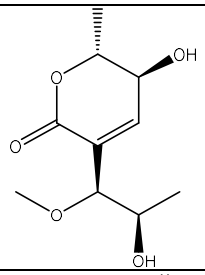
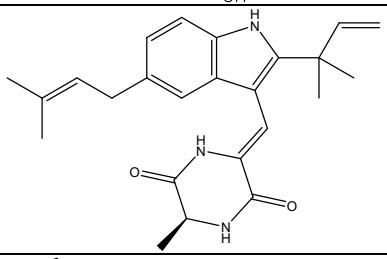
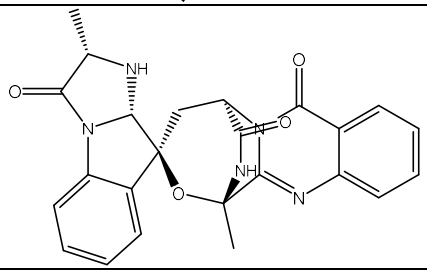
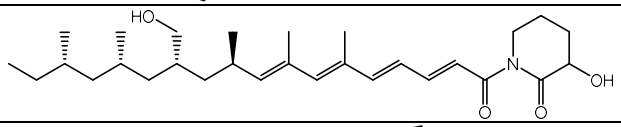
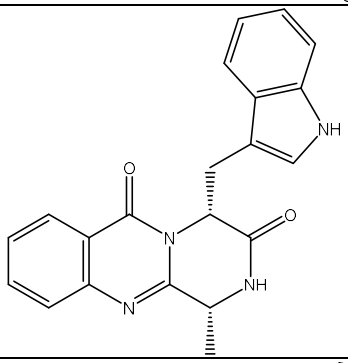
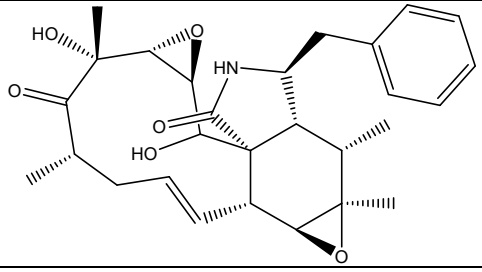
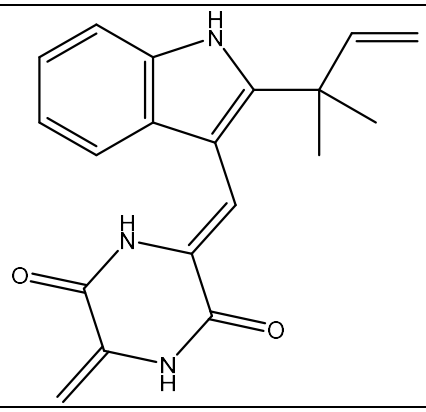
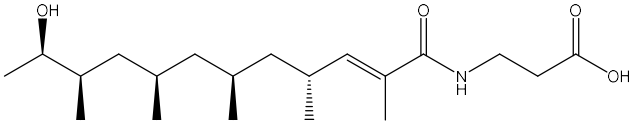
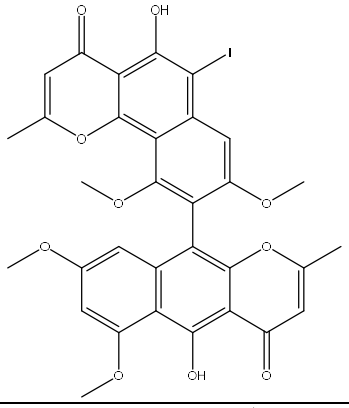
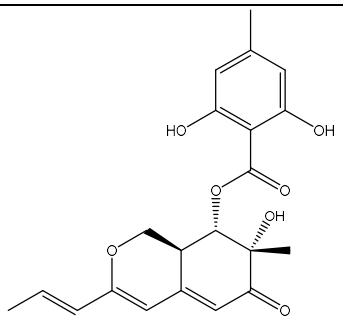
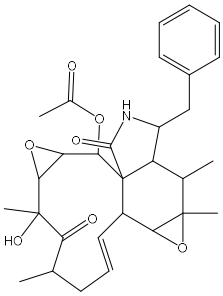
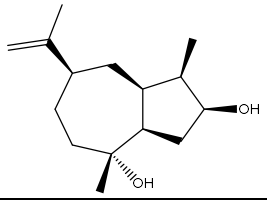
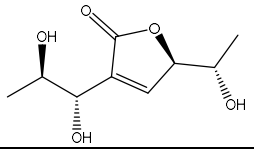
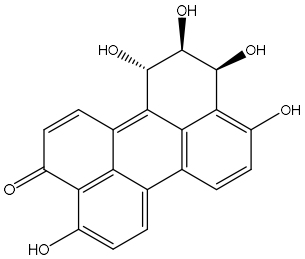
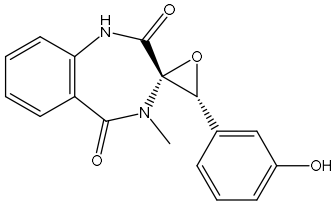
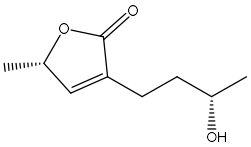
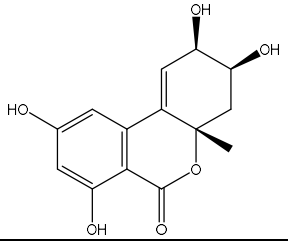
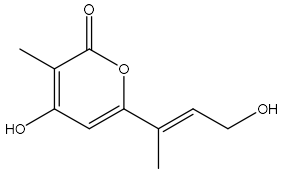
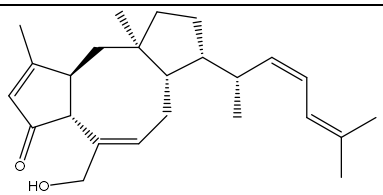
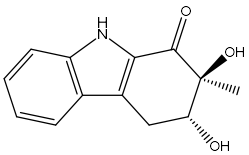
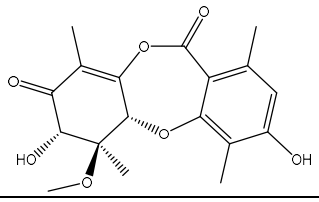
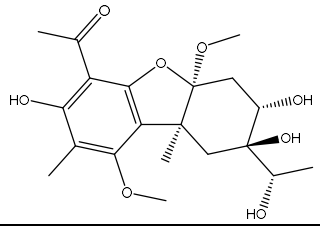
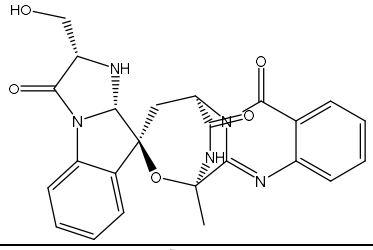
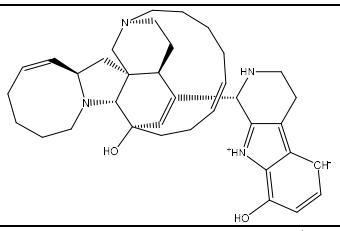
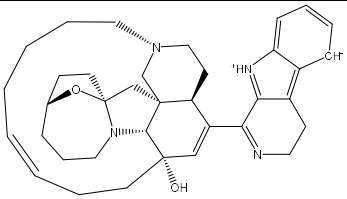
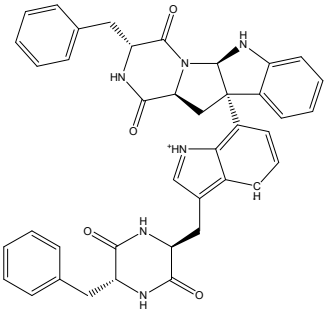
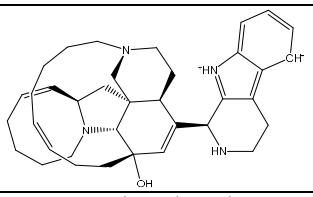
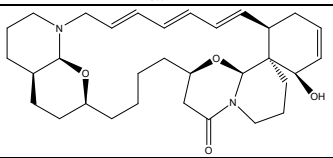
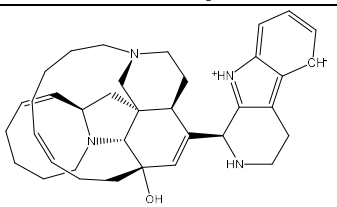
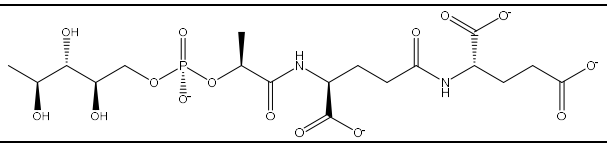
Table S1. The molecular docking scores of top docked deep-sea compounds and standard against *Mycobacterium tuberculosis* (Mtb) protein Rv1155

