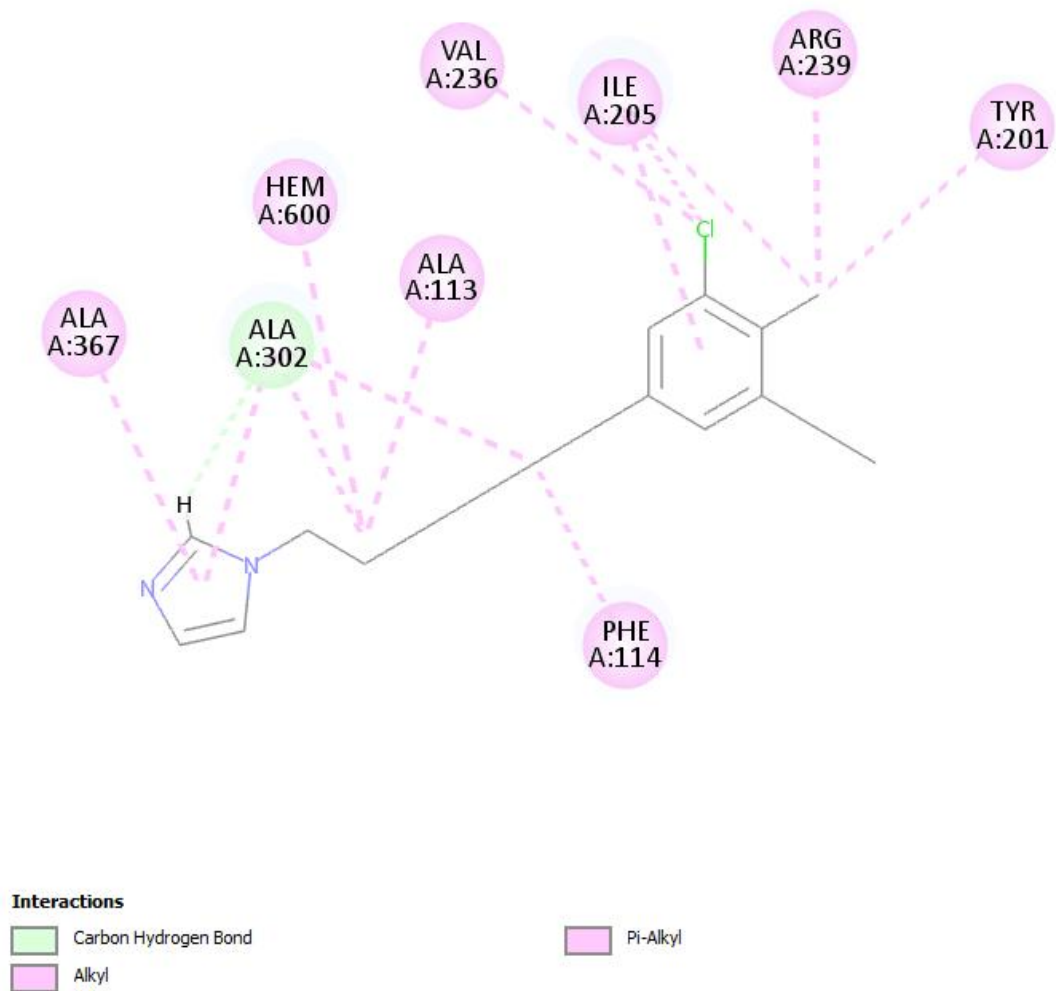
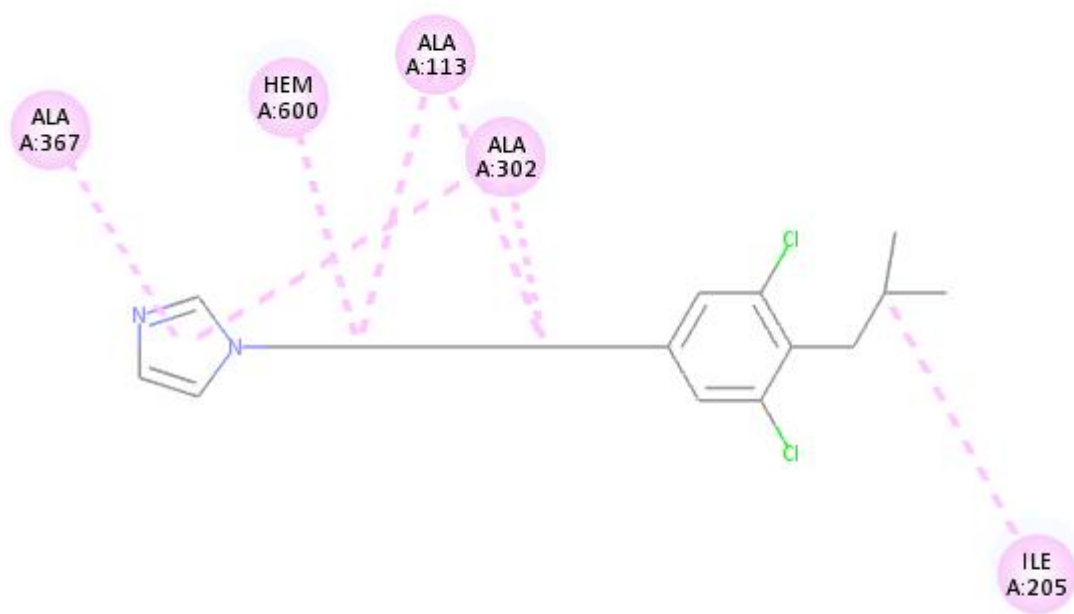


Supplementary Information



Supplementary Figure 1. 2D interactions of compound 52 within active pocket of 3ruk

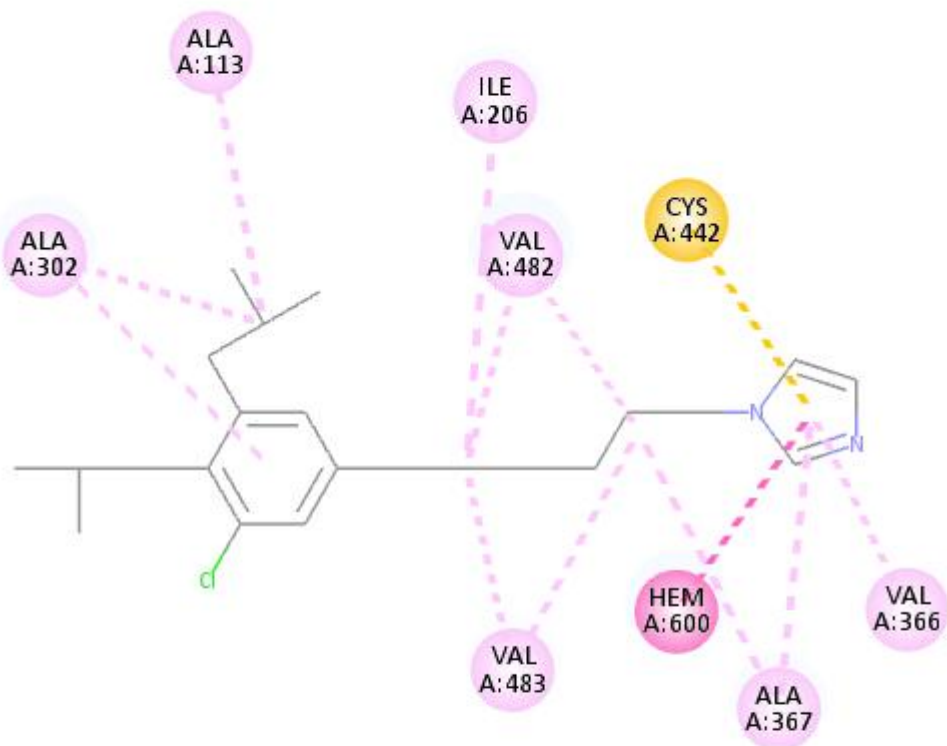


Interactions

Alkyl

Pi-Alkyl

Supplementary Figure 2. 2D interactions of compound 73 within active pocket of 3ruk

