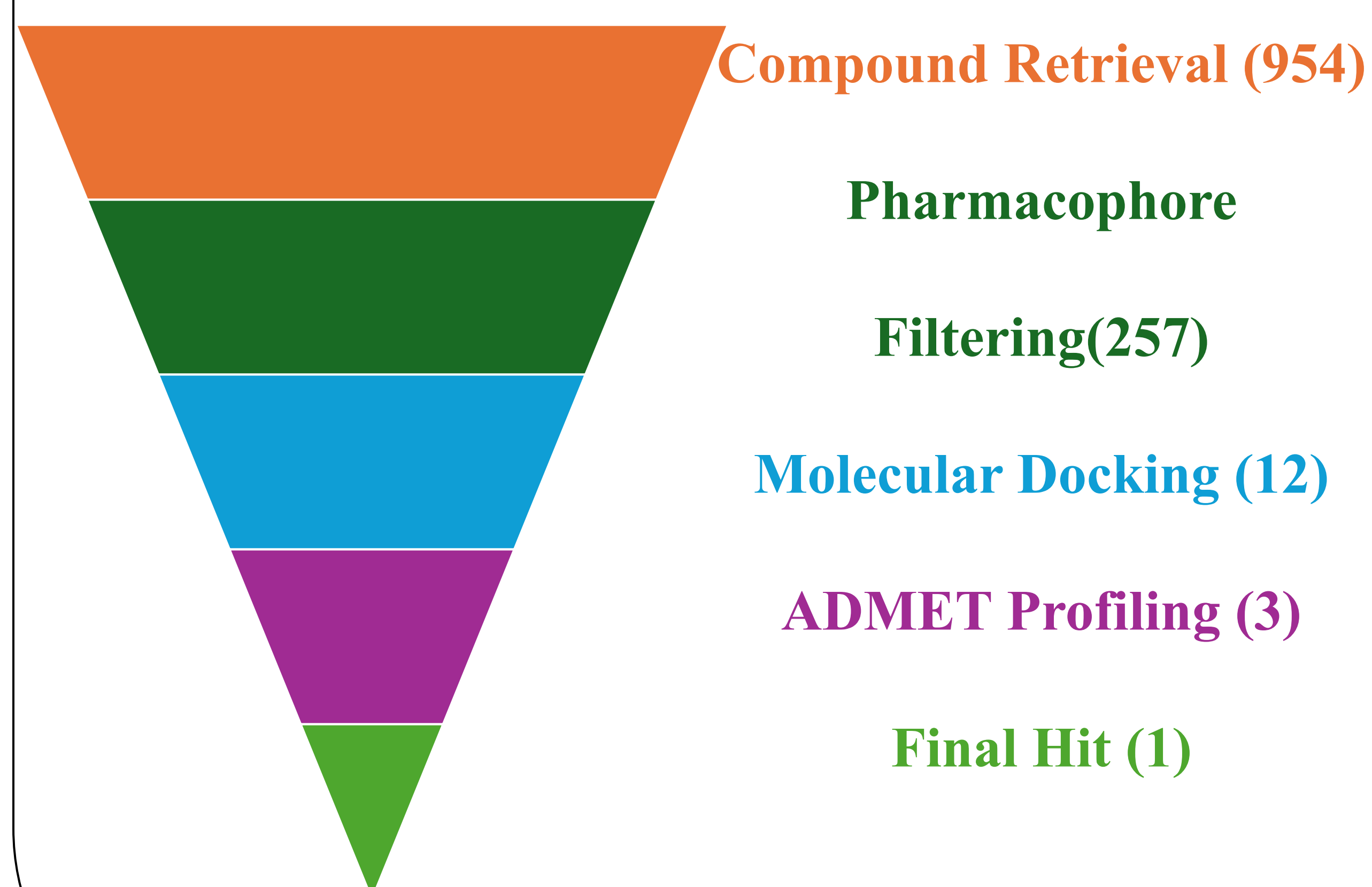


1. INTRODUCTION

- Anxiety disorder affects **284 million people globally**.
- Current treatments fail 30-40% of patients or cause significant side effects.
- The serotonin 5HT1A receptor (PDB ID:7E2Z) where partial agonism may provide anxiolytic effects with fewer side effects than full agonist or benzodiazepines.

