Quantum-Inspired Computing Digital Annealer

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Digital Annealer (DA) opens up new possibilities

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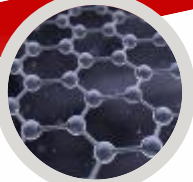
- A new digital circuit architecture which is inspired by quantum phenomena

General-purpose computer

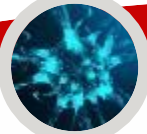
New architecture computer

Digital Annealer

Quantum computer



Neural computer



Applicable fields of combinatorial optimization problems

Chemistry

Finance

Transportation & Logistics

- Many of society's issues are combinatorial optimization problems that can be solved by DA, contributing to the creation of new business

Agenda

- Background
  - Computing evolution
  - Innovation of computer architecture
- Digital Annealer
  - Technology
  - Applications

Why Digital Annealer?

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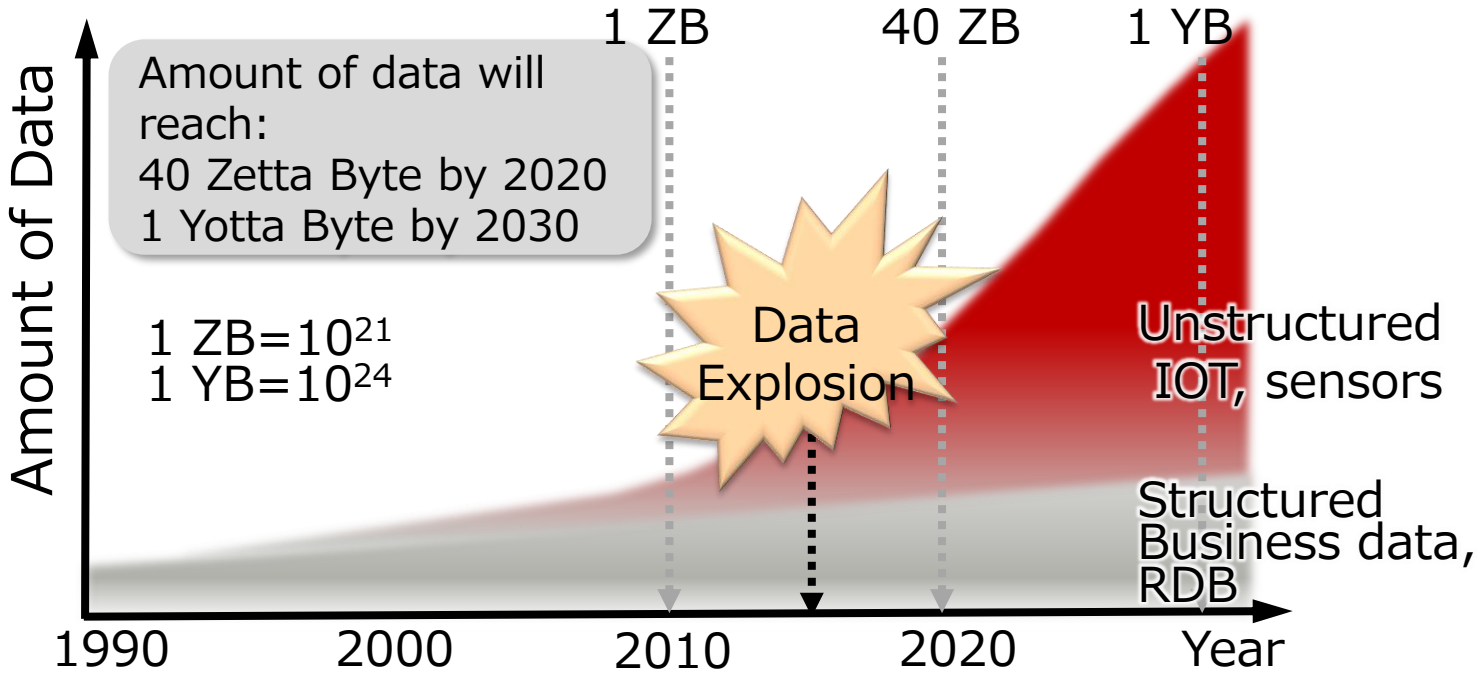
Computing evolution and innovation of computer architecture

～The demand change from high-speed computing to domain-specific computing～

Data explosion

- Amount of data exceeds capability of traditional IT
- Need to create valuable information from unstructured data



New computing architecture

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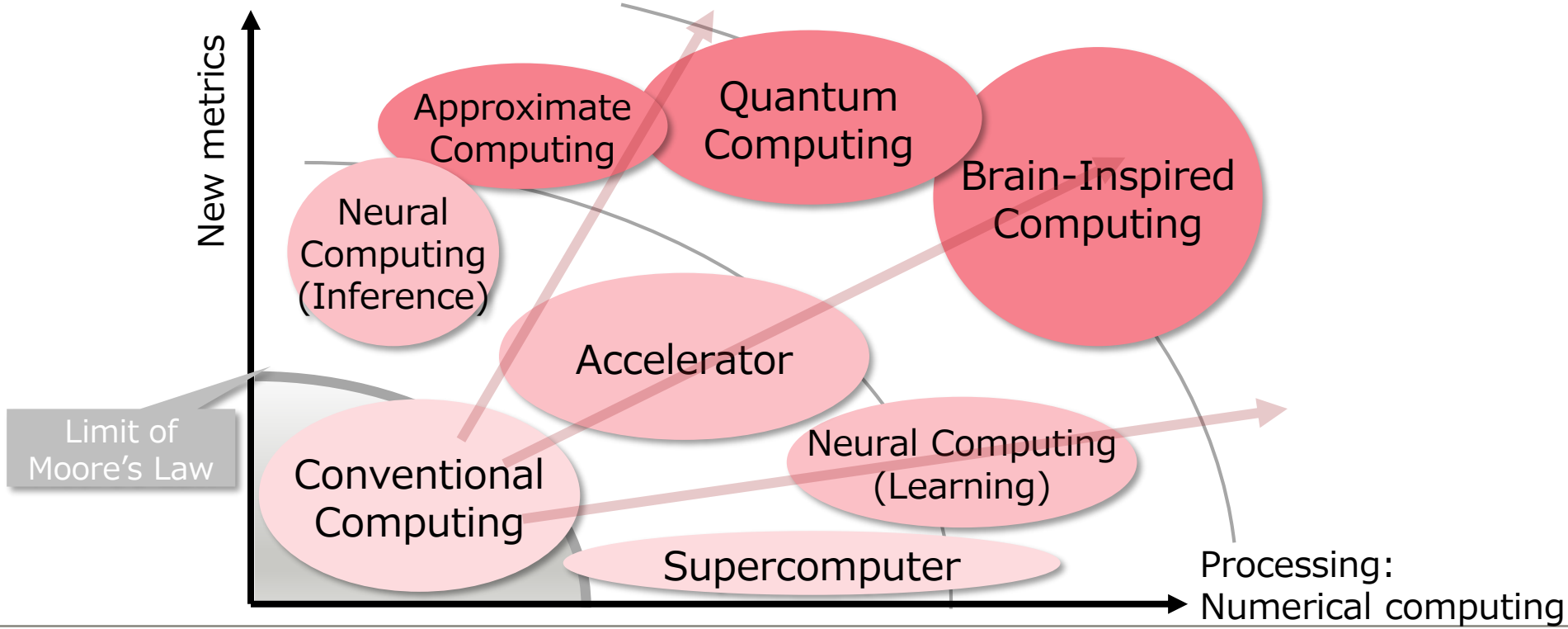
- Domain-specific computing taking care of new metrics
- New metrics: media processing, knowledge processing, intelligence processing



Direction of new computing architecture

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Conventional architecture		**New architecture**
General purpose core	→	**Designated simplified core**
Specialize the processing purpose, Eliminate waste		
Sequential processing	→	**Super-parallel processing**
Parallel processing of huge calculations		
Strict accuracy	→	**Demanded accuracy**
Efficient processing by “Irresponsible”		

