

2D & 3D interactions for top 10 compounds

2IOG - 5-removed waters - BT_ER_Tf

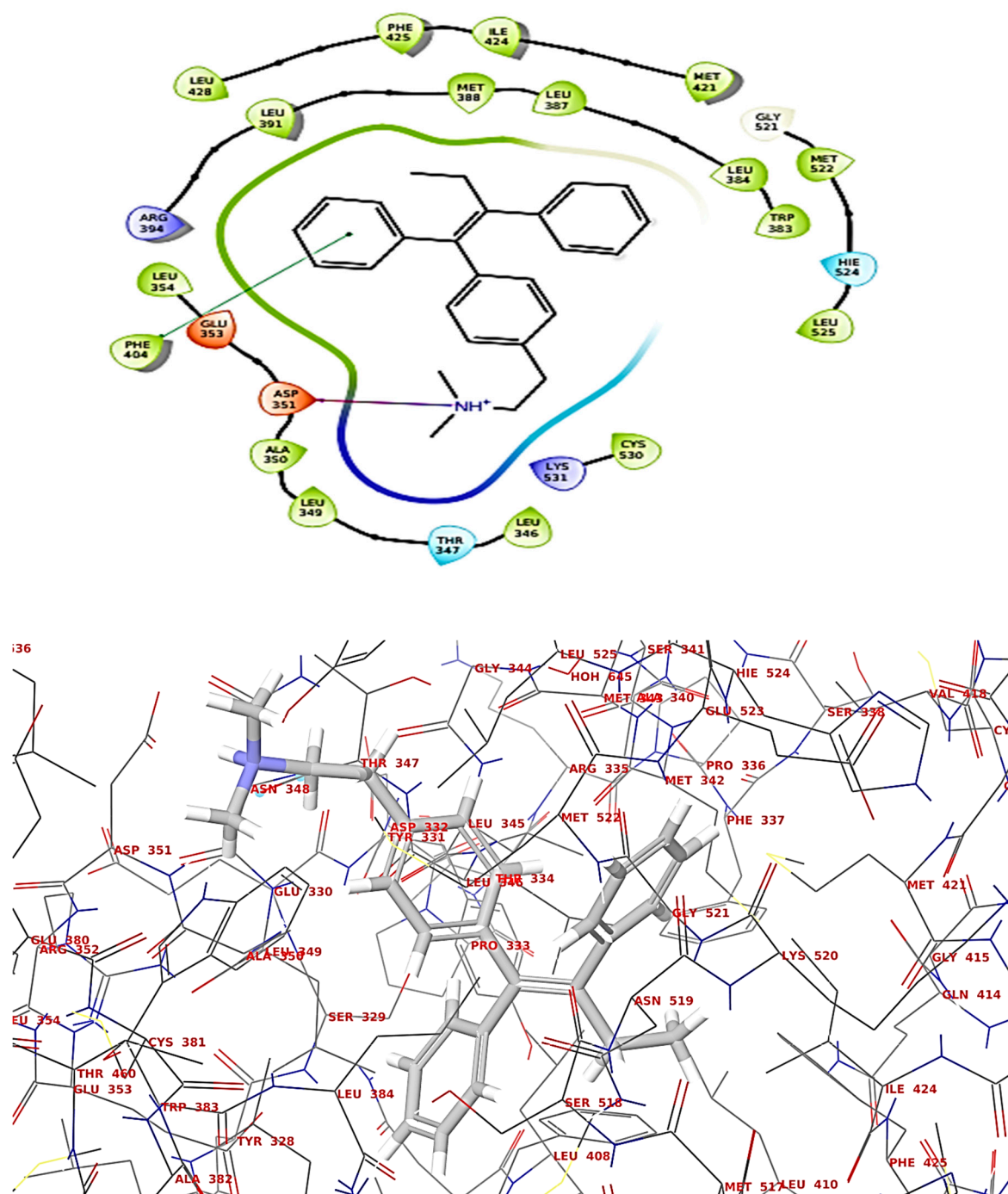
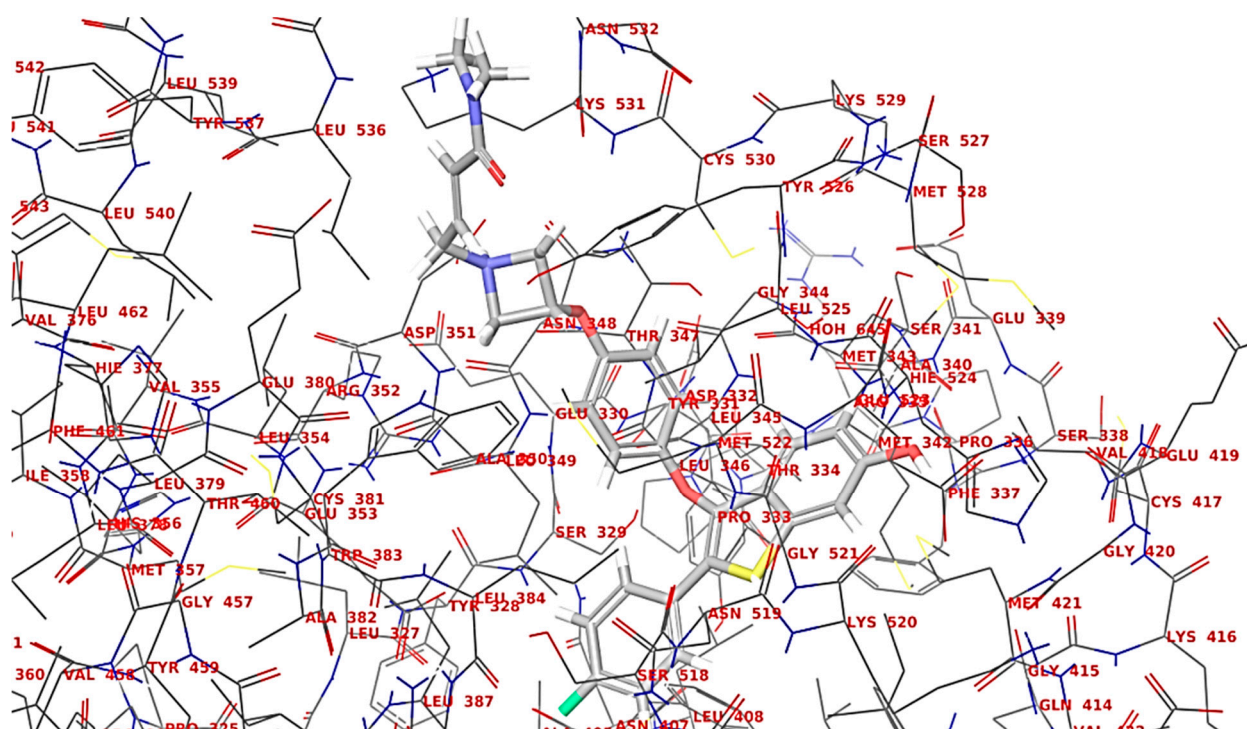