2. METHODOLOGY



3. RESULTS

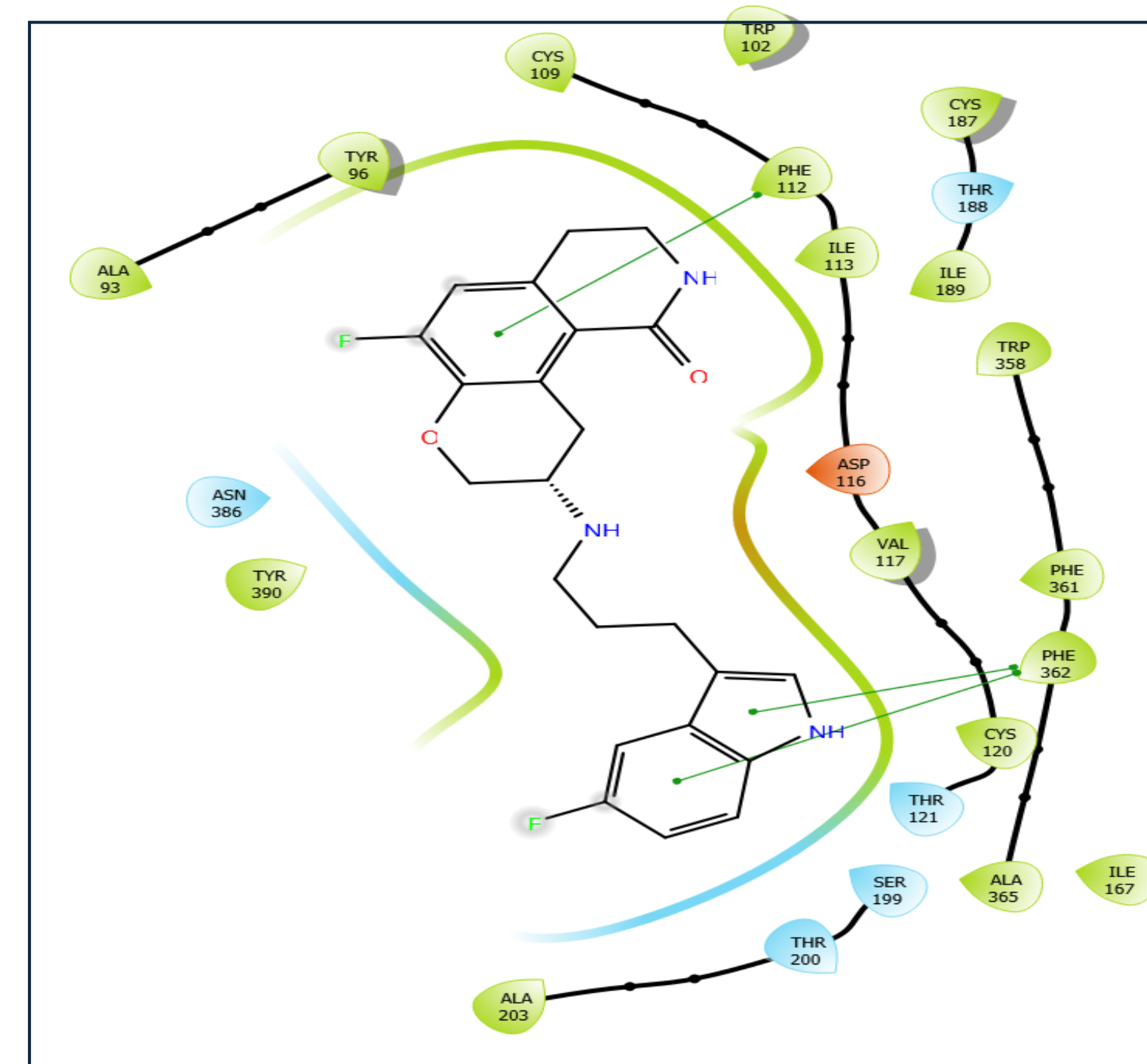


Figure 1: 2D interaction diagram of compound B3

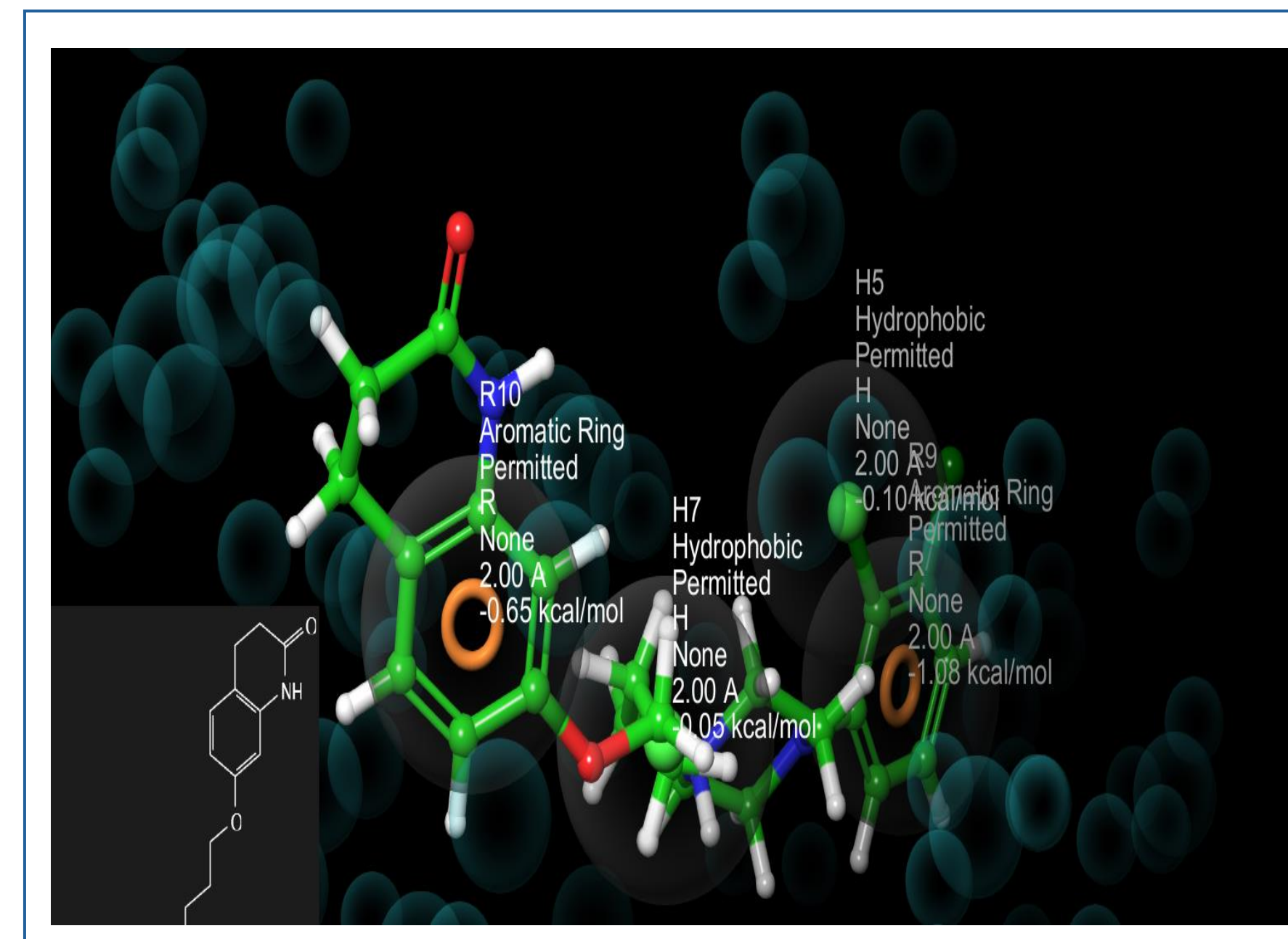


Figure 2: Pharmacophore hypothesis of serotonin receptor 5HT1A

Table 1: ADMET profiles of the top three(3) hits

S/N	Name	A1	A2	B3	Optimal Range
1	Log S	-4.252	-4.458	-3.912	-4 to 0.5 log mol/L
2	LogD	3.142	3.903	2.847	1 to 3 log mol/L
3	Log P	3.361	5.044	2.832	0 to 3 log mol/L
4	F(30%)	0.095	0.408	0.062	0–0.3
5	Caco-2	-5.092	-4.936	-5.129	>-5.15 log cm/s
6	MDCK	2.78E-5	2.03E-5	2.59E-5	2.0E-6 Log cm/s
7	HERG	0.843	0.931	0.782	0–0.3
8	AMES	0.667	0.537	0.704	0–0.3
9	QED	0.562	0.394	0.565	>0.67
10	SYNTH	3	2	3	≤ 6

