Accelerate Drug Development Using AI & ML

PHUSE Single Day Event – Chennai

Anoop P Ambika, Chief Executive Officer,
Genpro Research

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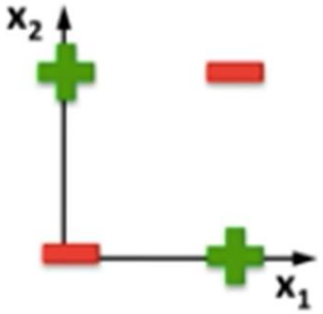
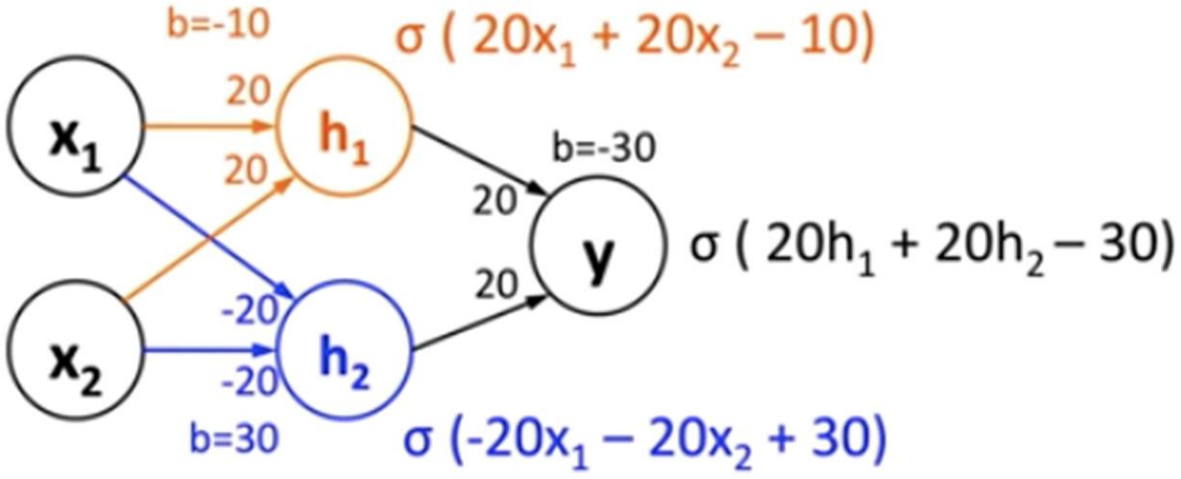
BASICS

Introduction to Machine Lea rning

Linear classifiers cannot solve this





σ(20*0 + 20*0 – 10) ≈ 0
σ(20*1 + 20*1 – 10) ≈ 1
σ(20*0 + 20*1 – 10) ≈ 1
σ(20*1 + 20*0 – 10) ≈ 1

σ (-20*0 – 20*0 + 30) ≈ 1
σ (-20*1 – 20*1 + 30) ≈ 0
σ (-20*0 – 20*1 + 30) ≈ 1
σ (-20*1 – 20*0 + 30) ≈ 1

σ (20*0 + 20*1 – 30) ≈ 0
σ (20*1 + 20*0 – 30) ≈ 0
σ (20*1 + 20*1 – 30) ≈ 1
σ (20*1 + 20*1 – 30) ≈ 1

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RESEARCH

Traditional Model of Dru g Discovery

Patient with a disease – was effectively treated as a black-box, and exposed to all manner of herbal mixtures and religious rituals.

