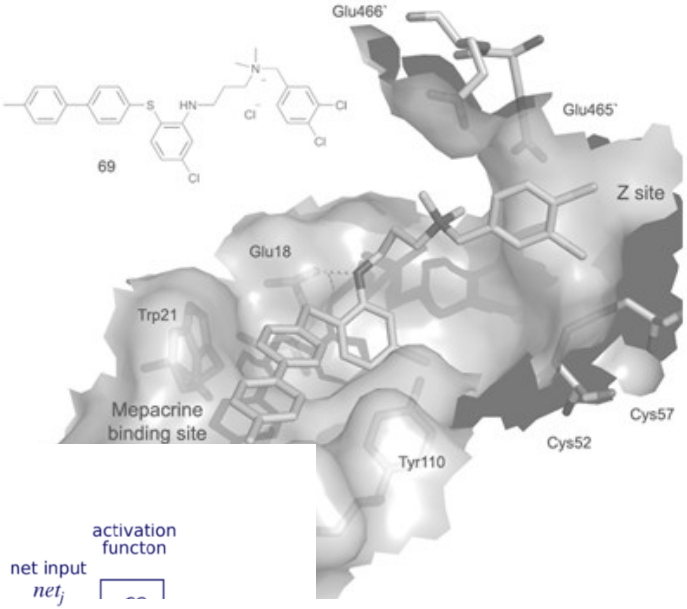
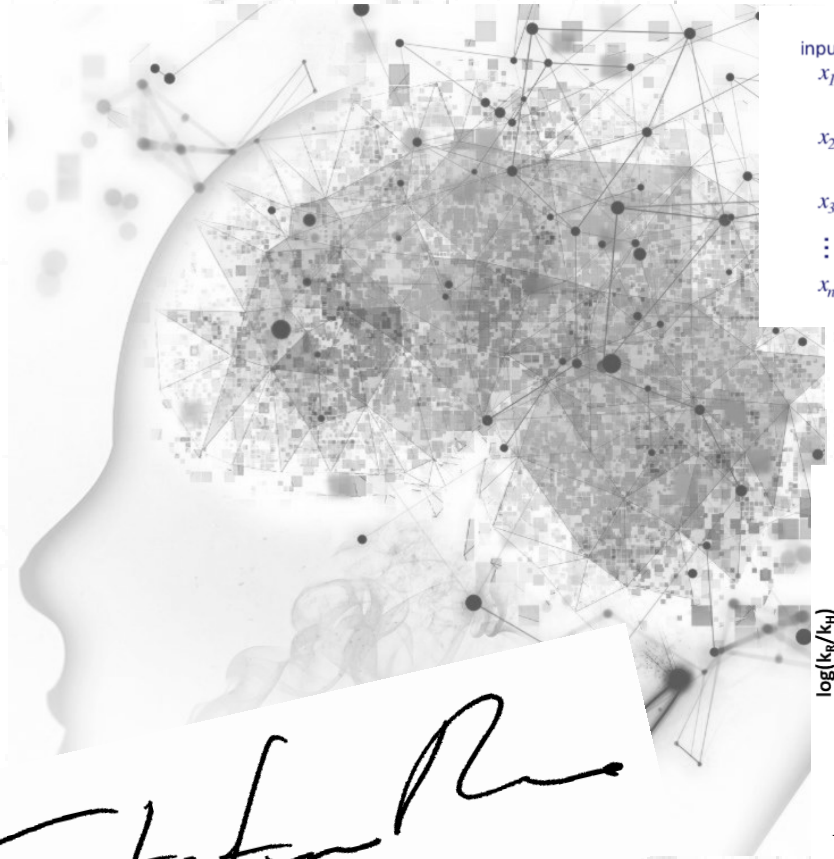
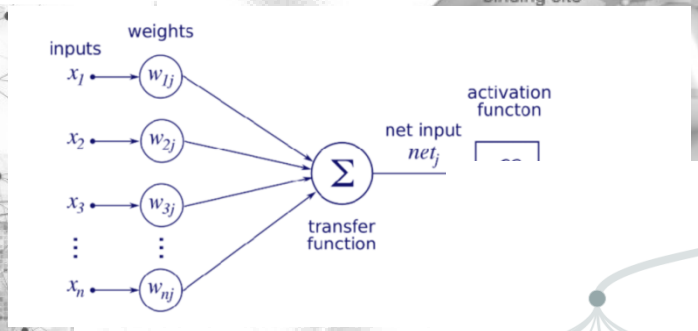
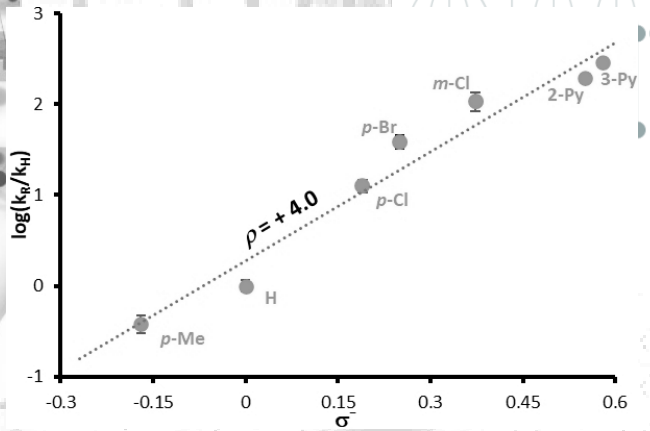
Introduzione ai metodi di Intelligenza Artificiale...









http://mms.dsfarm.unipd.it

https://unipd.zoom.us/j/82254597077

Ecco come organizzeremo il nostro viaggio…

http://mms.dsfarm.unipd.it

Cerca

UNIVERSITÀ DEGLI STUDI DI PADOVA

MMS Molecular Modeling Section

Department of Pharmaceutical and Pharmacological Sciences, University of Padova

Via Marzolo 5, 35131 Padova (Italy) - phone: +39 049 8275704, fax: +39 049 8275366

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News & Updates

MMS: Events

June-July, 2025
ESMEC 2025 - European School of Medicinal Chemistry – 44th Edition... *more*

MMS: Latest Hot Publication

Dodaro A et al. "Post-Docking Refinement of Peptide or Protein-RNA Complexes Using Thermal Titration Molecular Dynamics (TTMD): A Stability Insight." JCIM (2025) *more...*

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Cerca

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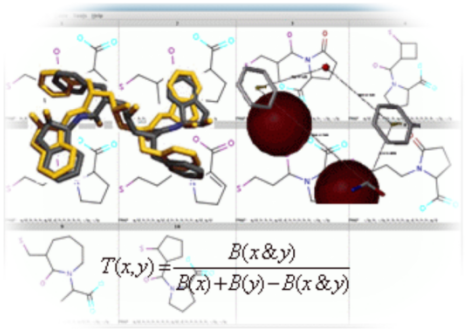
Obbiettivi del percorso formativo:

Il Corso si propone di fornire allo studente le conoscenze di base sulle moderne metodologie informatiche applicate alla chimica ed in particolare alla chimica farmaceutica che trovano oggigiorno una interessante applicazione nell'ambito della progettazione ed ottimizzazione di nuovi farmaci.