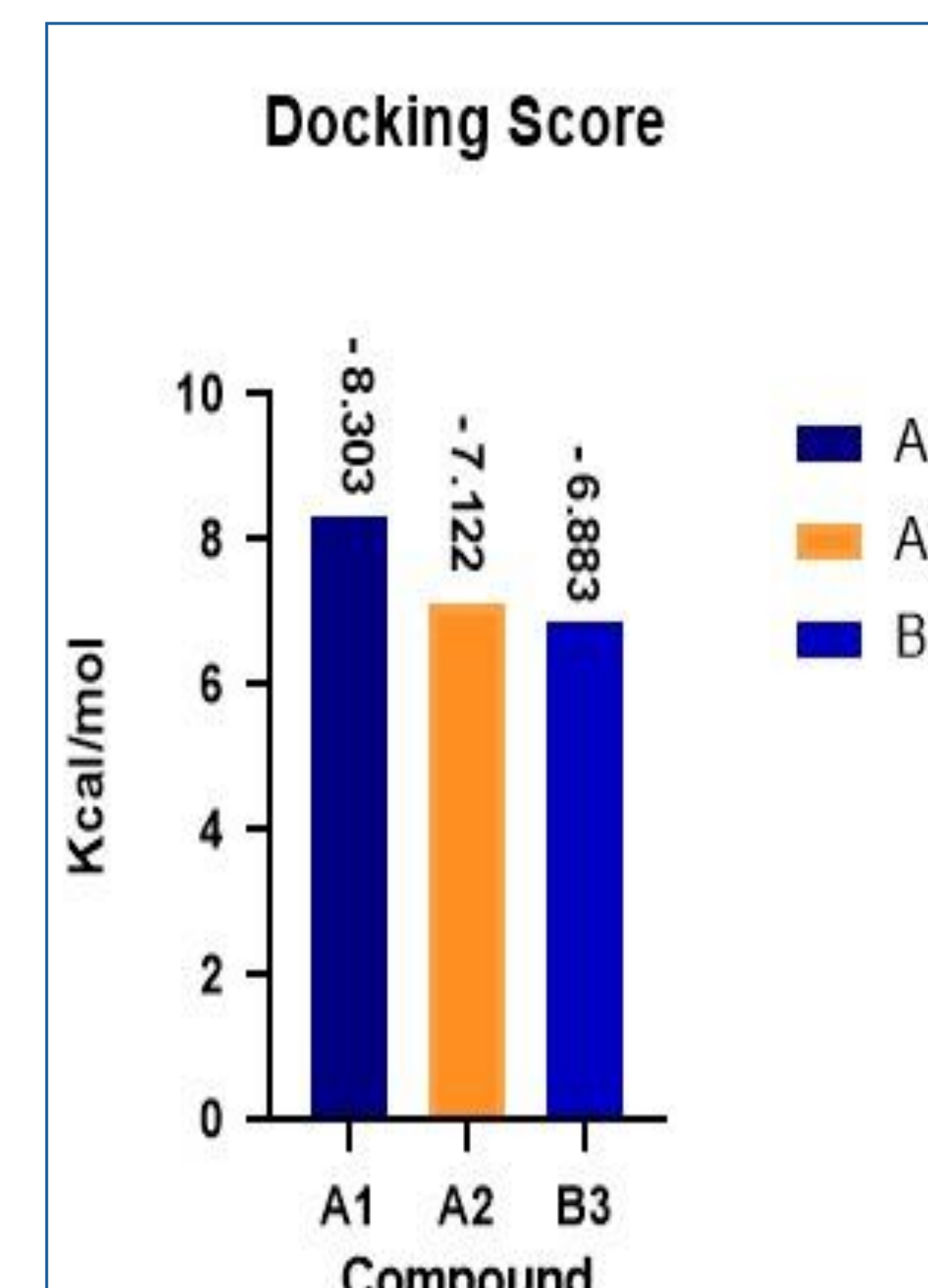


Figure 3: Docking scores of the top three (3) hits

4. CONCLUSION

This study shows that combining pharmacophore modeling, docking, and ADMET screening is an effective way to identify promising drug candidates. While no compound met every criterion perfectly, Compound **B3** stood out as the best overall choice balancing binding affinity and drug-likeness over Compound **A1**.

5. RECOMMENDATIONS

Future work will include through ligand efficiency guided scaffold hopping and multi parameter optimization of hit compound (**B3**) to improve its physicochemical and ADMET properties while also preserving binding potential to the 5HT1A receptor

6. REFERENCES

- Alshehri, A., Alshehri, B., Alghadir, O., Basamh, A., Alzeer, M., Alshehri, M., & Nasr, S. (2023). The prevalence of depressive and anxiety symptoms among first-year and fifth-year medical students during the COVID-19 pandemic: a cross-sectional study. *BMC medical education*, 23(1), 411. <https://doi.org/10.1186/s12909-023-04387-x>.
- Saliu, J. A. (2024). Machine Learning-Based Approach to Identify Inhibitors of Sterol-14-Alpha Demethylase: A Study on Chagas Disease. *Bioinformatics and Biology Insights*, 18. <https://doi.org/10.1177/11779322241262635>.