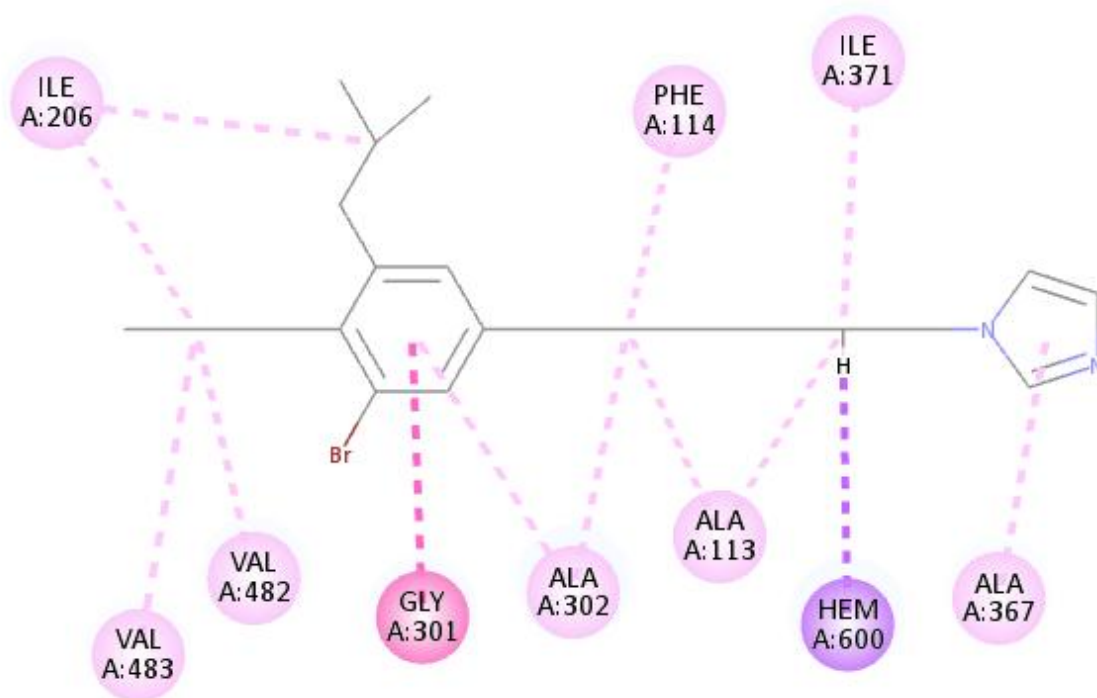


Interactions

- Pi-Sulfur
- Pi-Pi T-shaped

- Alkyl
- Pi-Alkyl

Supplementary Figure 3. 2D interactions of compound 81 within active pocket of 3ruk

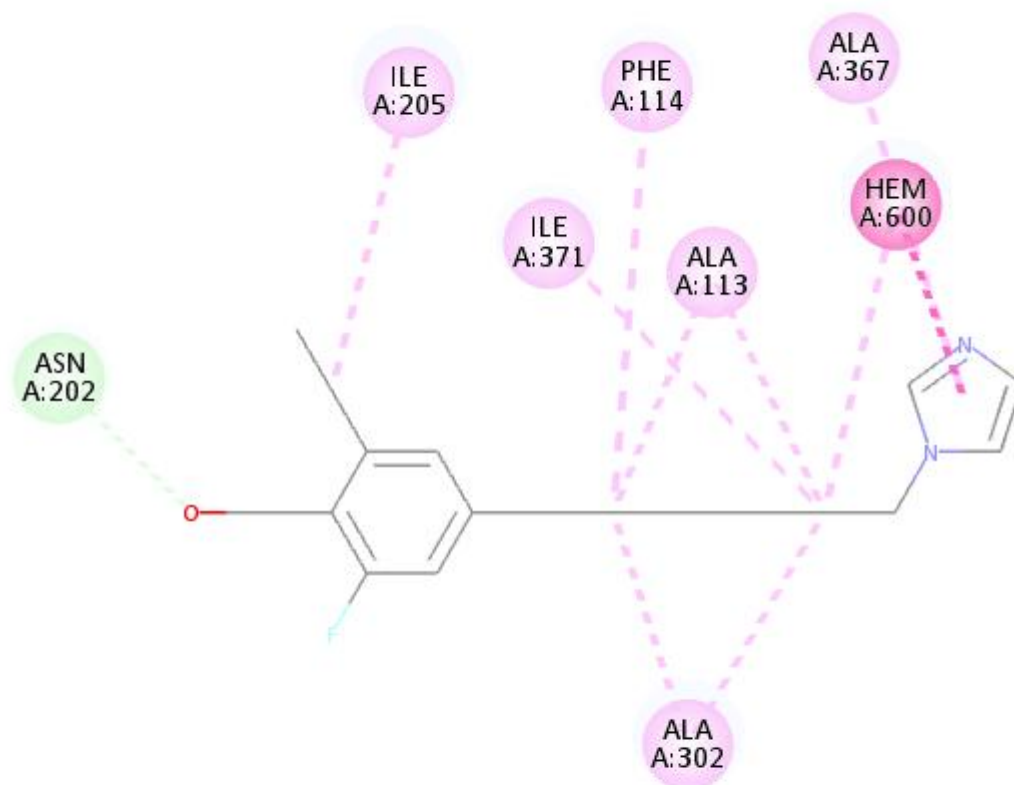


Interactions

- Pi-Sigma
- Amide-Pi Stacked

- Alkyl
- Pi-Alkyl

Supplementary Figure 4. 2D interactions of compound 153 within active pocket of 3ruk

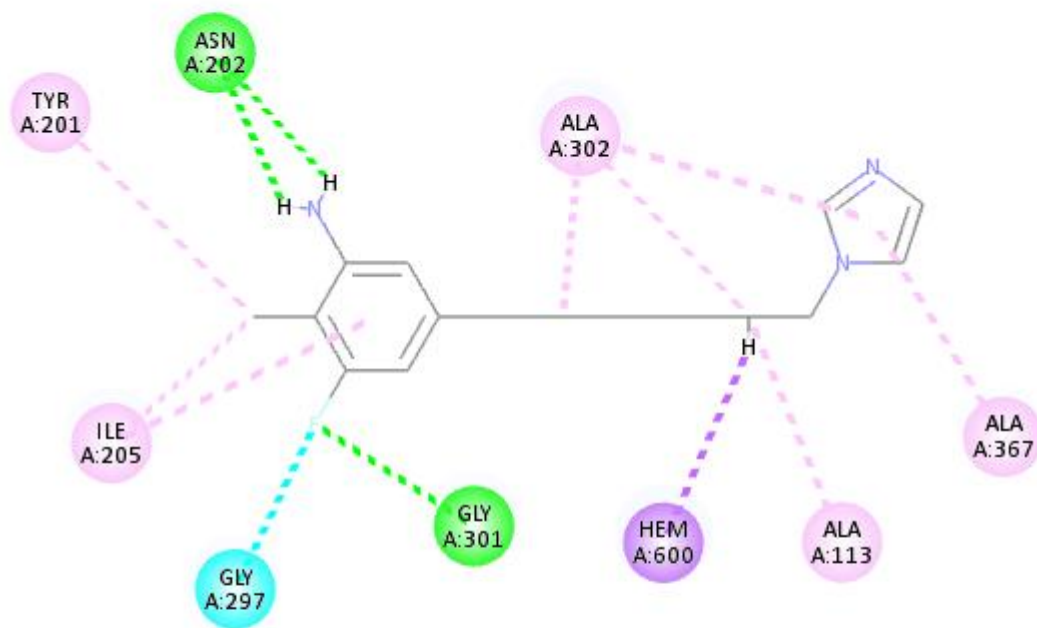


Interactions

Carbon Hydrogen Bond
 Pi-Pi Stacked

Alkyl
 Pi-Alkyl

Supplementary Figure 5. 2D interactions of compound 196 within active pocket of 3ruk