Figure S1a: 2D & 3D interactions for Compound BT_ER_Tf (Docking score -13.560)



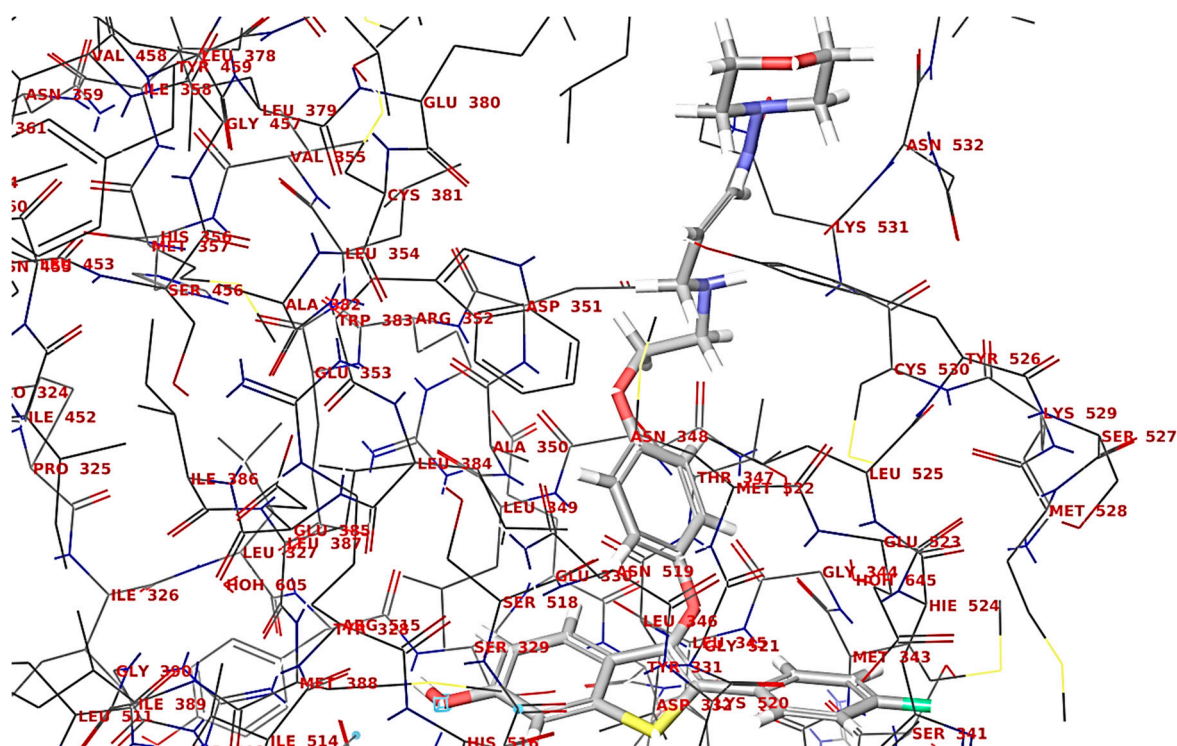


Figure S1c: 2D & 3D interactions for Compound BT ER 15e (Docking score -12.155)

