2022 7 116 2022 8 15

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Recursion Benevolent AI

Benevolent AI

Baricitinib [2]

Insilico Medicine 3CL

[2] Baricitinib Janus(JAK1/JAK2) Incyte Eli Lilly 2017 Olumiant

ADMET

AI +

AI +

AI

Ribonucleic Acid Sequencing RNA-seq

High-Throughput Sequencing HTS

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National

Center for Biotechnology Information NCBI

Gene Expression O

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PubChem

ChEMBL

Absorption, Distribution, Metabolism and Excretion ADME

DrugBank

LINCS L1000 PDB

Computer Aided Drug Design CADD ML DL

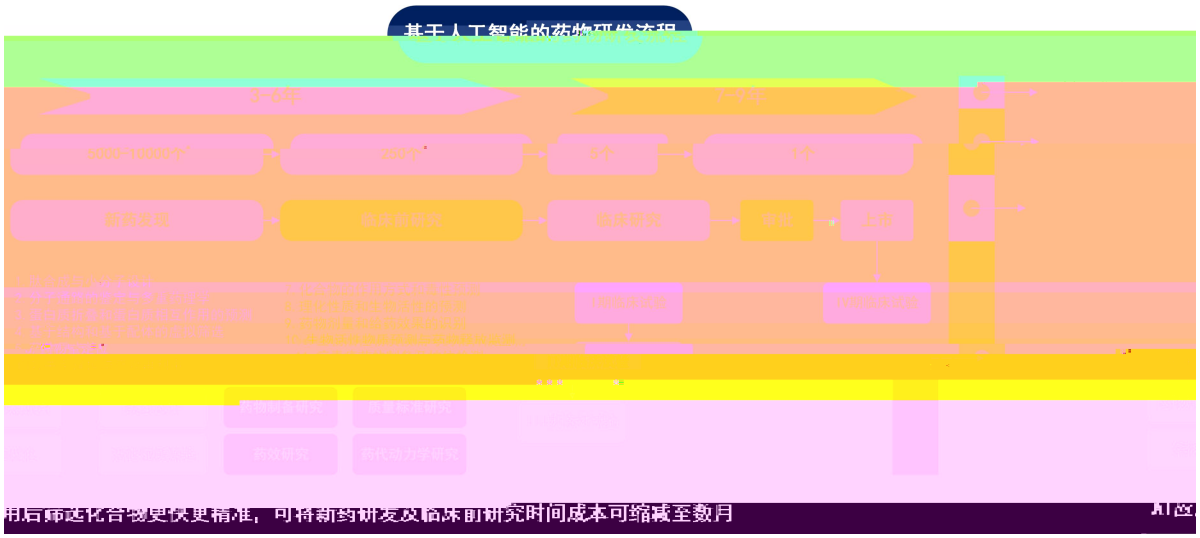
Quantitative Structure Activity Relationship QSAR

ML

①

②

2-1



2-1

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2-2

Yan [2] 2020 DL

Antimicrobial peptides AMPs Deep-AmPEP30

AmPEP30 Convolutional Neural Network, CNN

DeoxyriboNucleic Acid

DNA AMP

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AMPs

Zhavoronkov [3]