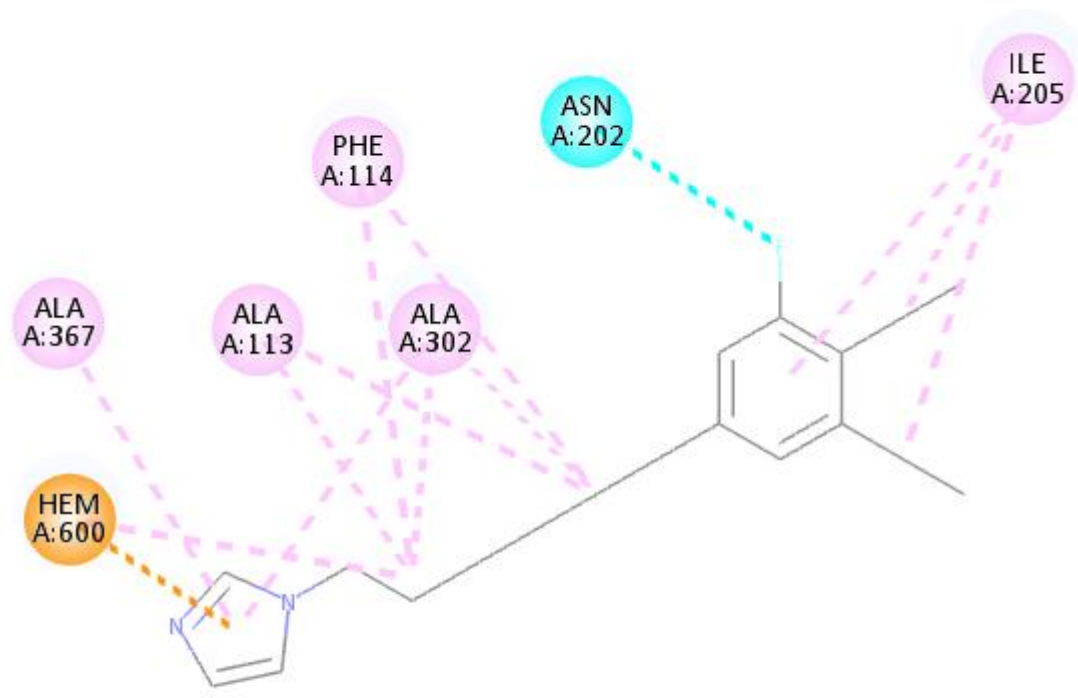


Interactions



- Conventional Hydrogen Bond
- Halogen (Fluorine)
- Pi-Sigma

- Alkyl
- Pi-Alkyl

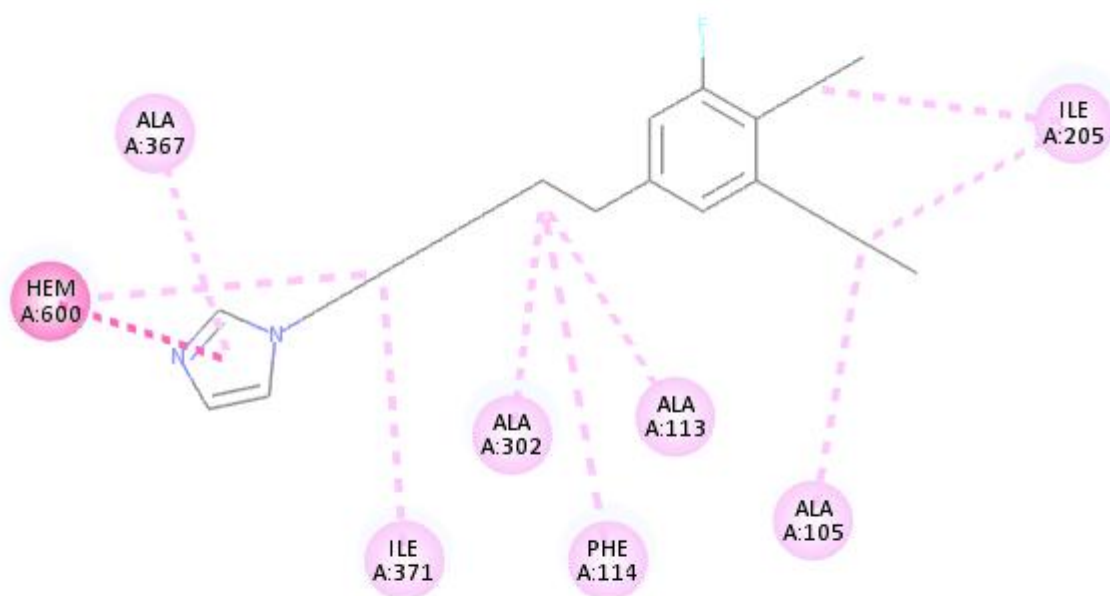
Supplementary Figure 6. 2D interactions of compound 212 within active pocket of 3ruk





Interactions

- | | | | |
|---|--------------------|---|----------|
|  | Halogen (Fluorine) |  | Alkyl |
|  | Pi-Cation |  | Pi-Alkyl |
|  | Pi-Pi Stacked | | |

Supplementary Figure 7. 2D interactions of compound 223 within active pocket of 3ruk

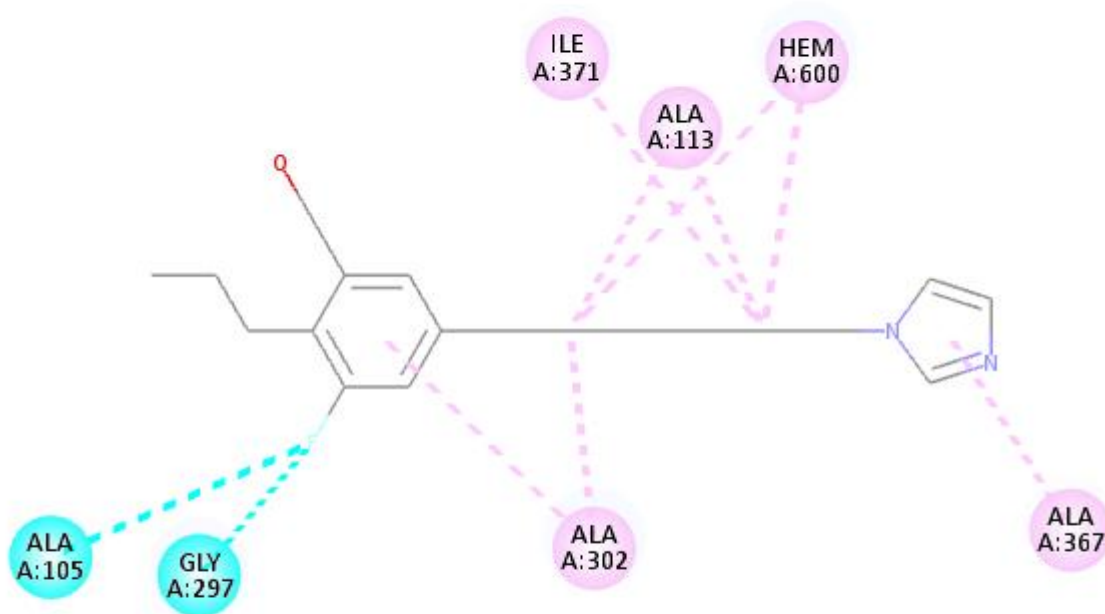


Interactions

 Pi-Pi Stacked
 Alkyl

 Pi-Alkyl

Supplementary Figure 8. 2D interactions of compound 224 within active pocket of 3ruk

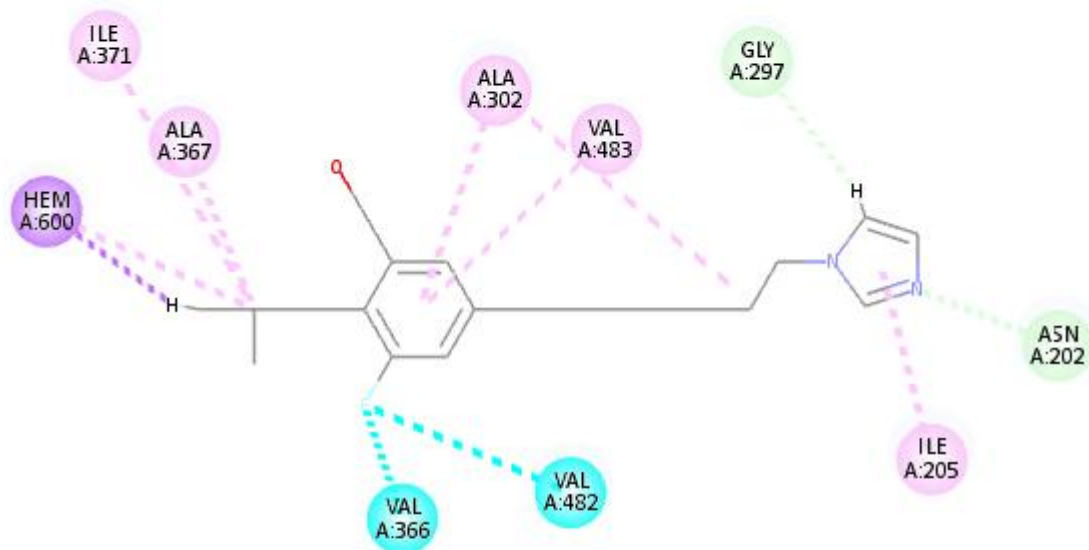


Interactions

 Halogen (Fluorine)
 Alkyl

 Pi-Alkyl

Supplementary Figure 9. 2D interactions of compound 229 within active pocket of 3ruk

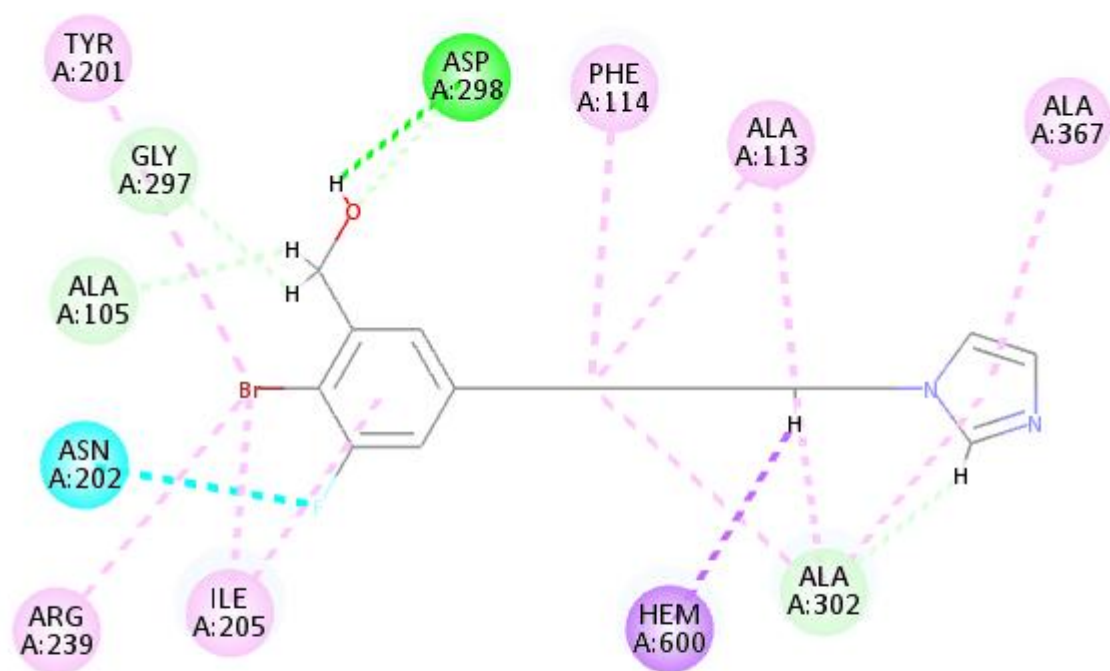


Interactions

- Carbon Hydrogen Bond
- Halogen (Fluorine)
- Pi-Sigma

- Alkyl
- Pi-Alkyl

Supplementary Figure 10. 2D interactions of compound 238 within active pocket of 3ruk