New computing architecture

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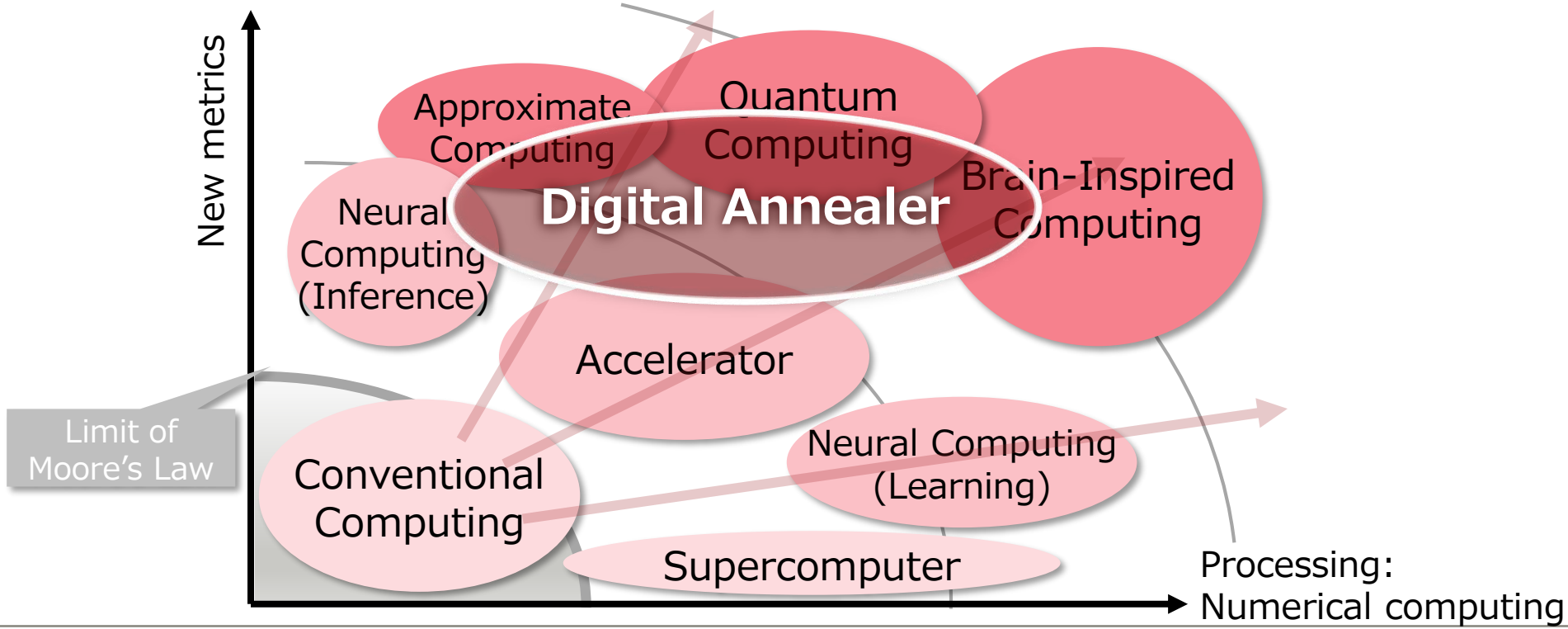
- Domain-specific computing taking care of new metrics
- New metrics: media processing, knowledge processing, intelligence processing



What is Digital Annealer?

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Quantum-inspired computing

Categories of quantum computing in a broad sense

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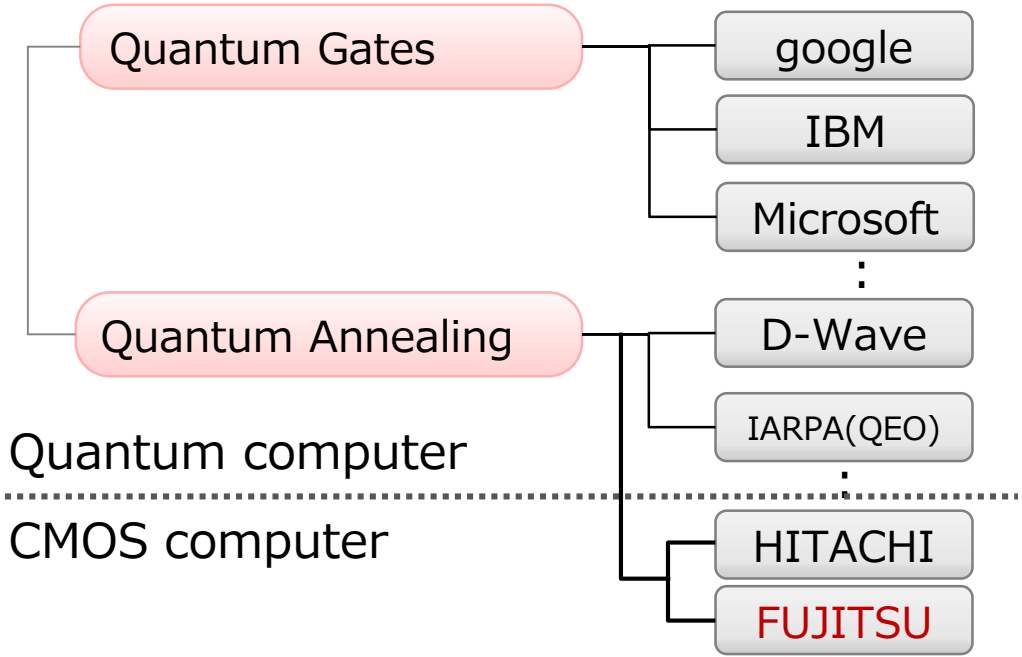
- Quantum computing, in a broad sense, consists of two categories
- Digital Annealer is in the quantum annealing category, not quantum computer, but computer using conventional CMOS devices

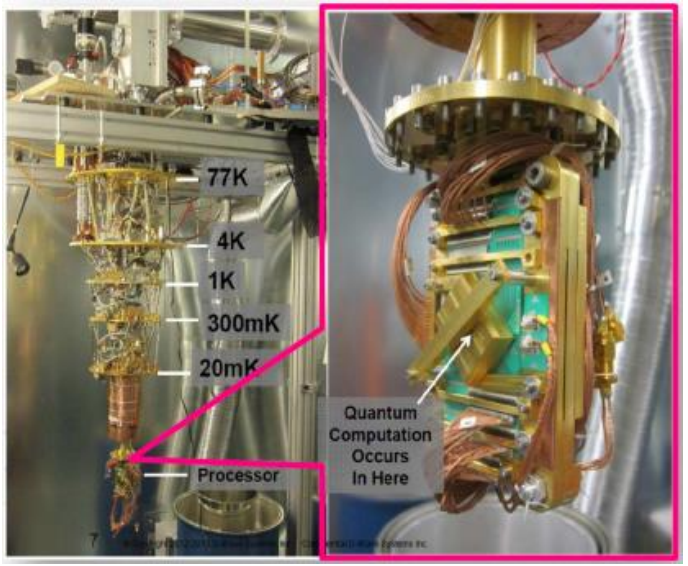


- Calculating by applying quantum gates for quantum bits with both states of 0 and 1
- Universal operations are executed like conventional computer

- Finding a global minimum status based on adiabatic theorem
- Combinational optimization problem is solved

Recent Announcements (quantum annealing)

- 3×3×3m magnetic shield and 15-mk refrigerator (~15mk)
  - 25kW power consumption including the cryogenic system



*D-Wave Systems Inc.（Burnaby, BC, Canada）

Digital Annealer: features

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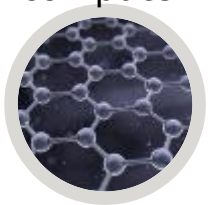
- New Architecture: Quantum-inspired digital circuits for solving complex combinatorial optimization problems

(Cloud service launched on May. 2018)
(On-Premise service launched on Jan. 2019)

Quantum computer



- Difficult to maintain quantum state
- Large-sized cooling equipment
- Partially connected architecture

- Stable calculation
- Small-sized hardware
- Fully-connected architecture

Digital Annealer is superior in usability

Roadmap of Digital Annealer

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Scale image of problems

Drug discovery (Finding stable structures)	Small molecule	Medium-sized molecule	Large molecule
Factory / Manufacturing (component picking)	One floor	Multiple floors	Entire factory
Traffic (Traffic volume optimization)	Tokyo bay area	Tokyo city	Entire Tokyo metropolitan area

1k 10k # of bits 100k 1M

First generation

- Scale: 1024 bits
- Precision: 16-bit (65536 levels)

15th May, 2018
Cloud service launched

Second generation

DAU: Digital Annealing Unit

- Scale: 8192 bits
- Precision: 64-bit (18 quintillion levels)

