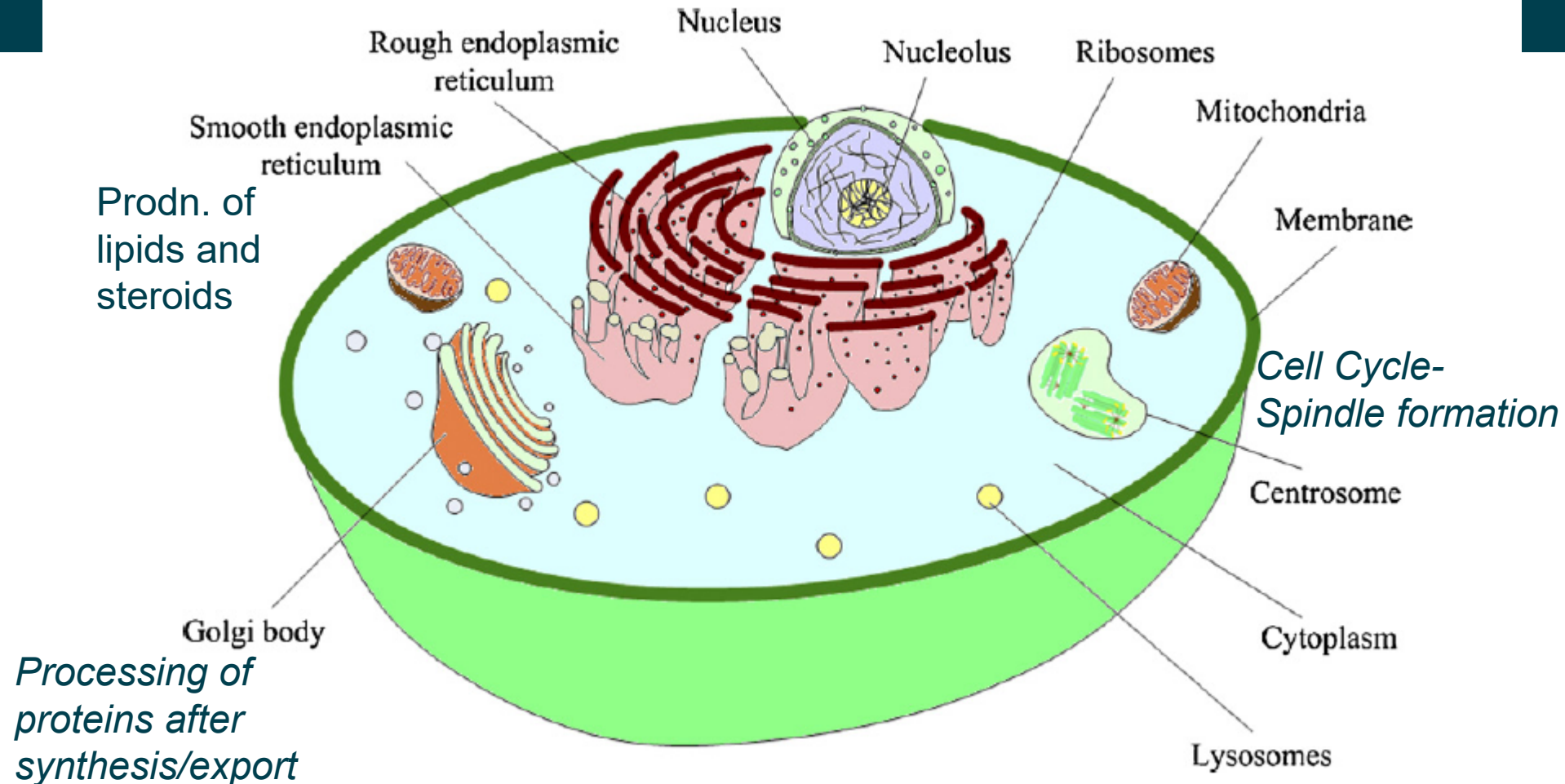




Basic Introduction to ML

Ravichandran Sarangan, Ph.D.,
BIDS, FNLCR, Frederick, MD 21701

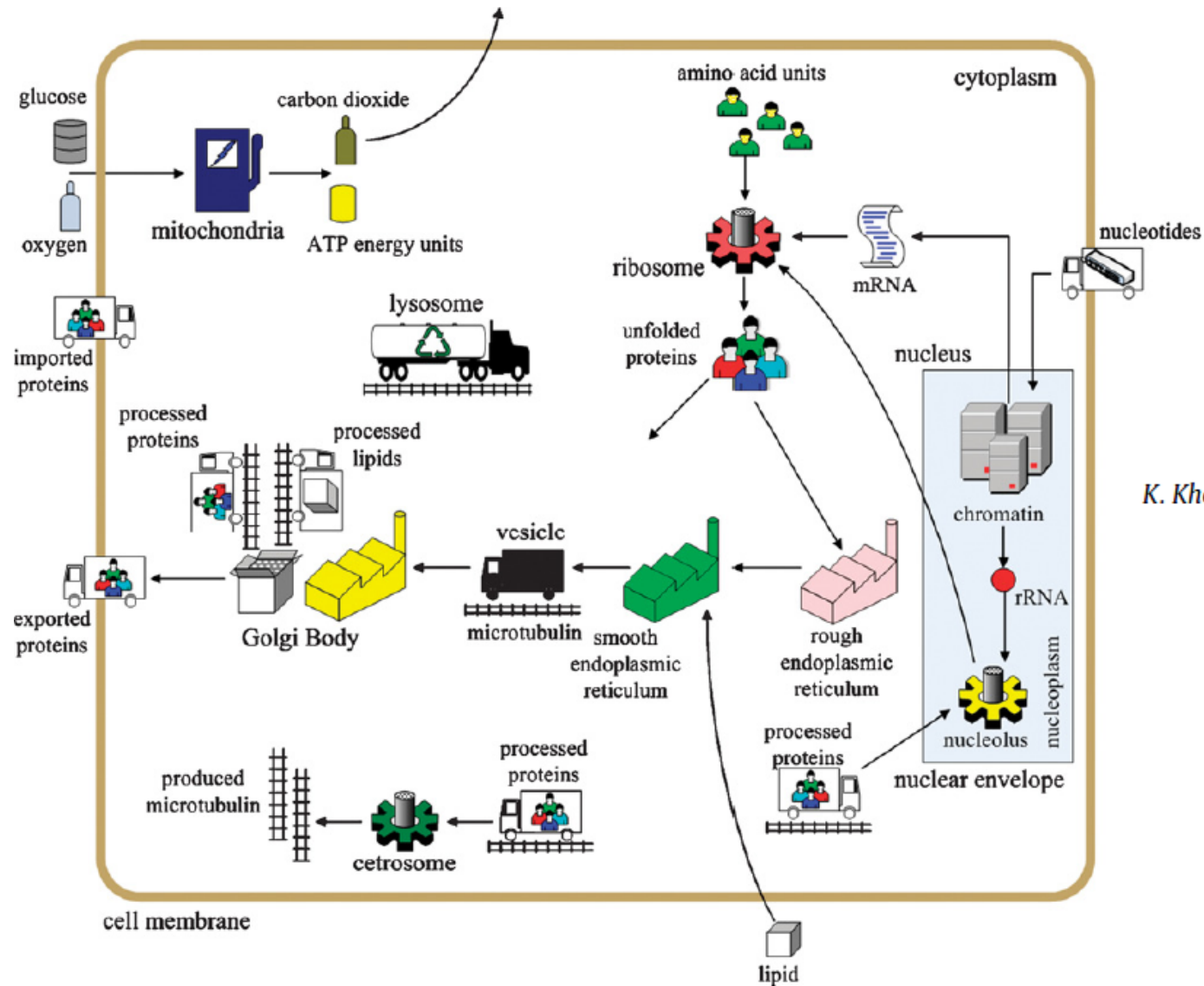
Cell As a Factory



Roughly 37.2 trillion cells in our body

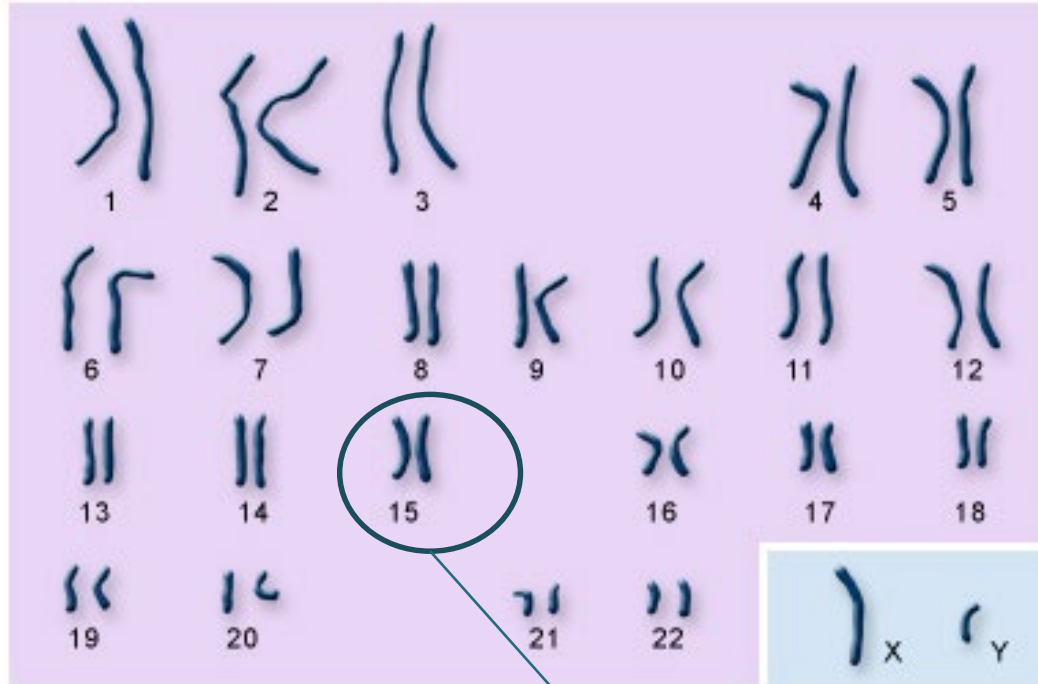
Typical cell (across length) $10 \times 10^{-6}\text{m}$

Cell As a Factory



K. Khoshmanesh et al. / Computational Biology and Chemistry 32 (2008) 315–331

Chromosome



autosomes

