
AIMS
African Institute for Mathematical Sciences
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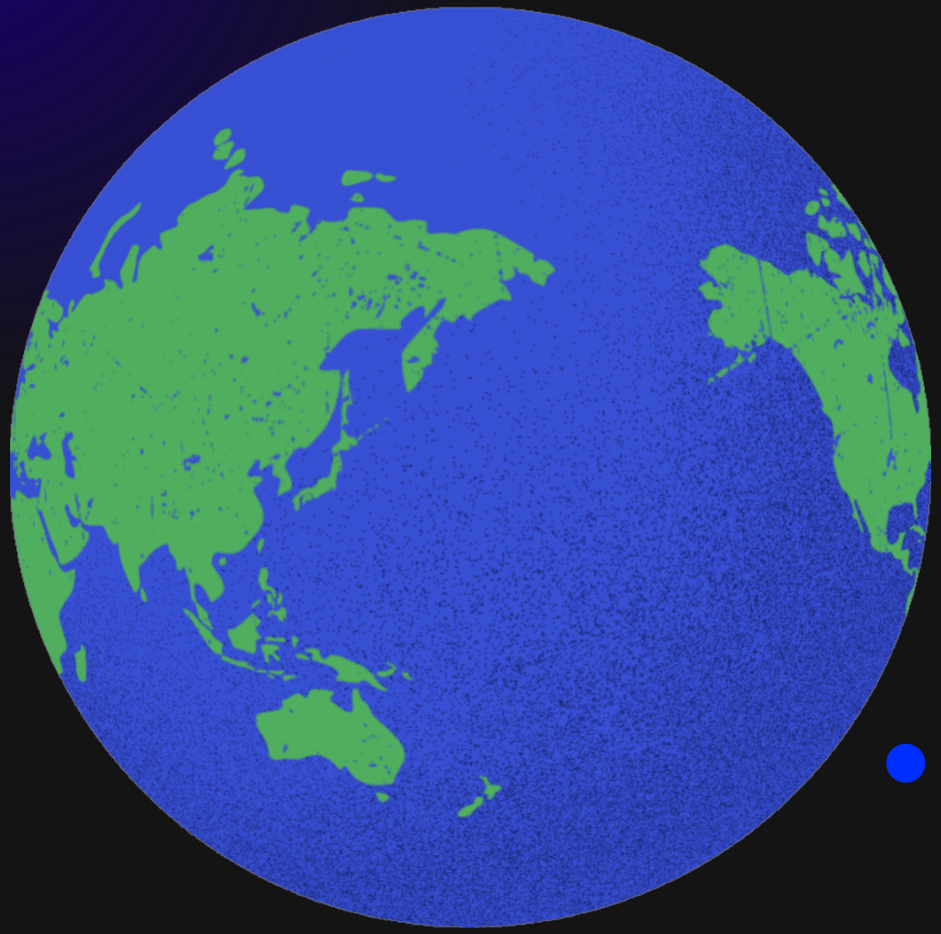
EDUCATION GLOBAL EVENT



263M+

cases

(Source: WMR 2024)

95% DEATHS

in Africa

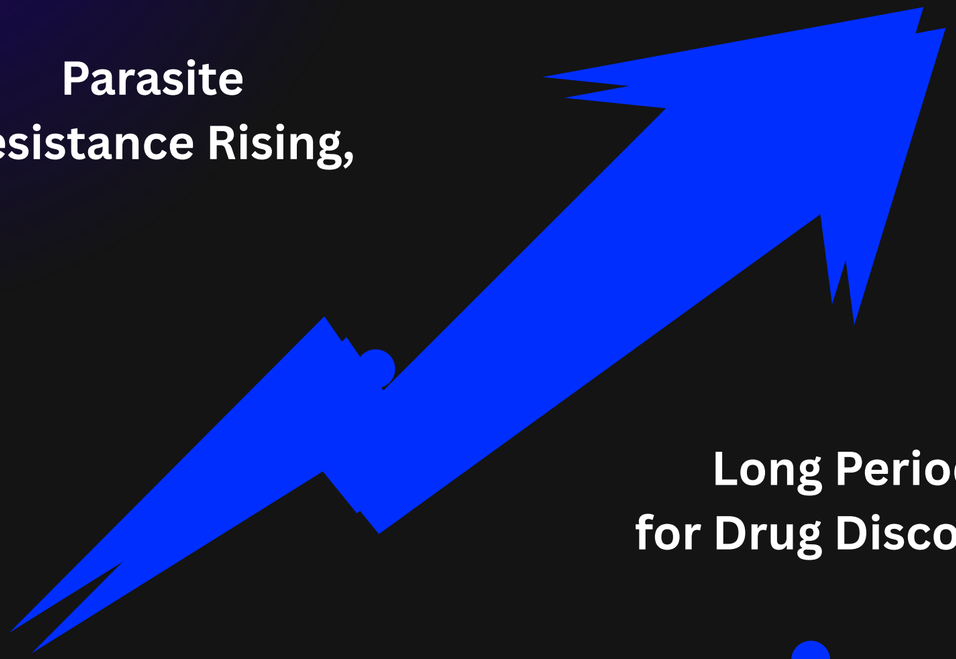
(Source: WMR 2024)

