ADMET

AI +

AI +

AI

Artificial Intelligence AI

“ ”

Machine Learning ML “AI ”

“AI ” ML

Decision Tree DT Hidden Markov Model HMM

20 Igor Aizenberg

Artificial Neural Network ANN “ Deep Learning DL ”

1-1

Ribonucleic Acid Sequencing RNA-seq

High-Throughput Sequencing HTS

1-2

National Center

for Biotechnology Information NCBI Gene

Expression Omnibus GEO The Cancer

Genome Atlas TCGA Arrayexpress

PubMed

ML

Han [1]

2019 DriverML ML

1-2

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

2-1

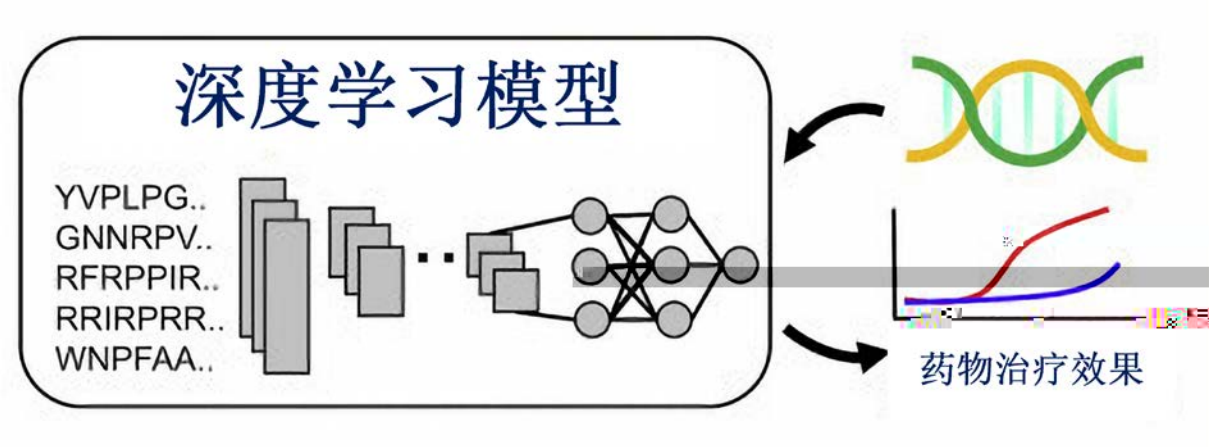
2-1

2 50

2-2

Yan [2] 2020 DL Antimicrobial peptides AMPs Deep-AmPEP30 AmPEP30 Convolutional Neural Network, CNN DeoxyriboNucleic Acid DNA AMP —AMPs

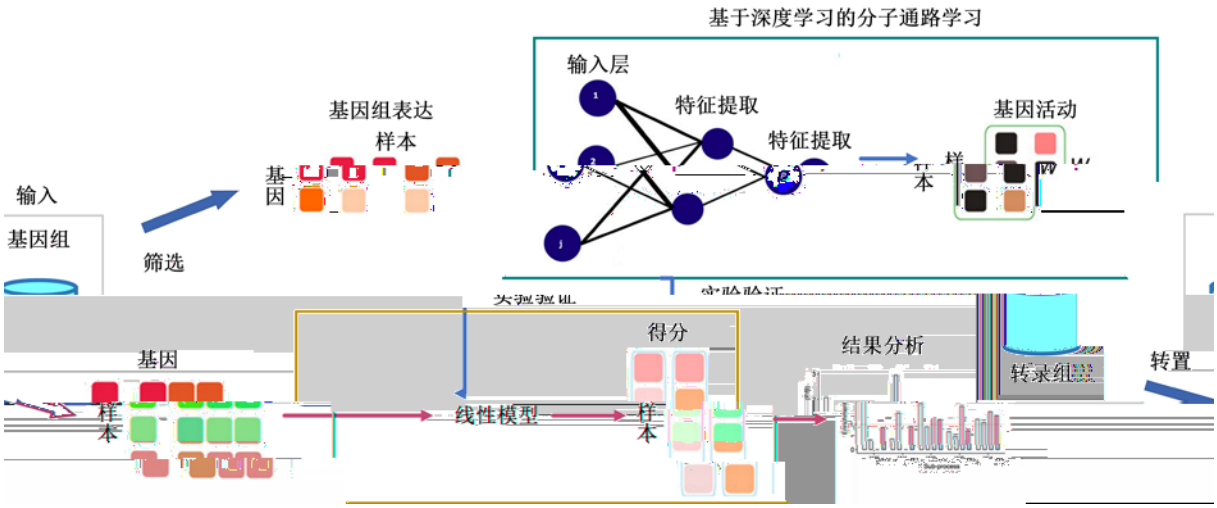
Zhavoronkov [3] GENTRL https://github.com/insilicomedicine/GENTRL DDR1 McCloskey [4] DNA DNA-Encoded small molecule Libraries DEL ML Xing [5] XGBoost