sex chromosomes

U.S. National Library of Medicine

Book of Life: 2 Multi-Volume Set



DAD

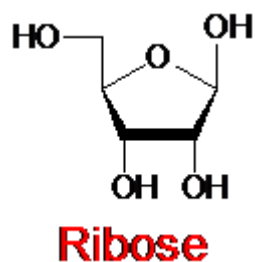
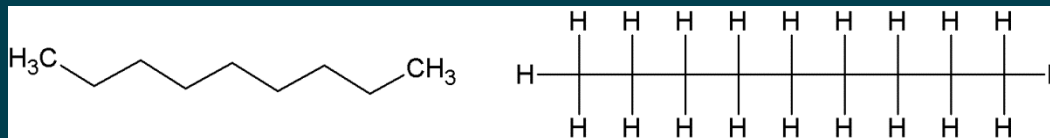


MOM

Brief Introduction

To understand the language of DNA, we need to understand some Chemistry/Biochemistry

Periodic Table



Periodic Table of Elements

1																	18	
H																	He	
2																		
Li	Be											B	C	N	O	F	Ne	
Na	Mg	3	4	5	6	7	8	9	10	11	12	Al	Si	P	S	Cl	Ar	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg								
		*	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	D
		**	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	T

General

NMR

Mass

Coloration

Characters :

Discoverer :

Name Origin :

Atomic Radius, A :

Electronegativity :

Ionization Potential, kJ/mol :

Electron Affinity, kJ/mol :

Density :

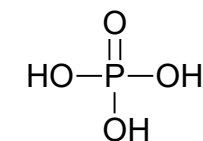
Melting Point, K :

Boiling Point, K :