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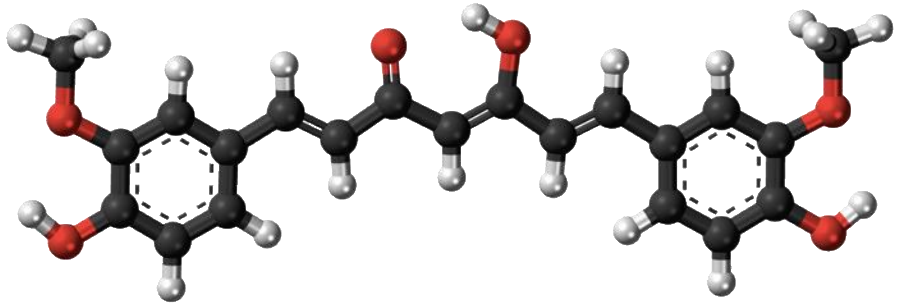
So what was happening



Drugs arising from herbal remedies typically acted by binding to a single receptor molecule

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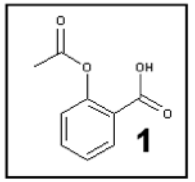
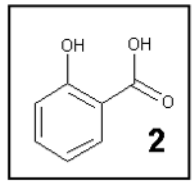
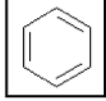
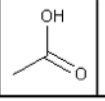
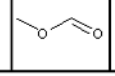
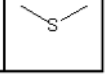
Reductionist Approach

Similarity Searching





1	1	1	0	1	1	0	1	0
2	1	1	0	1	0	0	0	0
								

A = Number of bits set in both = 3
B = Number of bits set in (1), but not in (2) = 2
C = Number of bits set in (2), but not in (1) = 0

TANIMOTO COEFFICIENT = A / (A + B + C)
= 3 / (3 + 2 + 0) = 0.6 or 60%

Search for a 'magic bullet' that binds specifically to a rationally chosen target

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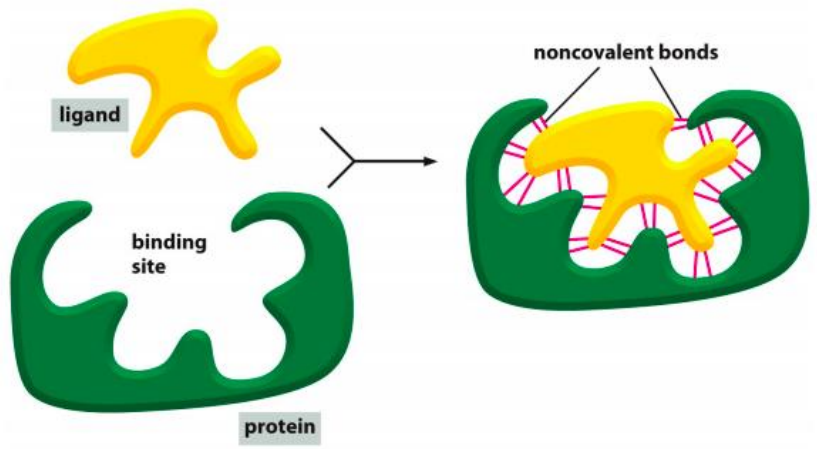
Drawbacks



Possibility of a designed molecule binding in places other than the target is often neglected until comparatively late in the discovery process, where many candidate drugs fail.