1. Introduzione alla chemoinformatica

2. Rappresentazione e archiviazione molecolare

3. Descrittori molecolari e introduzione relazioni quantitative struttura-attività (QSAR)

Per coloro che ancora non si fossero stressati abbastanza, ecco alcuni suggerimenti per procurarsi gratuitamente un "visualizzatore molecolare" per poter continuare a giocare anche in futuro:

1. Chimera (UCSF)	
2. DataWarrior	
3. ChatGPT	

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http://mms.dsfarm.unipd.it

Welcome to the **Molecular Modeling Section (MMS)** of the Department of Pharmaceutical and Pharmacological Sciences, at the University of Padova in Italy. Our mission is to develop and apply new IT and computational methodologies to speed up the identification and development of new drug candidates through the creation of collaborative interfaces with synthetic chemistry, biochemistry and biology, pharmacology, and different medical disciplines.

In the spirit of the motto "interdisciplinarity is dialog" the aim of the MMS is to face computational medicinal chemistry and therapeutic needs in collaboration with all field experts… not mixing our expertise but summing them up.

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I nostri compagni di viaggio:

… il mio personale suggerimento:

WIKIPEDIA
The Free Encyclopedia

ChatGPT

Menù (turistico) del nostro percorso di IA@DSF

•Parte prima: chemioinformatica

Rappresentazioni e descrittori molecolari; relazioni quantitative struttura-attività (QSAR): modelli lineari, modelli multivariati, alberi decisionali e approcci classificativi; approcci non lineari ; introduzione alle reti neurali e loro evoluzioni

•Parte seconda: applicazioni

…

Let's try to give a shared and shareable definition of "chemoinformatics": Indeed, better.. we use the one that Frank K. Brown gave in 1998.

*"Chemoinformatics is the mixing of those information resources to transform **data** into **information** and information into **knowledge** for the intended purpose of making **better** and **faster decisions** in the area of drug lead identification and optimization."*

F.K. Brown Chapter 35. Chemoinformatics: What is it and How does it Impact Drug Discovery. Annual Reports in Med. Chem., Ed. James A. Bristol, 1998, Vol. 33, pp. 375.

Before starting our adventure we must remember that: *Houston we've still had a problem!*

Drug discovery statistics:

https://www.nature.com/articles/d41573-025-00001-5

nature reviews drug discovery

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nature > nature reviews drug discovery > news > article

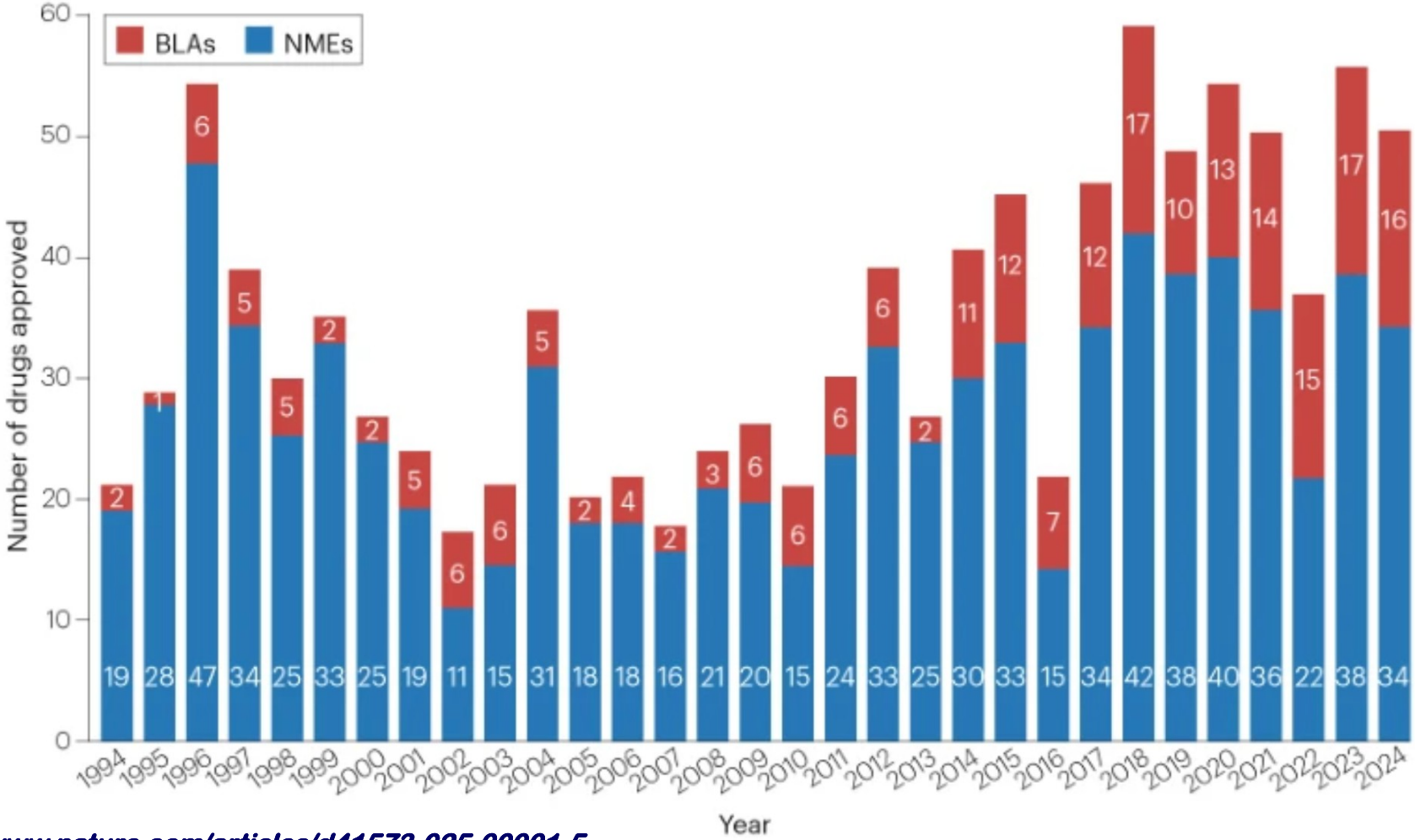
NEWS | 02 January 2025 | Update 20 January 2025

2024 FDA approvals

The FDA approved 50 new therapeutics in 2024, with green lights for a novel schizophrenia drug, a first NASH medicine and much more.

