



CSE



GRADUATION THESIS

AI-Powered Decision Support System for Antiviral Pharmaceutical Formulation

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Mr. Bang Ngoc Bao Tam, MEng

Student: Nguyen Quang Duc - 1810118



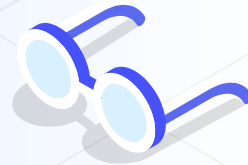
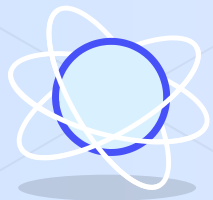


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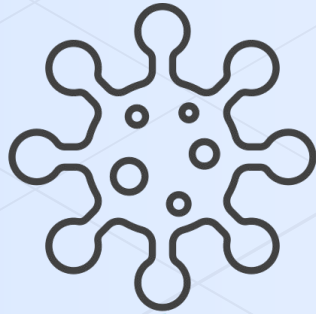
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CONCLUSION

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VIRUSES AND THEIR MAIN PROTEINS

VIR



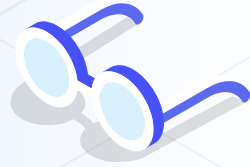
US



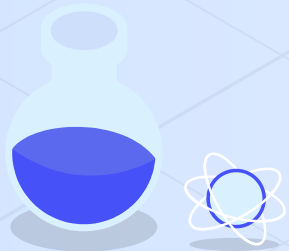
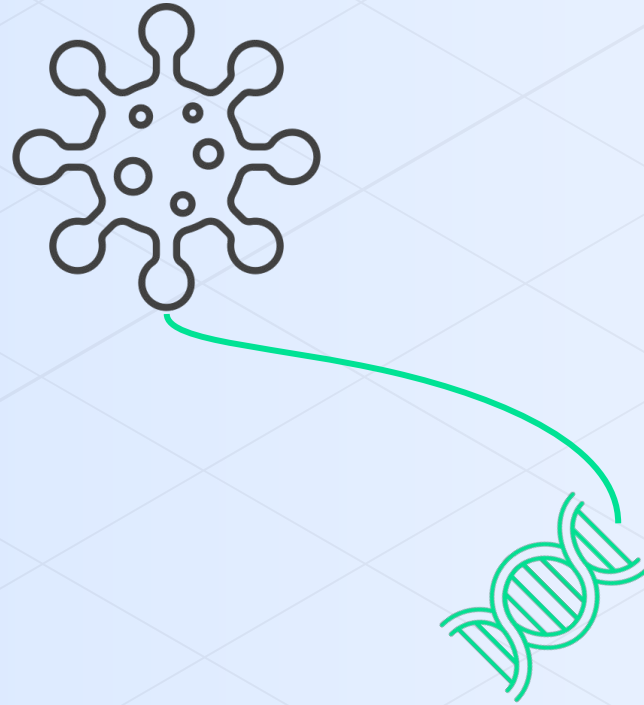
Protein A



Protein B



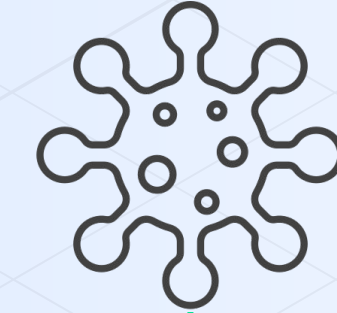
HOW DRUGS "KILL" VIRUSES?



HOW DRUGS "KILL" VIRUSES?



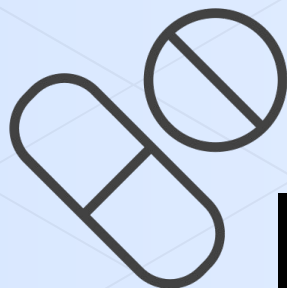
Ligand



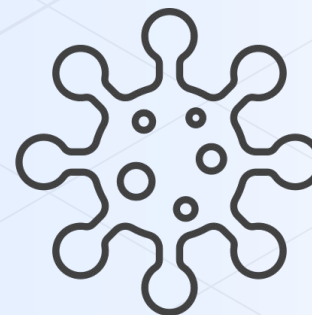
Protein



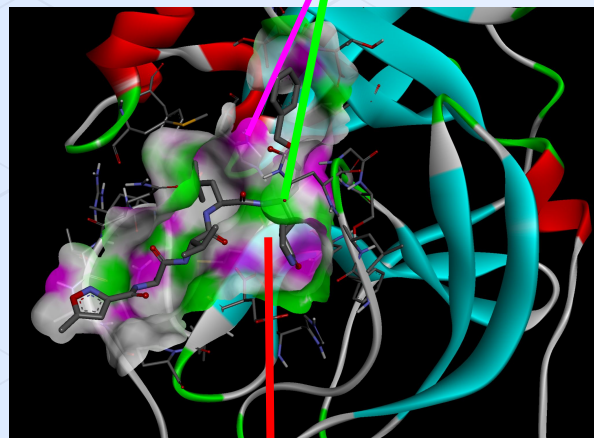
WHERE DOES LIGAND REALLY INTERACT?



Binding site



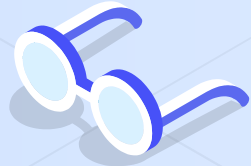
Ligand



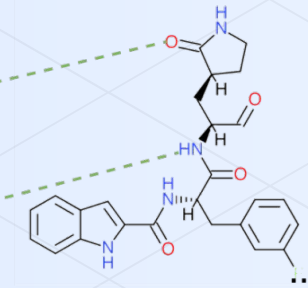
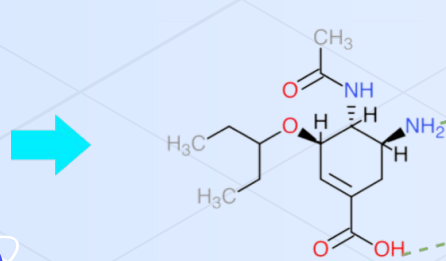
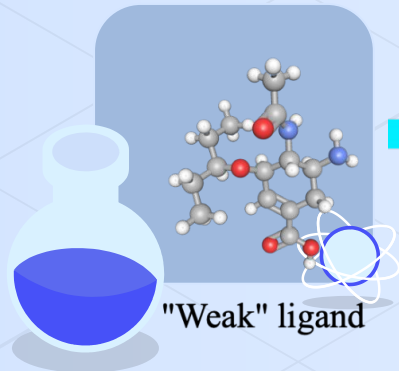
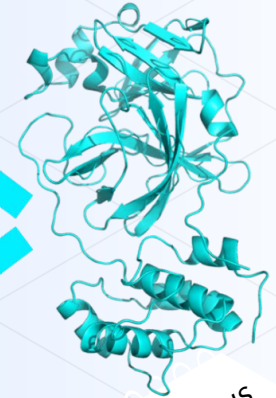
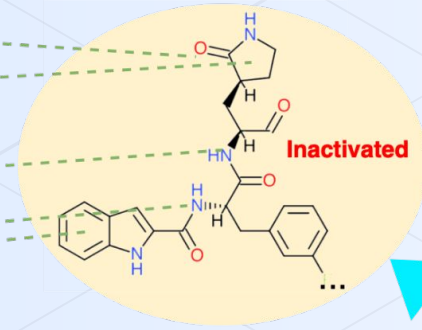
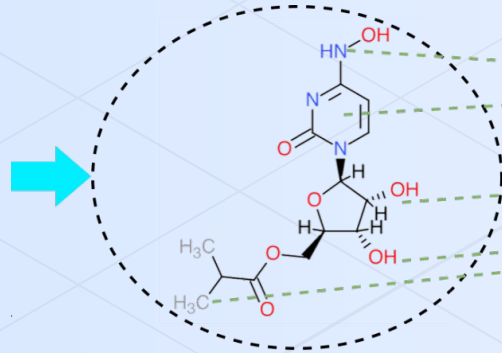
Cavity
(Pocket)



Protein

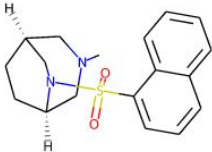
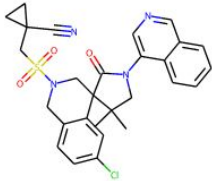


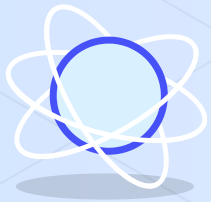
CAN ANY LIGANDS BECOME DRUGS?



DRUG DESIGN AT EARLY STAGE

“Designing strong ligands”

Image	Molecule	MW	cLogP	TPSA	Rotatable Bonds	Fraction sp3	HBA	HBD	Covalent Warhead
	<p>CLI-SEL-cf46d3af-1</p> <chem>CN1C[C@@H]2CC[C@H](C1)N(S(=O)(=O)c1ccccc3ccccc13)C2</chem> <p>Check Availability on Manifold</p>	330.14	2.55	40.62	2	0.44	3	0	false
	<p>ALP-POS-01611061-1</p> <p>Duplicate of: MAT-POS-50a80394-8</p> <chem>CC1(C)CN(c2cncc3cccc23)C(=O)C12CN(S(=O)(=O)CC1(C#N)CC1)C(c1ccc(C1)cc12)</chem> <p>3-aminopyridine-like</p> <p>Ordered</p> <p>Check Availability on Manifold</p>	534.15	4.65	94.37	4	0.39	5	0	false



