

The Role of Statistical Physics in Accelerating Drug Design and Development: From Simulations to Startup and beyond.

Daniel M Shadrack, PhD
Founder, Chairman & CEO,
iPhytos

Where physics meets pharmacy, and science meets impact

Physics Beyond the Blackboard

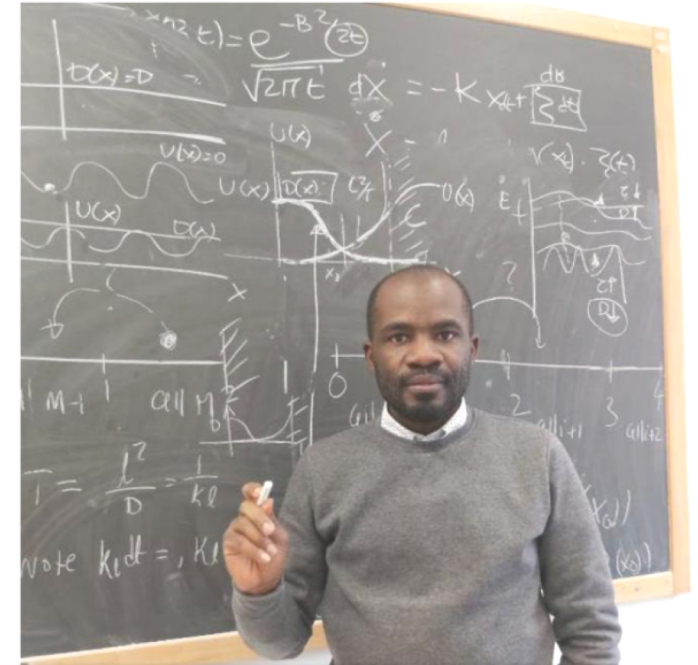
....What if I told you that the equations you solve today could save millions tomorrow?

$$p_i \propto \exp\left(-\frac{\epsilon_i}{kT}\right)$$

From biophysics to drug discovery: a personal journey

From Chemistry to Biophysics

ICTP alumnus Daniel Madulu Shadrack enriching science in Africa



How such equation could save life...??

Physics makes real-world impact.

Kinetics of protein-ligand unbinding
via smoothed potential molecular
dynamics simulations

Protein-ligand interactions

Protein folding

Statistical Physics and Life

Biological processes don't take single path, they Explore many configuration.

$$p_i \propto \exp\left(-\frac{\varepsilon_i}{kT}\right)$$

We can describe complex biological systems using probabilities

Statistical Physics and Life

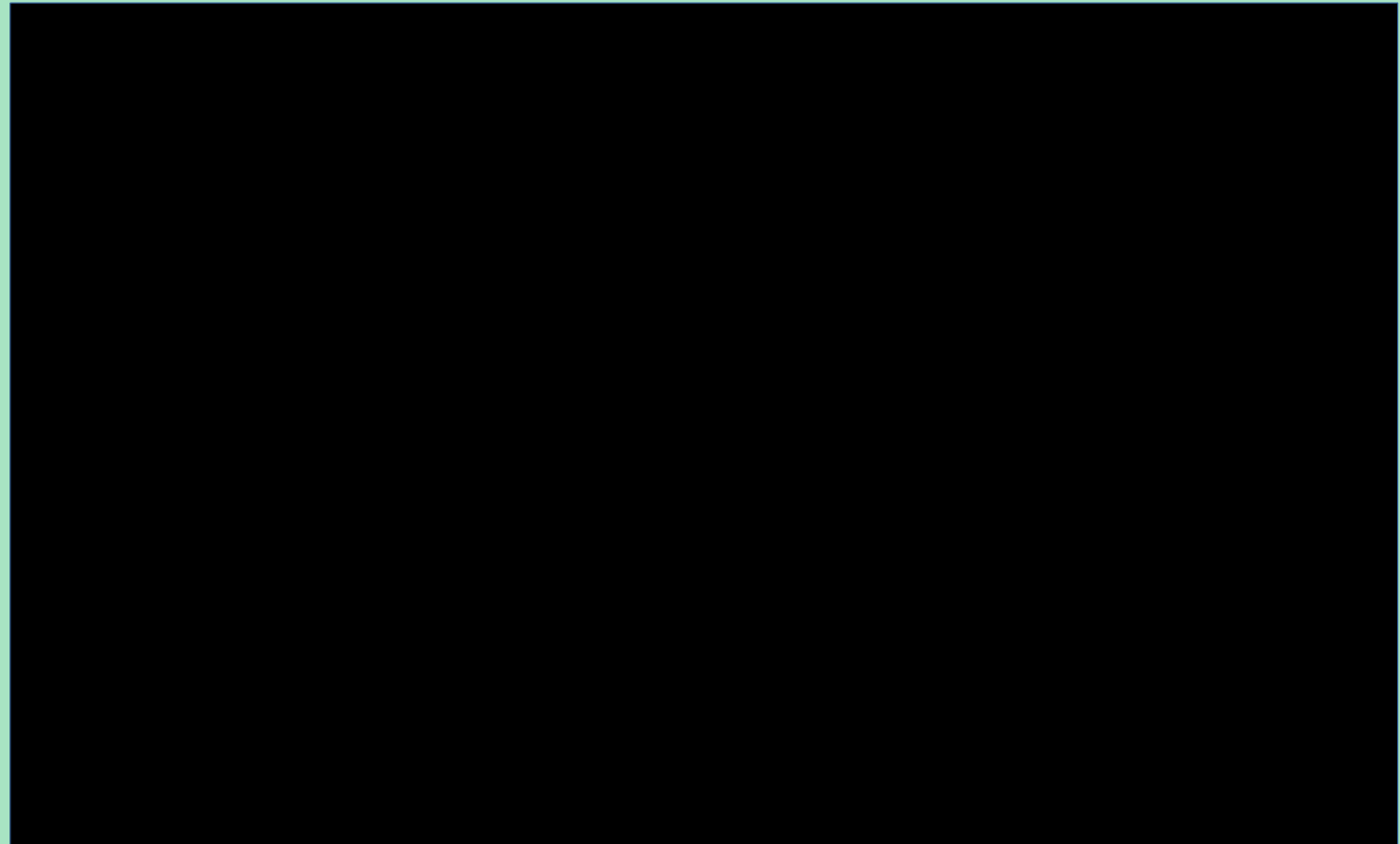
$$p_i \propto \exp\left(-\frac{\varepsilon_i}{kT}\right)$$