By Asher Mullard

Houston, we've had a problem here!



https://www.nature.com/articles/d41573-025-00001-5

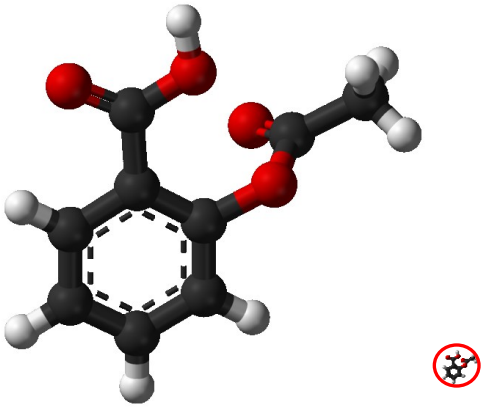
A very general introduction:

(I don't want to be offensive to show you this slide)

Vintage drugs

ASPIRINE

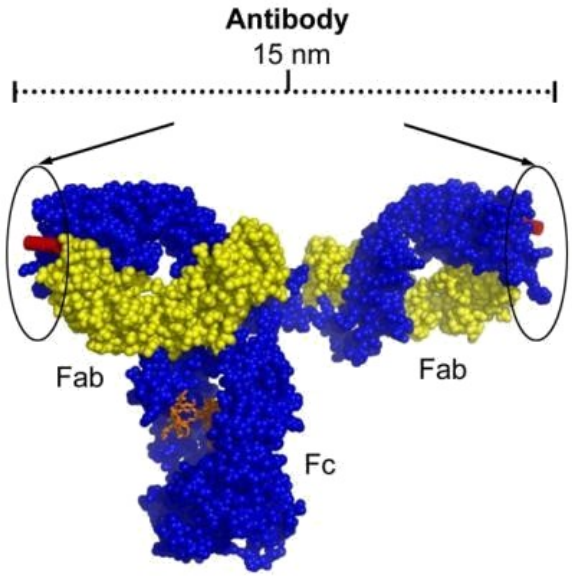
1. small molecule
2. 180 Da
3. 21 atoms
4. usually not immunogenic
5. usually chemically stable



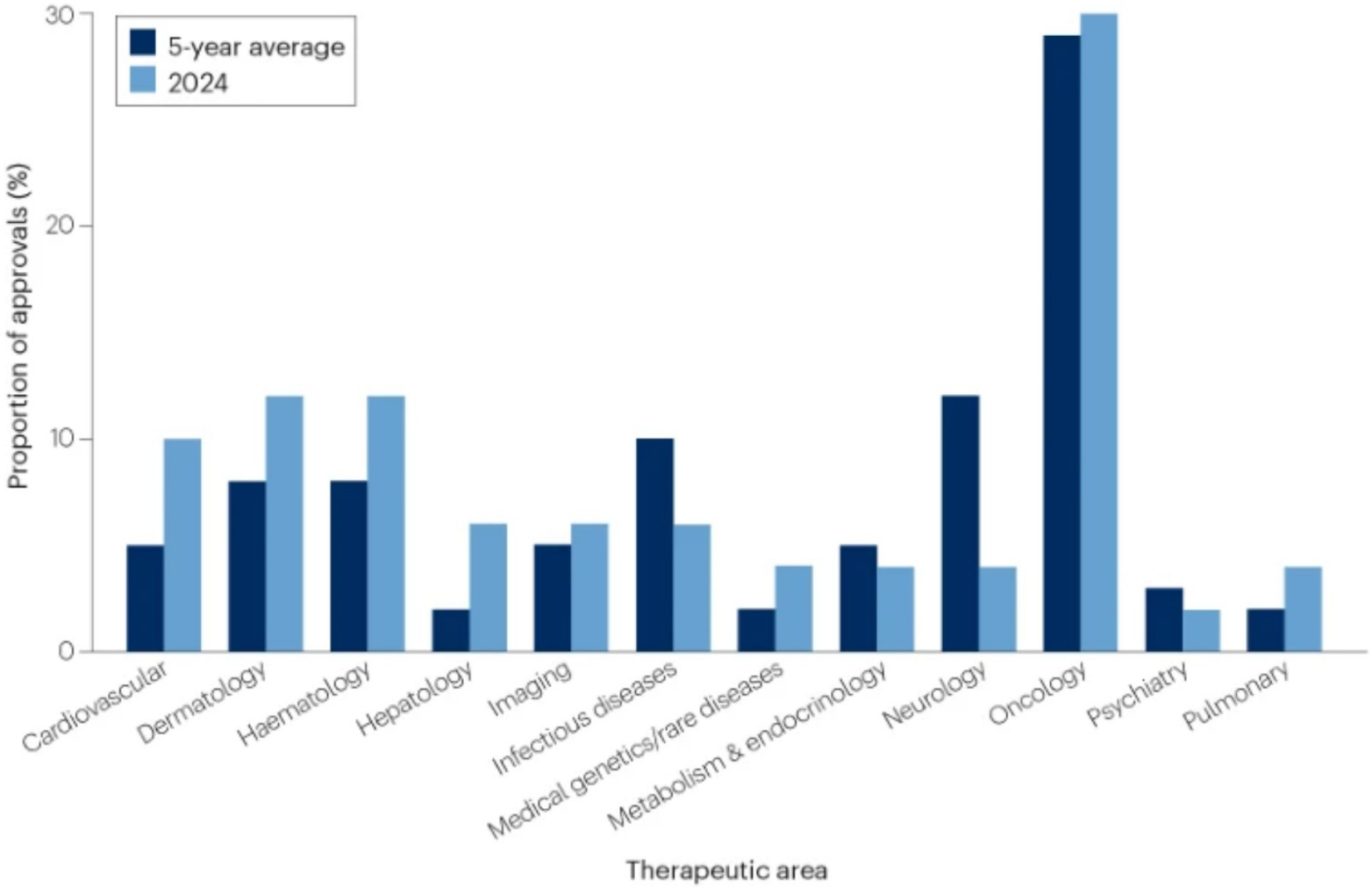
New age (biotech) drugs

MONOCLONAL ANTIBODY (mAb)