INTRODUCTION

Problem Definition and Solution Overview





CROWDSOURCING DRUG DESIGN

PURPOSE

Utilize the power of community

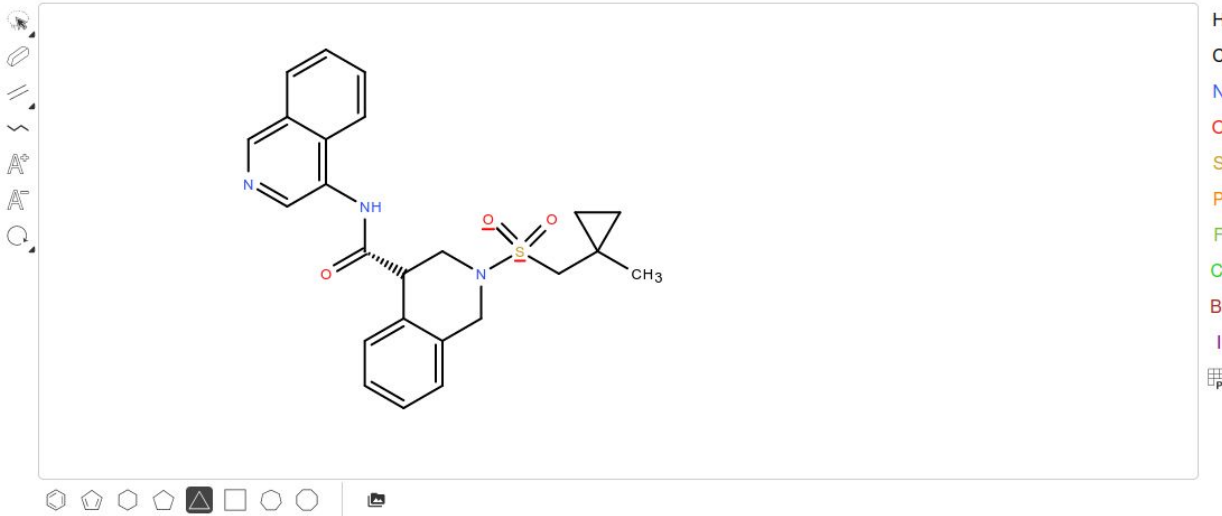
Draw or enter SMILES (add multiple by pressing "Add" after each entry)

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

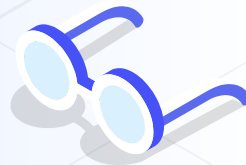
CC1(CS(=O)(=O)N2Cc3ccccc3C(C(=O)Nc3cncc4ccccc34)C2)CC1

Add

100%

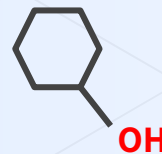
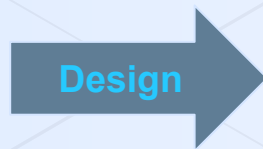


BUT THE PROBLEM IS...



NON-EXPERTS

A large number and has more time

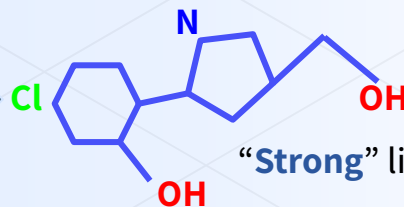


“Weak” ligands



EXPERTS

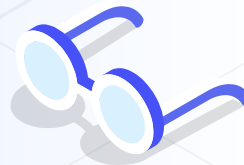
Not many experts and they do not have much time



“Strong” ligands

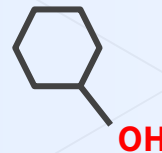
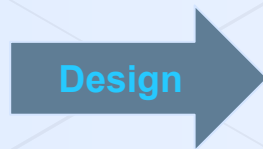


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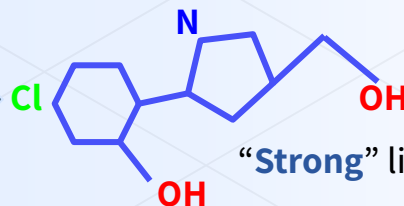
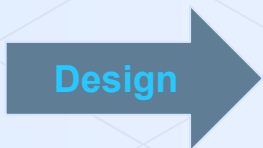


“Weak” ligands



EXPERTS

Not many experts and they do not have much time



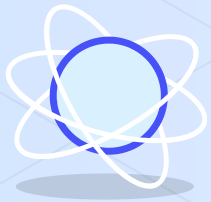
“Strong” ligands

HOW TO EFFECTIVELY UTILIZE COMMUNITY POWER?

AN INTELLIGENCE DECISION SUPPORT SYSTEM

To make the designed drugs
better and better





BACKGROUNDS

Computer Science Backgrounds



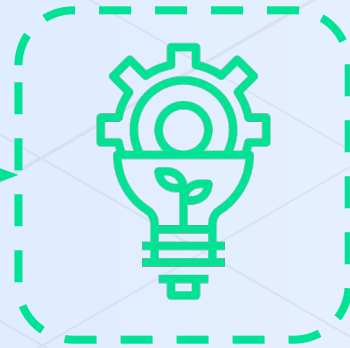
DECISION SUPPORT SYSTEM IN A NUTSHELL



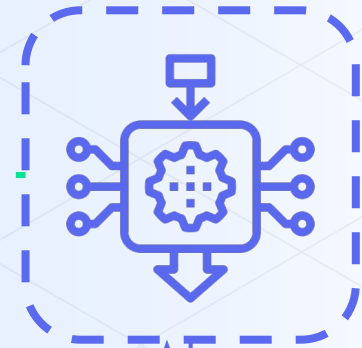
PREPARATION



KNOWLEDGE



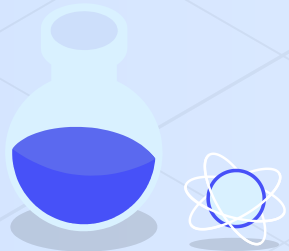
INFERENCE



Initial data

Queries

Suggestions



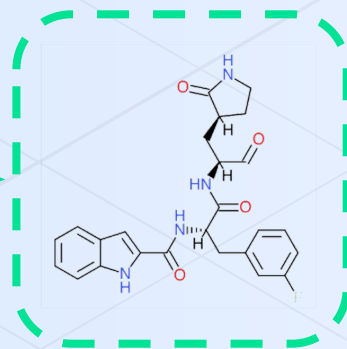
DECISION SUPPORT SYSTEM IN OUR SITUATION



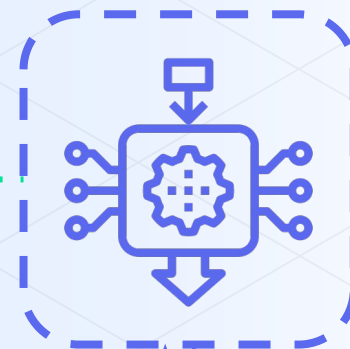
PREPARATION



CAVITY MODEL



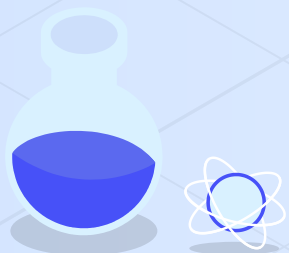
INFERENCE



**Ligand-Protein
complexes**

**Newly designed
ligands (docked)**

**Add/Replace
atom(s)**




THE INITIAL PROBLEM BREAKS INTO

PREPARATION

1. Identifying Drug-Protein Interactions

- Ligand-Protein complexes  Interactions

2. Building Cavity Model for Target Protein

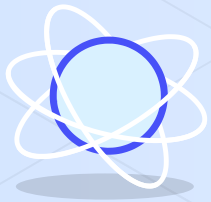
- Interactions  Cavity Model

INFERENCE

3. Building Algorithm for Recommending

- Newly Designed Ligands  Suggestions

Cavity Model



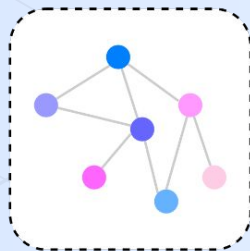
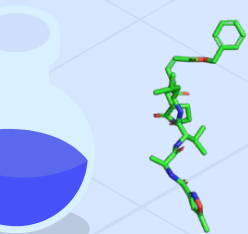
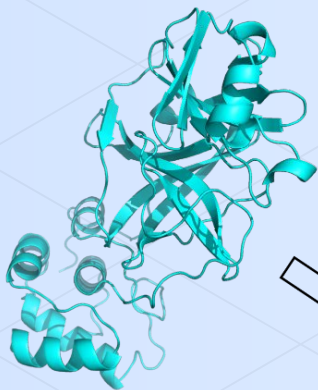
SOLUTIONS

Details of Designed System

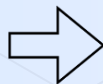


IDENTIFYING DRUG-PROTEIN INTERACTIONS

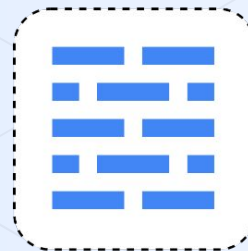
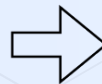
OVERALL PIPELINE