Relevance in biology:

Boltzmann distribution,

Entropy,

Partition functions.

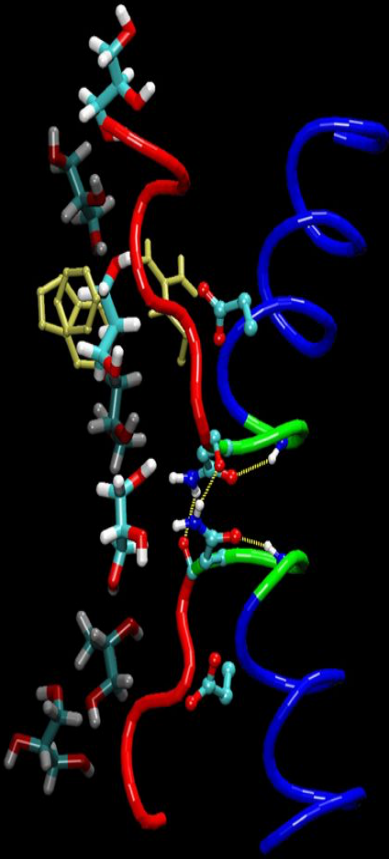


Simulating Nature – From Theory to Reality

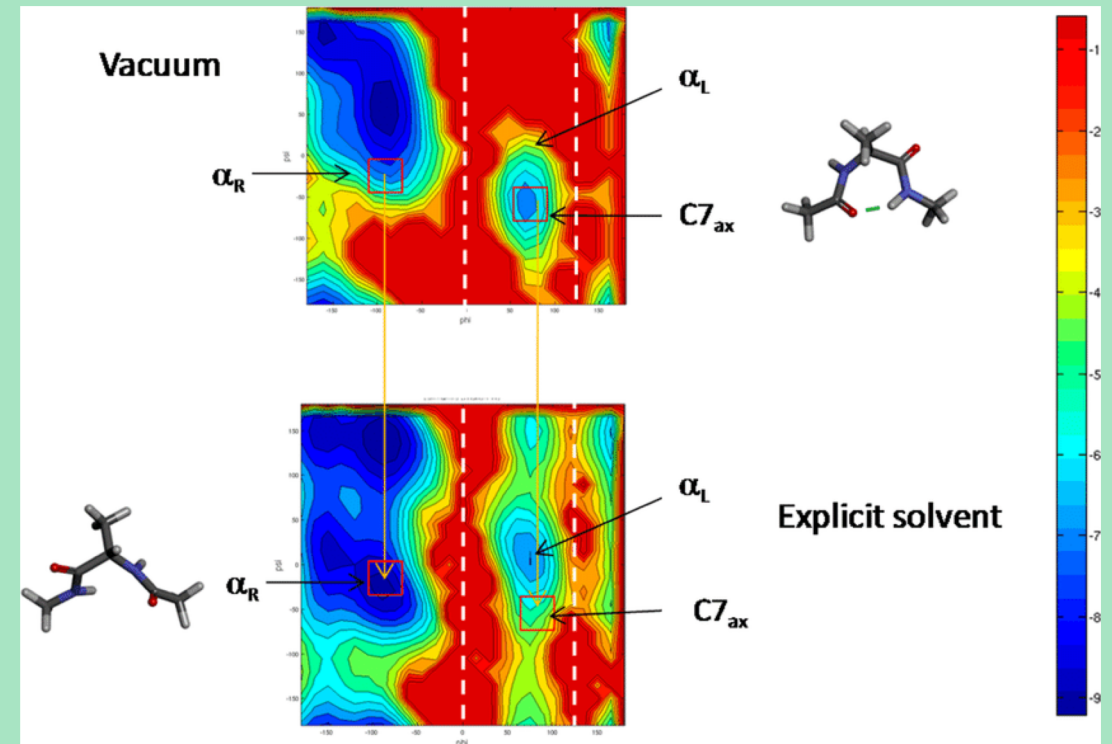
Molecular Dynamics Simulation

(a brief introduction)