or

Viagra gets invented

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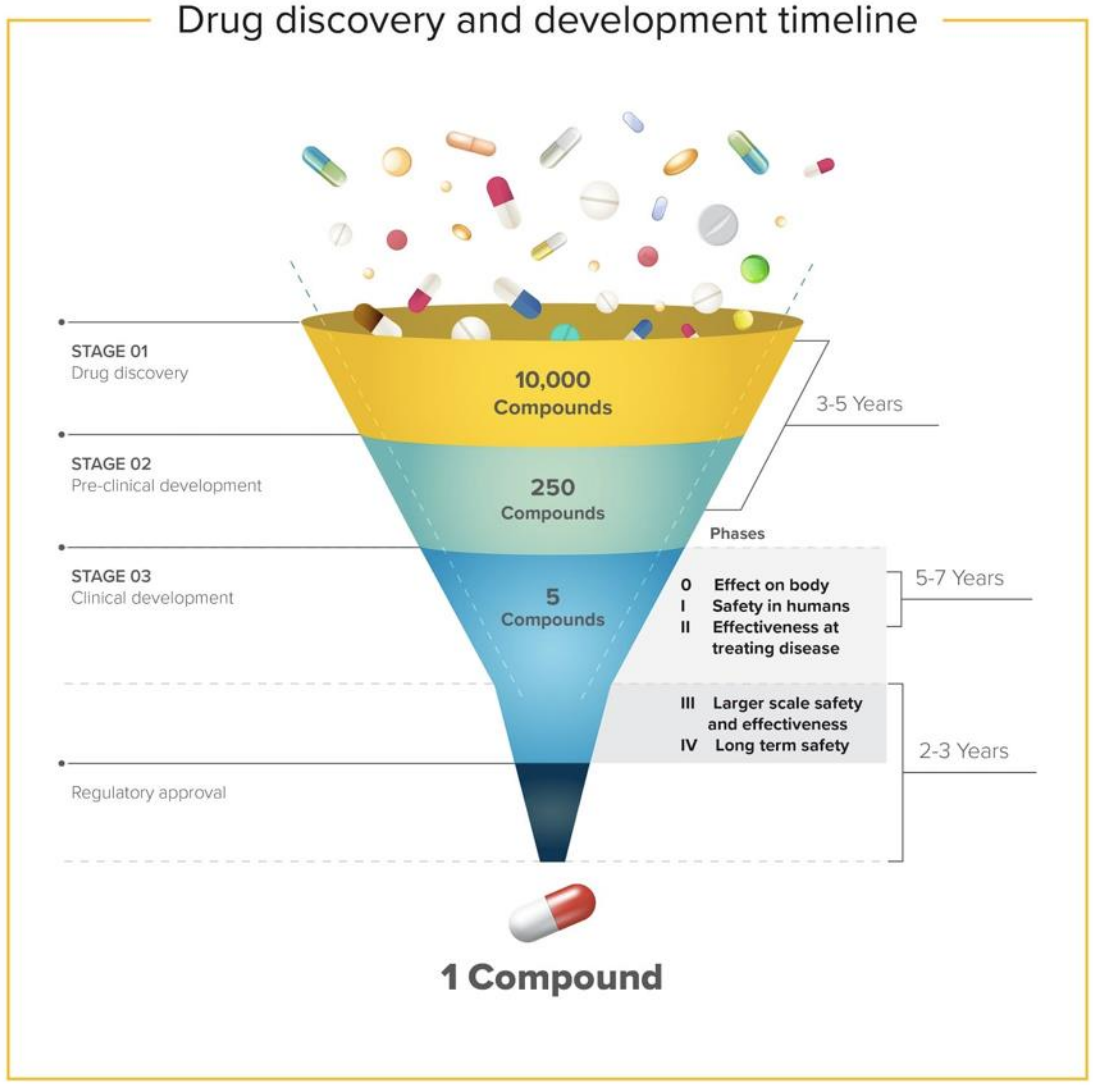
Current Timelines



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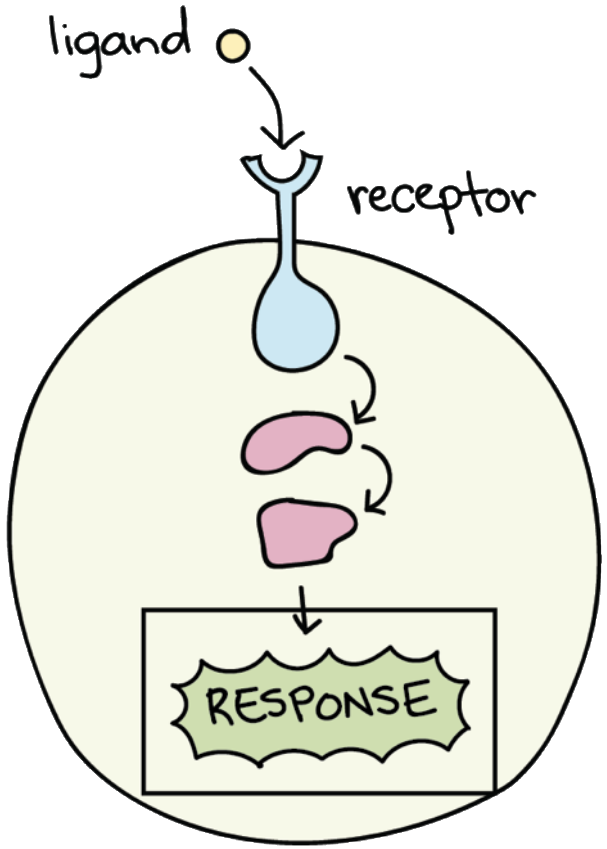
SIGNALING PATHWAYS



Cellular responses to signalling happen at both the *micro* and *macro* levels.

