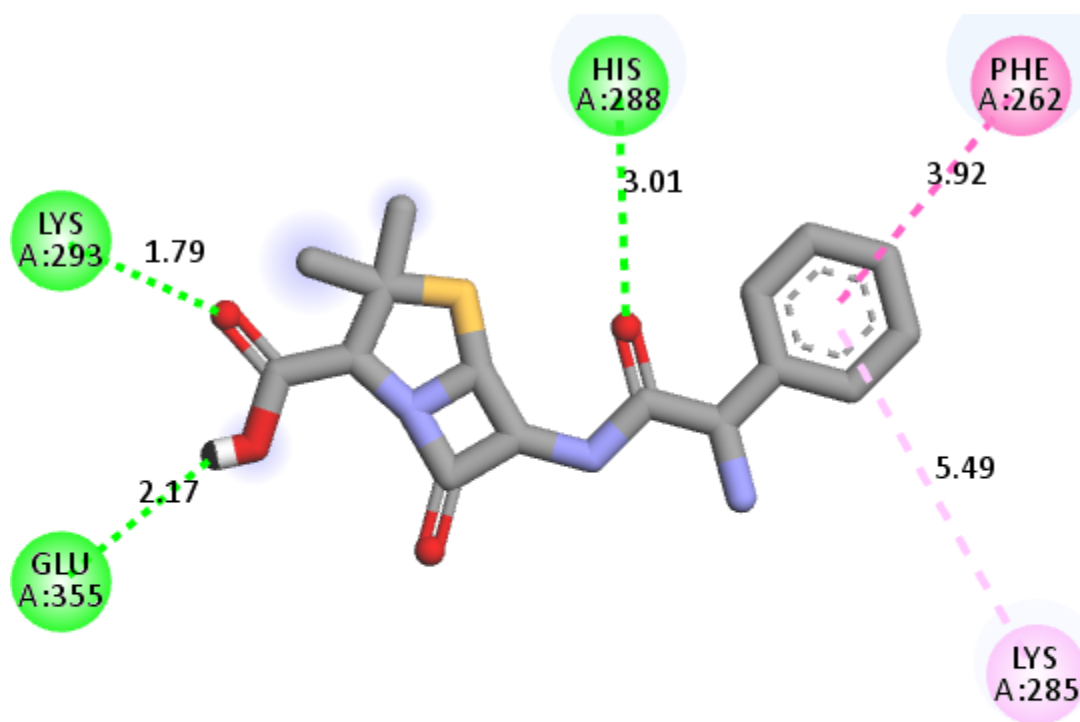





Experimental and Computational Insights of Schiff Base Copper(II) Complexes of Para-Substituted Benzaldehydes towards some Bacterial and Target Proteins



Interactions

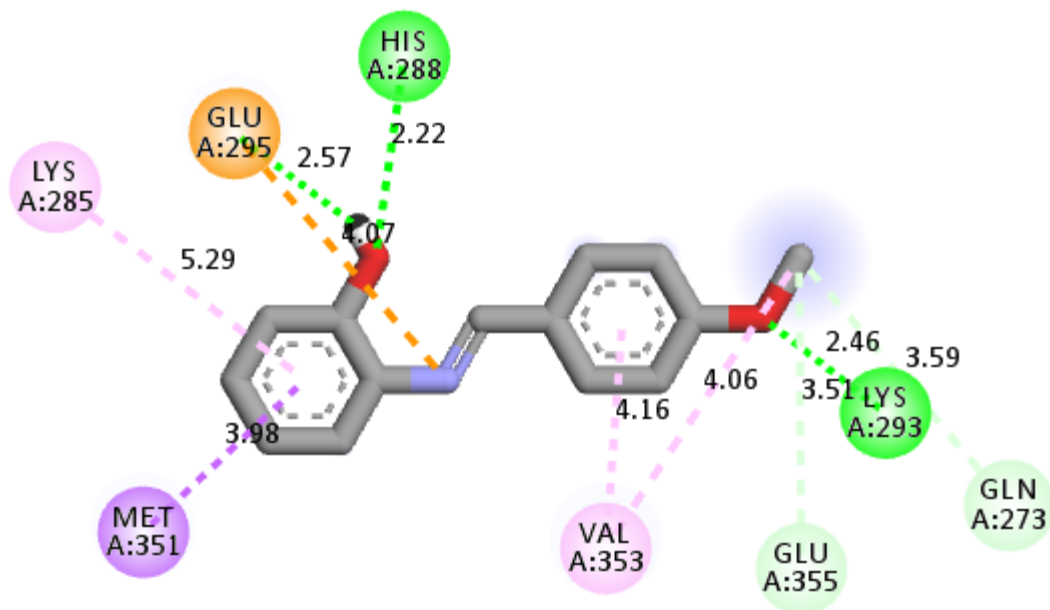
 Conventional Hydrogen Bond

 Carbon Hydrogen Bond

 Pi-Pi Stacked

 Pi-Alkyl

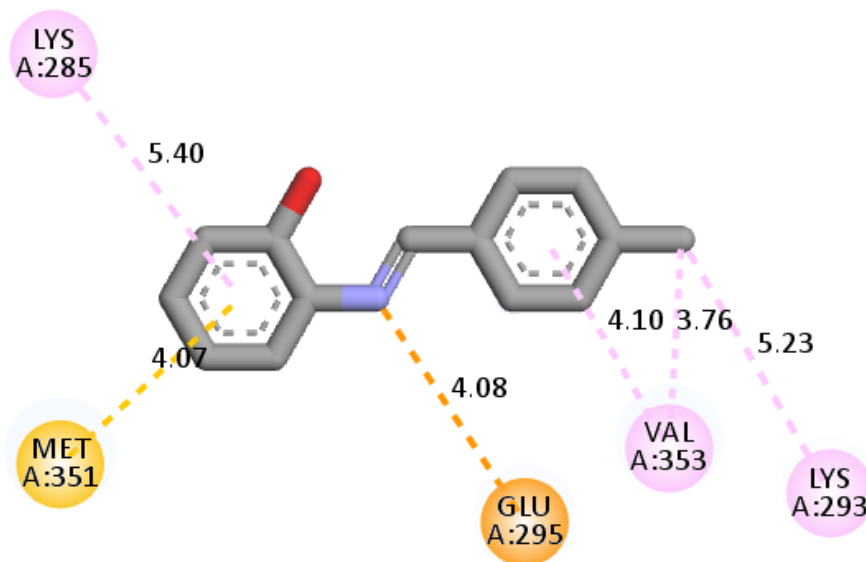
S1: Ampicillin-4YRD



Interactions

- Attractive Charge
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Sigma
- Pi-Sulfur
- Alkyl
- Pi-Alkyl

