Computer-aided Drug Design for Throat, Lung Gastrointestinal Infections

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ABSTRACT

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By and by the world is in a battle with throat and lung infections with no prompt medicines accessible. The scourge brought about by these infections is expanding step by step. A ton of researchers are continuing for the medication up-and-coming that could help the medical care framework in this battle. We present docking-based screening using a quantum mechanical scoring of a library built from approved drugs viz. Meropenem, Cefixime, Curcumin, Clindamycin, Cefaclor, Cefadroxil with Proteins of several infections causing microbes that could display antimicrobial activity against these infections. We hope that these findings may contribute to the rational drug design against these infections.

Keywords : Meropenem, Cefixime, Curcumin, Clindamycin, Cefaclor, Cefadroxil

I. INTRODUCTION

Lung, Throat and Gastrointestinal Infections leads to the greatest number of infection related mortalities worldwide . In 2020, nearly 120,00,00,00,000 newly diagnosed cases of Lung and Throat Infections were reported worldwide. The present study used a computer-aided drug design (CADD) approach to identify compounds for targeting proteins of the microbes causing these infections. The initial dataset was reduced to six compounds as selected ligands viz. Meropenem, Cefixime, Curcumin, Clindamycin, Cefaclor, Cefadroxil showing potential cure against these infections.

Lung Infections

Mycoplasma pneumoniae

PDB Id- 4X9M It catalyzes the oxidation of Glp by molecular oxygen to generate DHAP & hydrogen peroxide.

PDB Id -6QFP It is a cytotoxic nuclease that degenerates host DNA.

Human respiratory syncytial virus (hRSV)

PDB Id -6OJ7 It mediates the attachment of hRSV to the cell membrane and the fusion of F-proteins with the host membrane.

PDB Id- 4UCA [Nucleoprotein(N)] It is thought to protect viral RNA from nucleases

Streptococcus pneumoniae

PDB Id -4CP6 It is important for full virulence of streptococcus pneumoniae and its Amino acid sequence suggests that it may play a role in cellular adherence.

PDB Id -5LY6 It is a highly conserved membrane pore forming protein, located in cytoplasm but released into the medium during autolysis. It is a major virulence factor that exerts cytotoxic effects on epithelial cells and immune cells.

Throat Infection

Streptococcus pyogenes

PDB Id- 6OG4 (M protein) : It renders the streptococci resistant to phagocytosis and is involved in adherence to mammalian cells and immunoglobulins.

PDB Id- 1GVN Antitoxin component of a toxin-antitoxin (TA) module. Neutralizes the toxic effect of cognate zeta toxin.

Corynebacterium diphtheriae

PDB Id -1F0L : Diphtheria toxin, produced by a phage infecting Corynebacterium diphtheriae, is a proenzyme that, after activation, catalyzes the covalent attachment of the ADP ribose moiety of NAD to eukaryotic elongation factor 2 (eEF-2). Fragment A is the catalytic portion responsible for enzymatic ADP-ribosylation of elongation factor 2, while fragment B is responsible for binding of toxin to cell receptors and entry of fragment A.

PDB Id -1XDT : Diphtheria toxin, produced by a phage infecting Corynebacterium diphtheriae, is a proenzyme that, after activation, catalyzes the covalent attachment of the ADP ribose moiety of NAD to eukaryotic elongation factor 2 (eEF-2). Fragment A is the catalytic portion responsible for enzymatic ADP-ribosylation of elongation factor 2,

while fragment B is responsible for binding of toxin to cell receptors and entry of fragment A.

Gastro-intestinal Infection

Helicobacter pylori:

PDB id-3nv7: Reversibly transfers an adenylyl group from ATP to 4'-phosphopantetheine, yielding dephospho-CoA (dPCoA) and pyrophosphate.

E. coli

PDB id-5vwr Catalyzes the reversible transfer of amino group between aspartate and glutamate.

Salmonella sp.

PDB id-3ls6: Catalyzes the conversion of D-ribulose 5-phosphate to formate and 3,4-dihydroxy-2-butanone 4-phosphate.

Procedure:

1) ligand Screening

For the initial Ligand screening purposes, a web-based tool named SwissADME (<https://www.swissadme.ch/>) was used to eliminate a few compounds according to Lipinski's rule of five parameters. For a compound to qualify as ligand it should Have < 500 Da molecular weight, a high lipophilicity i.e. value of Log P being less than 5, hydrogen bond acceptors being less than 10 and H-bond donors less than 5. Any compound with more than 2 violations was ruled out for further study (Lipinski2004).

2) Protein Preparation and Active site Determination.

Required protein in pdb format was downloaded from the website **rcsb.org**, commonly known as the **Protein Data Bank**. 3D conformers of the ligand were downloaded from PubChem.