GENTRL

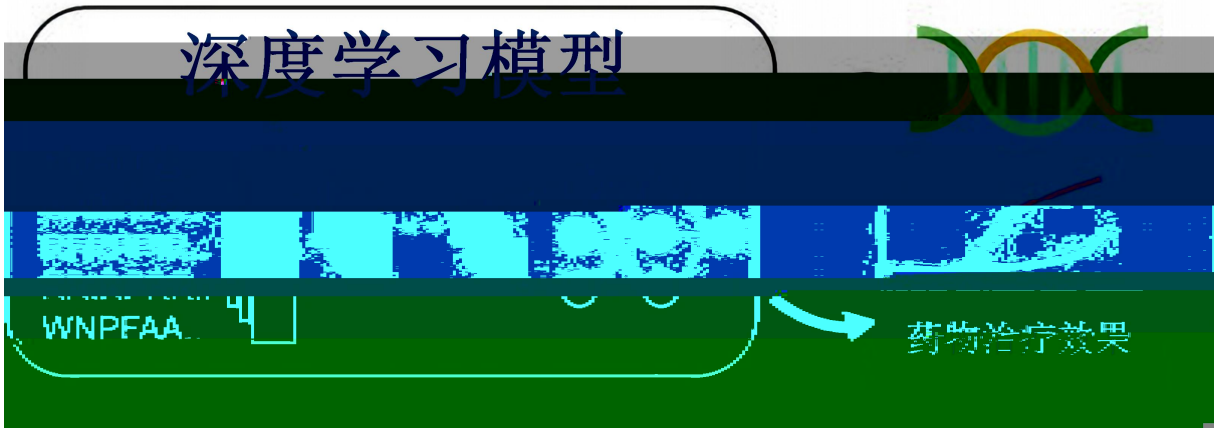
https://github.com/insilicomedicine/GENTRL

DDR1 McCloskey [4] DNA

DNA-Encoded small molecule Libraries DEL

ML

Xing [5] XGBoost



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— Protein-Protein Interaction, PPI

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Bayesian Network BN PPI

Gene Ontology GO

PPI BN

PCA

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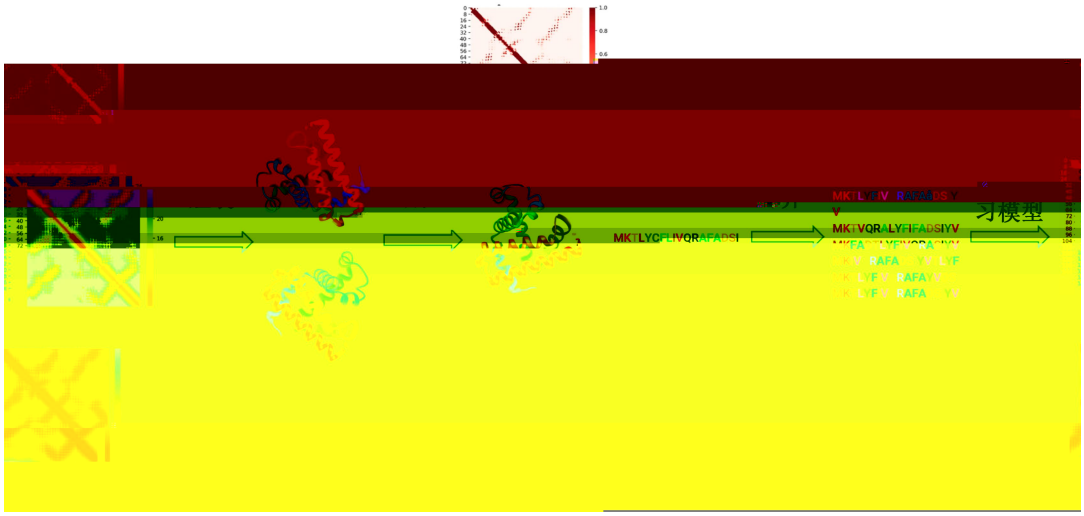
PPI