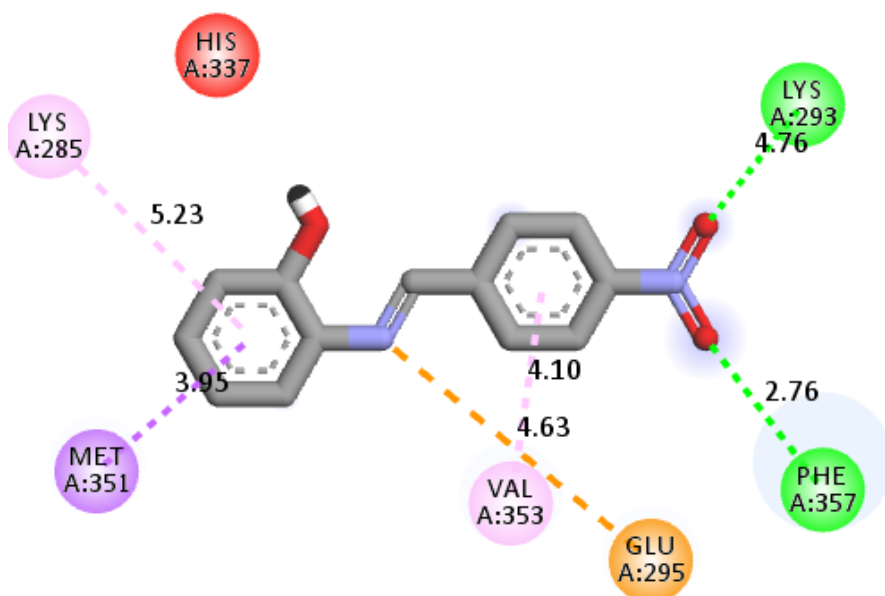
S2: F1-4YRD








Interactions

- Attractive Charge
- Pi-Sulfur
- Alkyl
- Pi-Alkyl

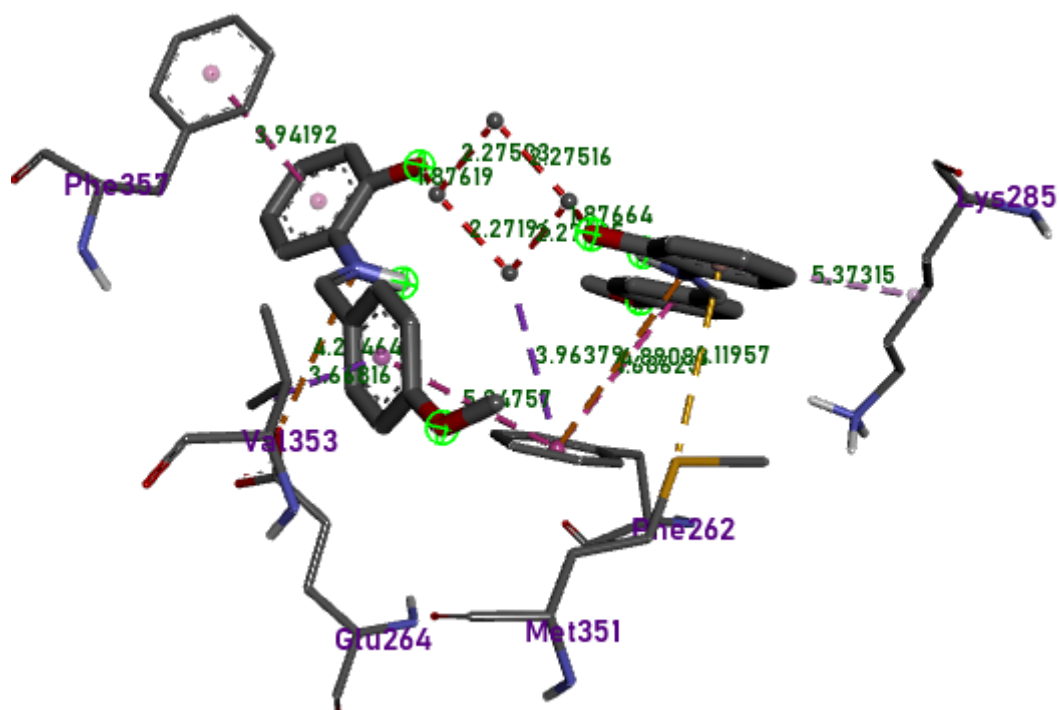
S3: F2-4YRD



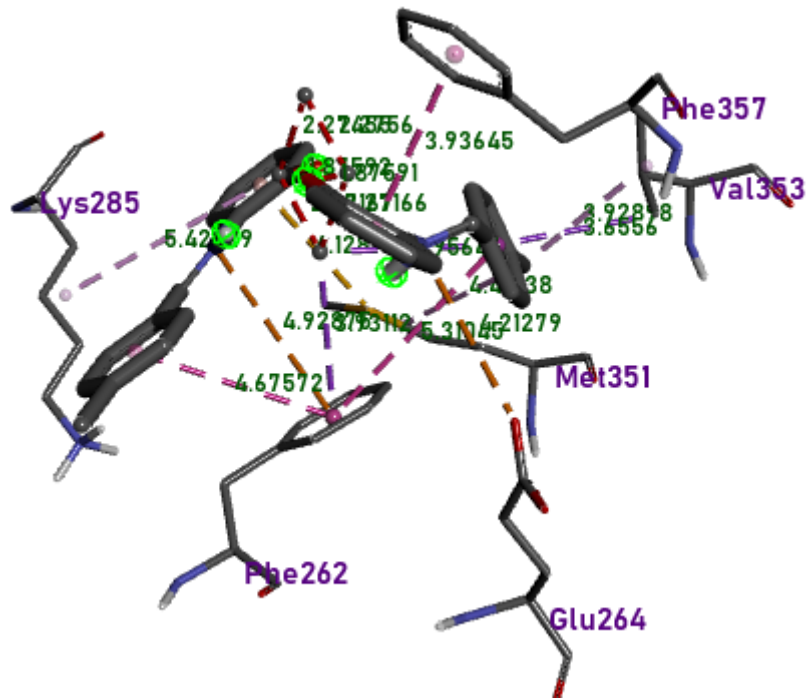
Interactions

- | | |
|--|---|
|  Attractive Charge |  Pi-Sulfur |
|  Conventional Hydrogen Bond |  Pi-Alkyl |
|  Pi-Sigma | |

