

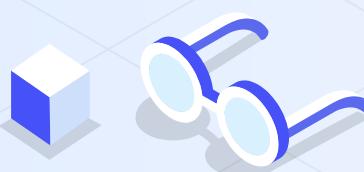
CSE

GRADUATION THESIS

AI-Powered Decision Support System for Antiviral Pharmaceutical Formulation

Advisors: Assoc. Prof. Quan Thanh Tho, PhD
Mr. Bang Ngoc Bao Tam, MEng

Student: Nguyen Quang Duc - 1810118



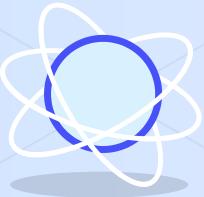


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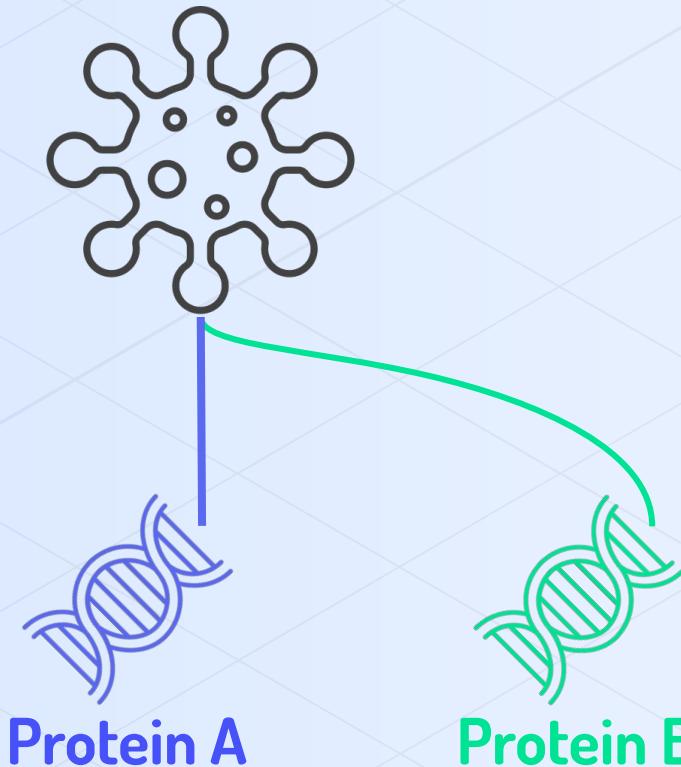
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Summary and Future
Developments



VIRUSES AND THEIR MAIN PROTEINS

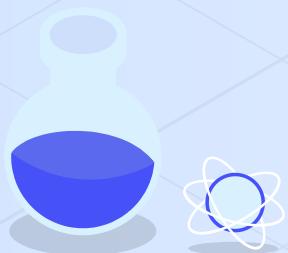
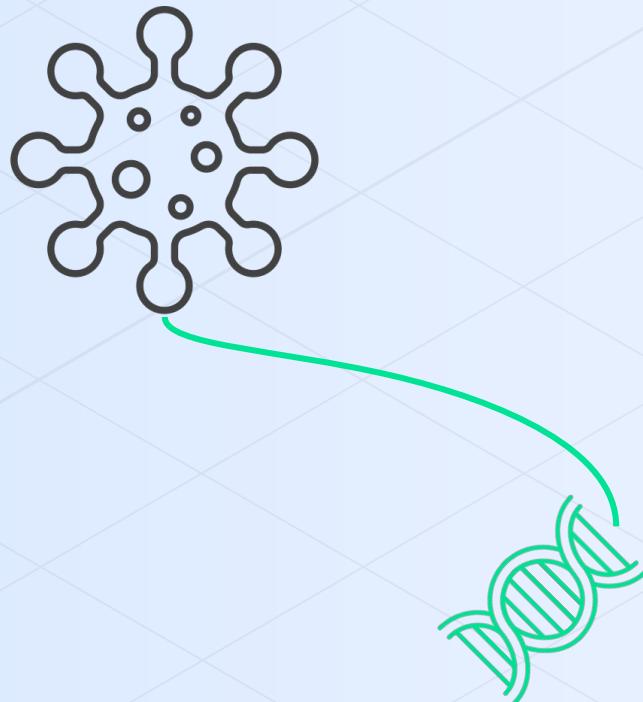
VI



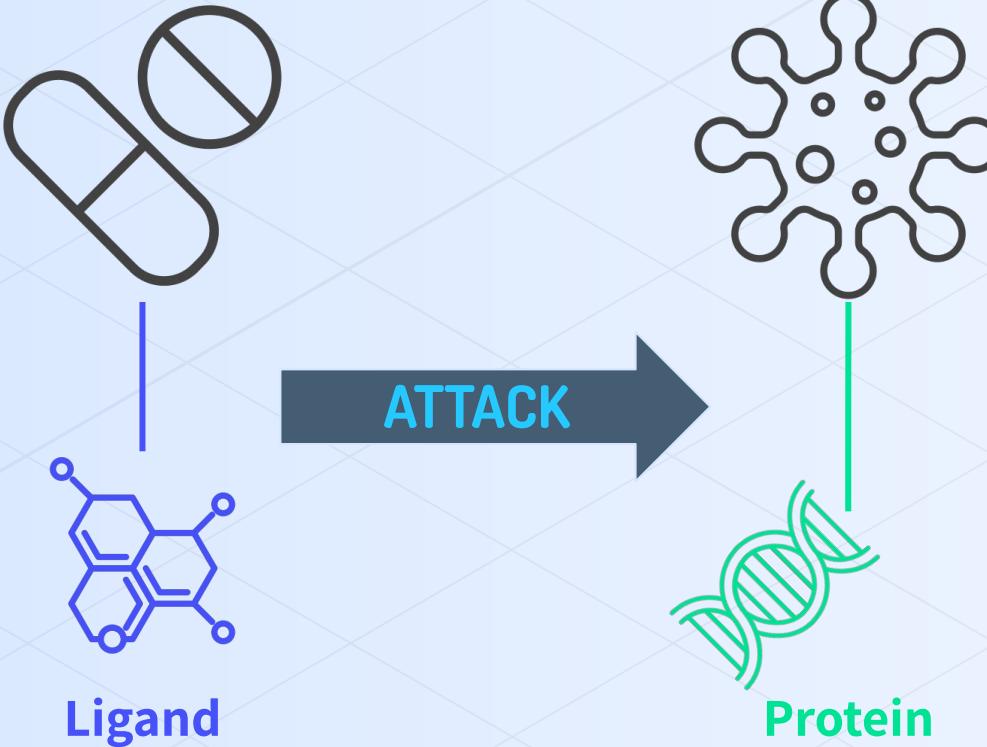
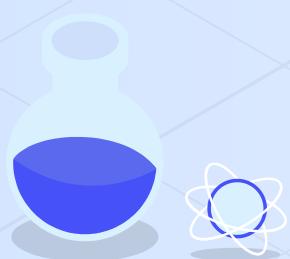
US



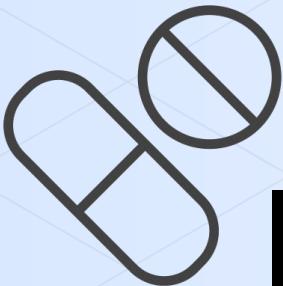
HOW DRUGS “KILL” VIRUSES?



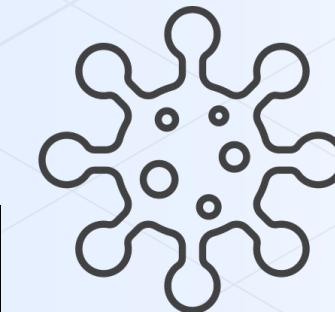
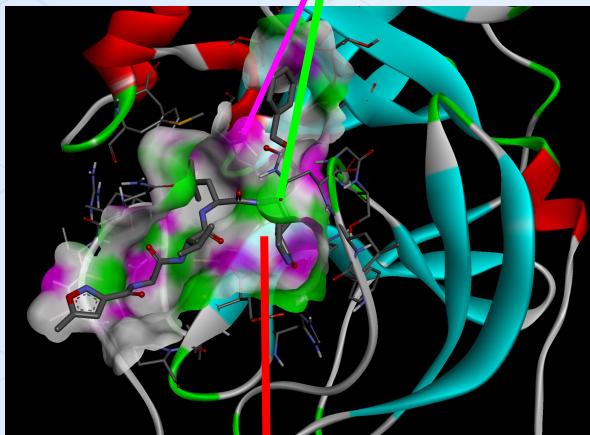
HOW DRUGS “KILL” VIRUSES?



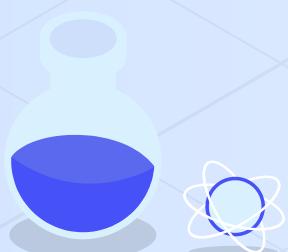
WHERE DOES LIGAND REALLY INTERACT?

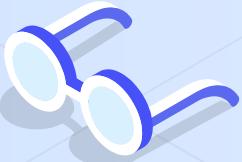


Ligand

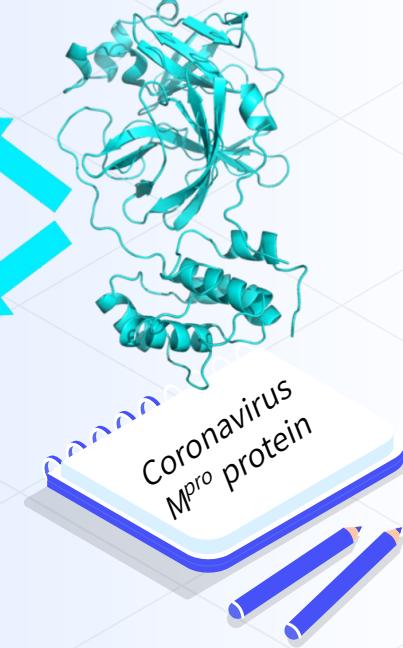
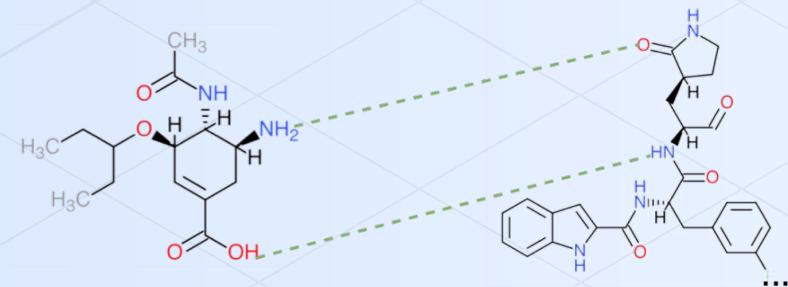
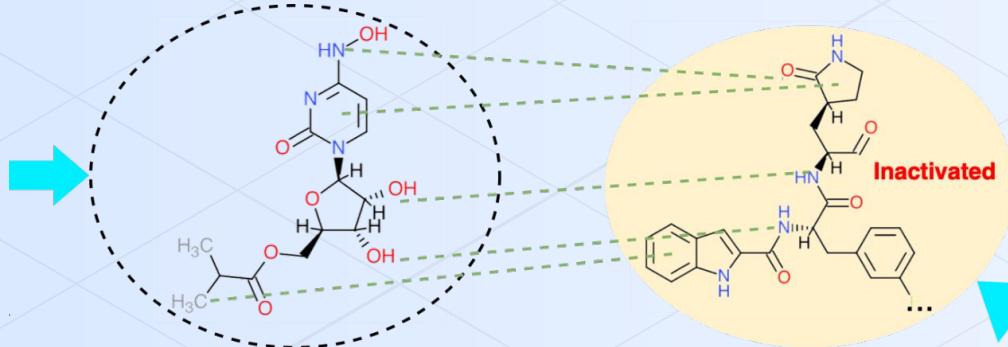
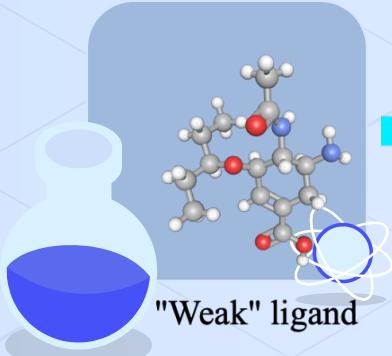
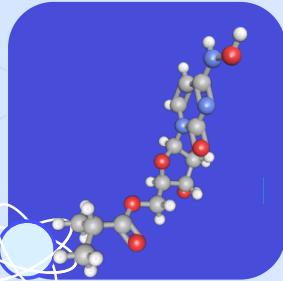


Protein



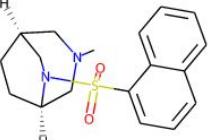
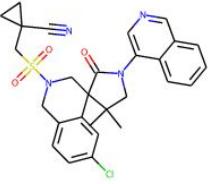


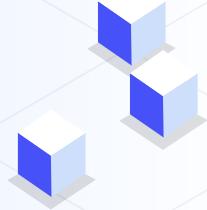
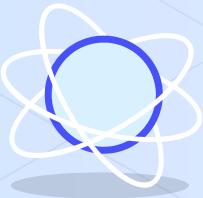
CAN ANY LIGANDS BECOME DRUGS?