by Giff Ransom

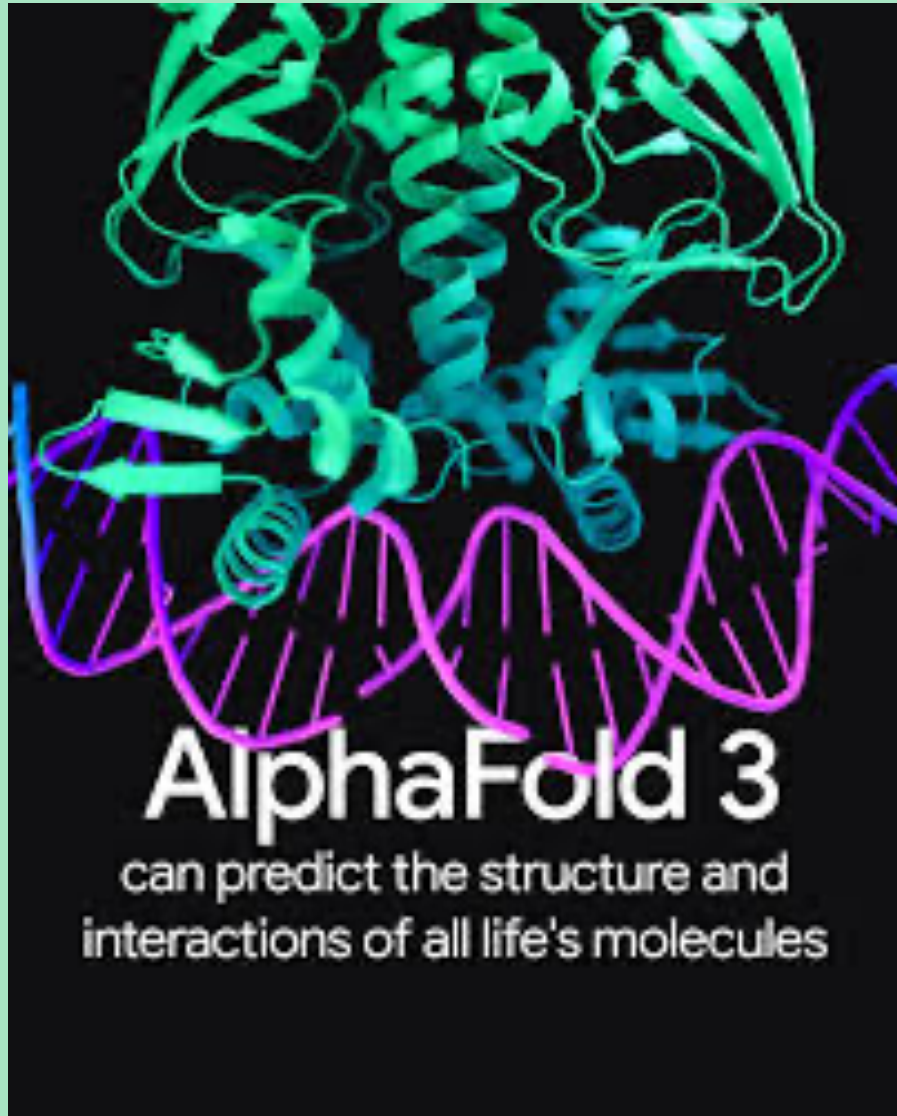


Molecular dynamics simulation



Free energy landscape

AI Meets Physics



AI in protein folding & molecular predication

Neural networks

Need for physical accuracy in AI predictions

The African Story – Birth of iPhytos

Overcoming challenges in African biotech



Challenging the status quo.
Thinking differently.