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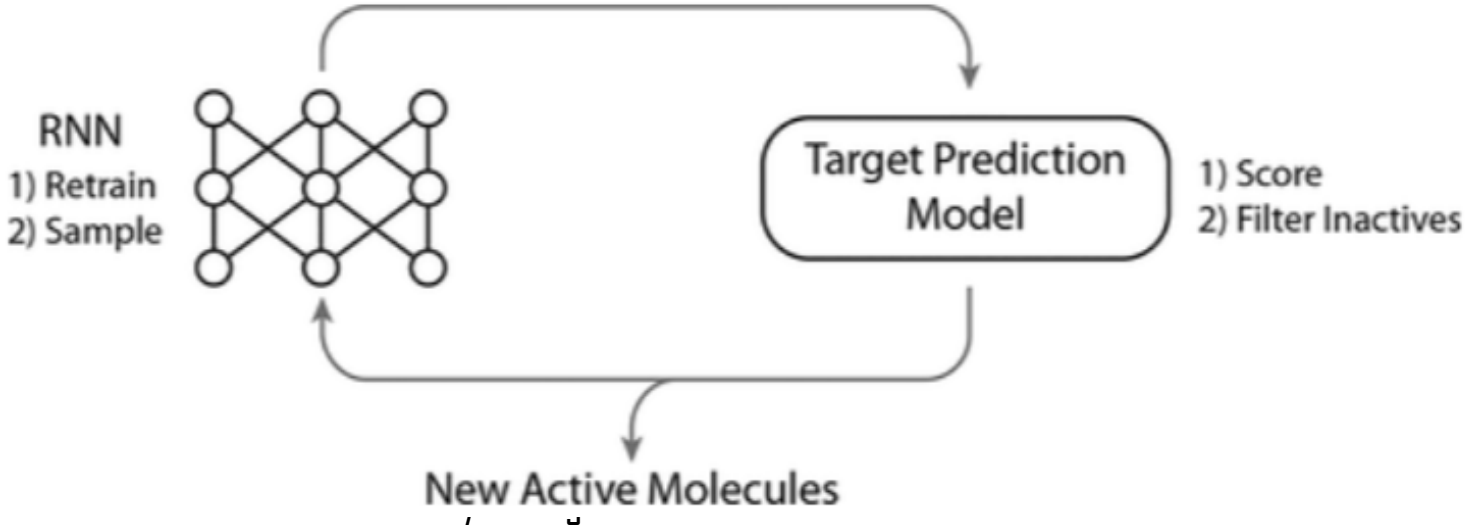
Molecule Design

