Supplementary Material of Molecular Docking and Dynamics of a Series of Aza-heterocyclic Compounds Against Effector Protein NleL

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Molecular Docking

The best conformation for each ligand of Figure 1, calculated from the molecular docking of AutoDock FR, is shown in Figure S1.

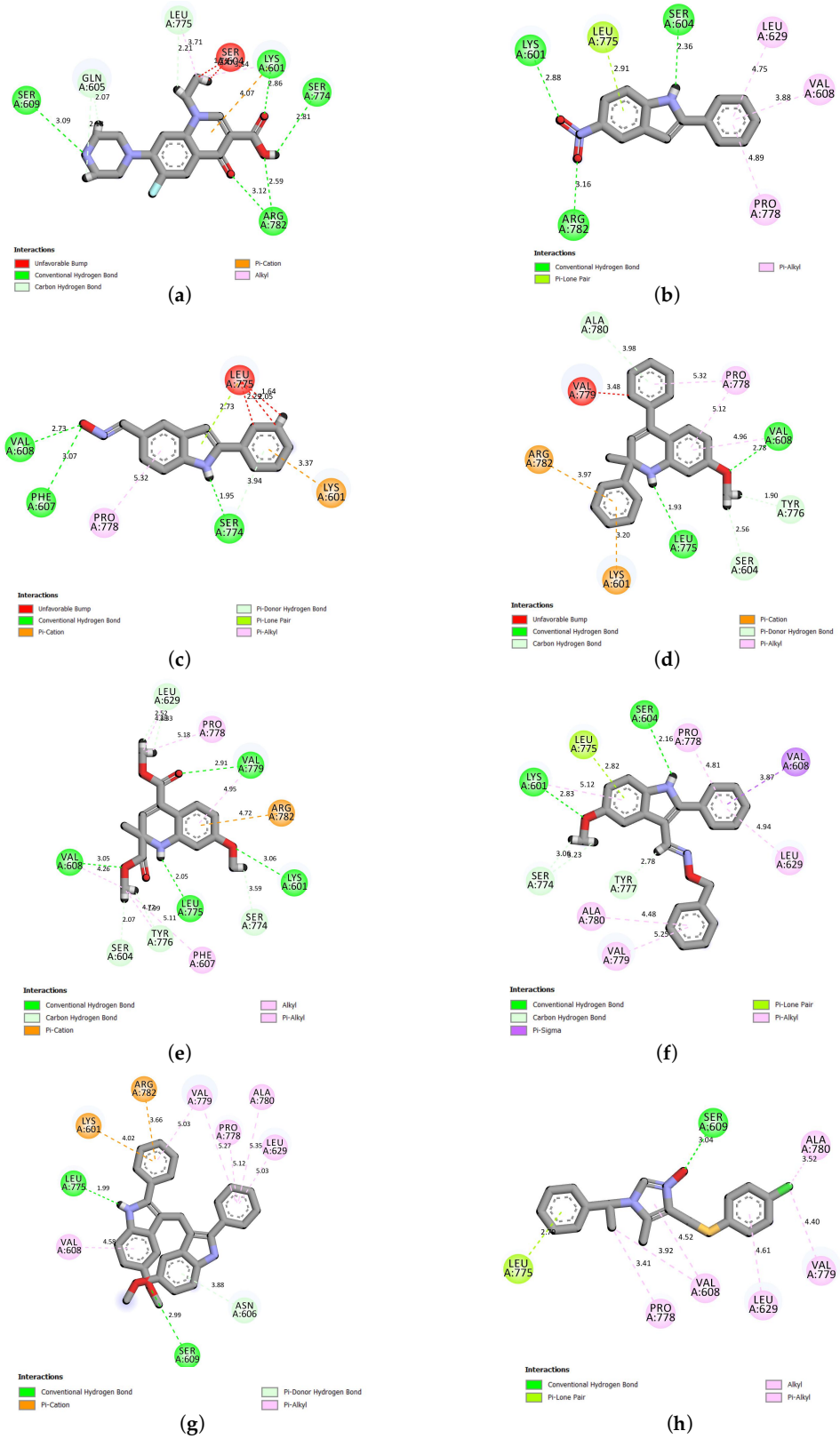

Figure S1. Interactions and distances (in Å) for ligands a) **1**, b) **2**, c) **3**, d) **4**, e) **5**, f) **6**, g) **7**, and h) **8** against the effector protein NleL.

Molecular Dynamics

Table S1 shows the average and maximum RMSD values for the receptor and the ligand aligned to the receptor for the 100 *ns* of simulation.

Table S1. Average and maximum RMSD (in Å) a) of the receptor and b) of the ligand aligned to the receptor for the 100 *ns*.

Ligand	RMSD Receptor average	RMSD Receptor maximum	RMSD Ligand average	RMSD Ligand maximum
1	3.149	5.073	6.732	27.938
4	2.883	6.625	3.052	7.463
6	3.339	6.931	5.564	11.134
7	3.246	5.716	2.830	6.187