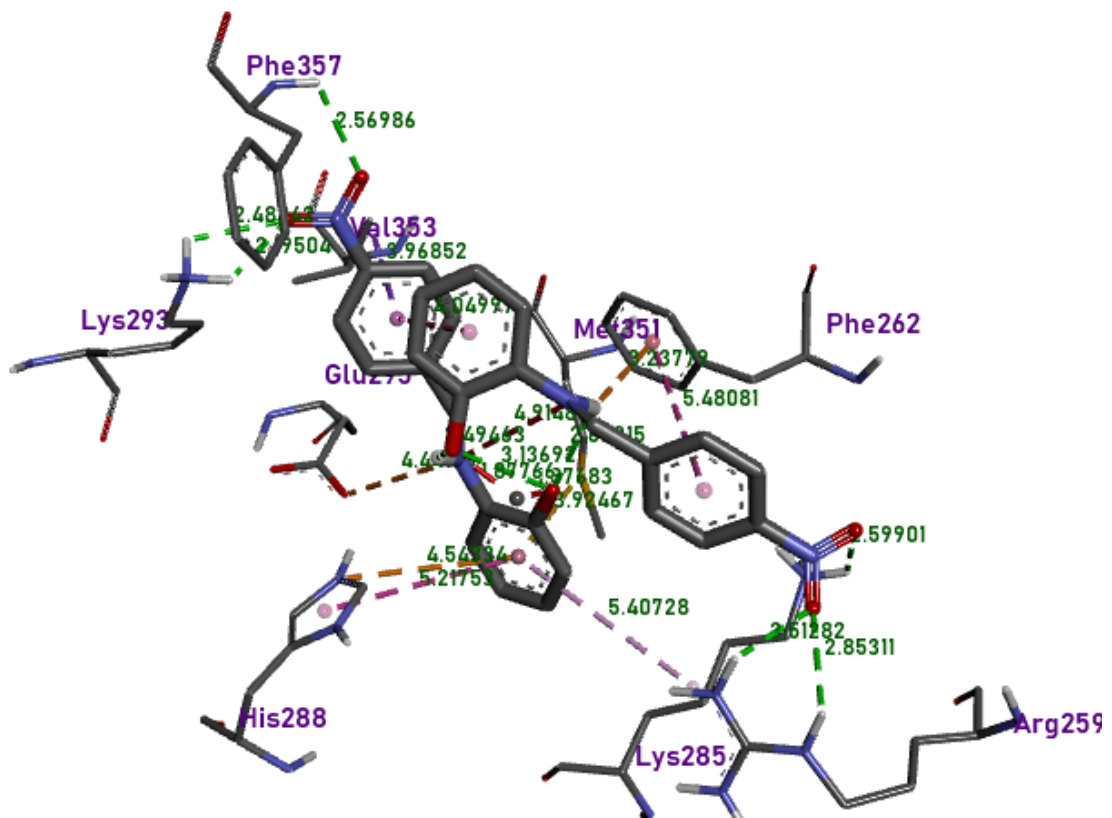
S4: F3-4yrd



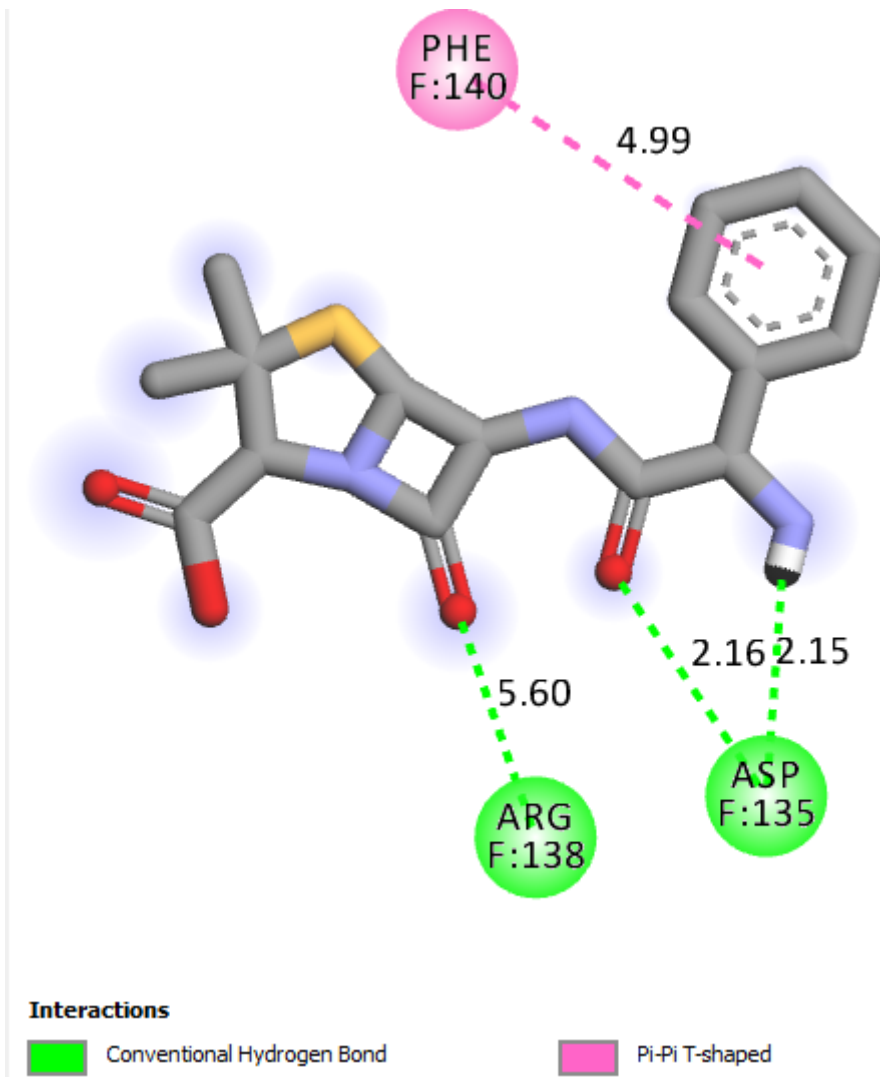
S5: F1-Cu-4YRD



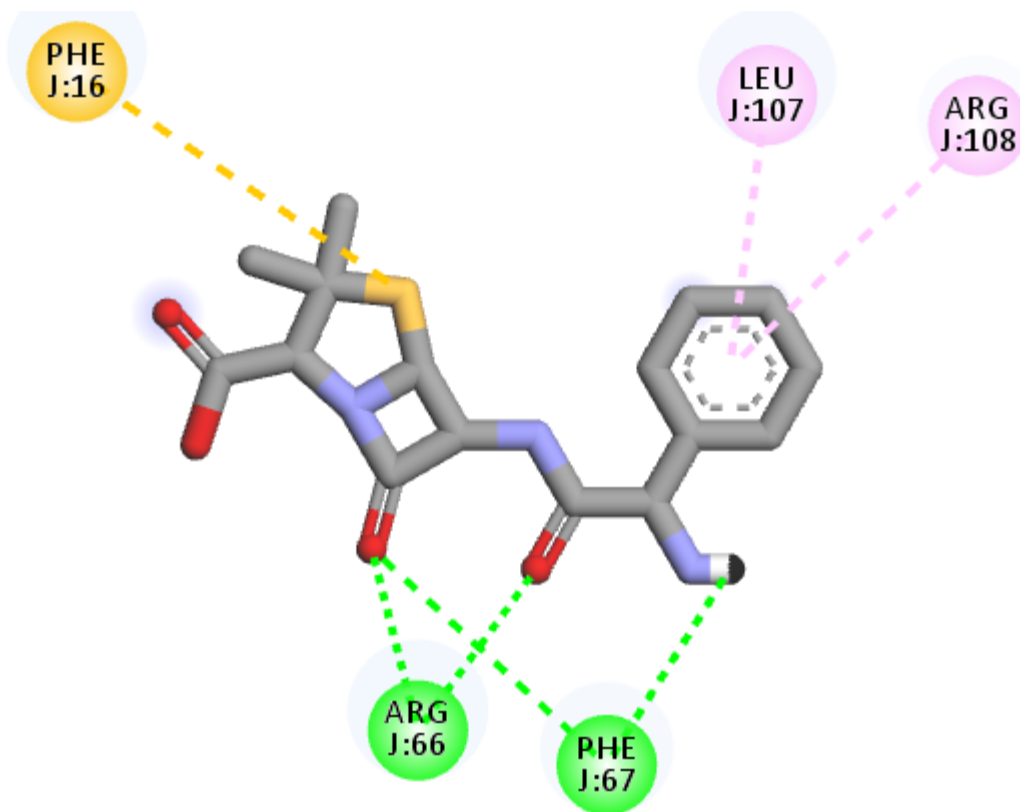
S6: F2-Cu-4YRD




S7: F3-Cu-4YRD




S8: Ampicillin-6KJ6-F



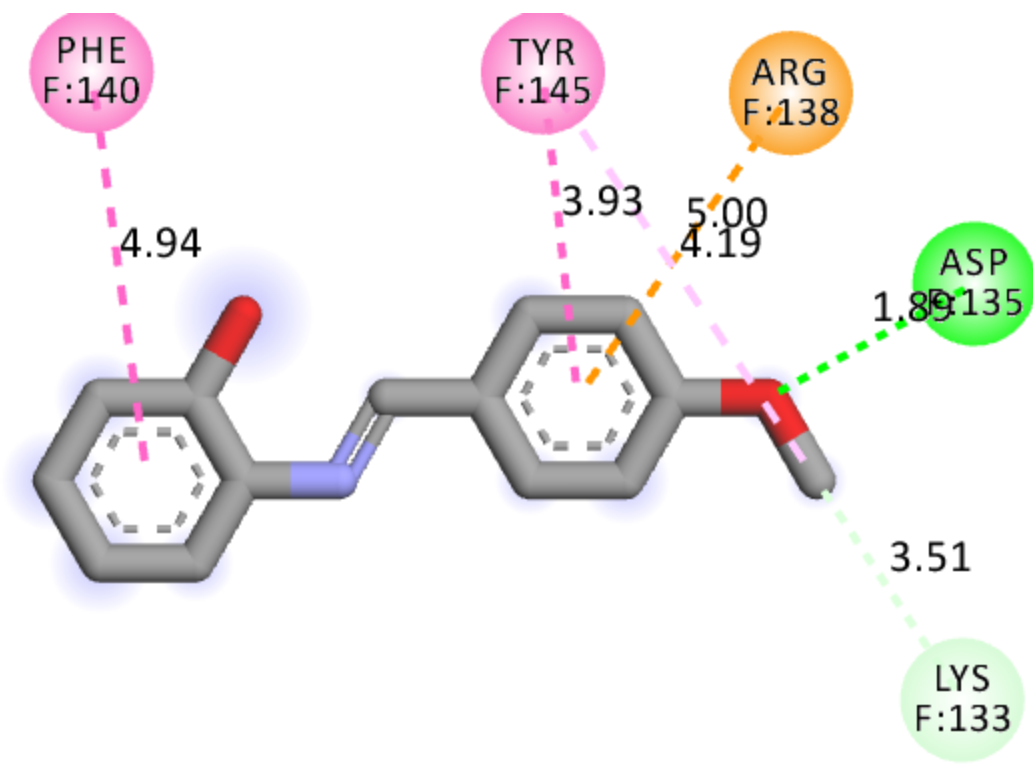
Interactions

 Conventional Hydrogen Bond

 Pi-Sulfur

 Pi-Alkyl

S9: Ampicillin-6KJ6-J

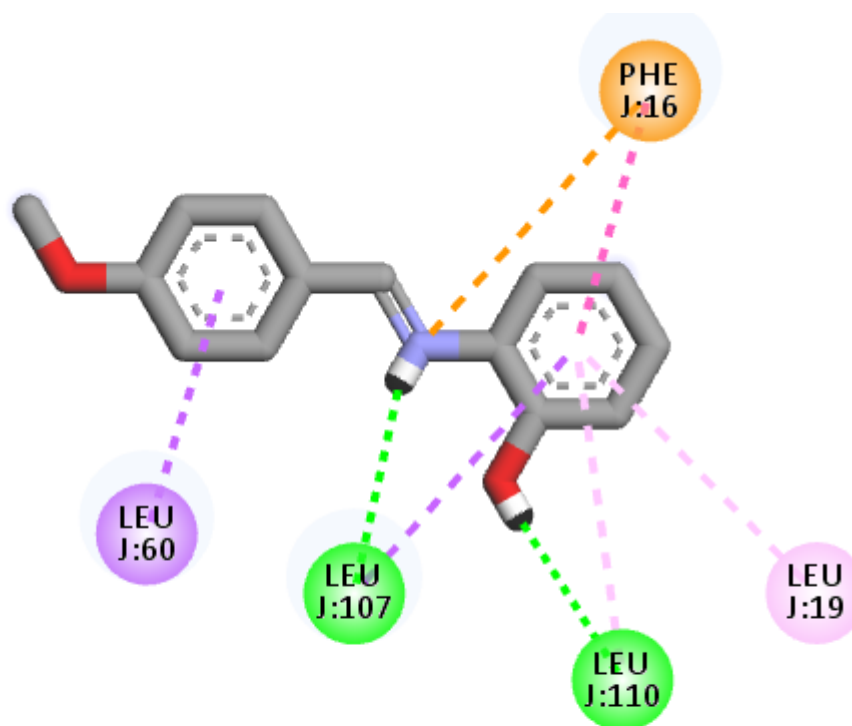