1. macromolecule
2. 150˙000 Da
3. 20˙000 atoms
4. usually immunogenic
5. usually chemically instable

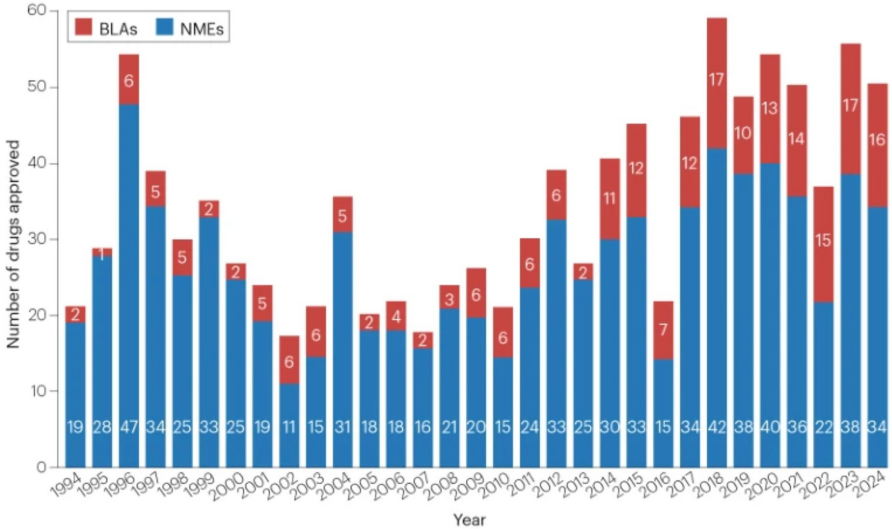


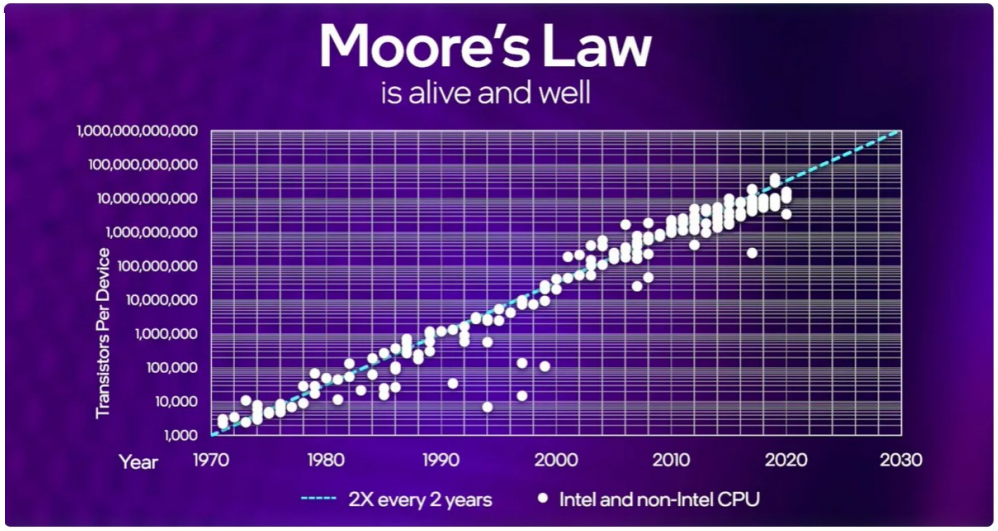
Houston, we've had a problem here!



https://www.nature.com/articles/d41573-025-00001-5

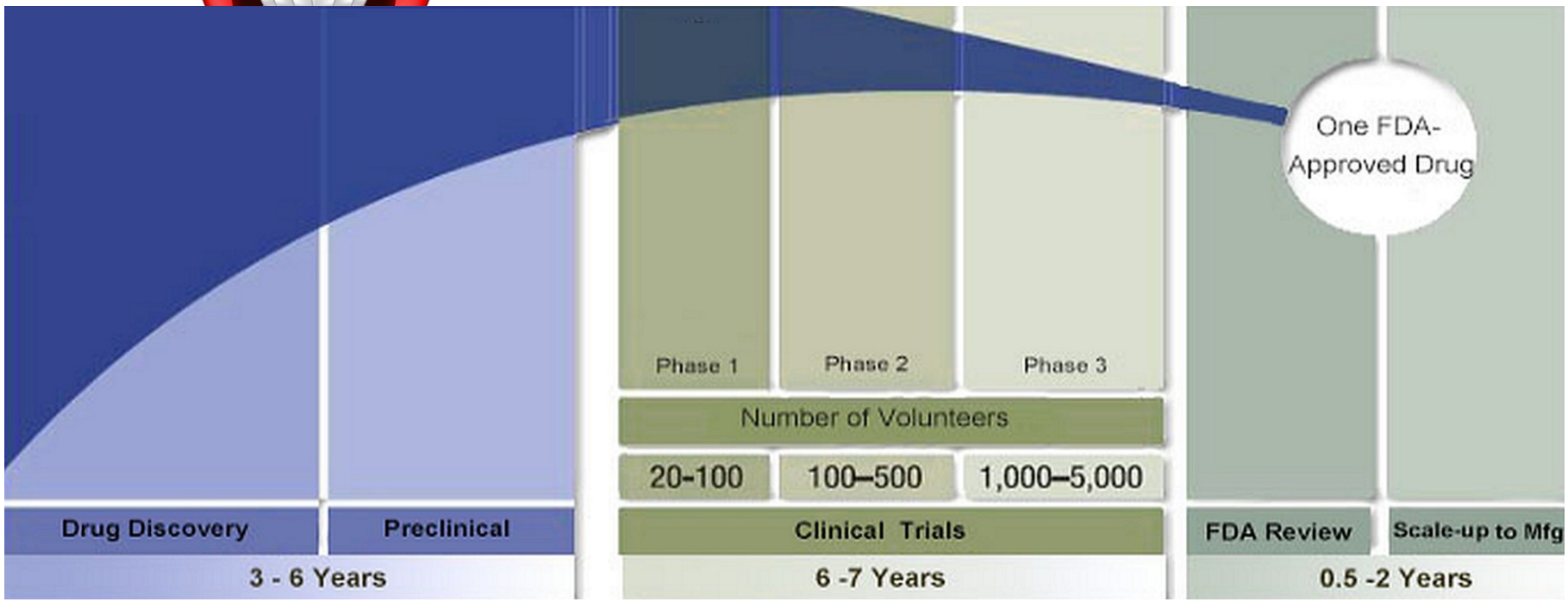
we can stop for a second and reflect together?





https://www.cnet.com/tech/computing/intel-will-outpace-moores-law-ceo-pat-gelsinger-says/

What you already know very very well: the long history of the birth of a drug…



Bringing a new drug to market can take 8-14 years and costs between $400 and $1000 million (even more!!!)

