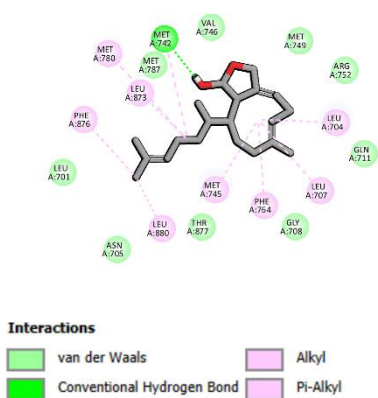
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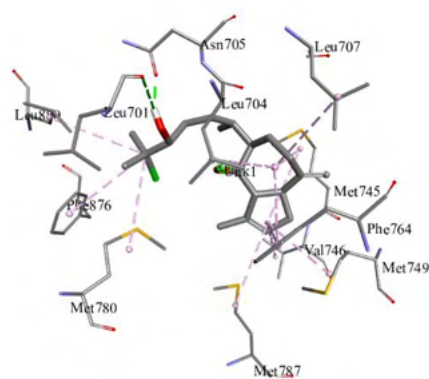
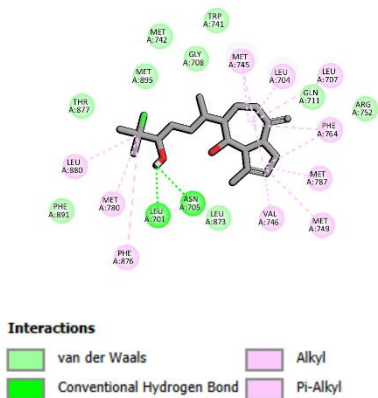
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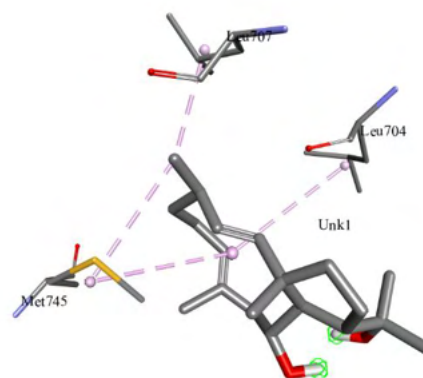
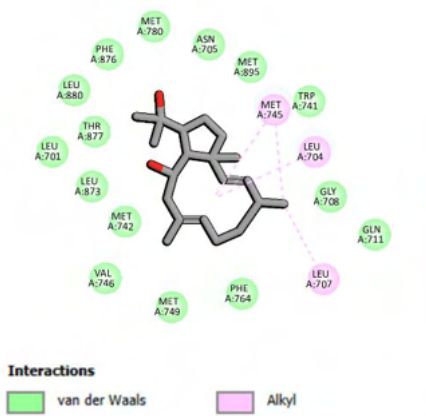
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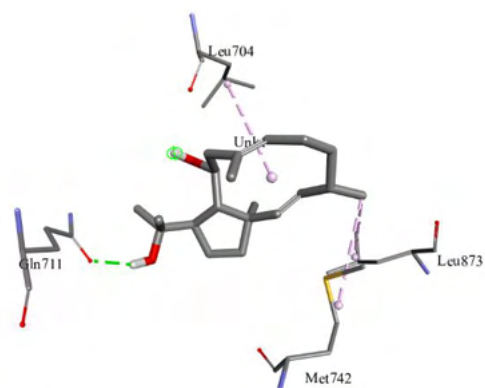
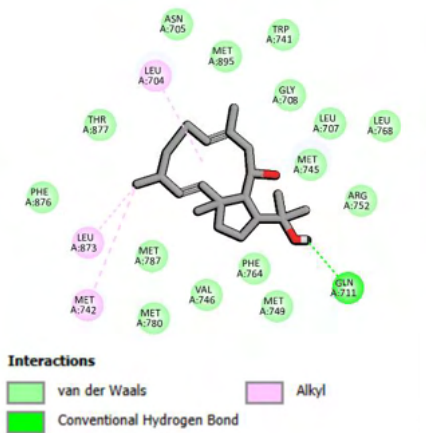
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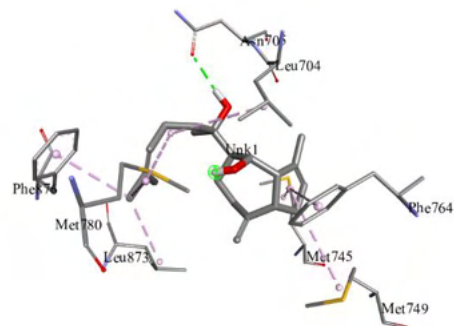
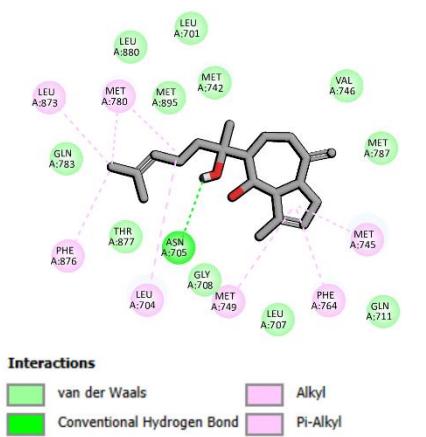
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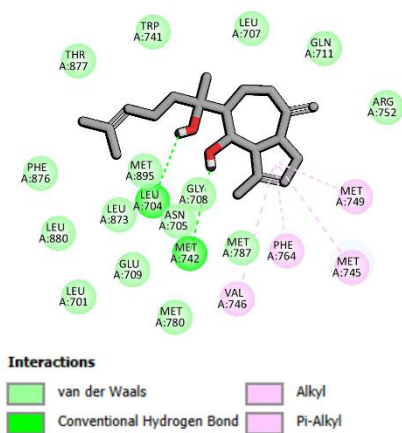
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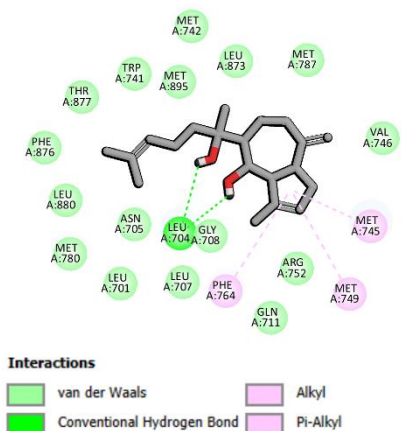
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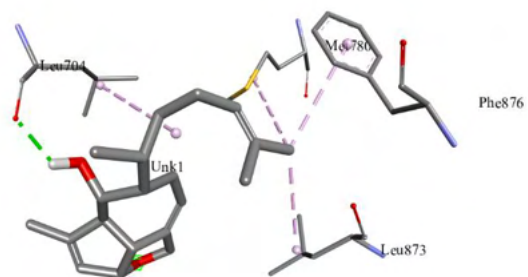
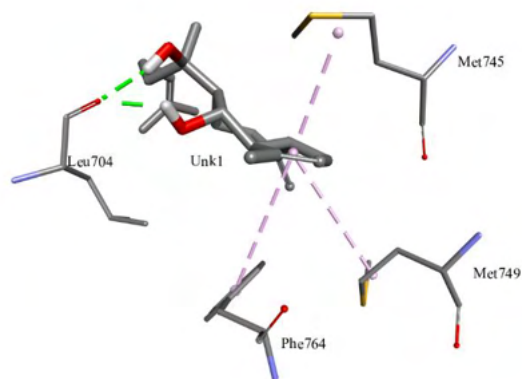
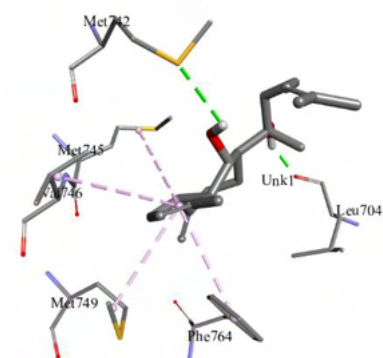
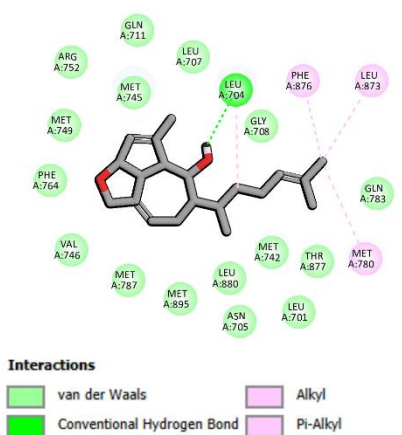
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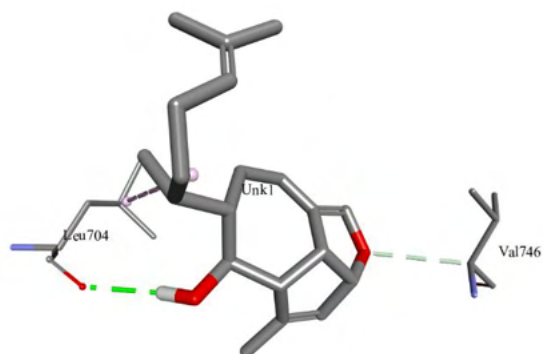
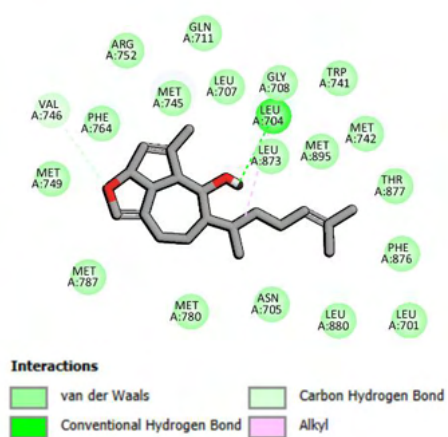
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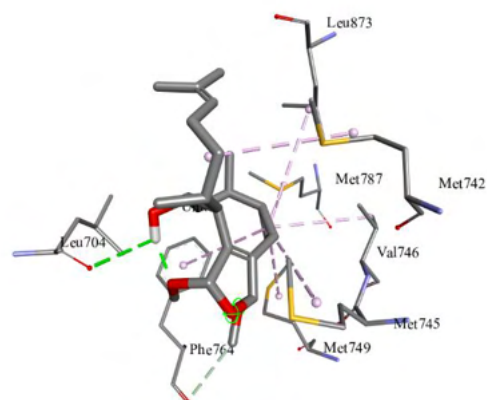