DRUG DESIGN AT EARLY STAGE

“Designing strong ligands”

Image	Molecule	MW	cLogP	TPSA	Rotatable Bonds	Fraction sp3	HBA	HBD	Covalent Warhead
	<chem>CLI-SEL-cf46d3af-1</chem> <chem>CN1C[C@H]2CC[C@H](S(=O)(=O)c1ccccc3cccc13)C2</chem> Check Availability on Manifold	330.14	2.55	40.62	2	0.44	3	0	false
	<chem>ALP-POS-01611061-1</chem> Duplicate of: <chem>MAT-POS-50a80394-8</chem> <chem>CC1(C)CN(c2cncc3cccc23)C(=O)C12CN(S(=O)(=O)CC1(C#N)CC1)Cc1ccc(Cl)cc1</chem> 3-aminopyridine-like Ordered Check Availability on Manifold	534.15	4.65	94.37	4	0.39	5	0	false



01

INTRODUCTION

Problem Definition and Solution Overview





CROWDSOURCING DRUG DESIGN

PURPOSE

Utilize the power of community

Draw or enter SMILES (add multiple by pressing "Add" after each entry)

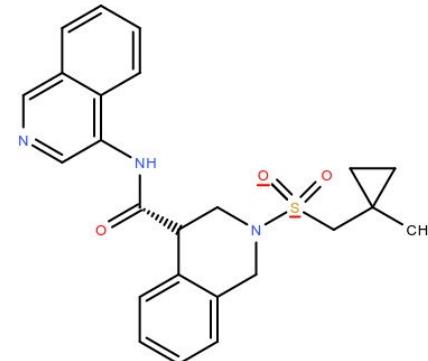
Warning: Structural alerts found (see below). Note: these are just warnings, you can still submit the molecule.

CC1(CS(=O)(=O)N2Cc3cccc3C(C(=O)Nc3cncc4cccc43)C2)CC1

Add



100%



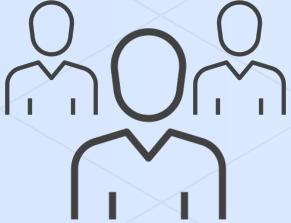
?

H
C
N
O
S
P
F
Cl
Br
I
PT





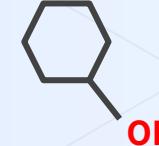
BUT THE PROBLEM IS...



NON-EXPERTS

A large number and has more time

Design



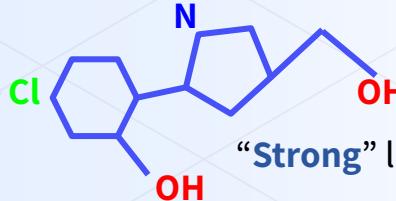
“Weak” ligands



EXPERTS

Not many experts and they do not have much time

Design

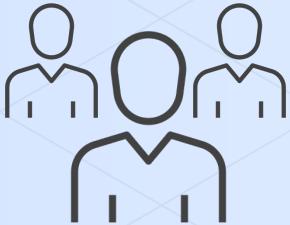


“Strong” ligands





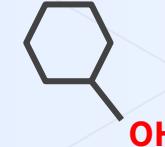
BUT THE PROBLEM IS...



NON-EXPERTS

A large number and has more time

Design



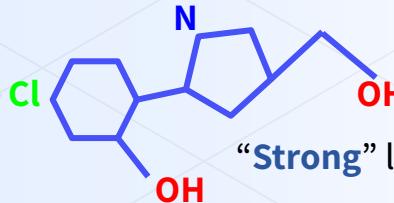
“Weak” ligands



EXPERTS

Not many experts and they do not have much time

Design



“Strong” ligands

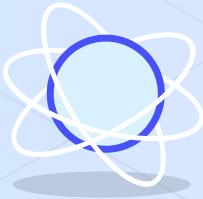
HOW TO EFFECTIVELY UTILIZE COMMUNITY POWER?



AN INTELLIGENCE DECISION SUPPORT SYSTEM

To make the designed drugs
better and better





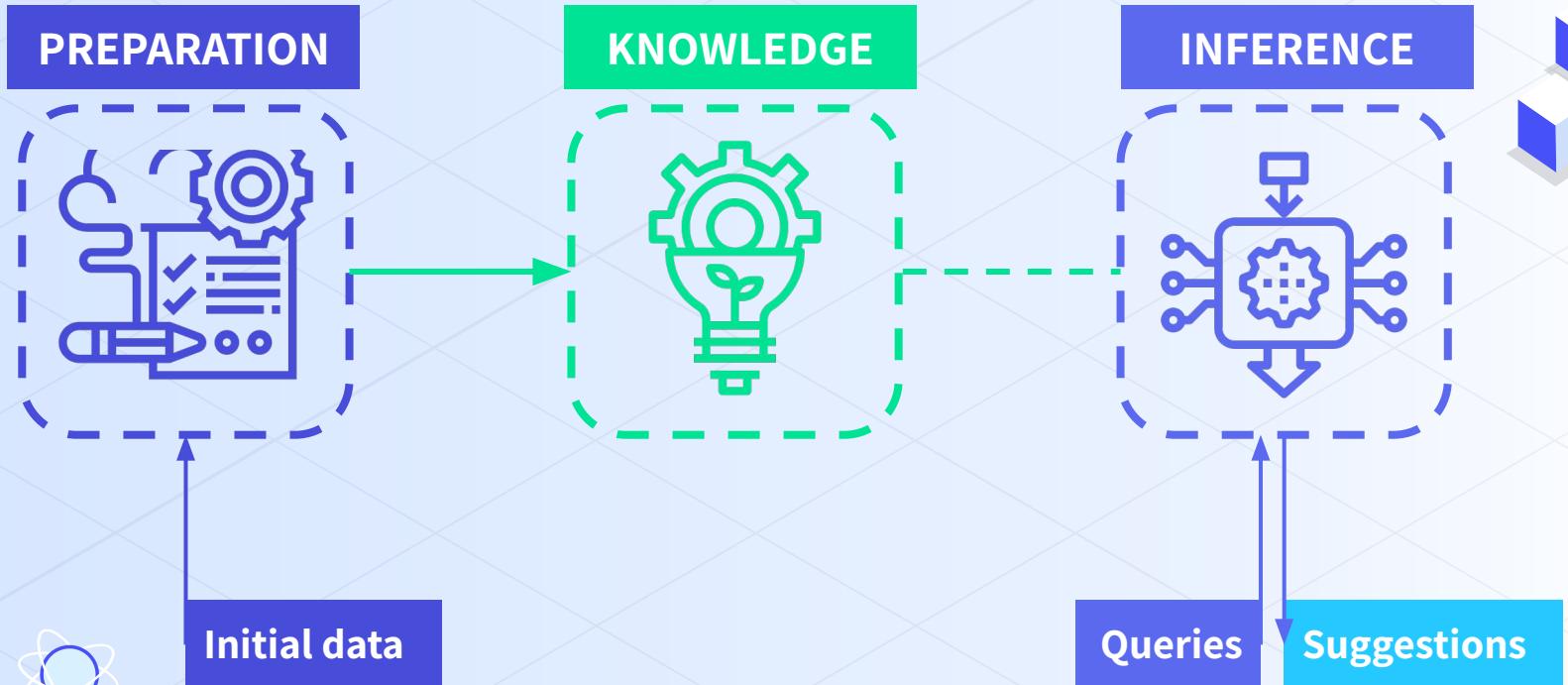
02

BACKGROUNDS

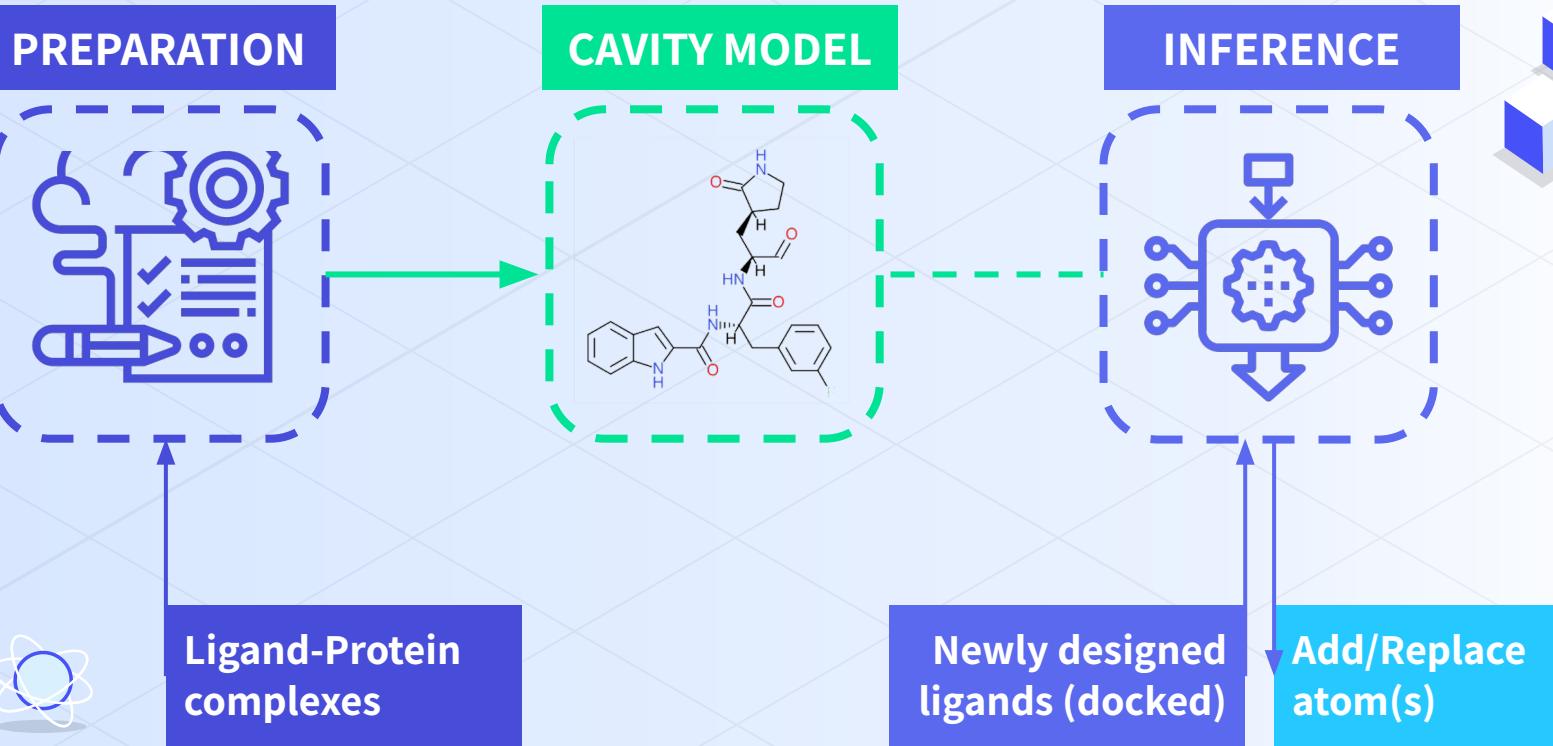
Computer Science Backgrounds



DECISION SUPPORT SYSTEM IN A NUTSHELL



DECISION SUPPORT SYSTEM IN OUR SITUATION



THE INITIAL PROBLEM BREAKS INTO



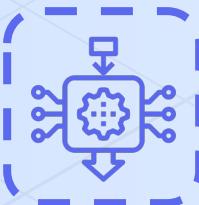
PREPARATION

1. Identifying Drug-Protein Interactions

- Ligand-Protein complexes → Interactions

2. Building Cavity Model for Target Protein

- Interactions → Cavity Model



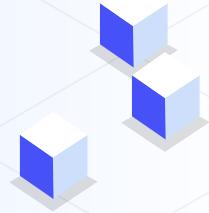
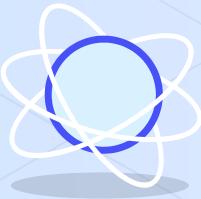
INFERENCE

3. Building Algorithm for Recommending

- Newly Designed Ligands → Suggestions

Cavity Model





03

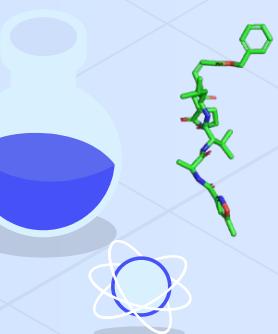
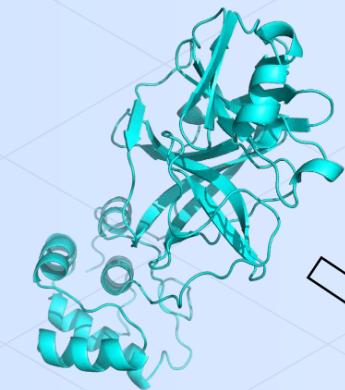
SOLUTIONS