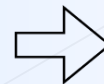
GNN-based Model









Ligand atom	Protein atom	Score
		0.9
		0.85
		0.92



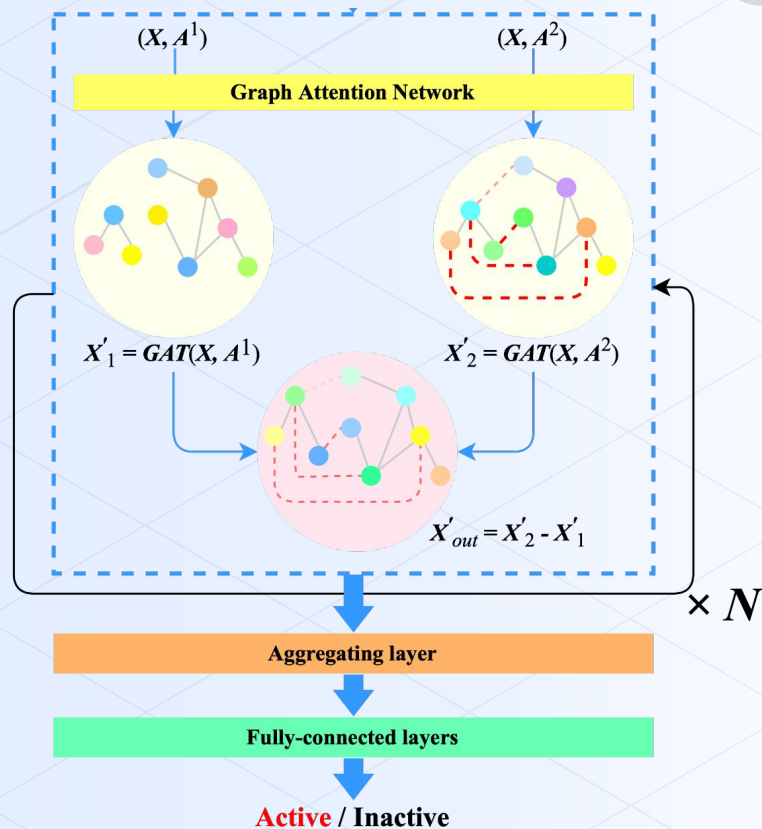
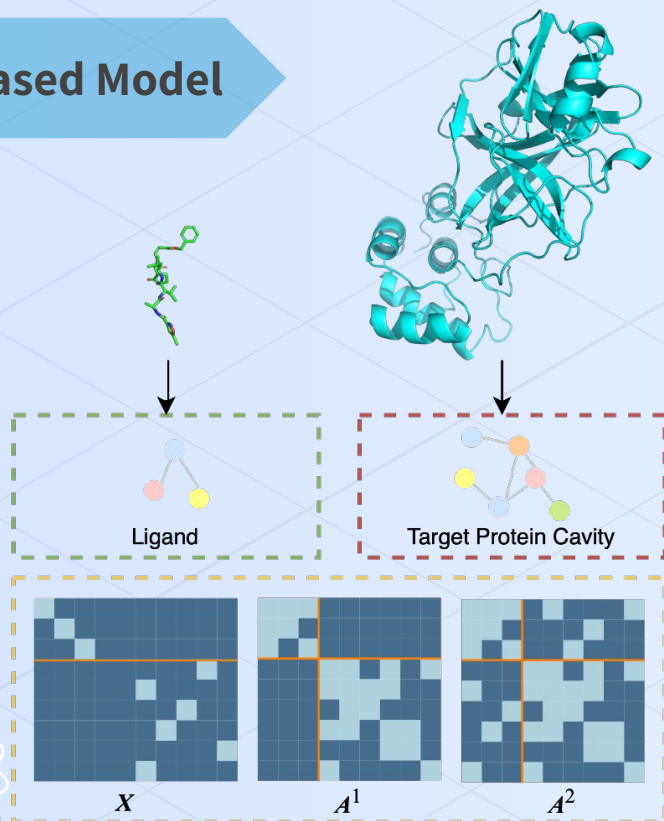
Knowledge-driven Algorithm



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

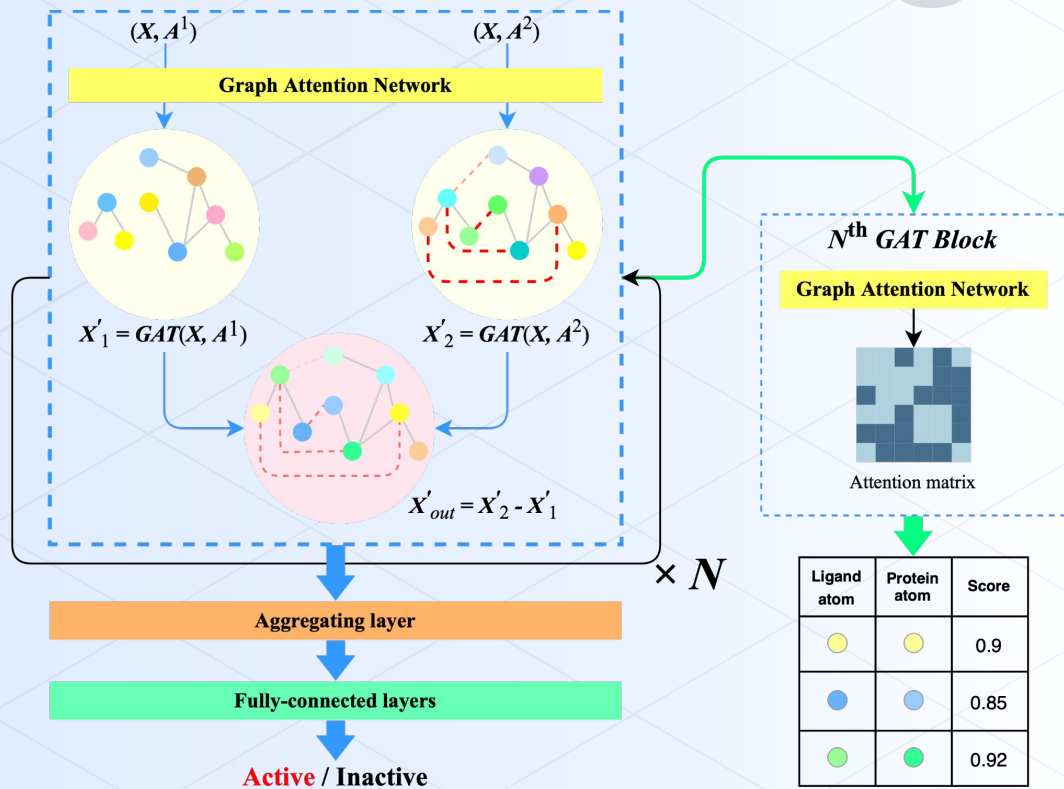
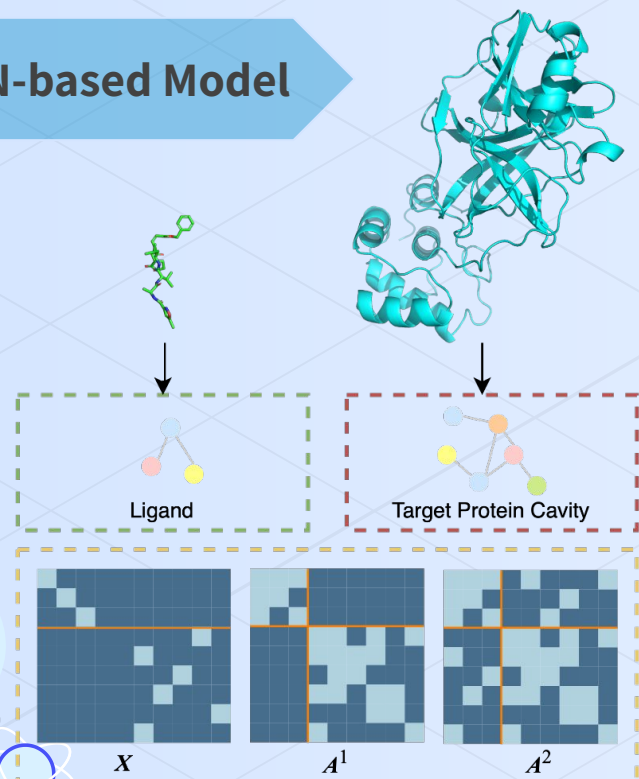
IDENTIFYING DRUG-PROTEIN INTERACTIONS