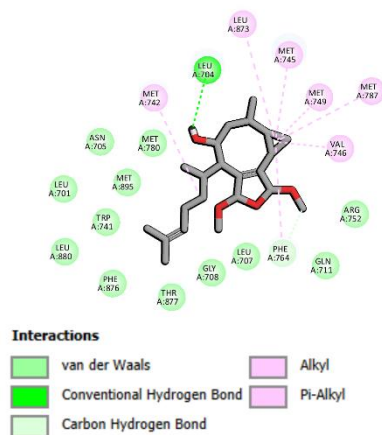
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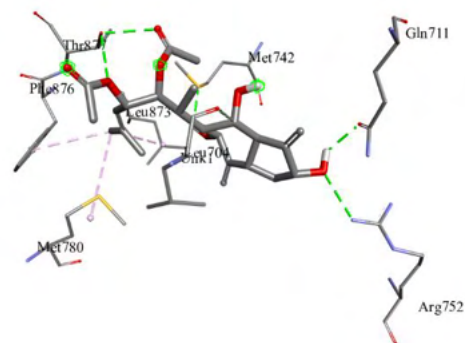
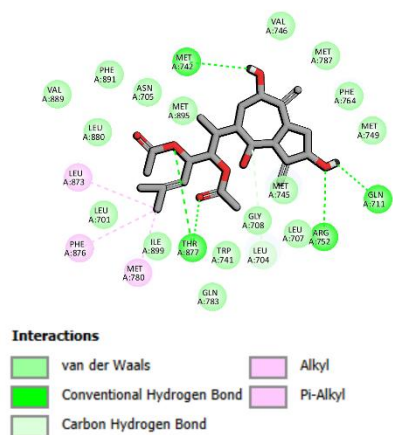
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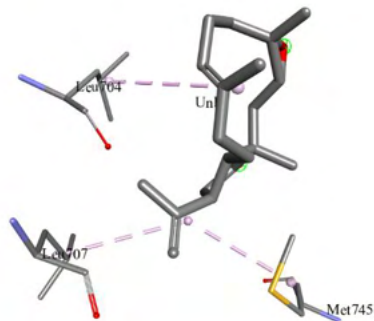
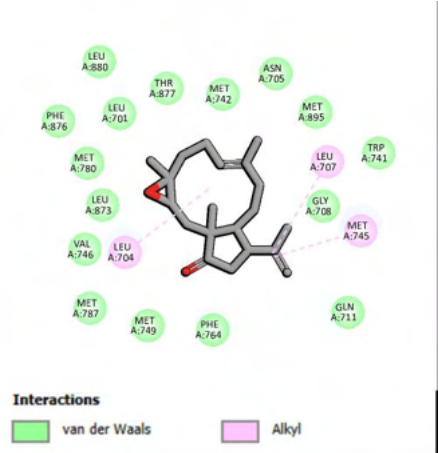
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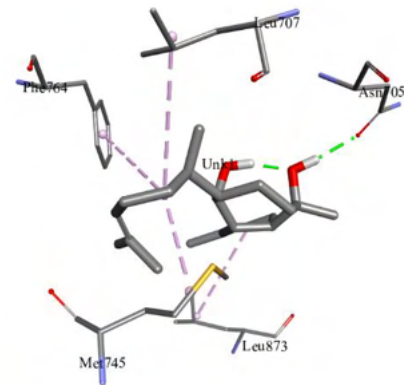
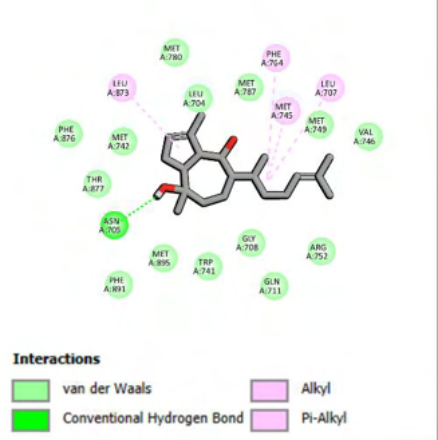
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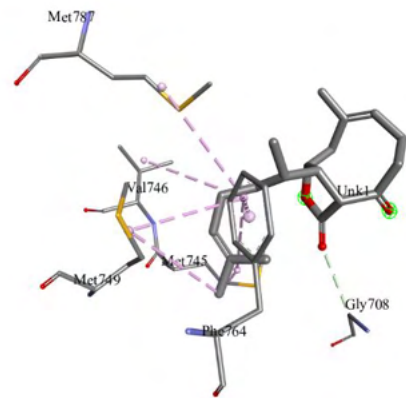
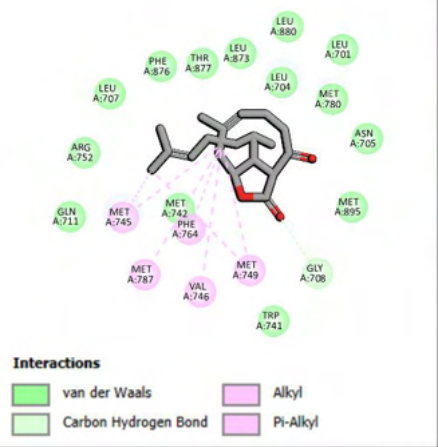
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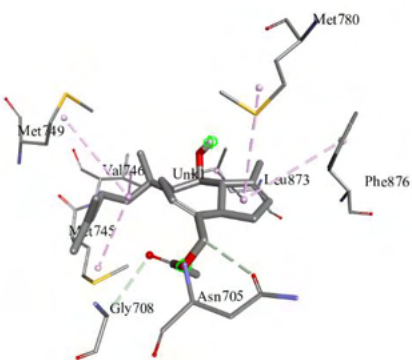
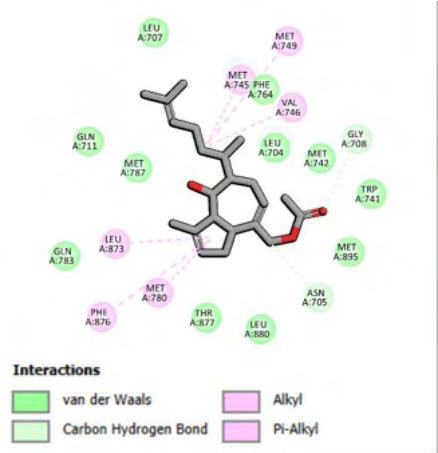
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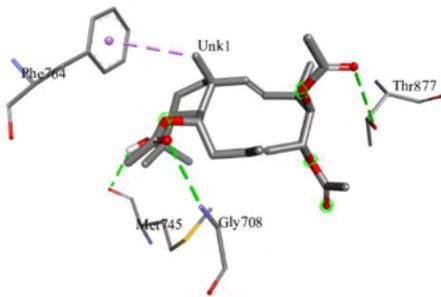
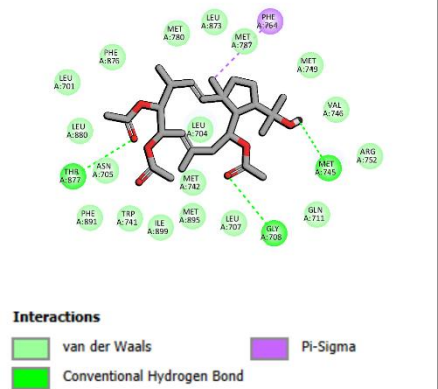
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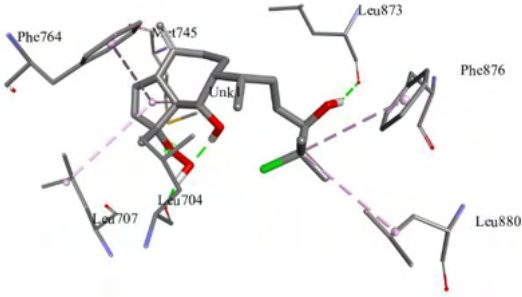
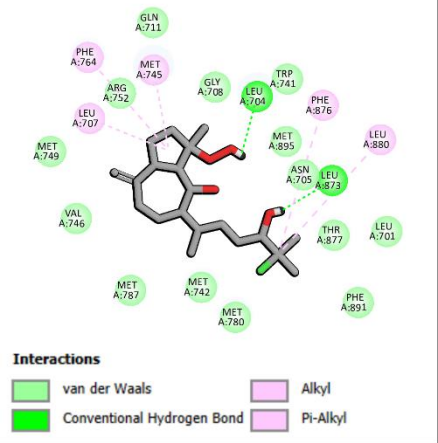
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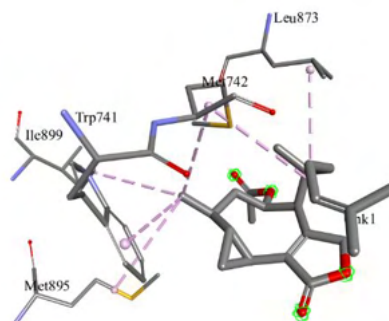
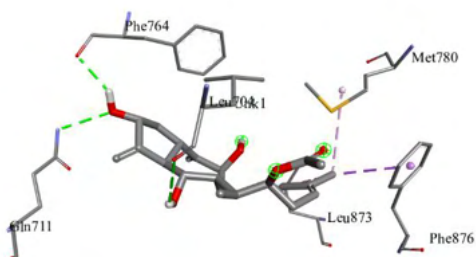
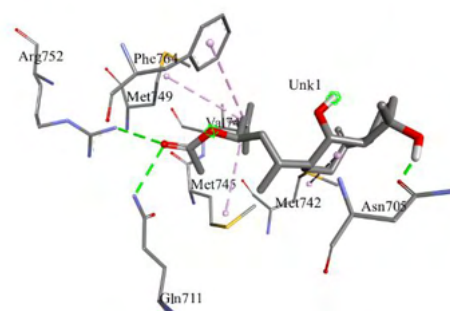