2IOG - 5-removed waters - BT_ER_15b

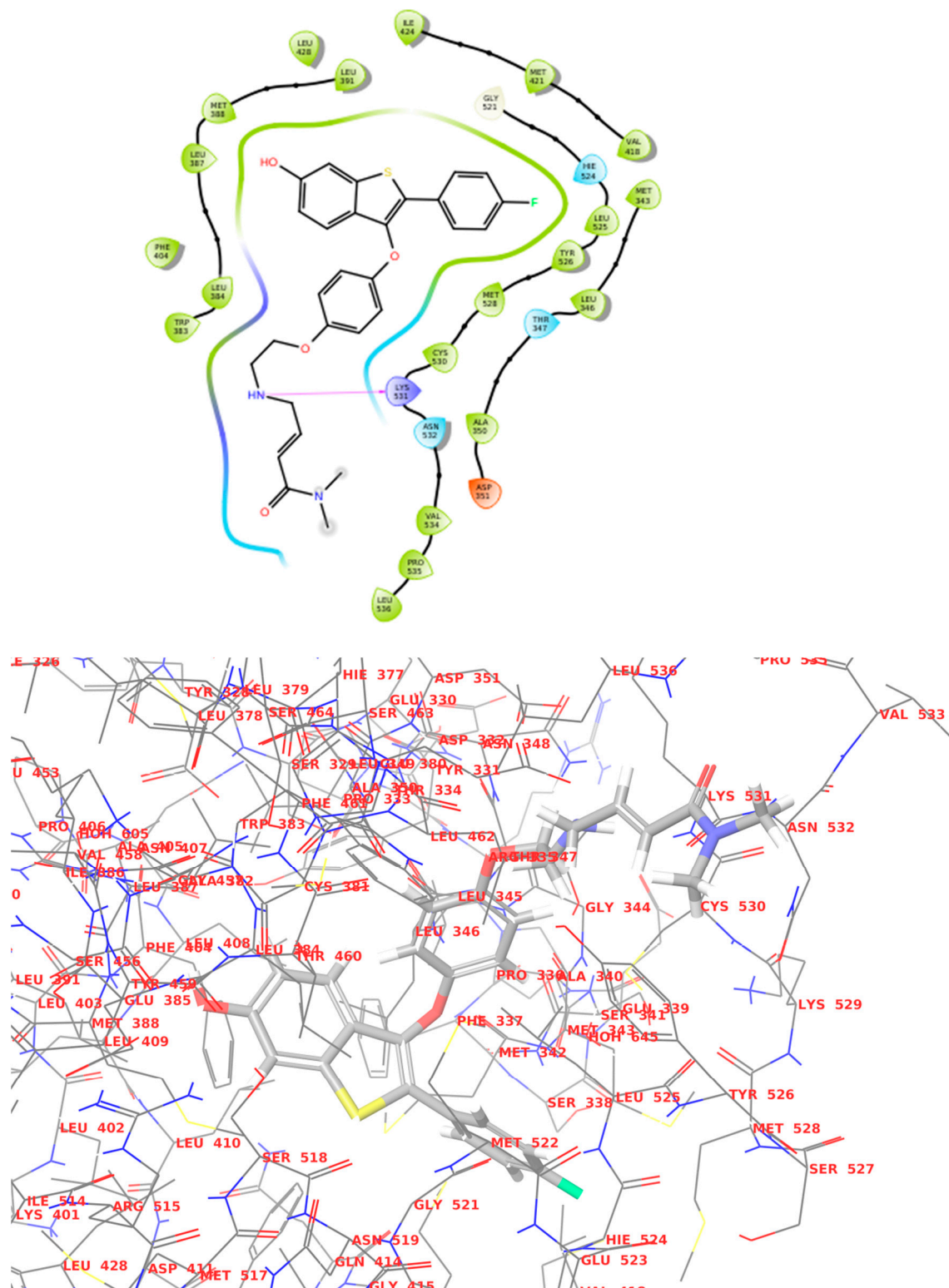


Figure S1d: 2D & 3D interactions for Compound BT ER 15b (Docking score -12.007)