OK

Cancel

Help



Phosphate

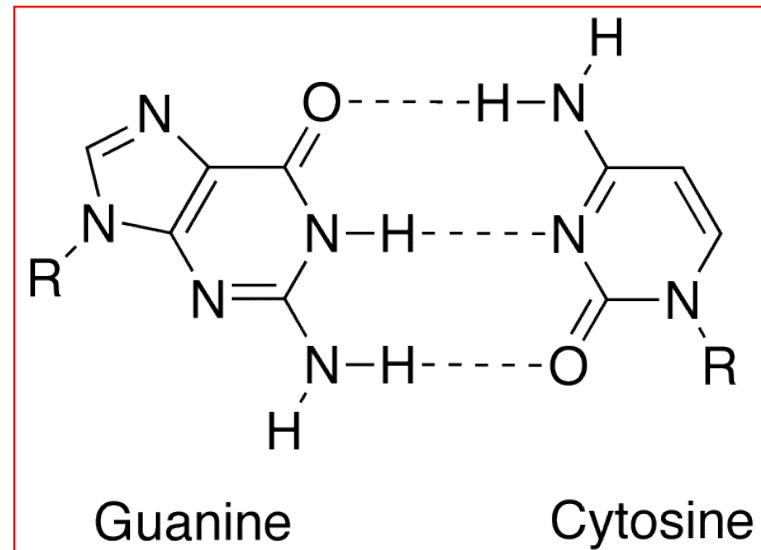
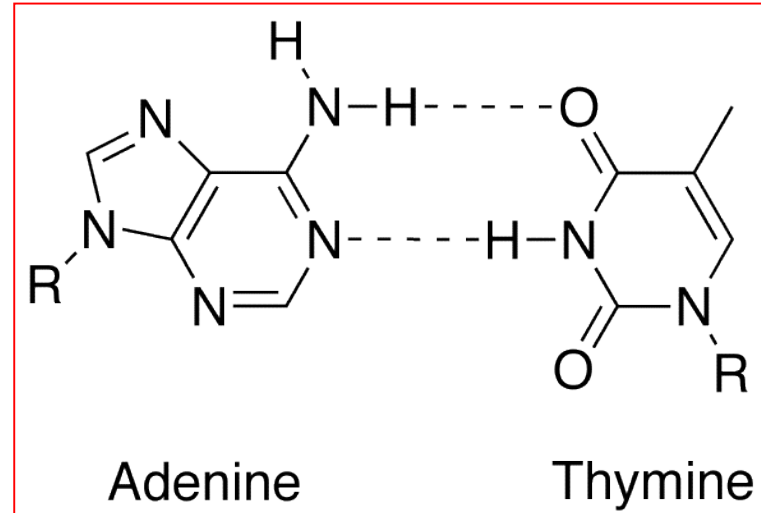
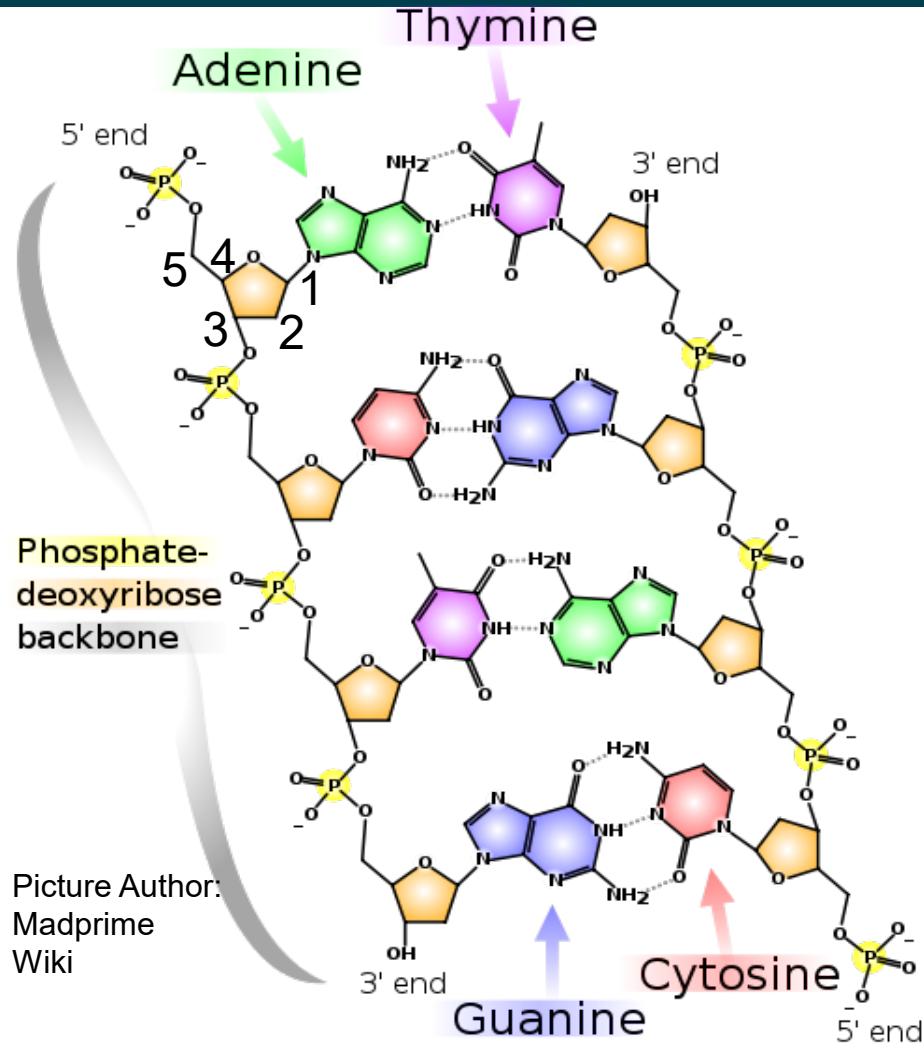
Chemistry:

Halogens

Some Ions

K, Li, K, Ca, Ni, Cu, Zn

DNA has direction



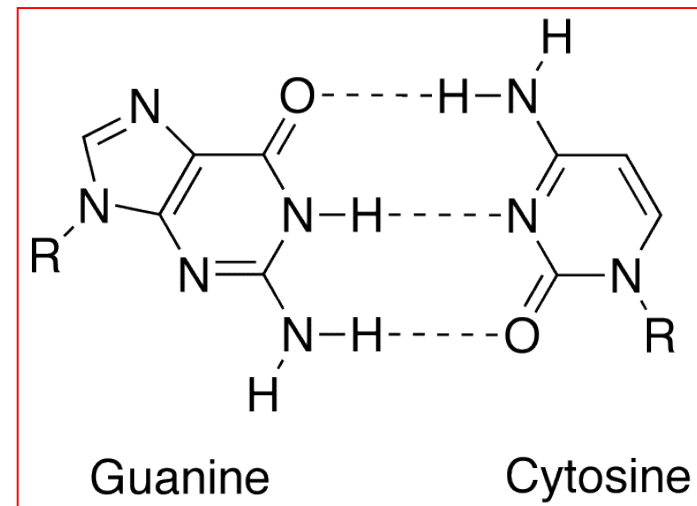
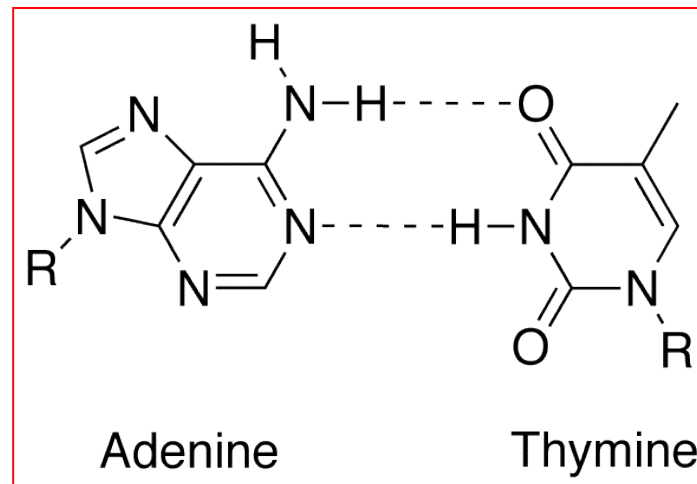
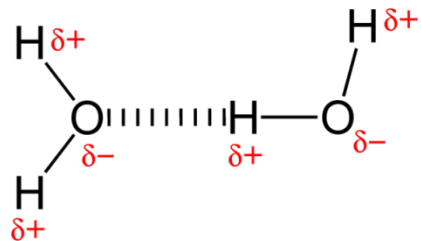
Biology is the chemistry that crawls

What holds the molecules together?



Atomic level: Chemistry Rules

- Bonded interactions
 - Covalent bonds
- Non-bonded interactions
 - H-bonds
 - Holds DNA
 - Makes drug binding work
 - Ionic, VDW etc.



H-bonds

Which pair is easy to break?