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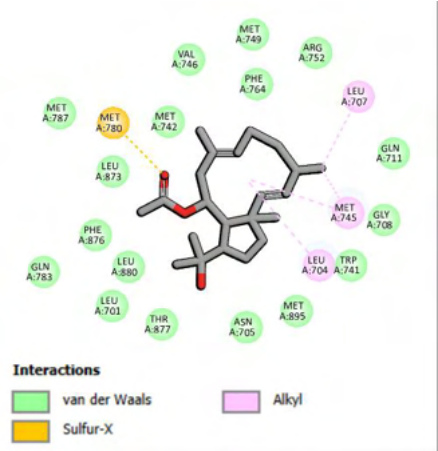


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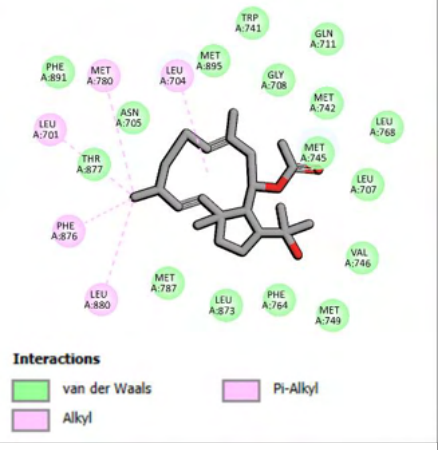




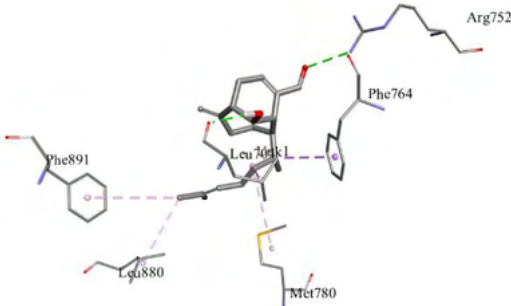
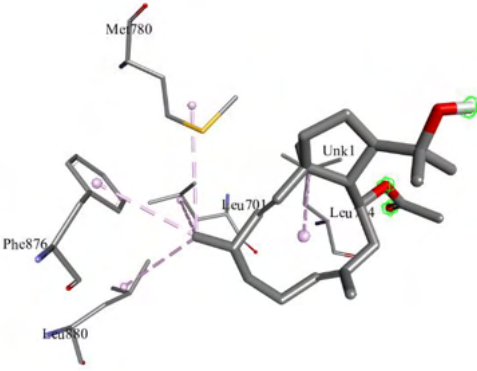
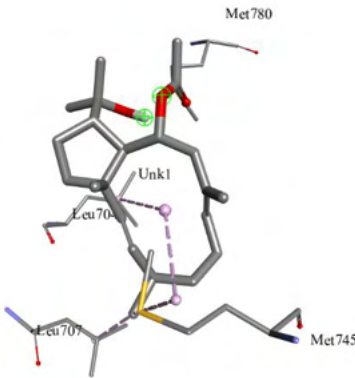
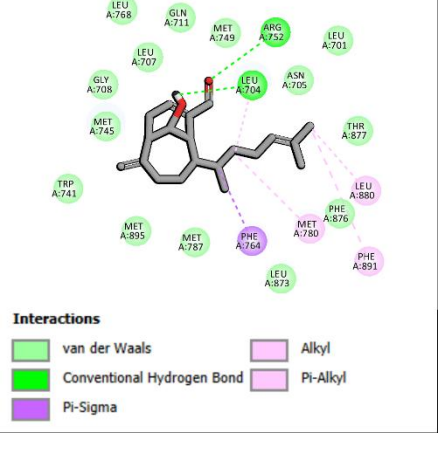
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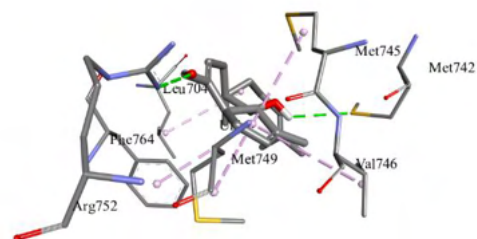
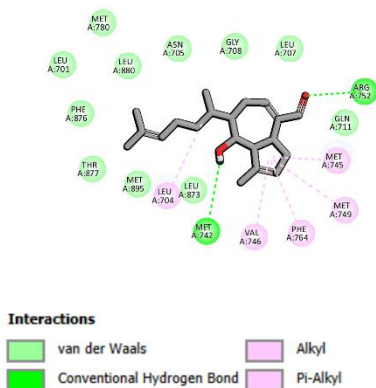
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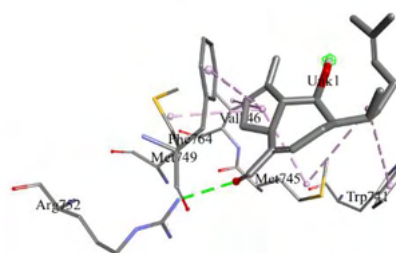
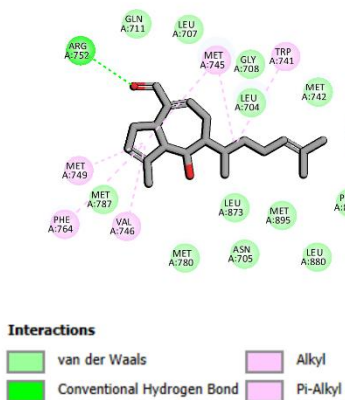
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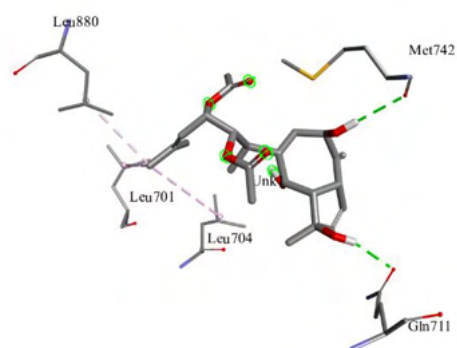
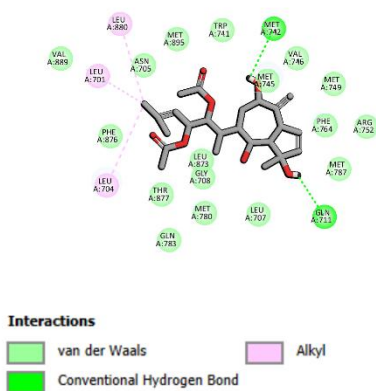
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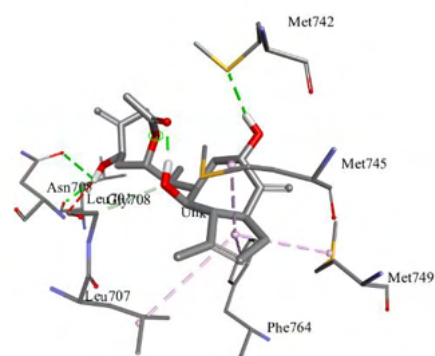
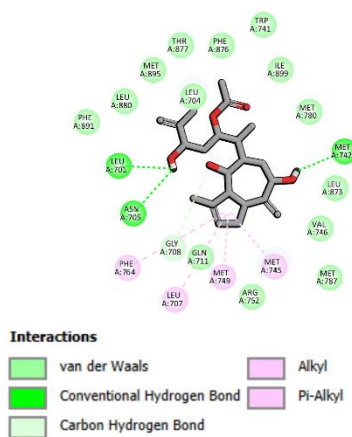
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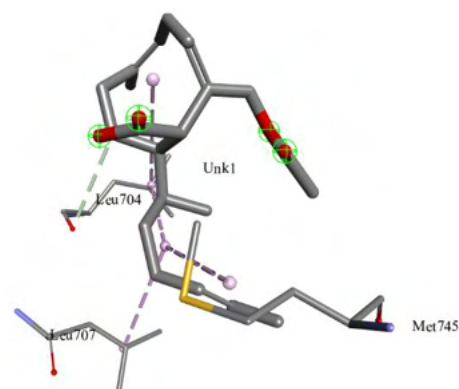
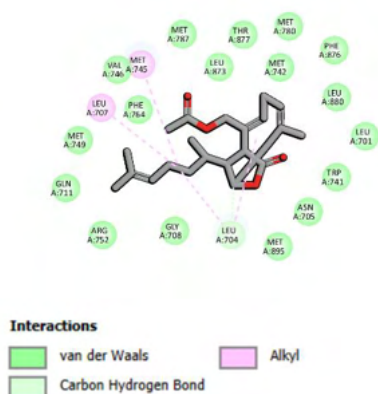
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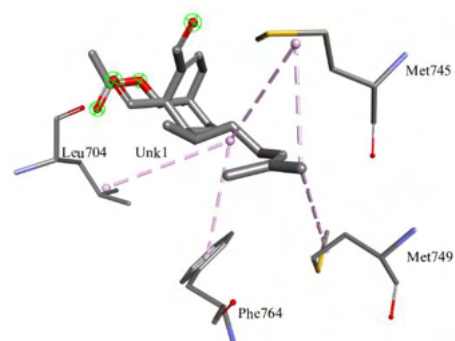
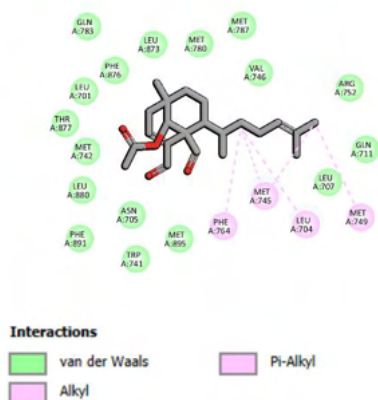
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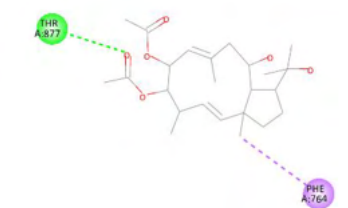
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S101