Interactions


- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Cation


- Pi-Pi Stacked
- Pi-Pi T-shaped
- Pi-Alkyl


S10: F1-6KJ6-F




Interactions

 Conventional Hydrogen Bond

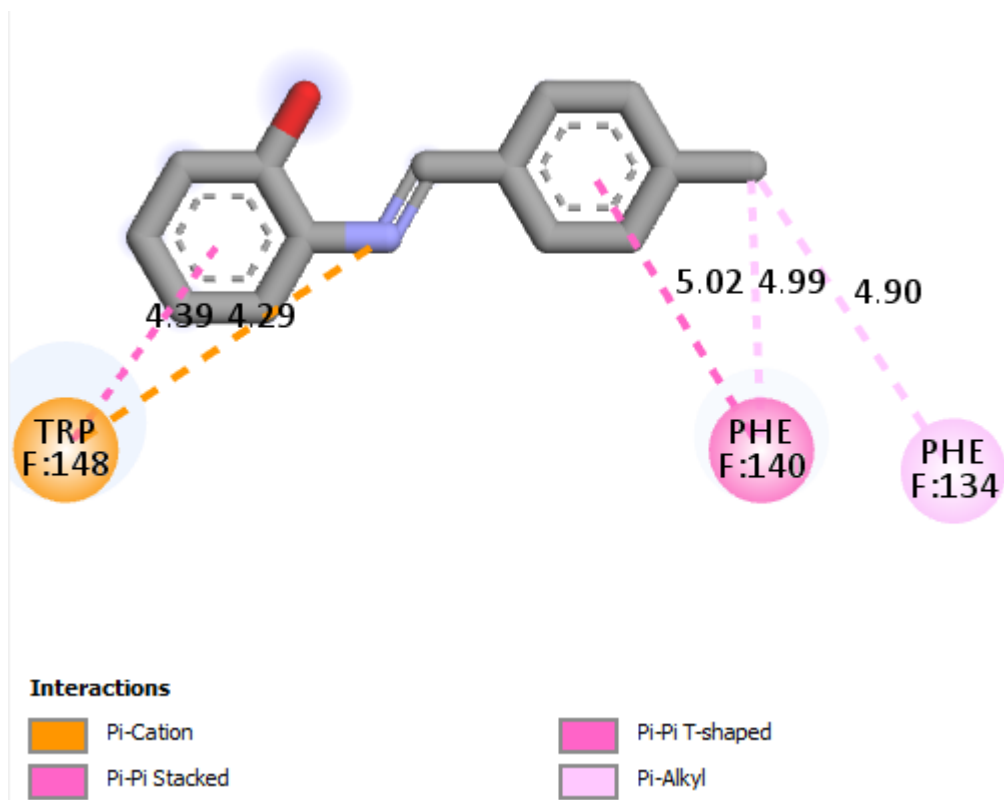
 Pi-Cation

 Pi-Sigma

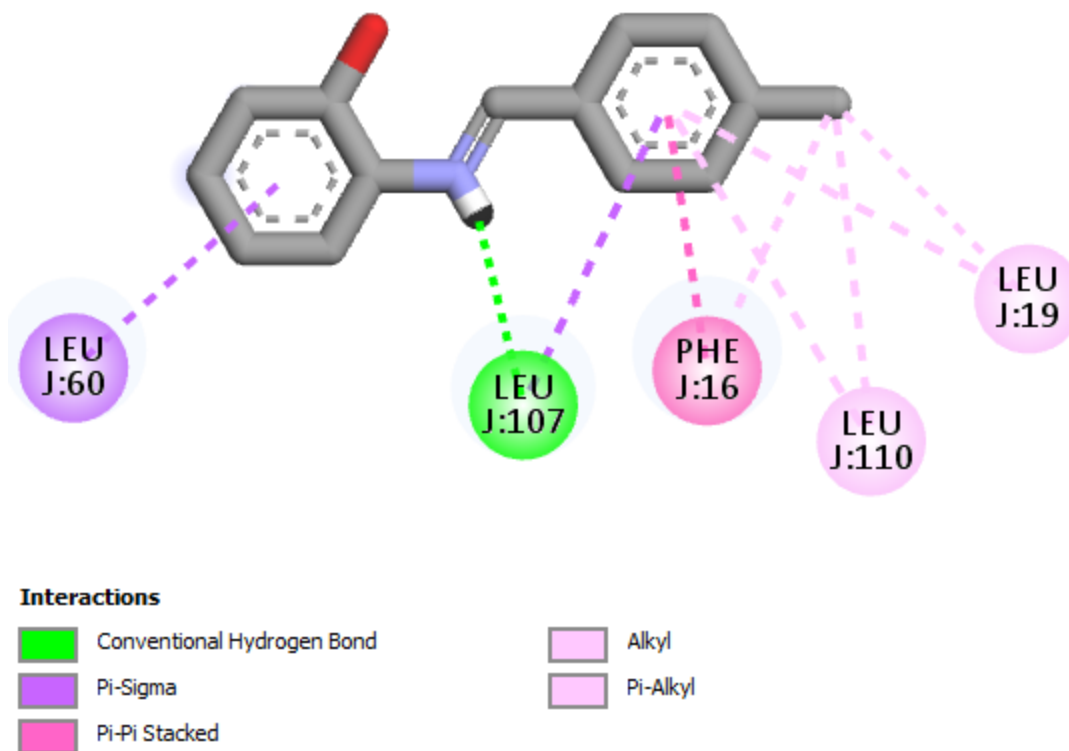
 Pi-Pi Stacked

 Pi-Alkyl

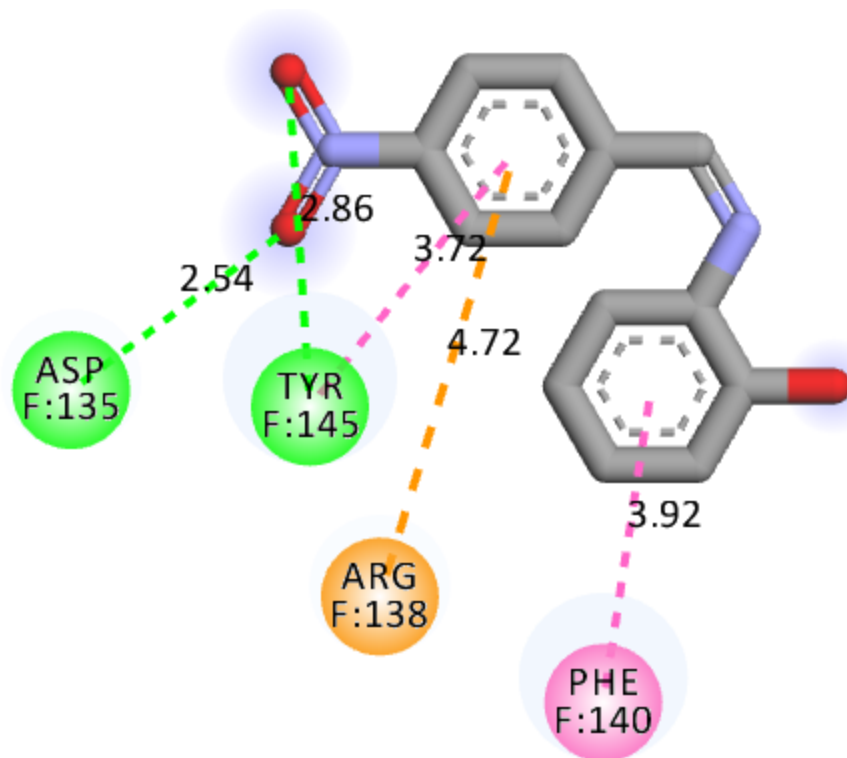
S11: F1-6KJ6-J