21th Dec., 2018
Cloud service launched

Next generation

- Large scale parallel processing
- Million-bit scale

Can be applied to 100-kbit-scale problems by using problem division techniques

FY 2018 FY 2019

Note: Road map is liable to change without notice

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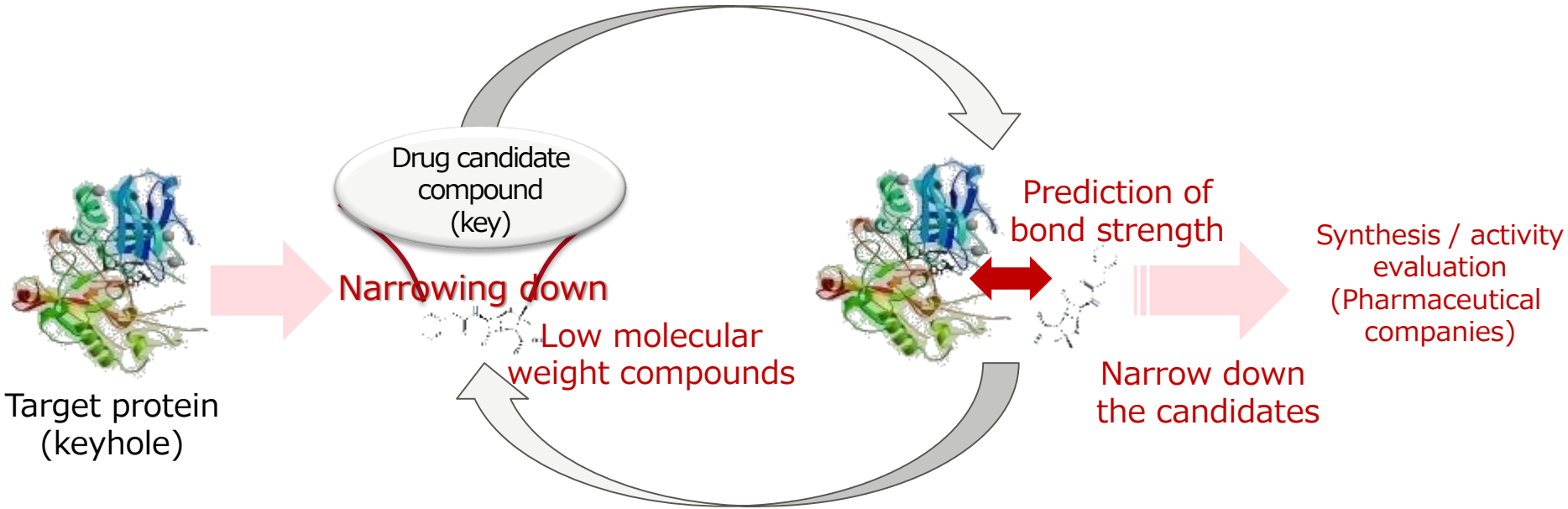
Applications

- Drug discovery (Chemistry)
- Medical care

Chemistry : Drug discovery by Digital Annealer

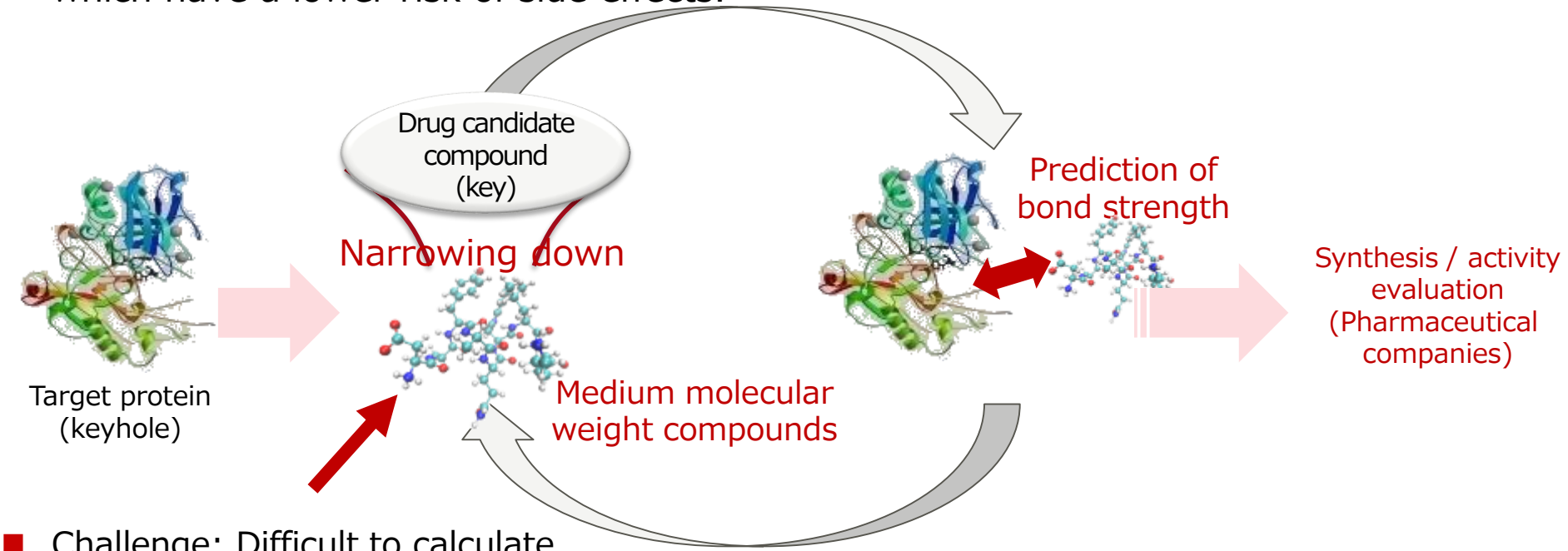
- Designing drug candidate compounds on a computer
- Efficacy can be estimated very accurately by predicting the bond strength between target proteins and drug candidate compounds



Creating drug candidates with high probability is available now (mostly low molecular weight).

Finding larger drug candidate with the Digital Annealer (DA)

- The development of medicines is shifting from low molecular compounds (with two to four amino acids) to medium molecular compounds (with five to fifty amino acids), which have a lower risk of side effects.



- Challenge: Difficult to calculate stable structures in an exhaustive search of all atoms

⇨ **Use DA to design drug candidate compounds**

Rapid Search for “Key Shapes” by using Digital Annealer

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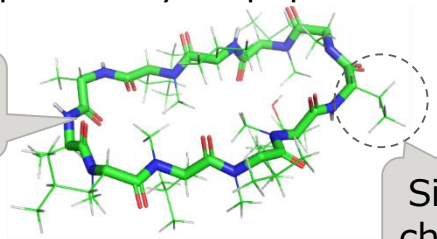
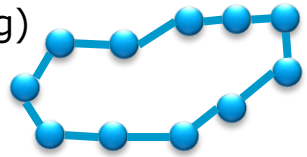
- Cyclic peptides (cyclic chains of amino acids) are promising compounds for medium-sized drugs

Example of a cyclic peptide

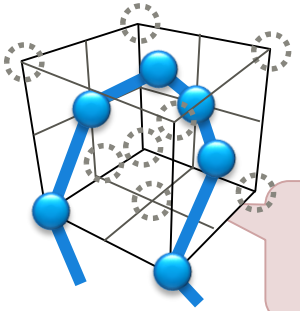


Modeling (Coarse graining)



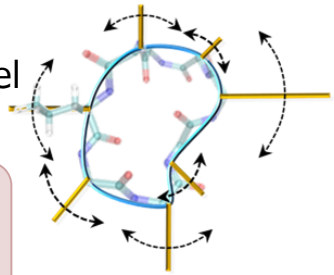
Modeling each amino acid as a bead on the lattice

1. Search for main-chain structure

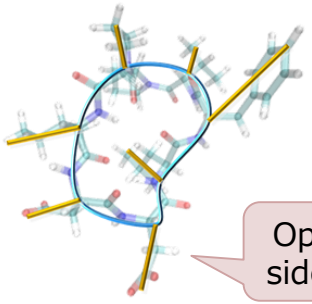


Optimization of the main-chain structure

Atomistic model



2. Search for side-chain structure



Optimization of the side-chain structure

The number of combinations for 1 and 2 is 1.9×10^{72}, for 15 amino acid residues