Details of Designed System

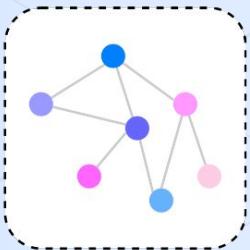




IDENTIFYING DRUG-PROTEIN INTERACTIONS

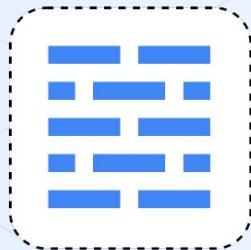


OVERALL PIPELINE



GNN-based Model

Ligand atom	Protein atom	Score
●	●	0.9
●	●	0.85
●	●	0.92



Knowledge-driven
Algorithm

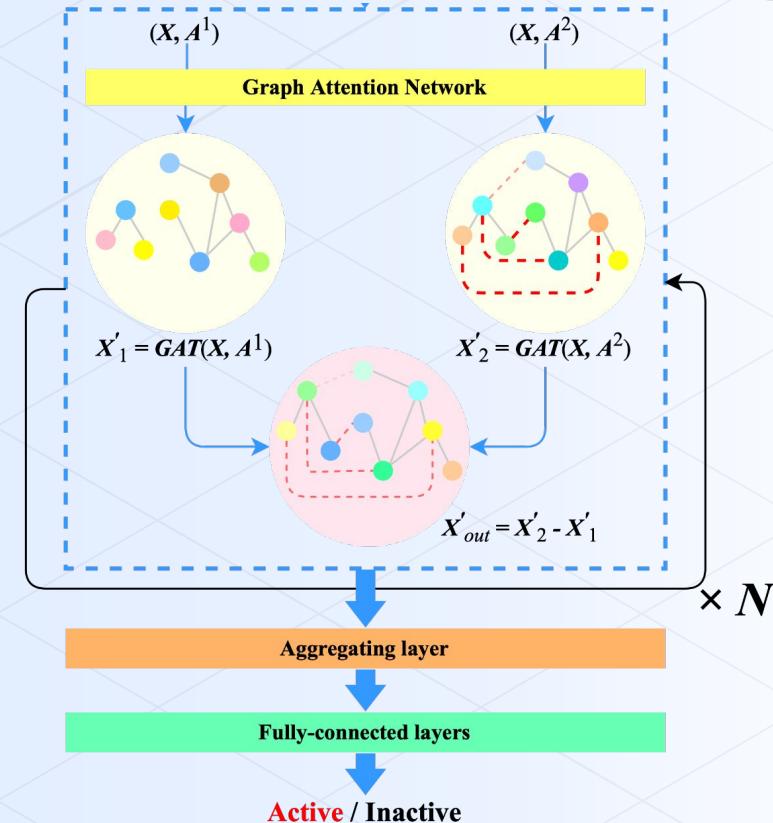
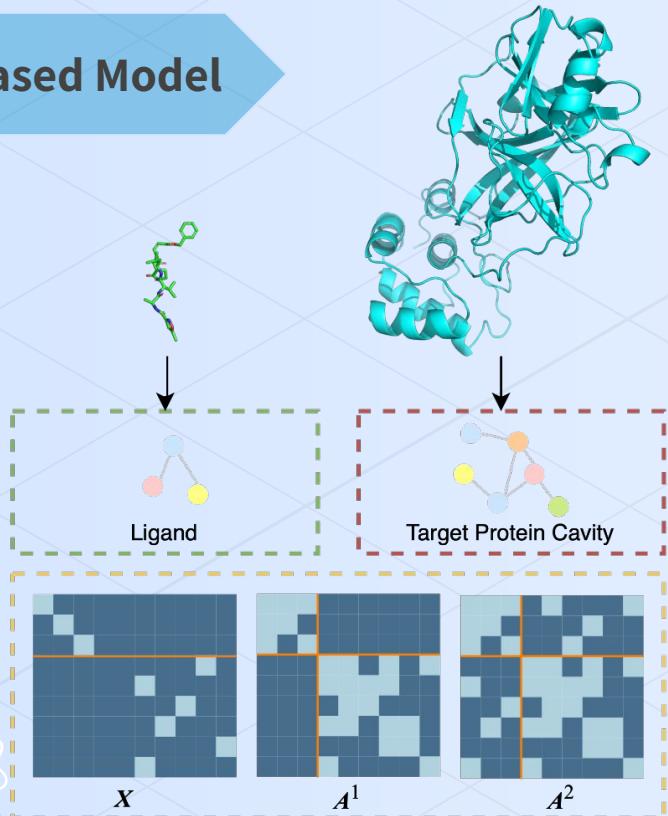
Ligand atom	Protein atom
H-Donor	H-Acceptor
H-Acceptor	H-Donor
Aromatic	Hydrophobe



IDENTIFYING DRUG-PROTEIN INTERACTIONS



GNN-based Model

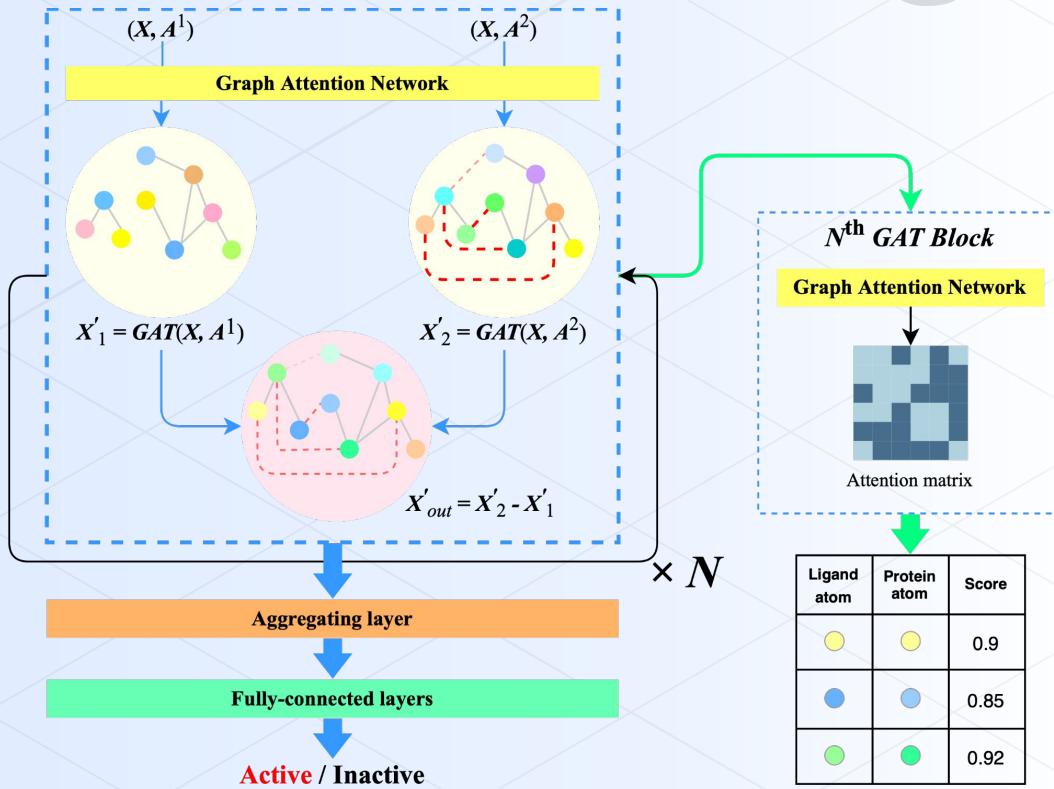
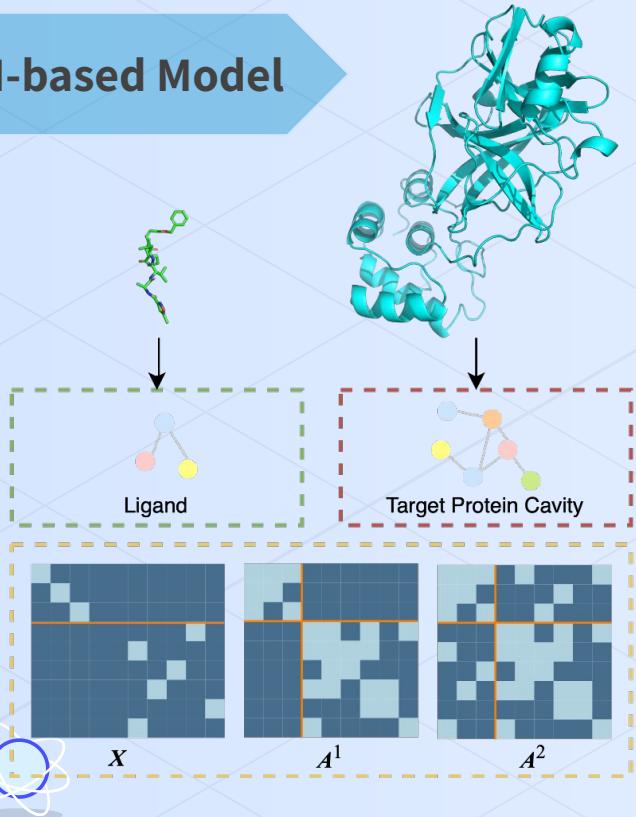