4 BILLION USD

(Source: WMR 2024)

Malaria Is Not Going Away

Parasite
Resistance Rising,



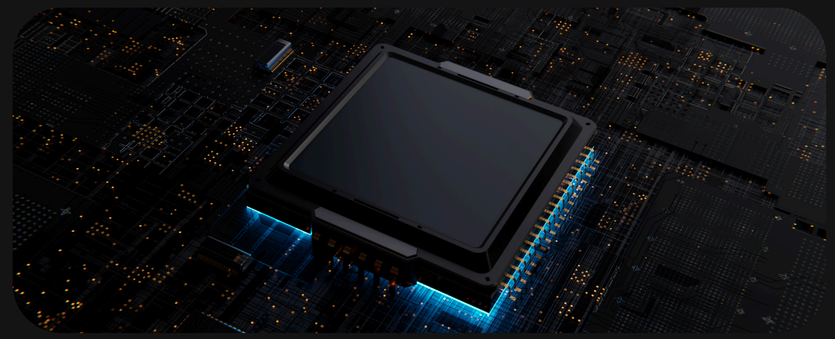
Long Period
for Drug Discovery

Treatments Failing.

(Source: WMR 2024)

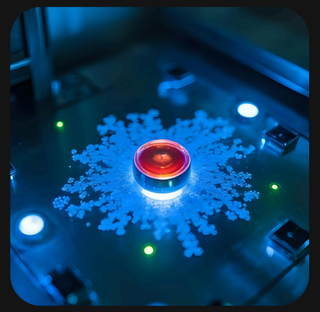
QUALARIA

QUANTUM LEAP AGAINST MALARIA



Reducing deaths by accelerating the identification of potential ligands for the dominant strain of malaria.

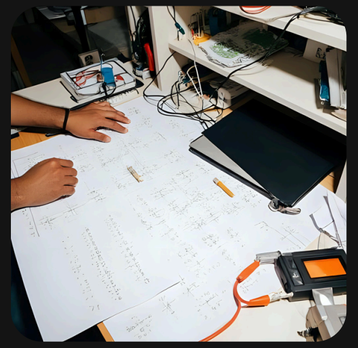
Quantum computers



Faster

Handles complex chemistry

More accurate



Can we accelerate the drug discovery process for malaria?

PROTEIN BINDS MOLECULE

USE CASE :

Plasmodium Falciparum

Over 98%

HOW???

Generate the PfEMP1 structure

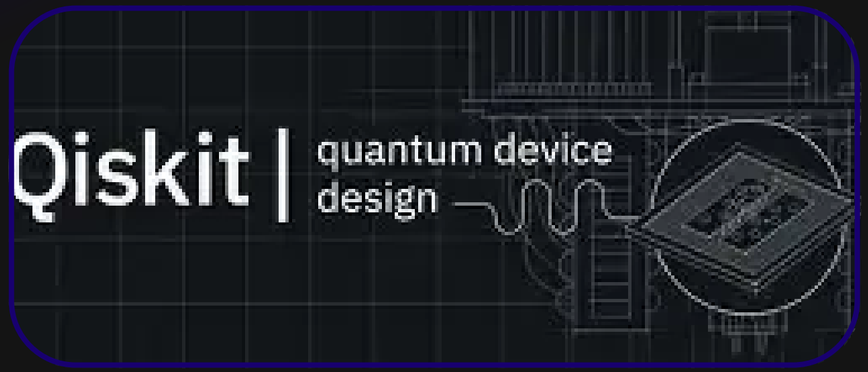
Target functional sites on the PfEMP1

Generate pocket–aware ligands (molecules)