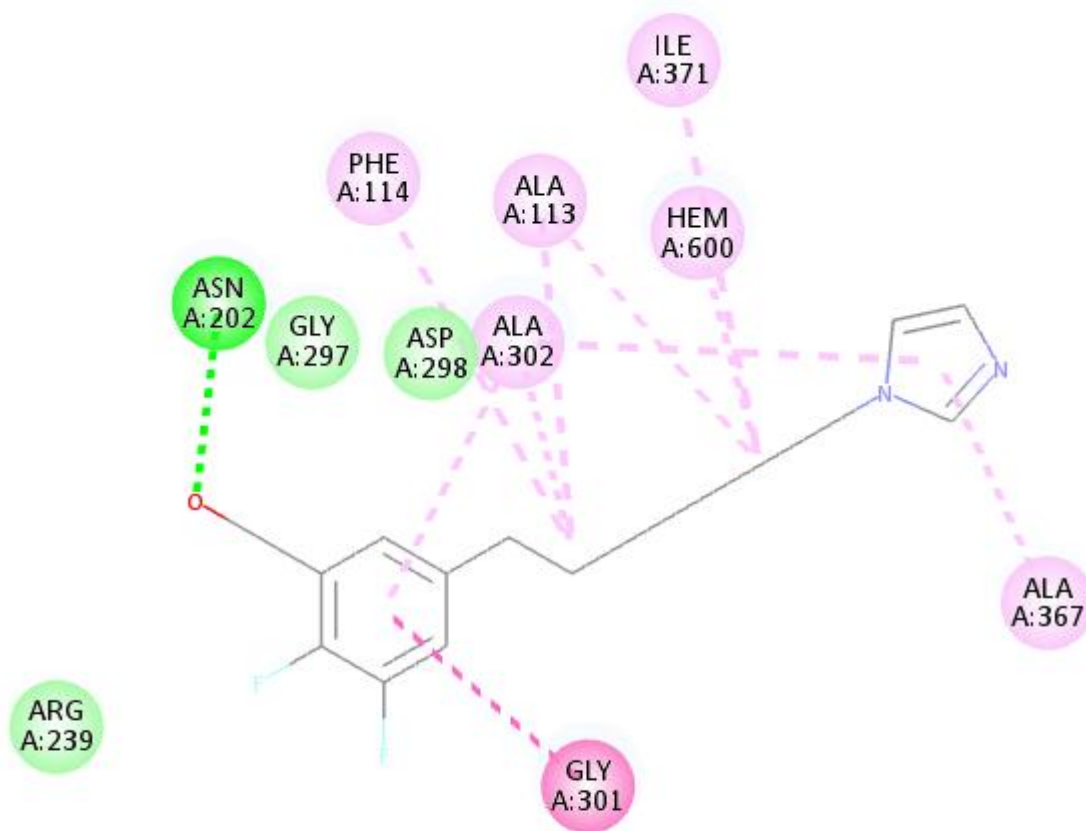


Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Halogen (Fluorine)

- Pi-Sigma
- Alkyl
- Pi-Alkyl

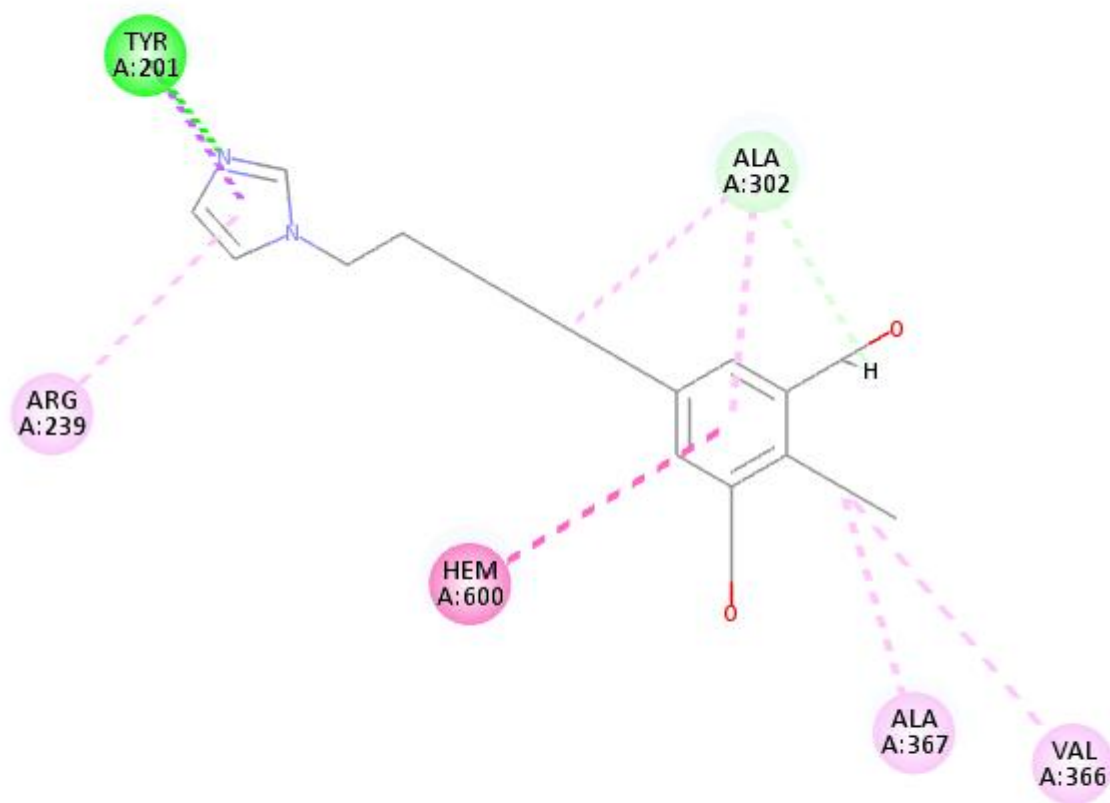
Supplementary Figure 11. 2D interactions of compound 255 within active pocket of 3ruk



Interactions

	van der Waals		Alkyl
	Conventional Hydrogen Bond		Pi-Alkyl
	Amide-Pi Stacked		

Supplementary Figure 12. 2D interactions of compound 264 within active pocket of 3ruk

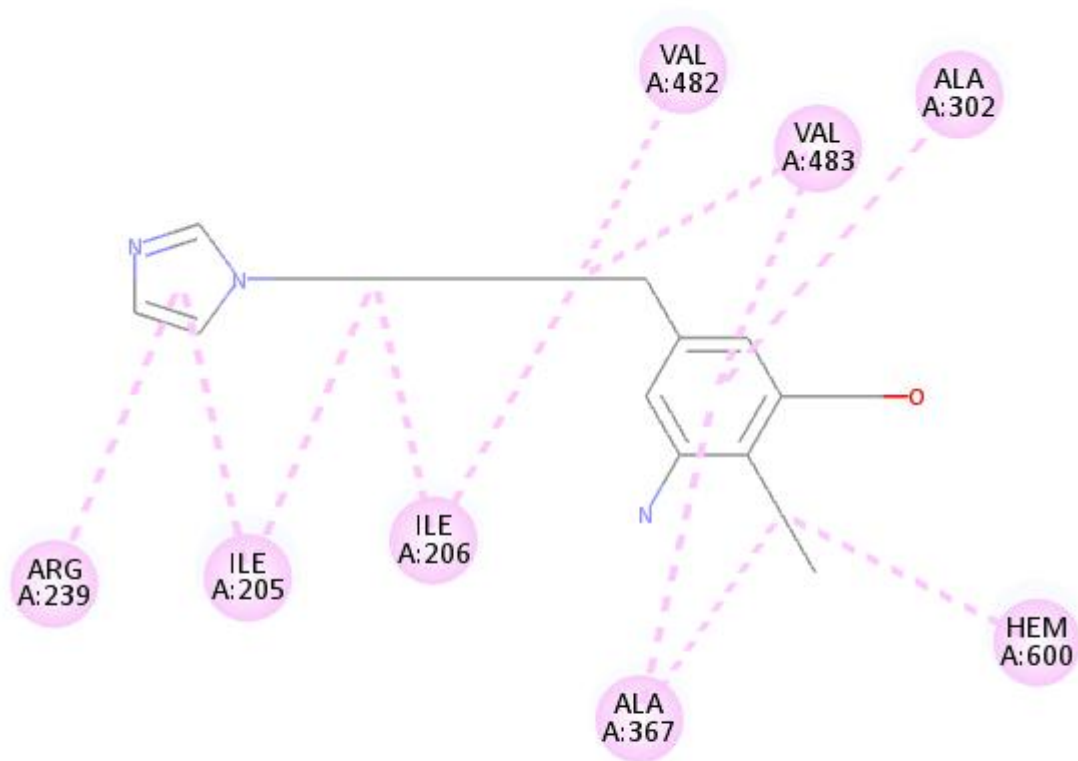


Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Sigma

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

Supplementary Figure 13. 2D interactions of compound 301 within active pocket of 3ruk