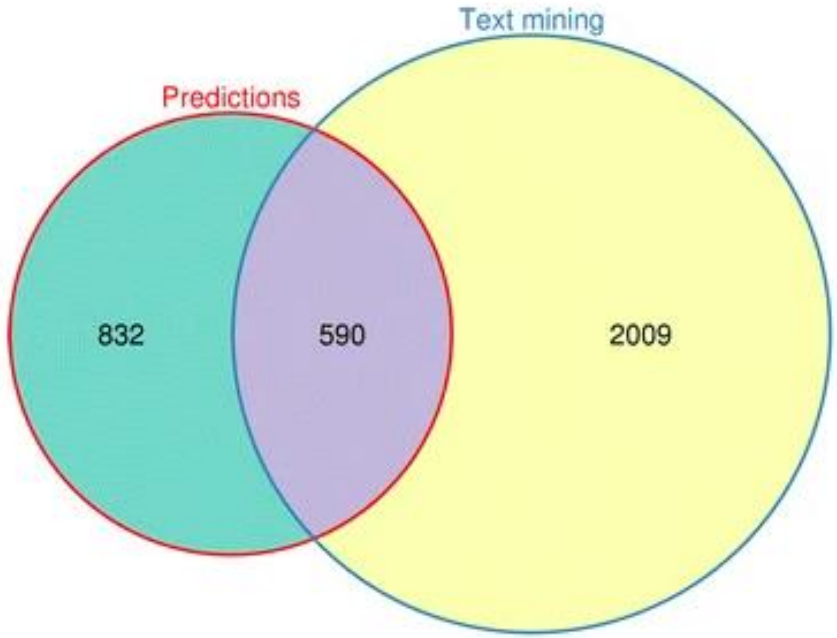
Much work has been done to apply DL methods, such as multi-task neural networks, to ligand-based virtual screening. Given a lead compound, compounds that have a similar chemical structure can be identified computationally.

TARGET IDENTIFICATION



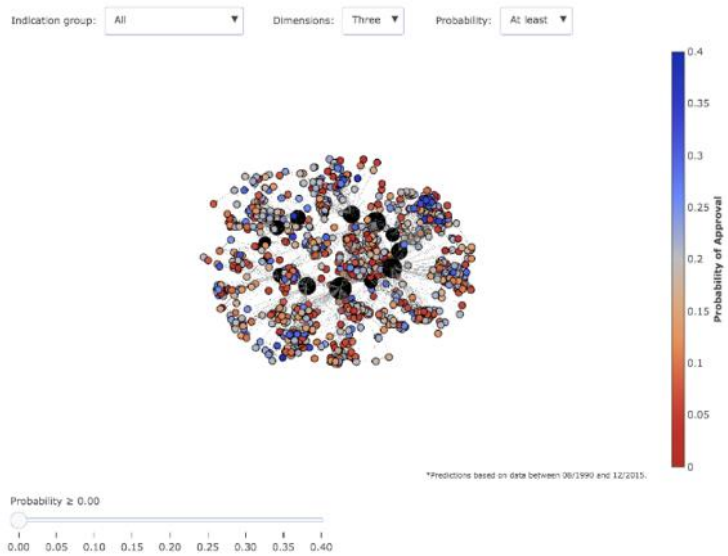
putative target to make predictions about potential causality, driven, for instance, by the properties of known true targets

NOVEL TARGETS



Understanding basic aspects of biology to identify therapeutic opportunities through alternate modalities or novel targets

Yes No



The holy grail for target identification or validation is the early prediction of future clinical trial success for a target-based drug discovery programme.

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Patient Recruitment

antidote

Where patients meet research

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Patient Engagement

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Computational Pathology

Deep learning frameworks can replace traditional handcrafted features in several basic pathology image-recognition tasks using image segmentation, detection of specific features or detection of a set of features used for classification.

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Artificial Intelligence algorithms for medical imaging

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Biomarker Discovery

ML-based biomarker discovery and drug sensitivity predictive models are demonstrated approaches to help improve clinical success rates, to better understand the mechanism of action of a drug and to identify the right drug for the right patients

OUR WORK

AI TOOLS THAT WE WORK ON

MOSS

QA system for Clinical Data Visualisation

VOODY

Enterprise search for the pharmaceutical industry

YESDTM

Automatically generate your SDTM specs and datasets

TFL AUTOMATION

Automate generation of safety tables and listings

PSEUDO

Data anonymization using machine learning

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Collaborations

INDUSTRY STARTUPS ACADEMIA NONPROFITS

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References

Applications of machine learning in drug discovery and development
Jessica Vamathevan, Dominic Clark, Paul Czodrowski, Ian Dunham, Edgardo Ferran, George Lee, Bin Li, Anant Madabhushi, Parantu Shah, Michaela Spitzer, and Shanrong Zhao

Machine Learning with Statistical Imputation for Predicting Drug Approvals
by Andrew W. Lo, Kien Wei Siah, and Chi Heem Wong

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