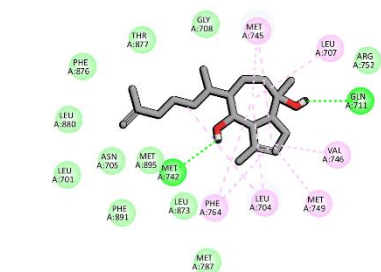


S102

**Interactions**

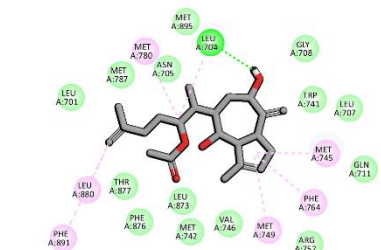
Conventional Hydrogen Bond Pi-Sigma

S103

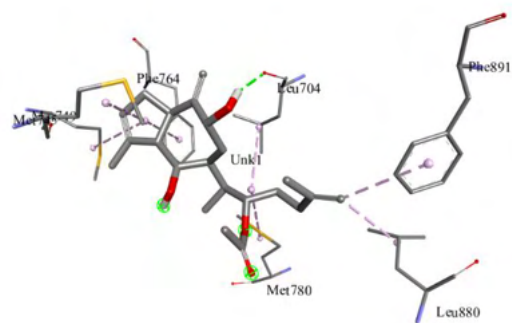
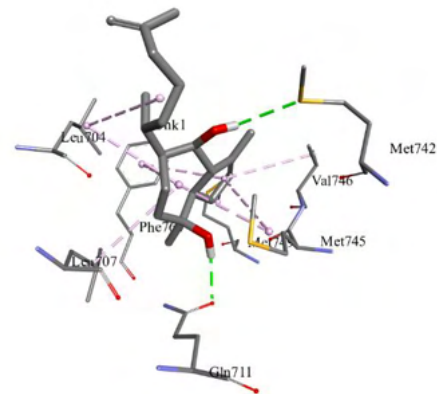
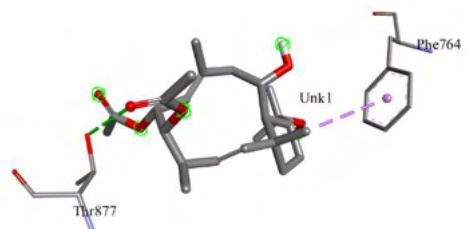
**Interactions**

van der Waals Conventional Hydrogen Bond Alkyl Pi-Alkyl

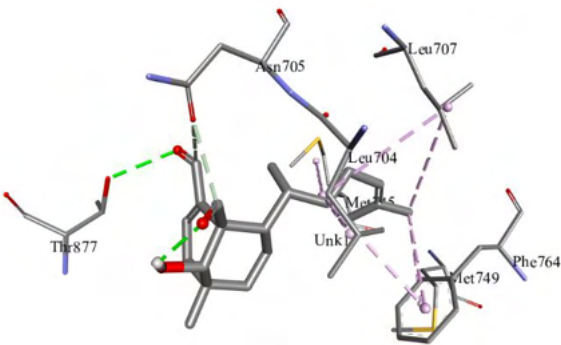
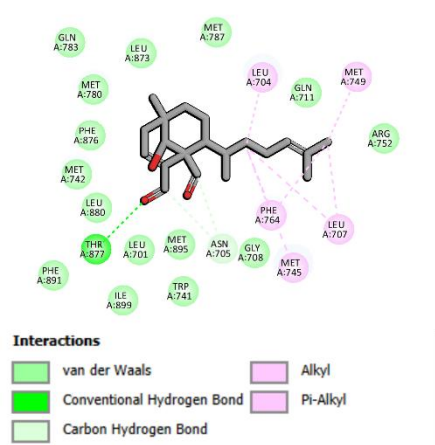
S105

**Interactions**

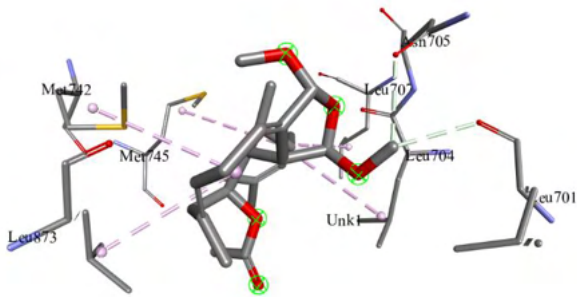
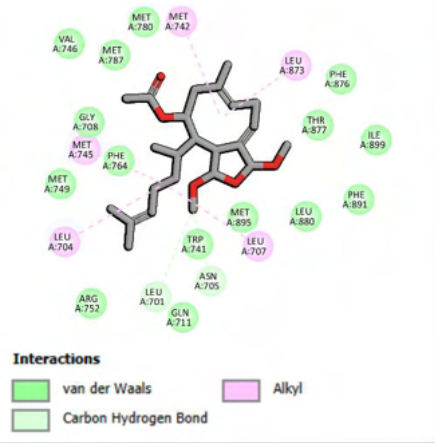
van der Waals Conventional Hydrogen Bond Alkyl Pi-Alkyl



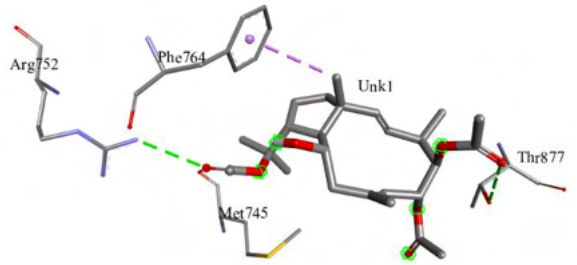
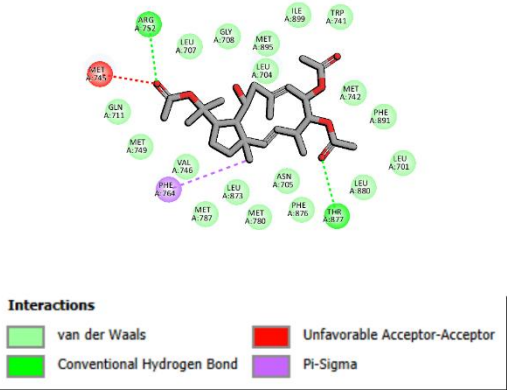
S106



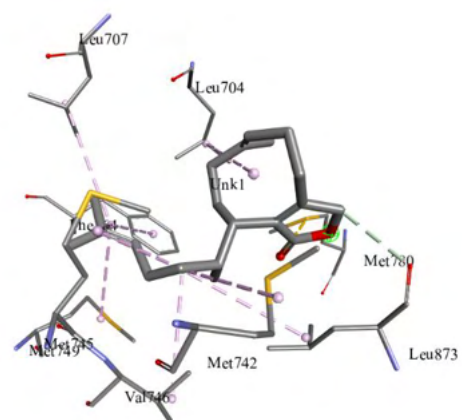
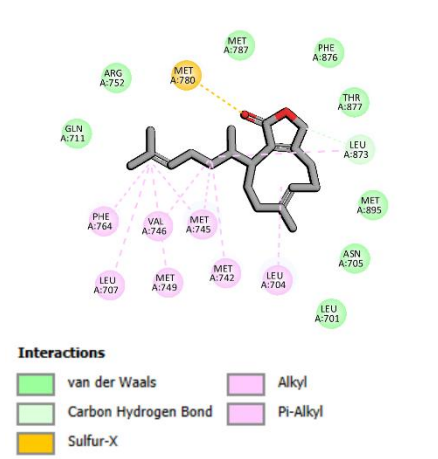
S111



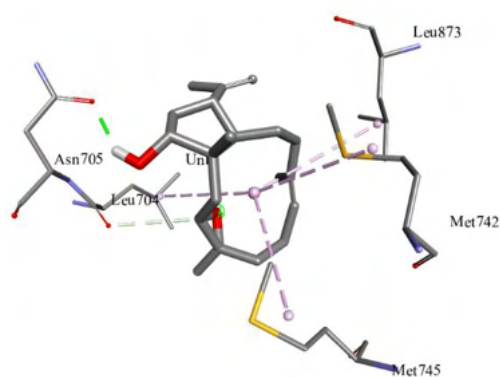
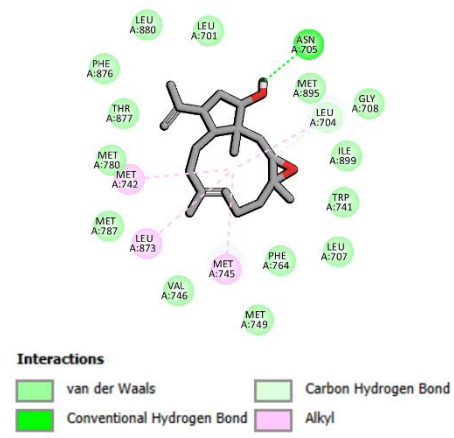
S112