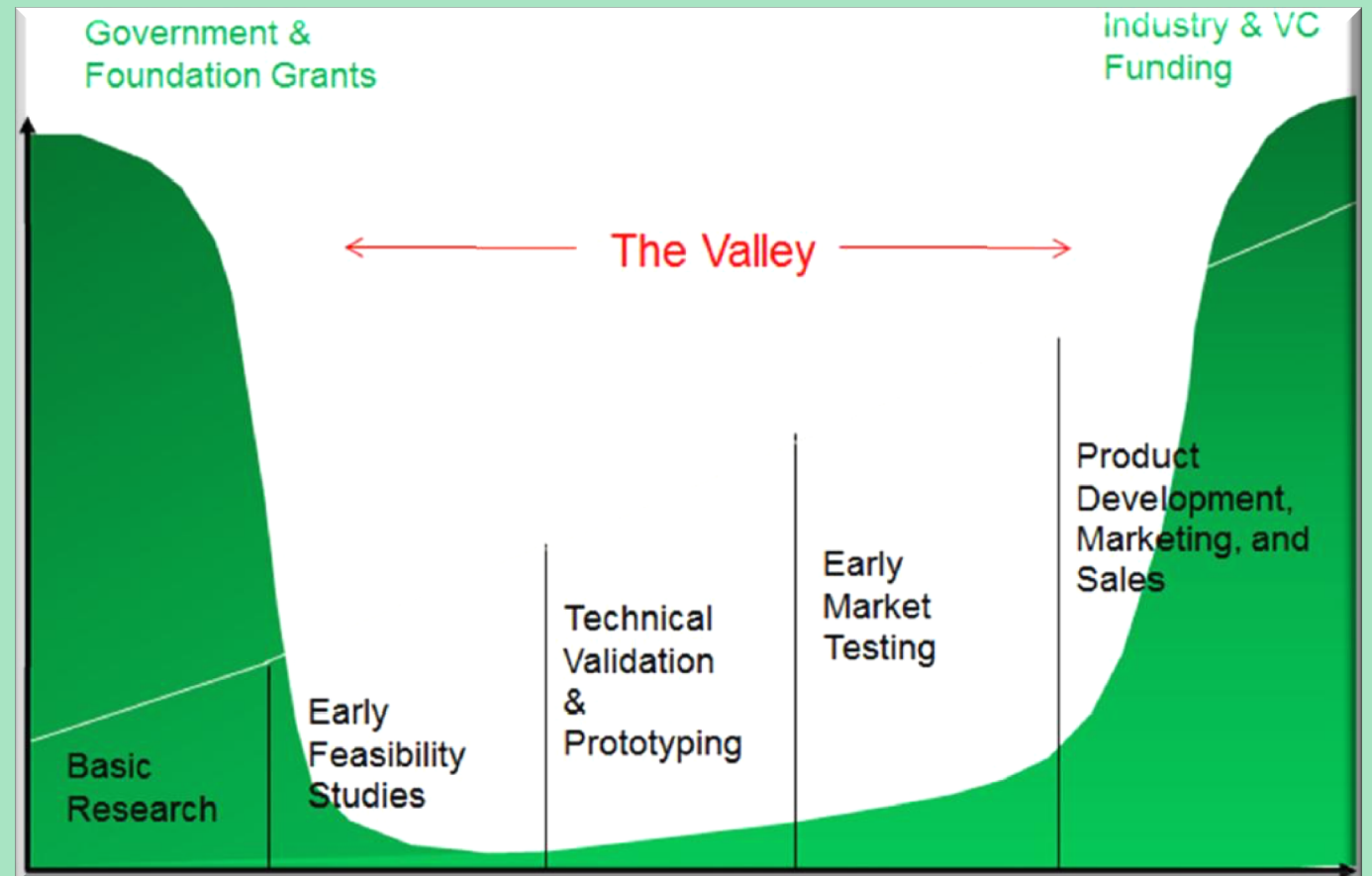
A NATIONAL INSILICO CLINICAL STAGE BIOTECH COMPANY

Dr. Daniel M Shadrack (PhD)
Founder, Chairman & CEO

Research ecosystem.

Imbalanced.

5% from LMICs.



Research ecosystem.

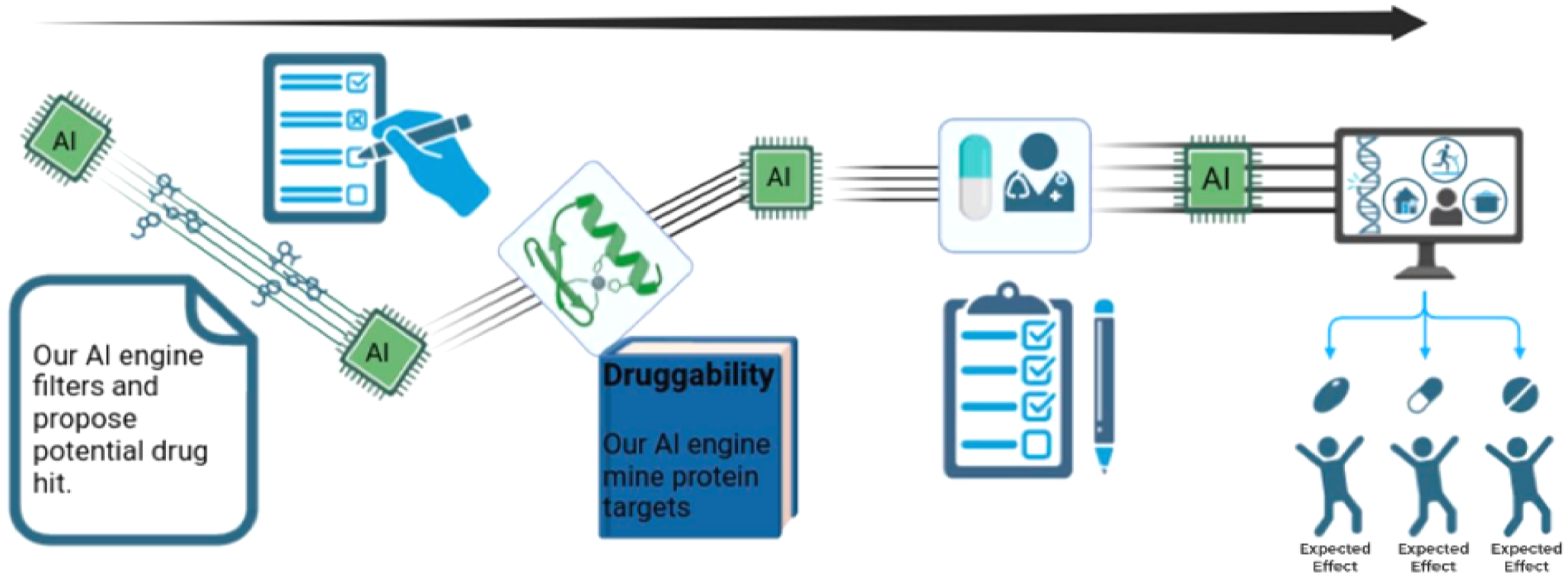
Imbalanced.

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Why Us

We believe in quality of life and precision treatment for every individual.



Advanced platform for Next Generation Phytotherapy



In-silico Drug Design



Pre-clinical Facility



Clinical Facility



Production Facility



VerdiaChem42

Molecular Intelligence platform analyzing compounds for drug-likeness, ADMET properties, toxicity, and synthetic accessibility.