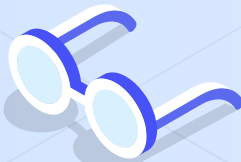
GNN-based Model



IDENTIFYING DRUG-PROTEIN INTERACTIONS

GNN-based Model





IDENTIFYING DRUG-PROTEIN INTERACTIONS



GNN-based Model

IMPROVEMENTS



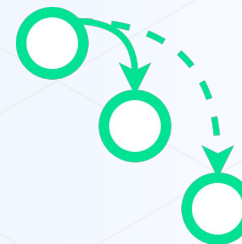
IMPROVEMENT 1

Enriched atom encoding



IMPROVEMENT 2

Total atom aggregation



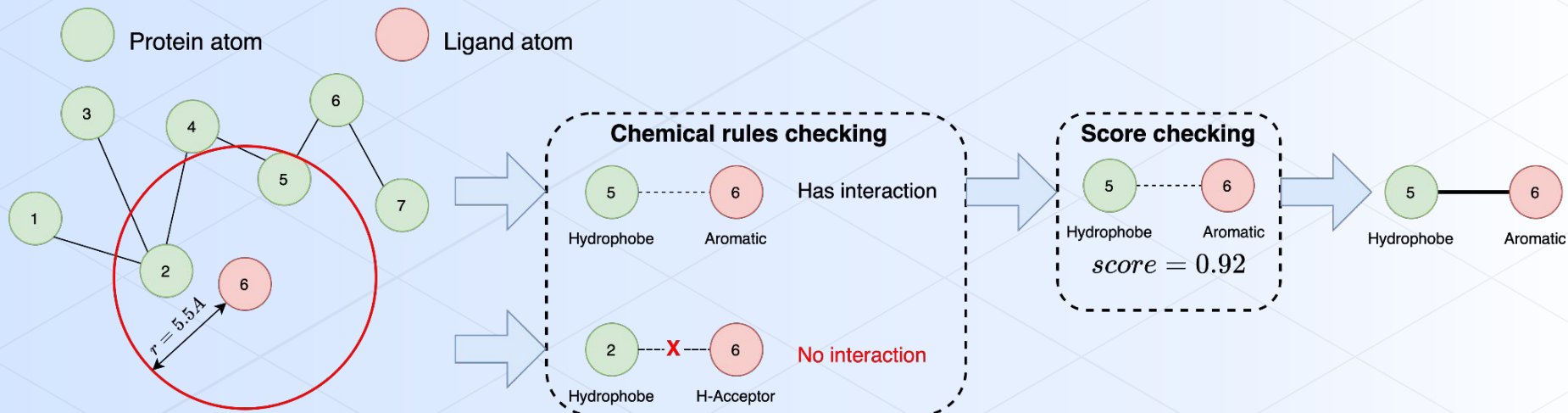
IMPROVEMENT 3

Multi-hop gating
mechanism

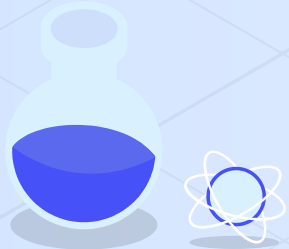
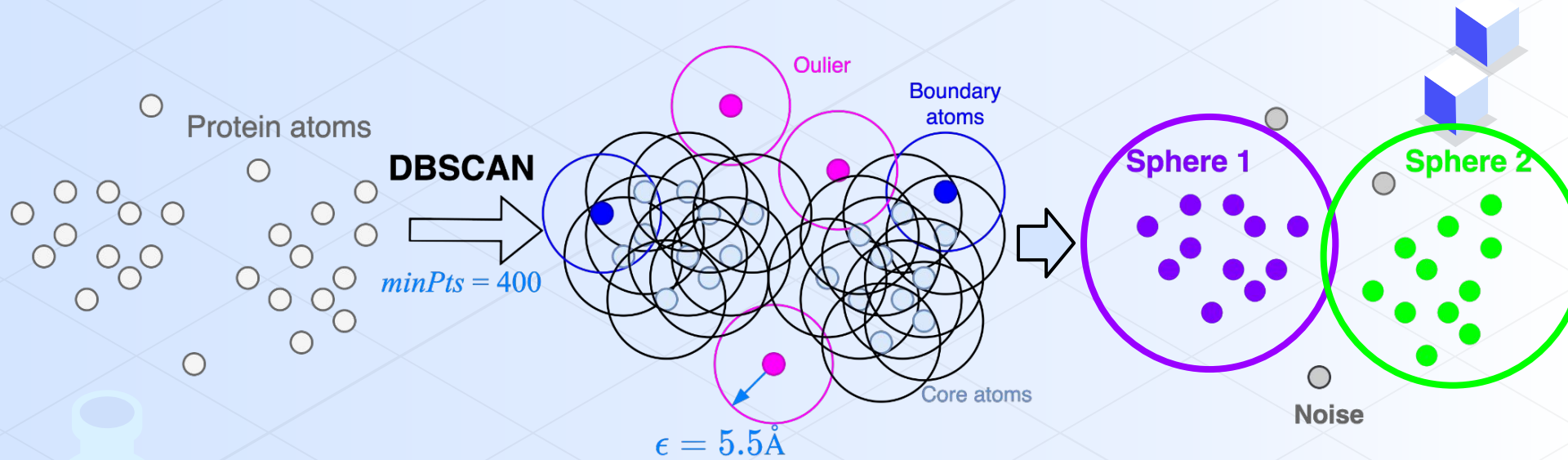


IDENTIFYING DRUG-PROTEIN INTERACTIONS

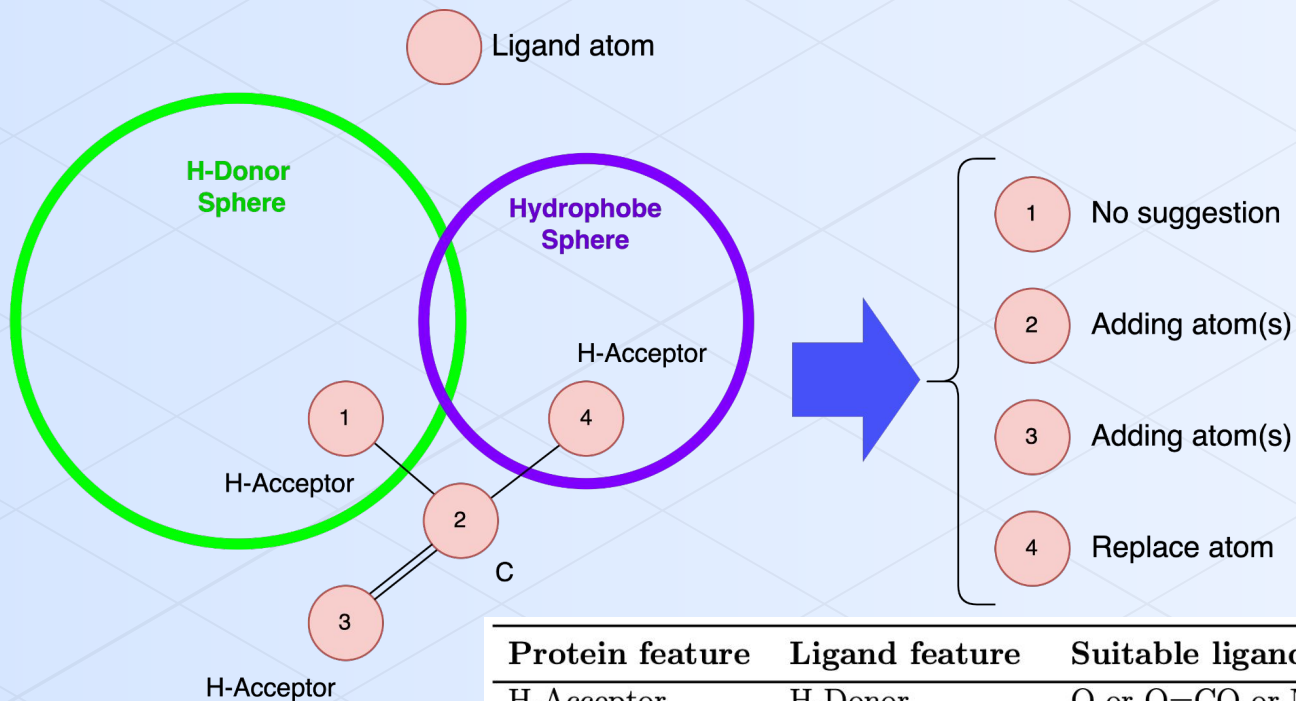
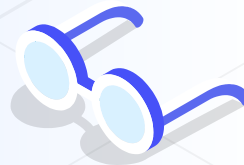
Algorithm



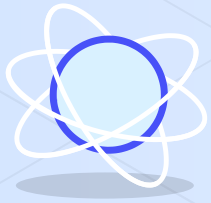
BUILDING CAVITY MODEL FOR TARGET PROTEIN



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 Cc1ccccc1 or C=Cc1ccccc1
Aromatic	Hydrophobic or C	C



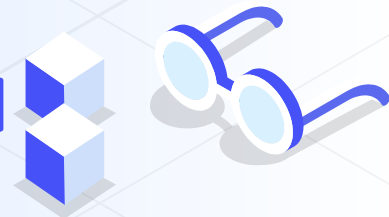
04

EXPERIMENTS

Evaluations of Designed System



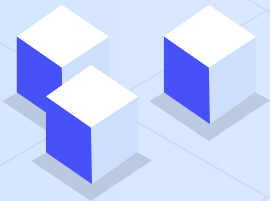
RESULTS OF INTERACTION IDENTIFICATION



20 complexes
manually annotated

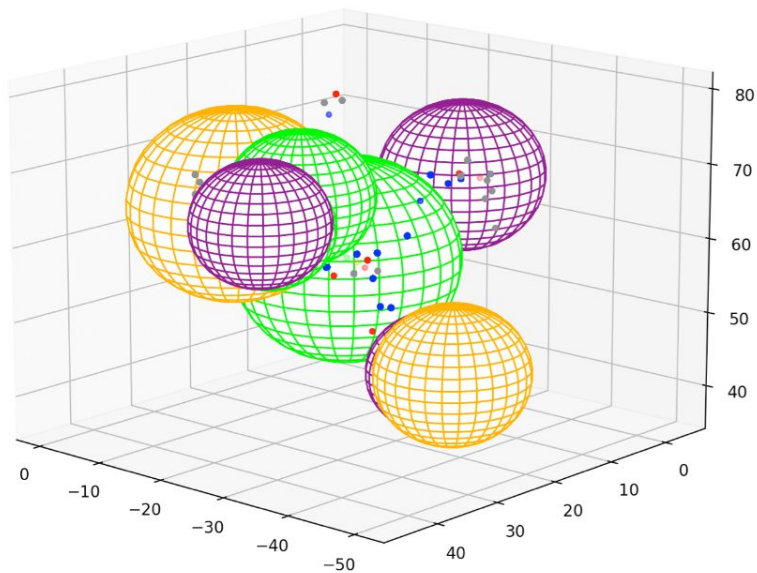
No.	Complex name	Recall	No.	Complex name	Recall
1	6LZE	0.82	11	6XQS	0.93
2	6M0K	0.58	12	7E19	0.73
3	6WTK	1.00	13	7JU7	0.21
4	6XA4	0.56	14	7KX5	0.86
5	6XBG	1.00	15	7L0D	0.86
6	6XBH	1.00	16	7LMD	0.50
7	6XBI	0.94	17	7LME	0.63
8	6XCH	1.00	18	7LMF	0.83
9	6XFN	0.40	19	7LMH	1.00
10	6XHM	0.88	20	7LMJ	1.00
Average Recall				0.79	