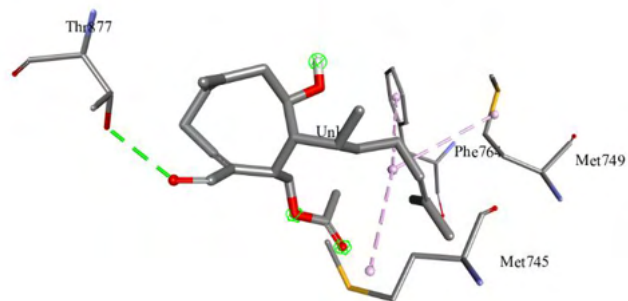
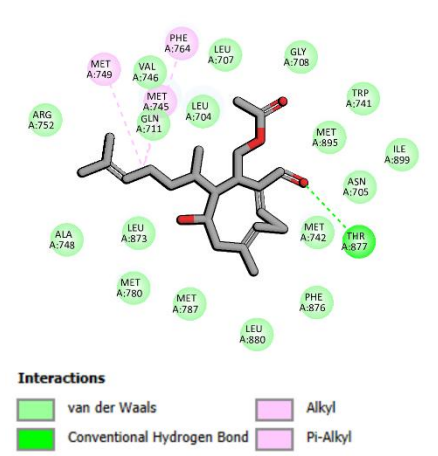
S113



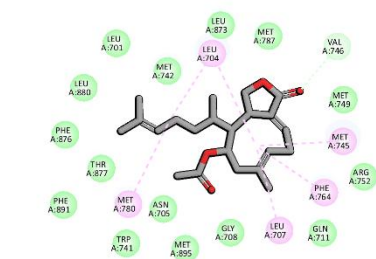
S114



S115

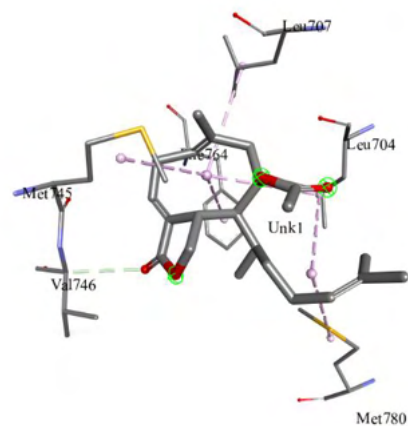


S116

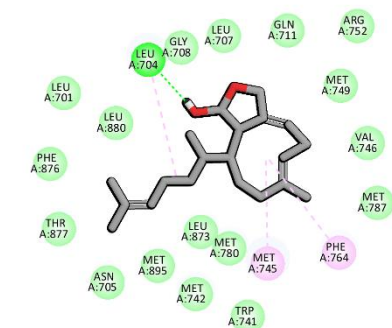


### Interactions

|                                                                                   |                      |                                                                                   |          |
|-----------------------------------------------------------------------------------|----------------------|-----------------------------------------------------------------------------------|----------|
|  | van der Waals        |  | Alkyl    |
|  | Carbon Hydrogen Bond |  | Pi-Alkyl |

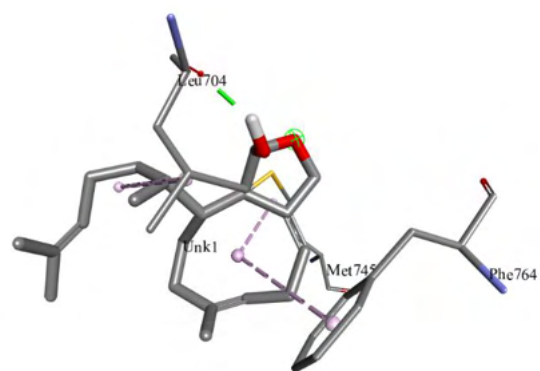


S117

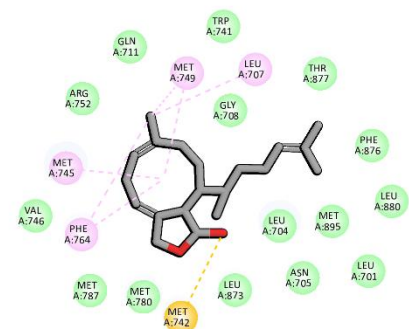


### Interactions

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

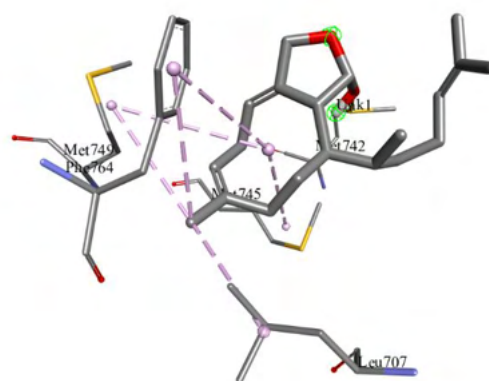


S118

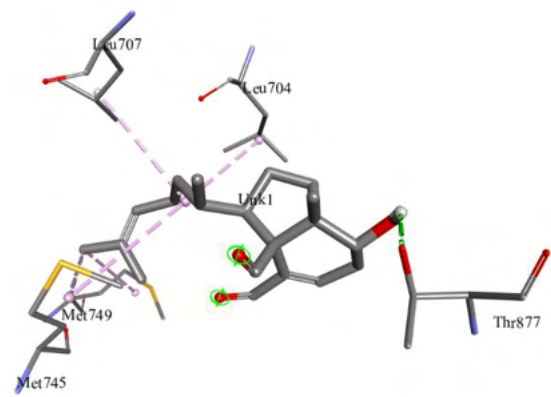
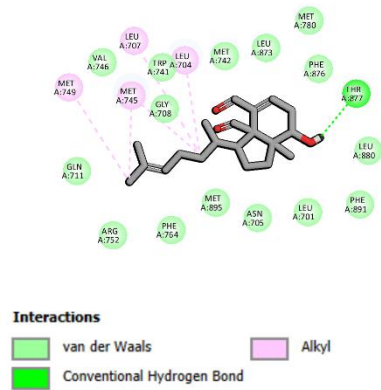


### Interactions

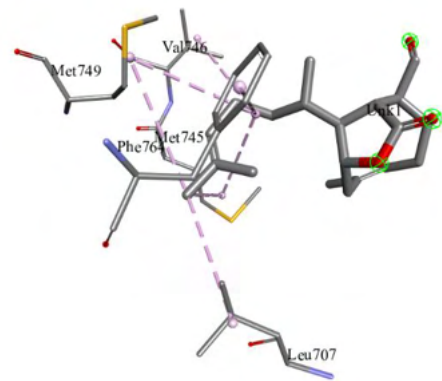
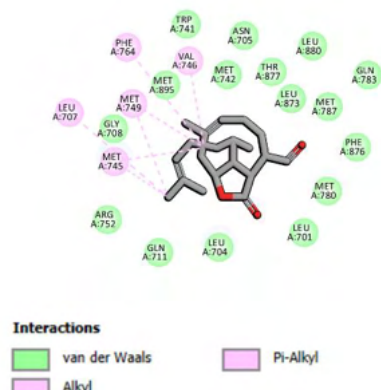
|                                                                                     |               |                                                                                     |          |
|-------------------------------------------------------------------------------------|---------------|-------------------------------------------------------------------------------------|----------|
|  | van der Waals |  | Alkyl    |
|  | Sulfur-X      |  | Pi-Alkyl |



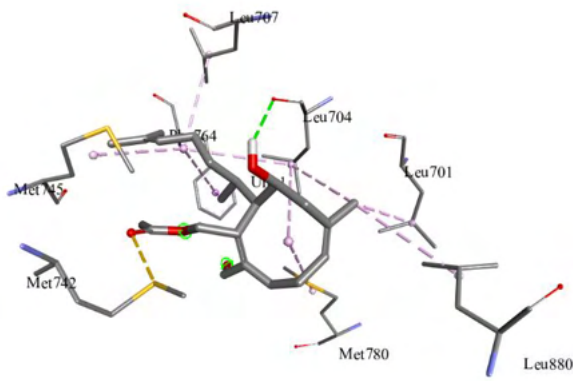
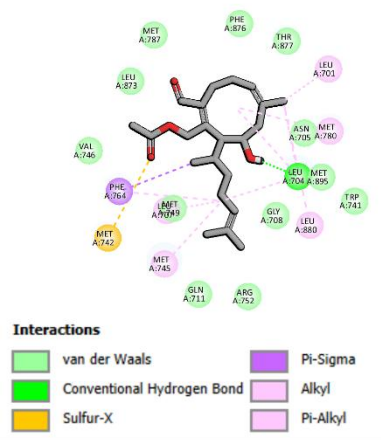
S119