[Learn more →](#)



VerdiaOmics

Network Pharmacology Engine mapping interactions between compounds, genes, proteins, and disease pathways.

[Learn more →](#)



VerdiaTrials

AI-Powered Clinical Outcome Prediction simulating real-world outcomes using patient data and disease models.

[Learn more →](#)

Advanced platform for Next Generation Phytotherapy



In-silico Drug Design



Pre-clinical Facility



Clinical Facility



Production Facility



Natural Products & Medicinal Chemistry Lab

Our extraction and compound testing lab focuses on isolating, purifying, and characterizing bioactive compounds from medicinal plants. Using both traditional and modern techniques, we evaluate phytochemical properties, stability, and biological activity to inform product development.



Animal Research Laboratory

Our licensed animal facility supports in vivo testing to assess the pharmacological effects, pharmacokinetics, and safety of herbal formulations. We follow strict ethical and regulatory guidelines in all preclinical studies.

- Pharmacokinetics & toxicity profiling
- Efficacy studies in disease models
- Dose optimization & safety assessment

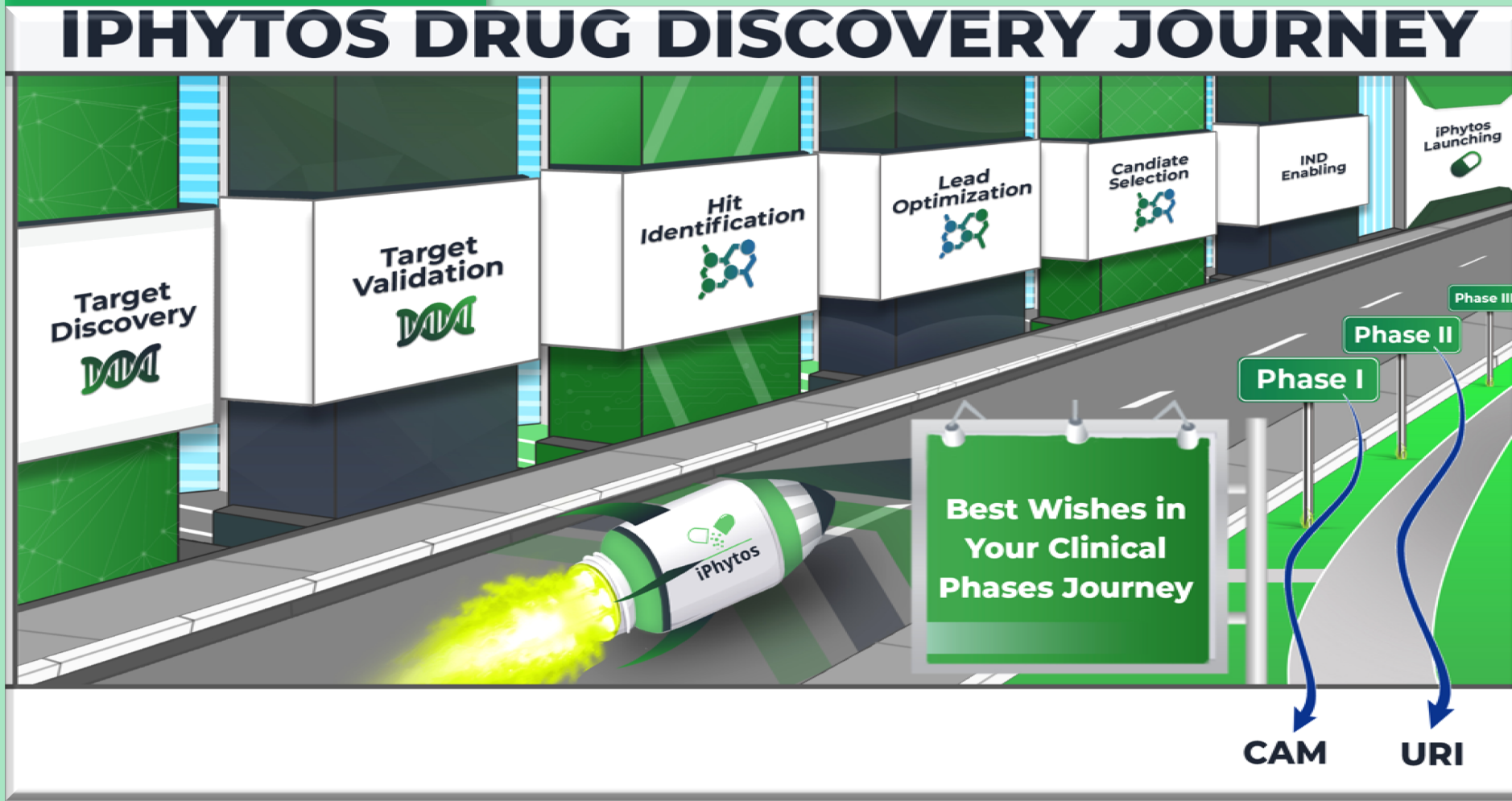


Product Development Lab

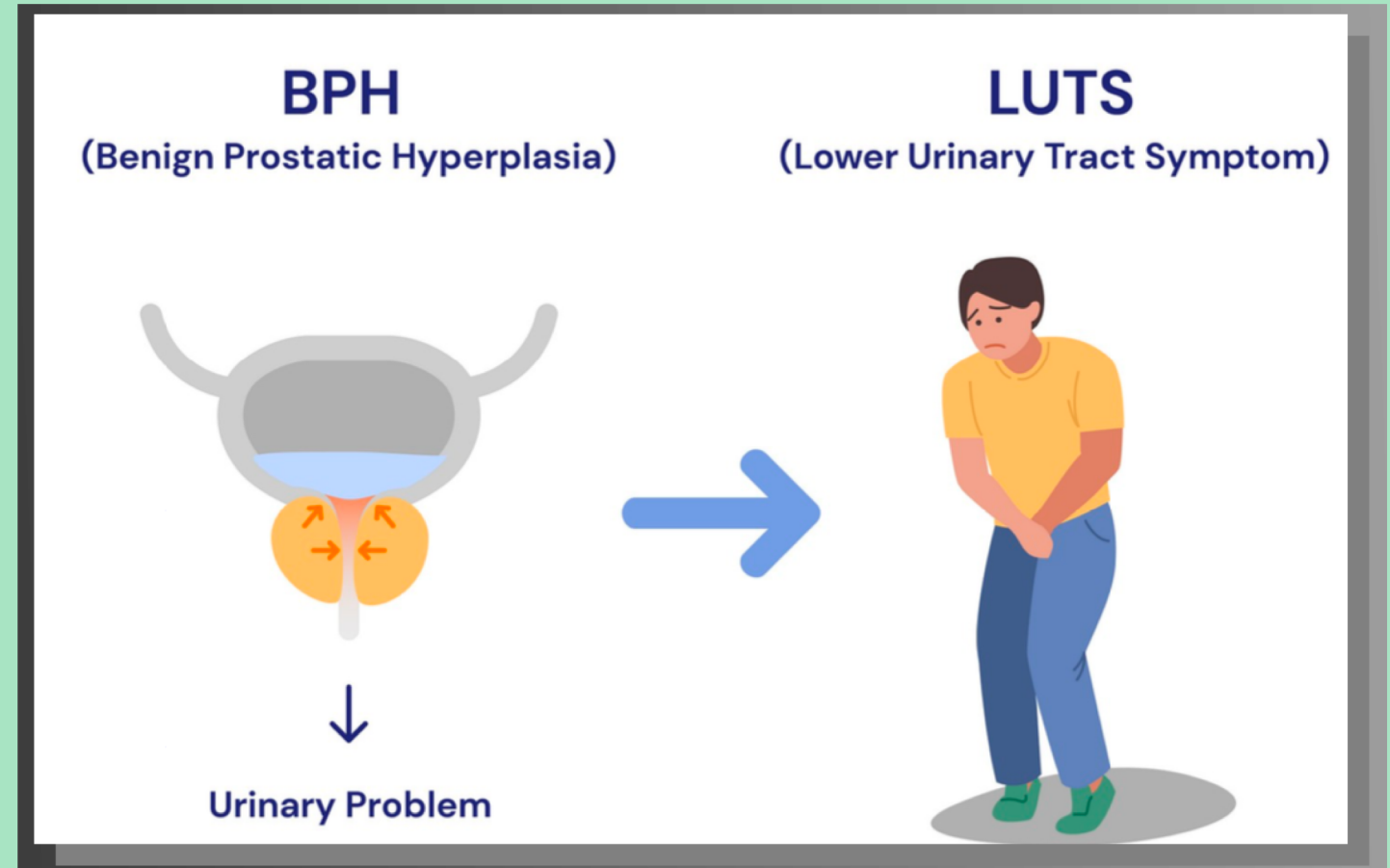
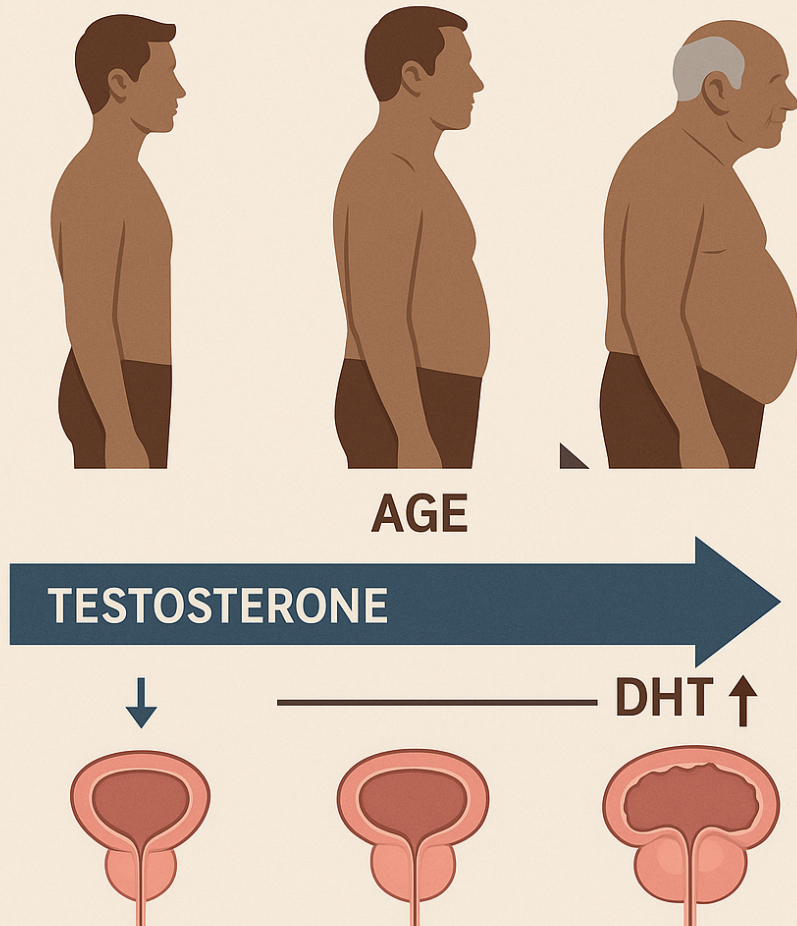
We translate active compounds into real-world formulations. Our formulation scientists work on creating stable, effective, and safe herbal medicines, guided by scientific validation and patient needs.