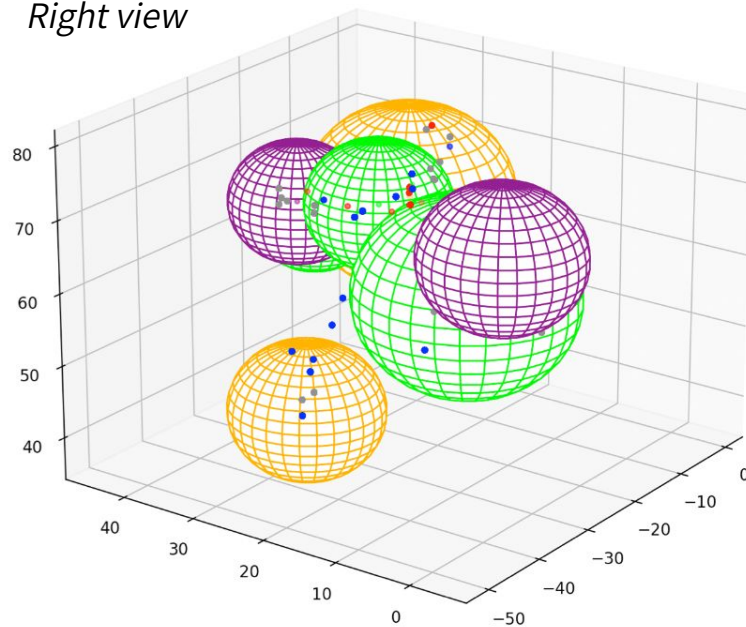



CAVITY MODEL FOR TARGET PROTEIN

Left view



Right view



 H-Donor

 H-Acceptor

 Hydrophobe

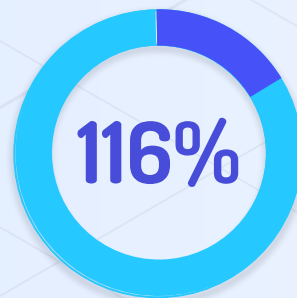
THE PERFORMANCE OF DESIGNED SYSTEM



With single suggestion

-0.76
kcal/mol

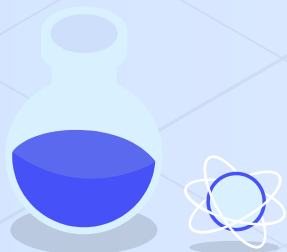
Binding Affinity

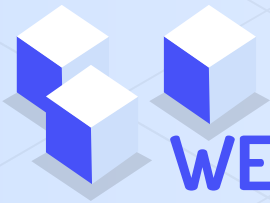


better than without any suggestions



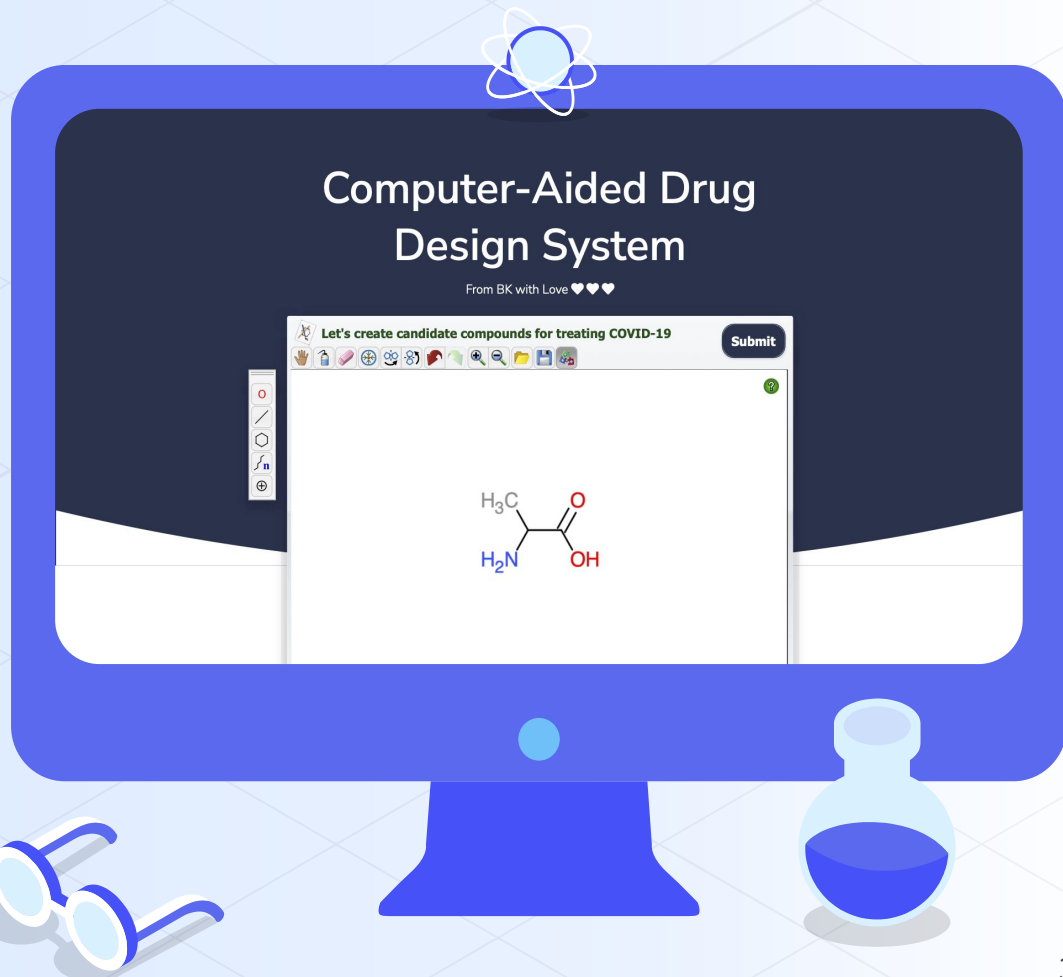
	W/O SUGGESTION	W SUGGESTIONS
Number of participants		26
Number of ligands	100	100
Mean docking score	-4.91	-5.67
Standard deviation of docking scores	1.46	1.41

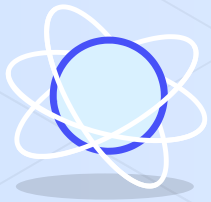




WEB APPLICATION

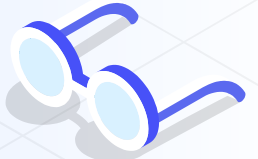
- ✓ Multiple OSs supported
- ✓ Responsive User Interface
- ✓ 5 minutes processing time





CONCLUSION


Summary and Future Developments





THE END

Thank You for Listening!



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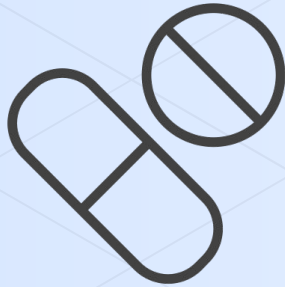
Antiviral Drugs?

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?

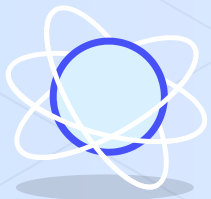


Ligand



Protein

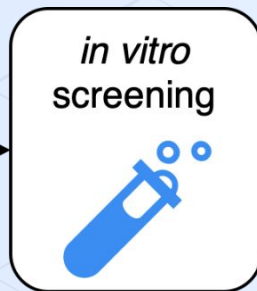
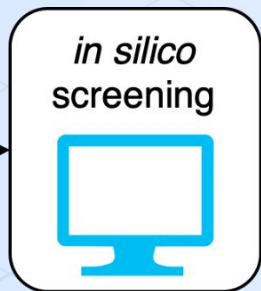




DRUG DISCOVERY PROCESS

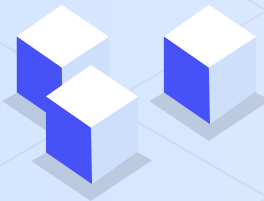


A huge amount of designed ligands



Final drugs





CROWSOURCING 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

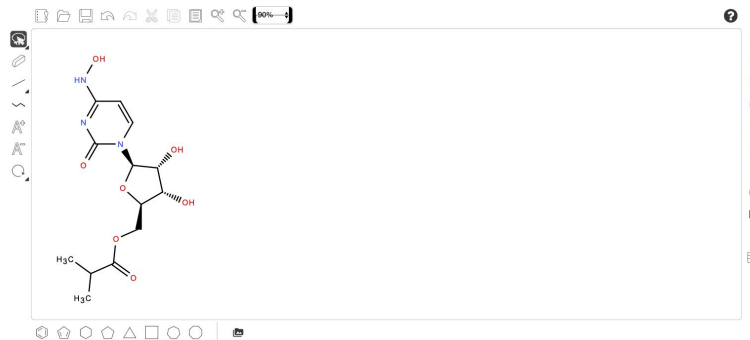
Discuss

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)C(=O)OC[C@H]1O[C@@H](n2ccc(NO)nc2=O)[C@H](O)[C@@H]1O

Add

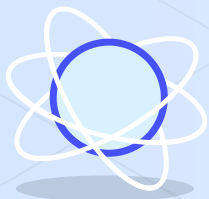


a) Welcome screen

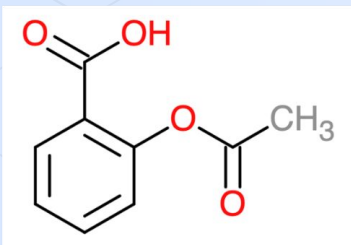
b) Design screen

a) Result screen

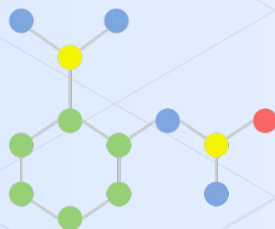
ViDok System



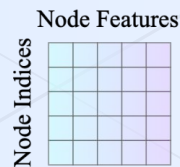
MOLECULAR PRESENTATION



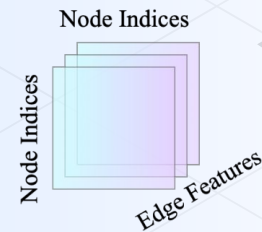
Kekulé Diagram



Molecular Graph



Node Feature Matrix



Adjacency Tensor

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



Fingerprint



CC(=O)Oc1ccccc1C(=O)O

SMILES string

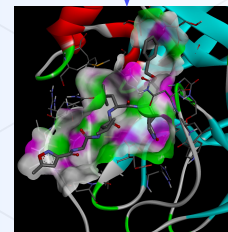
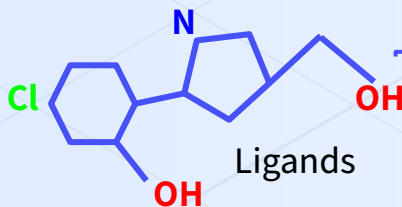
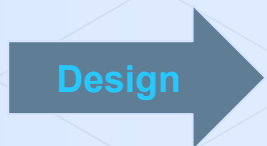
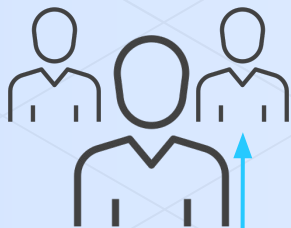
Tokenization
One-Hot Encoding