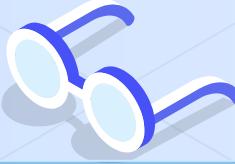


IDENTIFYING DRUG-PROTEIN INTERACTIONS



GNN-based Model

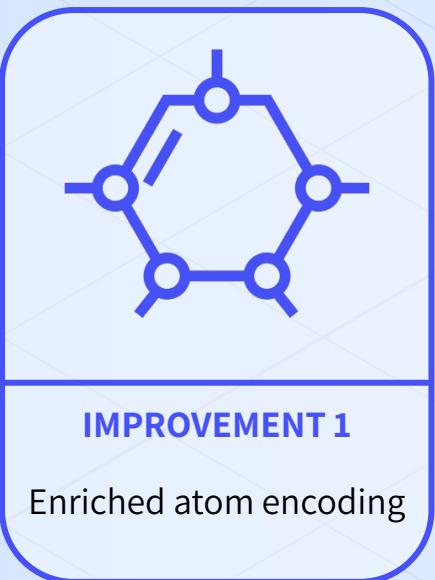




IDENTIFYING DRUG-PROTEIN INTERACTIONS

GNN-based Model

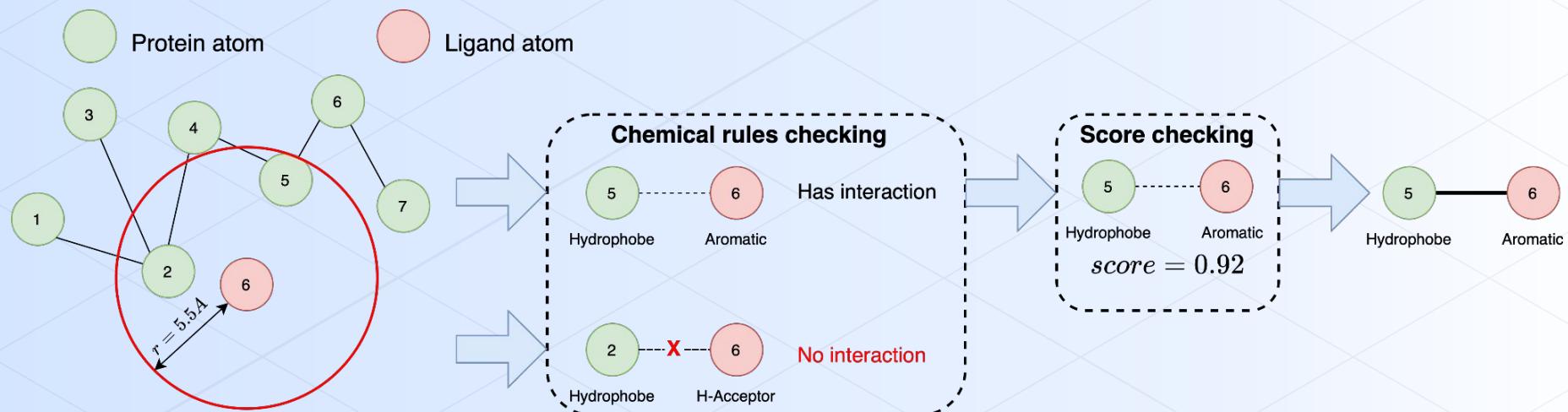
IMPROVEMENTS



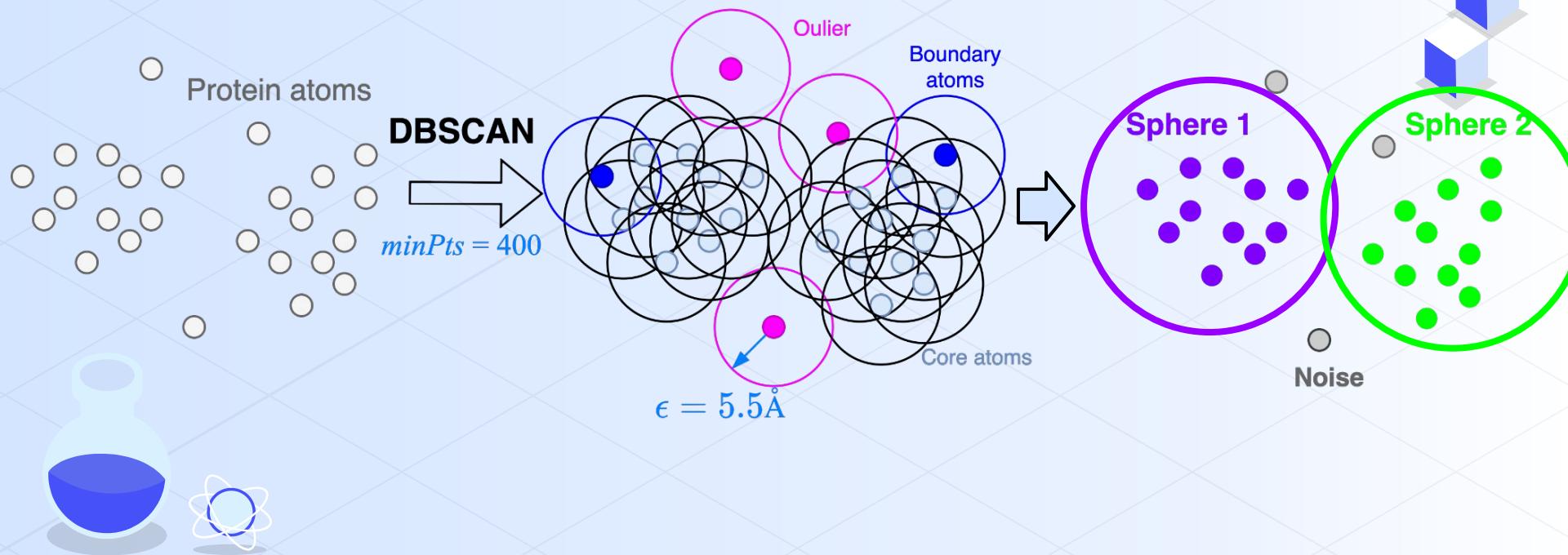


IDENTIFYING DRUG-PROTEIN INTERACTIONS

Algorithm

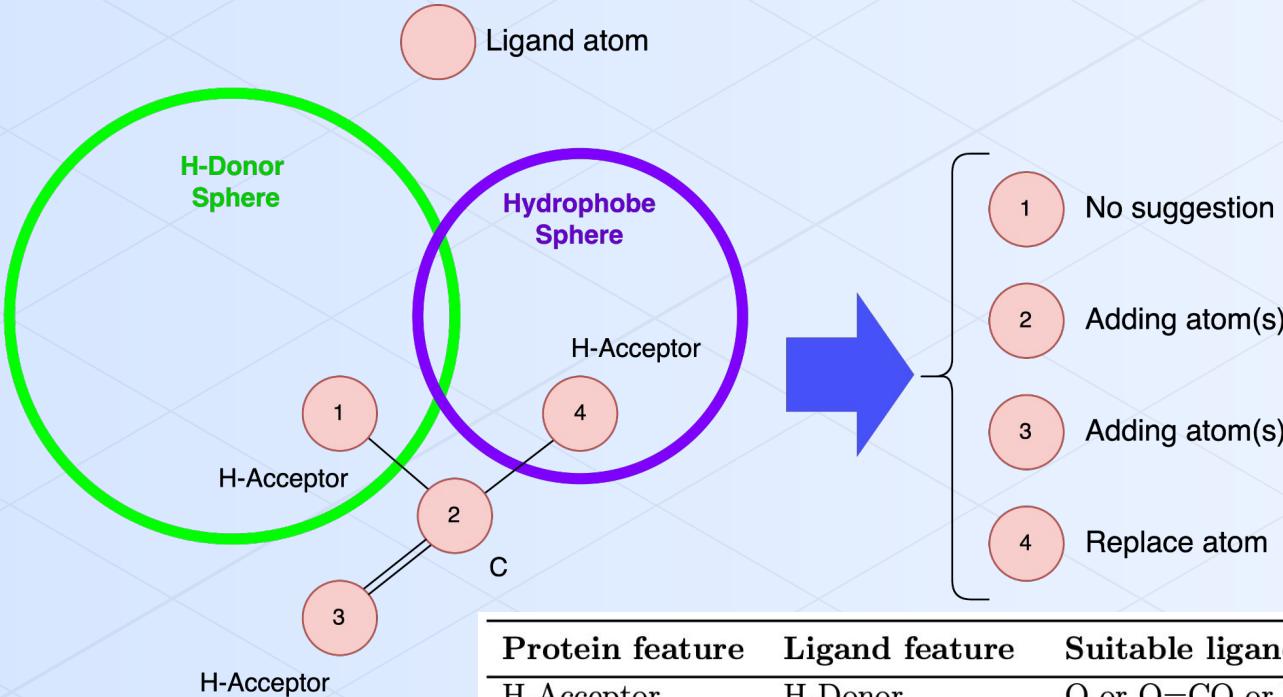


BUILDING CAVITY MODEL FOR TARGET PROTEIN

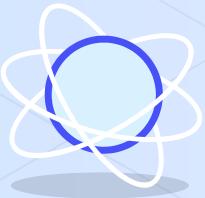




BUILDING ALGORITHM FOR RECOMMENDING



Protein feature	Ligand feature	Suitable ligand atom(s)
H-Acceptor	H-Donor	O or O=CO or N or NC=O
H-Donor	H-Acceptor	O=CO or NC=O or C=O
Hydrophobic or C	Aromatic	c1ccccc1 or Cc1cccc1 or C=Cc1cccc1
Aromatic	Hydrophobic or C	C



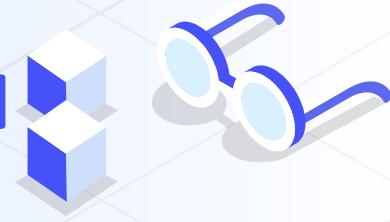
04

EXPERIMENTS

Evaluations of Designed System



RESULTS OF INTERACTION IDENTIFICATION



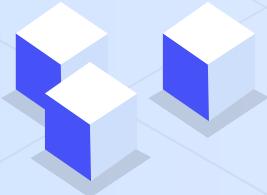
20 complexes
manually annotated



No.	Complex name	Recall	No.	Complex name	Recall
1	6LZE	0.82	11	6XQS	0.93
2	6M0K	0.58	12	7E19	0.73
3	6WTK	1.00	13	7JU7	0.21
4	6XA4	0.56	14	7KX5	0.86
5	6XBG	1.00	15	7L0D	0.86
6	6XBH	1.00	16	7LMD	0.50
7	6XBI	0.94	17	7LME	0.63
8	6XCH	1.00	18	7LMF	0.83
9	6XFN	0.40	19	7LMH	1.00
10	6XHM	0.88	20	7LMJ	1.00

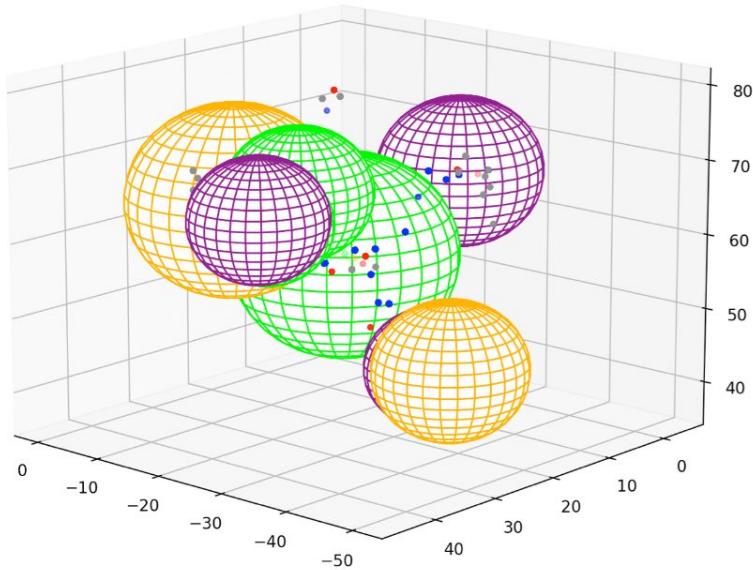
Average Recall

0.79

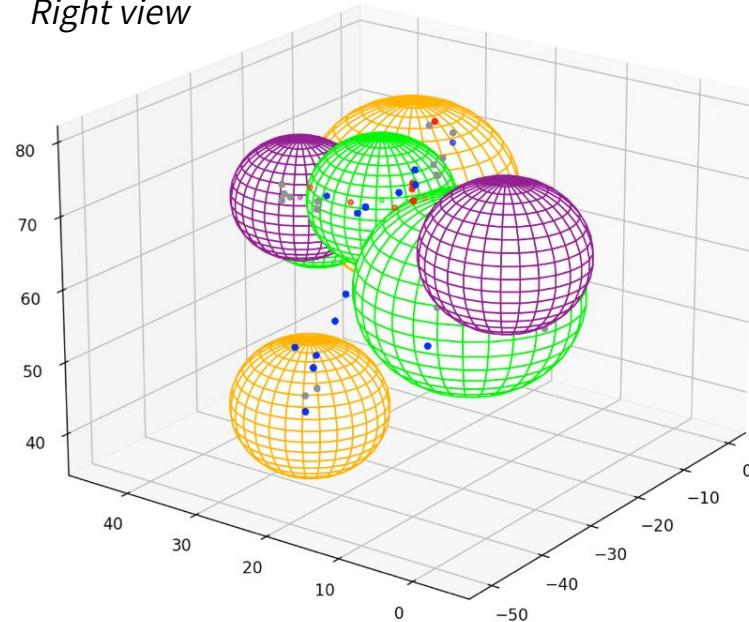


CAVITY MODEL FOR TARGET PROTEIN

Left view



Right view



H-Donor

H-Acceptor

Hydrophobe

THE PERFORMANCE OF DESIGNED SYSTEM



With single suggestion

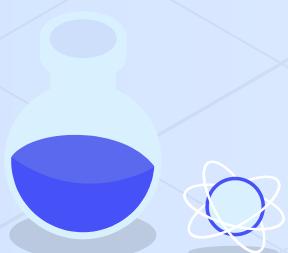
-0.76
kcal/mol

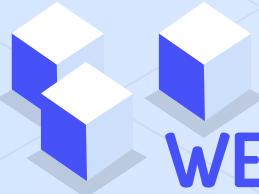
Binding Affinity



better than without any suggestions

	W/O SUGGESTION	W SUGGESTIONS
Number of participants	26	
Number of ligands	100	100
Mean docking score	-4.91	-5.67
Standard deviation of docking scores	1.46	1.41





WEB APPLICATION

- ✓ Multiple OSs supported
- ✓ Responsive User Interface
- ✓ 5 minutes processing time



The illustration features a computer monitor with a dark blue border. On the screen, there's a white interface titled "Computer-Aided Drug Design System" with a subtitle "From BK with Love ❤️❤️". The interface includes a toolbar with various icons, a sidebar with chemical symbols (O, /, C, N, S), and a central workspace showing a chemical structure: CC(C(=O)O)N. Below the monitor, there's a stylized blue balance scale and a flask containing blue liquid.