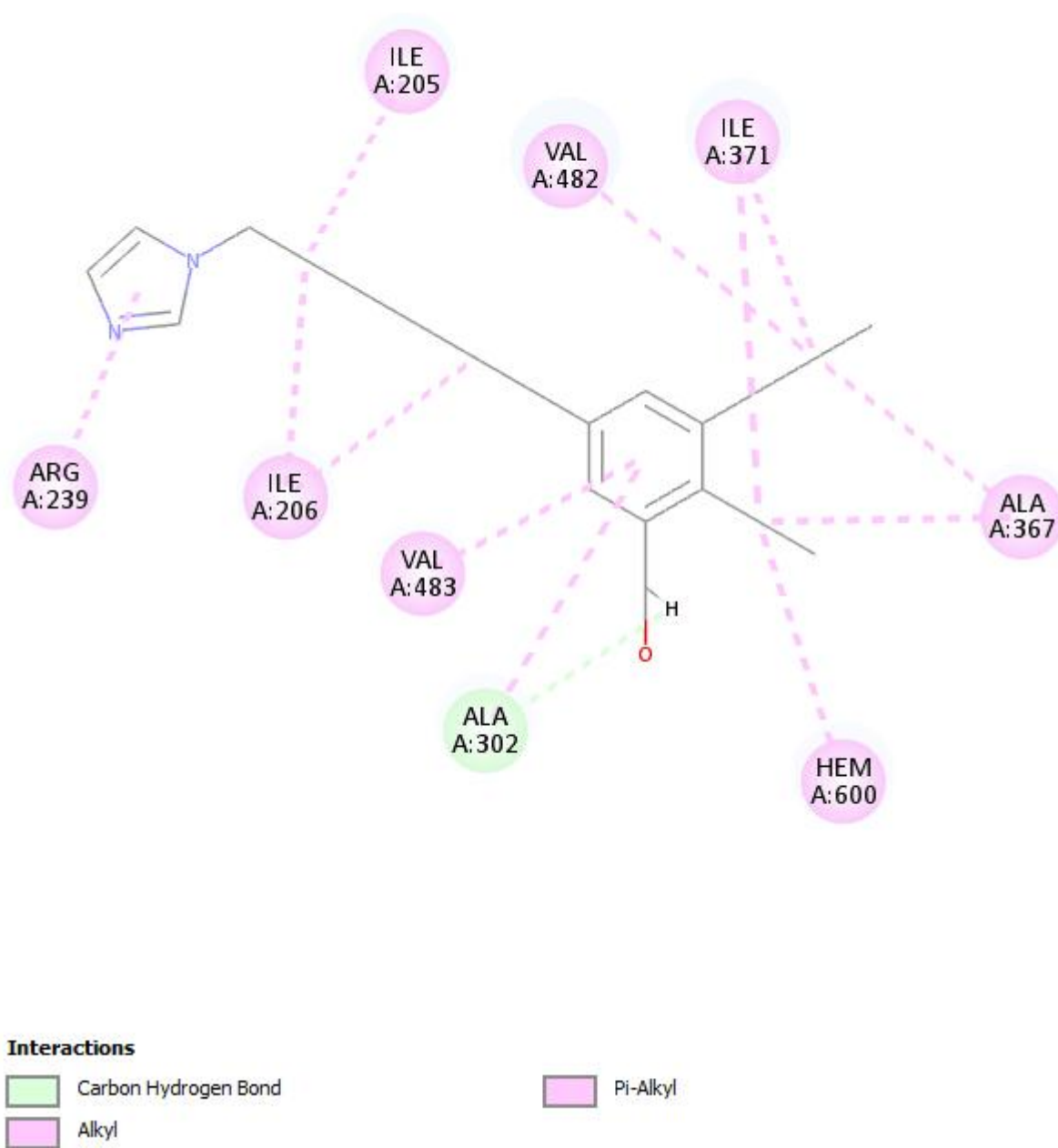


Interactions

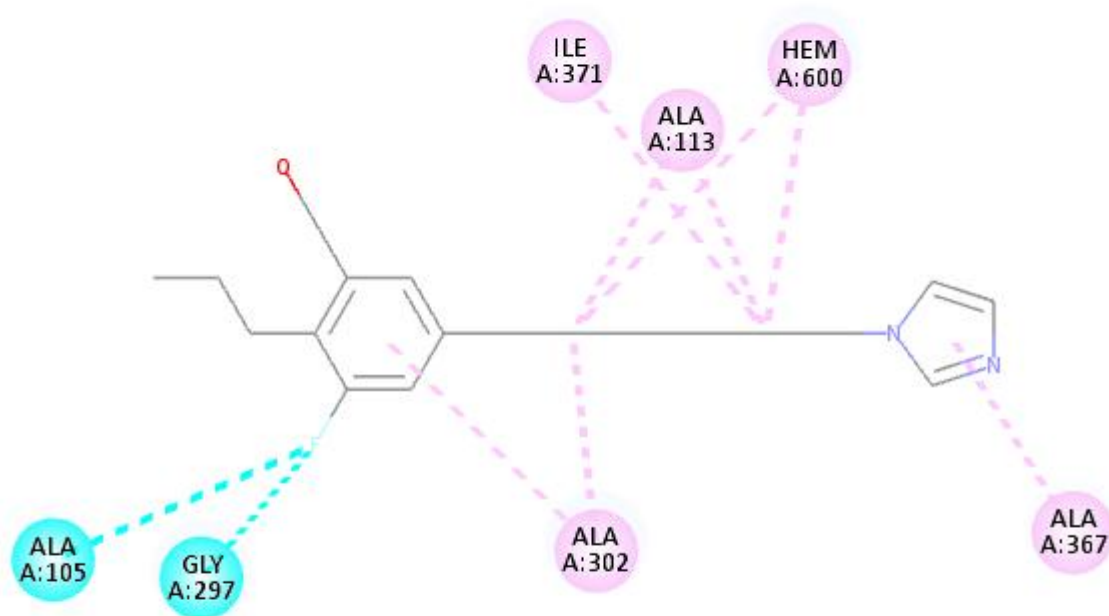
Alkyl

Pi-Alkyl

Supplementary Figure 14. 2D interactions of compound 302 within active pocket of 3ruk



Supplementary Figure 15. 2D interactions of compound 305 within active pocket of 3ruk

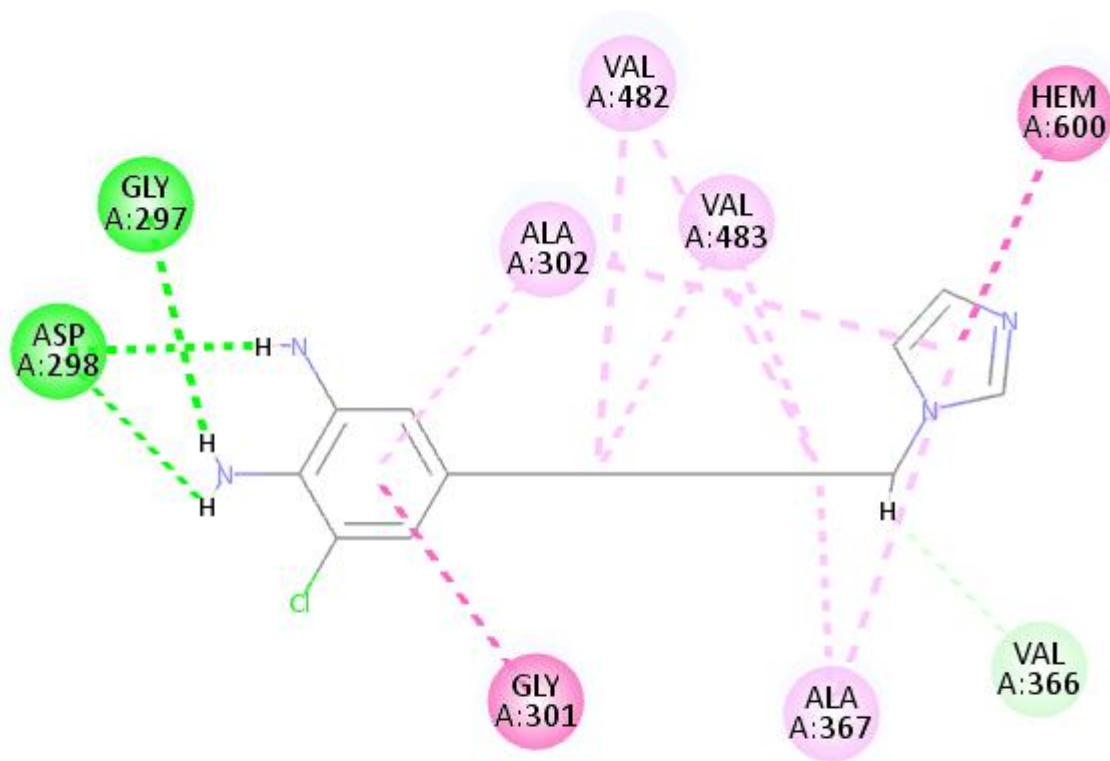


Interactions

 Halogen (Fluorine)
 Alkyl

 Pi-Alkyl

Supplementary Figure 16. 2D interactions of compound 309 within active pocket of 3ruk