Why we need *"chemoinformatics"* in pharma business?

xx.000 to 1?

Is this ratio really acceptable for a pharma company?

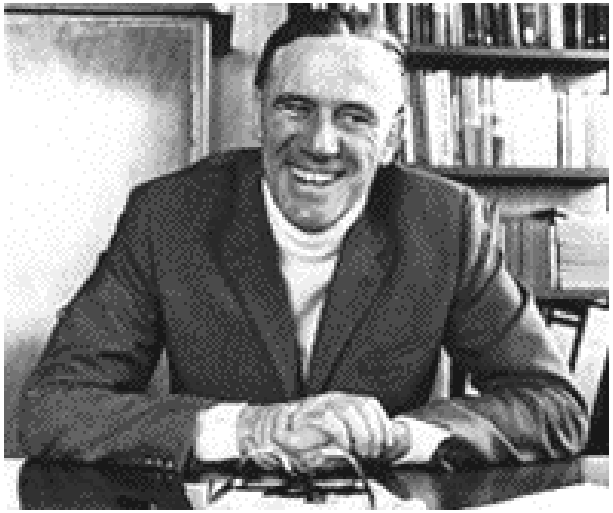
Indeed, better... we use the one that Frank K. Brown gave in 1998:

*"Chemoinformatics is the mixing of those information resources to transform **data** into **information** and information into **knowledge** for the intended purpose of making **better** and **faster decisions** in the area of drug lead identification and optimization."*

F.K. Brown Chapter 35. Chemoinformatics: What is it and How does it Impact Drug Discovery. Annual Reports in Med. Chem., Ed. James A. Bristol, 1998, Vol. 33, pp. 375.

again an egoistic definition of *informatics*:

In 1957 the German computer scientist Karl Steinbuch coined the word *Informatik* by publishing a paper called *"Informatik: Automatische Informationsverarbeitung" (Informatics: Automatic Information Processing).*



It is not sufficient to invent something. You need to recognize, that you have invented something.

Karl Steinbuch

K. Steinbuch: INFORMATIK: Automatische Informationsverarbeitung. SEG-Nachrichten Heft 4/1957

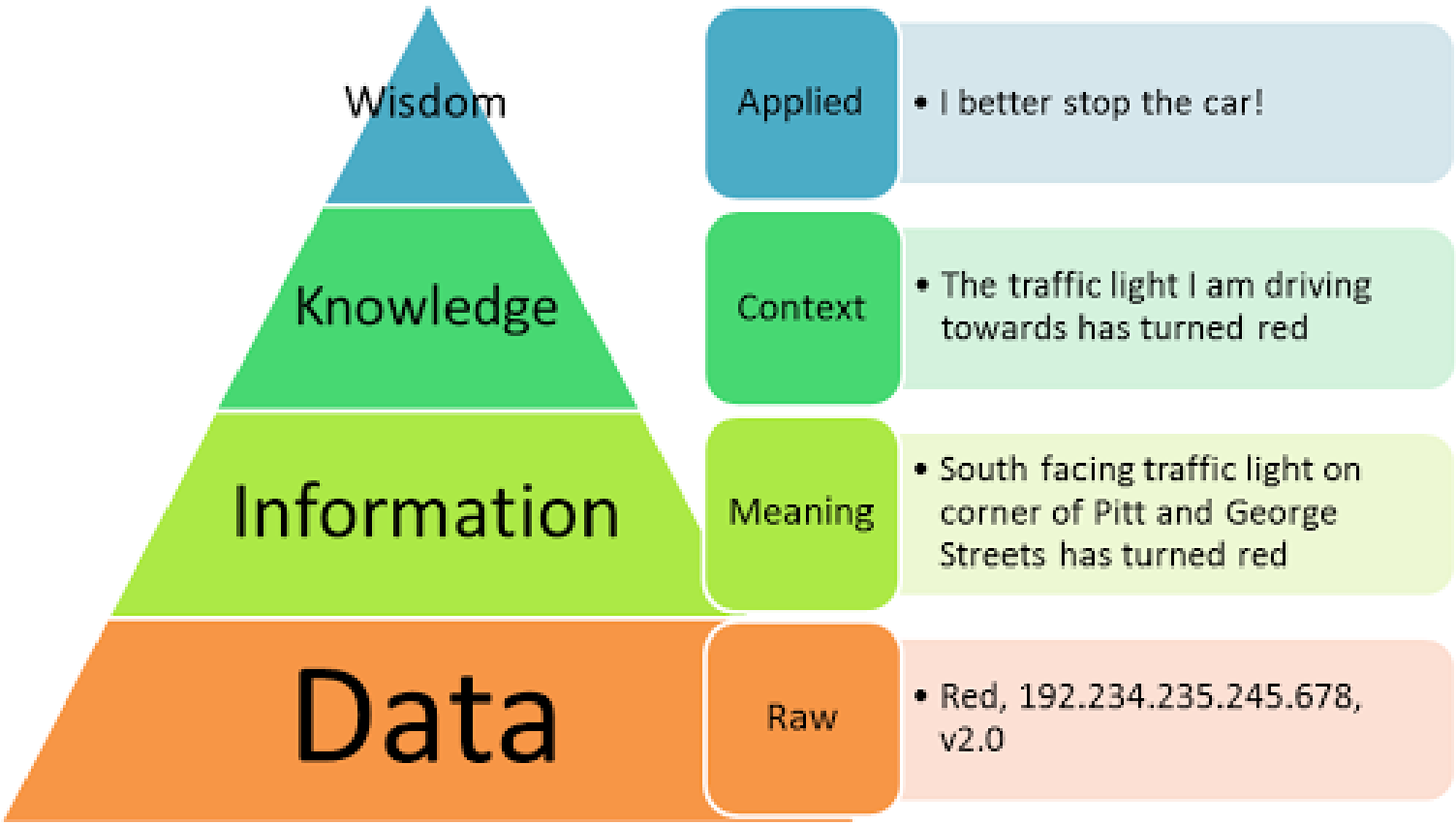
again an egoistic definition of informatics:

Informatics:

Informatics is, in its most general sense, the ***science of information***.