Gene Ontology GO

PPI

[7] —



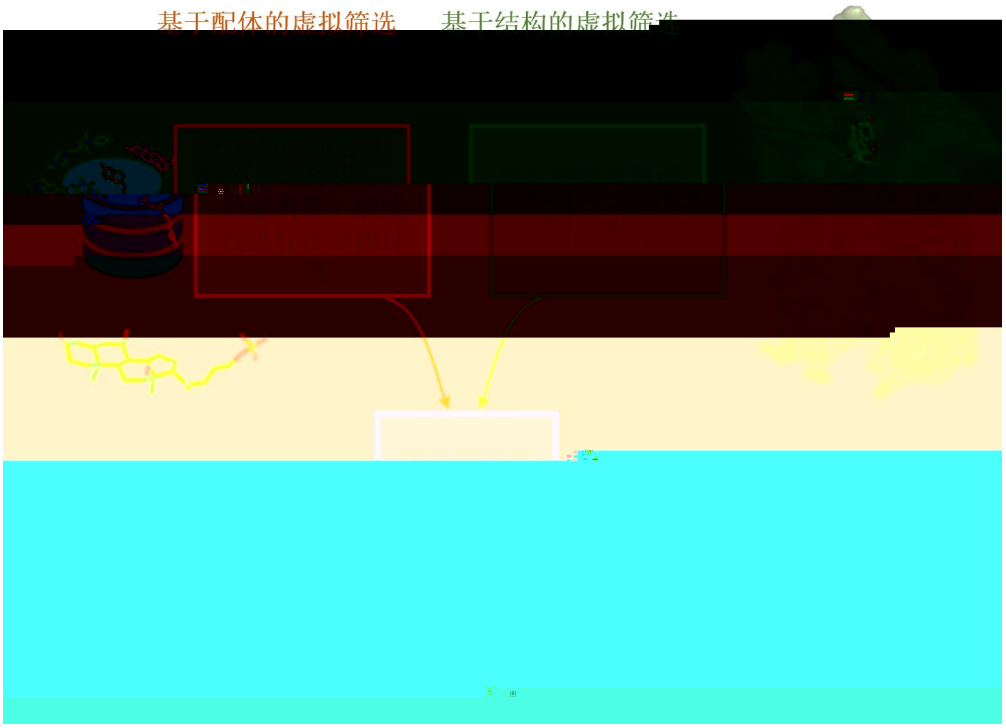
2-4

Virtual Screening VS

CADD

ML VS

ML VS VS



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VS 2-5 VS

Structural Based Virtual Screening SBVS VS

Ligand Based Virtual Screening LBVS

SBVS AI ML

[8] NNScore CScore SVR-SCORE ID-SCORE

SBVS SBVS

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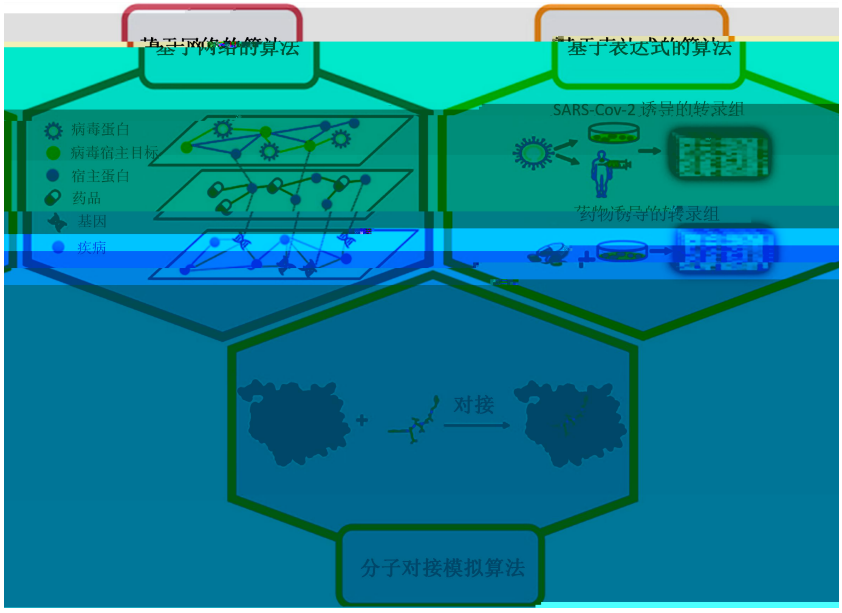
LBVS SwissSimilarity[9]

METADOCK[10] HybridSim-V[11]S AutoDock Bias[12]