2IOG - 5-removed waters - BT_ER_23c

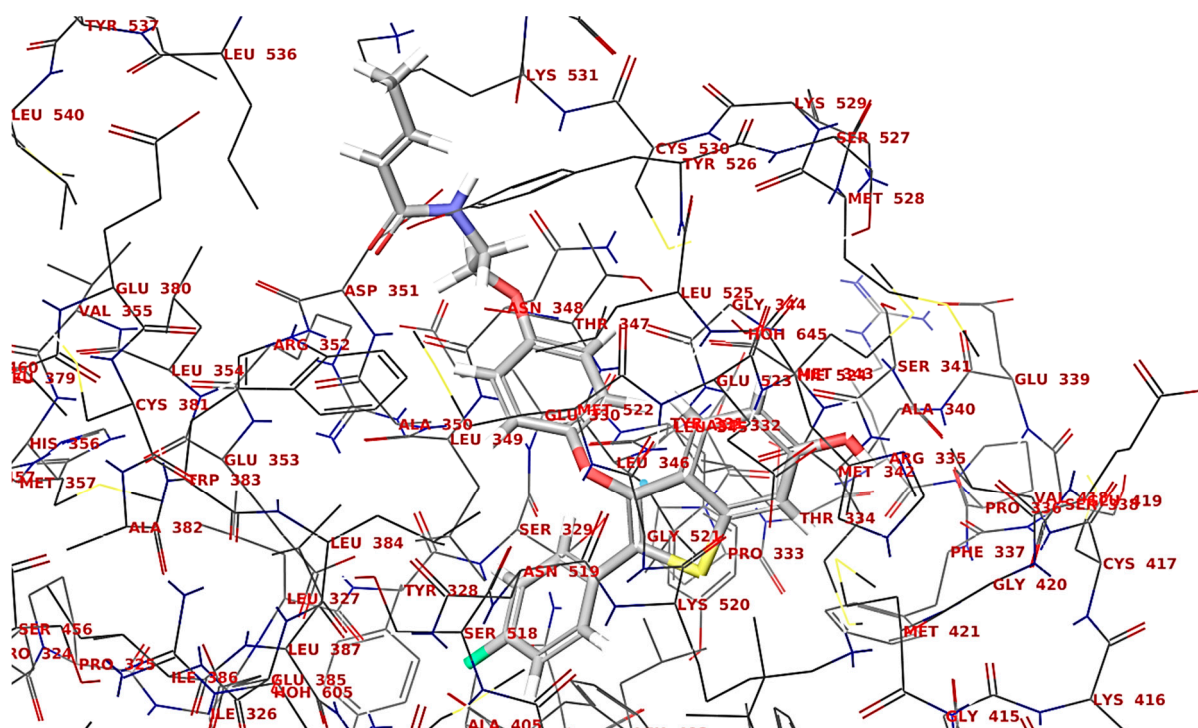
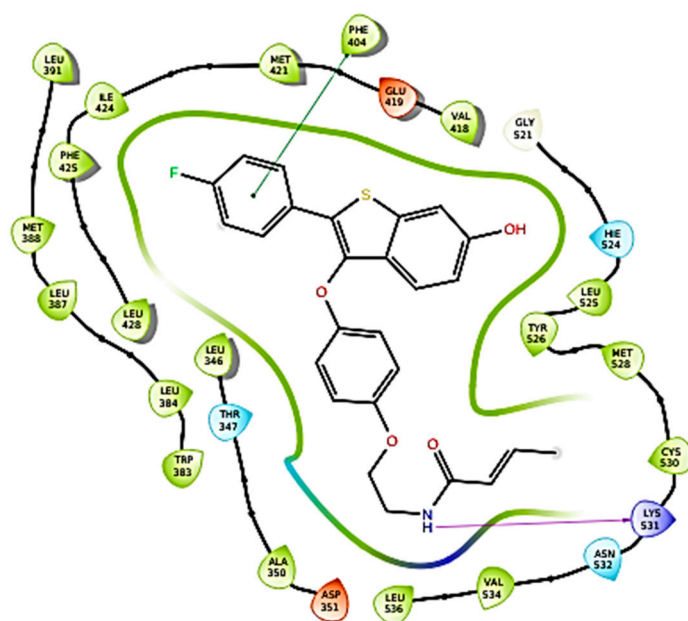


Figure S1e: 2D & 3D interactions for Compound BT ER 23c (Docking score -12.394)