| **Compound ID** | **Structure** | **Docking score (kcal/mol)** |
|---|---|---|
| **Compound_1749** |  | **-15.949** |
| Compound_1665 |  | -14.554 |
| Compound_1808 |  | -13.76 |
| Compound_1794 |  | -12.422 |
| Compound_1809 |  | -13.285 |
| Compound_1540 |  | -13.225 |

| | | |
|---|---|---|
| Compound_1786 |  | -14.035 |
| **Compound_1796** |  | **-14.402** |
| Compound_1552 |  | -12.82 |
| Compound_1799 |  | -13.022 |
| Compound_1539 |  | -12.538 |
| Compound_1529 |  | -12.495 |

| | | |
|---|---|---|
| Compound_1745 |  | -11.127 |
| Compound_1639 |  | -12.477 |
| Compound_1757 |  | -12.454 |
| Compound_1744 |  | -12.415 |
| Compound_1624 |  | -12.383 |
| Compound_1522 |  | -12.546 |
| Compound_1816 |  | -12.195 |
| Compound_1655 |  | -12.11 |
| Compound_1763 |  | -12.114 |

| | | |
|---|---|---|
| Compound_1654 |  | -12.118 |
| Compound_1802 |  | -12.861 |
| CMNPD _14553 |  | -11.544 |
| CMNPD _16909 |  | -10.98 |
| CMNPD _18363 |  | -11.688 |
| CMNPD _20213 |  | -11.297 |
| **CMNPD _22964** |  | **-11.935** |
| CMNPD _22967 |  | -11.322 |

| | | |
|---|---|---|
| Standard_F42202 |  | -6.385 |

Note: Bolded entries correspond to the three top-ranked hit candidates (Upenamide/CMNPD _22964 , Aspyronol/Compound_1749, and Fiscpropionate F/Compound_1796) selected for detailed molecular dynamics and MM-GBSA analyses.