C (= O) c 1



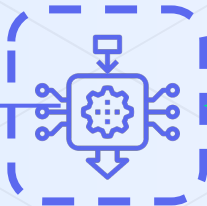
OVERVIEW BIG SYSTEM



DOCKING

Suggestions

INFERENCE



GNN-BASED MODEL

BASELINE MODEL COMPUTATION

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

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

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

GAT

$$x_i^h = \mathbf{W}_h x_i, \quad i = \overline{1, |V|}$$

$$e_{ij} = (x_i^h)^T \mathbf{W}_a x_j^h + (x_j^h)^T \mathbf{W}_a x_i^h, \quad i, j = \overline{1, |V|}$$

$$a_{ij} = \frac{\exp(e_{ij})}{\sum_{k \in C_i} \exp(e_{ik})} \mathbf{A}_{ij}, \quad i, j = \overline{1, |V|}$$

$$x_i^{temp} = \sum_{j \in C_i} a_{ij} x_j^h, \quad i = \overline{1, |V|}$$

$$z_i = \sigma(\mathbf{W}_o(x_i || x_i^{temp}) + b), \quad i = \overline{1, |V|}$$

$$x'_i = z_i x_i + (1 - z_i) x_i^{temp}, \quad i = \overline{1, |V|}$$

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

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

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

$\times N$

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

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

$\times L$

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

$\mathcal{M}(\mathbf{X}, \mathbf{A}^1, \mathbf{A}^2)$
 $\text{lastGATBlock} \leftarrow \text{GetLastGATBlock}(\mathcal{M})$
 $\mathcal{A} = \{a_{ij}\} \leftarrow \text{GetNormalizedAttentionMatrix}(\text{lastGATBlock})$
 $P \leftarrow \emptyset$

for i **in** $\text{Range}(0, M)$ **do**
 for j **in** $\text{Range}(i + 1, M)$ **do**
 if $a_{ij} + a_{ji} \geq 1$ **then**
 $P \leftarrow P \cup \{(i, j, \frac{a_{ij} + a_{ji}}{2})\}$
 end
 end
end
return 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:

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



Improved
Aggregation Layer:

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

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

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

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 $i = \overline{1, |V|}$

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

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

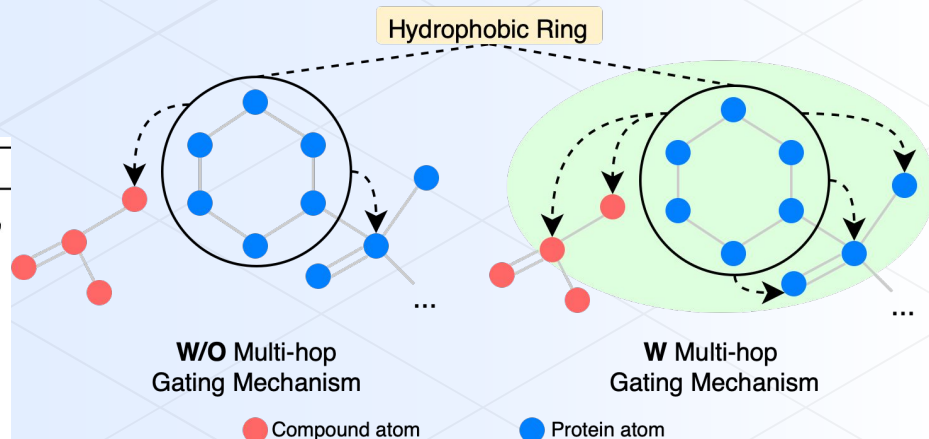
$$x_i^{temp} = \sum_{j \in C_i} a_{ij} x_j^{(k-1)}, \quad i = \overline{1, |V|}$$

$$z_i = \sigma(\mathbf{W}_o(x_i^{(0)} || x_i^{temp}) + b), \quad i = \overline{1, |V|}$$

$$x_i^{(k)} = z_i x_i^{(0)} + (1 - z_i) x_i^{temp}, \quad i = \overline{1, |V|}$$

end

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



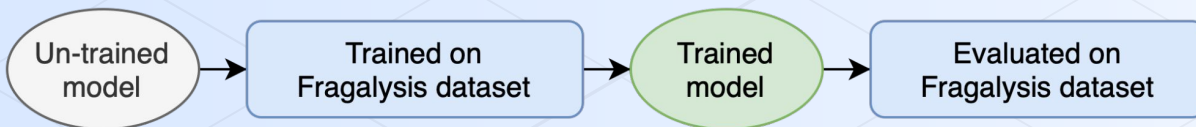


GNN-BASED MODEL

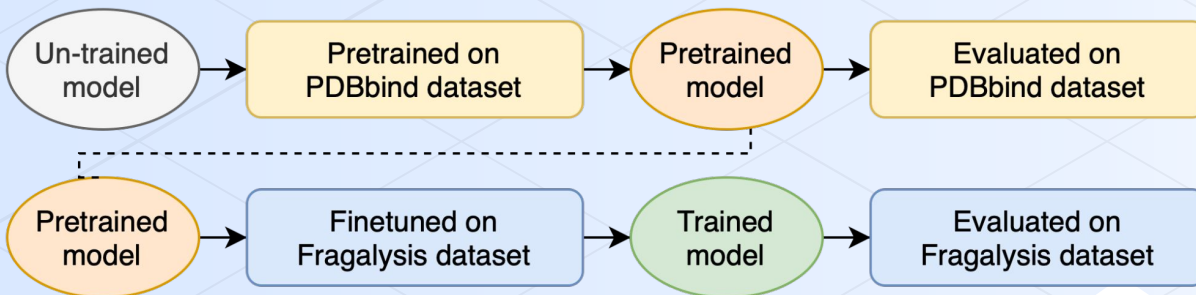
TRAINING AND TESTING FLOWS



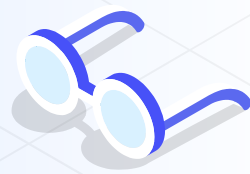
Normal flow



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-GCNet	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

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

Output: Interaction list

$I = \{(i, j, x_i, x_j) | i \in \text{ligand} \ \& \ j \in \text{protein} \ \& \ x \text{ is feature vector}\}$

$I \leftarrow \emptyset$

$\mathcal{N} \leftarrow \text{InitNearestNeighbor}(\text{protein} \rightarrow \text{atoms})$

for l_atom **in** ligand **do**

$listNearAtoms \leftarrow \text{GetNearAtoms}(\mathcal{N}, \epsilon_d, l_atom)$

for p_atom **in** $listNearAtoms$ **do**

$interaction \leftarrow \text{checkInteractionType}(\mathcal{R}, l_atom, p_atom)$

