Quantum computing – a new approach to study human disease patterns?

2019-11-21
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Bayer Group Structure

Board of Management

Pharmaceuticals

// Prescription drugs

Consumer Health

// Over-the-counter medicines, dietary supplements, dermatology products, foot care and sunscreen

Crop Science

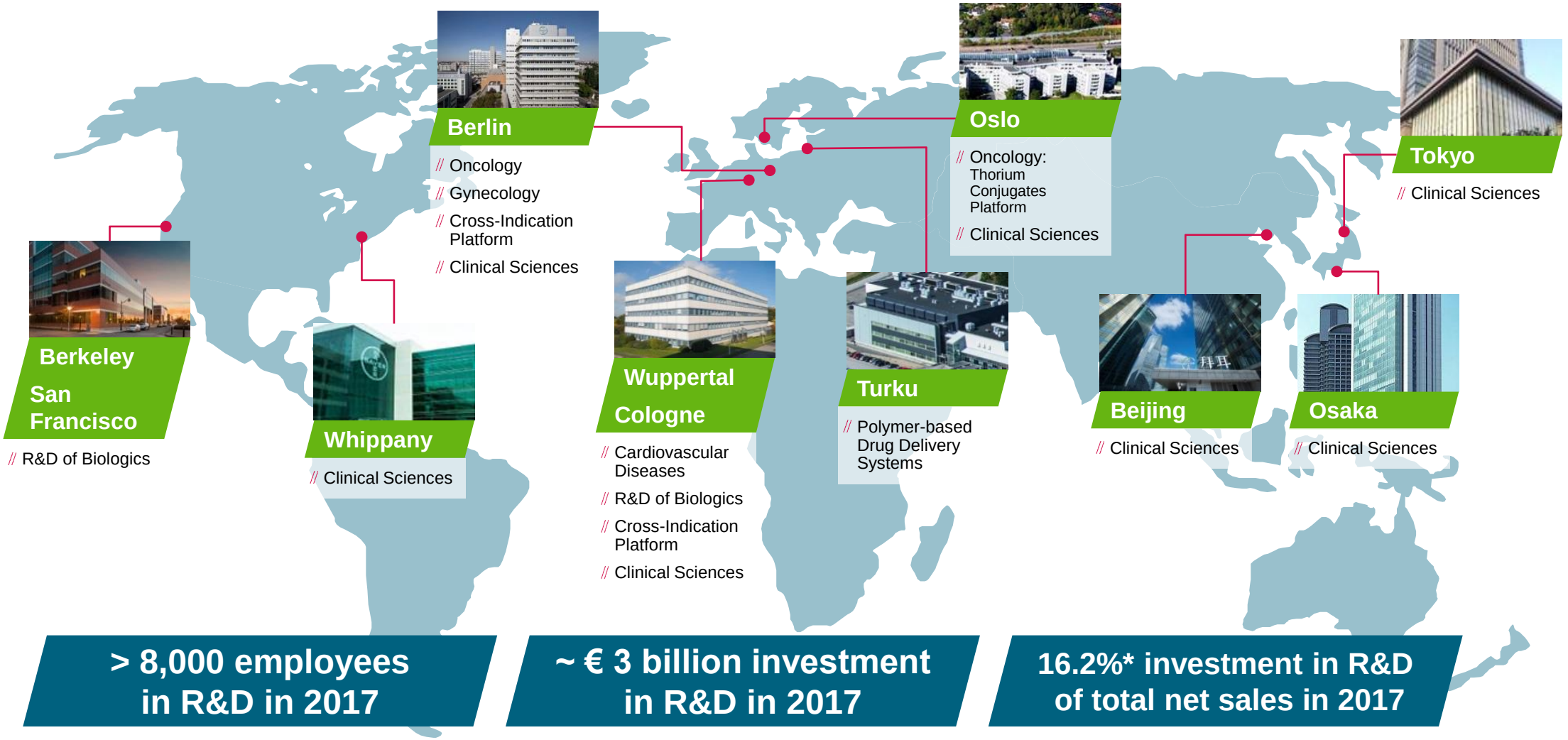
// Innovative chemical & biological crop protection, seeds & traits, digital technologies & services

Animal Health

Corporate Functions & Business Services

Currenta (60%)

Our global drug discovery network



Berlin
- // Oncology
- // Gynecology
- // Cross-Indication Platform
- // Clinical Sciences

Oslo
- // Oncology: Thorium Conjugates Platform
- // Clinical Sciences

Tokyo
- // Clinical Sciences

Berkeley
San Francisco
- // R&D of Biologics

Whippany
- // Clinical Sciences

Wuppertal
Cologne
- // Cardiovascular Diseases
- // R&D of Biologics
- // Cross-Indication Platform
- // Clinical Sciences

Turku
- // Polymer-based Drug Delivery Systems

Beijing
- // Clinical Sciences

Osaka
- // Clinical Sciences

> 8,000 employees in R&D in 2017

~ € 3 billion investment in R&D in 2017

16.2%* investment in R&D of total net sales in 2017

* Expenses before special items

Quantum computing – a new approach to study human disease patterns?

