



The figure is a complex scientific visualization, likely a manuscript page or a technical report, featuring a grid of panels. The top section contains a large table with multiple columns and rows of text and data. The bottom section contains a large table with multiple columns and rows of text and data. The middle section contains several smaller plots and diagrams, including a chemical structure of a protein-ligand complex.

**Table 1: Top Section Data**

Panel	Content
1	Figure 1: Overview of the study. The figure shows the structure of the protein-ligand complex and the results of the docking studies.
2	Figure 2: Docking studies. The figure shows the results of the docking studies, including the binding energy and the binding mode of the ligand.
3	Figure 3: Molecular dynamics simulations. The figure shows the results of the molecular dynamics simulations, including the root mean square deviation (RMSD) and the root mean square fluctuation (RMSF).
4	Figure 4: Free energy calculations. The figure shows the results of the free energy calculations, including the binding free energy and the free energy of activation.
5	Figure 5: Comparison of experimental and computational results. The figure shows the comparison of experimental and computational results, including the binding energy and the binding mode of the ligand.

**Table 2: Bottom Section Data**

Panel	Content
6	Figure 6: Docking studies. The figure shows the results of the docking studies, including the binding energy and the binding mode of the ligand.
7	Figure 7: Molecular dynamics simulations. The figure shows the results of the molecular dynamics simulations, including the root mean square deviation (RMSD) and the root mean square fluctuation (RMSF).
8	Figure 8: Free energy calculations. The figure shows the results of the free energy calculations, including the binding free energy and the free energy of activation.
9	Figure 9: Comparison of experimental and computational results. The figure shows the comparison of experimental and computational results, including the binding energy and the binding mode of the ligand.

**Chemical Structure:**

The chemical structure shown in the figure is a protein-ligand complex. The protein is represented by a ribbon diagram, and the ligand is represented by a stick model. The binding site is highlighted in yellow.