Table S2. Predicted ADMET parameters of the top scored deep-sea compounds and standard using ADMET 3.0

| **Compound ID** | **Molecular weight (g/mol)** | **Log P** | **HBD** | **HBA** | **TPSA (Å²)** | **Pfizer rule** | **Lipinski`s rule** | **PBB %** |
|---|---|---|---|---|---|---|---|---|
| **Compound_1749** | **216.1** | **-0.201** | **2** | **5** | **75.99** | **Pass** | **Pass** | **21.1** |
| Compound_1665 | 391.23 | 4.54 | 3 | 5 | 73.99 | Fail | Pass | 91.1 |
| Compound_1808 | 443.45 | 1.308 | 2 | 9 | 105.56 | Pass | Pass | 76.6 |
| Compound_1794 | 473.35 | 3.935 | 2 | 5 | 77.84 | Pass | Pass | 71.3 |
| Compound_1809 | 358.14 | 2.165 | 2 | 6 | 79.78 | Pass | Pass | 90.4 |
| Compound_1540 | 481.25 | 2.664 | 3 | 7 | 111.69 | Pass | Pass | 85.8 |
| Compound_1786 | 321.15 | 2.921 | 3 | 5 | 81.51 | Pass | Pass | 92.8 |
| **Compound_1796** | **355.27** | **2.895** | **3** | **5** | **86.63** | **Pass** | **Pass** | **49.6** |
| Compound_1552 | 696.05 | 4.764 | 2 | 10 | 137.8 | Pass | Pass | 97.6 |
| Compound_1799 | 386.14 | 3.39 | 3 | 7 | 113.29 | Pass | Pass | 98.3 |
| Compound_1539 | 523.26 | 1.884 | 2 | 8 | 117.76 | Pass | Pass | 88.9 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Compound_1529 | 238.19 | 3.078 | 2 | 2 | 40.46 | Fail | Pass | 67.7 |
| Compound_1745 | 202.08 | -0.632 | 3 | 5 | 86.99 | Pass | Pass | 11.2 |
| Compound_1639 | 350.08 | 2.364 | 5 | 6 | 118.22 | Pass | Pass | 92.9 |
| Compound_1757 | 310.1 | 1.762 | 2 | 6 | 82.17 | Pass | Pass | 74.3 |
| Compound_1744 | 170.09 | 0.308 | 1 | 3 | 46.53 | Pass | Pass | 53.4 |
| Compound_1624 | 278.08 | 0.558 | 4 | 6 | 107.22 | Pass | Pass | 85.8 |
| Compound_1522 | 196.07 | 0.152 | 2 | 4 | 70.67 | Pass | Pass | 64.7 |
| Compound_1816 | 368.27 | 5.036 | 1 | 2 | 37.3 | Fail | Pass | 94.7 |
| Compound_1655 | 231.09 | 2.272 | 3 | 4 | 73.32 | Pass | Pass | 88.2 |
| Compound_1763 | 348.12 | 1.247 | 2 | 7 | 102.29 | Pass | Pass | 93.3 |
| Compound_1654 | 396.18 | 2.069 | 4 | 8 | 125.68 | Pass | Pass | 84.8 |
| Compound_1802 | 459.15 | 1.046 | 3 | 10 | 125.79 | Pass | Pass | 57.1 |
| CMNPD_14553 | 568.38 | 3.076 | 3 | 6 | 71.33 | Fail | Pass | 83.7 |
| CMNPD_16909 | 566.36 | 3.418 | 1 | 6 | 60.66 | Fail | Pass | 89.8 |
| CMNPD_18363 | 664.28 | 3.434 | 4 | 10 | 132.0 | Pass | Pass | 97.4 |
| CMNPD_20213 | 552.38 | 3.597 | 2 | 5 | 51.1 | Fail | Pass | 88.9 |
| **CMNPD_22964** | **522.35** | **2.802** | **1** | **6** | **62.24** | **Fail** | **Pass** | **67.2** |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| CMNPD _22967 | 552.38 | 3.597 | 2 | 5 | 51.1 | Fail | Pass | 88.9 |
| Standard_F42202 | 546.15 | -1.674 | 9 | 17 | 286.55 | Pass | Fail | 29 |

Note: Bolded entries correspond to the three top-ranked hit candidates (Upenamide/CMNPD _22964 , Aspyronol/Compound_1749, and Fiscpropionate F/Compound_1796) selected for detailed molecular dynamics and MM-GBSA analyses.