A-T

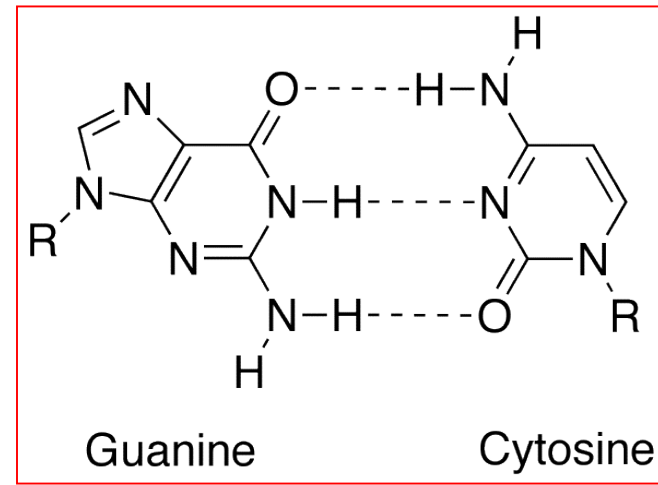
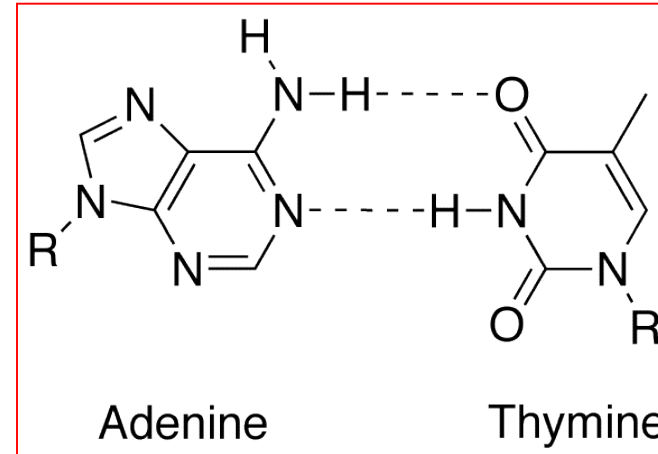
Or

G-C

of H-bonds

Can we think of A-T being the site for
DNA actions such as
double-stranded → single-stranded

Replication and Transcription etc.



Drug Discovery Cost

[cost-of-clinical-trials-for-new-drug-FDA-approval](#)

September 24, 2018

Cost of Clinical Trials for New Drug FDA Approval Are Fraction of Total Tab

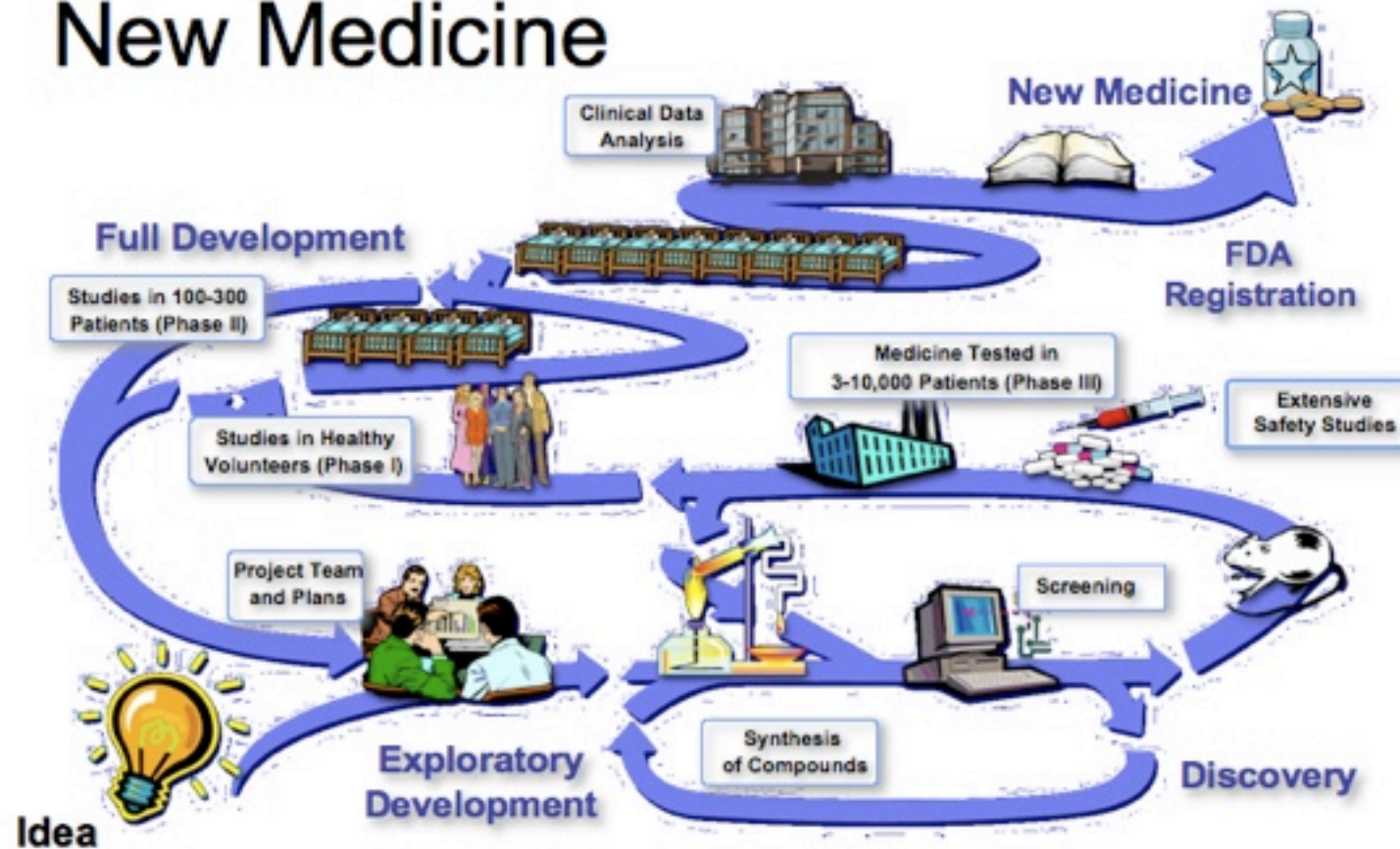
CLINICAL TRIALS TO OBTAIN FDA APPROVAL TYPICALLY ACCOUNT FOR SMALL PROPORTION OF TOTAL DRUG RESEARCH AND DEVELOPMENT COSTS, STUDY SUGGESTS.