I didn't fond a better (and egoistic) representation of this definition that this:

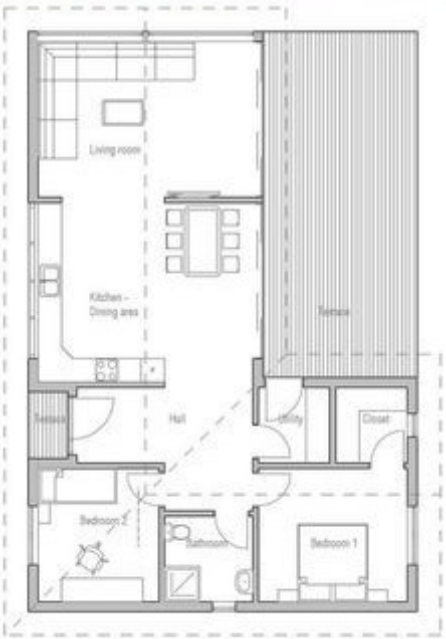
The DIKW pyramid… intriguing!



Rowley, Jennifer (2007). "The Wisdom Hierarchy: Representations of the DIKW Hierarchy". Journal of Information and Communication Science. 33 (2): 163–180.

Informatics is the basic science of any *virtualization* process:

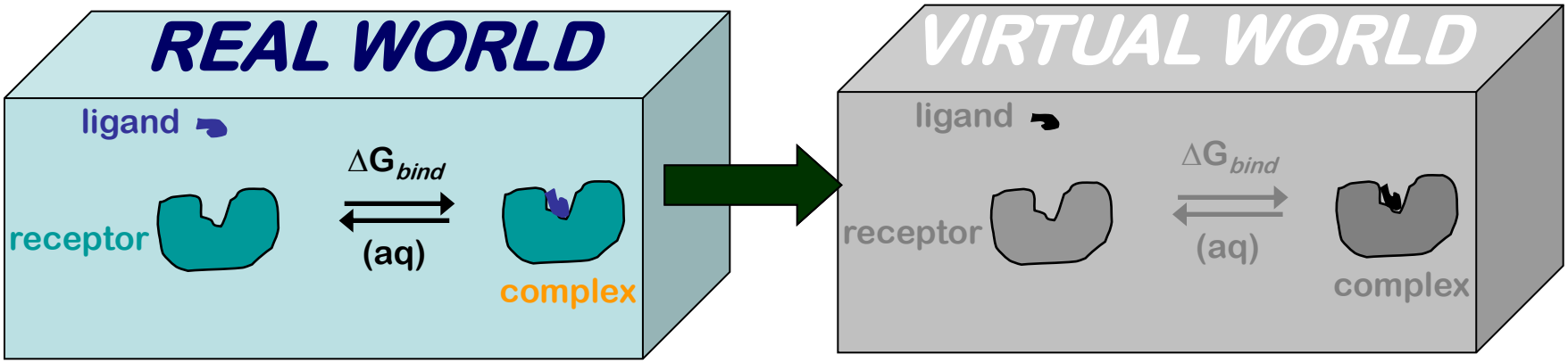
REAL WORLD



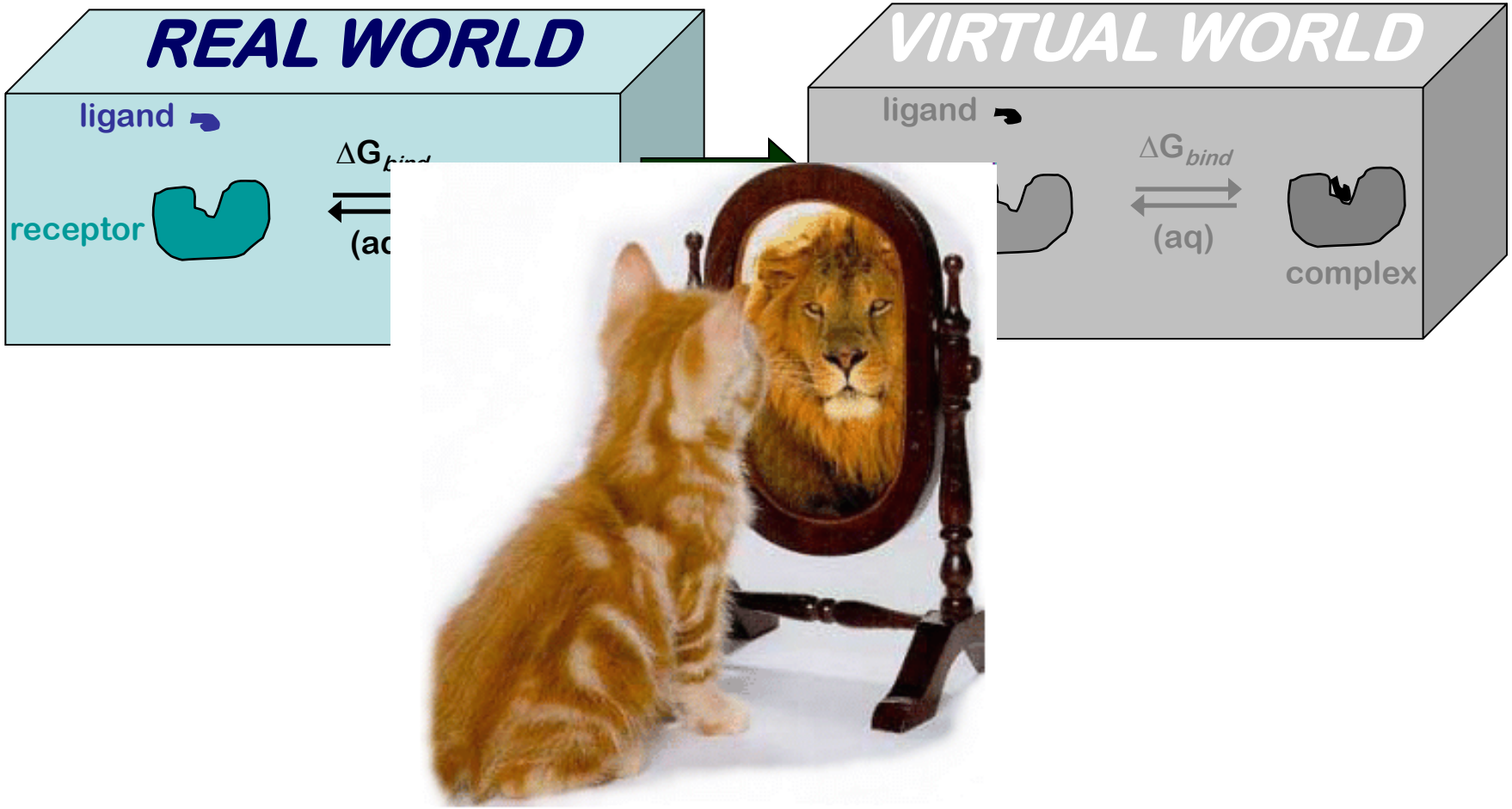
VIRTUAL WORLD

Informatics is the basic science of any *virtualization* process:

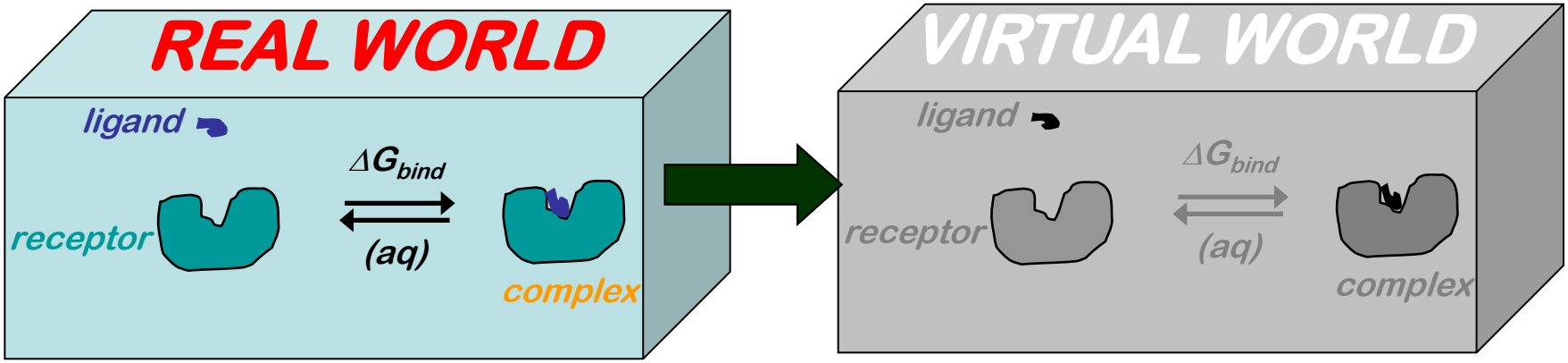
From an informatics point of view, any compu tool is a *virtualization process*: the creation of a virtual version of the real process.

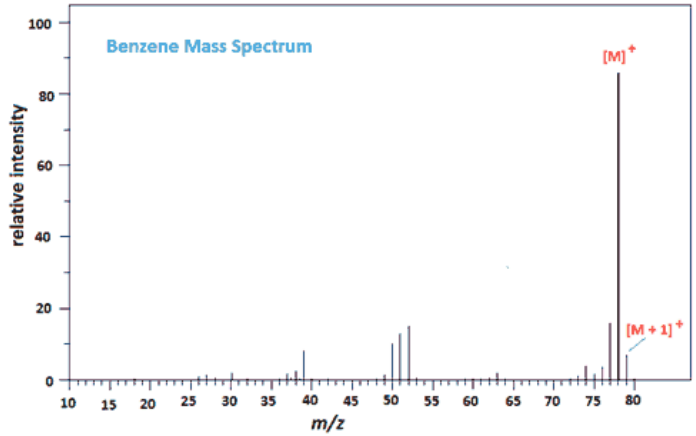


The *accuracy* of this virtualization process is crucial:



My favorite example:





Q: determine the molecular weight of benzene?

A:

C6H6

Hydrogen (H) 1.00794 atomic mass

Carbon (C) 12.0107 atomic mass

Molecular weight calculation:

*12.0107*6 + 1.00794*6*

= 78.11184 g/mol

Now, in what informatics has influenced more in our daily life?

Well, we probably summarize the answer in only one word:

Time

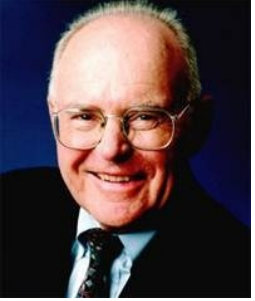
couple of concrete example…

Informatics helps us to solve simple problems a number of times:

Calculate the molecular weight is trivial thing, calculate 10 millions … less!

or solve very complex problems:

Anticipate, the human hepatotoxicity (liver toxicity) of a chemical (drug candidate)!



Informatics as synonymous of speed?

Moore, Gordon E. (April 19, 1965). "Cramming more components onto integrated circuits" (PDF). intel.com. Electronics Magazine. Archived (PDF) from the original on March 27, 2019. Retrieved April 1, 2020.