if $interaction$ **is** Hydrogen **then**

$x_i, x_j \leftarrow \text{CalculateFeature}(l_atom, p_atom)$

$I \leftarrow I \cup \{(l_atom, p_atom, x_i, x_j)\}$

end

if $interaction$ **is** Hydrophobic **then**

$hasHighProb \leftarrow \text{HasHighProb}(P, l_atom, p_atom)$

if *not* $hasHighProb$ **then**

 continue

end

$x_i, x_j \leftarrow \text{CalculateFeature}(l_atom, p_atom)$

$I \leftarrow I \cup \{(l_atom, p_atom, x_i, x_j)\}$

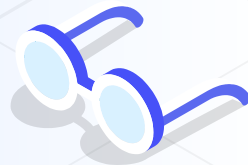
end

end

end

return I

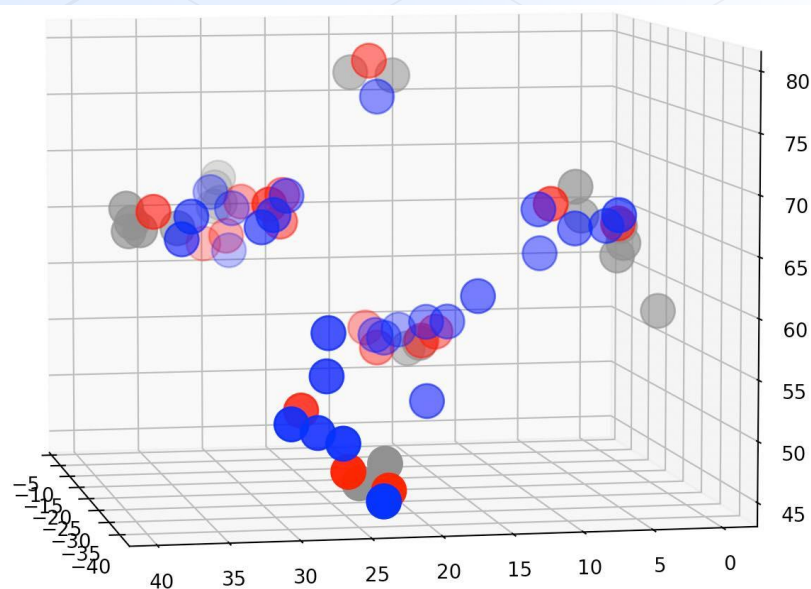


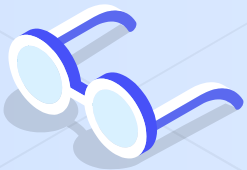


DETECTED INTERACTIONS

- **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





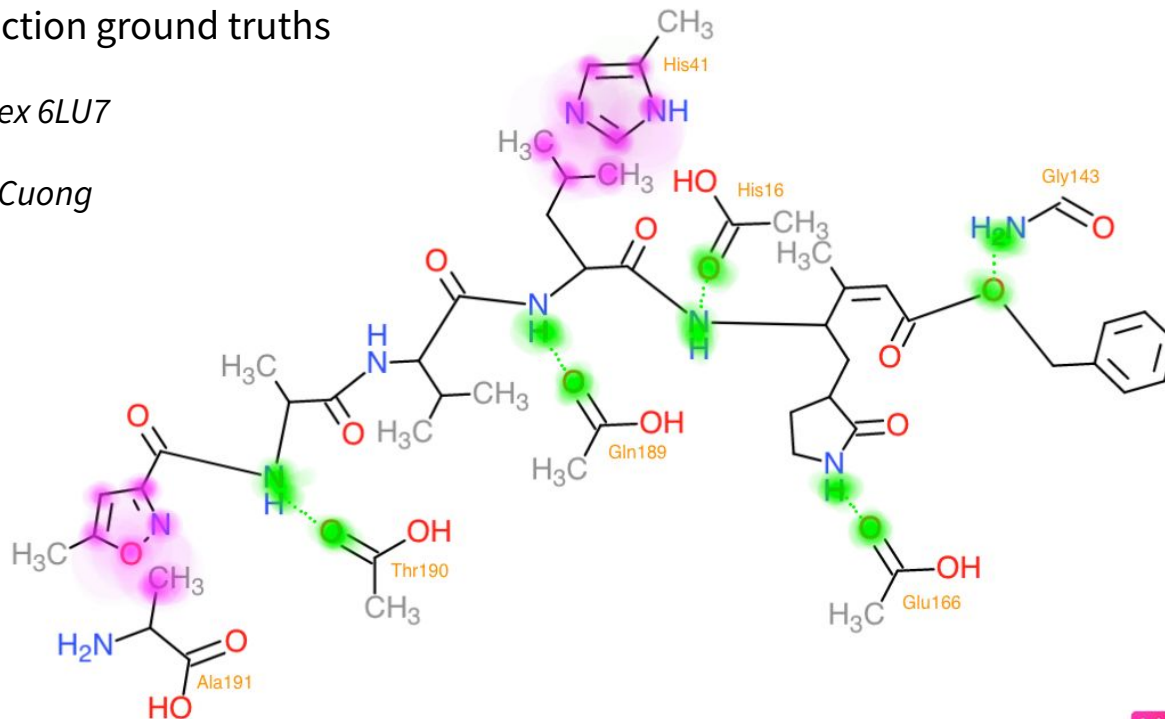
PAIRWISE INTERACTION EXAMPLES



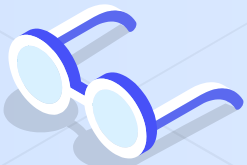
Interaction ground truths

Complex 6LU7

By Mr. Cuong



Point X lite



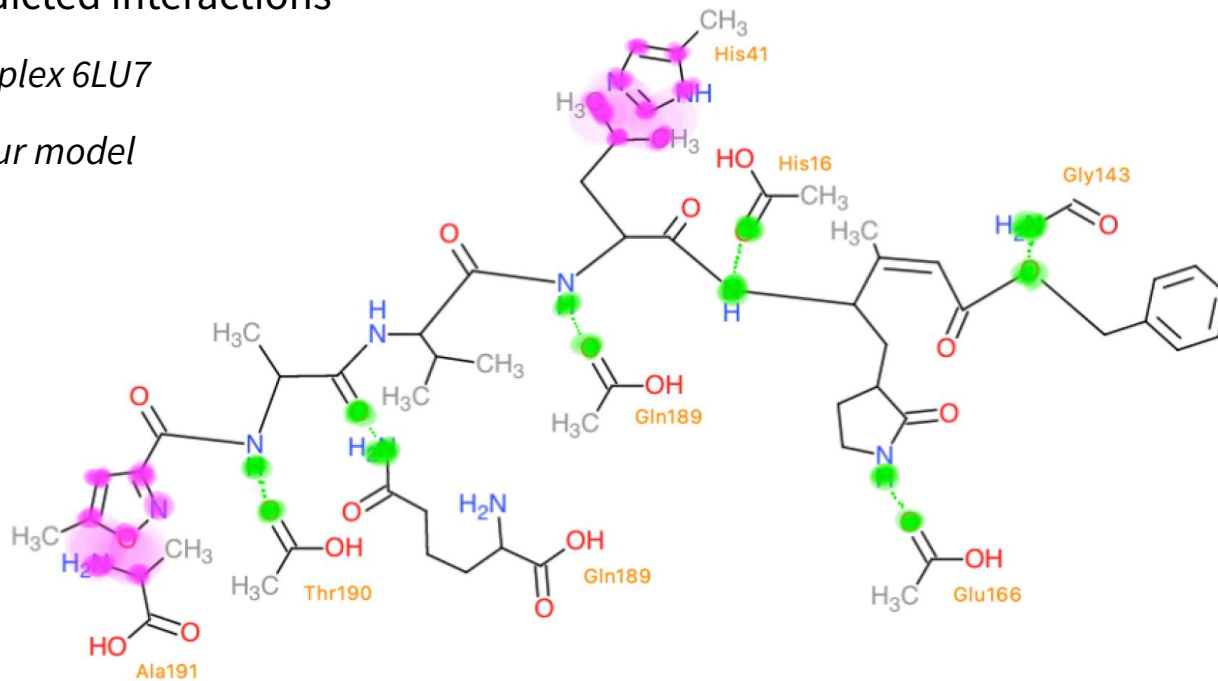
PAIRWISE INTERACTION EXAMPLES



Predicted interactions

Complex 6LU7

By our model



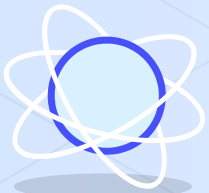


CAVITY MODEL FOR TARGET PROTEIN

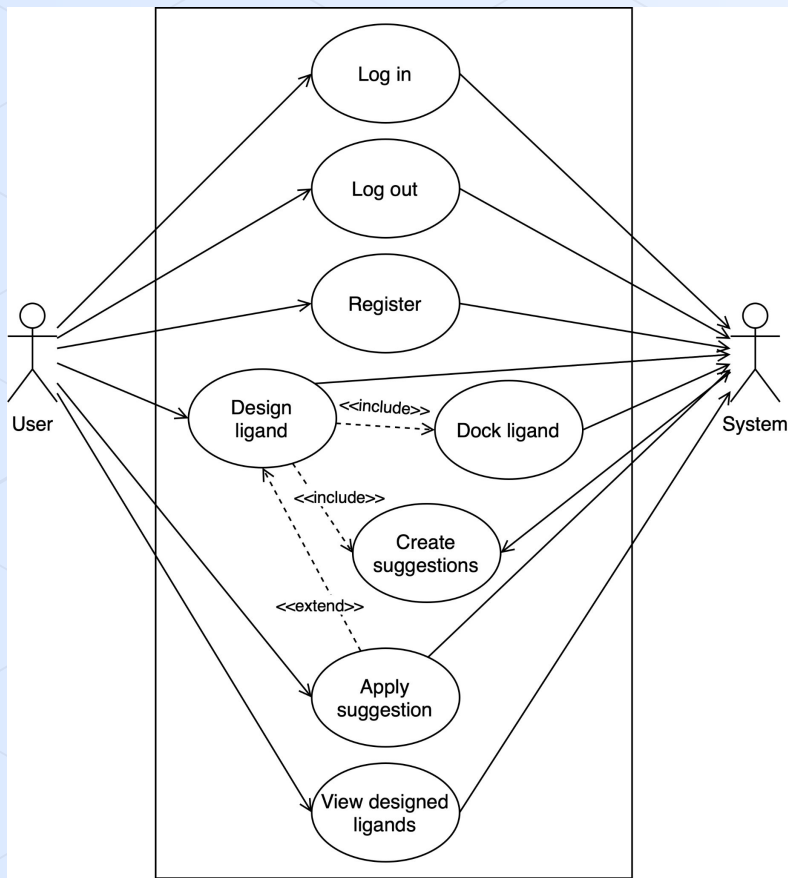
SPHERE LIST OF PHARMACOPHORE MODEL

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



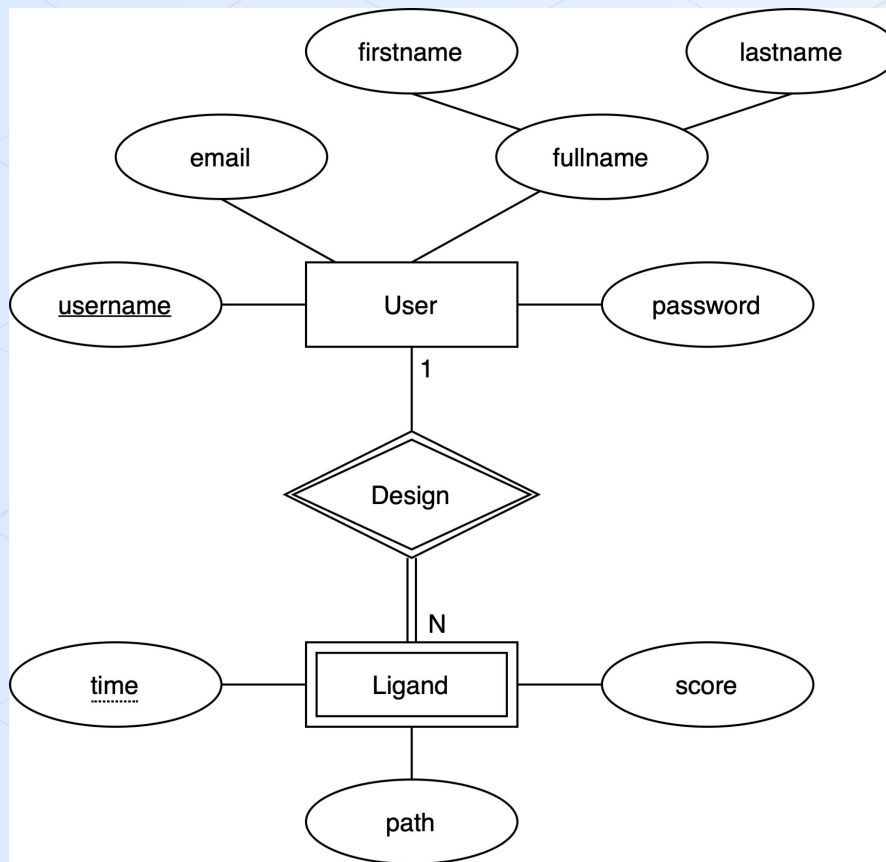


APPLICATION USECASES

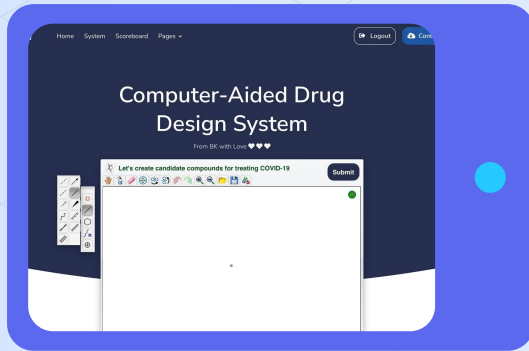




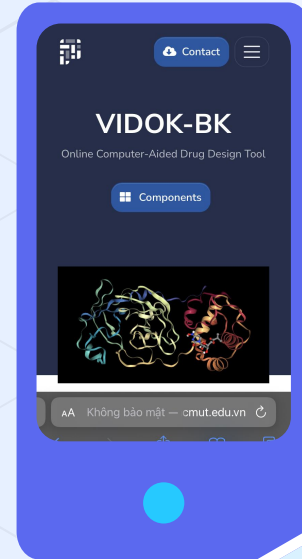
DATABASE DESIGN



TABLET AND MOBILE APPLICATIONS

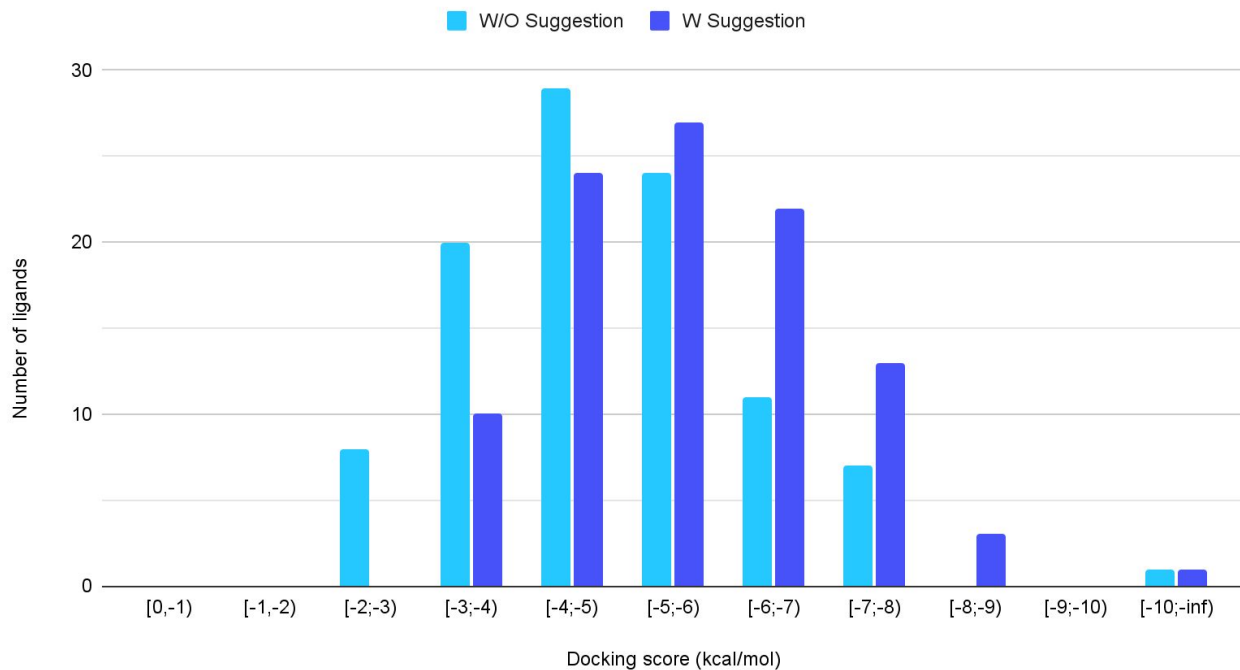


- Multiple OSs
- Multiple browsers



HISTOGRAM OF DOCKING SCORES

Histogram of docking score of designed ligand with and without suggestion



THE PERFORMANCE OF DESIGNED SYSTEM



The screenshot displays a web browser window with the URL `ura.hcmut.edu.vn/vidok/`. The website header includes a logo, navigation links (Home, System, Scoreboard, About), and buttons for Logout and Contact. The main content area features the title "VIDOK-BK" and the subtitle "Online Computer-Aided Drug Design Tool", with a prominent "Design Now" button.