Aiming to search more than hundreds of times faster than conventional simulation

Main chain optimization

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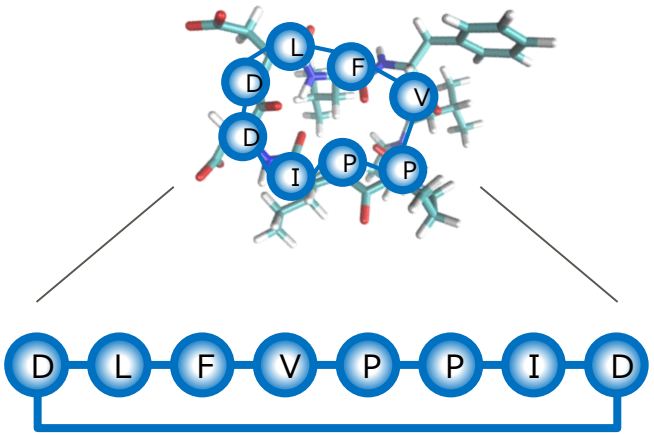
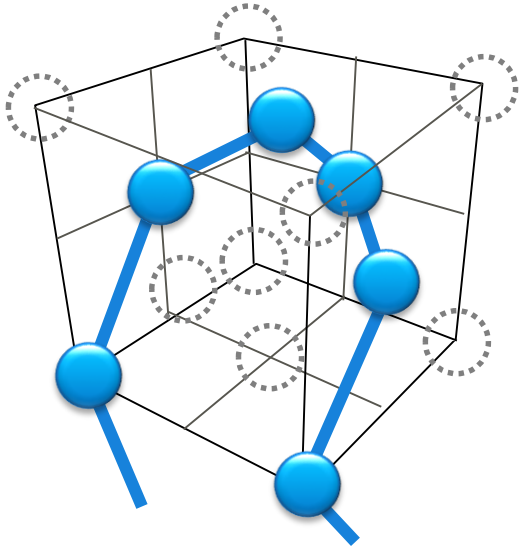
- Example: Cyclic peptide consisting of 8 amino acids