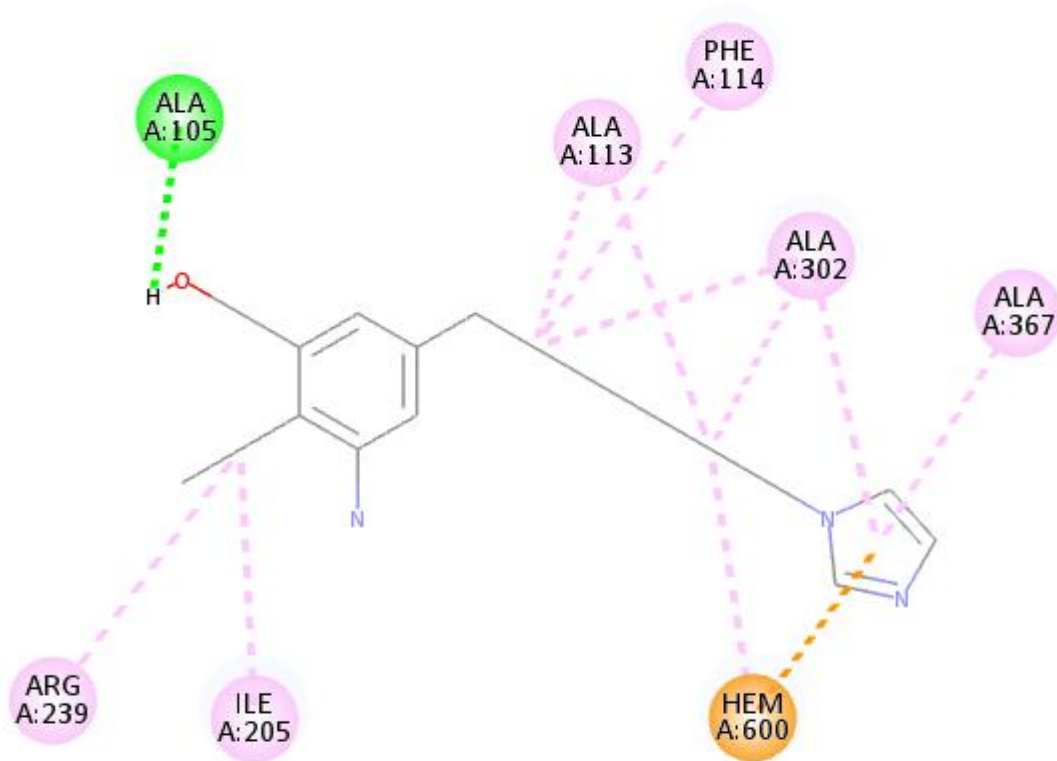


Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Pi T-shaped

- Amide-Pi Stacked
- Alkyl
- Pi-Alkyl

Supplementary Figure 17. 2D interactions of compound 361 within active pocket of 3ruk

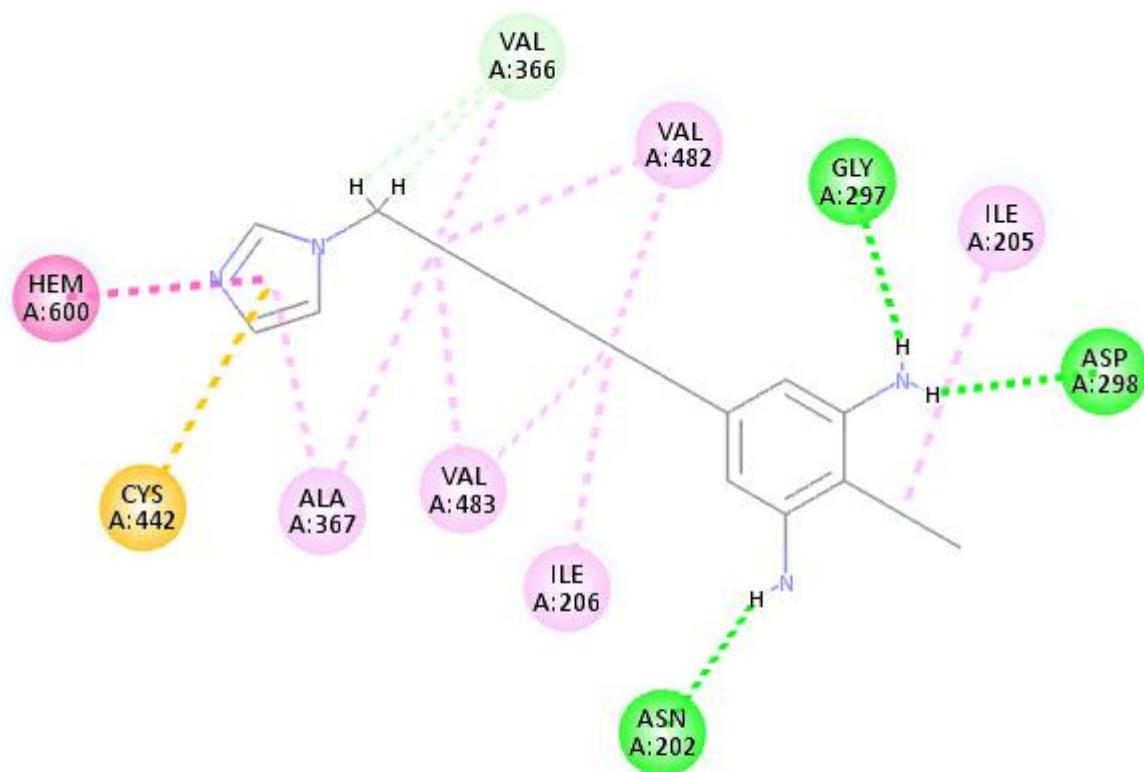


Interactions

- Conventional Hydrogen Bond
- Pi-Cation
- Pi-Pi Stacked

- Alkyl
- Pi-Alkyl

Supplementary Figure 18. 2D interactions of compound 382 within active pocket of 3ruk

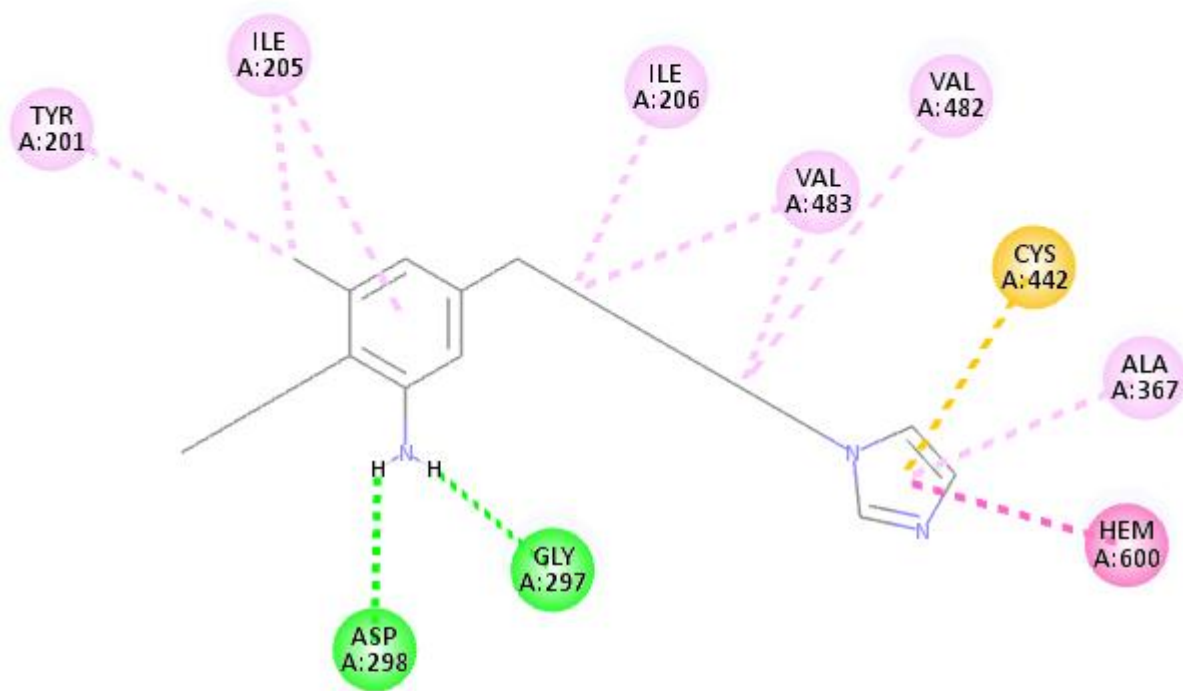


Interactions


- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Sulfur

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


Supplementary Figure 19. 2D interactions of compound 383 within active pocket of 3ruk