1.06

Logistic



2-6 AI ML

COVID-19

2 SARS-CoV-2

COVID-19

COVID-19

AI ML COVID-19

2-6 2-

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2-1 AI ML

AI ML		
[13]	SARS-CoV-2	https://github.com/Murali-group/SARS-CoV-2-network-analysis
[14]	-	
[15]	MT-DTI	
[16]	-	
[17]		https://github.com/ChengF-Lab/CoV-KGE
[18]		https://github.com/yejinjkim/drug-repurposing-graph
[17]		https://github.com/FangpingWan/NeoDTI
[19]		https://github.com/FangpingWan/CoV-DTI
[20]	-	https://github.com/Barabasi-Lab/COVID-19
- InfinityPhenotype[21]		

		https://[illegible]hub.com/[illegible]lab/covid19_re[illegible]rposing
[illegible]2]		https://g[illegible]ub.com/[illegible]993/DeepCE
[24]		
[14]		
		https://github.com/ekraka/SSnet
[26]		

[27,28]

S

[illegible]

[illegible] [13]

(Regularized Laplacian RL) [illegible]

FDA SARS-CoV-2

[29] Zhu [21] AI InfinityPhenotype

FDA

Liquiritin I

COVID-19

[30]

AI ML Nguyen

[24] MathPose MathDL

SARS-CoV-2 3CL —

MathPose

MathDL

COVID-19 15

AI ML [31–33]

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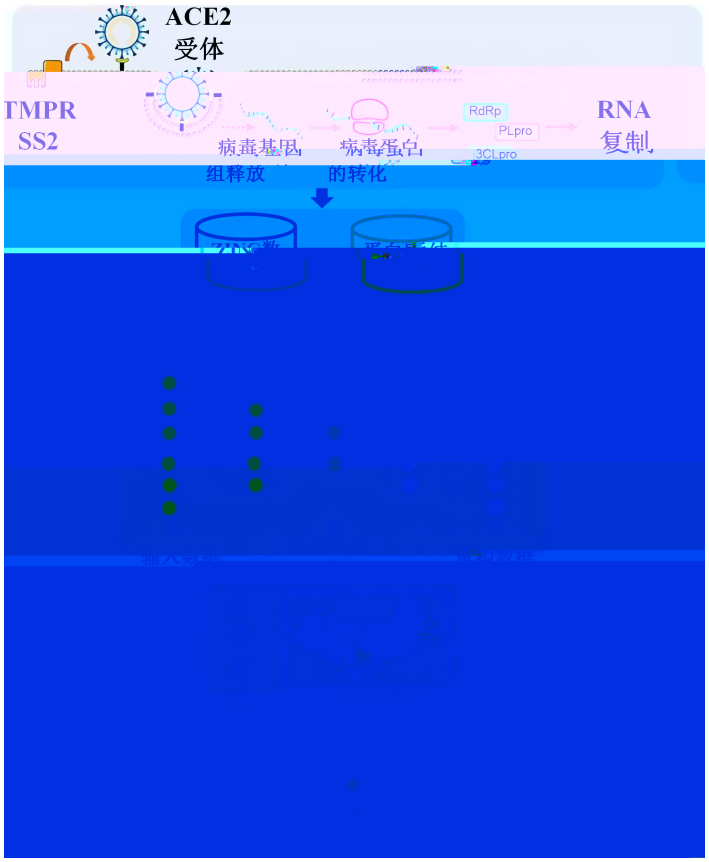
[34] Zhavoronkov [35]

COVID-19

Srinivasan [36]

COVID-19



2-7 AI ML

2-2 AI ML

AI ML		
[35]		
Q [37]		https://github.com/tbwxmu/2019-nCov
[38]		

Hooshmand [45]