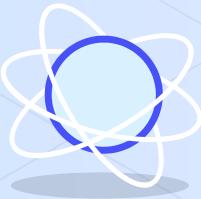
Computer-Aided Drug Design System

From BK with Love ❤️❤️

Let's create candidate compounds for treating COVID-19

Submit

CC(C(=O)O)N



05

CONCLUSION

Summary and Future Developments

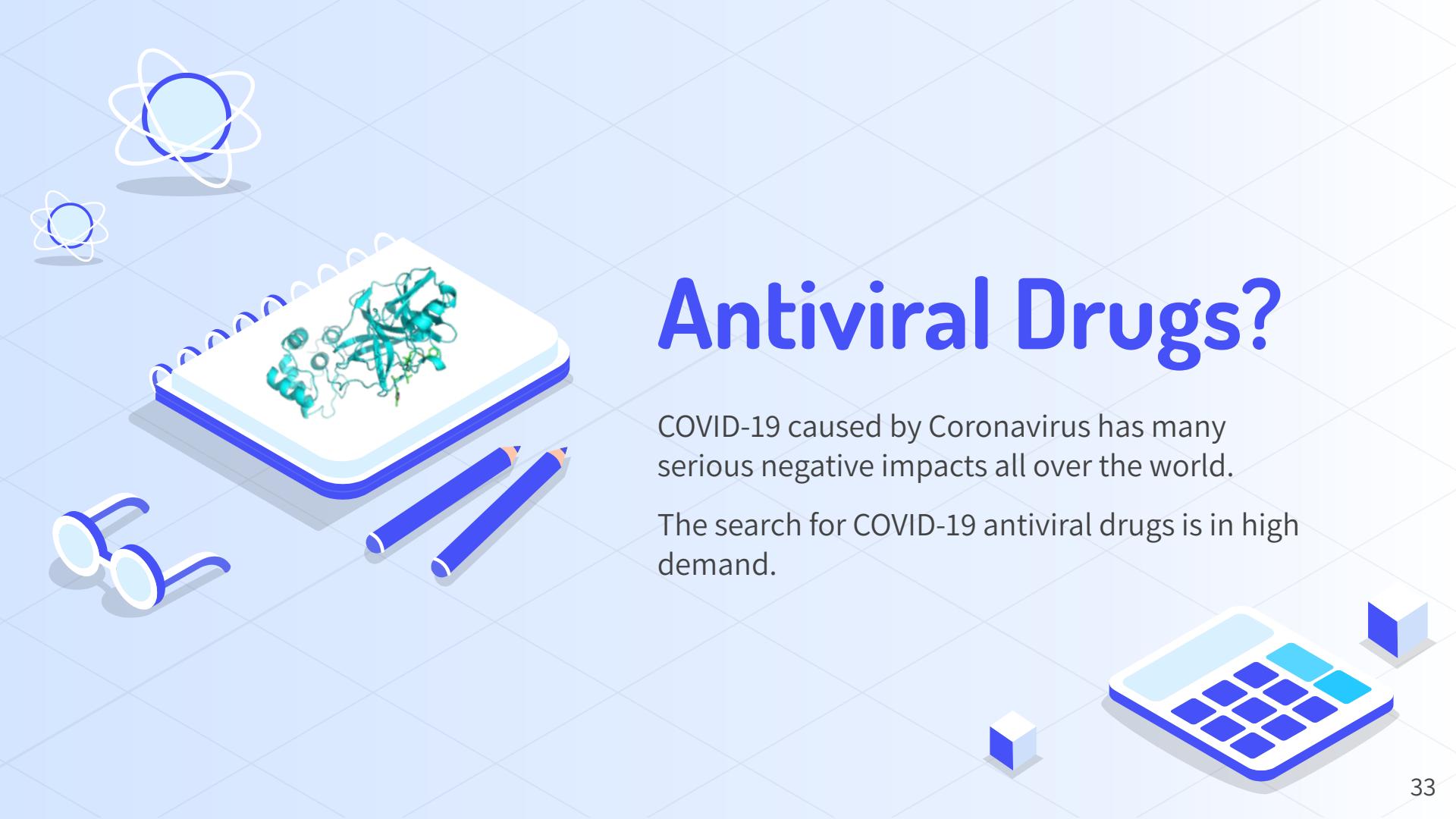


THE END

Thank You for Listening!

Nguyen Quang Duc (Mr.) | Faculty of Computer Science and Engineering
Ho Chi Minh City University of Technology | www.cse.hcmut.edu.vn | Skype: nguyenquangduc2000
A3 Building, 268 Ly Thuong Kiet Street, Ward 14, District 10, Ho Chi Minh City, Vietnam
M (+84) 898 986 370 | E duc.nguyenquang@hcmut.edu.vn



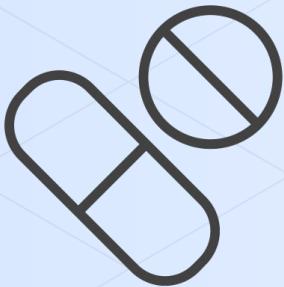
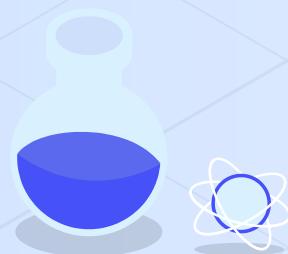


Antiviral Drugs?

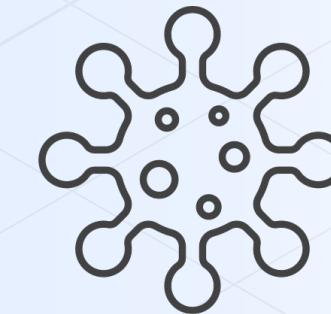
COVID-19 caused by Coronavirus has many serious negative impacts all over the world.

The search for COVID-19 antiviral drugs is in high demand.

HOW DRUGS “KILL” VIRUSES?

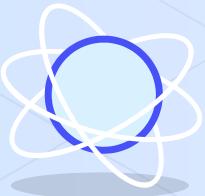


Ligand

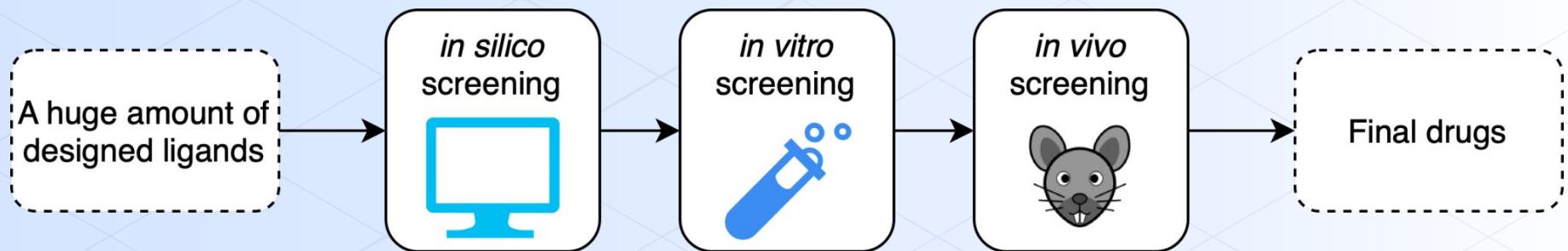
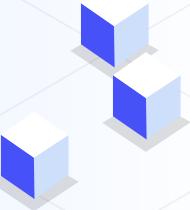


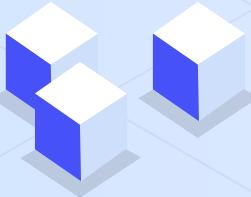
Protein





DRUG DISCOVERY PROCESS





CROWDSOURCING DRUG DESIGN SYSTEMS

COVID Moonshot System →

PostEra

Submit Submissions About Discuss

COVID Moonshot

Read About the Story

CONTRIBUTE YOUR DESIGNS

We will prioritize compounds and send them out
for synthesis and testing.

Track the status of previously submitted
molecules.

Join the discussion with scientists around the
world on our forum.

Methodology

Compound Tracker

Discuss

Draw or enter SMILES (add multiple by pressing "Add" after each entry)

Warning: Structural alerts found (see below). Note: these are just warnings, you can still submit the molecule.

CC(C(=O)OC[C@H]1O[C@H](n2ccc(N)nc2=O)[C@H](O)[C@@H]1O)Add

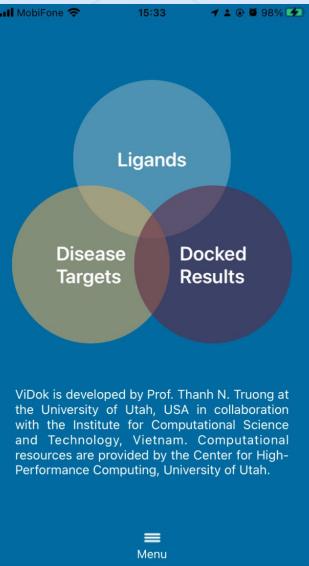
Back Disease Target Docked Results

New Run My Results Share

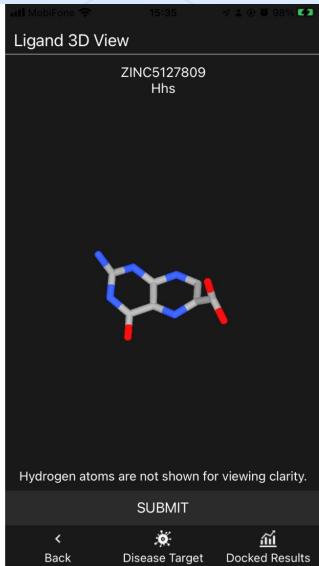
≡

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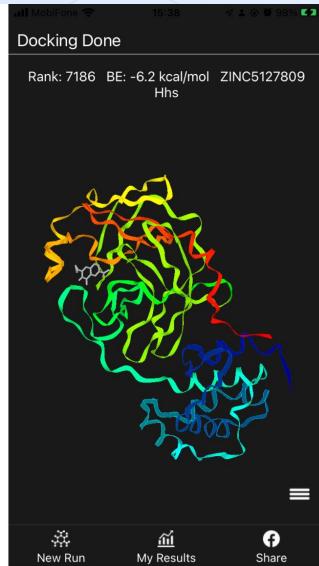
H C N O S P F Cl Br I PT



a) Welcome screen

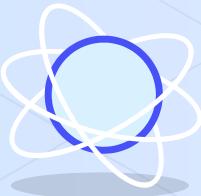


b) Design screen

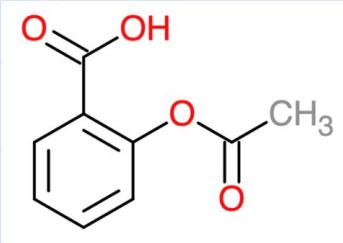


a) Result screen

ViDok System



MOLECULAR PRESENTATION

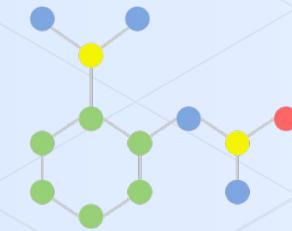


Kekulé Diagram

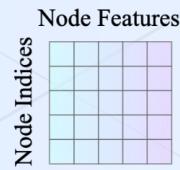
[0 0 0 1 ... 0 0 0 0 1]



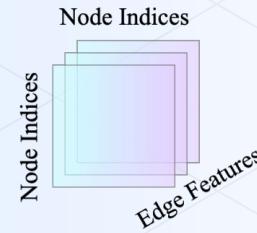
Fingerprint



Molecular Graph



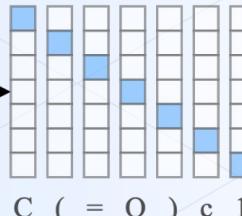
Node Feature Matrix



Adjacency Tensor

CC(=O)Oc1ccccc1C(=O)O → Tokenization → One-Hot Encoding

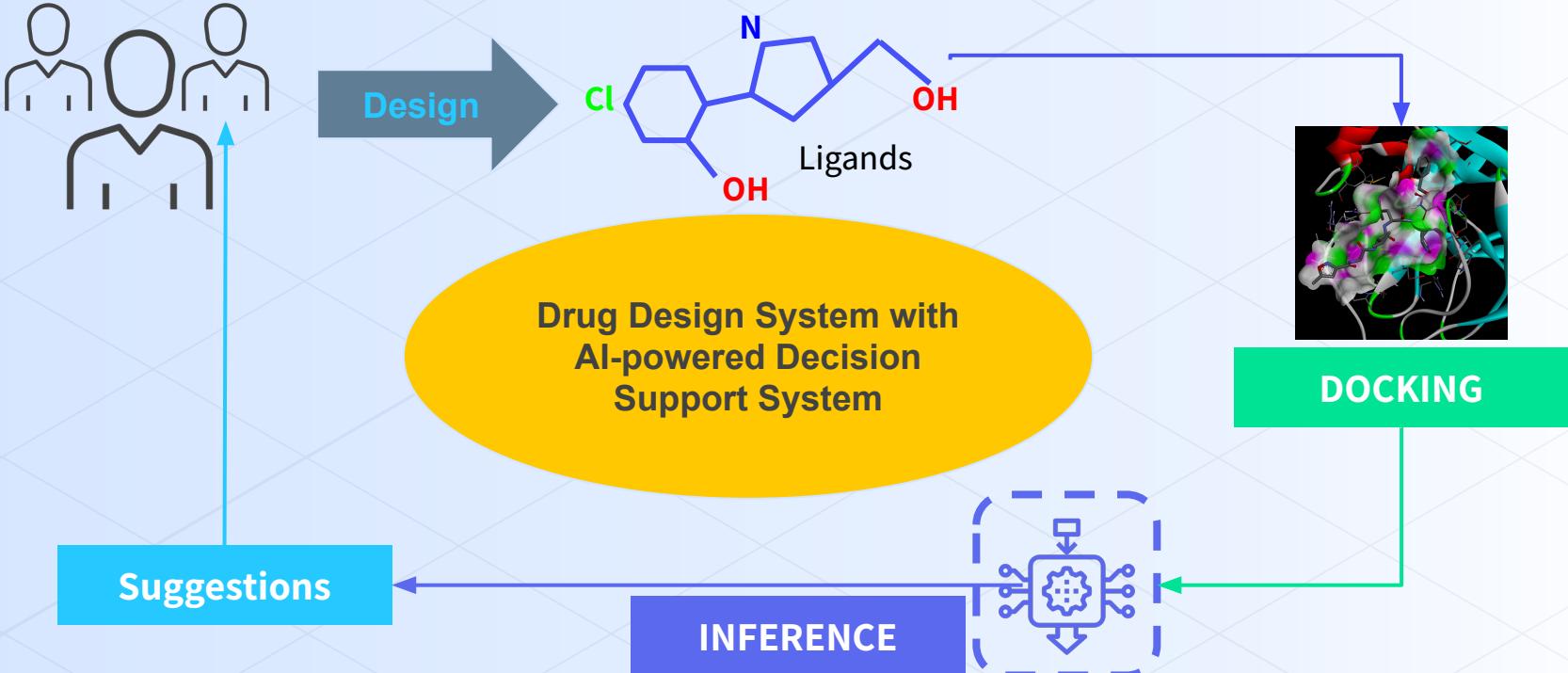
SMILES string



C (= O) c 1



OVERVIEW BIG SYSTEM



GNN-BASED MODEL

BASELINE MODEL COMPUTATION

$$\mathbf{X} = \{x_1, x_2, \dots, x_M\} \text{ with } x_i \in \mathbb{R}^F$$

$$\mathbf{A}_{ij}^1 = \begin{cases} 1 & \text{if } i \text{ and } j \text{ are connected by covalent bond or } i = j \\ 0 & \text{otherwise} \end{cases}$$