- Capsule, tablet, syrup, and ointment formulation
- Stability and shelf-life testing
- Pilot batch production for clinical readiness

Our processes.



The problem we are solving....



Our success: From pre-clinical to clinical

In-silico

in vitro/ in vivo

Human



A novel in-silico designed
phytotherapy for treatment of BPH

URIPHYTOL[®]-500 mg
Capsules

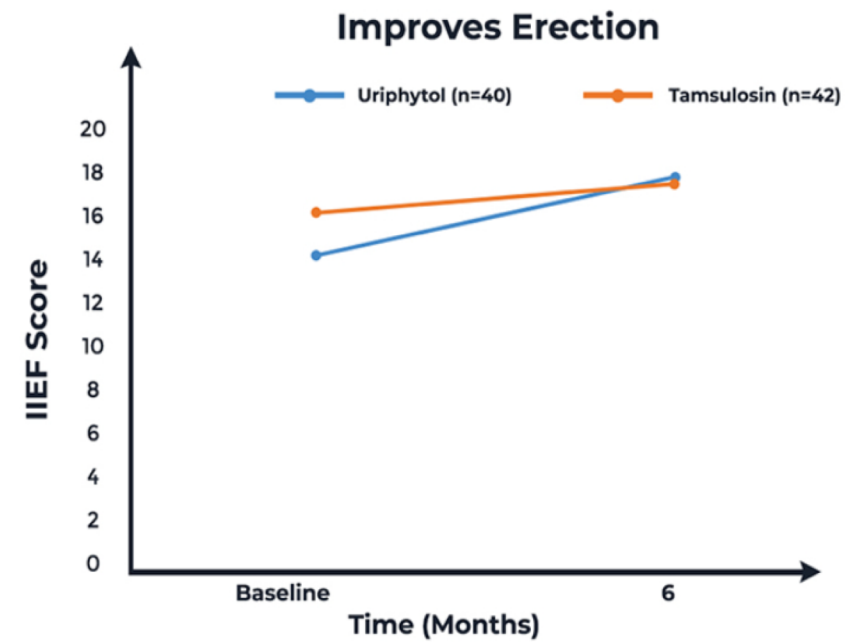
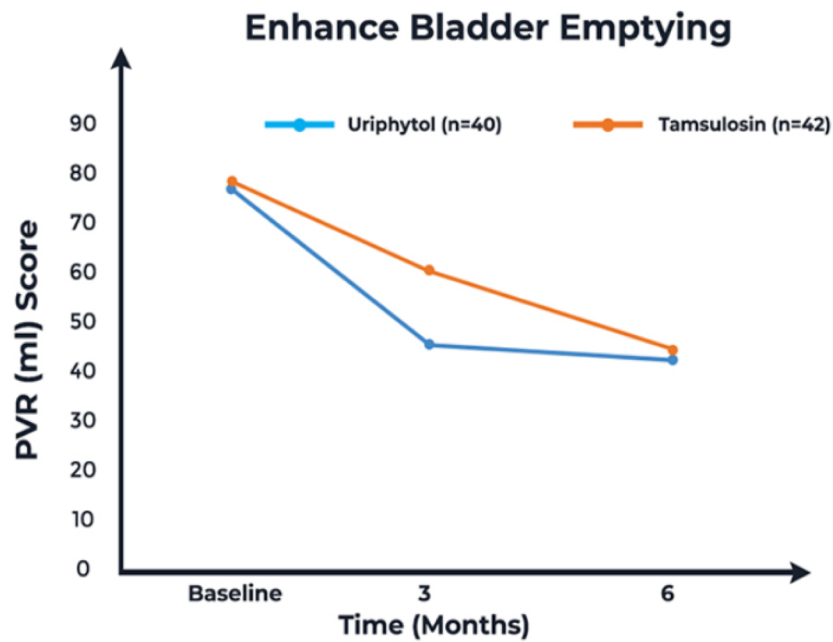
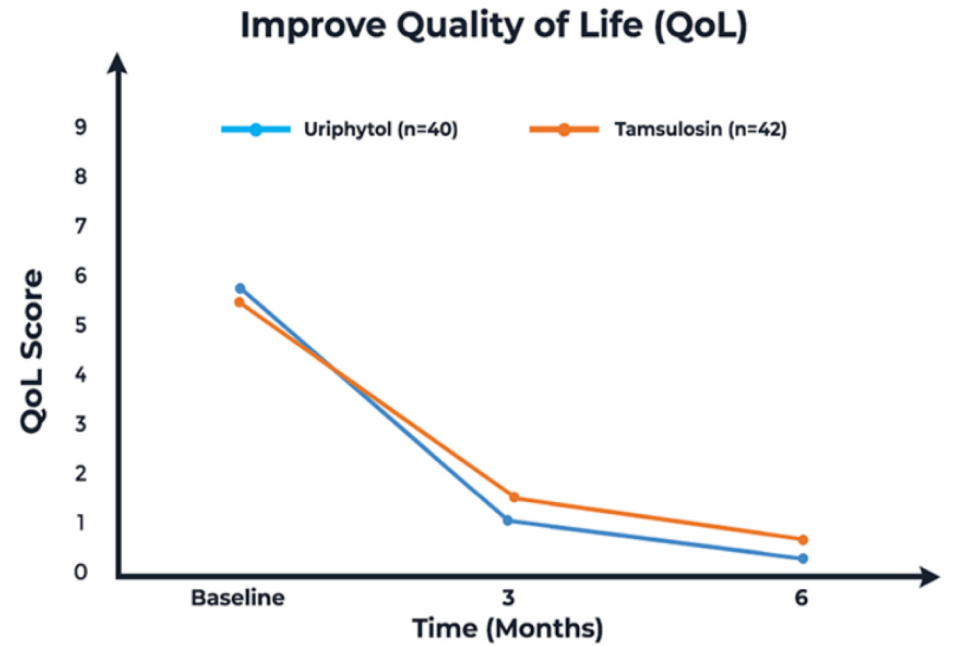
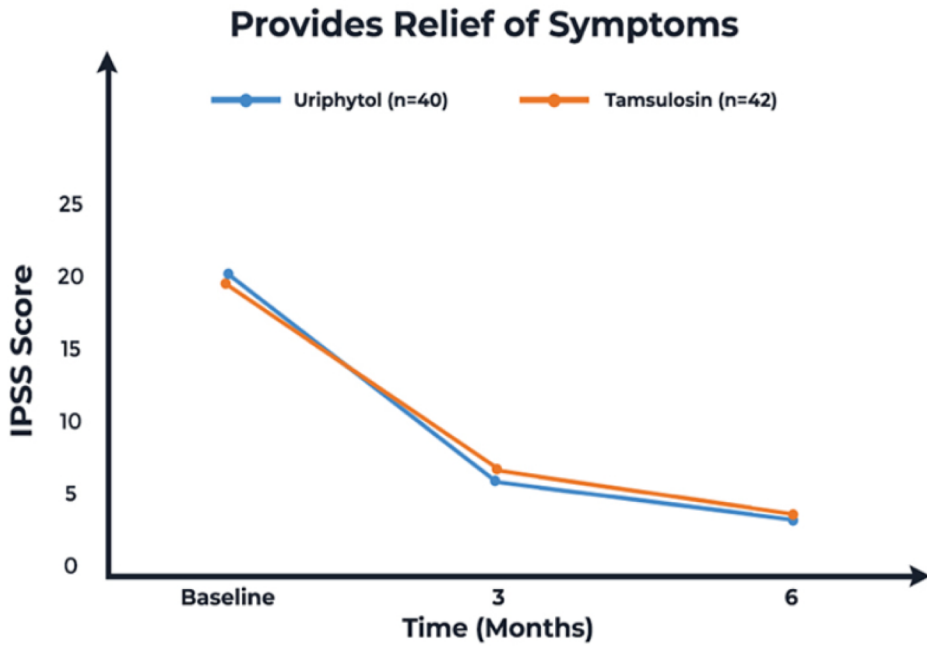
R_x