2-2

2-3 DisGeNET STRTCH STRING

Gu [6] 2020 197 DisGeNET



2-3

Neurodegenerative Diseases NDDS

ML

ML

Protein-

Virtual Screening VS

CADD

ML VS

ML VS VS

2-5

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

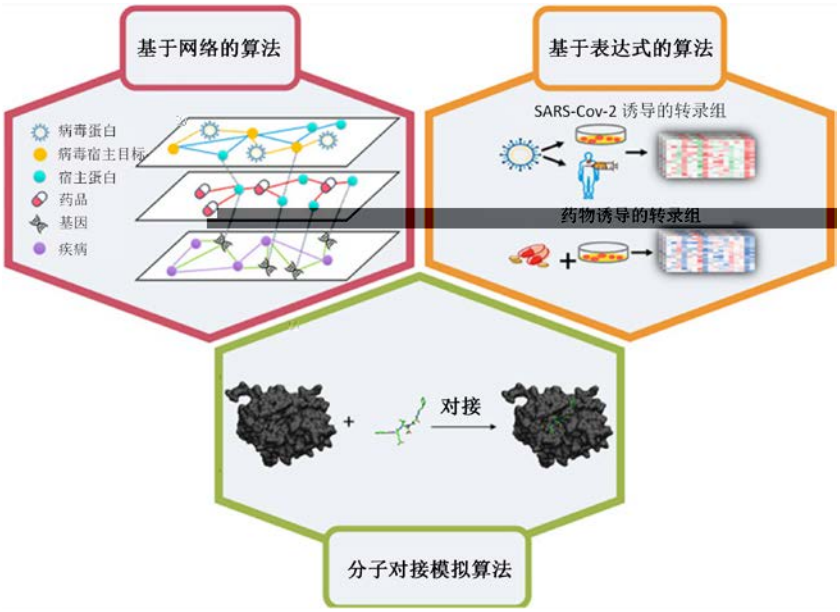
SBVS SBVS

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-

1

2-1 AI ML

AI ML		
[13]	SARS-CoV-2	https://github.com/Murali-group/SARS-CoV-2-network-analysis

[14]5 Yï ”QC04x0X’ÒØ ’9ÓQ À†

[22]		https://github.com/uhlerlab/covid19_repurposing

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]

2-7

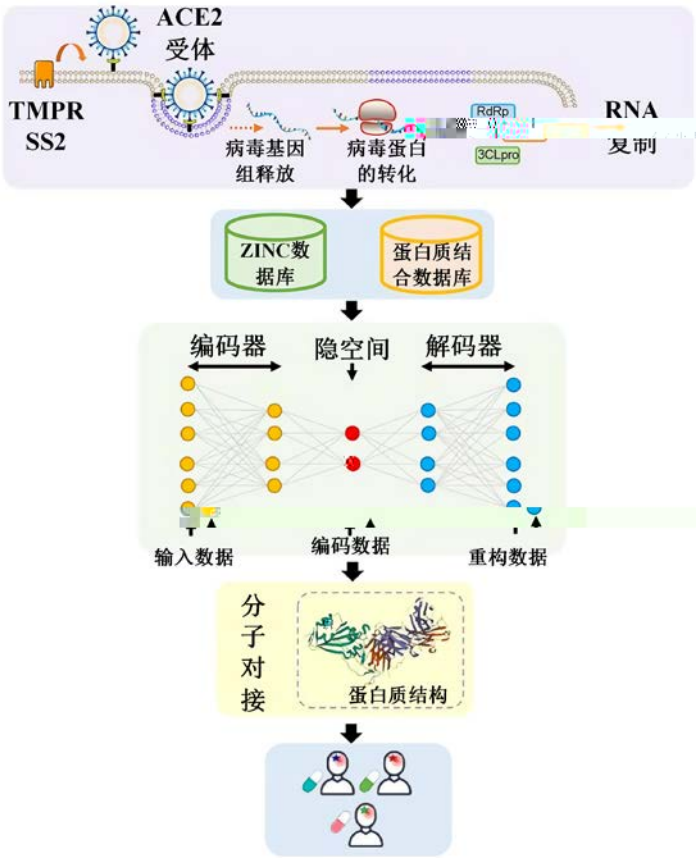
2-2

[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]		
[39]	SMILES	
[40]		
[41]		https://github.com/pkuwangsw/COVIDVS
[36]		