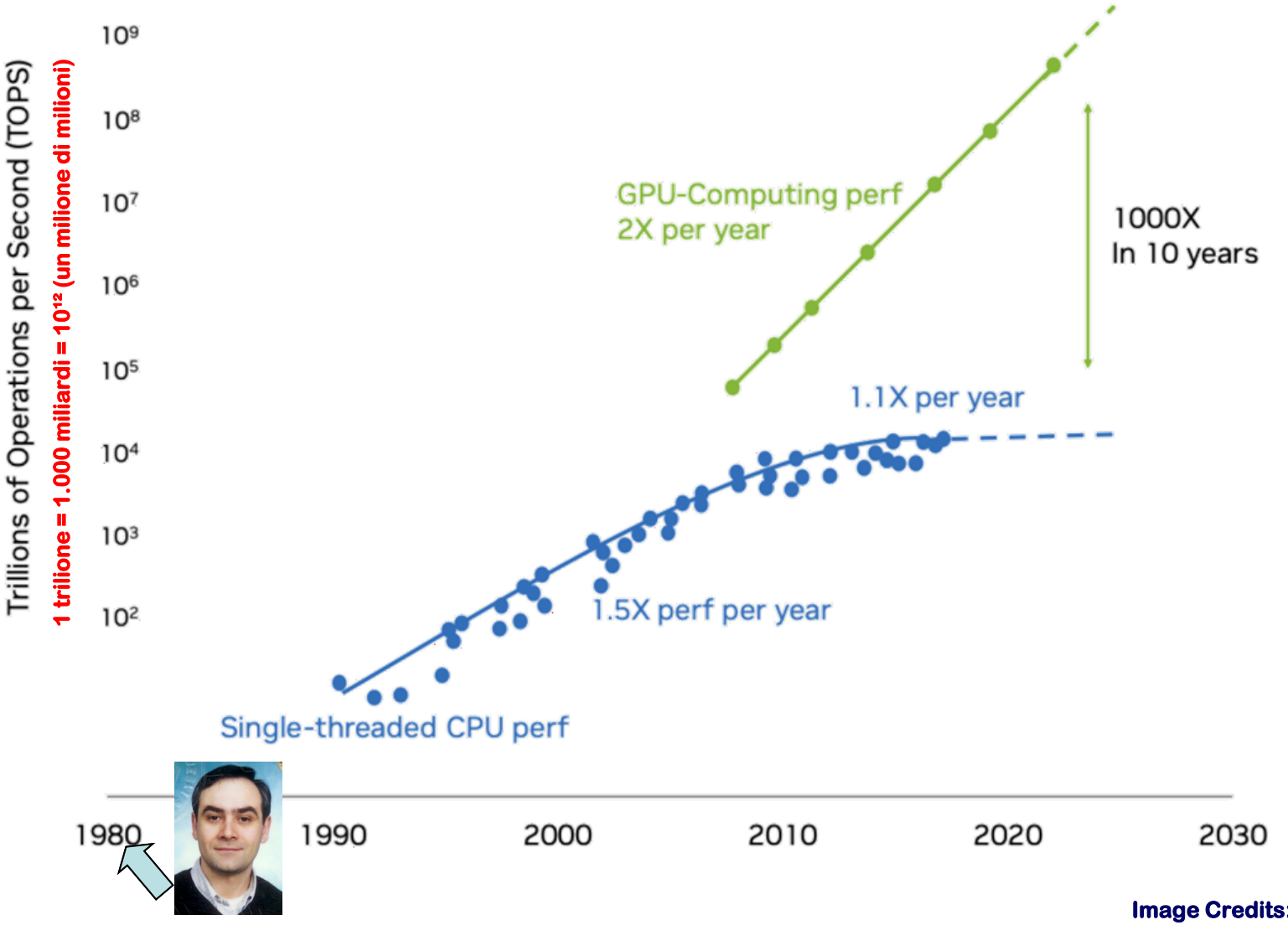


Image Credits: Nvidia

This was my first PC… and as a monitor I used my TV !!!

just for informatics addicted!

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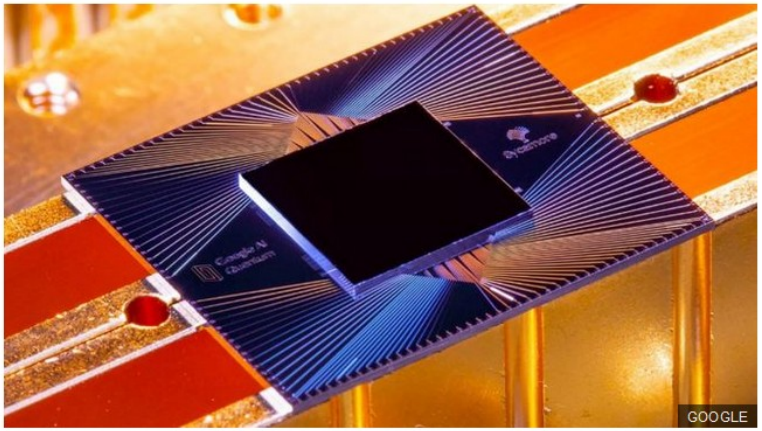
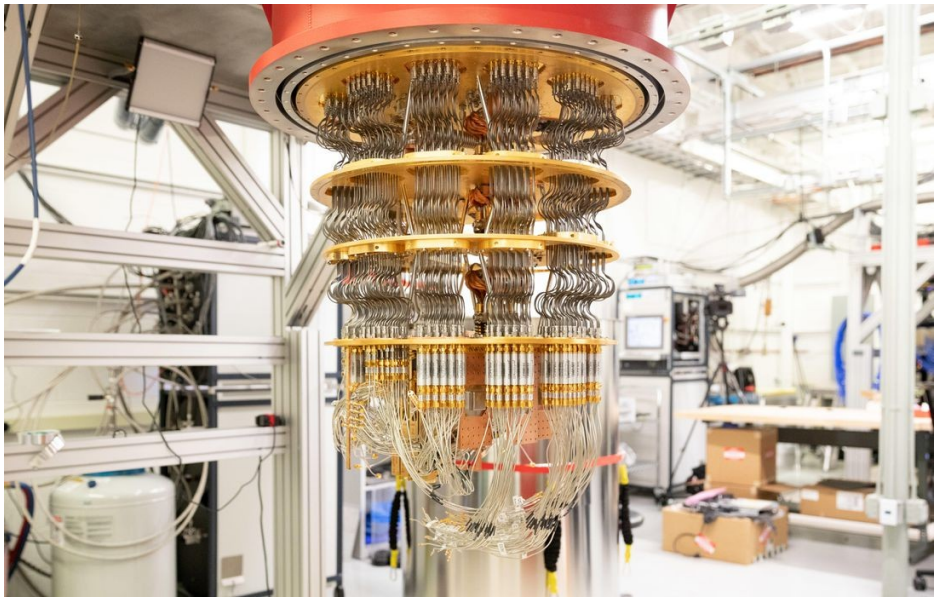
Science & Environment

Google claims 'quantum supremacy' for computer

By Paul Rincon
Science editor, BBC News website

23 October 2019 | Share





The technology giant's Sycamore quantum processor was able to perform a specific task in 200 seconds that would take the world's best supercomputer 10,000 years to complete.

To be update: https://thequantuminsider.com/

and remember… “Time is money!”

Some details about costs:

Experiment Typical Cost per Compound (€)

Computer modeling	7
Biochemical assay	270
Cell culture assay	2.700
Rat acute toxicity	8.100
Protein crystal structure	68.000
Animal efficacy trial	200.000
Rat 2-year chronic oral toxicity	550.000
Human clinical trial	3.500.000

You understand why it is so attractive to the pharmaceutical industry?

TITLE
“INTRODUZIONE ALLA IA NELLE SCIENZE DEL FARMACO”
DIRECTOR
Stefano Moro
CAMERA
Dipartimento di Scienze del Farmaco
DATE
SCENE
TAKE