S12: F2-6KJ6-F




S13: F2-6KJ6-J

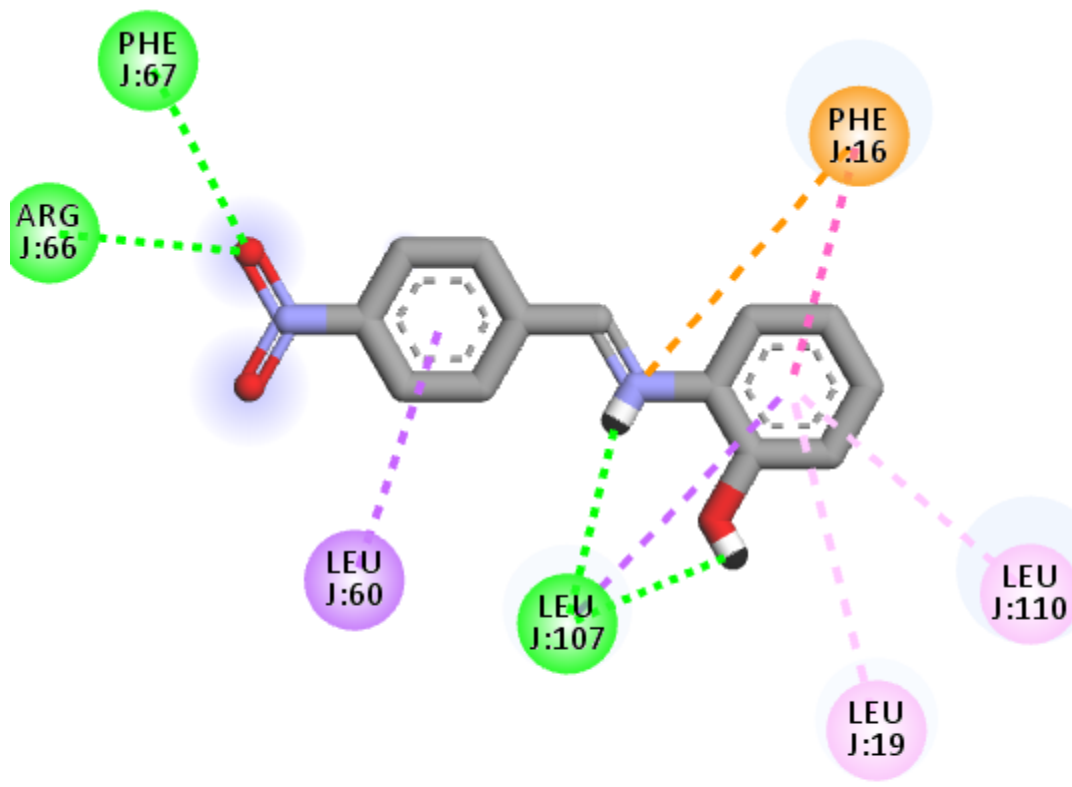


Interactions






 Conventional Hydrogen Bond
 Pi-Cation

 Pi-Pi Stacked

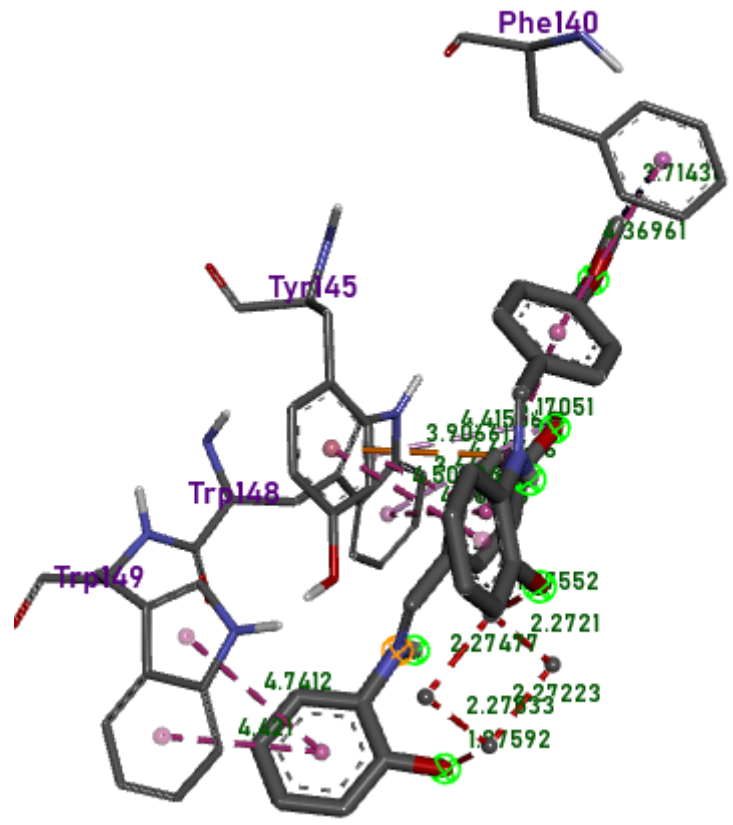
S14: F3-6KJ6-F



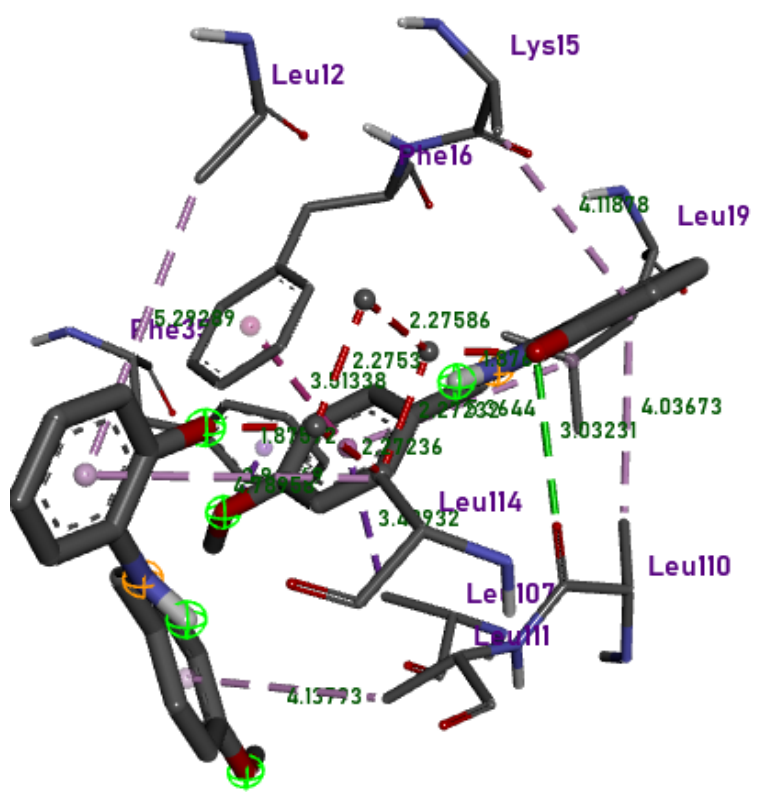
Interactions

- | | |
|--|---|
|  Conventional Hydrogen Bond |  Pi-Pi Stacked |
|  Pi-Cation |  Pi-Alkyl |
|  Pi-Sigma | |