Comparative data analysis using HPC and QC to evaluate its potential advantages in structural learning

Better understand disease evolution of patients with more than one disease

Real world evidence generation and QC

Call for Urgency

Current challenges in HealthCare

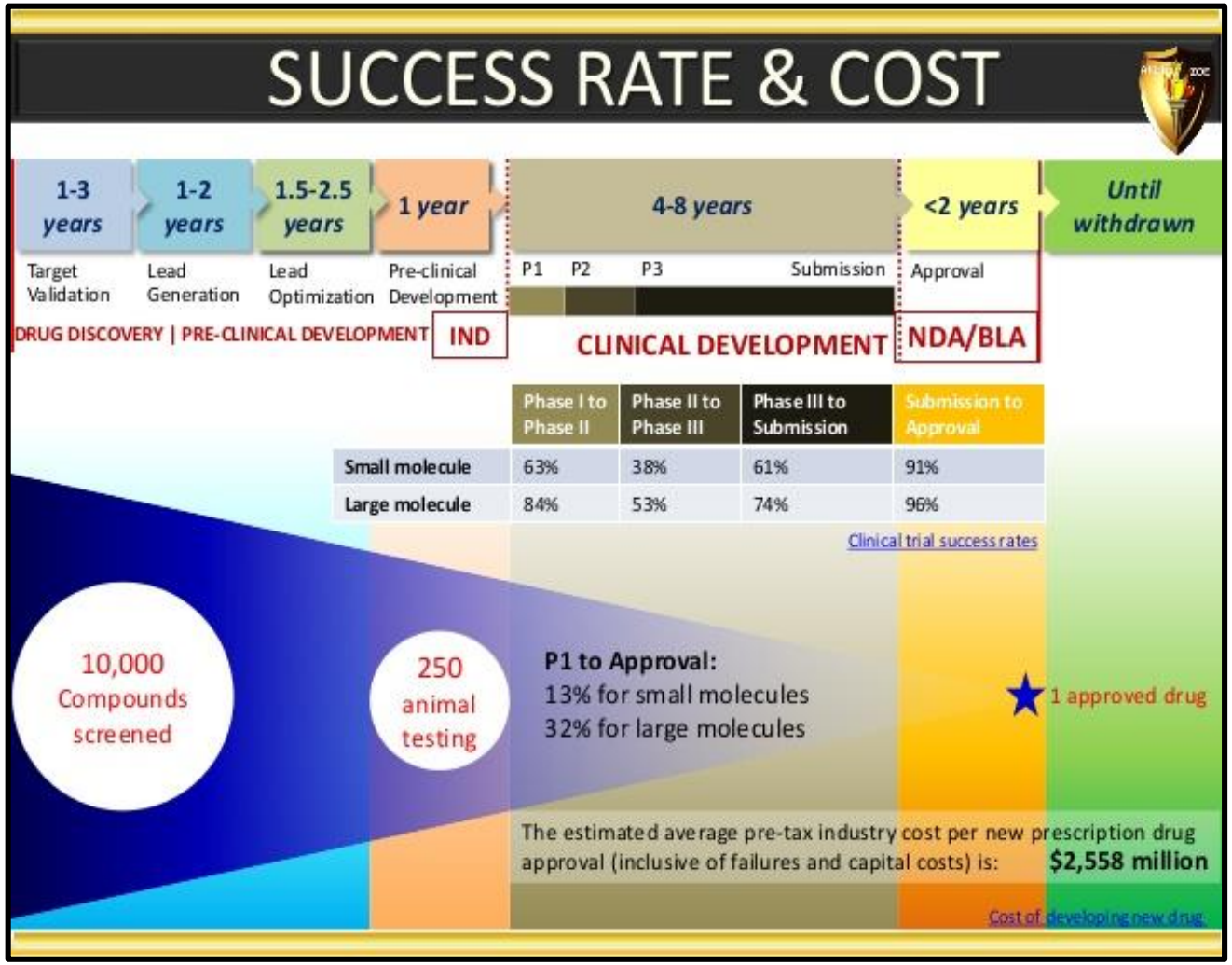
High costs

Probability of success from research to market approval: <1%

Lengthy development process

Late stage failures

3 types of drug responses (beneficial, neutral, harmful) leading to adverse events due to lack of differentiation