Interactions

 Conventional Hydrogen Bond

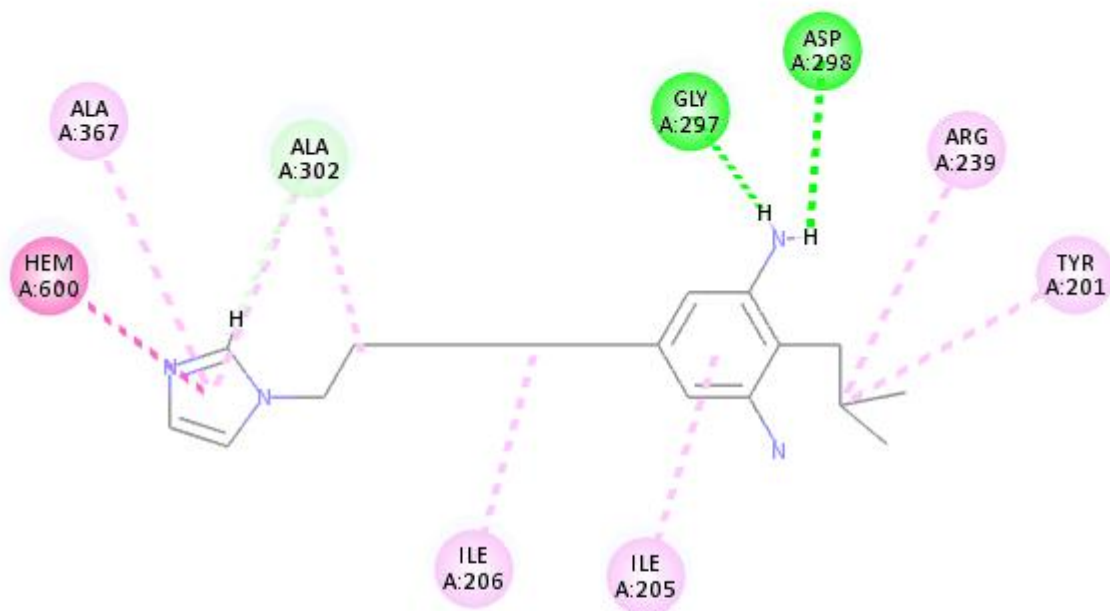
 Pi-Sulfur

 Pi-Pi T-shaped

 Alkyl

 Pi-Alkyl

Supplementary Figure 20. 2D interactions of compound 393 within active pocket of 3ruk

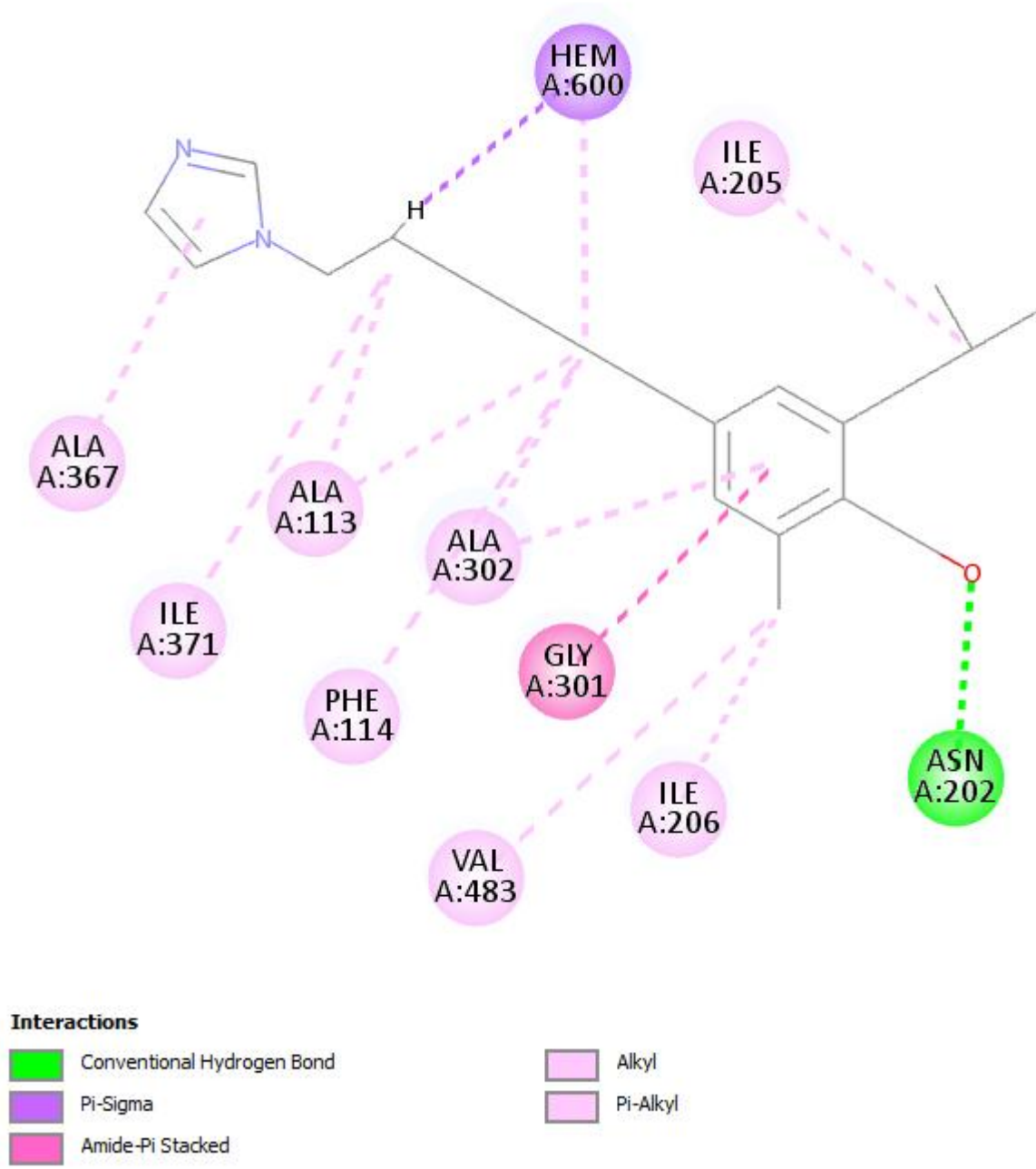


Interactions

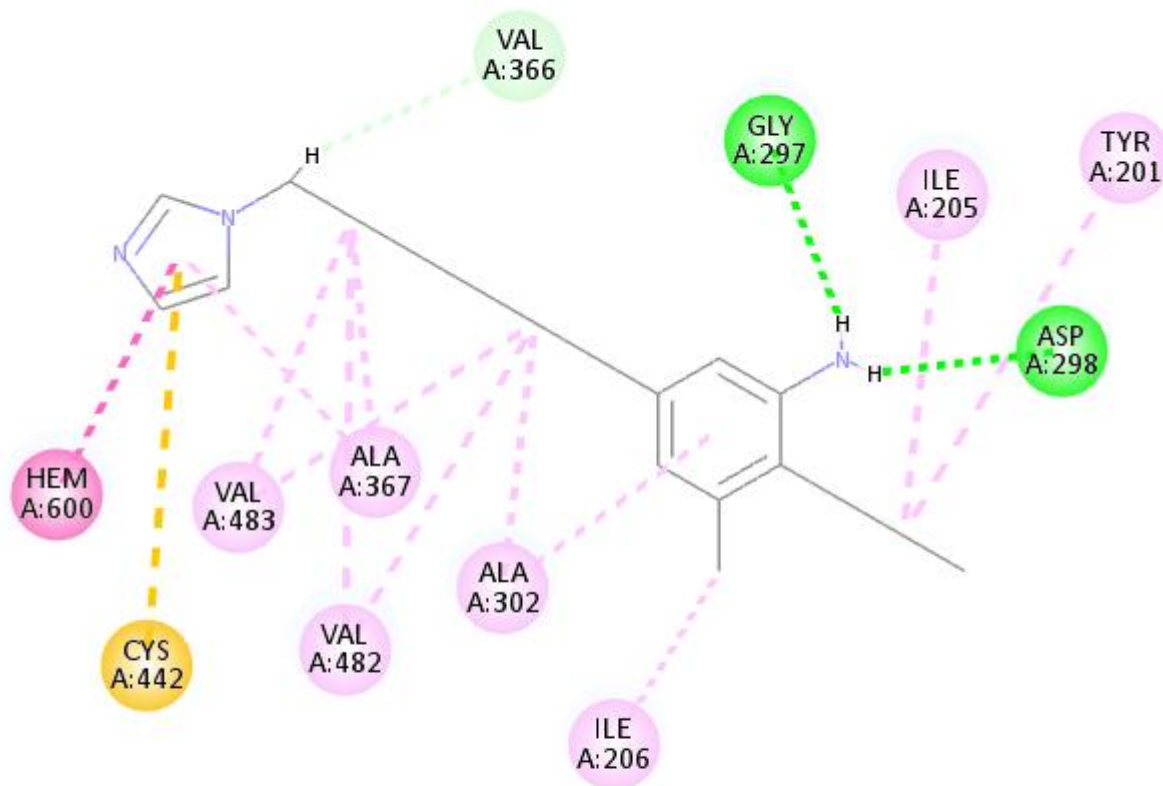
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Pi T-shaped