16 HCoV

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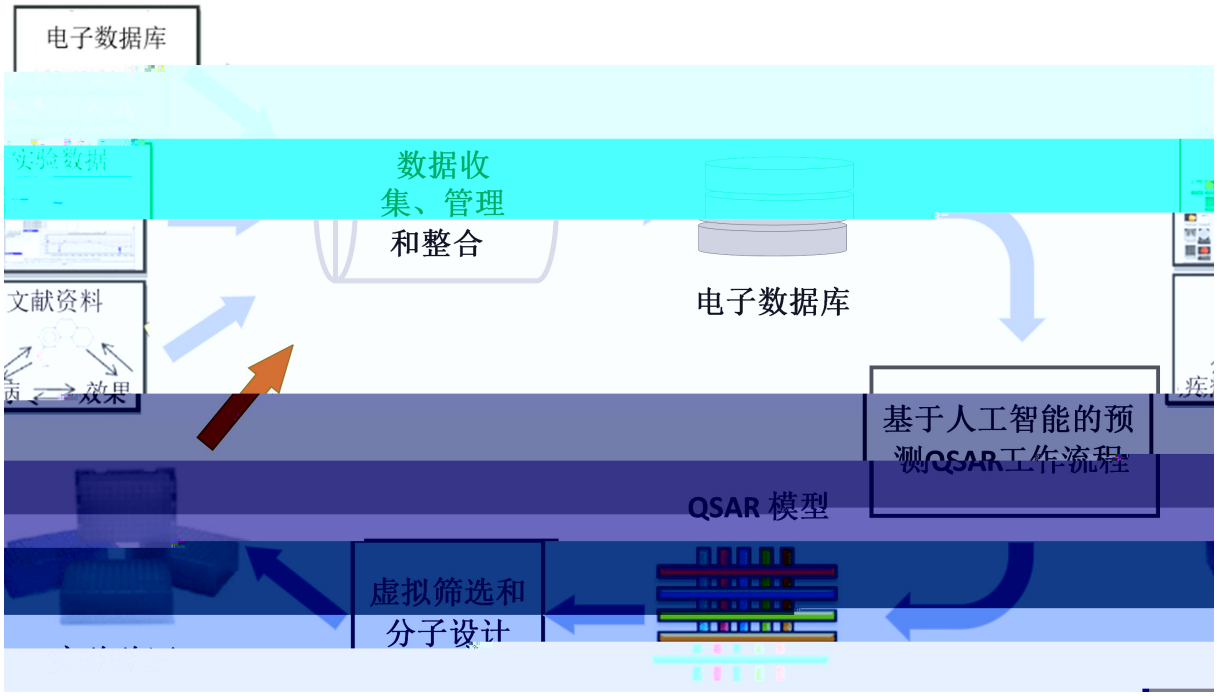