Source: Valdova, Veronika. (2015). The potential of utilization of Systems Theoretic Accident Model and Processes (STAMP) in drug development: Hazard identification and risk minimization.. 10.13140/RG.2.1.1925.2242.

Call for Urgency

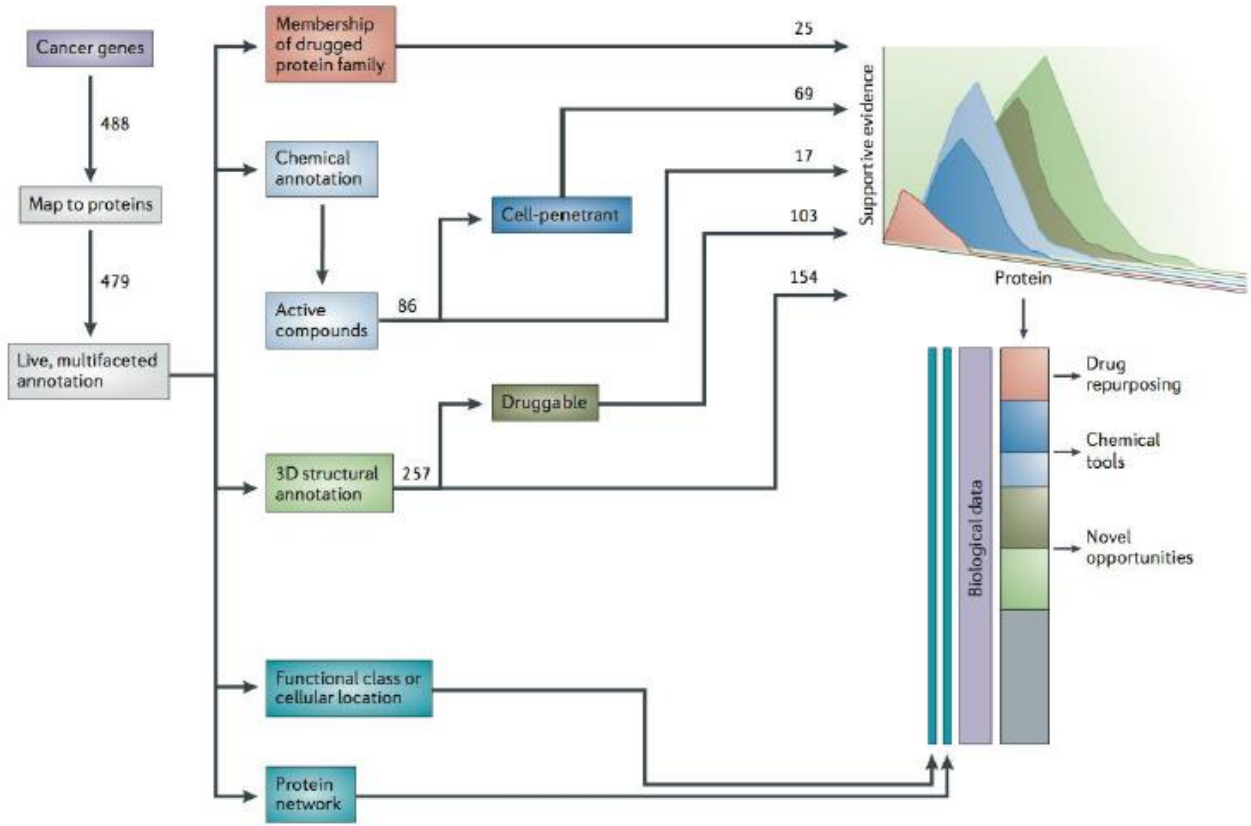
Challenges in HealthCare

DRUGGABILITY AND DRUG DEVELOPMENT

// Complex coordination of biological and chemical frame conditions

// Risk averse approach lead only to small improvements of known molecules cohort