Quantitative Structure-Activity Relationship QSAR

QSAR

Gaussian Process GPs

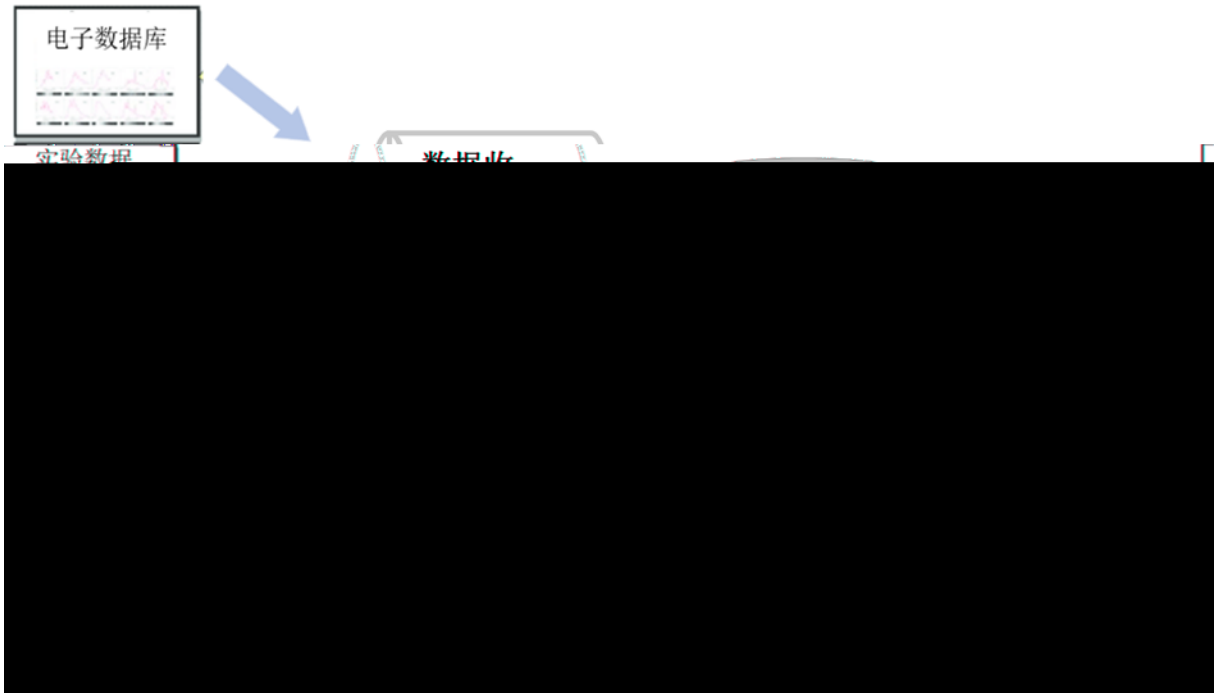
Vega (https://www.vega-qsar.eu/) QSAR-Co[42] Transformer-CNN[43] Chemception (https://github.com/Abdulk084/Chemception) QSAR

N C L tqsW. Á >-i£ $ ‰ðaE4A3Dj <0431BE6>-8 4 Td/M

Hooshmand [45]