BT_ER_15d - 2IOG - 5-removed waters

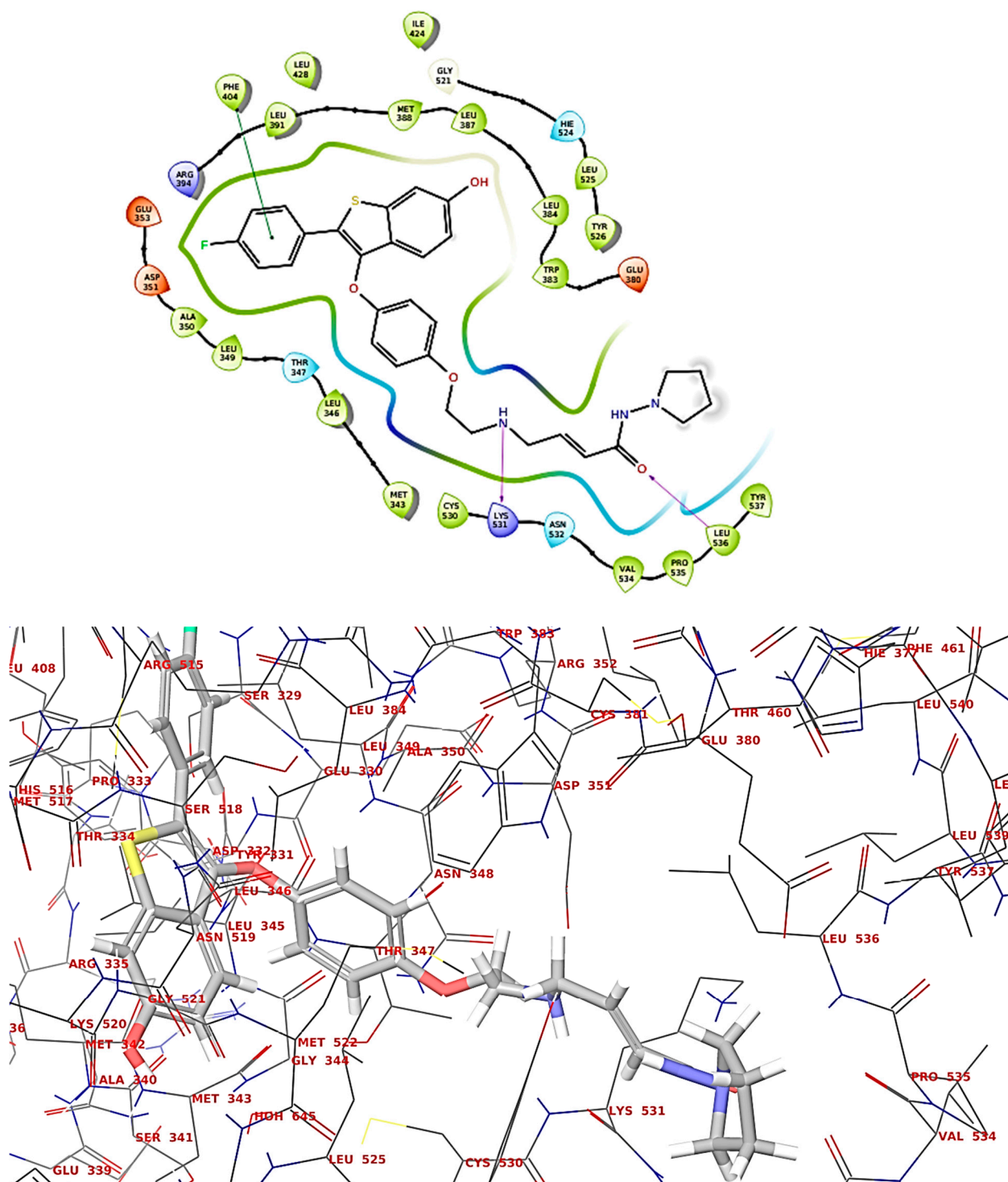


Figure S1f: 2D & 3D interactions