2-8

2-9

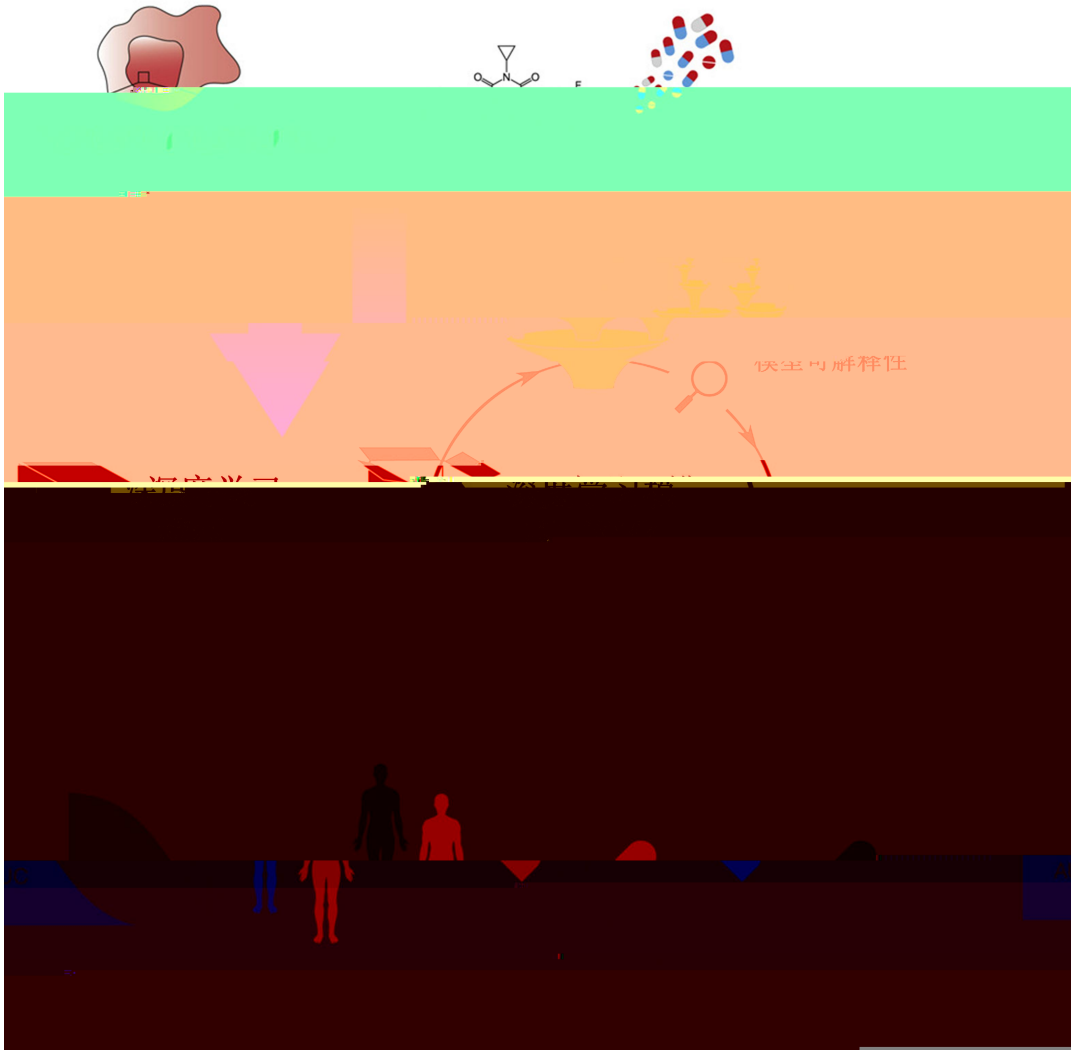
Web LimTox pkCSM admetSAR Toxtree DeepTox[46] PrOCTOR[47]

Robledo-Cadena [48]