Clinical /human. (Part II)

The chemistry & pharmacology

Pilot Observational @ KCMC with
a team of UROLOGISTS





In human The chemistry & pharmacology: PK/PD

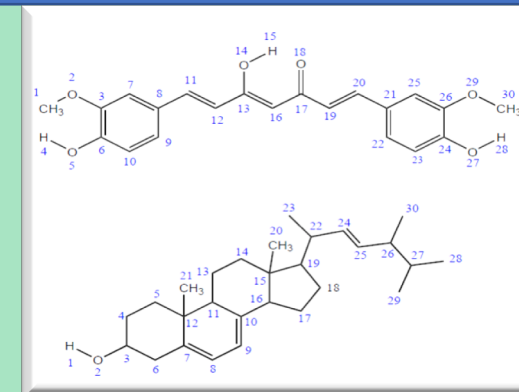


Generally,

- Strength: 500 mg capsules
- Dose: 500 mg TDS x 4/12 (some patients goes up to 6)
- Improved bioavailability, solubility and easily absorbed
- Natural with higher safety profile > 2000 mg / day still safe
- Toxicity: No renal or liver toxicity
- Contraindicated: Warfarin.

Warning:

**Not to be taken on empty stomach for patient with PUD
(peptic ulcer diseases)**



URIPHYTOL[®]-500 mg
Capsules

R_x



Acts Faster Within
30
Days



Available also in several private hospitals and pharmacies across the country.

URIPHYTOL is distributed by the government in 14 Regional Referral Hospitals (RRH)

The impact and call to young scientists

The impact

Drug candidate and collaboration

Building scientific capacity in Africa
(schools, internship positions),
14 employments

The Call

Learn, start small, build bold.
Africa's potential in biotech





Explaining the science behind URIPHYTOL to the Director General of TMDA



Explaining URIPHYTOL to the former minister of health (left side) and to the deputy minister of health (right side).

ASANTENI SANA



**Statistical physics gave me the tools. Africa gave me the reason.
AI gave me the wings**

**Challenging the status quo.
Thinking differently.**