Target Discovery need Multidisciplinary Data Analysis



Source: Patel et al Nature Reviews Drug Discovery (2013) 12:35-50

Call for Urgency

Current challenges in HealthCare

PHARMA INVENTIVENESS AT PLATEAU

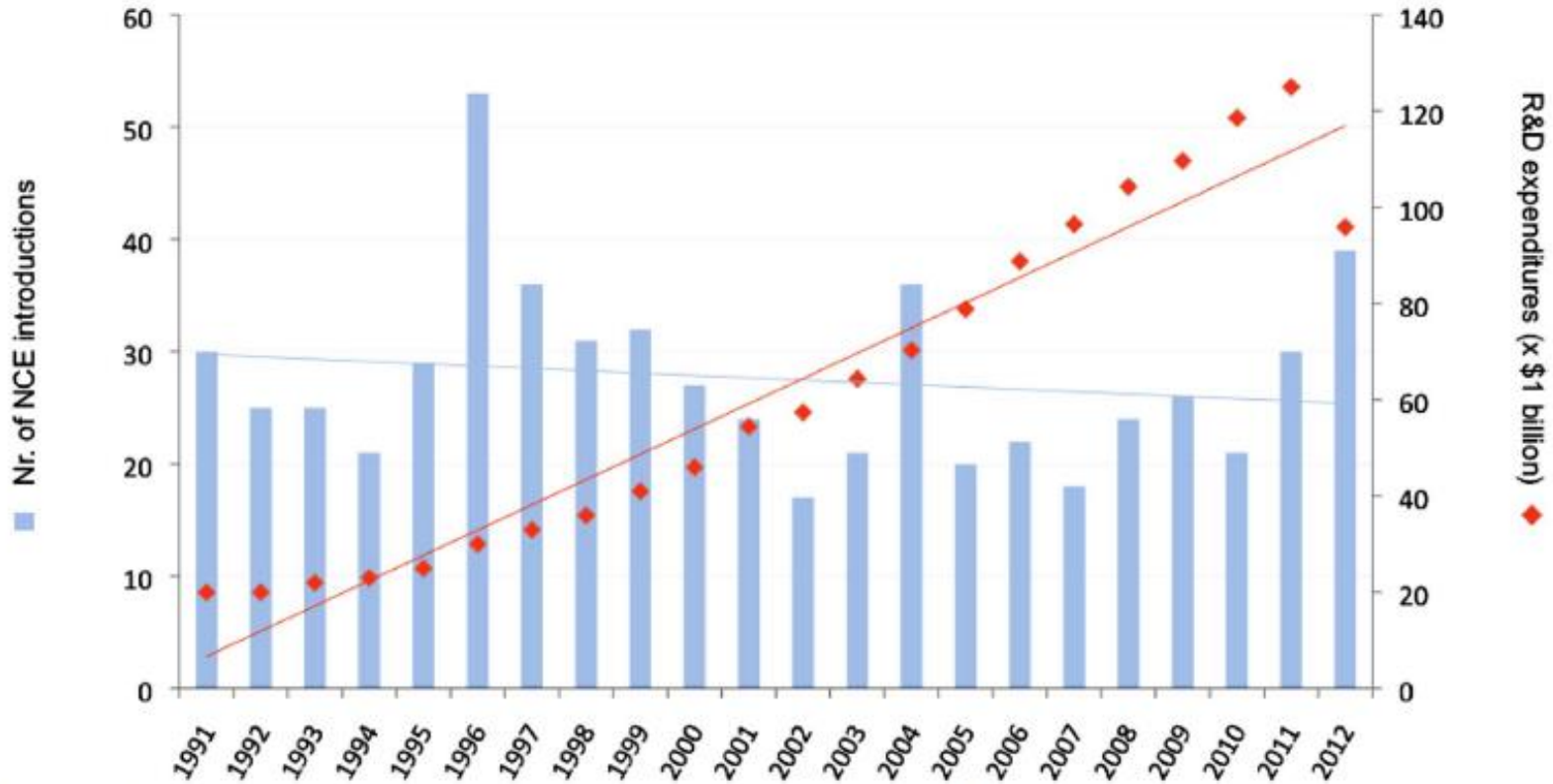


Figure 1. The pharmaceutical "productivity gap"; the considerable rise of R&D expenditures versus a stagnant pattern of New Chemical Entity (NCE) introductions (Data obtained from fda.gov, Medtrack and literature (Drews, 1998; EFPIA)).