16 HCoV

12



2-8

2-9

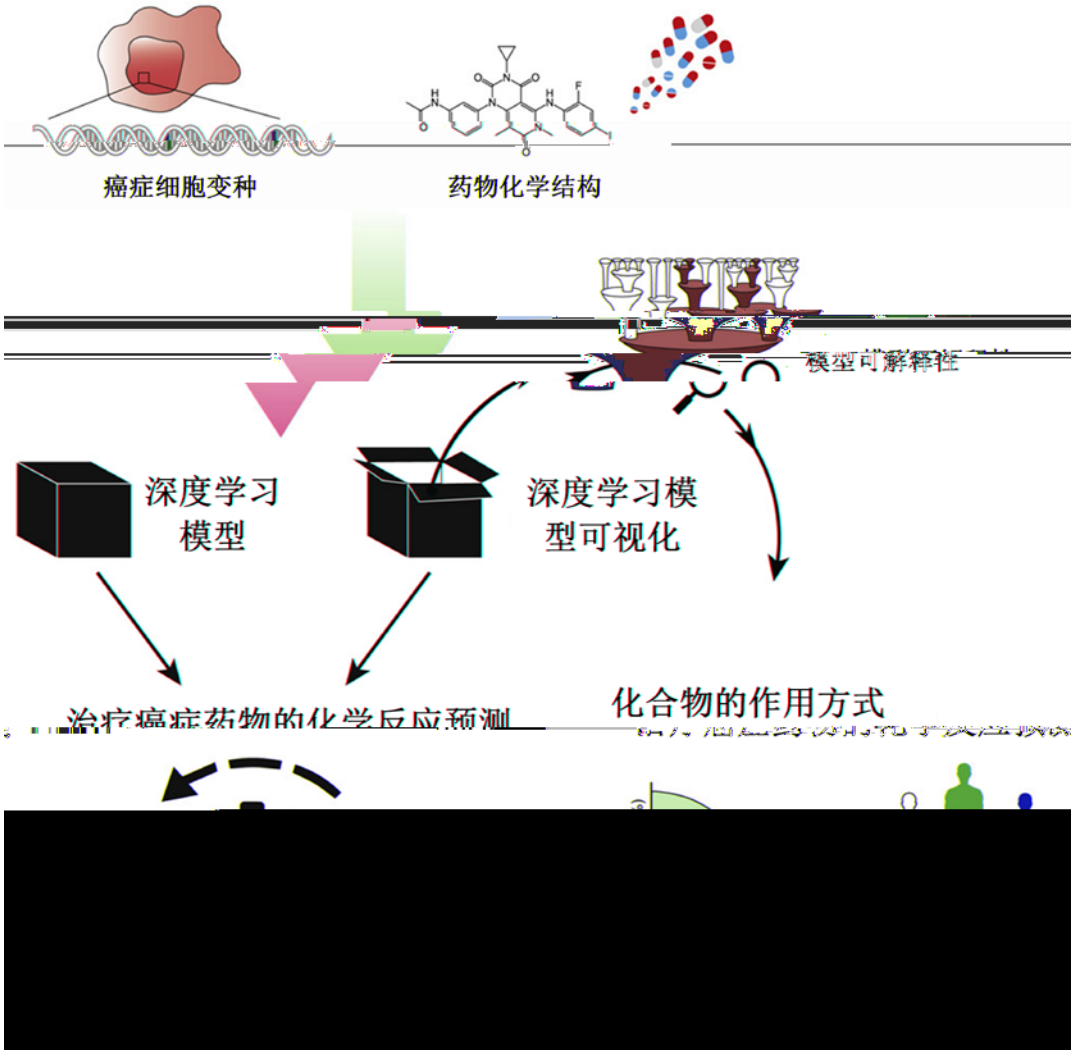
Web LimTox pkCSM admetSAR Toxtree DeepTox[46] PrOCTOR[47]

Robledo-Cadena [48]

PrOCTOR

2,576

16 2

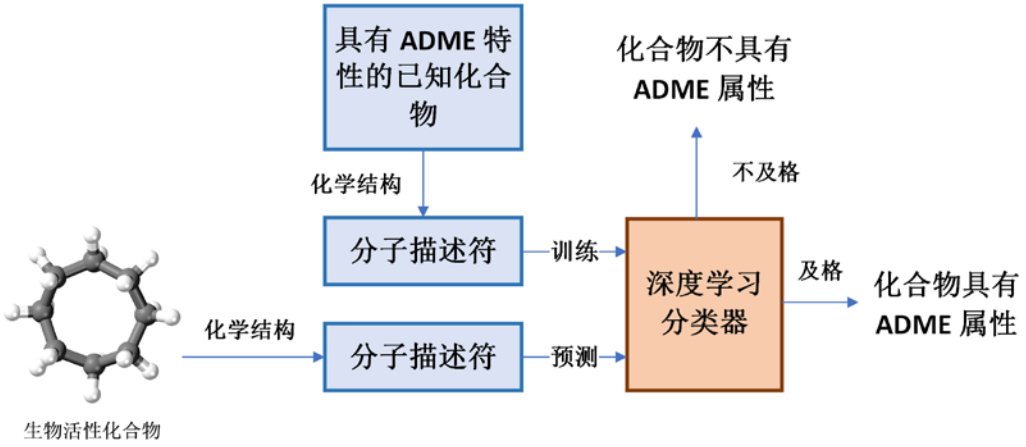


2-9

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

Parabolic

Response Curve PRC

10 HIV

AI-PRS 33%

Tang [51]