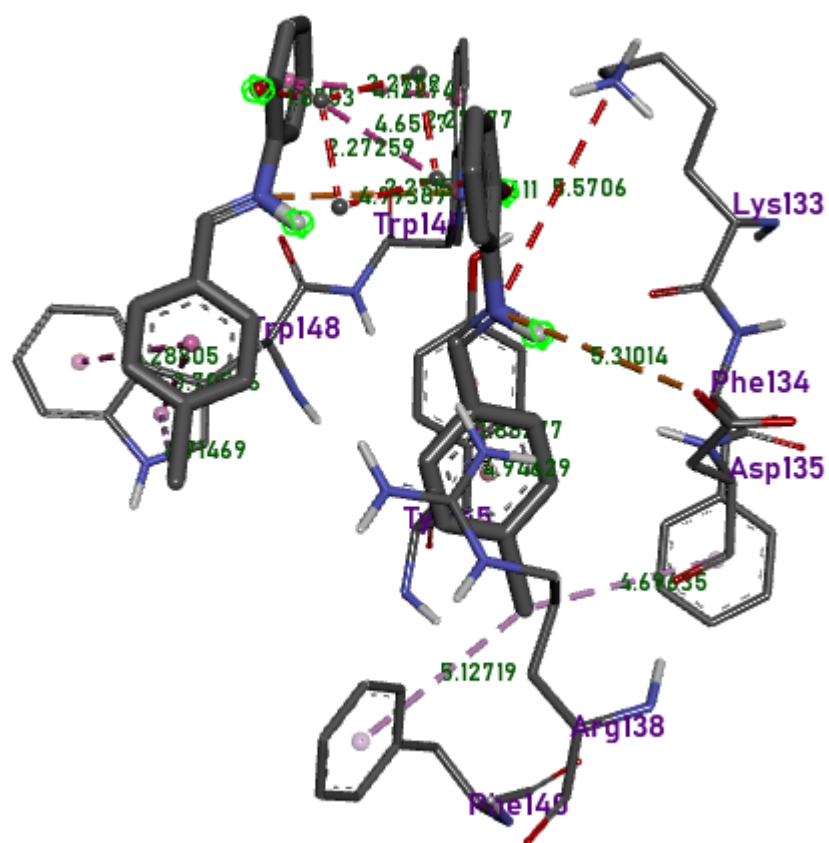
S15: F3-6KJ6-J



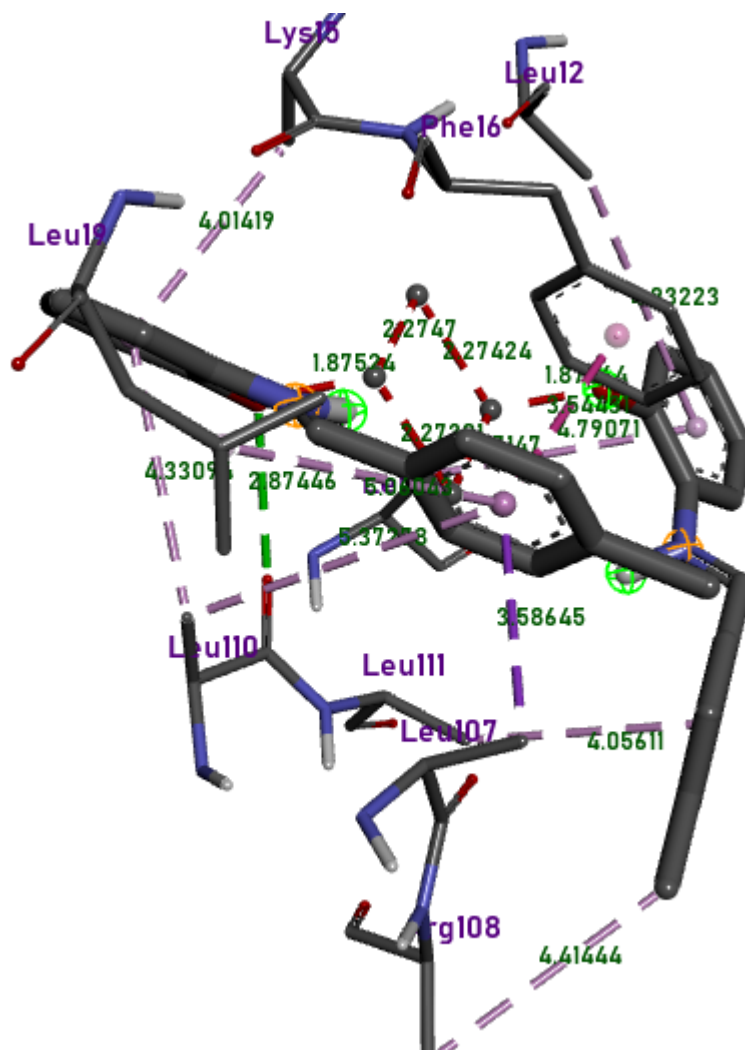
S16: F1-Cu-6KJ6-F



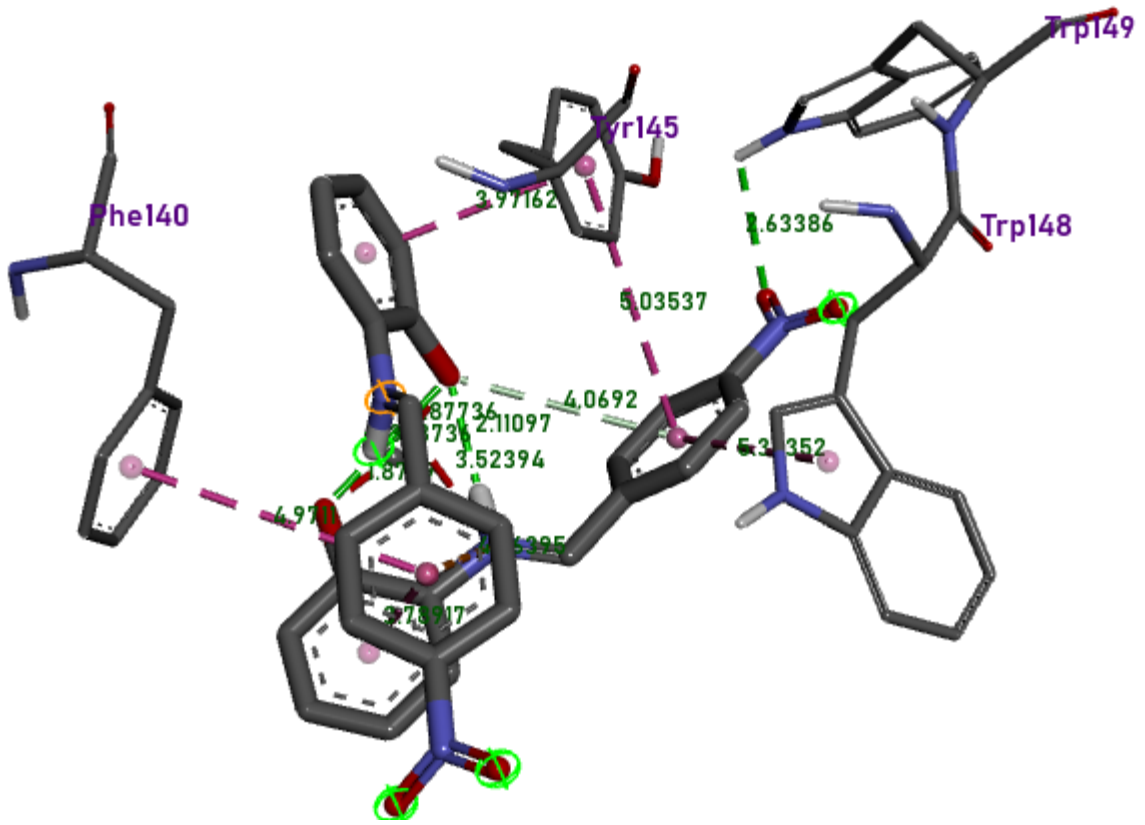
S17: F1-Cu-6KJ6-J



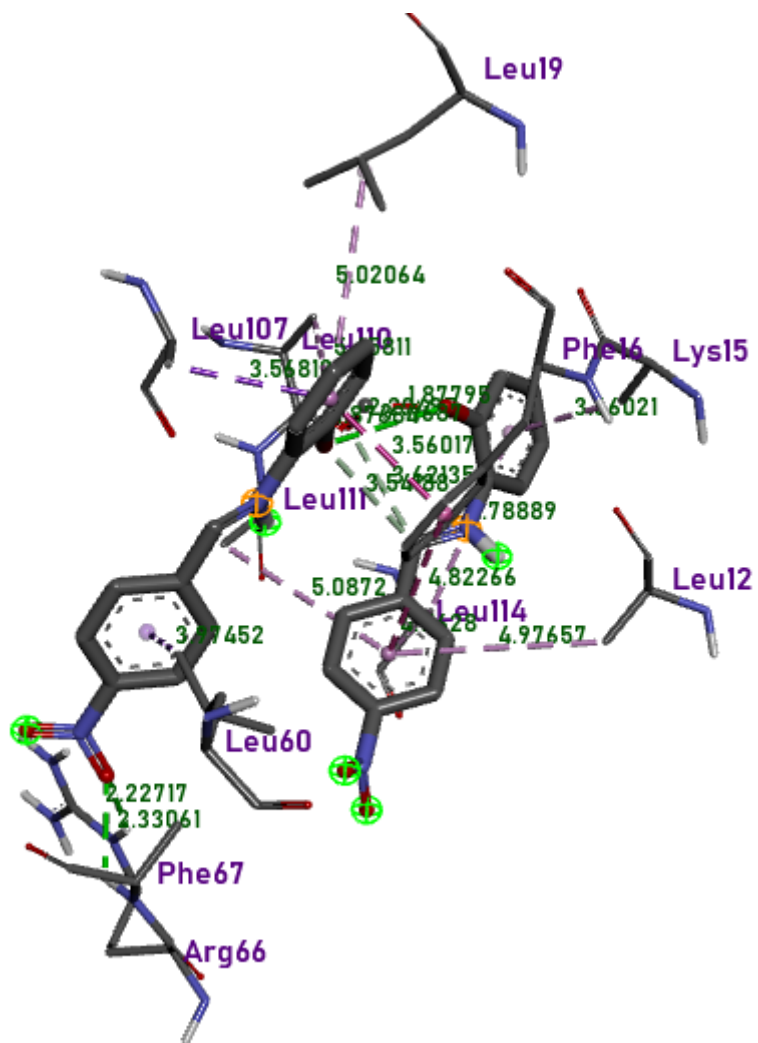
S18: F2-Cu-6KJ6-F



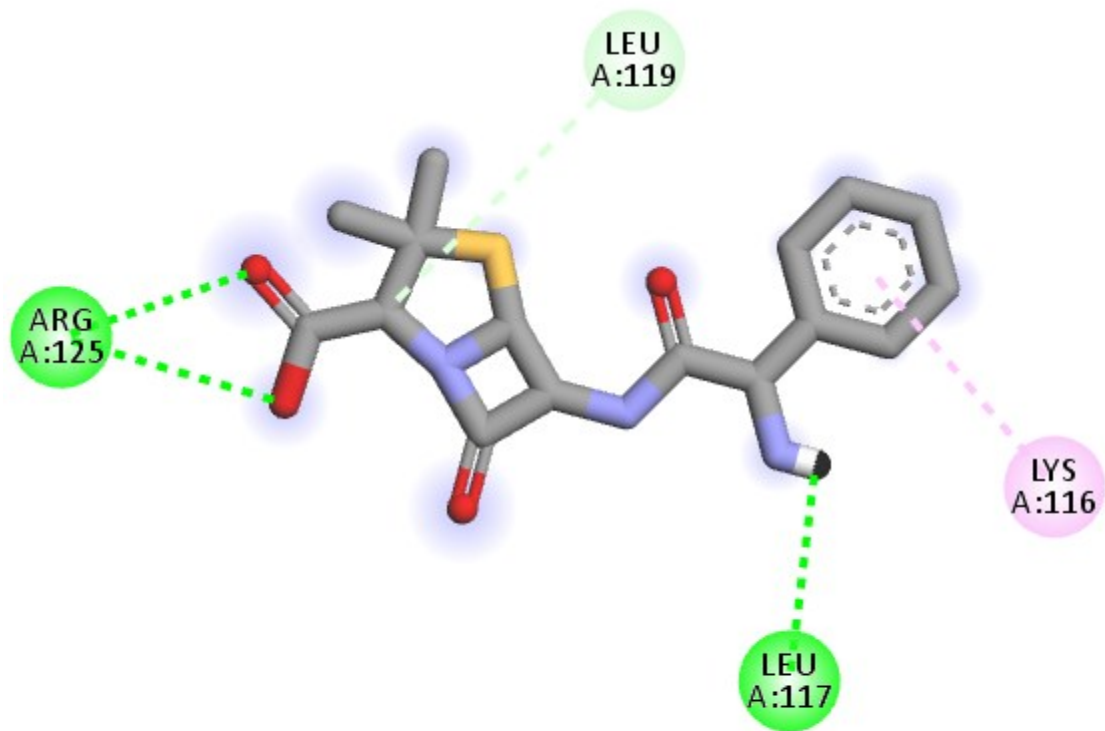
S19: F2-Cu-6KJ6-J




S20: F3-Cu-6KJ6-F




S21: F3-Cu-6KJ6-J



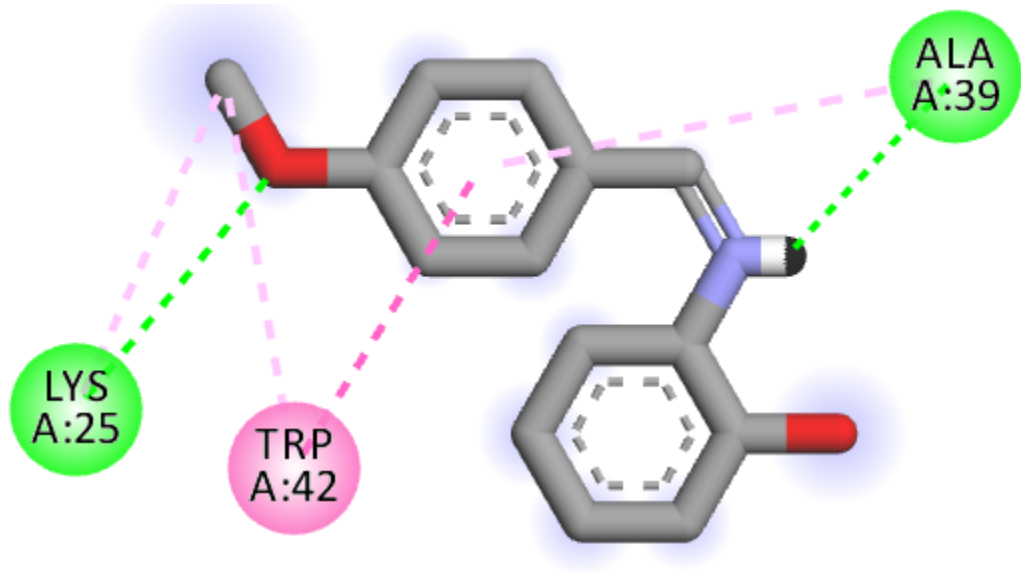
Interactions

 Conventional Hydrogen Bond