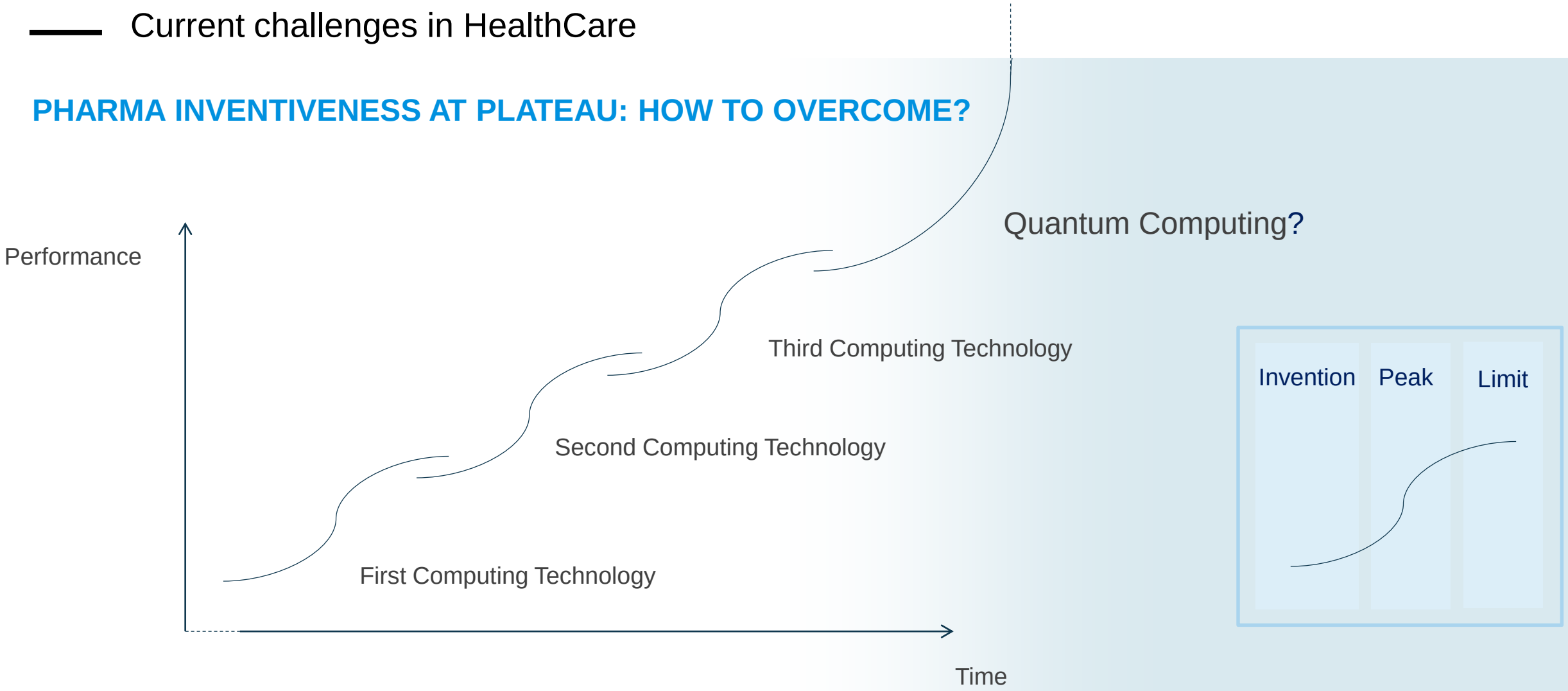
Cost per drug increasing

Source: K. D. S. FERNALD *ET AL*. ***Technology and Investment*, 2013, 4, 168-178**

Call for Urgency

Current challenges in HealthCare

PHARMA INVENTIVENESS AT PLATEAU: HOW TO OVERCOME?



What is QC and why it will change the world?

Google may have just ushered in an era of 'quantum supremacy'

'The first computation that can only be performed on a quantum processor'