Using **PyMOL (Version 2.4.1)** software water molecules as well as native ligands from the protein

were removed, defined as cleaning/purification of the protein for further application. **Using a web server called DeepSite** Active Pockets of the proteins were calculated. The results calculated by the web server were in the form of different ids, centers and scores.

Scoring In deepsite was using neural networking based on following instructions using DCNN architecture.

<https://academic.oup.com/bioinformatics/article/33/19/3036/3859178> Center values for the grid were selected keeping score greater than 0.98.

UCSF Chimera (Version 1.14) was used to prepare the receptor using DockPrep function. **Dock Prep** prepared structures for Docking using these functions:

- deleting water molecules
- repairing truncated sidechains
- adding hydrogens
- assigning partial charges
- writing files in Mol2 format

3) In silico Docking Using Autodock Vina

Auto dock Vina (Version 1.1.2) along with UCSF Chimera (Version 1.14) was used for molecular **Docking Studies**. Center values and size of the grid of different scores were used from **DEEPSITE** calculations done above.

Following Parameters were set in auto dock vina.

Receptor options –

- **Add hydrogens in Chimera (true/false)** – whether to add hydrogens in Chimera before calling the script. The receptor prep script will check for hydrogens and add them if they are missing. AutoDock Vina needs the polar (potentially H-bonding) hydrogens to identify atom types for scoring purposes.

- **Merge charges and remove non-polar hydrogens (true/false)** – note AutoDock Vina does not use charges or nonpolar hydrogens, so this setting is not expected to affect results except for the presence or absence of nonpolar hydrogens in the processed receptor
- **Merge charges and remove lone pairs (true/false)** – note AutoDock Vina does not use charges or lone pairs, so this setting is not expected to affect results except for the presence or absence of lone pairs in the processed receptor (and there may not have been any lone pairs to start with)
- **Ignore waters (true/false)**
- **Ignore chains of non-standard residues (true/false)** – ignore chains composed entirely of residues other than the 20 standard amino acids.
- **Ignore all non-standard residues (true/false)** – ignore all residues other than the 20 standard amino acids.

For Ligands

- **Merge charges and remove non-polar hydrogens (true/false)** – note Auto Dock Vina does not use charges or nonpolar hydrogens, so this setting is not expected to affect results except for the presence or absence of nonpolar hydrogens in the ligand output files
- **Merge charges and remove lone pairs (true/false)** – note AutoDock Vina does not use charges or lone pairs, so this setting is not expected to affect results except for the presence or absence of lone pairs in the ligand output files (and there may not have been any lone pairs to start with)

Docking parameters

- **Number of binding modes (1-10, 10)** – maximum number of binding modes to generate
- **Exhaustiveness of search (1-8, 8)** – thoroughness of search, roughly proportional to time

- **Maximum energy difference (kcal/mol) (1-3,3)** – maximum score range; binding modes with scores not within this range of the best score will be discarded.

The docking results were calculated by Autodock vina using it's Scoring function and results were displayed in the form of Scores and RMSD values. Docking results with the highest value score accompanied by negative sign and least RMSD values were chosen for further studies.

4) Residue Analysis

PyMOL was used for visualization of interactions of the docked structure at the ligand sites. **Discovery Studio 2020** was used to study the ligand interactions

and total number of residues. It was also used to plot the 2D structure of the interactions and residues.

5) Statistical Analysis: Descriptive, estimation and Hypothesis testing with confidence interval of 95% was applied to data

II. Results and Discussion

Bioavailability Radar: Further analysis included six selected ligands viz. Meropenem, Cefixime, Curcumin, Clindamycin, Cefaclor, Cefadroxil. A more illustrated and comprehensive study was done using bioavailability radar. Bioavailability radar is a descriptive tool to investigate the drug-likeness of the ligands based on six physicochemical properties. The radar that fits the shaded area is Orally bioavailable.

Fig 1 shows the bioavailability radar of selected compounds.

Molecular Docking

The docking result was obtained from Autodock vina in the form of Dock score for all the proteins docked with above mentioned ligands, average docking Score of each ligand aggregated to average dock score. Standard deviation and Confidence interval was calculated, based on the confidence interval minimum value of dock score for each ligand was calculated. All the dock scores above the minimum score were considered for further evaluations.