8 amino acids sequence



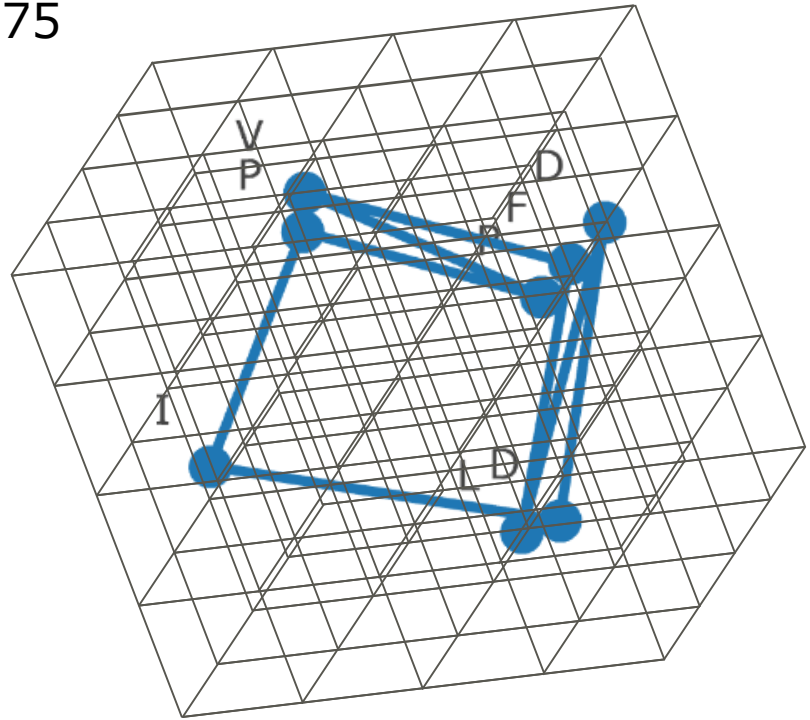
Lattice model



Start annealing

Early stage of annealing

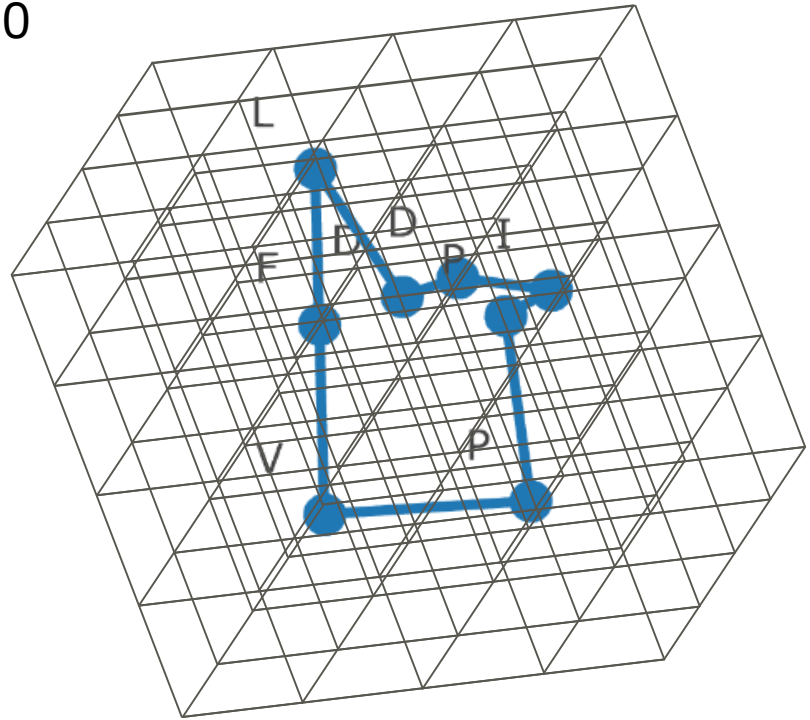
Interaction energy: 675



Many constraint violation, Unstable structure

Middle stage of annealing

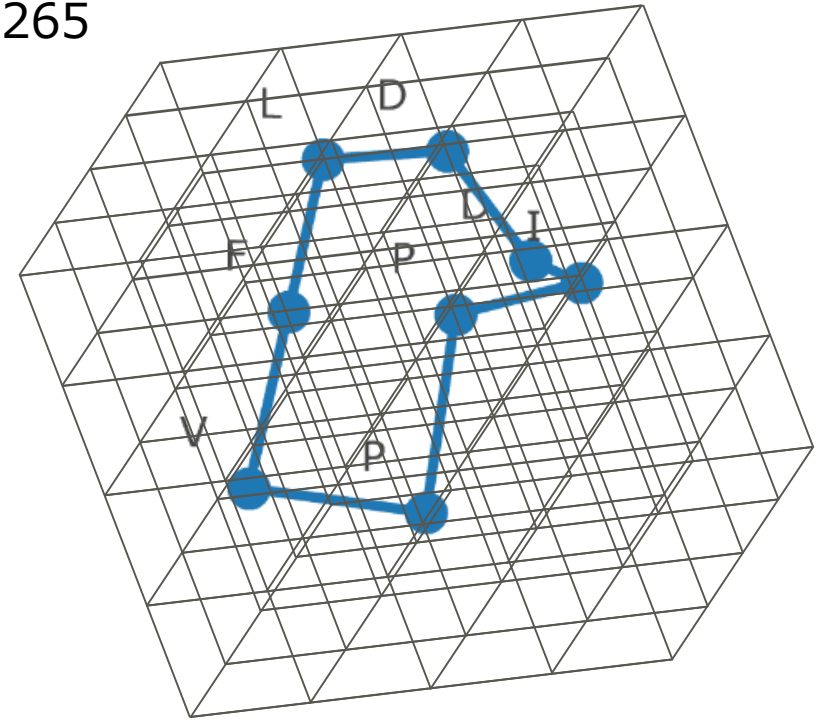
Interaction energy: 10



Many constraint violation, Unstable structure

Late stage of annealing

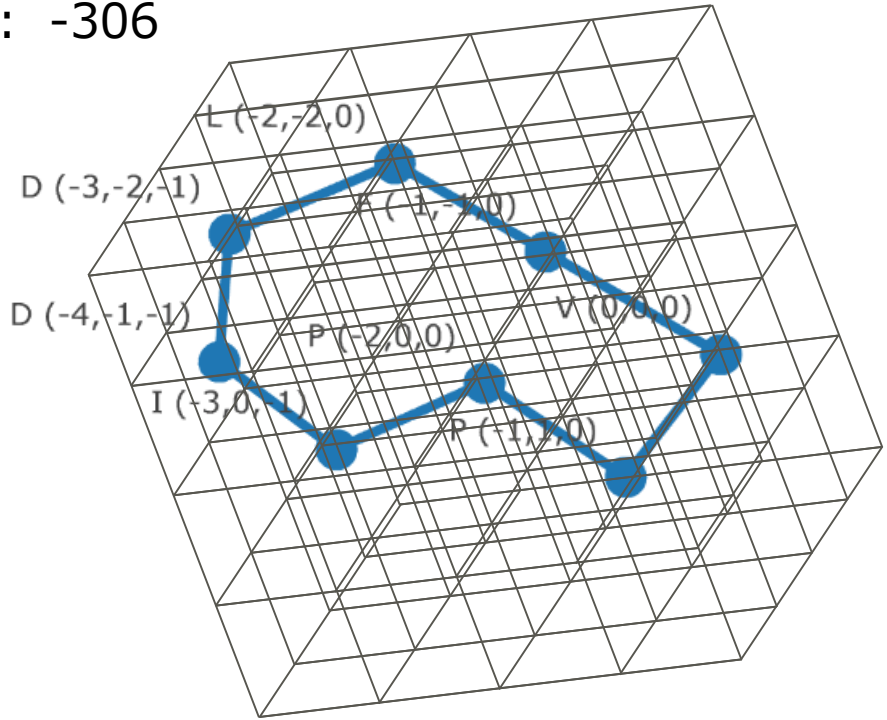
Interaction energy: -265



No constraint violation, Relatively stable structure

After annealing

Interaction energy: -306

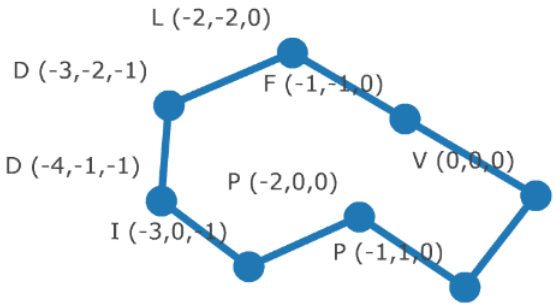


Converge most stable structure

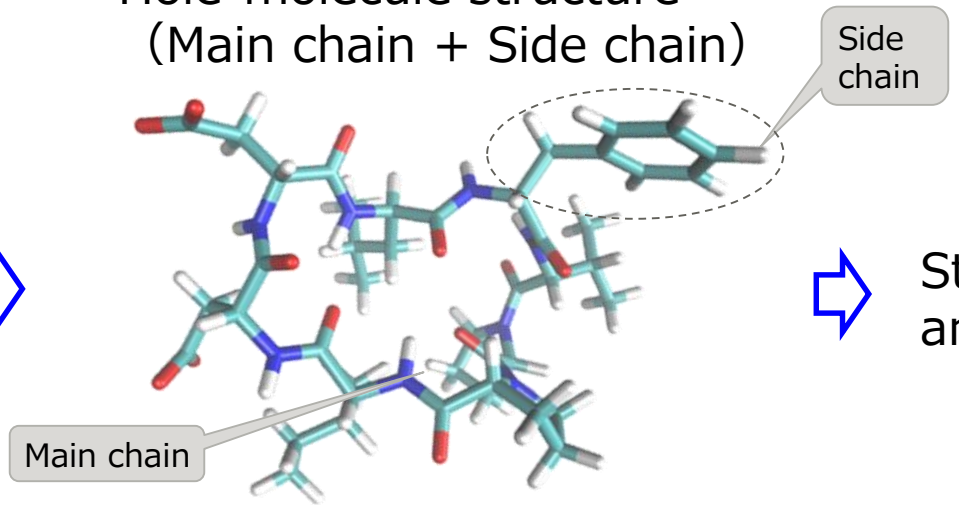
Side chain optimization

- After conversion from the lattice model to hole-molecule structure, add the side chains to main chain extracted
- Treat side chains as rotamers, Optimize rotamer's angle by using DA

Optimized lattice model



Hole-molecule structure (Main chain + Side chain)



Start annealing

Early stage of annealing

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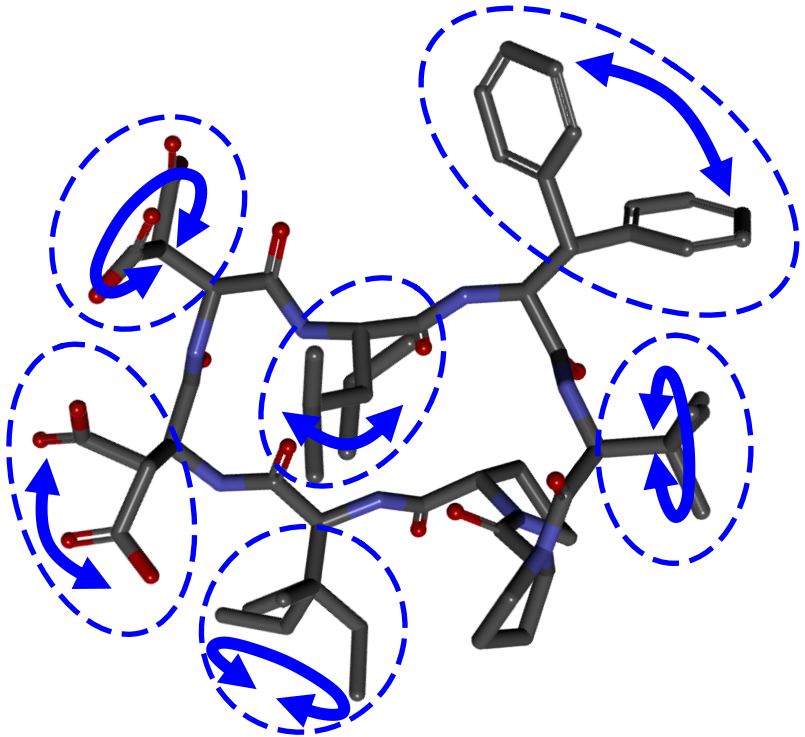
Energy: 107.7



Many unstable structure of side chains

Middle stage of annealing

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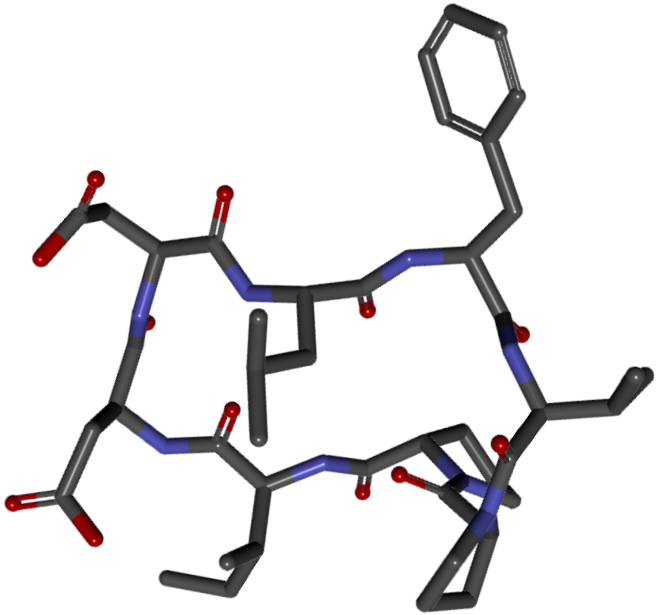
Energy: 74.3



Many unstable structure of side chains

Late stage of annealing

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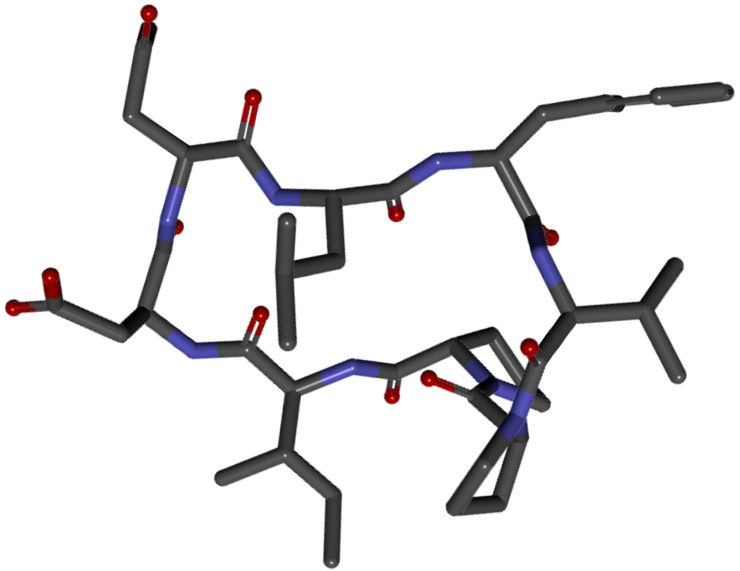
Energy: 67.3