Clinical trials that support FDA approvals of new drugs have a median cost of \$19 million, according to a new study by a team including researchers from Johns Hopkins Bloomberg School of Public Health.

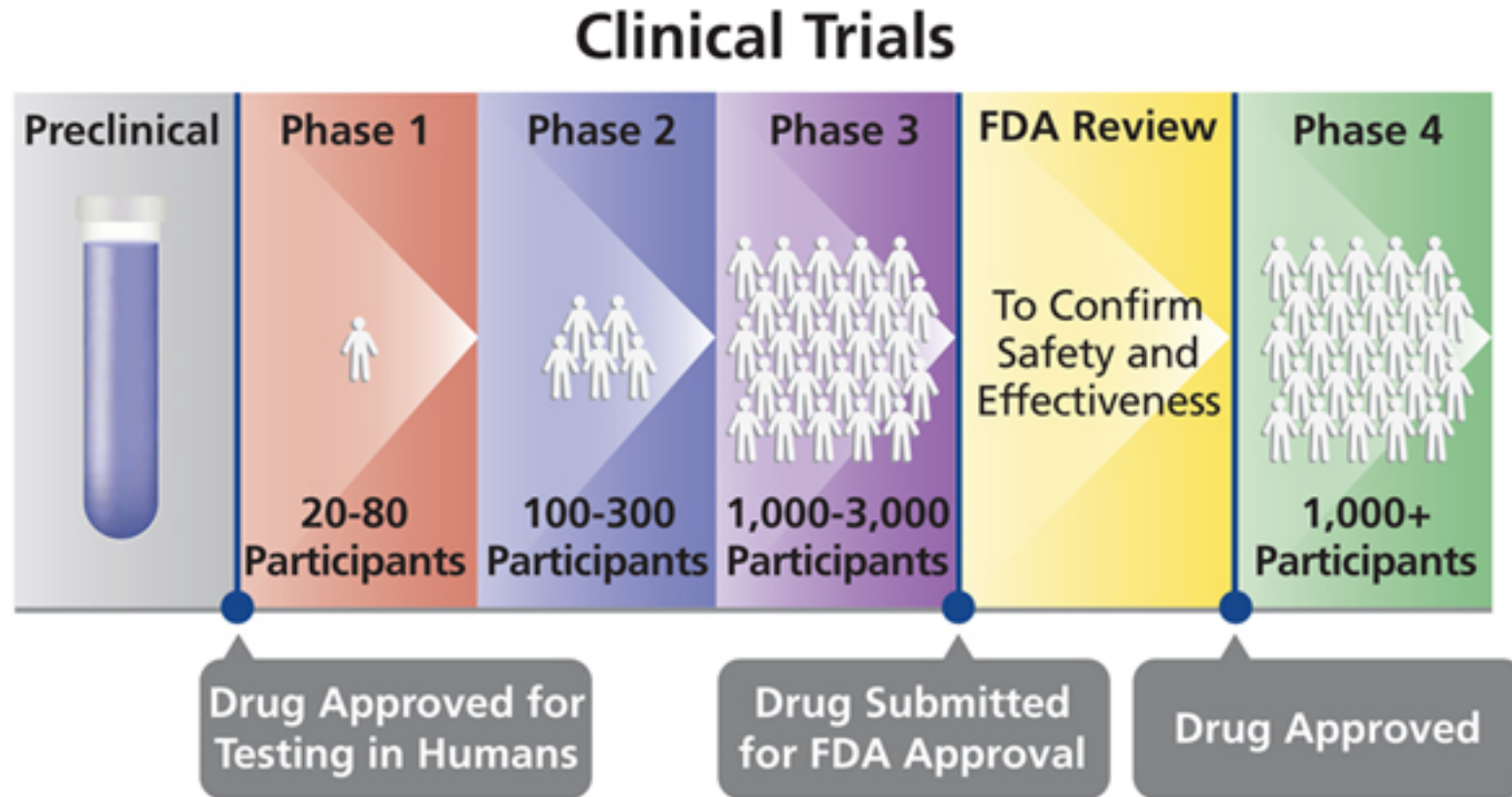
The \$19 million median figure represents less than one percent of the average total cost of developing a new drug, which in recent years has been estimated at between \$2 to \$3 billion.