Lung Infections:

S.No	Score	Protein	Ligand	Interactions	Remark
1	-7	4CP6	CEFADROXIL	<p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Sigma Pi-Alkyl 	Effective
2	-6.9	4CP6	CURCUMIN	<p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Anion Pi-Sigma Alkyl Pi-Alkyl 	Effective

3	-8.7	4X9M	CEFADROXIL	<p>Interactions</p> <ul style="list-style-type: none"> Conventional Hydrogen Bond Carbon-Hydrogen Bond Pi-Sulfur Pi-Alkyl 	Effective
4	-8.8	4X9M	CURCUMIN	<p>Interactions</p> <ul style="list-style-type: none"> Van der Waals Conventional Hydrogen Bond Carbon-Hydrogen Bond Unfavorable Donor-Donor Pi-Donor Hydrogen Bond Pi-Sigma Amide-Pi Stacked Alkyl Pi-Alkyl 	Effective
5	-10	4X9M	MEROPENEM	<p>Interactions</p> <ul style="list-style-type: none"> Conventional Hydrogen Bond Carbon-Hydrogen Bond Pi-Sulfur Pi-Alkyl 	Effective

6	-7.3	5LY6	CEFADROXIL	<p>Interactions</p> <ul style="list-style-type: none"> Conventional Hydrogen Bond Carbon Hydrogen Bond Unfavorable Acceptor-Acceptor Pr-Allyl 	Effective
7	-7.4	5LY6	CURCUMIN	<p>Interactions</p> <ul style="list-style-type: none"> Conventional Hydrogen Bond Carbon Hydrogen Bond Pr-Cation Pr-Allyl Pr-Allyl 	Effective
8	-6.5	60J7	CURCUMIN	<p>Interactions</p> <ul style="list-style-type: none"> Conventional Hydrogen Bond Pr-Cation Pr-Allyl Pr-Allyl 	Non-Effective

9	-6	6QFP	CEFADROXIL		Non-Effective
10	-5.7	6QFP	MEROPENEM		Non-Effective

Table 1 shows the interactions of proteins of lung Infection causing bacteria with selected ligands along with max docking score selected based on the above-mentioned statistical data.

Throat Infection

S.No	Score	Ligand	Protein	Interactions	Remark
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1	-8.9	curcumin	1F01	<p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Carbon-Hydrogen Bond Pi-Pi Stacked Pi-Pi T-shaped Aromatic-Pi Stacked Alkyl Pi-Alkyl 	Effective
2	-8	cefaclor	1F01	<p>Interactions</p> <ul style="list-style-type: none"> Conventional Hydrogen Bond Pi-Sulfur Pi-Pi Stacked Alkyl 	Effective
3	-7.5	clindamycin	1F01	<p>Interactions</p> <ul style="list-style-type: none"> Conventional Hydrogen Bond Pi-Sigma Pi-Sulfur Pi-Alkyl 	Effective

4	-8.2	cefixime	1F01	<p>Interactions</p> <ul style="list-style-type: none"> Conventional Hydrogen Bond Pi-Sulfur Pi-Pi Stacked Alkyl Pi-Alkyl 	Effective
5	-8.2	curcumin	1gvn	<p>Interactions</p> <ul style="list-style-type: none"> Conventional Hydrogen Bond Carbon Hydrogen Bond Unfavorable Donor-Donor Pi-Alkyl 	Effective
6	-8.2	cefaclor	1gvn	<p>Interactions</p> <ul style="list-style-type: none"> Conventional Hydrogen Bond Carbon Hydrogen Bond Unfavorable Acceptor-Acceptor Alkyl Pi-Alkyl 	Effective

7	-8.1	clindamycin	1gvn		Effective
8	-8	cefixime	1gvn		Effective
9	-6.8	curcumin	1xdt		Effective

10	-7.3	cefaclor	1xdt	<p>Interactions</p> <ul style="list-style-type: none"> Carbon-Hydrogen Bond Pi-Allyl 	Effective
11	-6.8	clindamycin	1xdt	<p>Interactions</p> <ul style="list-style-type: none"> Conventional Hydrogen Bond Carbon-Hydrogen Bond Pi-Allyl 	Effective
12	-7	cefixime	1xdt	<p>Interactions</p> <ul style="list-style-type: none"> Conventional Hydrogen Bond Carbon-Hydrogen Bond Unfavorable Donor-Donor Pi-Sulfur Pi-Pi Stacked Allyl Pi-Allyl 	Effective

13	-7.4	curcumin	6og4		Effective
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Table 2 shows the interactions of proteins of Throat Infection causing bacteria with selected ligands along with max docking score selected based on the above-mentioned statistical data.

Gastro-Intestinal Infection

S.No	Score	Ligand	Protein	Interactions	Remark
1	-7.2	curcumin	3NV7		Effective

2	-9.5	curcumin	5vwr		Effective
3	-6.8	curcumin	3LS6		Effective

Table 3 shows the interactions of proteins of GI Infection causing bacteria with selected ligands along with max docking score selected based on the above-mentioned statistical data.

Conclusion :

All six ligands were studied using bioavailability radar. Our results proposed showed best docking result of Meropenem, Cefixime, Curcumin, Clindamycin, Cefaclor, Cefadroxil with studied organisms and their targeted proteins. To find the effectiveness and to propose the exact mechanism in-vitro studies can be encouraged on Meropenem, Cefixime, Curcumin, Clindamycin, Cefaclor, Cefadroxil to find a potent cure for the Infection causing bacteria.

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