Use VQE to select molecule with less binding energy

Possible Drugs

Powered by



qBraid

OUR SOLUTION

```
Selected top 5 ligands:
O=C(O)CCc1cccc(CO)c1 | QED: 0.73 | MW: 180.20
COc1ccc2c(O)cccc2c1 | QED: 0.72 | MW: 174.20
COC1CCc2c(O)cccc2C1 | QED: 0.71 | MW: 178.23
O=C(O)COc1ccccc1 | QED: 0.71 | MW: 152.15
O=C(O)c1cccc(C(=O)O)c1 | QED: 0.69 | MW: 166.13


Ligand: O=C(O)CCc1cccc(CO)c1 | QED: 0.73

=== GROUND STATE ENERGY ===

* Electronic ground state energy (Hartree): -0.871042191872
  - computed part:      -0.871042191872
  - ActiveSpaceTransformer extracted energy part: 0.0
~ Nuclear repulsion energy (Hartree): 739.098911444657
> Total ground state energy (Hartree): 738.227869252784

=== MEASURED OBSERVABLES ===

  0:  # Particles: 2.000 S: 0.000 S^2: 0.000 M: 0.000

=== DIPOLE MOMENTS ===

~ Nuclear dipole moment (a.u.): [41.43867035  -10.90560946  11.58005272]

  0:
  * Electronic dipole moment (a.u.): [-3.409651212445  3.774015032041  -0.329081922888]