PrOCTOR

2,576

16 2

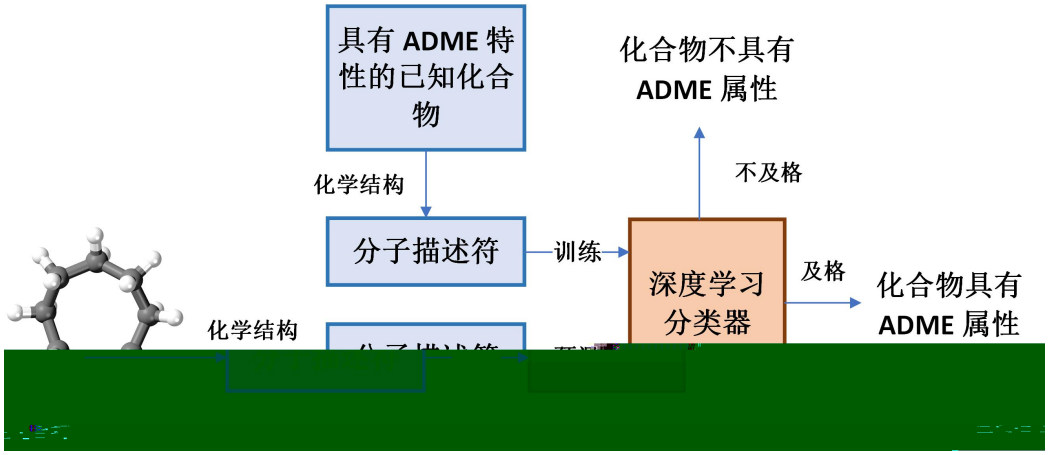


2-9

2-10 SMILES

Coulomb matrices

Deep Neural Networks DNN



2-10

ChemMapper

ML DL

[49] KronRLS SimBoost DeepDTA Padme

ML

DL 2-11 Shen

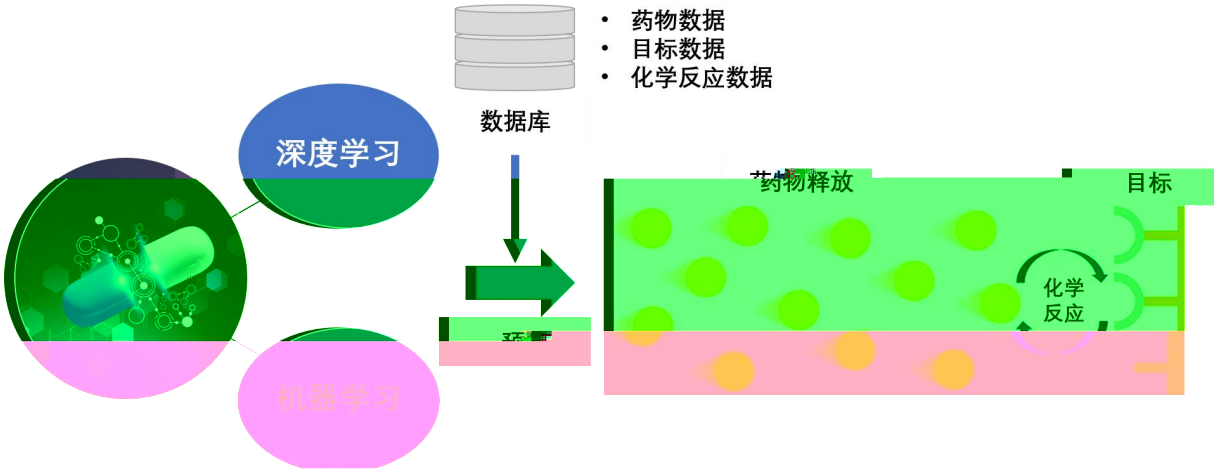
[50] AI-PRS

AI-PRS

Wu DL RF WDL-RF (https://zhanglab.ccmb.med.umich.edu/WDL-RF/)

G G Protein-Coupled Receptors GPCRs Cichonska [54]

pairwiseMKL https://github.com/aalto-ics-kepaco [55]



2-12

2-13 2-3 COVID-19

[56] Fast [57]

MARIA NetMHCPan4

SARS-CoV-2 T B 405 T

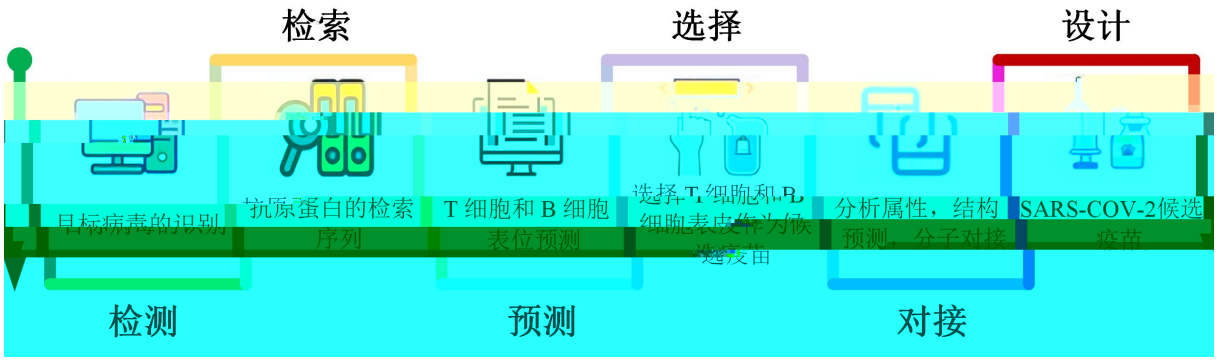
MHC-I MHC-II

S B

COVID-19

2-3 AI ML

AI ML		
[57]	SARS-CoV-2 T B	
XGBoost[58]		
[59]	SARS-CoV-2 HLA	
[60]		https://github.com/zikunyang/DCVST