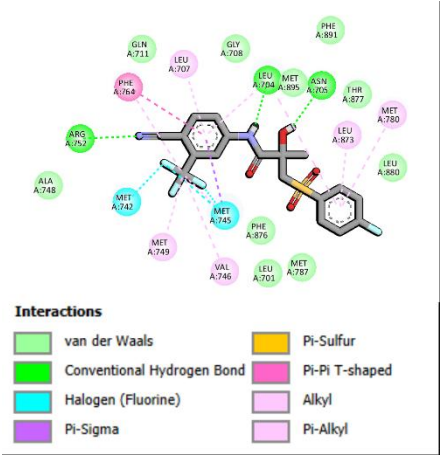
S120



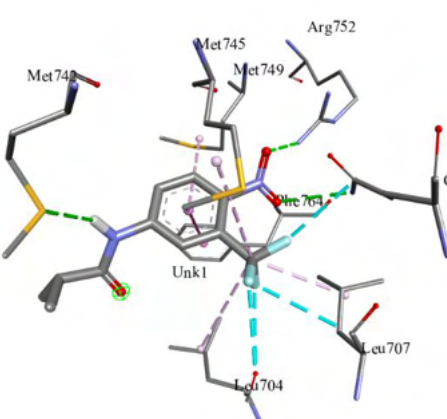
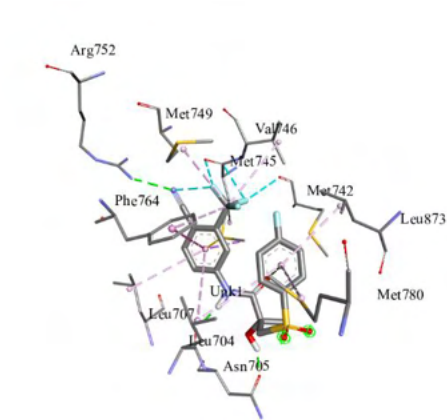
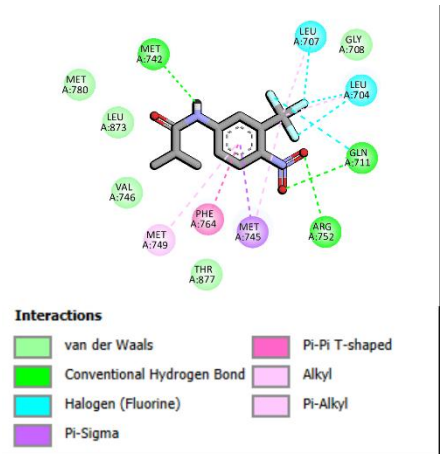
S122

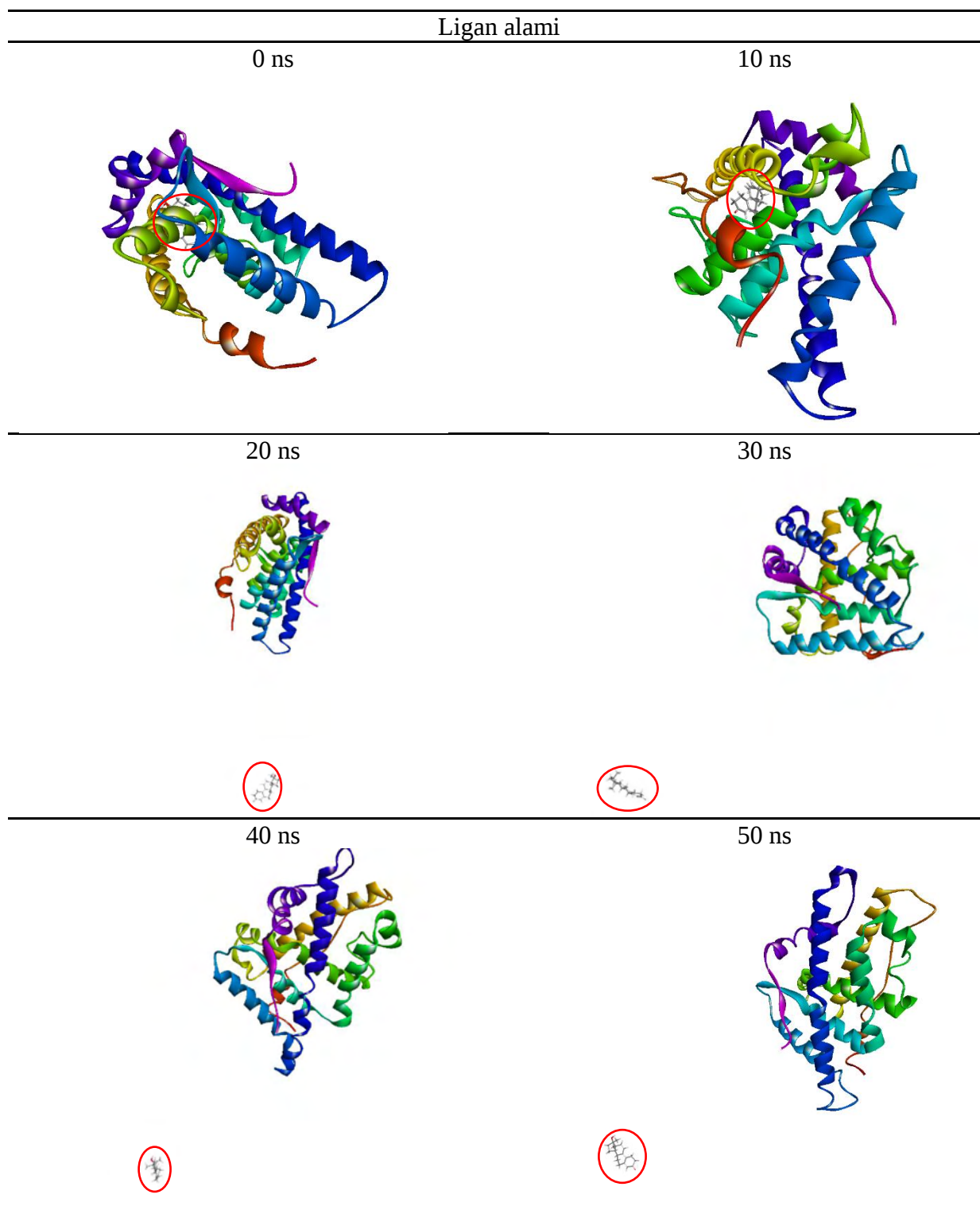


SBC

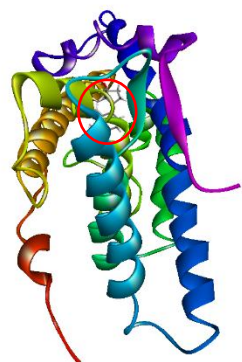


SFL



**Lampiran 8.** Pergerakan ligan alami, ligan uji, dan obat pembanding per-ns

---

60 ns

70 ns



A ribbon diagram of a protein structure at 70 ns. The protein is shown in a similar rainbow-colored ribbon representation. A red circle highlights a small molecule or ligand bound to the protein, located near the bottom center of the structure.

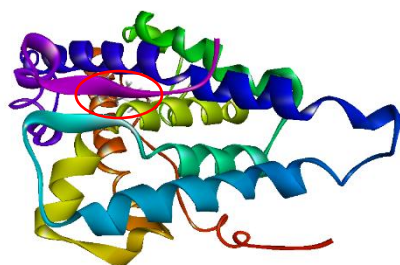
80 ns



90 ns



---

100 ns

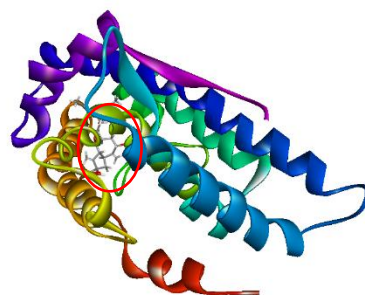
---

*S77*

---

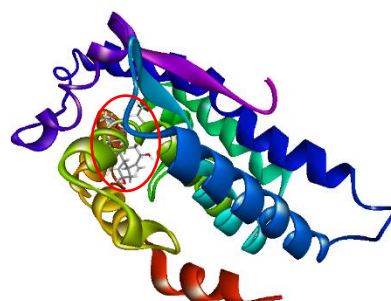
0 ns

10 ns



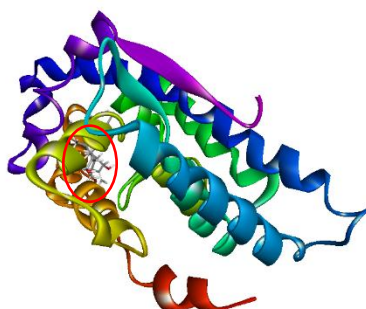
20 ns

30 ns

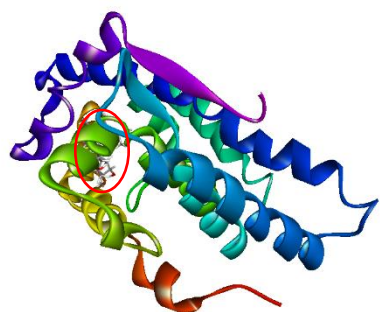


40 ns

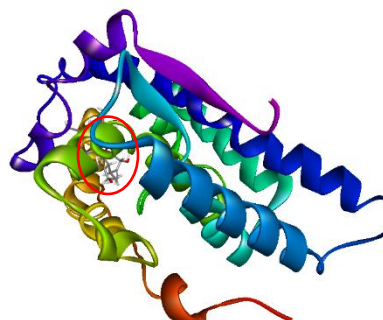
50 ns



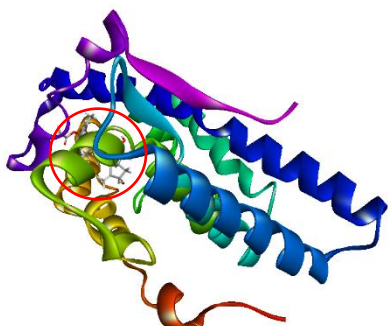
---

60 ns

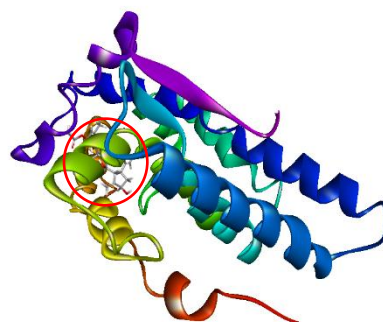
70 ns



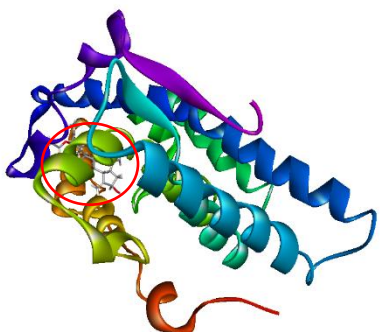
---

80 ns

90 ns



---

100 ns

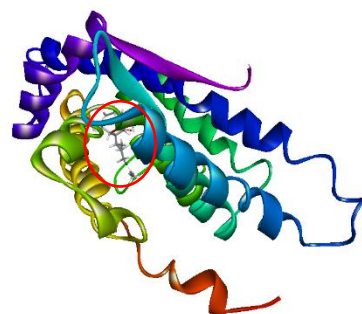
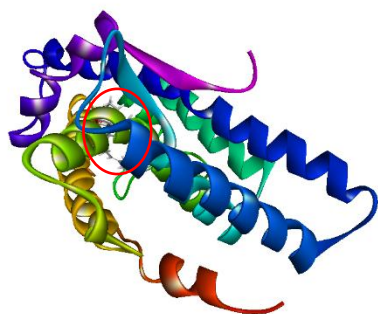
---