    - computed part:      [-3.409651212445  3.774015032041  -0.329081922888]
    - ActiveSpaceTransformer extracted energy part: [0.0  0.0  0.0]
  > Dipole moment (a.u.): [44.848321562445  -14.679624492041  11.909134642888]  Total: 48.669197755236
                 (debye): [113.99305230048  -37.311880225944  30.269998093686]  Total: 123.704749962833

Running time: 0.255784273147583 seconds
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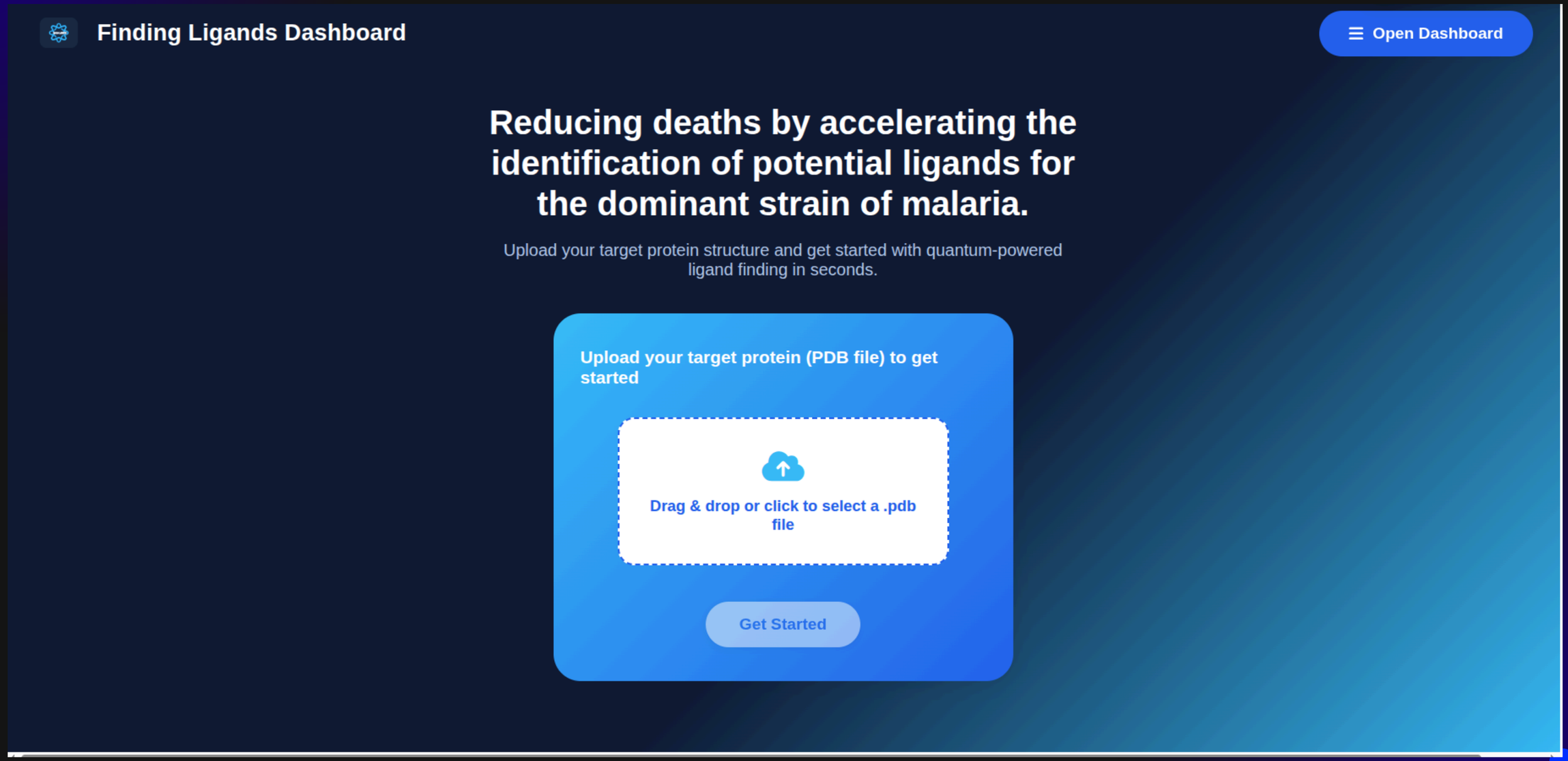
Finding Ligands Dashboard
Open Dashboard
Reducing deaths by accelerating the identification of potential ligands for the dominant strain of malaria.
Upload your target protein structure and get started with quantum-powered ligand finding in seconds.
Upload your target protein (PDB file) to get started
Drag & drop or click to select a .pdb file
Get Started

Qualaria

Filter

Search Molecule

- Molecule Ranking
- Uploads
- Process