$$\mathbf{A}_{ij}^2 = \begin{cases} \mathbf{A}_{ij}^1 & \text{if } i, j \in \text{protein or } i, j \in \text{ligand} \\ e^{-(d_{ij}-\mu)^2/\sigma} & \text{if } i \in \text{protein and } j \in \text{ligand,} \\ & \text{or if } i \in \text{ligand and } j \in \text{protein} \\ 0 & \text{otherwise} \end{cases}$$

$$\mathbf{X}'_1 = \mathbf{GAT}(\mathbf{X}, \mathbf{A}^1)$$

$$\mathbf{X}'_2 = \mathbf{GAT}(\mathbf{X}, \mathbf{A}^2)$$

$$\mathbf{X}'_{out} = \mathbf{X}'_2 - \mathbf{X}'_1$$

$\times N$

$$\mathbf{GAT} \left\{ \begin{array}{l} x_i^h = \mathbf{W}_h x_i, \quad i = \overline{1, |V|} \\ e_{ij} = (x_i^h)^T \mathbf{W}_a x_j^h + (x_j^h)^T \mathbf{W}_a x_i^h, \quad i, j = \overline{1, |V|} \\ a_{ij} = \frac{\exp(e_{ij})}{\sum_{k \in C_i} \exp(e_{ik})} \mathbf{A}_{ij}, \quad i, j = \overline{1, |V|} \\ x_i^{temp} = \sum_{j \in C_i} a_{ij} x_j^h, \quad i = \overline{1, |V|} \\ z_i = \sigma(\mathbf{W}_o(x_i || x_i^{temp}) + b), \quad i = \overline{1, |V|} \\ x'_i = z_i x_i + (1 - z_i) x_i^{temp}, \quad i = \overline{1, |V|} \end{array} \right.$$

$$x^{complex} = \sum_{i \in \text{ligand}} x_i$$

$$y = \sigma(\mathbf{W}_c x + b)$$

$\times L$

GNN-BASED MODEL

ATTENTION INFERENCE ALGORITHM

Algorithm 1: Attention Inference

Input : GNN-based model with attention mechanism \mathcal{M} ,

Input for GNN-based model $(\mathbf{X}, \mathbf{A}^1, \mathbf{A}^2)$,

The total number of atoms M .

Output: List of high interaction probability pairs

$$\mathbf{P} = \{(i, j, s) | i \in \text{ligand} \& j \in \text{protein} \& s \geq 0.5\}$$

$$\mathcal{M}(\mathbf{X}, \mathbf{A}^1, \mathbf{A}^2)$$

$$\text{lastGATBlock} \leftarrow \text{GetLastGATBlock}(\mathcal{M})$$

$$\mathcal{A} = \{a_{ij}\} \leftarrow \text{GetNormalizedAttentionMatrix}(\text{lastGATBlock})$$

$$\mathbf{P} \leftarrow \emptyset$$

for i in Range($0, M$) **do**

for j in Range($i + 1, M$) **do**

if $a_{ij} + a_{ji} \geq 1$ **then**

$\mathbf{P} \leftarrow \mathbf{P} \cup \{(i, j, \frac{a_{ij} + a_{ji}}{2})\}$

end

end

end

return \mathbf{P}

GNN-BASED MODEL

IMPROVEMENT 1

Feature	Value
<i>Original</i>	
Atom type	C,N,O,S,F,P,Cl,Br,B,H (onehot)
Degree of atom	0, 1, 2, 3, 4, 5, 6 (onehot)
Number of H atoms attached	0, 1, 2, 3, 4 (onehot)
Implicit valence electrons	0, 1, 2, 3, 4, 5 (onehot)
In aromatic	0 or 1
<i>Added in Improvement 1</i>	
Hydrogen D/A	[is_donor, is_acceptor]
Pos/Neg Ionizable	[is_pos, is_neg]
In lumped hydrophobe	0 or 1

GNN-BASED MODEL

IMPROVEMENT 2

Old Aggregation Layer:

$$x^{complex} = \sum_{i \in ligand} x_i$$



$$x^{complex} = (x^{ligand} || x^{protein})$$

$$x^{ligand} = \sum_{i \in ligand} x_i$$

Improved
Aggregation Layer:

$$\begin{cases} x^{protein} = \sum_{i \in P} x_i \\ P = \{x_p, p \in protein | \exists c \in ligand : dist(p, c) < 5.5\text{\AA}\} \end{cases}$$

GNN-BASED MODEL

IMPROVEMENT 3

Algorithm 2: Multi-hop gating mechanism

Input : Normalized attention coefficients a_{ij} , where $i, j = \overline{1, |V|}$,
Atom feature vectors x_i^h , where $i = \overline{1, |V|}$,
Number of hops K .

Output: Refined atom feature vectors $x_i^{(K)}$, where $i = \overline{1, |V|}$

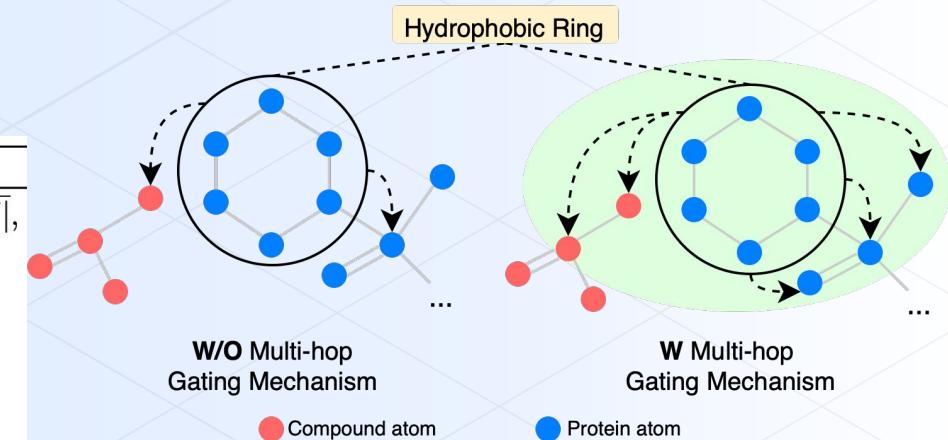
$$x_i^{(0)} = x_i^h, i = \overline{1, |V|}$$

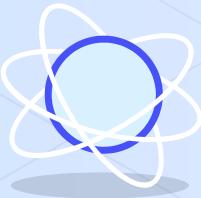
for k in Range($1 \dots K$) **do**

$$\left| \begin{array}{l} x_i^{temp} = \sum_{j \in C_i} a_{ij} x_j^{(k-1)}, i = \overline{1, |V|} \\ z_i = \sigma(\mathbf{W}_o(x_i^{(0)} || x_i^{temp}) + b), i = \overline{1, |V|} \\ x_i^{(k)} = z_i x_i^{(0)} + (1 - z_i) x_i^{temp}, i = \overline{1, |V|} \end{array} \right.$$

end

return $\mathbf{X}^{(K)} = \{x_i^{(K)} | i = \overline{1, |V|}\}$

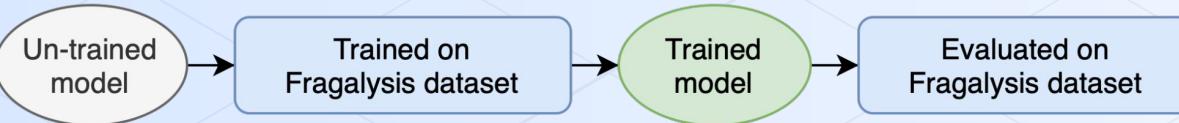




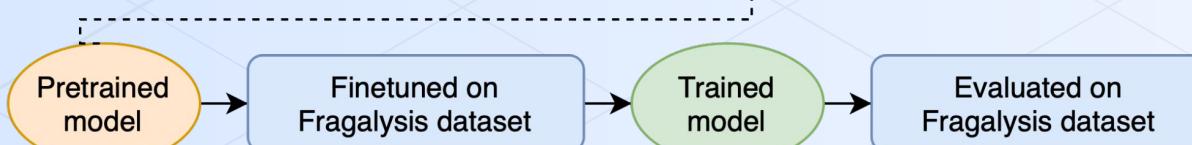
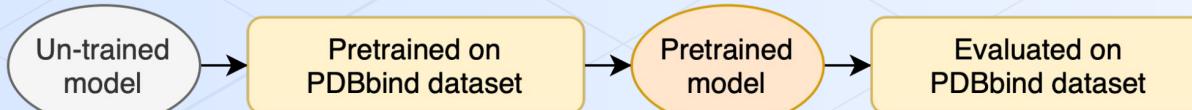
GNN-BASED MODEL

TRAINING AND TESTING FLOWS

Normal flow



Transfer learning flow



	PDBbind			Fragalysis		
	Active	Inactive	Total	Active	Inactive	Total
Training	10037	5237	15274	75	125	200
Testing	2530	1287	3817	35	54	89

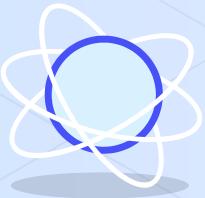


GNN-BASED MODEL

RESULTS OF PREDICTING PHARMACOLOGICALLY ACTIVE

Model with settings	Directly trained on Fragalysis	Pretrained on PDBbind	Finetuned on Fragalysis
<i>String-based representation</i>			
DeepDTA	0.870	0.849	0.862
<i>String-based + Feature matrix representation</i>			
DrugVQA	0.853	0.819	0.820
<i>Graph-based + String-based representation</i>			
GraphDTA-GINConvNet	0.885	0.838	0.874
GraphDTA-GATNet	0.886	0.814	0.890
GraphDTA-GCNNet	0.868	0.836	0.862
GraphDTA-GAT_GCN	0.874	0.835	0.874
<i>Graph-based representation</i>			
Baseline model	0.841	0.758	0.859
Baseline + Ipmt 1	0.865	0.787	0.896
Baseline + Ipmt 2	0.877	0.785	0.915
Baseline + Ipmt 3	0.870	0.793	0.936
Baseline + Ipmt 1,2	0.822	0.813	0.930
Baseline + Ipmt 1,2,3	0.868	0.820	0.938





KNOWLEDGE-DRIVEN ALGORITHM

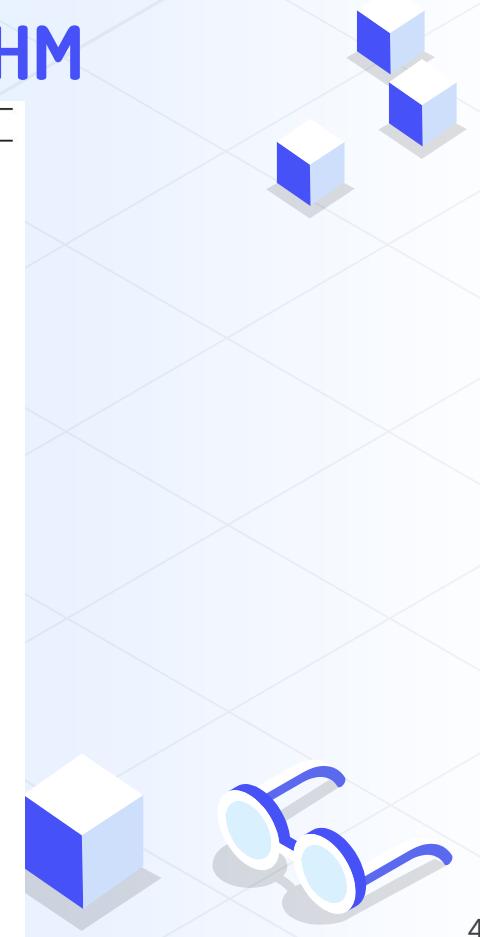
Algorithm 3: Nearest Neighbors combined with chemical rules

Input : High interaction probability pairs

$P = \{(i, j, s) | i \in ligand \& j \in protein \& s \geq 0.5\}$,
ligand, protein,
Distance threshold ϵ_d ,
Chemical rules \mathcal{R} .