for Compound BT_ER_15d (Docking score -11.524)

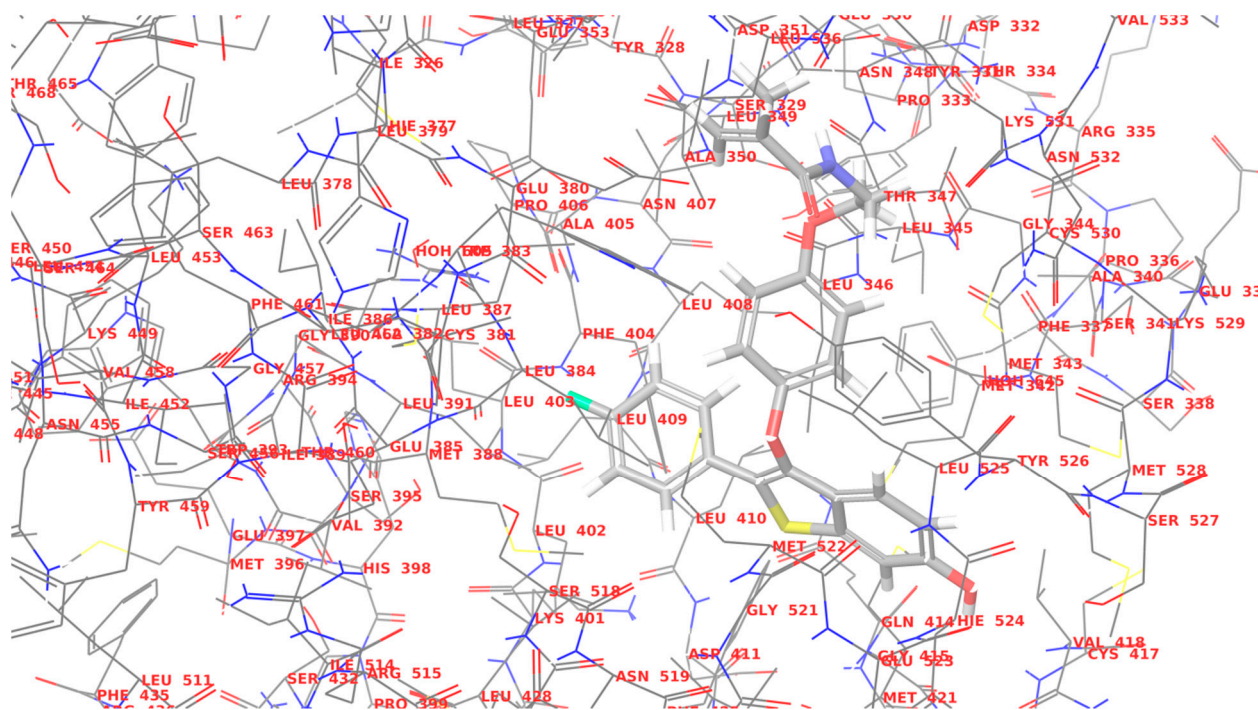
[illegible]