Relatively stable structure of side chains

After annealing

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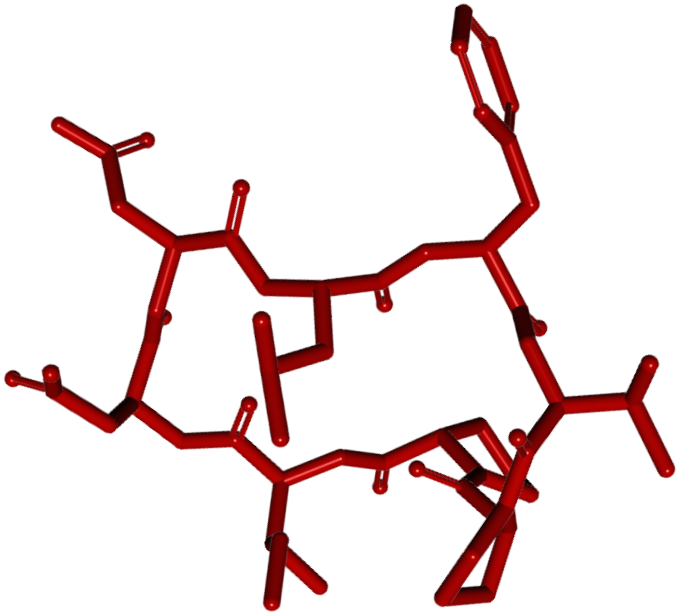
Energy: 56.1



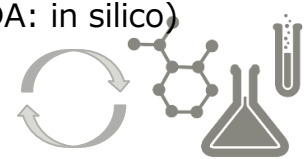
Converge most stable structure

Co-creation with PeptiDream

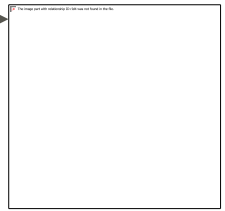
- PeptiDream Inc. is a biopharmaceutical company employing their proprietary and highly-innovative **Peptide Discovery Platform System** (PDPS).

1. Collaboration between DA and PDPS will enable drastic speedup of "**Generation and optimization of candidate compounds**" process.
2. Providing **pharmaceutical companies** with our DA technology directly or through PeptiDream will develop into co-creation with you

Stable structures
(DA: in silico)



Experimental data
(PDPS: in vivo)



- Pharmaceutical company A
- One of you, B
- One of you, C
- One of you, D
- Pharmaceutical company X
- Pharmaceutical company Y
- Pharmaceutical company Z

- Partners: 19 companies

Applying our technology in the field of practical peptide discovery to verify its effectiveness

Process of Drug Discovery and Our Challenges

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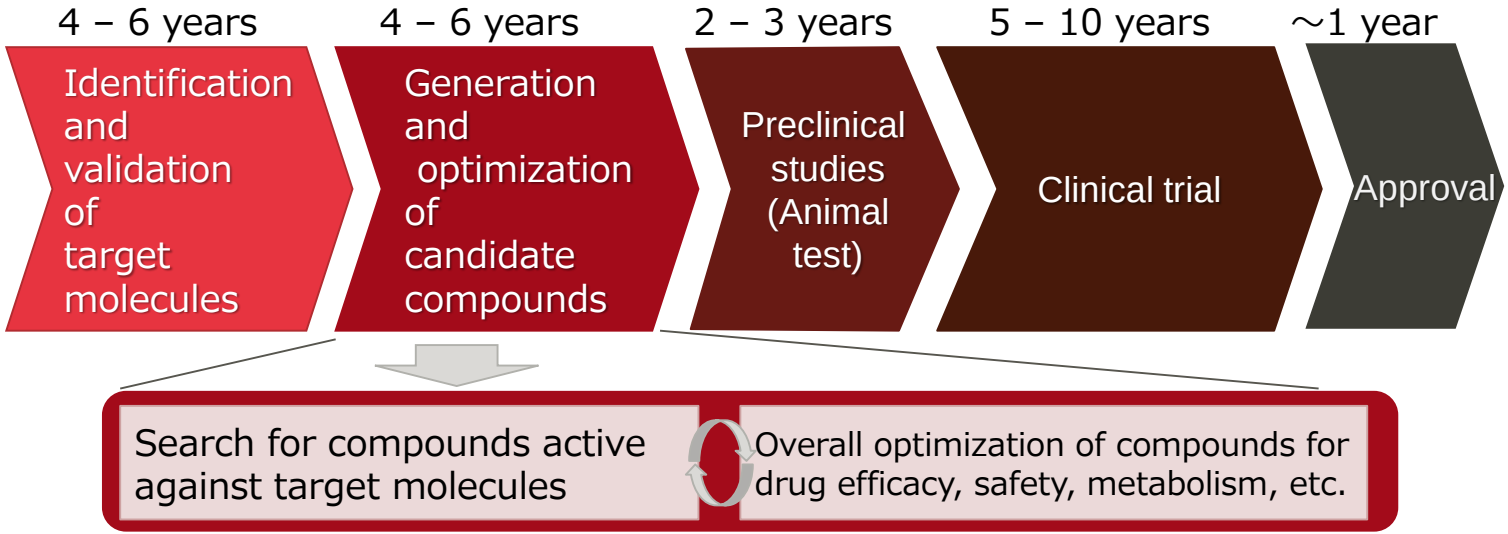
- Drug discovery is a lengthy process that usually takes more than 10 years



- Stable molecular structure (= key shape) is important for narrowing down the list of candidate compounds
  - Medium-sized molecules, however, have too many possible shapes, and we cannot simulate stable structures in a practical period of time with conventional simulation technology

Rapid search for stable structures by Digital Annealer will dramatically improve efficiency of the narrowing down

Medical care : Radiation Therapy

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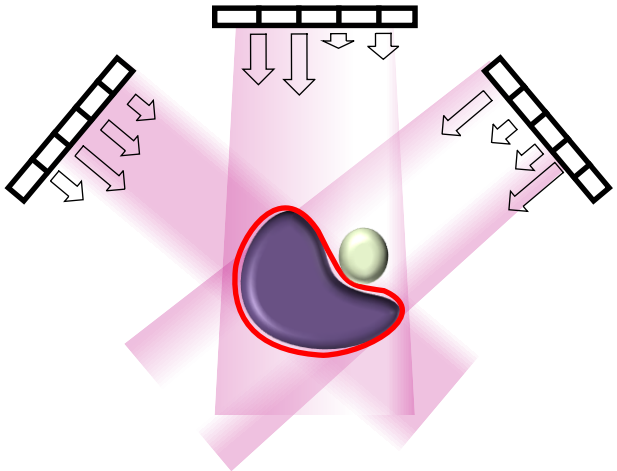
- Intensity Modulated Radiotherapy (IMRT)

  is now becoming an increasingly popular cancer treatments.

  IMRT uses several beams onto the cancers without or minimizing damage to normal organs.

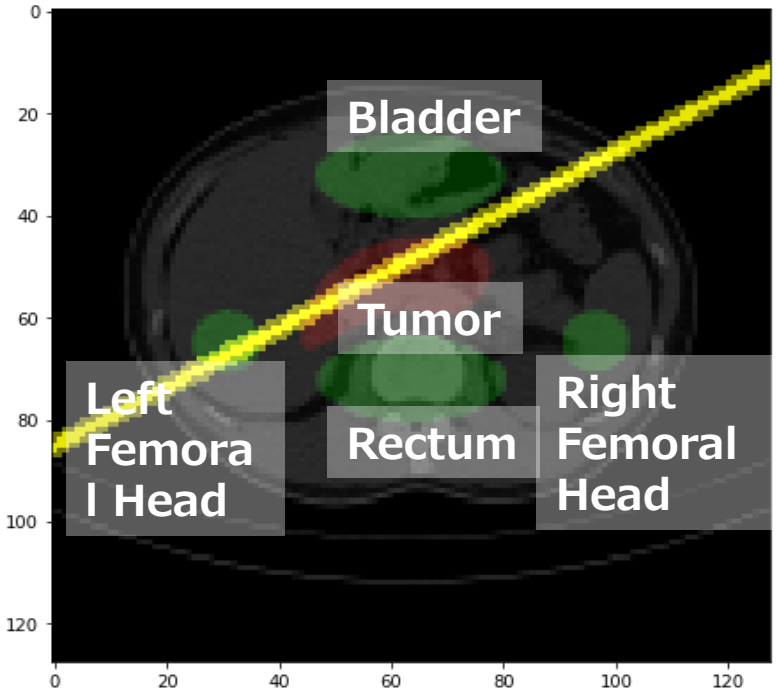
  - Adequate treatment, by optimizing patterns and intensity of radiation
- Large amount of calculation is required for optimization
  - Usually up to several days are required → Use DA to reduce calculation time