Google's 53 Qubits Quantum Computer

https://www.cnet.com/news/ibm-new-53-qubit-quantum-computer-is-its-biggest-yet/

Quantum Computing

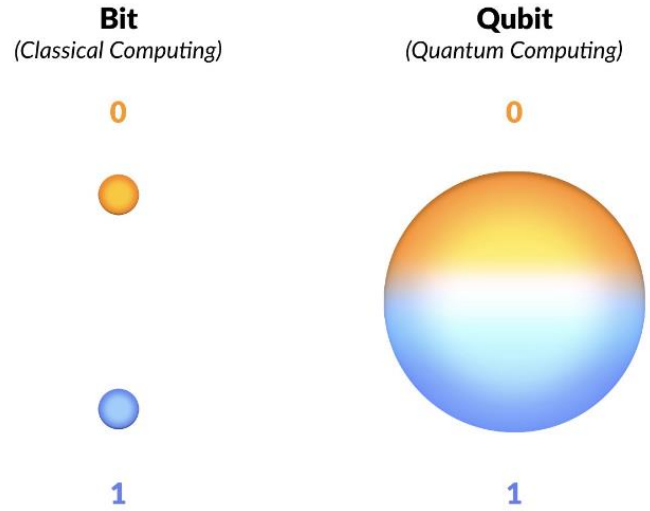
What is QC and what's its potential value?

USP QUANTUM COMPUTING:

- Extreme parallel, by this, Quantum computers could solve problems (optimization, simulation, ML) that in principle could be solved by conventional computing, but only with an unrealizable amount of time.

- Operating at Quantum Level under Quantum mechanics
  - **Superposition**
  - Entanglement
  - Tunneling

DOING IN MINUTES WHAT WOULD OTHERWISE TAKE THOUSANDS OF YEARS



Quantum Computing

Basics

QC BASICS: OPERATING AT QUANTUM LEVEL UNDER QUANTUM MECHANICS

Three approaches:

QC Annealing

- nodes to be optimized for every problem
- Up to 2000 qubits (unit not comparable to gate based qbits) [D-Wave]

Universal (Gate based) QC

- “comparable” to todays integrated circuit approach
- Up to 72 qubits today, (not sufficient today to solve “error problem” during calculation) [Google]

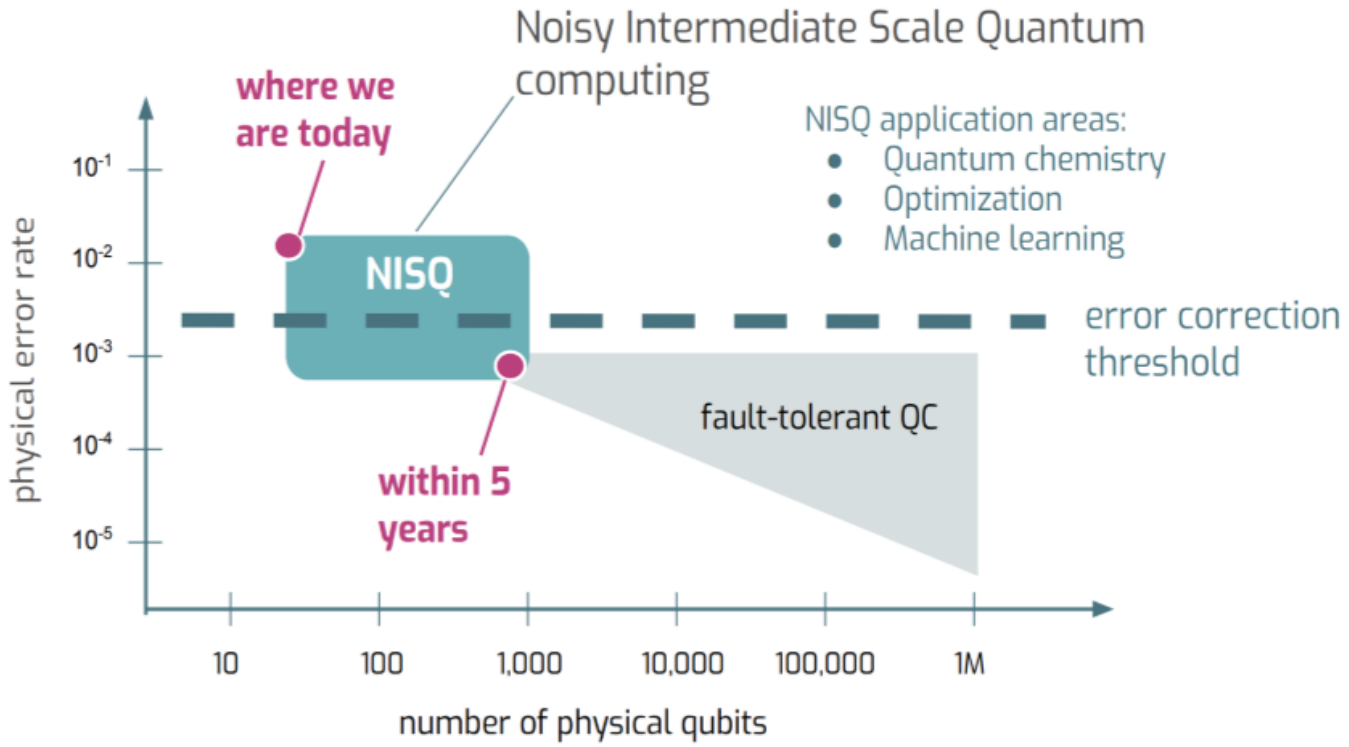
QC Simulation

- Developing future QC algorithms and applications today
- Up to 40 qubits [Atos]

Quantum Computing

Where are we today?