S100

---

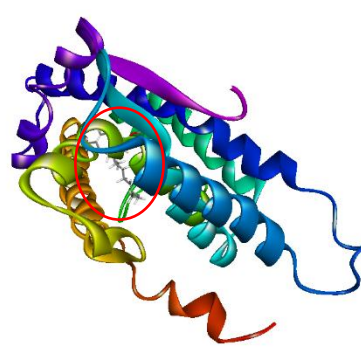
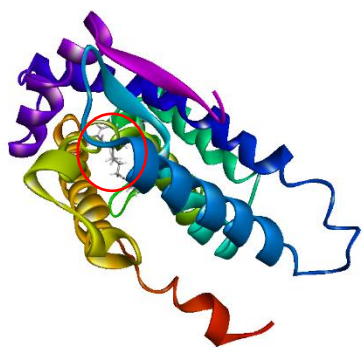
0 ns

10 ns



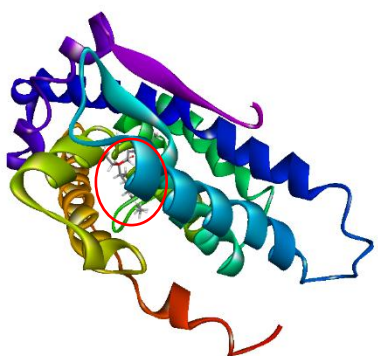
20 ns

30 ns

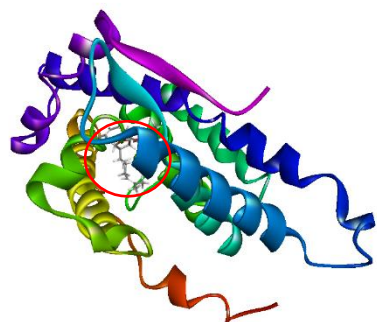


40 ns

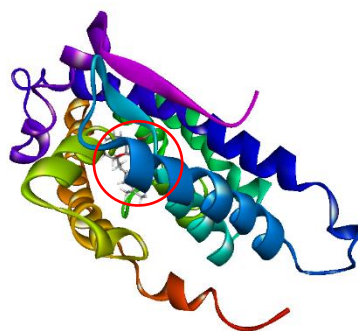
50 ns



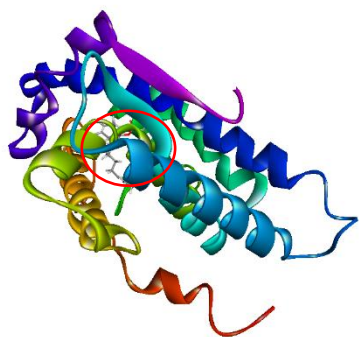
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60 ns

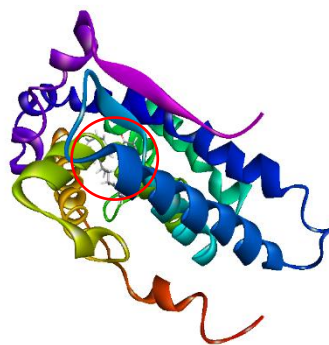
70 ns



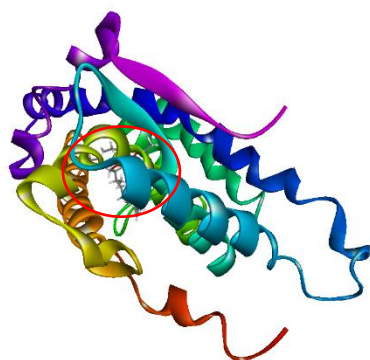
---

80 ns

90 ns



---

100 ns

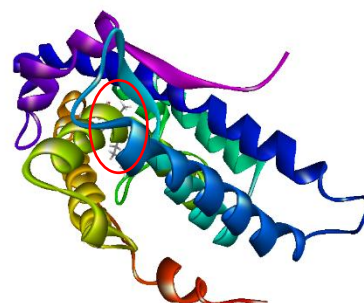
---

S116

---

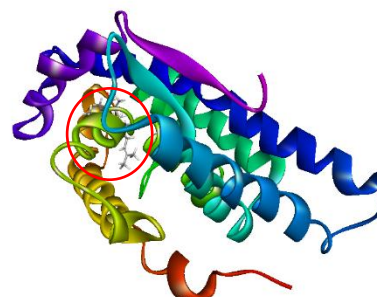
0 ns

10 ns



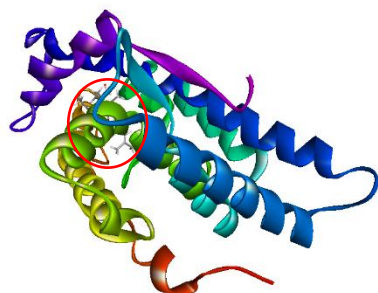
20 ns

30 ns

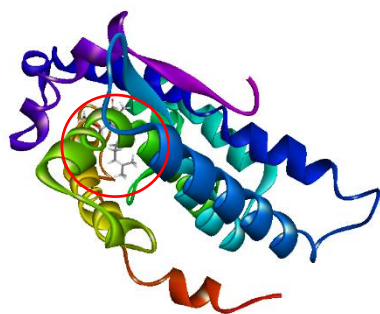


40 ns

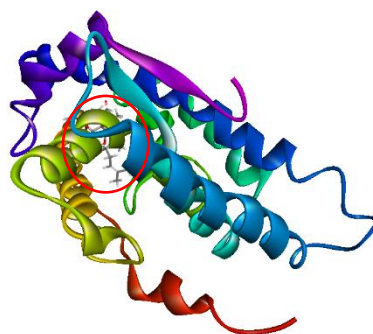
50 ns



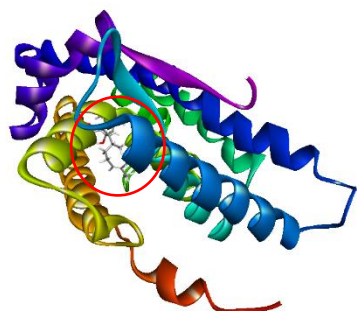
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60 ns

70 ns



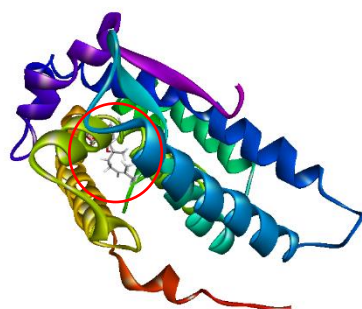
---

80 ns

90 ns



---

100 ns

---

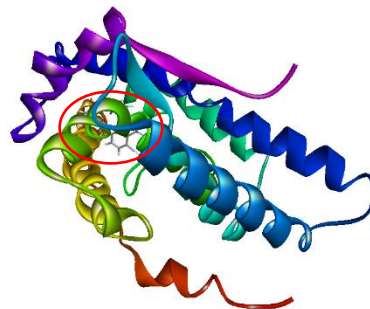
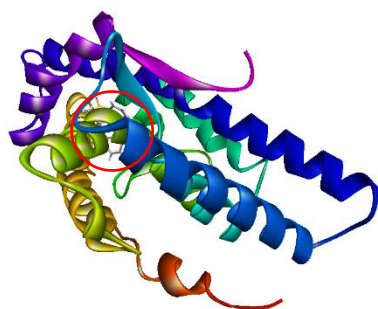
---

Bicalutamide

---

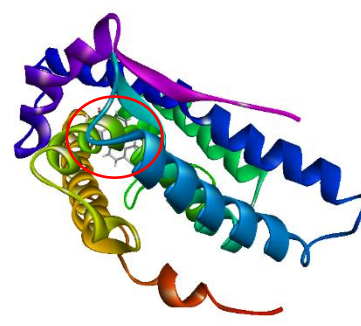
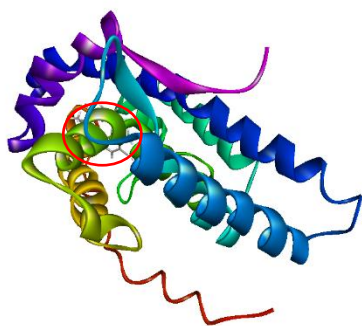
0 ns

10 ns



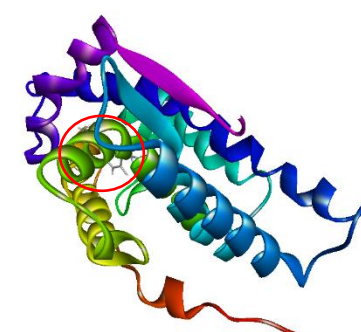
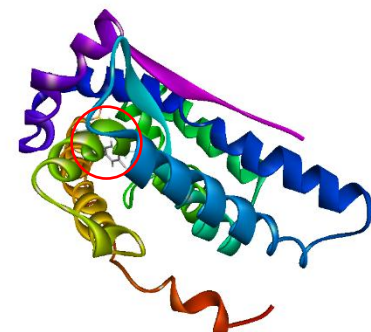
20 ns