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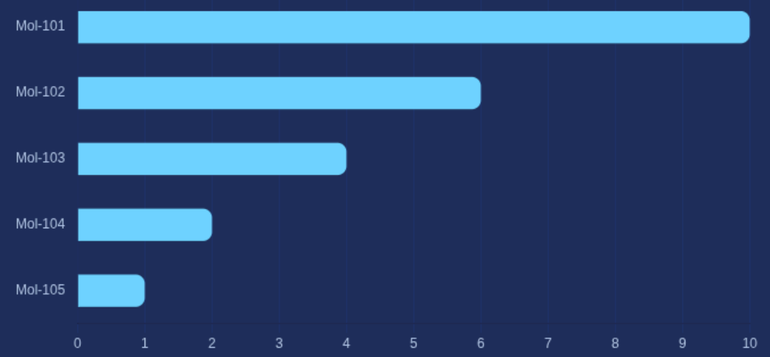
Molecule Rankings

Molecules	Target Protein	Binding Energy	Stability
Mol-101	PfEMP1	-7.2	High
Mol-102	PfEMP1	-6.8	Medium
Mol-103	PfEMP1	-6.5	Low
Mol-104	PfEMP1	-5.9	Medium
Mol-105	PfEMP1	-5.2	High

Binding Energy Distribution



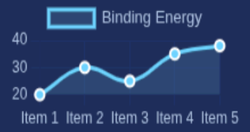
Molecule 101

Molecule Details

Algorithm	VQE
Optimizer	COBYLA
Computation	Quantum
Qubits	6

Details

Energy Decomposition

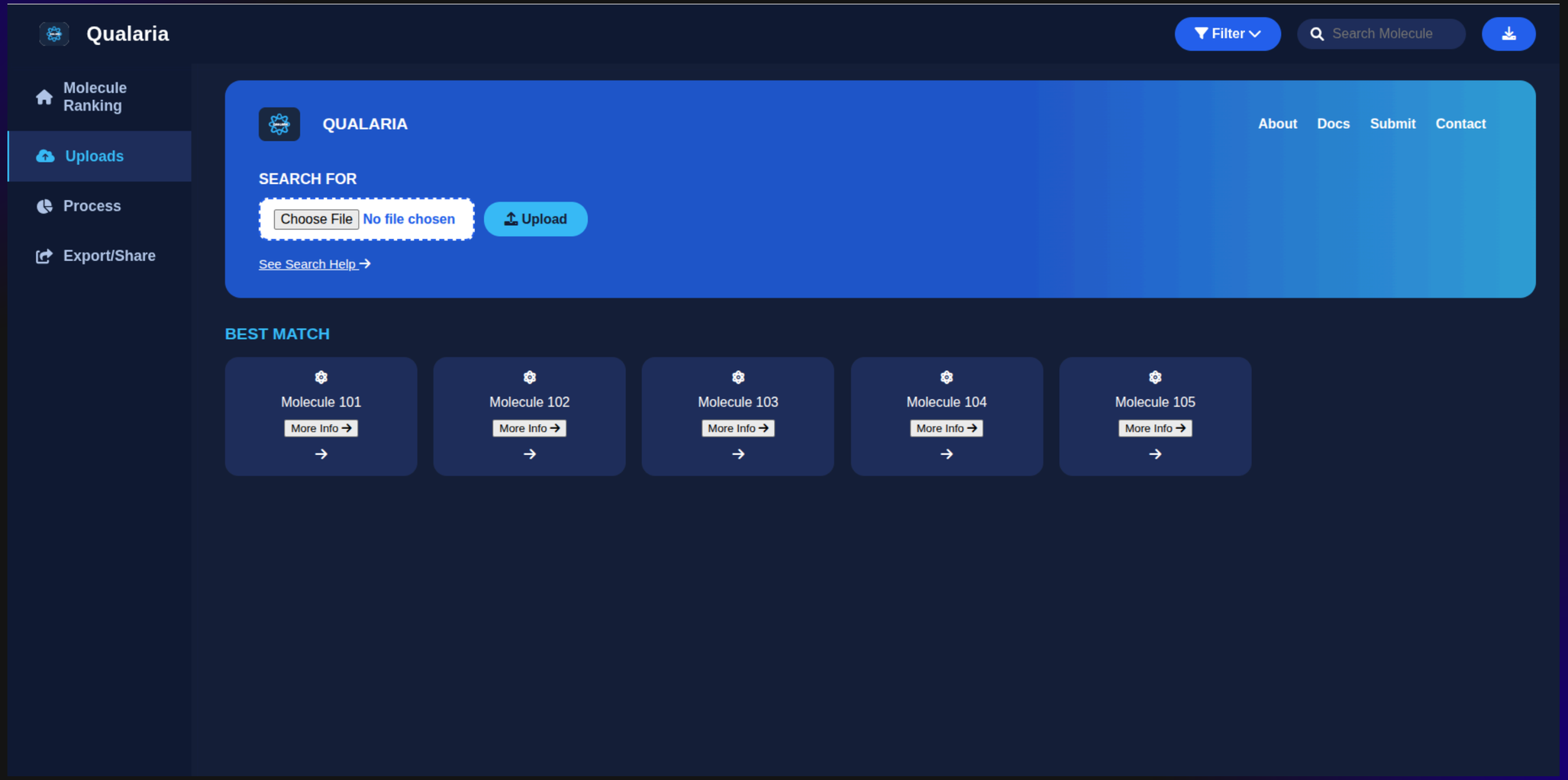


About the Simulation

Quantum Computing using advanced algorithms like VQE to enhance malaria ligand finding by precisely predicting binding energies of ligands to proteins.

More Info

Algorithm Ligand Protein Binding Energy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QUALARIA
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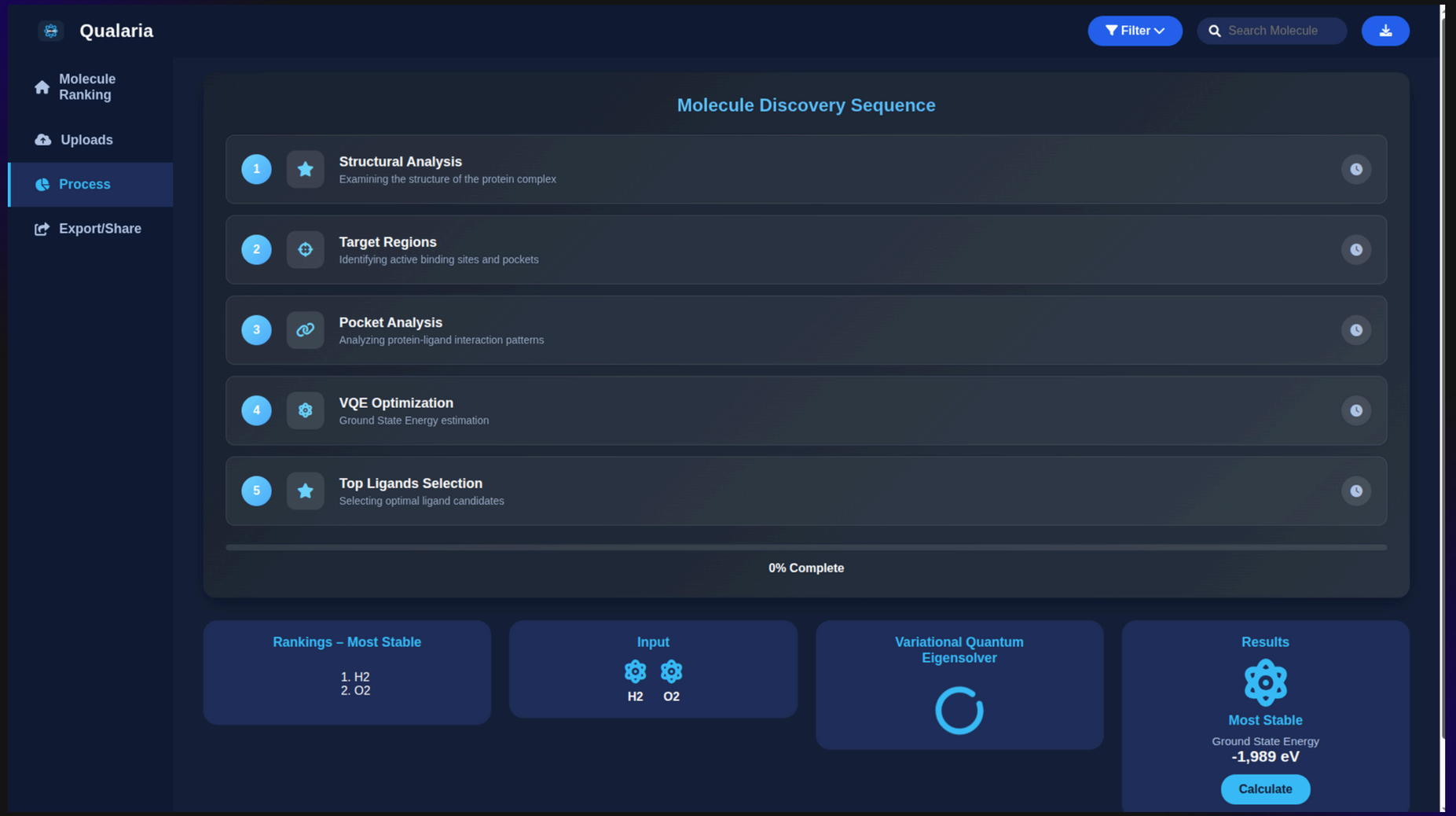
Docs
Submit
Contact
SEARCH FOR
Choose File