Quantum advantage could be achieved in the next 2-5 years



CBINSIGHTS Source: Rigetti Computing *Quantum advantage is the potential ability of quantum computing devices to solve problems faster than classical computers.

Quantum Computing

Basics – Maturity Grade / Performance

QUANTUM COMPUTERS MATURITY

2018	*128 qubits, Rigetti, US. (announced 8/2018, expected by late 2019)*
2018	72 qubits, Google, US.
2017	50 qubits, IBM, US.
2017	17 qubits, IBM, US.
2006	12 qubits, Institute for Quantum Computing, Perimeter Institute for Theoretical Physics, and MIT.
2000	7 qubits, Los Alamos National Laboratory, US.
2000	5 qubits, Technical University of Munich, Germany.
1998	2 qubits, IBM, UC Berkeley, Stanford University, and MIT, US.
1998	2 qubits, Oxford University, UK.

Source:; MIT, Qubit Counter;

Quantum Computing

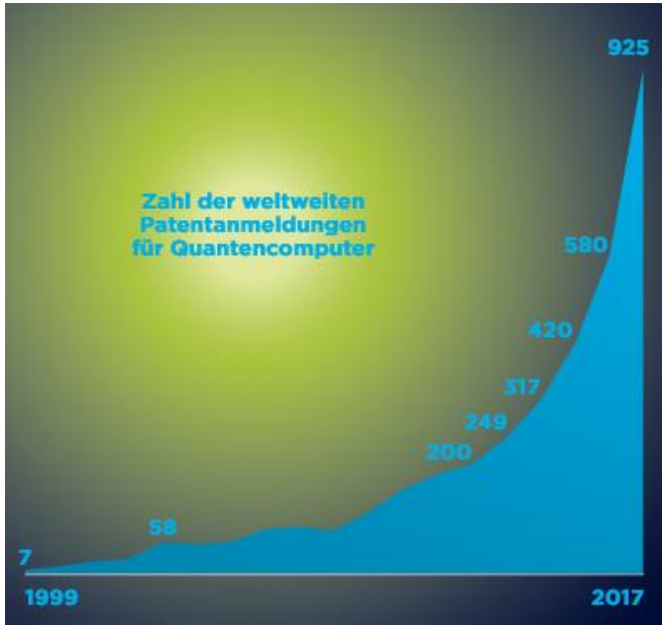
Why should we care?

A noise-free 300-qubit QC could perform more calculations at once (compare more combinations in parallel) than there are atoms in the observable universe*.
These general purpose quantum computer may become available in 5 to 10 years, but Noisy Intermediate-Scale Quantum (NISQ) computer starts to be useful today…drug development and many other optimization problems will be transformed massively:

- trial-and-error approach to identify targets replaced by much more efficient simulation of chemical/biological reactions
- HR: different competencies needed and others to be phased out
- IT infrastructure, needs to be quantum ready for tackling computational hard problems

Companies with access to QC will have tremendous advantage over those being late to the game!

Number of worldwide patent applications for quantum computers



https://www.handelsblatt.com/technik/digitale-revolution/mobilitaet-vw-will-mit-quantencomputern-den-verkehrskollaps-verhindern/25140834.html

*https://www.scientificamerican.com/article/quantum-leaps-in-quantum-computing/

Quantum Computing

Governments are investing in Quantum Computing

- The **United States**: The new National Quantum Initiative Act will give America a national master plan for advancing quantum technologies with a **1.2 billion dollar** fund to promote quantum information science.
  - The National Quantum Coordination Office which is part of the White House Office of Science and Technology is looking to keep America at the forefront of the quantum revolution. The plan is to create new research Centers that brings together academics from different disciplines and large companies to pool their knowledge and resources in joint research efforts with government institutes.
- **China**: has been investing heavily in quantum technology and sees the field as an opportunity to leapfrog the US.
- The **European Union**: has launched a **1.1 billion euro** quantum master plan. European Quantum Computing and Simulation Infrastructure Program started (JUNIQ). EU industry workshop to prepare C(EO)-level round with Commisioner to foster QC in industry.