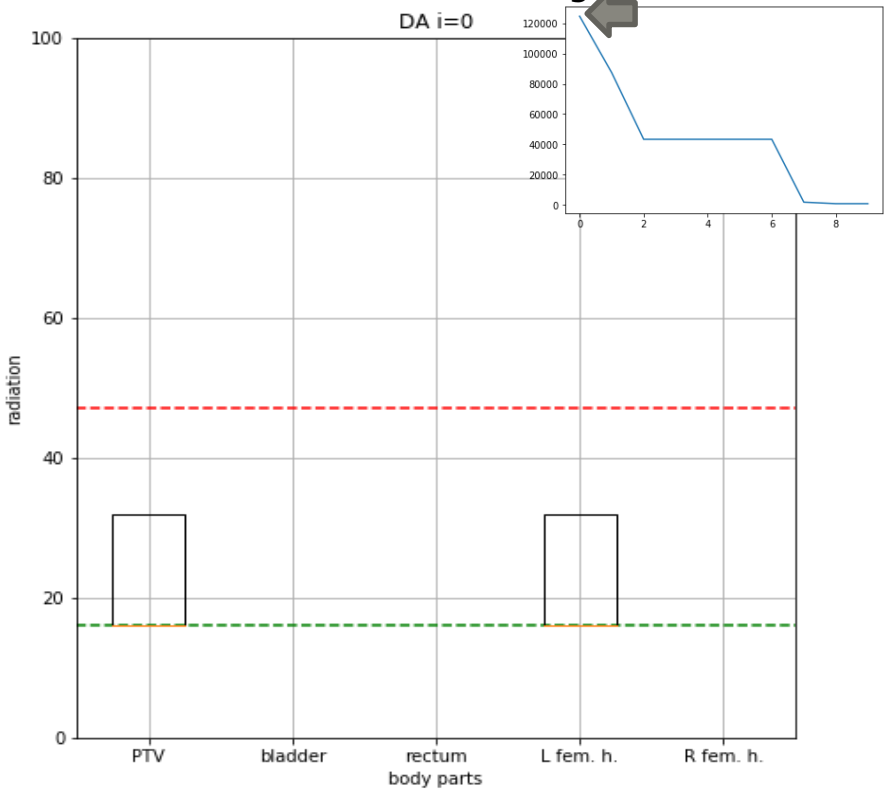


Medical care : Radiation Therapy demo(1)

Goal: to damage the tumor at the level around the red line and limit the damage to the other organs to the level around or below the green line

Initial State

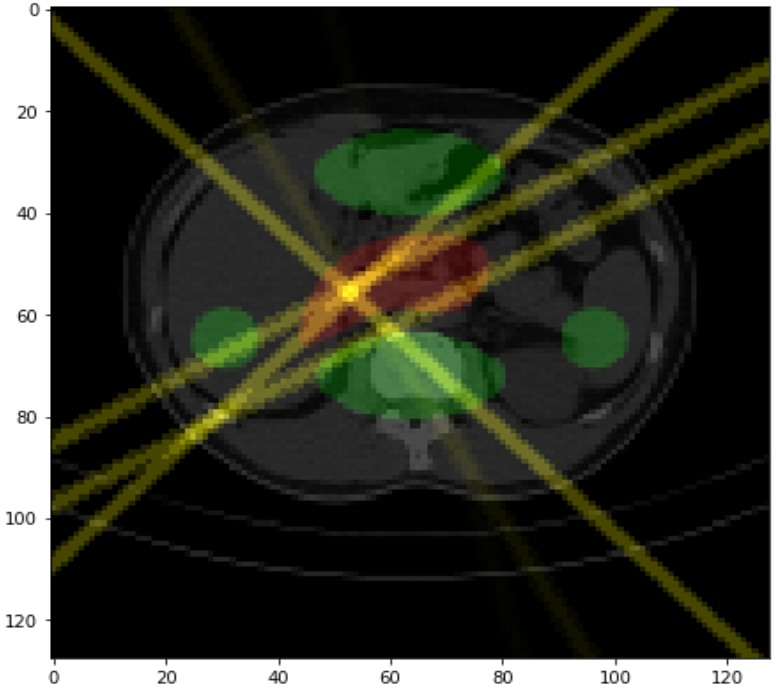


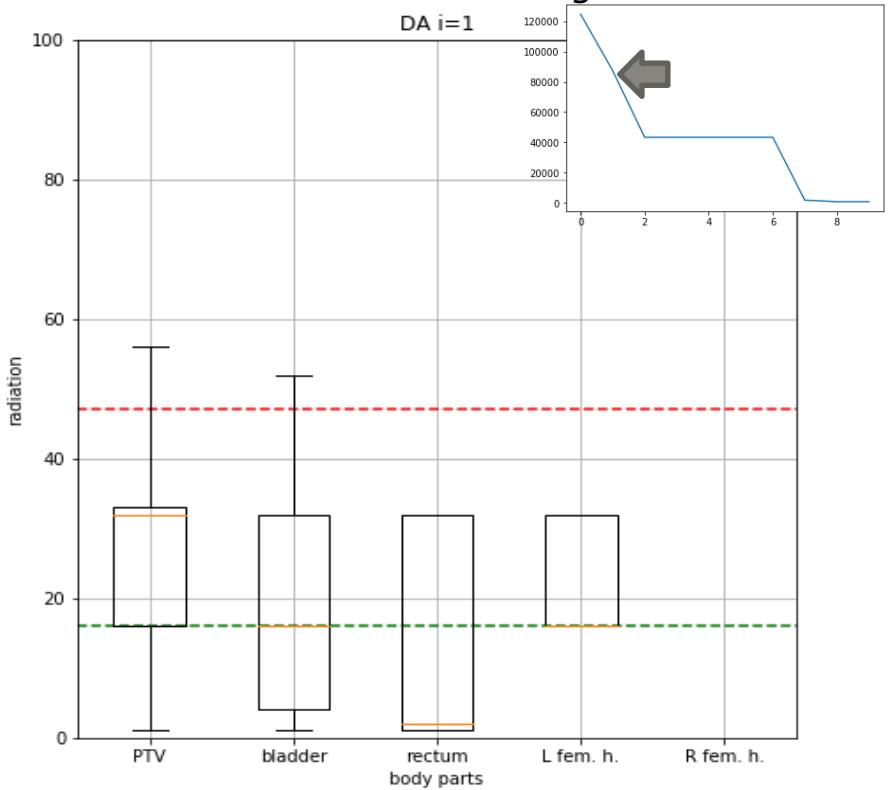


Medical care : Radiation Therapy demo(2)

Goal: to damage the tumor at the level around the red line and limit the damage to the other organs to the level around or below the green line