 Pi-Alkyl

BLU  Carbon Hydrogen Bond

S22: Ampicillin-6p8o

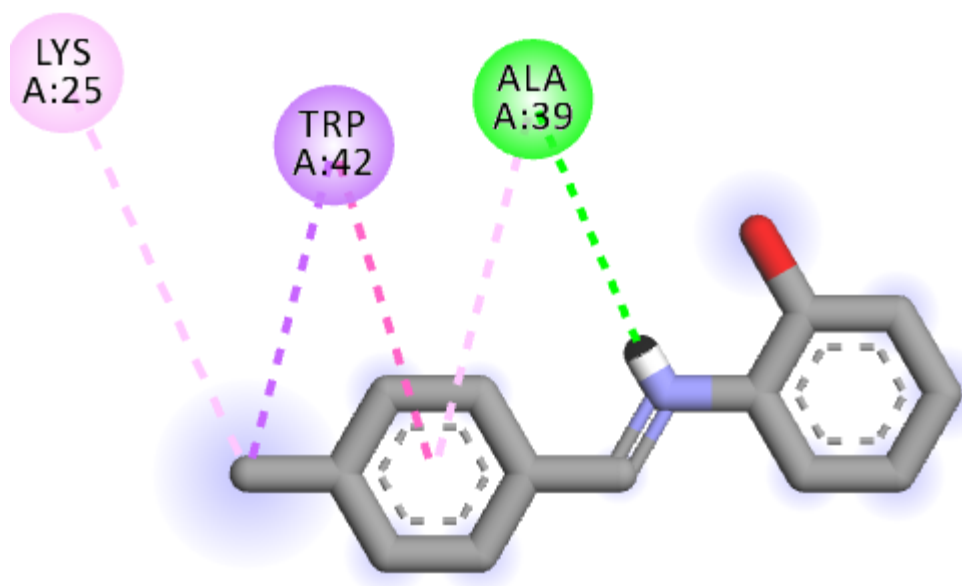


Interactions






- Conventional Hydrogen Bond
- Pi-Pi Stacked

- Alkyl
- Pi-Alkyl

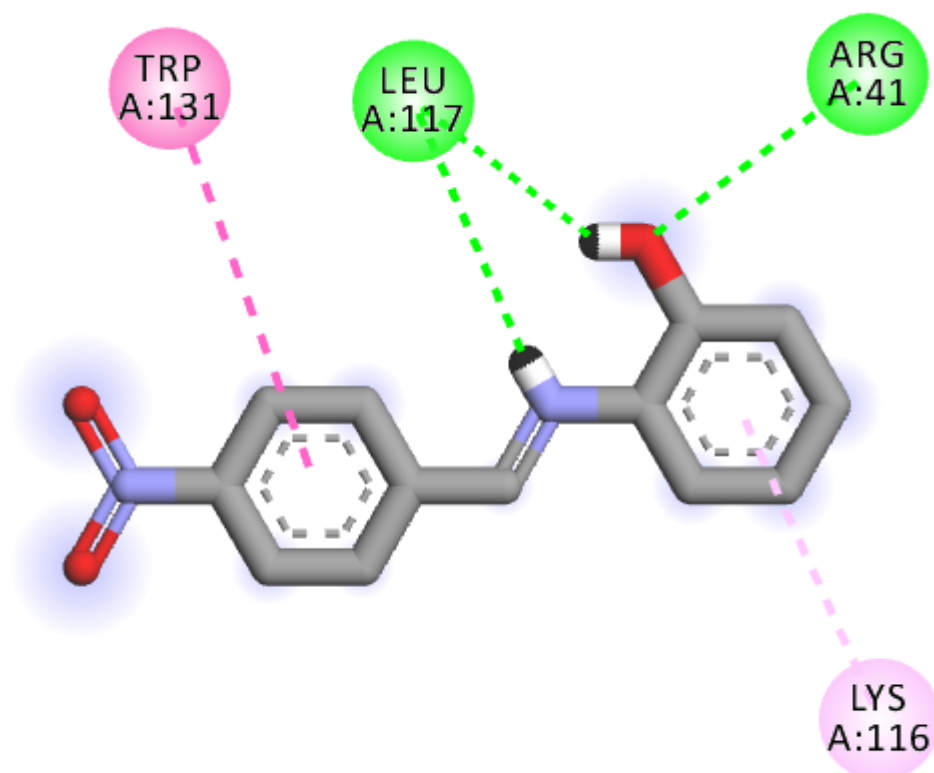
S23: F1-6P8O




Interactions


- | | | | |
|--|----------------------------|---|----------|
|  | Conventional Hydrogen Bond |  | Alkyl |
|  | Pi-Sigma |  | Pi-Alkyl |
|  | Pi-Pi Stacked | | |