- Alkyl
- Pi-Alkyl

Supplementary Figure 21. 2D interactions of compound 401 within active pocket of 3ruk



Supplementary Figure 22. 2D interactions of compound 441 within active pocket of 3ruk

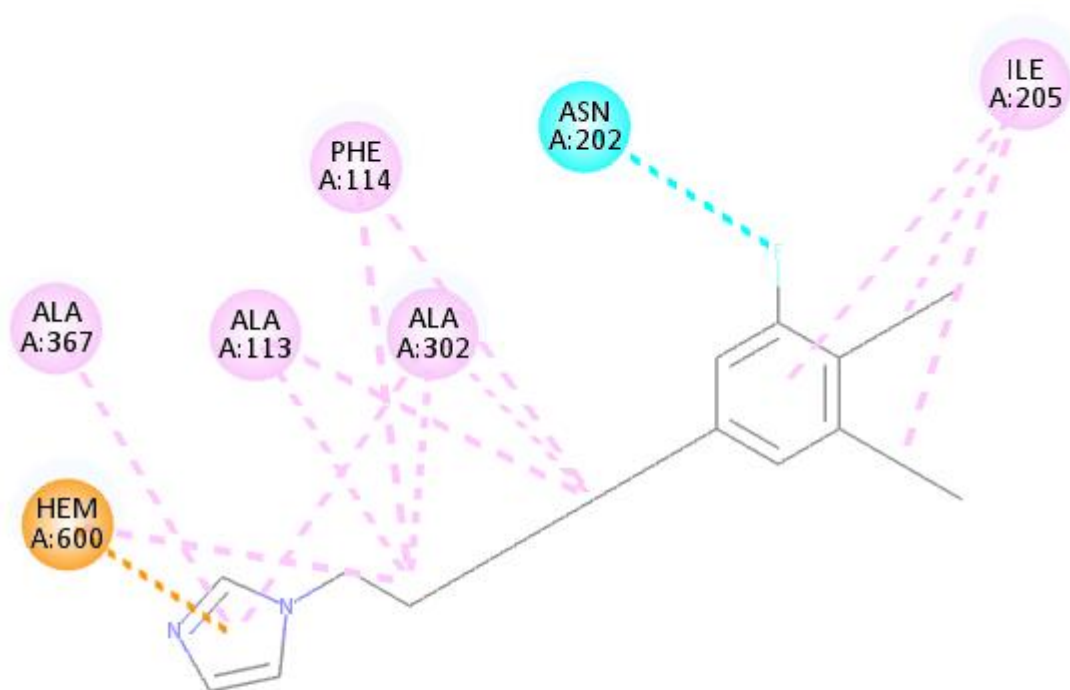


Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Sulfur


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


Supplementary Figure 23. 2D interactions of compound 473 within active pocket of 3ruk



Interactions

 Halogen (Fluorine)

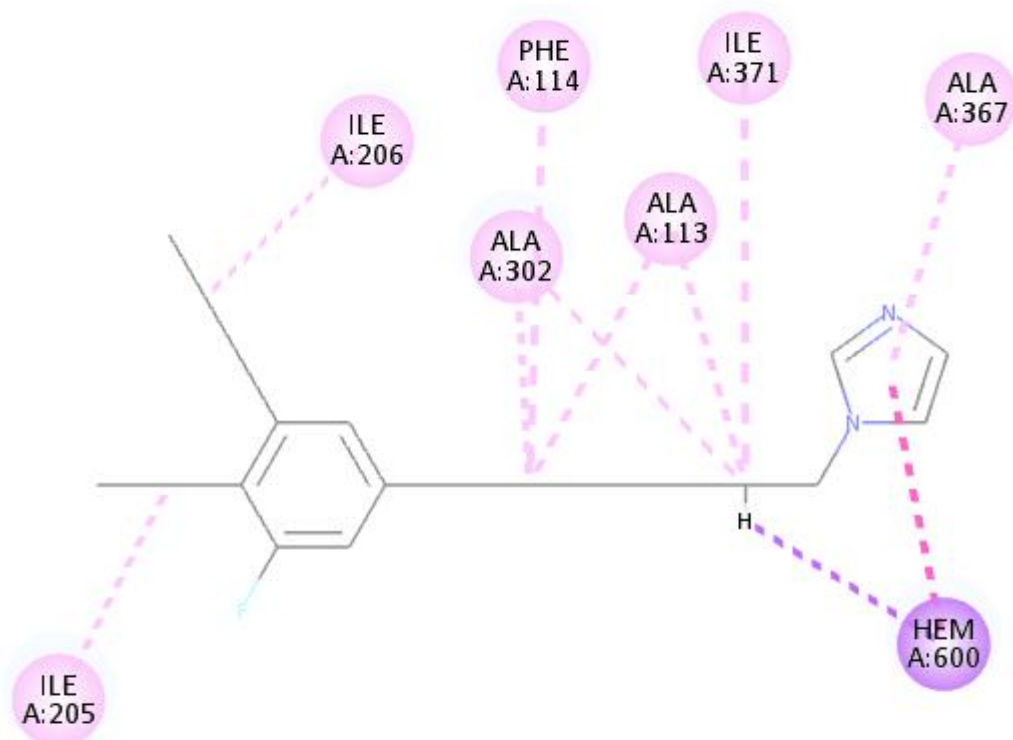
 Pi-Cation

 Pi-Pi Stacked

 Alkyl

 Pi-Alkyl

Supplementary Figure 24. 2D interactions of compound 543 within active pocket of 3ruk

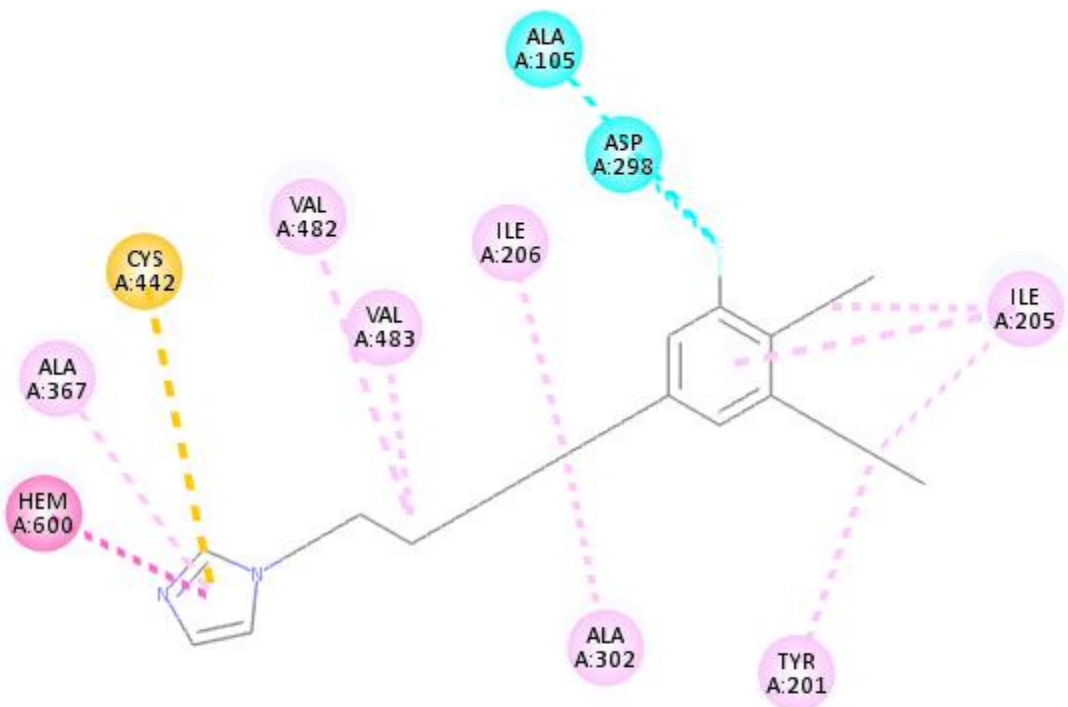


Interactions

- Pi-Sigma
- Pi-Pi Stacked

- Alkyl
- Pi-Alkyl


Supplementary Figure 25. 2D interactions of compound 624 within active pocket of 3ruk



Interactions

 Halogen (Fluorine)

 Pi-Sulfur

 Pi-Pi T-shaped

 Alkyl

 Pi-Alkyl

Supplementary Figure 26. 2D interactions of compound 953 within active pocket of 3ruk