Figure S1h: 2D & 3D interactions for Compound BT ER 23b (Docking score -11.622)

2IOG - 5-removed waters - SL_TN_56

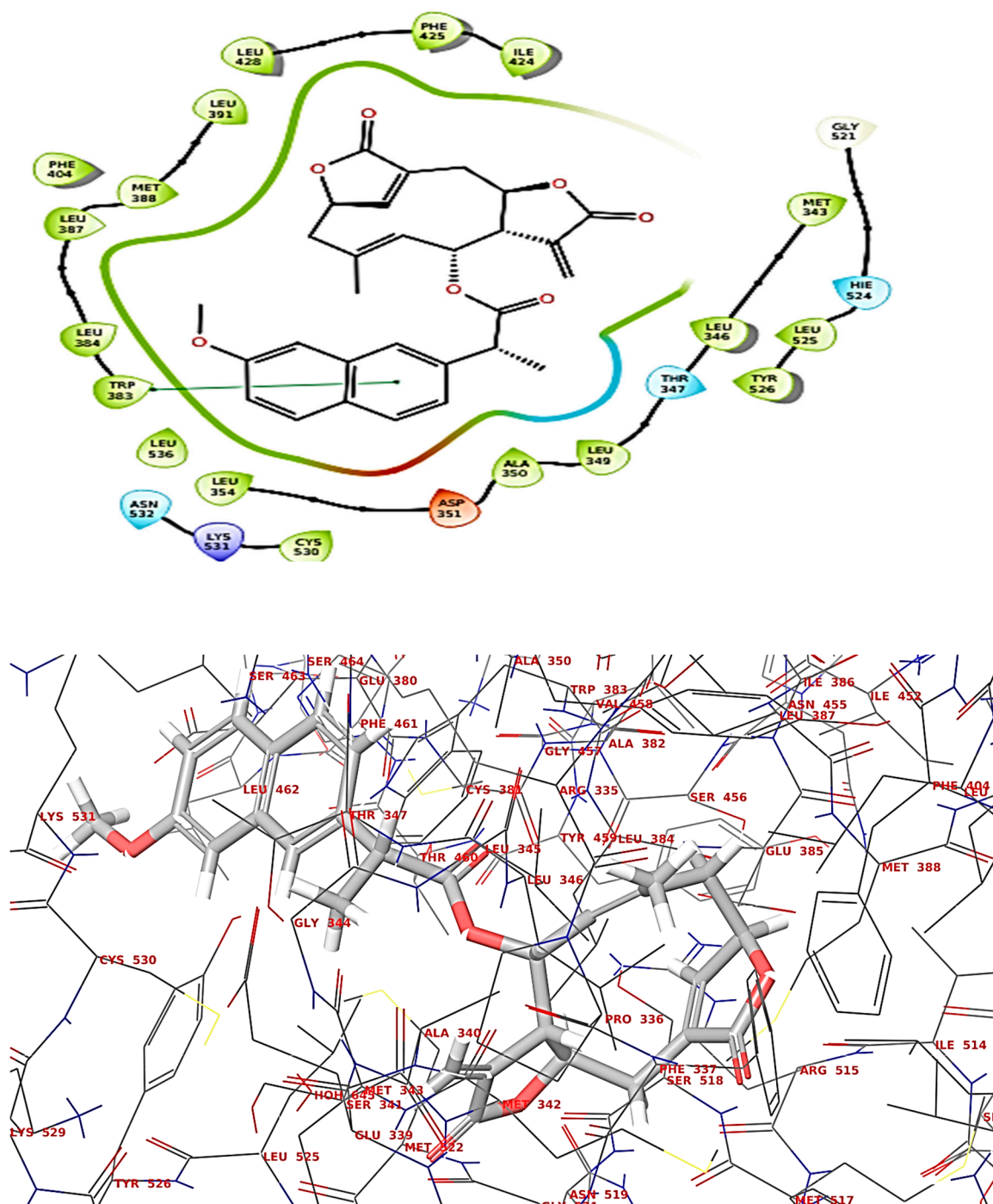


Figure S1i: 2D & 3D interactions for Compound SL TN 56 (Docking score -10.962)

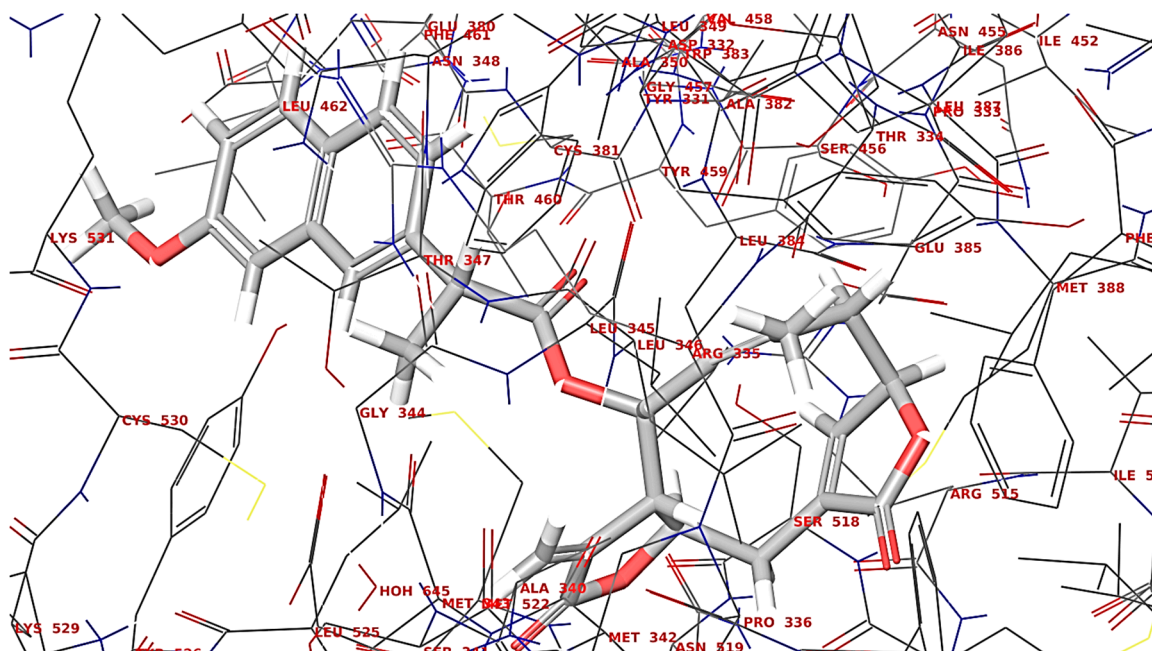


Figure S1j: 2D & 3D interactions for Compound SL TN 55 (Docking score -10.962)