Source: https://www.technologyreview.com/f/612679/president-trump-has-signed-a-12-billon-law-to-boost-us-quantum-tech/

Quantum Computing

AI Machine Learning / Deep Learning @ Life Science

BUSINESS IMPACT

Machine learning drives improvements and new solutions to business problems across a vast array of business and social scenarios. QC potentially enables the next level of AI / ML:

- Automation
- Drug research
- CRM
- Supply chain optimization
- Predictive maintenance
- Operational effectiveness
- Workforce effectiveness
- Fraud detection
- Automated vehicles
- Chemical processes optimization
- Resource optimization

Quantum Computing

Problems & Challenges in Quantum Computing

QC NASCENT

- Lack of software and hardware ecosystem
- Ecosystem underdeveloped
- Tools available for MS, IBM, Intel
- Problem of scale (system is very sensitive to environment; operated at 15 milli Kelvin in highly isolated env., colder than outer space)
- This leads to I/O problem
- How to reduce error during manipulating the qbits
- Different technology approaches, think about technology hedging (i.e. hw agnostic provision)

Quantum Computing

Use cases

USE CASES - ASSUMPTIONS, TO BE VERIFIED

General:

- Optimization problems (“Traveling Sales Man Problem”)
- Molecular dynamics simulation (today limited, due to numerous interactions and dependencies: i.e. electron – electron interface, electron – proton interface a.s.f.)

HealthCare:

- Drug design, precision medicine, Real World Evidence

Quantum Computing

PoC Approach

POC QC APPROACH: APPLY USE CASE, THAT ALLOWS TO JUDGE ON RESULTS

Use Case: Identification of Virtual Patient Models using QC

- Using a “simple” public available dataset (MIMIC3) and apply to an “clustering problem”
- Compare results to parallel “classical” HPC approach

Target:

- Find hints for disease evolution

Underlying Problem:

- Real World Data data does not reflect disease evolution, as they are captured after disease diagnosis. Only poor insights gained via analytics today (too many false positives)

Quantum Computing

Current Use Cases at Bayer

1. Identification of Virtual Patient Models using QC

- Using a “simple” public available dataset (MIMIC3) and apply to an “clustering problem” – root cause analysis of multi comorbidities – Project with RWTH Aachen and Atos
- Results: => Assessment of cluster identification strategies shows a clear overall superiority of models based on QC based clustering technique ✓

Atos, Bayer and RWTH Aachen University use Atos Quantum Learning Machine to study human disease patterns

2. Cancer Cell Proliferation

- Learning of the pathogenesis of tumor cell types out of the observed distribution of mutation and genetic aberration profiles.

BAYER RWTH AACHEN UNIVERSITY Atos

Quantum Computing

What's feasible for near-term QCs (todays NISC's)

- Structure-based algorithms
  - Binding side identification
  - Pharmacophore modeling
  - De novo protein modeling
  - Docking / virtual screening
  - Molecular dynamics / FEP
  - Protein-protein docking
- Ligand-based algorithms
  - Ligand similarity search / scaffold hopping
  - Conformational search
  - Ligand-based virtual screening
  - Library design
  - QSAR
- Quantum chemistry, structural biology algorithms and machine learning
  - ADME/Tox prediction
  - pKaprediction
  - Membrane permeability
  - Decision-making algorithms
  - Statistical modeling
  - Electronic structure calculations
  - Sequence alignment / homology modelling
  - Crystal structure prediction

Source: ProteinQure

Quantum Computing (QC)

Summary

PHARMA INVENTIVENESS AT PLATEAU

PRECISION MEDICINE IS COMING

GENE THERAPY IS COMING

AI IS COMING

AI IS A MUST HAVE

⇒ Quantum Computing offers “Next level of AI”

⇒ right time to act *NOW!*

⇒ *1. Perform QC Experiment* ✓

⇒ *2. Develop QC Strategy*

Quantum Computing

Best practices

LESSONS LEARNED IN POC SO FAR

// Look for QC experts in your company, you may have more than you think

// Drive classical approach in parallel in order to judge on QC results

// Use “high quality data” for PoC

// Fine tuning of parameters takes time, be patient

// Visualize it, otherwise your experts may talk different languages

Thank you!

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