Drug Discovery

The Long Road to a New Medicine



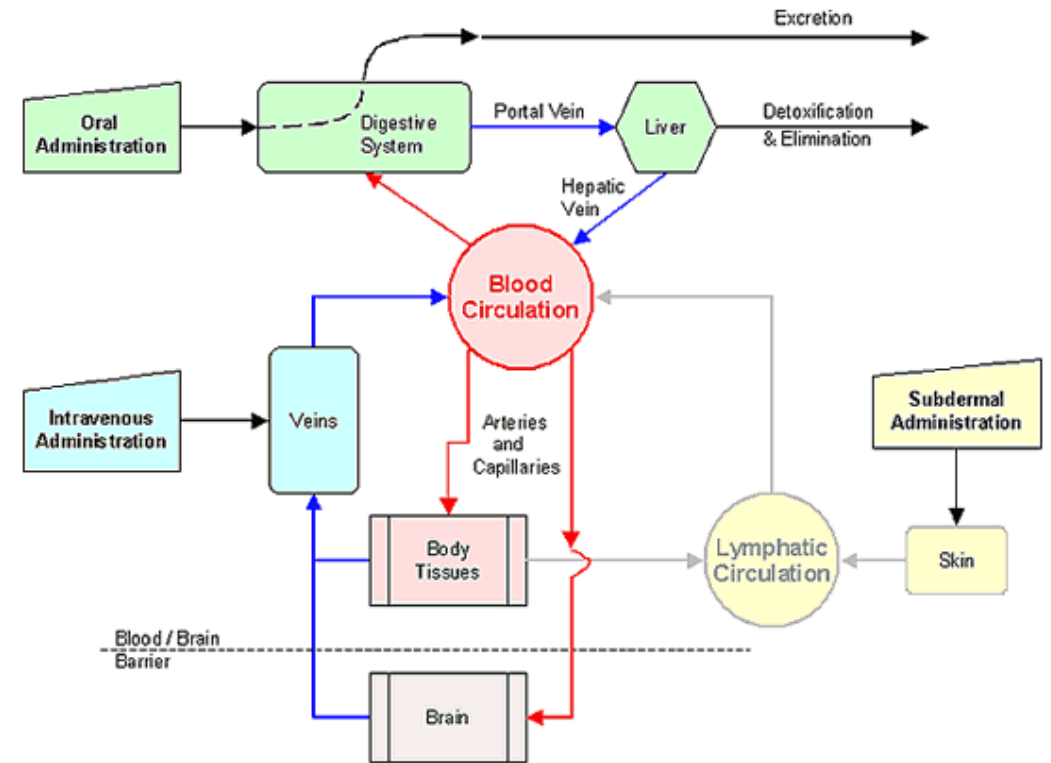
Clinical Trials



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Drug Binding Basics

- Receptor
 - $R + L \leftrightarrow R.L$
- Enzyme (cofactors, ions ..)
 - $E + A + B \leftrightarrow E + C + D$
 - inhibitors: nb binding
- Drugs
- **A**dsorption, **D**istribution, **M**etabolism and **E**limination



Methods of Drug Delivery
Copyright © CLL Topics, Inc., 2003

Drug-sized molecule bound to a protein