Output: Interaction list

```
 $I = \{(i, j, x_i, x_j) | i \in ligand \& j \in protein \& x \text{ is feature vector}\}$ 
 $I \leftarrow \emptyset$ 
 $N \leftarrow InitNearestNeighbor(protein \rightarrow atoms)$ 
for  $l\_atom$  in ligand do
     $listNearAtoms \leftarrow GetNearAtoms(N, \epsilon_d, l\_atom)$ 
    for  $p\_atom$  in  $listNearAtoms$  do
         $interaction \leftarrow checkInteractionType(\mathcal{R}, l\_atom, p\_atom)$ 
        if  $interaction$  is Hydrogen then
             $x_i, x_j \leftarrow CalculateFeature(l\_atom, p\_atom)$ 
             $I \leftarrow I \cup \{(l\_atom, p\_atom, x_i, x_j)\}$ 
        end
        if  $interaction$  is Hydrophobic then
             $hasHighProb \leftarrow HasHighProb(P, l\_atom, p\_atom)$ 
            if not  $hasHighProb$  then
                | continue
            end
             $x_i, x_j \leftarrow CalculateFeature(l\_atom, p\_atom)$ 
             $I \leftarrow I \cup \{(l\_atom, p\_atom, x_i, x_j)\}$ 
        end
    end
end
return  $I$ 
```





DETECTED INTERACTIONS

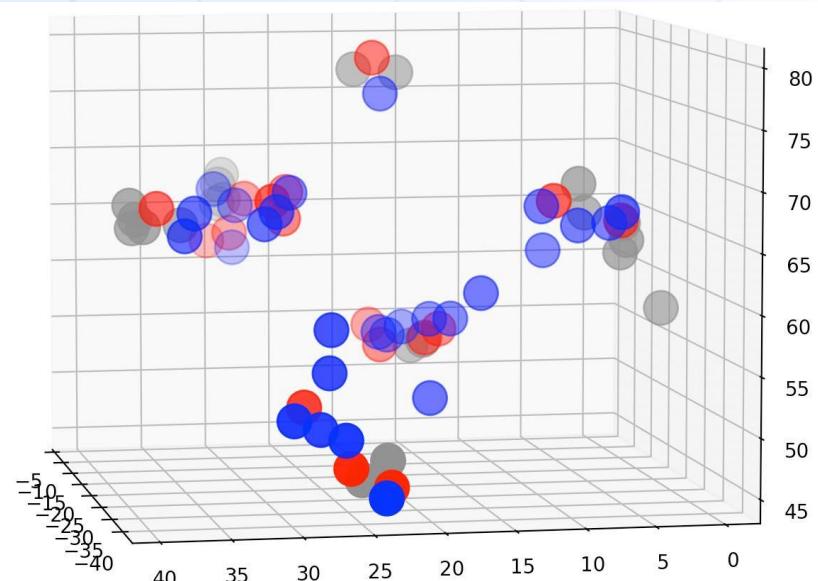
- **Crawled from ViDok:** Top 1000
- **After processed (usable):** 918
- **Classification results:**

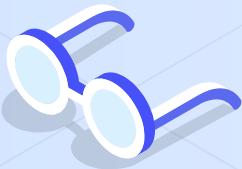
- **Active:** 915
- **Inactive:** 3

-
- **Interaction protein atoms detected from 915 active complexes:**

- **H-Donor:** 9150
- **H-Acceptor:** 599
- **Hydrophobe:** 4831

Interaction protein atoms detected from top 1000 designed ligand-protein complexes on ViDok system





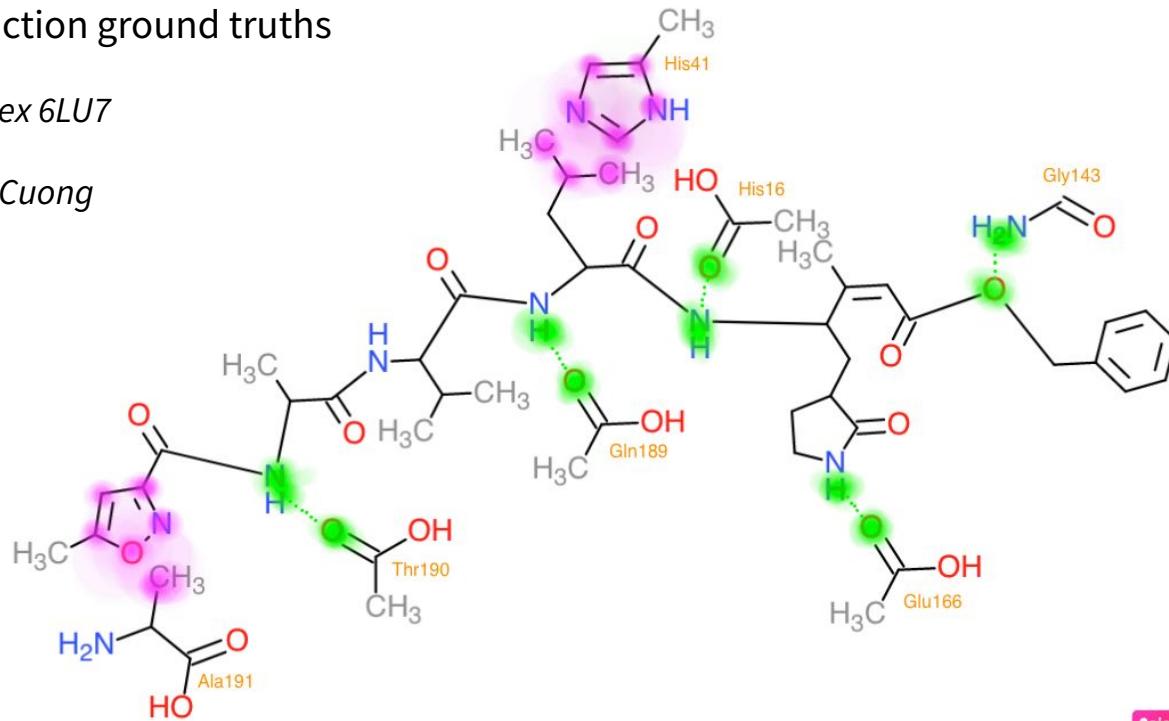
PAIRWISE INTERACTION EXAMPLES

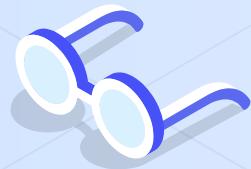


Interaction ground truths

Complex 6LU7

By Mr. Cuong





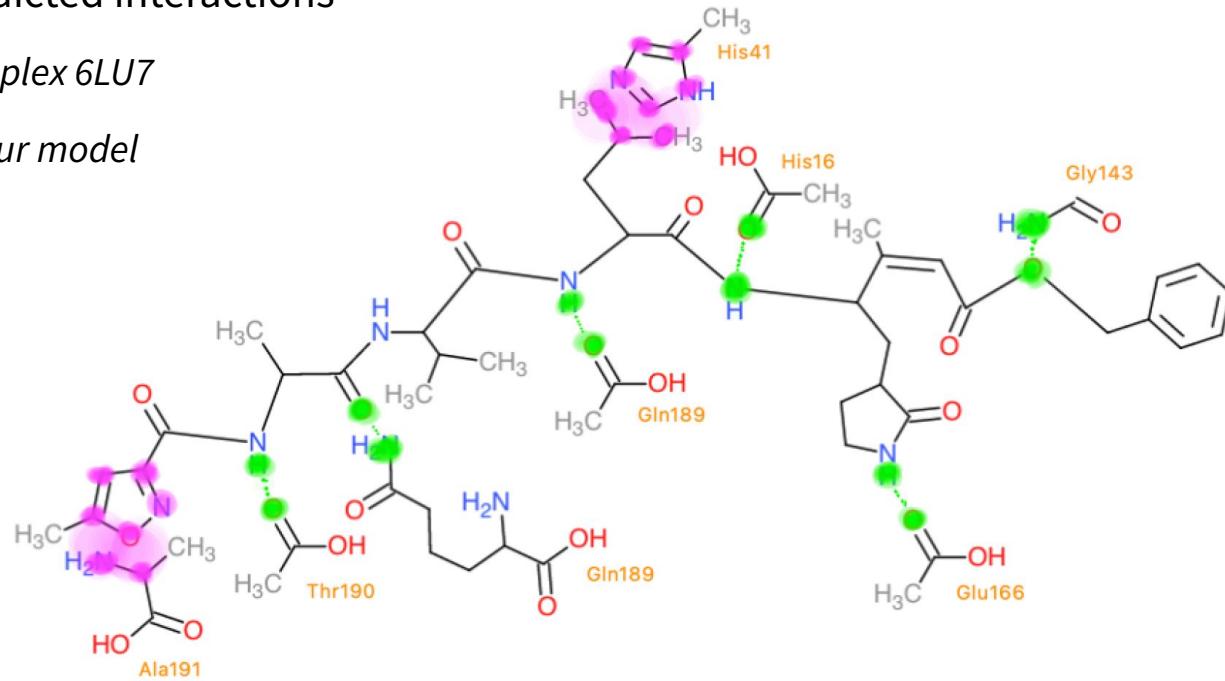
PAIRWISE INTERACTION EXAMPLES



Predicted interactions

Complex 6LU7

By our model



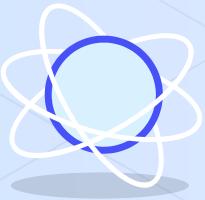


CAVITY MODEL FOR TARGET PROTEIN

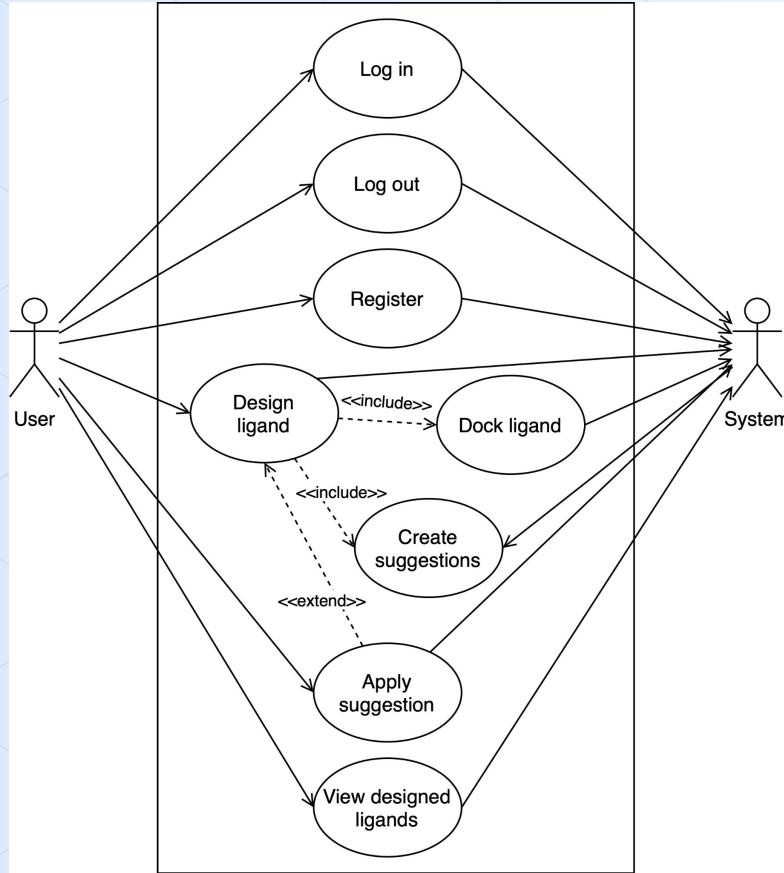
SPHERE LIST OF PHARMACOPHORE MODEL

Feature	X	Y	Z	Radius
Hydrogen Donor	-30.225	3.831	66.757	5.5
Hydrogen Donor	-19.0313	16.6303	56.0029	13.623
Hydrogen Donor	-21.6388	27.2708	66.9083	8.8003
Hydrogen Donor	-24.0361	34.8547	64.6313	7.628
Hydrogen Donor	-11.6326	29.4802	66.0156	7.2845
Hydrogen Donor	-8.198	28.631	61.431	5.5
Hydrogen Acceptor	-41.5963	23.2133	46.3095	9.1333
Hydrogen Acceptor	-20.4093	16.358	55.6273	11.5058
Hydrogen Acceptor	-12.8375	28.9957	64.8636	12.7014
Hydrophobic	-40.0793	24.85	46.7966	7.7066
Hydrophobic	-27.6896	5.9601	66.6768	9.9262
Hydrophobic	-24.5747	36.9257	65.9457	8.211
Hydrophobic	-20.9697	17.4683	54.4411	9.3026
Hydrophobic	-7.5645	29.226	65.6474	7.8231