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Prachar [59] 174 SARS-CoV-2 11 HLA SARS-CoV-2 HLA SARS-CoV-2

COVID-19 Yang [60]

DeepVacPred

DeepVacPred 694aa 16 B

82 CTL 89 HTL SARS-CoV-2 RNA

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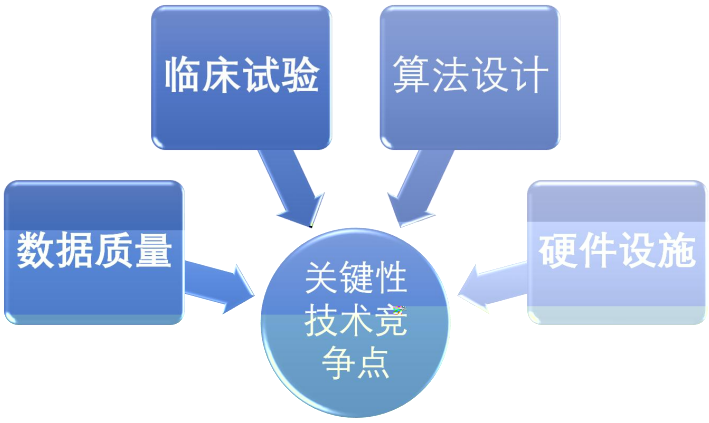

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Graphic Processing Unit GPU

Tensor Processing Unit TPU

Central Processing Unit CPU GPU

Field Programmable Gate Array FPGA

AI/ML

2014

Generative Adversarial Networks GANs

2014 2015 AI

AI Exscientia

Insilico Medicine

AI

AI

2016 2017 AI

AI

2018 AI

AI Exscientia Atomwise Recursion Insilico Medicine

AI AI

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Benevolent AI				Baricitinib
Exscientia				Exscientia AI

Atom

Recursion

NME

2019 Recursion

Takeda 60

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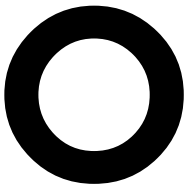

Insilico
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IND-enabling COVID-19

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AI 2019

AI Benevolent AI Atomwise Recursion

3-2

AI

3-2 AI

Benevolent AI	2019 9 17 - BenevolentAI 9000 2018 4 19 - BenevolentAI 1.15 2015 8 26 - BenevolentAI 8700
Exscientia	Exscientia 9 4.744 2022 1 10 IPO 2022 1 10 IPO - Exscientia 1 2021 7 8 Grant - Exscientia 150 2021 4 20 D - Exscientia 2.25 * https://www.crunchbase.com/organization/exscientia/company_financials
Atomwise	2020 09 17 D - 9000 - MSD Partners Octave Group Shumway Capital TpTfOCV Partners OMX Ventures Avenir Growth 2019 08 22 C 5300 – Shumway Capital TPTF OCV Partners 2018 03 1 B 3600 - Shumway Capital Morgan Noble Avenir Growth Capital
Recursion	2019 7 15 Recursion Pharmaceuticals 1.21 C Baillie Gifford Scottish Mortgage Investment Trust Intermountain Ventures University of Minnesota Texas Tech University System
Insilico Medicine	Insilico Medicine 10 3.063 2022 1 11 Venture - Series Unknown 2022 1 11 - Insilico Medicine 2021 6 22 C - Insilico Medicine 2.55 2020 4 20 B -Insilico Medicine * https://www.crunchbase.com/organization/insilico-medicine/company_financials
	2 2021 2 19 SciClone Pharmaceuticals 1.34 2021 2 19 - SciClone Pharmaceuticals 1.34

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	2018 7 3 SIG 2020 3 16 1000 A
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3-3 AI

	AI DrugSpaceX ModelArts		
	80%		
	CPCR CPCR		
	DNA 2021 10 MindSpore AlphaFold2 2 3		
	1.5		

	2019 11 FDA		

Artificial Intelligence AI

— **Protein-Protein Inte**

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Exscientia Atomwise Recursion Insilico Medicine

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