No file chosen
Upload
See Search Help
BEST MATCH
Molecule 101
More Info
Molecule 102
More Info
Molecule 103
More Info
Molecule 104
More Info
Molecule 105
More Info


Qualaria
Filter
Search Molecule
Molecule Ranking
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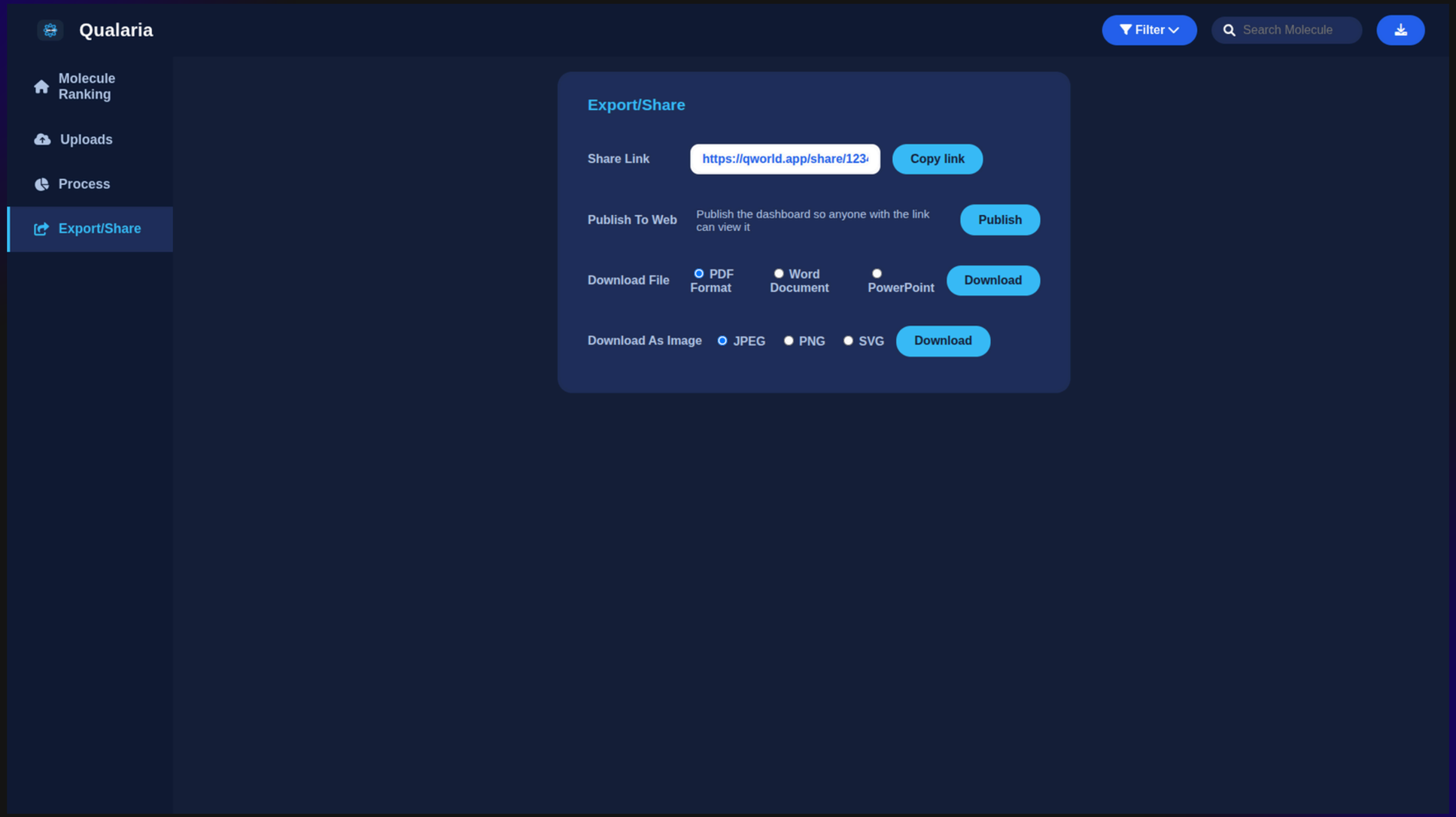
Molecule Discovery Sequence
1
Structural Analysis
Examining the structure of the protein complex
2
Target Regions
Identifying active binding sites and pockets
3
Pocket Analysis
Analyzing protein-ligand interaction patterns
4
VQE Optimization
Ground State Energy estimation
5
Top Ligands Selection
Selecting optimal ligand candidates
0% Complete
Rankings – Most Stable
1. H2
2. O2
Input
H2
O2
Variational Quantum Eigensolver
Results
Most Stable
Ground State Energy
-1,989 eV
Calculate

PROTOTYPE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Molecule Ranking
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Process
Export/Share
Export/Share