30 ns

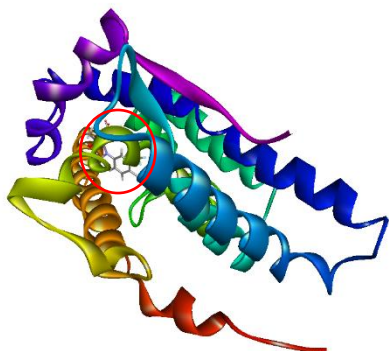


40 ns

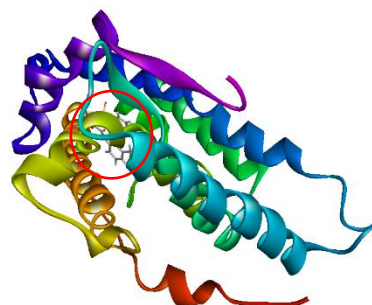
50 ns



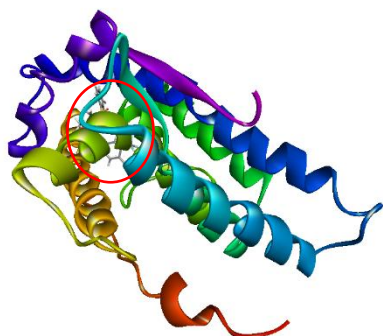
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60 ns

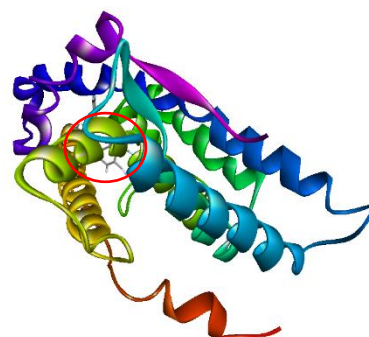
70 ns



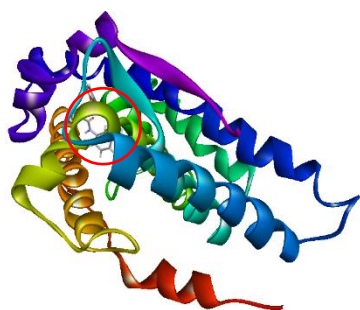
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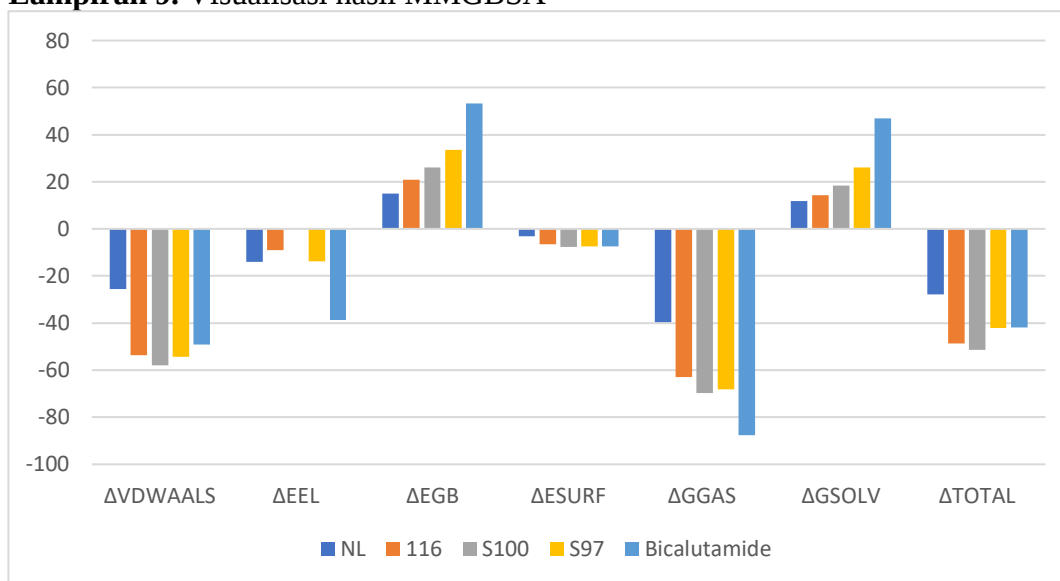
80 ns

90 ns



---

100 ns

**Lampiran 9.** Visualisasi hasil MMGBSA

## Lampiran 10. Hasil turnitin

|                               |                                                                                                                                                                                                                                  |              |                |
|-------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------|----------------|
| prinkomprefinal-1749998929073 |                                                                                                                                                                                                                                  |              |                |
| ORIGINALITY REPORT            |                                                                                                                                                                                                                                  |              |                |
| 12%                           | 11%                                                                                                                                                                                                                              | 6%           | 6%             |
| SIMILARITY INDEX              | INTERNET SOURCES                                                                                                                                                                                                                 | PUBLICATIONS | STUDENT PAPERS |
| PRIMARY SOURCES               |                                                                                                                                                                                                                                  |              |                |
| 1                             | bidd.group<br>Internet Source                                                                                                                                                                                                    | 6%           |                |
| 2                             | Submitted to University of Wolverhampton<br>Student Paper                                                                                                                                                                        | 3%           |                |
| 3                             | www.bidd.group<br>Internet Source                                                                                                                                                                                                | 1%           |                |
| 4                             | Trent E. Balius, Mayukh Chakrabarti, Y. Stanley Tan. "DOCK 6: Incorporating hierarchical traversal through precomputed ligand conformations to enable large-scale docking", American Chemical Society (ACS), 2023<br>Publication | 1%           |                |
| 5                             | Submitted to University of KwaZulu-Natal<br>Student Paper                                                                                                                                                                        | <1%          |                |
| 6                             | D. Thirumal Kumar, M.S. Shree Devi, S. Udhaya Kumar, Annie Sherlin et al. "Understanding the activating mechanism of the immune system against COVID-19 by                                                                       | <1%          |                |

## Lampiran 11. Kartu bukti bimbingan

| No | Tanggal          | Dosen Pembimbing                     | Topik                                    | Disetujui | Aksi                                                                                                                                                                        |
|----|------------------|--------------------------------------|------------------------------------------|-----------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1  | 27 Februari 2025 | Dr Aiyyi Asnawi, M.Si                | Jejaring Farmakologi                     | ✓         |       |
| 1  | 13 Maret 2025    | Dr. apt. Fauzan Zein Muttaqin, M.Si. | Pelatihan penambatan molekul             | ✓         |       |
| 2  | 23 April 2025    | Dr. apt. Fauzan Zein Muttaqin, M.Si. | Skrining Senyawa Uji                     | ✓         |       |
| 2  | 4 Maret 2025     | Dr Aiyyi Asnawi, M.Si                | Skrining Senyawa Uji                     | ✓         |       |
| 3  | 11 Maret 2025    | Dr Aiyyi Asnawi, M.Si                | Preparasi senyawa uji                    | ✓         |       |
| 3  | 3 Mei 2025       | Dr. apt. Fauzan Zein Muttaqin, M.Si. | Laporan kemajuan 2                       | ✓         |       |
| 4  | 5 Mei 2025       | Dr. apt. Fauzan Zein Muttaqin, M.Si. | Evaluasi residu asam amino penting       | ✓         |       |
| 4  | 17 April 2025    | Dr Aiyyi Asnawi, M.Si                | Validasi penambatan molekul              | ✓         |       |
| 5  | 30 April 2025    | Dr Aiyyi Asnawi, M.Si                | Penambatan molekul senyawa uji           | ✓         |       |
| 5  | 7 Mei 2025       | Dr. apt. Fauzan Zein Muttaqin, M.Si. | Evaluasi hasil penambatan molekul        | ✓         |       |
| 6  | 6 Mei 2025       | Dr. apt. Fauzan Zein Muttaqin, M.Si. | Visualisasi hasil penambatan molekul     | ✓         |       |
| 6  | 21 Mei 2025      | Dr Aiyyi Asnawi, M.Si                | simulasi dinamika molekul                | ✓         |       |
| 7  | 12 Mei 2025      | Dr Aiyyi Asnawi, M.Si                | evaluasi hasil simulasi dinamika molekul | ✓         |       |
| 7  | 21 Mei 2025      | Dr. apt. Fauzan Zein Muttaqin, M.Si. | simulasi dinamika molekul                | ✓         |       |
| 8  | 28 Mei 2025      | Dr. apt. Fauzan Zein Muttaqin, M.Si. | Hasil dan Analisis Data                  | ✓         |       |
| 8  | 28 Mei 2025      | Dr Aiyyi Asnawi, M.Si                | Hasil dan Analisis Data                  | ✓         |   |

## Lampiran 12. Daftar Riwayat Hidup



### Data Pribadi

|                           |                                                                                                   |
|---------------------------|---------------------------------------------------------------------------------------------------|
| Nama                      | : Robi Adrian                                                                                     |
| Alamat                    | : Kp. Seke RT/RW 002/006 Desa<br>Cikasungka Kec. Cikancung Kab.<br>Bandung Jawa Barat             |
| Kode pos                  | : 40396                                                                                           |
| Nomor Telepon             | : 0896-6165-2525                                                                                  |
| Email                     | : adrianrobi248@gmail.com                                                                         |
| Jenis kelamin             | : Laki-laki                                                                                       |
| Tempat, Tanggal Kelahiran | : Bandung, 06 Juli 2003                                                                           |
| Warga Negara              | : Indonesia                                                                                       |
| Agama                     | : Islam                                                                                           |
| Pendidikan                | : SDN 2 CIKASUNGKA<br>SMPN 1 CIKANCUNG<br>SMK GUNA DHARMA NUSANTARA<br>UNIVERSITAS BHAKTI KENCANA |