Below the website content, a Lighthouse performance audit is visible. The audit results are as follows:

Metric	Score
Performance	91
Accessibility	100
Best Practices	92
SEO	100
PWA	—

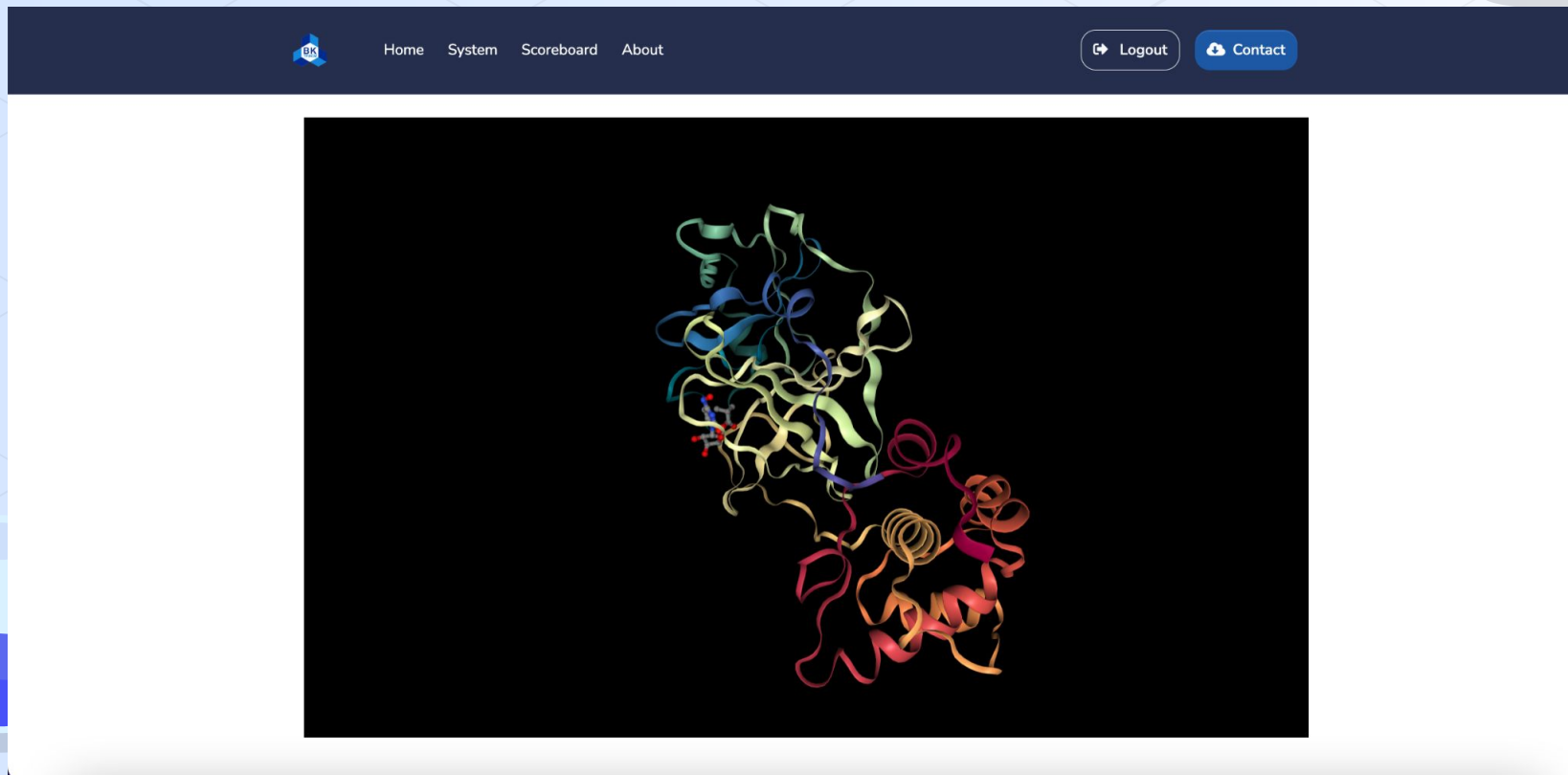


APPLICATION SCREENSHOTS



The screenshot displays the main interface of the Computer-Aided Drug Design System. At the top, a dark blue navigation bar contains a logo on the left, followed by links for Home, System, Scoreboard, and About. On the right side of this bar are buttons for Logout and Contact. The central area features the title "Computer-Aided Drug Design System" in large white font, with the tagline "From BK with Love" and three hearts below it. A white rectangular window is overlaid on the main interface, titled "Let's create candidate compounds for treating COVID-19". This window includes a toolbar with various chemical drawing tools, a large empty canvas for drawing, and a "Submit" button in the top right corner. A small green question mark icon is visible in the top right of the canvas. At the bottom of the window, the text "ChemDoodle" and "Copyright © 2000-2022 MyCompany. All Rights Reserved." is visible. A green footer bar at the very bottom of the screenshot contains the text "Include some updating calculations here".

APPLICATION SCREENSHOTS



APPLICATION SCREENSHOTS



Navigation: Home System Scoreboard About Logout Contact

Suggestions

Reset

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

APPLICATION SCREENSHOTS



[Home](#) [System](#) [Scoreboard](#) [About](#)

[Logout](#)

[Contact](#)

Scoreboard

View top deisgned ligands

Designed Ligands

Ligands per page

10

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