Early stage

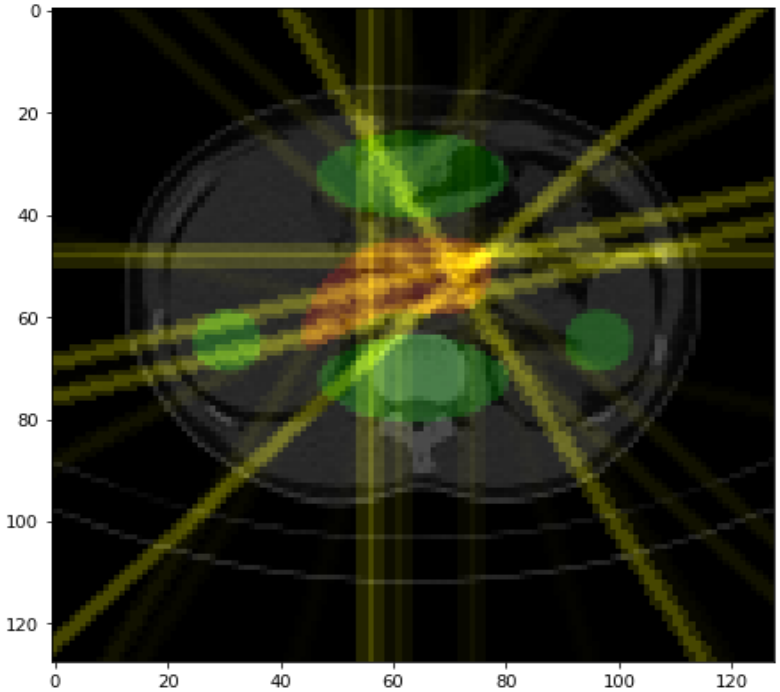


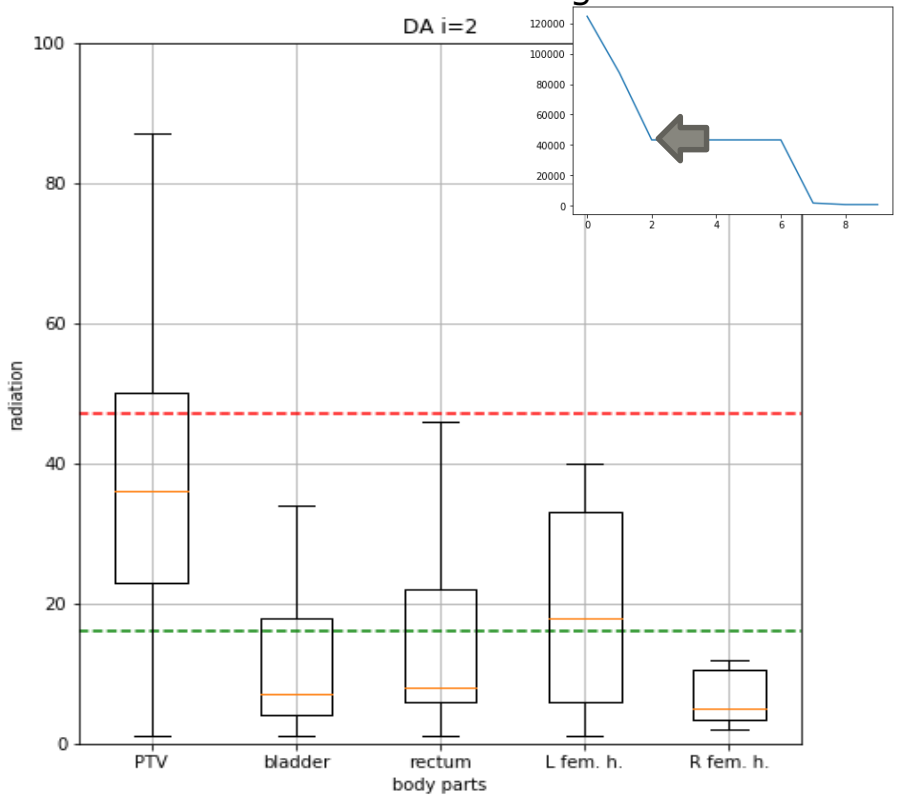


Medical care : Radiation Therapy demo(3)

Goal: to damage the tumor at the level around the red line and limit the damage to the other organs to the level around or below the green line

Middle stage

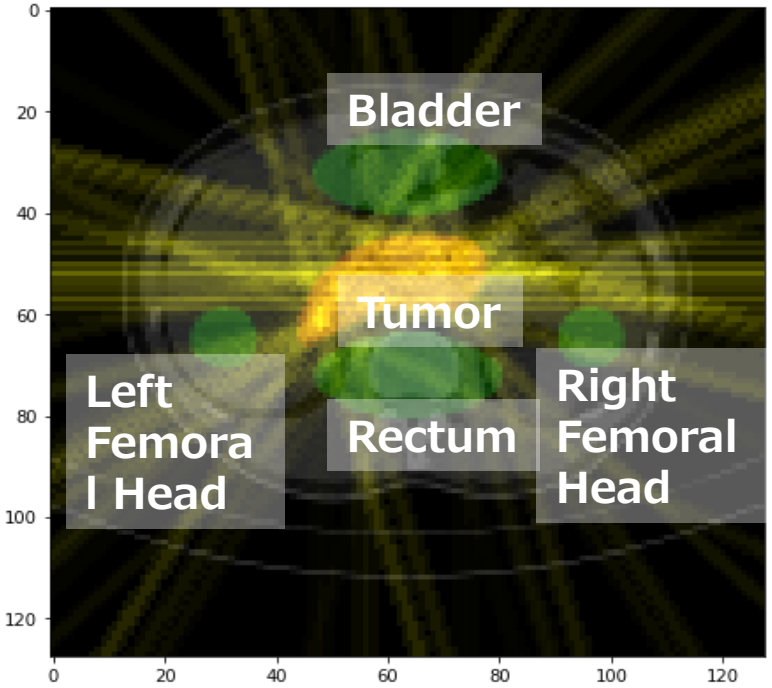


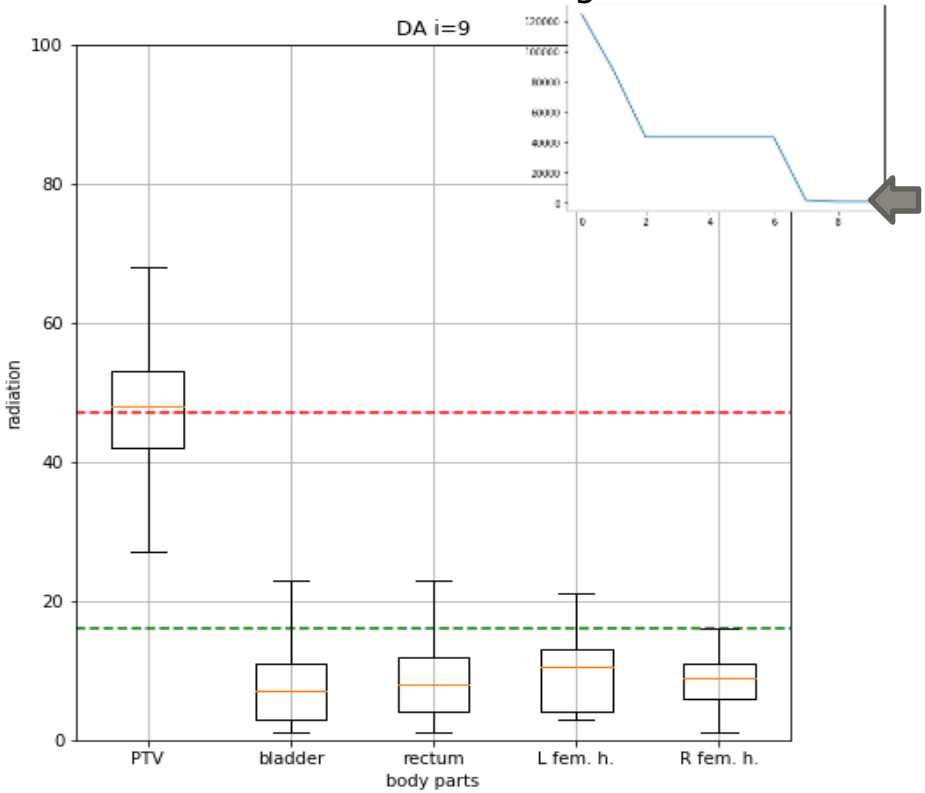


Medical care : Radiation Therapy demo(4)

Goal: to damage the tumor at the level around the red line and limit the damage to the other organs to the level around or below the green line

Completed





Expansion of applicable fields

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We are forming community and co-create with to customers and partners to develop application of DA, and develop global markets

Chemistry Drug discovery | Finance | Digital marketing | Transportation Logistics | Medical care | Energy

Social issues
Core business

Field Expansion

Digital Annealer

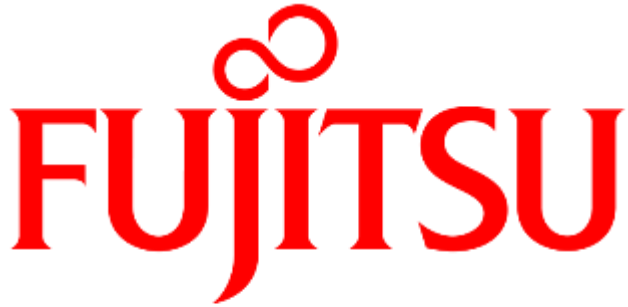
Co-creation with customers

Chemistry, Material, Drug discovery, Finance, Logistics, Transportation, Medical care

Partners

UNIVERSITY OF TORONTO
WASEDA University 早稲田大学
1QBit

FUJITSU
Business unit Laboratory



shaping tomorrow with you