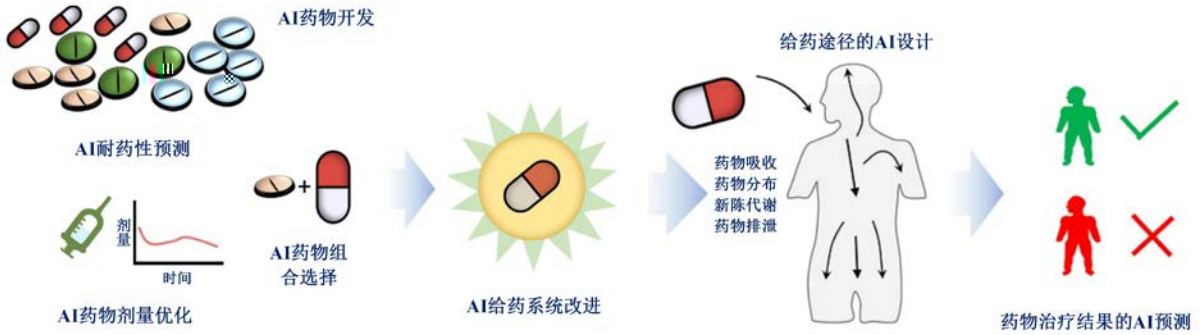
ML

Hu [52]

K ML

Digoxin Imai [53]

Vancomycin



2-11

2-12

CATALYST

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

2-13

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

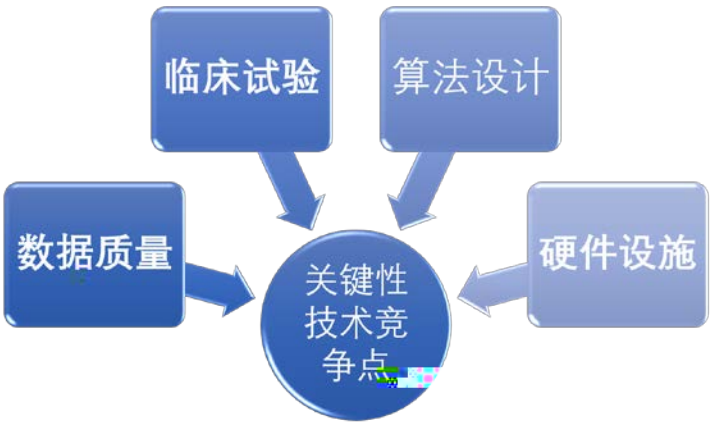
COVID-19 Yang [60] DeepVacPred

DeepVacPred 694aa 16 B

82 CTL 89 HTL SARS-CoV-2 RNA

3.5

1



3-1

3

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

3-1

3-1

Benevolent AI				Baricitinib
Exscientia				Exscientia AI

Atomwise				
Recursion				NME 2019 Recursion Takeda 60 6
Insilico Medicine				7 IND-enabling COVID-19 3CL MAT2A USP1 “ ” 0 1
				rCARD GPU NVIDIA Clara Discovery Pipeline GROMACS Autodock-GPU
				AI AI

				PandaOmics Chemistry42
				“ ”
				AI
				AI

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 - 1aÁ•34bD!\ >8700 2022 1 ò 10 -

	2 2021 2 19 SciClone Pharmaceuticals 1.34 2021 2 19 - SciClone Pharmaceuticals 1.34 2016 12 21 -Healenvoy 300
	1 2000 2020 7 9 2020 7 9 2000
	2018 7 3 SIG 2020 3 16 1000 A
	2021 08 4 D IMO Ventures Neumann Capital Artisan Partners Artisan Partners 2020 9 3.188 C 2 Mirae Asset IMO Ventures Parkway SIG
	2021 10 20 2022 06 22 A 5

3-3

3-3 AI

	AI DrugSpaceX ModelArts		
	80%		
	CPCR CPCR		
	DNA 2021 10 MindSpore		

	AlphaFold2 2 3		
	1.5 2019 11 FDA		

Artificial Intelligence AI

Artificial Neural Network ANN

Computer Aided Drug Design CADD

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Convolutional Neural Network CNN

Deep Learning DL

Machine Learning ML

Protein-Protein Interaction, PPI

Quantitative Structure-Activity Relationship QSAR

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Exscientia

Atomwise Recursion Insilico Medicine

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