Screening FDA-approved drugs against three *Leishmania* targets

A student research project in computational drug repurposing

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The question

I am a high school student who wants to be a doctor. I used molecular docking to look for repurposing candidates for visceral leishmaniasis among ~1,800 FDA-approved drugs, focusing on a disease that gets little research attention.

Method

- Docking with **AutoDock Vina-GPU-2.1**; binding pockets found with **fpocket**; drug library from **DrugCentral**.
- Three receptors: PTR1 (PDB 1E92), trypanothione reductase (TR, PDB 2YAU) and CYP51 (PDB 3L4D).
- Pocket selection cross-checked against literature-reported binding-site residues where available.
- Every top-10 hit per target got a rendered pose check against the known pocket, not just a raw score.

Top predicted hit per target

Target	Top hit	Predicted affinity	What the site records about it
CYP51	Digitoxin	−13.0 kcal/mol	Its aglycone digitoxigenin has a confirmed IC50 = 6.9 µg/mL against *L. infantum* itself (selectivity index 42.8). Specificity gap 2.47.
PTR1	Alectinib	−12.1 kcal/mol	No direct *Leishmania* precedent found. Specificity gap 1.47.
TR	Ergotamine	−10.5 kcal/mol	Strong on all three targets, clearest on TR; classed “mixed, leaning sticky” (gap 0.97).

A check on the method

The same drugs kept appearing near the top of more than one target’s results. To tell a real fit from a scoring function that likes a molecule everywhere, I z-scored each drug’s affinity per target and computed a **specificity gap** across the three unrelated pockets.

Of 25 drugs examined, 8 were confirmed generically “sticky” and 4 were genuinely pocket-specific. That analysis also made me walk back my own earlier claim about ergotamine, and the correction is on the site.

What this does and does not show

These are **computational hypotheses**. A docking score is evidence that an interaction is physically plausible; it is not evidence that a drug works or is safe, and nothing here is medical advice.

I have no wet lab, cell culture or assay access, so the natural next step is an enzyme-inhibition or parasite growth-inhibition assay run by someone who does.

HOW AI WAS USED

I build this project with Claude Code, and say so on every page. It helped with the docking scaffolding, the statistics pipeline and the write-ups. Choosing the targets, designing the specificity-gap method and every interpretation are mine. If I can run 3 miles on my own, a bike lets me ride 30, and the bike is worth writing about.

Full write-ups, charts and pose renders: biomedbound.com → Molecular Docking

Data, receptor prep files and docking configs available on request