Share Link
https://qworld.app/share/123
Copy link
Publish To Web
Publish the dashboard so anyone with the link can view it
Publish
Download File
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Business Model

50,000 USD
Startup

Partners

Pharmaceutical companies developing antimalarial drugs.

Academic research institutions studying malaria.

Global health organizations (e.g., WHO, Gates Foundation).

Revenue Streams

Licensing of drug candidates to pharmaceutical companies.

Collaborative R&D partnerships and milestone payments.

Platform-as-a-Service (PaaS) for quantum drug discovery simulations.

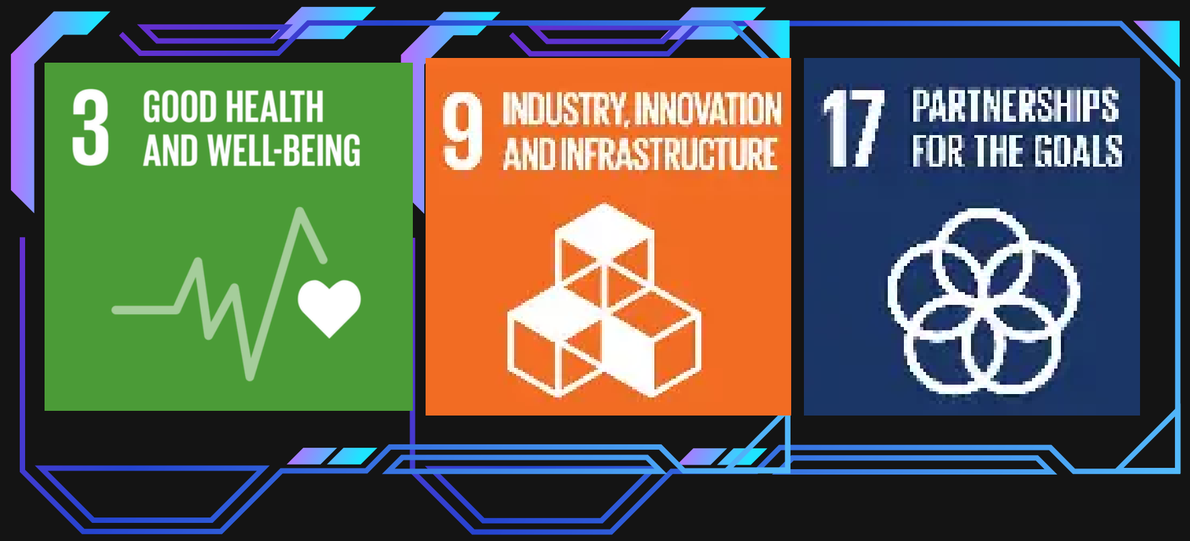
The broader anti-malarial drugs market is forecast to achieve USD 6.54 billion by 2033 (CAGR 4.6% from 2026 to 2033)

Drug Discovery Process

Focus Here

IMPACT ????

Contributes to SDG Goals



- Reducing deaths
- Lower reinfection
- Affordable development pipeline

Thank You

Let’s reduce malaria deaths with quantum power.

Category	Estimated Allocation	Purpose
Lab Supplies & Reagents	$12,000	Chemicals, assay kits, basic consumables for ligand screening
Computational Resources	$7,000	Software licenses (cheminformatics, molecular modeling), cloud compute
Contract Research (CROs)	$8,000	Outsourced screening, ADME/Tox profiling, or specialized assays
Salaries/Stipends	$10,000	Part-time scientist(s)/consultant(s) or student stipends
Business Development	$3,000	Market research, grant writing, IP searches, regulatory consulting
Networking/Travel	$2,500	Conferences, meetings with partners or funders
Legal & IP	$2,500	Incorporation, basic IP filings, contracts
Operational Overhead	$5,000	Rent (shared/lab incubator), utilities, insurance, admin

https://www.verifiedmarketreports.com/product/drugs-for-malaria-market/

The broader anti-malarial drugs market is forecast to achieve USD 6.54 billion by 2033 (CAGR 4.6% from 2026 to 2033)