S24: F2-6P8O



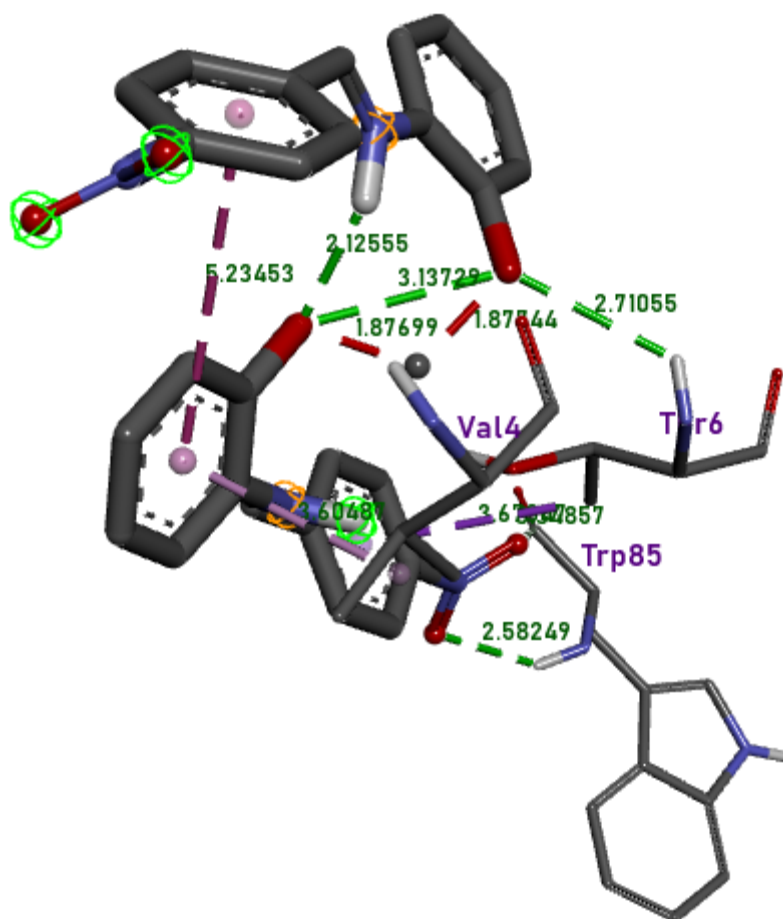
Interactions

 Conventional Hydrogen Bond

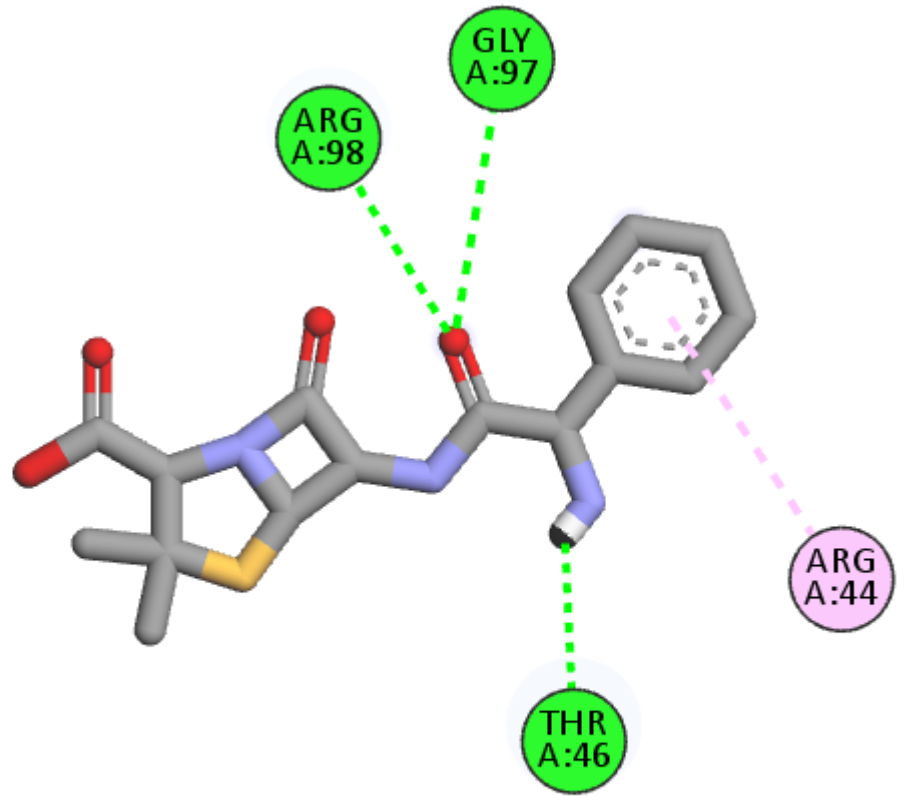
 Pi-Pi T-shaped

 Pi-Alkyl


S25: F3-6P80



S28: F3-Cu-6P8O

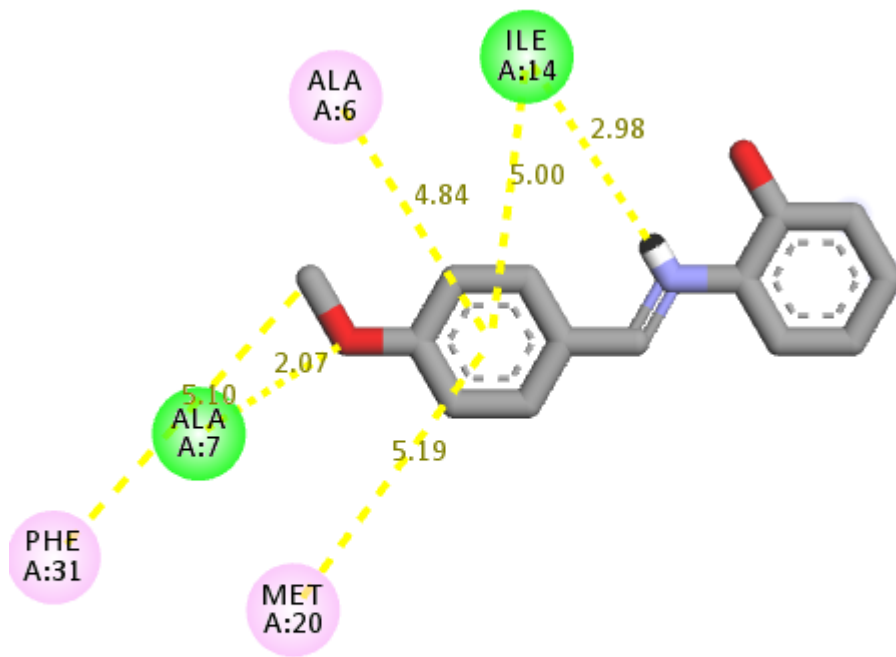


Interactions


 Conventional Hydrogen Bond

 Pi-Alkyl

S29: Ampicillin-4OSG

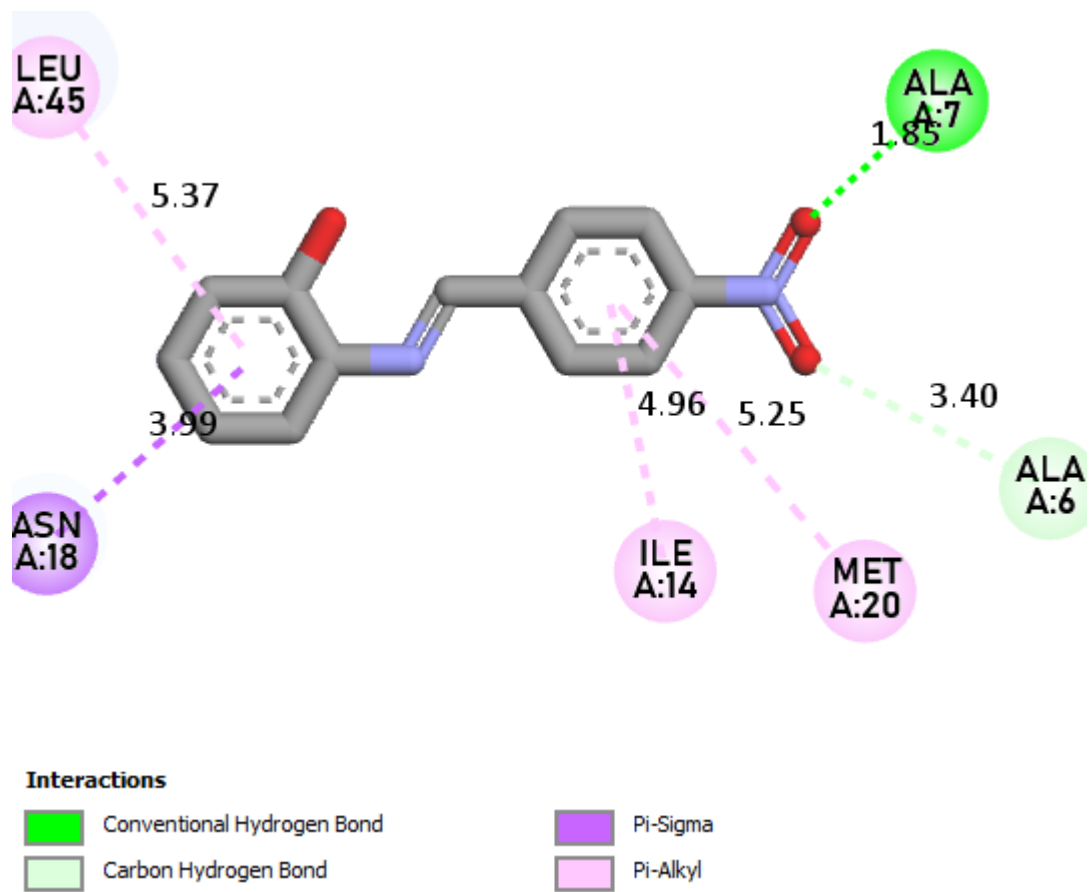


Interactions

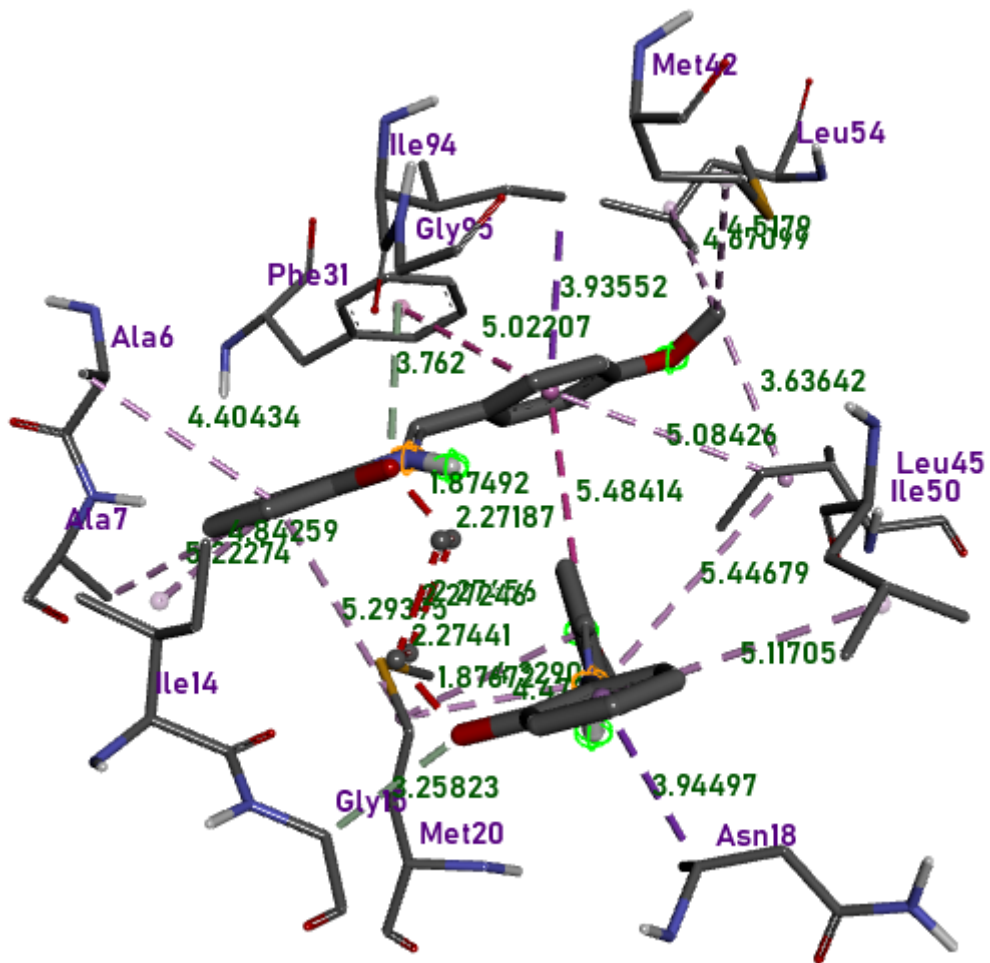
 Conventional Hydrogen Bond

 Pi-Alkyl

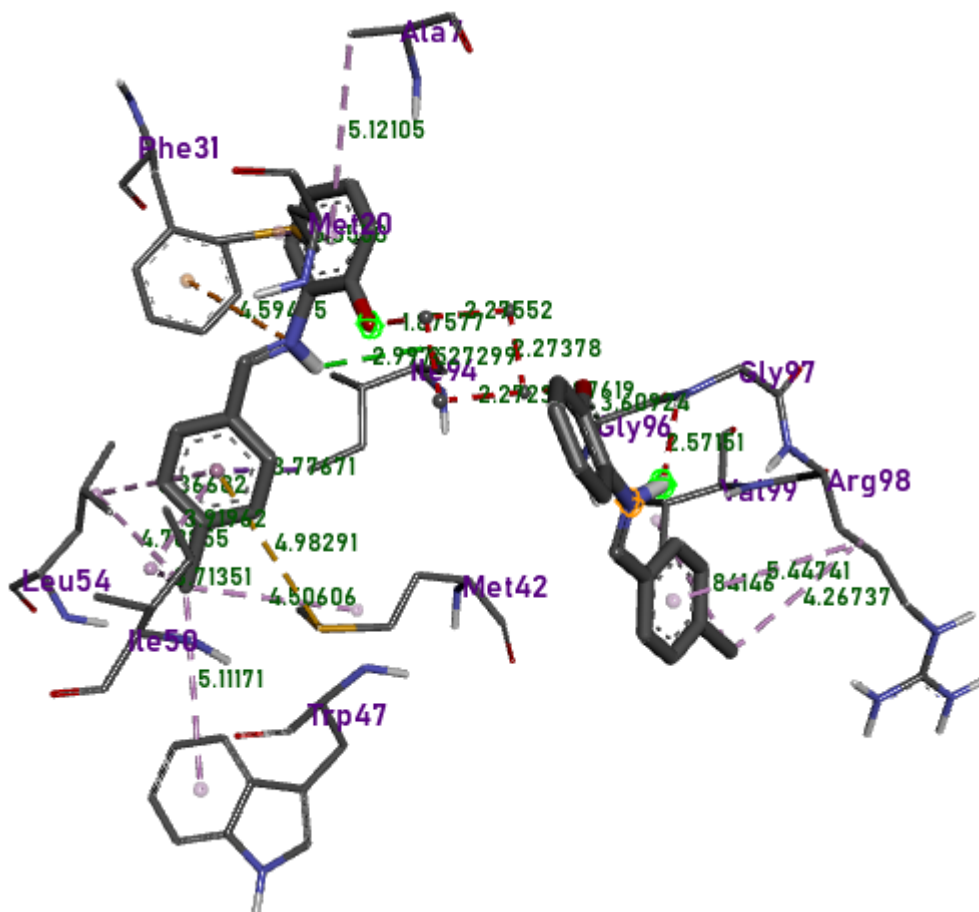
S30: F1-4OSG



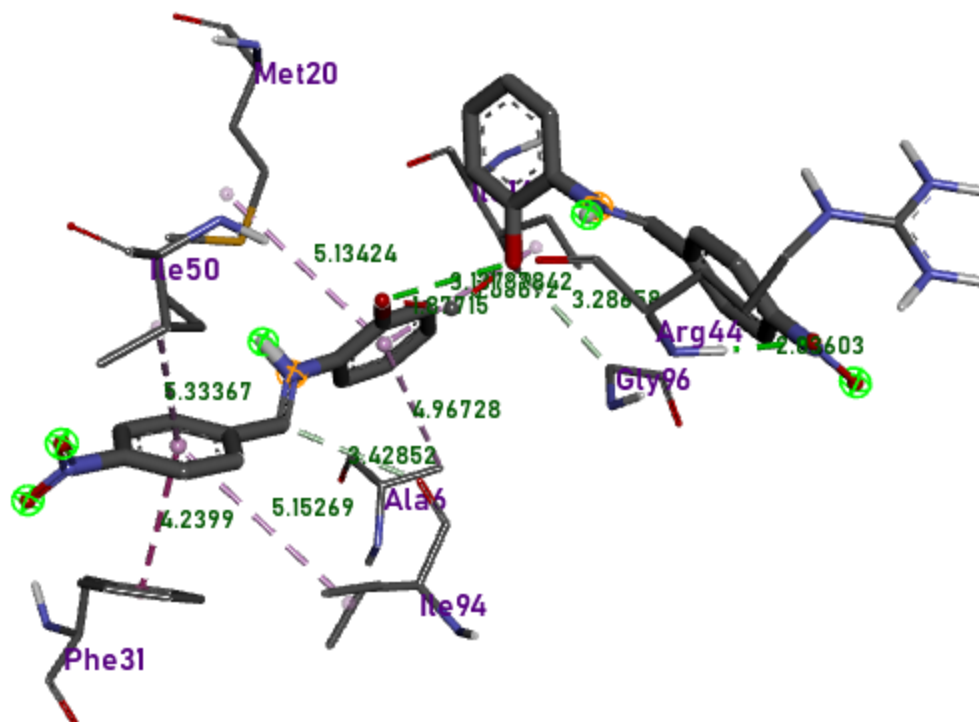
S31: F3-4OSG



S32: F1-Cu-4OSG



S33: F2-Cu-4OSG



S34: F3-Cu-4OSG