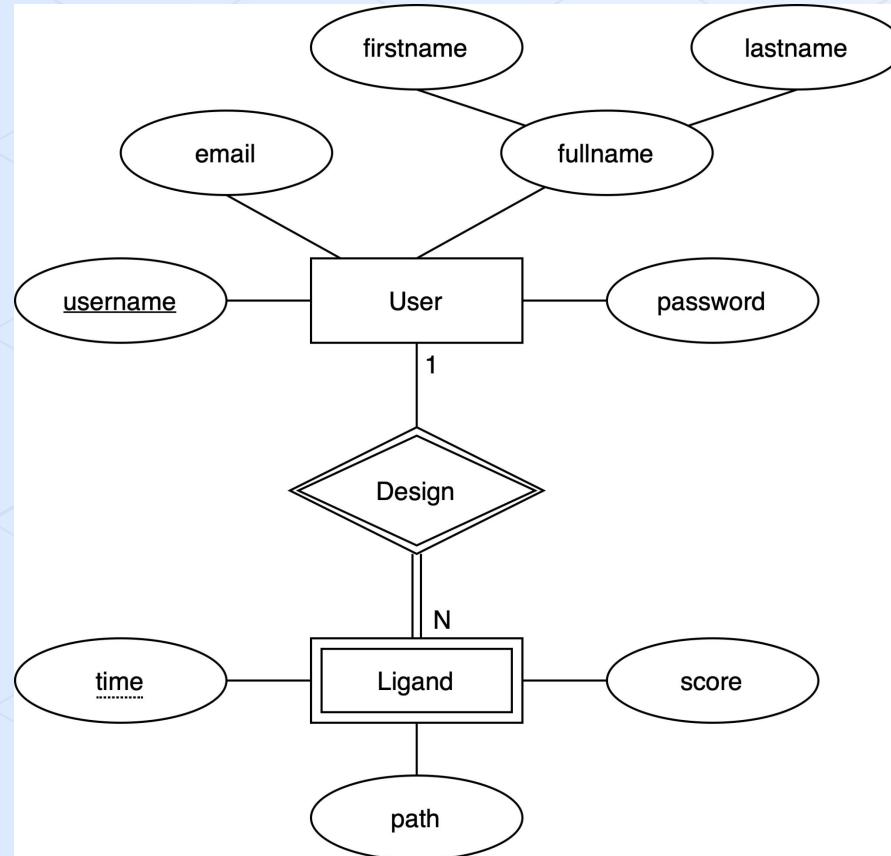




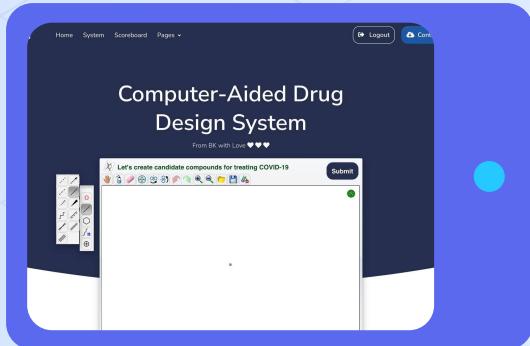
APPLICATION USECASES



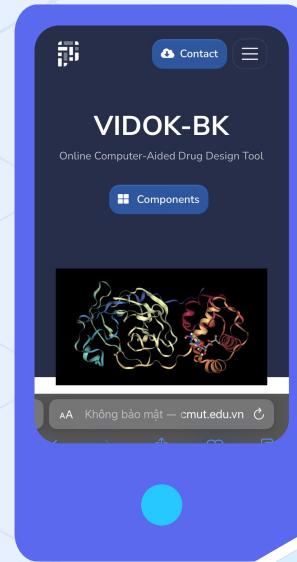
DATABASE DESIGN



TABLET AND MOBILE APPLICATIONS

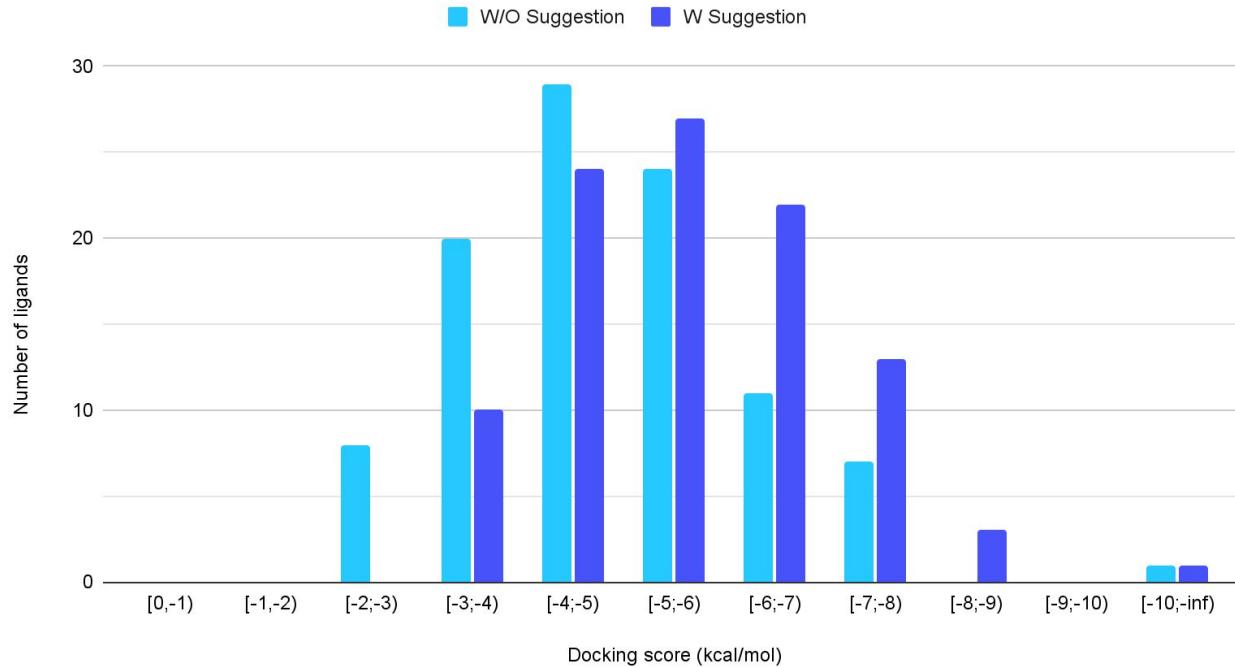


- Multiple OSs
- Multiple browsers



HISTOGRAM OF DOCKING SCORES

Histogram of docking score of designed ligand with and without suggestion



THE PERFORMANCE OF DESIGNED SYSTEM



← → ⌛ Not Secure | ura.hcmut.edu.vn/vidok/

Home System Scoreboard About

Logout Contact

VIDOK-BK

Online Computer-Aided Drug Design Tool

Design Now

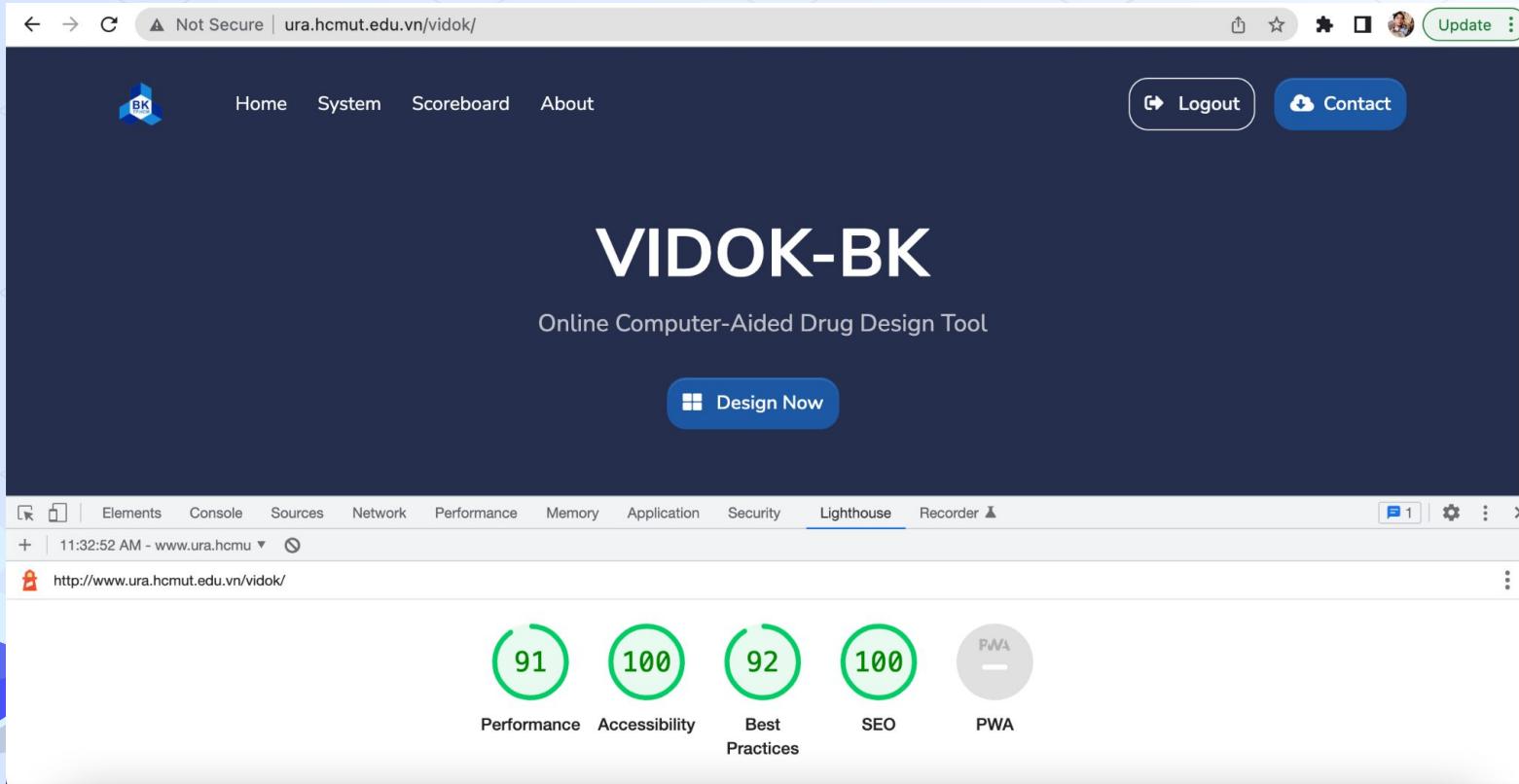
Elements Console Sources Network Performance Memory Application Security Lighthouse Recorder

+ 11:32:52 AM - www.ura.hcmu

http://www.ura.hcmut.edu.vn/vidok/

91 100 92 100 PWA

Performance Accessibility Best Practices SEO PWA



APPLICATION SCREENSHOTS

The screenshot displays the homepage of the "Computer-Aided Drug Design System". The header features a logo with "BK" and navigation links for Home, System, Scoreboard, and About. On the right are Logout and Contact buttons. The main title "Computer-Aided Drug Design System" is centered, followed by a message "From BK with Love ❤️❤️❤️". A central window titled "Let's create candidate compounds for treating COVID-19" contains a toolbar with various icons and a "Submit" button. The ChemDoodle interface is visible at the bottom, with a text input field that says "Include some updating calculations here". The ChemDoodle logo and copyright information are at the bottom right.

Home System Scoreboard About

Logout Contact

Computer-Aided Drug Design System

From BK with Love ❤️❤️❤️

Let's create candidate compounds for treating COVID-19

Submit

Include some updating calculations here

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APPLICATION SCREENSHOTS

A screenshot of a web-based application interface. At the top, there is a dark blue header bar with the following elements from left to right: a small logo icon, the text "Home", "System", "Scoreboard", and "About", and two buttons on the far right: "Logout" and "Contact". Below the header is a large black rectangular area containing a 3D ribbon model of a protein structure. The protein is composed of several distinct domains, each represented by a different color (blue, green, yellow, red, orange) and shown as a twisted ribbon. The background of the main content area is black, making the colored protein structure stand out.

APPLICATION SCREENSHOTS

The screenshot shows a user interface for a molecular modeling or simulation application. The main title "APPLICATION SCREENSHOTS" is displayed prominently at the top center. Below the title is a dark header bar containing the application logo, navigation links (Home, System, Scoreboard, About), and user account links (Logout, Contact). A large, light gray rectangular box labeled "Suggestions" is centered on the page. Inside this box, there is a "Reset" button and a table with the following data:

No.	Type	Atom index(es)	New Atom(s)	Apply
0	add	0	O=CO	<button>Apply</button>
1	add	0	C=O	<button>Apply</button>
2	add	0	NC=O	<button>Apply</button>
3	add	15	O=CO	<button>Apply</button>
4	add	15	C=O	<button>Apply</button>
5	add	15	NC=O	<button>Apply</button>
6	add	15	O	<button>Apply</button>
7	add	15	N	<button>Apply</button>

APPLICATION SCREENSHOTS

The screenshot shows a dark-themed web application interface. At the top left is a logo with a blue 'BK' monogram. To its right are navigation links: Home, System, Scoreboard, and About. On the far right are Logout and Contact buttons. The main title 'Scoreboard' is centered above a subtitle 'View top deisgned ligands'. The background features abstract geometric shapes.

This screenshot shows a table of 'Designed Ligands' with four entries. The columns are labeled: No., Name, Score, User, and Download. Each entry includes a 'Download' button. The table is styled with alternating row colors. Above the table, there are filters for 'Ligands per page' (set to 10) and 'Only me'.

No.	Name	Score	User	Download
1	DOCKED2022-05-09T08:43:29Z.mol	-11.92	cuong	Download
2	DOCKED2022-05-09T08:42:37Z.mol	-11.402	cuong	Download
3	DOCKED2022-05-11T20:27:29Z.mol	-11.147	Duy Phuoc	Download
4	DOCKED2022-05-11T20:26:44Z.mol	-10.841	Duy Phuoc	Download

HISTOGRAM OF PROCESSING TIME

Histogram of processing time for scoring designed ligands with and without suggestion

